A New Dynamic Approach for Statistical Optimisation of GNSS Radio Occultation Bending Angles

A thesis submitted in fulfilment of the requirements for the degree of Doctor of Philosophy

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Declaration

I certify that except where due acknowledgement has been made, the work is that of the author alone; the work has not been submitted previously, in whole or in part, to qualify for any other academic award; the content of the thesis is the result of work which has been carried out since the official commencement date of the approved research program; any editorial work, paid or unpaid, carried out by a third party is acknowledged; and, ethics procedures and guidelines have been followed.

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Abstract

Climate change has become a serious issue for our society. It is of great importance to accurately monitor climate change and provide reliable information to the society so that proper actions can be taken to alleviate the significant change of climate. Global Navigation Satellite Systems (GNSS) based radio occultation (RO) is a new satellite remote sensing technique that can provide high vertical resolution, long-term stable and global coverage atmospheric profiles of the Earth’s atmosphere. However, the quality of the retrieved atmospheric profiles decreases above about 30 km due to a low signal-to-noise ratio of GNSS signals at these high altitudes, since errors in bending angle profiles are propagated to refractivity profiles through an Abel integral and subsequently propagated to other atmospheric profiles through the hydrostatic integral. It is therefore important to carefully initialise the bending angles at high altitudes to minimise these error propagation effects and thereby optimise the climate monitoring utility of the retrieved profiles.

Statistical optimisation is a commonly used method for this purpose. This method combines the observed bending angle profile and background bending angle profile based on their error covariance matrices to determine “optimised” bending angle profile. The focus of this thesis is to investigate an advanced statistical optimisation algorithm, which dynamically estimates both background and observation error covariance matrices, for the best determination of RO optimised bending angle profile. In this new algorithm, background bending angle profiles and their associated error covariance matrices are estimated using bending angles from multiple days of the European Centre for Medium-range Weather Forecasts (ECMWF) short-term (24h) forecast and analysis fields as well as the averaged observed bending angle. The background error covariance matrices are constructed with geographically varying background error estimates on a daily-updated basis. The observation error covariance matrices are estimated using multiple days of RO data with geographically varying observation errors for an occultation event. The most distinctive advantage of the new algorithm is that both background and observation error covariance matrices are realistically estimated using large ensemble of climatological and observed data, while existing algorithms use crude formulations to estimate both error matrices.

The new algorithm developed is evaluated against the algorithm used by the Wegener Center Occultation Processing System version 5.4 (OPSv5.4) by calculating statistical errors of retrieved atmospheric profiles relative to their reference profiles. Since the background errors at different heights are highly correlated and their covariance matrix is critical for the resulting optimised bending
angles, the dynamically estimated background error covariance matrix is first used in statistical optimisation to retrieve atmospheric profiles from simulated MetOp as well as observed CHAMP and COSMIC RO events on single days. The dynamically estimated observation error covariance matrix is then used in the statistical optimisation together with the estimated background error covariance matrix to retrieve atmospheric profiles using the same test data.

It can be concluded from the evaluation that if the estimated background error covariance matrix is solely used for the statistical optimisation, it can significantly reduce random errors and generate less or similar residual systematic errors (biases) in the optimised bending angles. The subsequent refractivity profiles and atmospheric (dry temperature) profiles retrieved are benefitted from the improved error characteristics of bending angles. If both observation and background error covariance matrices estimated from the new approach are used, the standard deviations of the optimised bending angles are only further reduced for simulated MetOp data, while for the observed CHAMP and COSMIC data, large random errors of bending angles are found at higher altitudes (e.g. > 50 km). This is likely to be that the observation errors are underestimated at high altitudes, where bending angles are largely affected by ionospheric effects and observation errors, and more weights are given to the noisy observed bending angles in the estimation of the optimised bending angles. Errors in CHAMP and COSMIC observed bending angles are further transferred downwards to their subsequently retrieved refractivity and dry temperature profiles, the quality of which is also degraded.

The effects of the estimated background and observation error correlations on the atmospheric retrievals are investigated using simulated MetOp data. It is found that these realistically estimated correlations alone can reduce the random errors of the optimised bending angles significantly and improve the quality of the subsequent refractivities and temperatures. The performance of the new approach that uses only the new background matrix in the statistical optimisation on monthly occultation data is evaluated. The results show that the monthly errors are similar to those from single days, but in a smoother manner.
Acronyms and Abbreviations

A
ABL Atmospheric Boundary Layer
AMSU Advanced Microwave Sounding Unit
atmPrf Atmospheric profiles without moisture information
ATS Applications Technology Satellite

C
C/A-code Coarse/Acquisition code
CCR CHAMPCLIM Retrieval
CDAAC COSMIC Data Analysis and Archive Center
CHAMP CHAllenging Minisatellite Payload
CIRA COSPAR International Reference Atmosphere
CMA China Meteorological Administration
COMS Communication, Ocean and Meteorological Satellite
COSMIC Constellation Observing System for Meteorology, Ionosphere, and Climate
CORS Continuously Operating Reference stations

D
DLR Deutsches Zentrum für Luft- und Raumfahrt
DMI Danish Meteorological Institute
DMSP Defense Meteorological Satellite Program
DoD Department of Defence
DOY Day of Year

E
ECMWF European Centre for Medium-Range Weather Forecasts
EDA Ensemble of Data Assimilation
EOS Earth Observing System
EGOPS End-to-End Generic Occultation Performance Simulation and Processing System
EUMETSAT European Organisation for the Exploitation of Meteorological Satellite
F
FedSat Federation Satellite
FoMod Forward Modelling
FY FengYun

G
C/A-code Coarse/Acquisition code
GCM Global Circulation Model
GFZ German Research Centre for Geosciences
GLONASS Global Navigation Satellite System (Russian constellation)
GNSS Global Navigation Satellite System (general constellation)
GO Geometric Optics
GOES Geostationary Satellite System
GPS Global Positioning System
GPS/MET Global Positioning System/Meteorology
GRACE Gravity Recovery and Climate Experiment
GRAS Global Navigation Satellite System Receiver for Atmospheric Sounding
GTS Global Telecommunications System

H
HY HaiYang

I
IGRA Integrated Global Radiosonde Archive
ILW Integrated Liquid Water
IPCC Intergovernmental Panel on Climate Change
IWV Integrated Water Vapour
InRet Inversion and Retrieval

J
JMA Japan Meteorological Agency
JPL Jet Propulsion Laboratory

K
KMA Korea Meteorological Administration
L
LIO  LEO-LEO Infrared-laser Occultation
LEO  Low Earth Orbit
LMIO  LEO-LEO Microwave occultation and the LEO-LEO Infrared-laser Occultation
LMO  LEO-LEO Microwave Occultation

M
MetOp  Meteorological Operational Satellite Programme
MSU  Microwave Sounding Unit
MSIS  Mass Spectrometer and Incoherent Scatter Radar
MAnPI  Mission Analysis and Planning

N
NASA  National Aeronautics and Space Administration
NCAR  National Center for Atmospheric Research
NCEP  National Centers for Environmental Prediction
NHP  Northern hemisphere Polar
NHSM  Northern Hemisphere Subtropics and Mid-latitudes
NOAA  National Oceanic and Atmospheric Administration
NSOAS  National Satellite Ocean Application Service
NWP  Numerical Weather Prediction

O
OL  Open Loop
OP5v4  Occultation Processing System version 5.4
OSMod  Observation System Modelling

P
PBL  Planetary Boundary Layer
P-code  Precision code
PLL  Phase Locked Loop
POD  Precise Orbit Determination
PRN  Pseudo-Random Noise
PW  Perceptible Water
R
R.M.S Root-Mean-Square
RO Radio Occultation
ROPPE Radio Occultation Processing Package
RosHydroMet Russian Federal Service for Hydrometeorology and Environmental Monitoring

S
SAC-C Satélite de Application Científicas C
SGP4 Simplified General Perturbations version 4
SHP Southern Hemisphere Polar
SHSM Southern Hemisphere Subtropics and Mid-latitudes
Sim-MetOp Simulated MetOp
SMS Synchronous Meteorological Satellite
SO Statistical Optimisation
SUNSET Stellenbosch University Satellite
Suomi-NPP Suomi National Polar-orbiting Partnership

T
TGRS TriG (Tri-GNSS) GNSS Radio-occultation system
TIROS Television Infrared Observation Satellite

U
UCAR University Corporation for Atmospheric Research
U.S. United States
USA United States of America
UTLS Upper Troposphere and Lower Stratosphere
UTC Universal Time Coordinated

W
WEGC Wegener Center for Climate and Global Change
WO Wave Optics
WMO World Meteorology Organization
WVRs Water Vapour Radiometers

Z
ZWD Zenith Wet Delay
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Chapter 1. Introduction

Global climate change has become a serious issue for our society since the beginning of the industrial revolution in the mid-18th century. According to the fourth assessment report from the Intergovernmental Panel on Climate Change (IPCC), the global-mean surface temperature rose by 0.74ºC ± 0.18 ºC over the 100-year period from 1906 to 2005, and the rate of temperature change over the second half of the period is twice as those over the 100-year period [Trenberth et al., 2007]. In addition, the lower-tropospheric temperatures were found having slightly greater warming rates than those of the surface temperatures over the period 1958 to 2005, the areas of droughts enlarged and the areas of cryosphere shrank [Trenberth et al., 2007]. All of these changes have affected the biology of the Earth and human activities. As a result, it is of great importance to monitor climate changes accurately and take proper actions to prevent these changes.

1.1 Background

1.1.1 The climate system

Climate is usually defined as “average weather” and is described in terms of the mean and variability of atmospheric parameters, such as temperature, precipitation and wind over a period of time that ranging from months to millions of years [Treut et al., 2007]. The climate system consists of five components: the atmosphere, hydrosphere, cryosphere, land surface and biosphere.

The atmosphere is composed of nitrogen (78.09% N\textsubscript{2}), oxygen (20.95% O\textsubscript{2}), argon (0.93%, Ar), carbon dioxide (0.039%) and some other gases. According to the values of vertical temperature, the atmosphere can be divided into the troposphere, stratosphere, mesosphere, thermosphere and exosphere. The troposphere is the lowest part of the Earth’s atmosphere. It starts from the surface of the Earth to about 9 km at the poles and 17 km at the equator. The lowest part of the troposphere is known as the Atmospheric Boundary Layer (ABL) and is directly influenced by the activities on the Earth’s surface. The ABL is also often called Planetary Boundary Layer (PBL). The troposphere part above the ABL is the free atmosphere where only some internal air turbulences exist. The top boundary of the troposphere is known as the tropopause and its height is an indicator of the tropospheric warming. Within the troposphere, the temperature decreases with height and the value at the tropopause is usually the lowest in troposphere. From the tropopause upwards till about 50 km is the stratosphere. In the stratosphere, the temperature increases with height. Although the climate change of stratosphere does not directly affect the biology of the Earth, it may affect the height of the
tropopause and thus affect the warming or the cooling of the troposphere. The mesosphere starts from the top of the stratosphere to about 85 km. In the mesosphere, the temperature decreases with height. The top of the mesosphere is known as the mesopause and is the coldest layer of the Earth’s atmosphere. From the mesopause to about 700 km is the thermosphere. In the thermosphere, the temperature increases with height. Above the thermosphere is the exosphere, this layer is the outermost layer of the Earth’s atmosphere. Since this layer is close to the Sun, the temperature is rather high. Gases in this layer are almost not affected by the Earth’s gravity anymore, thus their atoms and molecules can move into the outer space. A special region of the Earth’s atmosphere is the ionosphere. The ionosphere starts from about 60 km to about 1500 km, and it includes the thermosphere and parts of the mesosphere and exosphere. The ionosphere contains free electrons of the gases in the atmosphere that are ionised by the Sun’s radiation.

The hydrosphere includes all water resources of the Earth, such as lakes, rivers and oceans. About two-thirds of the Earth’s surface is covered by these water resources, especially oceans which occupy about 97% of the Earth’s water supply. The oceans play an important role in the climate system as it stores most of the Sun’s energy that reaches the Earth. Due to the large amount of plants in the ocean, the oceans are also important sources for releasing O₂. In addition, the oceans also play a key role in the weather system since many weather events are linked with the air convention between the oceans and continents [Herr and Galland, 2009].

The cryosphere describes water in a solid form on the Earth’s surface. It includes sea ice, glaciers and ice sheets etc. The cryosphere is of great importance in balancing the Earth’s energy cycle. It prevents the Earth from becoming too warm by reflecting a high percentage of the sunlight.

The land surface includes all the continents on the Earth’s surface. It absorbs solar energy and transfers the energy to the atmosphere by latent heat, sensible heat and long wave radiation etc. The land surface is important for energy exchange in the climate system.

The biosphere includes all life on the Earth, including human beings as well as closed and self-regulating ecosystems. Compared to other components of the climate, the biosphere affects the Earth’s climate the most, e.g., the combustion of fossil fuels by human beings breaks the balance of the carbon cycle in climate system and increase the amount of CO₂ in the atmosphere.

1.1.2 Climate change

The main energy source for our Earth is the radiation from the Sun. About 30% of the energy reaching the top of the Earth’s atmosphere is reflected back to the space mainly due to clouds, small particles in the atmosphere and Earth’s surface. The rest of the energy is absorbed by the atmosphere and the surface of the Earth. To keep the energy balance, the absorbed energy is then emitted back to space in the form of long-wave radiation by the Earth itself. The reason that the Earth is kept warm is
the existence of greenhouse gases in the atmosphere preventing the long-wave from the Earth radiating back to space [Treut et al., 2007]. Due to this energy cycle, the climate system of the Earth stays stable for a long time in old days.

Since the beginning of industrial revolution in the mid-18th century, climate has been observed changed significantly. As mentioned at the beginning of this chapter, both the surface temperature and troposphere temperature has risen quickly. The global sea level has risen at a fast rate (about 1.7 mm/yr over the 20th century) [Church and White, 2006; Holgate and Woodworth, 2004]. The area of the cryosphere has shrunk, the melting of the glaciers and the collapse of the ice shelves in polar regions were also noticeable [Hock, 2005; Lemke et al., 2007]. The oceans are also found acidulated [Leatherman et al., 2000].

Although the aforementioned climate change could be caused by natural reasons, such as eruption of volcanos, the main contributions to the change are from the anthropology factors. Among all anthropological factors, the most important one is the combustion of fossil fuels, which results in the increase in the amount of greenhouse gases in the atmosphere. One of the most common greenhouse gases is carbon dioxide (CO2) which is of the largest percentage in the total amount of greenhouse gases. Other common greenhouse gases are methane (CH4) and nitrous oxide (N2O), fluorinated gases (F-gas) etc. Many studies have shown that greenhouse gas emissions substantially rose over the past century [Meinshausen et al., 2009; Peters et al., 2012]. The increased greenhouse gas effects from the increase of the gases break the energy balance of the Earth’s system which results in the increase of atmospheric temperature. If the greenhouse gas emissions are not constrained, the atmospheric temperature will rise quickly in the future and the Earth’s climate will change then [Meinshausen et al., 2009].

1.1.3 Observing the Earth’s atmosphere

Two of the conventional and often used atmospheric observation methods are radiosondes and weather satellites. Radiosondes provide high vertical resolution and accurate atmospheric profiles. However, radiosondes are expensive to be launched and typically restricted to launches from land based weather stations. These two reasons results in radiosonde data are sparse, especially in oceanic and polar regions. Weather satellites could provide global coverage datasets. However, atmospheric data from weather satellites are usually of low vertical resolution and contains large uncertainties [e.g., Ladstädter et al., 2011].

The Global Navigation Satellite System (GNSS) radio occultation (RO) technique has become a robust technique for sensing the properties of the Earth’s atmosphere since the early 1990s [Hajj et al., 2002; Kursinski et al., 1996]. This technique sets specially designed GNSS receivers on Low Earth Orbit (LEO) satellites to receive GNSS signals. Due to the inhomogeneity of atmospheric
density, GPS signals are bent along their propagation path through the atmosphere. The bending angles can be calculated and further used to derive atmospheric profiles such as refractivity, temperature, density and pressure. Currently, only GNSS signals from the U.S. Global Positioning System (GPS) are utilised in the RO technique. Signals from other satellite navigation systems like the European Galileo or the Russian Global Navigation Satellite System (GLONASS) are proposed to be received in the near future. Therefore, only GPS is mentioned in the following description of this thesis. The uses of other GNSS system in RO and also in other meteorology applications are similar to GPS.

The RO technique exhibits several beneficial characteristics: First of all, its measurements are self-calibrated and long-term stable which make RO data highly consistent and can be combined together without the need of inter-calibration [Foelsche et al., 2009; Foelsche et al., 2011; Hajj et al., 2004; Schreiner et al., 2007]. Secondly, RO measurements can be obtained under all-weather conditions and are available globally. Furthermore, the retrieved atmospheric profiles have high agreements with atmospheric profiles provided by other methods in the upper troposphere and lower stratosphere (UTLS) region, and the data also have high vertical resolution in the same atmospheric regions [Kursinski, 1997; Zhang et al., 2011b].

Due to these characteristics, the GPS RO technique has become a useful tool for climate monitoring [Anthes et al., 2000; Leroy et al., 2006] and has been widely used for the study of the Earth’s climate and weather [Anthes, 2011]. For example, RO data have been used to study the climate trends and variability [Anthes, 2011; Foelsche et al., 2009; Steiner et al., 2001; Steiner et al., 2011; Zhang et al., 2011] and the obtained results are found to be consistent with other observation data records. The RO data has also been used for the study of the tropopause [Borsche et al., 2007; Schmidt et al., 2010; Schmidt et al., 2005; Xu et al., 2011], atmospheric boundary layer [Sokolovskiy et al., 2006; von Engeln et al., 2005] and diurnal tides [Pirscher et al., 2010; Zeng et al., 2008]. The RO data is also useful for severe weather prediction [Chien and Kuo, 2010; Kuo et al., 2012]. The RO data has also demonstrated their usefulness in numerical weather prediction (NWP) systems. Research shows that, after the RO data are assimilated in the NWP systems, the quality of the weather forecast products, especially in the polar and oceanic regions are improved [Cucurull and Derber, 2008; Cucurull et al., 2007; Healy and Eyre, 2000; Healy and Thépaut, 2006]. In addition to the uses in neutral atmosphere, RO data have been successfully used for the study of the ionosphere and also space weather [Carter et al., 2013; Hajj et al., 2000; Pavelyev et al., 2012; Yue et al., 2010; Yue et al., 2012].

Due to the important role of the RO technique plays in climate monitoring and weather forecasting, it is therefore selected as the main research topic of this thesis. More specifically, this thesis focuses on the application of the RO technique in the neutral atmosphere. It is expected that the
outcomes from this thesis can make some contributions to the areas of RO research and applications by improving the quality of RO retrieved atmosphere results.

1.2 Objectives

Before introducing the aim and objectives of this thesis, it is necessary to briefly introduce the fundamentals of RO data processing here, focusing on aspects needed as a background for this thesis (altitudes > 20 km of interest, dry air retrieval only); more details on the data processing can be found in Chapter 3.

RO raw measurements include GNSS phases and amplitudes. After the clock errors of the receiver and transmitter and other observation errors are corrected, excess phases are derived based on the raw measurements. These excess phases are further used for obtaining Doppler shifts from which, together with precise orbit information of both GNSS and LEO satellites, bending angle profiles are derived. The obtained bending angles contain both ionospheric and neutral atmospheric contributions. It is the neutral atmospheric contribution that is useful for retrieving atmospheric profiles. Thus, the ionospheric contribution is an error in this context. To correct for the ionospheric effects on the derived atmospheric parameters, a linear combination of bending angles retrieved from both GPS frequencies is applied [Ladreiter and Kirchengast, 1996; Vorob’ev and Krasil’nikova, 1994] for eliminating the first-order ionospheric effects on the bending angles, while small residual ionospheric errors still remain [Bassiri and Hajj, 1993; Danzer et al., 2013; Liu et al., 2013; Mannucci et al., 2011; Rocken et al., 2009; Syndergaard, 2000].

The next step of the RO data processing is to use the ionosphere-corrected bending angle to calculate refractivity through the Abel integral, and the refractivity is then used to calculate pressure and temperature through the hydrostatic integral and the equation of state. The ionosphere-corrected bending angles, however, are not directly suitable for deriving good quality refractivity and temperature, since they contain observational noise and residual ionospheric errors that are especially relevant at high altitudes above about 30 km, where the signal-to-noise ratio becomes increasingly small [Ramsauer and Kirchengast, 2001; Rieder and Kirchengast, 2001; Steiner and Kirchengast, 2005]. These errors are transferred down to refractivity through the Abel integral and further down to pressure and temperature through the hydrostatic integral. In order to obtain statistically optimised bending angles to initialise the Abel integral, current major RO data processing centres combine the ionosphere-corrected bending angles with background bending angles through a statistical optimisation process, the latter typically derived from a climatological model [Ho et al., 2012; Steiner et al., 2013]. The obtained optimised bending angles are then used for the calculation of refractivity and temperature.
The statistical optimisation is a generalized least squares approach [Rodgers, 1976; 2000], weighting the bending angles by their inverse error covariance matrices. The more accurate the estimated error covariance matrices, the better quality the obtained bending angles. However, the difficult of this method is the obtaining of accurate error covariance matrices, especially for background error covariance matrix since it is neither supplied by climatological models nor is its construction a straightforward task. Therefore, current approaches usually crude formulate both background and observation error covariance matrices using empirical values for the errors and analytical functions for the error correlations.

In order to avoid the crude formulation, this thesis develops an advanced statistical optimisation algorithm, which statistically and realistically estimate both background and observation error covariance matrices, to optimise RO observed bending angles. To achieve this aim, several objectives are listed as follows:

1) To develop a daily background error-field for the dynamic estimation of background error covariance matrix for the day, and the resulting matrix is dependent on latitude, longitude, altitude and day of year;

2) To dynamically and realistically estimate background error covariance matrix using a large ensemble of bending angles ECMWF short-range forecast and analysis fields together with averaged-observed bending angles, and to correct the biases in background bending angles;

3) To dynamically estimate the observation errors dependent on altitude;

4) To estimate correlation of observation errors using large ensemble of RO observed bending angles;

5) To evaluate the new algorithm using single days and monthly RO observations.

As can be seen from the objectives, the distinctive advantage of the new approach is that it uses large ensemble of climatological data and real observed data to statistically estimate both background and observation error covariance matrices, and the biases in the background bending angles are also corrected. Therefore, the estimated matrices are believed close to the “true” values and characteristics of both background and observation information. It is expected that using this new approach, the quality of the optimised bending angles and the subsequently retrieved refractivity and atmospheric profiles can be improved, which can in turn be helpful for accurate climate monitoring and weather forecasting.

1.3 Thesis outline
Chapter 2 introduces currently commonly used atmospheric observation methods, and advantages and disadvantages of these methods, and the development as well as the current status of the GPS RO technique. Chapter 3 presents fundamentals of GPS RO data processing. Chapter 4 gives an overview of existing high altitude initialisation and statistical optimisation algorithms as well as other initialisation methods, and then introduces a new statistical optimisation approach. Chapter 5 firstly evaluates the performance of the background error covariance matrix estimated in the new statistical optimisation using single days RO observations. After that, the performance of the complete new approach that uses both estimated background and observation error covariance matrices is evaluated using the same single days’ data. In Chapter 6, the performance of background matrix estimated in the new statistical optimisation approach is evaluated using two months’ RO data. Summary and recommendations are given in Chapter 7.
Chapter 2. Atmospheric Observation Methods

In this chapter, the two most commonly used atmospheric observation methods, i.e. radiosondes and weather satellites, are introduced first. The applications of GPS in meteorology are then discussed. GPS meteorology can be roughly categorised into ground-based GPS technique and space-based GPS RO technique. The ground-based GPS RO technique mainly provides spatial distribution of water vapour. The GPS RO technique provides vertical atmospheric profiles and is the focus of this study. The GPS RO technique has weaknesses in retrieving atmospheric profiles in moist atmospheric regions. Therefore, this chapter also discusses a generalisation of the RO technique, i.e., the LMIO technique. The LMIO includes LEO-LEO microwave occultation and the LEO-LEO infrared-laser technique. The former can retrieve accurate atmospheric profiles in moist atmospheric regions and the latter allows the calculation of greenhouse gases. In the final part of this chapter, atmospheric data assimilation, which combines different types of observations together to obtain an optimal estimate of the atmospheric parameters, is discussed. The products from atmospheric data assimilation are rather important since they are believed to be optimal and often used as references for other independent atmospheric observation methods.

2.1 Radiosonde

The radiosonde technique has been one of the most important upper-air observation methods for weather prediction since the 1940s. This method suspends several atmospheric sensors and a radio transmitter on a weather balloon inflated with hydrogen or helium gas. As the balloon ascends, the sensors measure the properties of the atmosphere, such as temperature, pressure and humidity. In addition, the wind direction and speed can also be determined by tracking the position of the radiosonde [Durre et al., 2006]. The measurements are sent back to a ground station through the radio transmitter for data recording and analyses. As the balloon ascends, atmospheric pressure decreases, so the size of the balloon becomes larger. When the balloon arrives at a height between 20 km to 30 km, the diameter of the balloon reaches a maximum size and the balloon bursts. To avoid the damage of the lives and properties on the Earth’s surface, a parachute is used to slow down the descending of the balloon. The maximum height that a radiosonde balloon can reach is determined by the diameter and the thickness of the balloon. Although, with special design, the balloon can reach even higher, the measurements above 30 km are not accurate anymore and the cost of the combustion of the hydrogen
or helium gas would be considerable. As a result, most of current radiosondes are only designed to reach at a height between 20 km to 30 km. The radiosonde sounding takes about one to two hours each time. Its precision of temperature and relative humidity are approximately 0.2 °C and ~3.5% respectively [Elliot and Gaffen, 1991].

For data sharing, the observations obtained at most of the radiosonde stations around the world are transferred to various meteorological centres through the Global Telecommunications System (GTS). The largest radiosonde data archive is the Integrated Global Radiosonde Archive (IGRA) operated by National Oceanic and Atmospheric Administration (NOAA) in the USA. This data archive receives data from 1500 quality-assured radiosonde stations [Durre et al., 2006]. Figure 2.1 shows the distribution of the radiosonde stations covered by the IGRA in the world:

![Figure 2.1 The distribution of the radiosonde stations providing data for IGRA (from [Durre et al., 2006])](image)

The oldest atmospheric data records from these stations were from 1938, however, most of the radiosonde data records were available from 1970s. Two thirds of these stations release radiosondes two or four times a day. Most of the measured radiosonde profiles have at least 100 hPa vertical resolution. Unlike many other atmospheric observation methods, that measure non-atmospheric variables and convert these variables into atmospheric variables based on some assumptions, radiosondes provide in situ measurements of the atmosphere. Therefore, the radiosonde measurements in the lower troposphere are more accurate than many other atmospheric observation techniques.
Radiosonde data have been widely used in climate monitoring [McCarthy et al., 2009; Seidel et al., 2010], and validation of other observation data [Rocken et al., 1997; Spencer and Christy, 1992].

The disadvantages of the radiosonde technique are also obvious. First of all, radiosonde stations can only be built on land, thus, radiosonde datasets are missing in the oceanic and polar regions. Secondly, the cost on the maintenance of radiosonde stations and the launch of radiosonde balloons are considerable, which again imposes limitations on both spatial and temporal resolutions of radiosonde data and results. The third problem is the large uncertainty in radiosonde data records introduced by hardware of different sensors and this affects the accuracy in determining the trends in climate change [Sherwood et al., 2005].

Numerous efforts have been made to improve the utility of radiosonde data, such as building more radiosonde stations, developing methods for mitigating the uncertainty in the radiosonde records [Durre et al., 2005; Haimberger et al., 2012; McCarthy et al., 2008]. With these efforts, the uncertainties in radiosonde data have been properly mitigated to a large extent. However, the considerable cost of launching radiosondes and also the limited coverage of the data records of this technique cannot be easily solved. As a result, the utility of radiosonde for global climate monitoring is limited. In addition, the atmospheric profiles from radiosondes can only reach up to about 25 km height, so this technique cannot be used for the meteorological study for the middle and upper stratosphere.

2.2 Weather satellites

The advent of weather satellites allows the observation of the Earth’s atmosphere from space, which yields a large and even global coverage of dataset. These satellites carry high-resolution cameras to produce images of the Earth and atmospheric sensors to provide quantitative atmospheric profiles [Kidd et al., 2009; Smith et al., 1986]. The first weather satellite launched and achieved success is TIROS-1 from the program of the Television Infrared Observation Satellite (TIROS) in 1960 by the National Aeronautics and Space Administration (NASA) of the United States [Fritz and Wexler, 1960; Stroud, 1960]. Before the TIROS-1 satellite, the use of satellites for meteorology was unproven. The success of TIROS-1 convinced the uses of satellites in meteorology and proved the possibility of observing the atmosphere from space.

According to the height and direction of the satellite orbit, weather satellites could be classified into three categories: sun-synchronous polar-orbiting satellites, geostationary satellites and other close polar-orbiting satellites. The first category of the satellites, i.e. the sun-synchronous polar-orbiting satellite circulates the Earth from north to south in Low Earth Orbit (LEO) every 98 minutes, passing over the poles during their flight [Kidd et al., 2009]. The typical altitude of the polar-orbiting satellite is about 850 km and their orbit is synchrony with the Sun, which allows the observation of the whole
globe. Currently, this type of satellites in operation include NOAA-18, NOAA-19 from National Oceanic and Atmospheric Administration (NOAA) [Davis, 2007], the MetOp-A and MetOp-B satellites from the Meteorological Operational Satellite programme (MetOp) operated by the European Organisation for the exploitation of Meteorological Satellite (EUMETSAT) [Klaes and Schmetz, 2007], and the FY-3A (FengYun – 3A) and FY-3B satellites from China Meteorological Administration (CMA) [Jin et al., 2010] etc. Table 2.1 lists some of current operational sun-synchronous polar-orbiting satellites based on the information from the World Meteorology Organization (WMO).

<table>
<thead>
<tr>
<th>Satellite name</th>
<th>Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMSP-F16, DMSP-F18</td>
<td>DoD</td>
</tr>
<tr>
<td>NOAA-18, NOAA-19</td>
<td>NOAA</td>
</tr>
<tr>
<td>MetOp-A, MetOp-B</td>
<td>EUMETSAT</td>
</tr>
<tr>
<td>FY-3B</td>
<td>CMA</td>
</tr>
<tr>
<td>Suomi-NPP</td>
<td>NASA</td>
</tr>
</tbody>
</table>

The main advantage of the polar-orbiting satellite is its high resolution of the Earth’s images and the global coverage of the datasets. However, it does not allow continuous observation of a weather event. The advent of geostationary satellites complements the polar-orbiting satellites by allowing continuous observations of short-period weather events. This type of satellite is in earth-synchronous orbit with a typical altitude of approximately 36,000 km. The geostationary satellites are at a fixed location above the Earth enabling a continuous observation of weather events, providing information on local storms and tropical cyclones, and providing real-time information of these events. Using geostationary satellites, many severe weather events have been predicted and tracked to ensure the safety of people and avoids severe economic loss.

The first geostationary satellite was ATS-1 from the program of Applications Technology Satellite (ATS) and was launched in 1966 by NASA. The successful launch and operation of this satellite demonstrated the utility of the earth-synchronous satellite in meteorology. After ATS-1, two other satellites launched from the program of Synchronous Meteorological Satellite (SMS) further demonstrated the uses of this type of satellites for meteorological research. Shortly after the SMS satellites, a series of geostationary satellites were launched from the program of Geostationary Satellite System (GOES) [Davis, 2007]. These satellites provided large amount of data for weather forecasting, severe weather events tracking, environmental monitoring as well as other meteorological
studies. Current operational geostationary satellites include the GOES series satellites from NOAA, the Meteosat series from EUMESAT [Stuhlmann et al., 2005], the FY series satellites from CMA [Dong et al., 2009; Jin et al., 2010], etc. Table 2.2 lists most of the currently operational geostationary satellites.

**Table 2-2** Current operational geostationary satellites

<table>
<thead>
<tr>
<th>Satellite name</th>
<th>Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>GOES-12, GOES-13, GOES-14, GOES-15</td>
<td>NOAA</td>
</tr>
<tr>
<td>Meteosat-7, Meteosat-8, Meteosat-9, Meteosat-10</td>
<td>EUMETSAT</td>
</tr>
<tr>
<td>Electro-L N1</td>
<td>RosHydroMet</td>
</tr>
<tr>
<td>FY-2D, FY-2E, FY-2F</td>
<td>CMA</td>
</tr>
<tr>
<td>COMS-1</td>
<td>KMA</td>
</tr>
<tr>
<td>Himawari-6, Himawari-7</td>
<td>JMA</td>
</tr>
</tbody>
</table>

The main disadvantage of geostationary satellite is their images are of low vertical resolution due to their high orbital altitudes. In addition, the datasets from this type of weather satellites are only able to cover a certain area.

In addition to these sun-synchronous polar-orbiting and geostationary satellites, many other LEO satellites have also been launched for the purpose of monitoring climate. For example, the USA carried out the Earth Observing System (EOS) programme with the aim of modelling climate change. Many satellites have been launched from this programme to sense climate including ocean, greenhouse gases, ozone, etc [Edwards et al., 2004; Lombard et al., 2007; Ramapriyan et al., 2010; Schoeberl et al., 2004]. The EOS programme has also developed a set of space-borne instruments and a data system to obtain highly accurate, frequent, and global measurements of geophysical properties of land, oceans, and the atmosphere [Justice et al., 1998; Waters et al., 2006]. In addition to the satellites from the EOS programme, many other satellites have been launched and operated by other organisations. For example, the HaiYang-1 (HY-1) and HY-2 satellites from the Chinese National Satellite Ocean Application Service (NSOAS) , were launched for the purpose of ocean monitoring [Jin et al., 2010]; the Gravity Recovery and Climate Experiment (GRACE) were launched by NASA and DLR (Deutsches Zentrum für Luft- und Raumfahrt – German Centre for Aerospace) to study the gravity of the Earth and the profiling of the temperature and humidity of the Earth’s atmosphere in March 2002. All of these LEO satellites provide us opportunities to study climate from multiple disciplines.
The most distinctive advantage of weather satellites is their global/large-scale coverage of data records. However, the atmospheric data provided by them usually contain large uncertainties/errors. For example, the quality of data records from Microwave Sounding Unit (MSU) or its advanced instrument (AMSU), which is the most commonly used sensors by weather satellites, is largely affected by the errors of orbital decay, diurnal cycle drift effects, inter-satellite bias removal and merging procedure [Fu and Johanson, 2004; Wentz and Schabel, 1998; Zou et al., 2009]. Although numerous efforts have been made to mitigate the uncertainties of the MSU/AMSU data [Zou et al., 2006; Zou et al., 2009], data records from MSU/AMSU still contain larger uncertainties than many other observation data. For example, Ladstädt er. et. al. [2011], assessed the differences in lower stratospheric temperature records from MSU/AMSU, radiosondes and GPS RO and found that, after correcting the sampling errors, the data records from radiosonde and GPS RO are highly consistent. The differences between the data records from MSU/AMSU and those from other two observation methods were found large. This is due to the fact that the MSU/AMSU data are of lower vertical resolution (typically more than 5 km) than the other two types of data, and the low vertical resolution further results in missing important features of the vertical atmospheric structure. In addition, the MSU/AMSU data are also not suitable for tropopause study which requires observation data of high vertical resolution.

2.3 GPS and its applications in meteorology

2.3.1 Introduction of GPS

The GPS is a US–owned utility that provides users with positioning, navigation, and timing services. The system consists of three segments: the space, control and user segments. The space segment is composed of 24 satellites within six equally-spaced orbital planes surrounding the Earth (see Figure 2.2). These satellites circulate the Earth twice a day with an altitude of about 20, 200 km. The design of the constellation ensures that at least four satellites can be observed anywhere on the Earth. The requirement for four satellites is the minimum observation requirements for positioning. Apart from these 24 satellites, there are several other satellites in the system and they are used to replace the decommissioned satellites when necessary [Hofmann-Wellenhof et al., 1997].

The GPS control segment includes a master station, 16 monitoring stations and four GPS ground antennas. The master control station performs the primary control segment functions, providing command and control of the GPS constellation. It also generates and uploads navigation messages and ensures the health and accuracy of the satellite constellation. The monitoring stations are mainly used for tracking GPS satellites and send the tracked information to the master control station. The ground antennas are used for the communication with the GPS satellites for command and control purposes.
The user segment includes GPS receivers and other related observation instruments. The receivers use the signals from the GPS satellites and then calculate positions at the users’ end.

GPS measurements are based on two stable carrier signals in L-band, denoted as L1 and L2, the frequencies of which are 1575.42 MHz and 1227.60 MHz respectively. The wavelengths of L1 and L2 are 19.0 cm and 24.4 cm. Two Pseudo-Random Noise (PRN) codes are modulated onto the carrier signals: the coarse/acquisition code (C/A-code) and the precision code (P-code). The P-code is modulated on both L1 and L2 signals, while the C/A code is only modulated on the L1 signal. The power of C/A code is 3dB stronger than the power of the P-code. These two codes are used in measuring the distances from the GPS satellites to the receiver. In addition to these two codes, the navigation message, which include the satellites’ orbits, GPS clock error, ionospheric error as well as other information, are also modulated onto the two signals.

In concept, the GPS observables are ranges deduced from measured time or phase differences based on a comparison between emitted signals and received signals. Receivers can generate replica signals which have the same frequency and the same fractional phase of the GPS signals at the emission time. Using the replica signals, and the signals received at the user’s end, the range between the observed GPS satellite and the receiver could be determined. The determination of a range uses the clocks of the GPS transmitter and the receiver. Since both of the two clocks are biased from the time defined by the GPS system, the resulting ranges are also called pseudoranges. Measurements rely on measured time are called code pseudoranges and measurements rely on measured phase differences are called phase pseudoranges.
A code pseudorange is calculated by multiplying the time difference $\Delta t$ with the speed of light $c$:

$$R = c\Delta t = c(t_R - t^S)$$  \hspace{1cm} (2.1)

where $t_R$ is the reading of the receiver clock at signal reception time and $t^S$ is the reading of the satellite clock at signal emission time. Due to the instabilities of transmitter and receiver clocks, their time readings are biased from the time of the GPS system. Accounting the clock errors, Eq. (2.1) can be rewritten as:

$$R = c(t_R(GPS) - \delta_R) - (t^S(GPS) - \delta^S) = c(t_R(GPS) - t^S(GPS)) + c(\delta^S - \delta_R) = \rho + c\Delta \delta$$  \hspace{1cm} (2.2)

where $t_R(GPS)$ and $t^S(GPS)$ are the emission and reception time based on time of GPS system, respectively. $\delta_R$ and $\delta^S$ are the delays of the transmitter and receiver clocks with respect to the GPS system time; $\Delta \delta = \delta^S - \delta_R$ denotes the total clock error, $\rho$ is the geometric distance between the transmitter and the receiver and is calculated by the coordinates of both transmitter and receiver.

Equation. (2.2) is also called the observation equation. In fact, the range $R$ is also affected by other effects in terms of the ionospheric delay, neutral atmospheric delay, etc. These errors are not included in the observation Eq. (2.2), but they are needed to be accounted for in using the range for GPS applications. For the detail of the effects of these errors on the range observations and the mitigation approaches for these errors, Hofmann-Wellenhof et al., [1997] can be consulted. In GPS positioning, which is one of the conventional GPS applications, the coordinates of the receivers are unknowns and they can be derived by using several observation equations from different GPS satellites.

The calculation of phase pseudorange starts from calculating beat phase ($\varphi^S_R$) which is the difference between the phases at the emission time and the reception time. If no loss of signal occurs, the beat phase can be expressed by the measureable fractional beat phase and an unknown initial integer number ($N$):

$$\varphi^S_R(t) = \Delta \varphi^S_R |_{t_0} + N$$  \hspace{1cm} (2.3)

where $\Delta \varphi^S_R |_{t_0}$ denotes the measureable fractional phase at epoch $t$ augmented by the number of integer cycles since the initial epoch to $t_0$. Based on the beat phase, the phase pseudorange ($\Phi$) can be expressed as:

$$\Phi = -\Delta \varphi^S_R$$
$$= \frac{1}{\lambda} \rho + \frac{c}{\lambda} \Delta \delta + N$$  \hspace{1cm} (2.4)
Equation (2.4) is the observation equation for the phase pseudorange. The phase pseudorange is much more accurate than the code pseudorange. The observables of the phase pseudorange and the code pseudorange are the basis for the applications of the GPS. The phase pseudorange is used in the GPS RO and the detail of how to use it in RO is elaborated in Section 3.2.

2.3.2 Ground-based GPS technique

The ground-based GPS technique has been used to remote sensing water vapour since the early 1990s. Before this technique, two commonly used methods for water vapour sensing are radiosondes and radiometers. The radiosonde can provide humidity information with high vertical resolution. However, as mentioned in Section 2.1, due to the limited coverage of radiosonde data, measurements from radiosonde are only suitable for regional water vapour study. Radiometer is a device for sensing the water vapour. According to the location, radiometer can be categorised into ground-based, upward-looking water vapour radiometers (WVRs) and the space-based downward-looking WVRs. The ground-based WVRs measure the background microwave radiation produced by atmospheric water vapour using radio signals. The measured frequency dependence sky brightness temperature allows the calculation of integrated water vapour (IWV) and integrated liquid water (ILW) along a given line of sight. Since the sky brightness temperature varies with season and site, the algorithm for the retrieval of IWV and ILW is complicated and the results may not be accurate. The space-based WVRs have some similarities in retrieving IWV and ILW with the ground-based WVRs. The difference is, the ground-based WVRs measure water vapour emission lines against the cold background of space, while the space-based WVRs measure the corresponding absorption lines in the radiation from the hot background provided by the Earth. Due to the significant variation of temperature over land, the retrieval of IWV is complicated and rather inaccurate. Over the oceans, where the changes of temperature are less, the results are better. Both the ground-based and space-based WVRs are not robust in atmospheric regions where there are heavy clouds.

The principle of the ground-based GPS technique is to utilise the delay of the GPS signals caused by the neutral atmosphere to calculate a time-varying zenith wet delay (ZWD) through a stochastic filtering process. Given surface temperature and pressure readings at the GPS receivers, the obtained ZWD can be transformed with very little additional uncertainty into an estimate of IWV overlying that receiver which later allows for the calculation of perceptible water (PW) [Bevis et al., 1994; Rocken et al., 1995]. The IWV and PW retrieved from the ground-based GPS meteorology has been proved to be a useful source of humidity information for NWP systems [Deblonde et al., 2005; Kuo et al., 1993].

Due to the robustness that the ground-based GPS technique has shown in studying the distribution of water vapour, many networks of continuously operating reference stations (CORS) are being
constructed around the world nowadays [Adams et al., 2011; Bock et al., 2007]. The number of CORS stations is much larger than the number of radiosonde stations in the world. For example, in the state of Victoria, Australia, there are about 110 ground-based GPS CORS stations, while there are only two radiosonde stations in the same area. The large number of the ground-based CORS stations enables scientists to study water vapour distribution in a larger geographical scale with a dense horizontal resolution.

2.3.3 Space-based GPS RO technique

The RO technique is a limb sounding technique to provide atmospheric profiles of a planet. This technique exploits the atmospheric refraction of the signals to retrieve atmospheric profiles. The RO technique was initially applied to probe the atmosphere of Venus, Titan and other outer planets [Fjeldbo et al., 1971; Kliore and Patel, 1980; Lindal et al., 1983]. With the advent of the first satellite navigation system, i.e. GPS, the RO technique was then used to sense the properties of the Earth’s atmosphere.

The first opportunity to demonstrate the RO technique for the Earth’s atmosphere was the MicroLab-1 satellite from the GPS/Meteorology (GPS/MET) experiment in 1995 [Hocke, 1997; Ware et al., 1996]. The altitude of this satellite is about 750 km and it circulates the Earth every 100 minutes. This experiment provides about 150 occultation events per day. The retrieved atmospheric profiles have demonstrated the properties of high vertical resolution which is about 1.5 km in the stratosphere and from 0.1 km to 0.5 km in the lower troposphere [Hocke, 1997; Rocken et al., 1997; Steiner et al., 1999]. The horizontal resolution of the retrieved atmospheric profiles is about 300 km. The atmospheric profiles also reveal high quality in the Upper Troposphere and Lower Stratosphere (UTLS) regions. Comparing atmospheric profiles retrieved from GPS/MET observations with other observation data, it has been shown that the mean agreement of temperature profiles between GPS/MET data and other observation data is about 1 K in the altitude range from 1 km to 40 km [Rocken et al., 1997]. Researches have shown that the assimilation of GPS/MET bending angles improves the temperature and specific humidity analysis above 850 mbar [Liu et al., 2001]. The success of the GPS/MET experiment reveals the potential usage of the RO technique in observing the Earth’s atmosphere.

Although the GPS/MET experiment is very successful, it still has some weaknesses. For example, the presence of significant amount of water vapour in the lower troposphere prone to be lost track in that region, and the number of occultation events per day is insufficient for meteorological study. These weaknesses are improved by following-on RO missions, which not only largely increase the number of occultation events but also improve the quality of the RO results. In the following paragraphs, some commonly used RO missions are introduced.
CHAMP The CHAllenging Minisatellite Payload (CHAMP) satellite was launched in July, 2000 by Germany and US [Reigber et al., 2002]. It carries a BlackJack receiver developed by the Jet Propulsion Laboratory (JPL), which is more powerful than the receiver on the MicroLab-1 satellite and enables sounding well in the lower troposphere. The CHAMP satellite provides about 230 RO events per day and 150 of them are of good quality. The retrieved atmospheric profiles are of good quality in the UTLS regions. The mean temperature biases of CHAMP profiles with respect to the climatology data are less than 0.4 K in the height range from 10 km to 35 km and their standard deviations are about 1 K at 10 km, and 2 K at 30 km [Wickert et al., 2001; Wickert et al., 2004]. Research show that the assimilation of the CHAMP retrieved atmospheric profiles has positive impacts on the products from atmospheric data assimilation and also NWP system [Aparicio and Deblonde, 2008; Healy et al., 2005; Lösch et al., 2006]. Figure 2.3 shows the global distribution of CHAMP RO events for an example day of 15 July, 2008. This picture is plotted based on the atmospheric profiles without moisture information (atmPrf) provided by CDAAC. It should be noted that, the number of RO events is in fact much more than that shown in Figure 2.3. However, some of the RO measurements are rather noisy and are discarded. The events shown in Figure 2.3 are those with good quality and can be used for climate study.

Figure 2.3 The distribution of occultation events from CHAMP satellite on 15 July, 2008

GRACE The Gravity Recovery and Climate Experiment (GRACE) mission was carried out in 2002. Figure 2.4 shows the distribution of GRACE satellites for an example day on 15th January, 2008. Both CHAMP and GRACE satellites, formed as a satellite configuration, produce more than 300 occultation events per day. Research shows that the combination of CHAMP and GRACE
profiles agree well with the climatology model data since only little refractivity bias with a small standard deviation is found in the altitude range from 5 km to 30 km [Wickert et al., 2005; Wickert et al., 2006]. Both CHAMP and GRACE missions have two ground stations that receive GPS signals for double-difference process to remove satellites’ clock errors on the RO observations [Beyerle et al., 2005; Wickert et al., 2002].

![Figure 2.4 The distribution of occultation events from GRACE satellite on 15 July, 2008](image)

Although, the RO results from CHAMP and GRACE satellites have been improved, there still exist many problems. Firstly, the total number of occultation events is still too small for accurate meteorological study. For the atmospheric study and also weather prediction, the more the number of occultation events in a certain region (e.g., 5°×5° lat/lon cells) is, the more accurate the data in the meteorological study. However, as can be seen from Figures 2.3 and 2.4, many regions are still not covered by occultation events. Secondly, the retrieved atmospheric profiles from CHAMP and GRACE are still rather noisy, especially in the lower troposphere. These problems limit the usage of RO data in climate monitoring and weather prediction.

**COSMIC** The Constellation Observing System for Meteorology Ionosphere & Climate (COSMIC) satellites were launched by Taiwan and US in 2006 [Anthes et al., 2008; Rocken et al., 2000; Wu et al., 2005]. This mission includes a constellation of six satellites with orbits of about 800 km. The six satellites provide about 2500 profiles per day which largely increase the number of occultation events per day [Anthes et al., 2008]. Figure 2.5 shows the distribution of occultation events from COSMIC satellites for the same example day as Figures 2.3 and 2.4.
The COSMIC mission also implements an open-loop (OL) technique to track GPS signals in the lower troposphere [Kuo et al., 2004; Sokolovskiy, 2001]. Using the OL tracking technique, RO soundings are significantly improved in the lower troposphere than the Phase Locked Loop (PLL) which is used by many previous missions. It was also found that the negative refractivity biases in lower troposphere presented in previous missions using PLL tracking is significantly reduced in the refractivity retrievals from the COSMIC mission [Anthes et al., 2008]. More than 70% of the COSMIC soundings are able to penetrate below 1 km over the sea surface and also in tropics where a large amount of water vapour exists. The COSMIC RO retrievals have also been used to determine the depth of the planetary boundary layer and the results are consistent with those obtained from ECMWF analysis fields [Guo et al., 2011]. This again proves that the penetration of COSMIC RO soundings is excellent since the height of PBL usually ranges from 100 m to 3 km which is rather low. In addition, COSMIC mission is the only mission currently available that is dedicated to the RO purpose only.

**MetOp** The Meteorological Operational Satellite programme (MetOp) includes three satellites: MetOp-A, MetOp-B and MetOp-C. The MetOp-A and MetOp-B satellites were launched in October 2006 and September 2012, respectively. The MetOp-C satellite is proposed to be launched in 2016. RO data records now available at CDAAC only include those from MetOp-A. The MetOp series satellites, as mentioned in Section 2.2, are sun-synchronous polar-orbiting weather satellites, and they carry the AMSU and other instruments for weather sounding. However, these satellites also carry GPS receivers to sense the Earth’s atmosphere using the RO technique. This is similar to many other LEO satellites, e.g., CHAMP and GRACE, these satellites were not only used for sensing the

![Figure 2.5 The distribution of occultation events from COSMIC satellites on 15 July, 2008](image)
atmosphere using the RO technique, but are also used for Earth’s gravity field study. A satellite can usually carry many different instruments for different meteorology studies.

The MetOp satellites use the GRAS (Global Navigation Satellite Receiver for the Atmospheric Sounding) instrument to receive GPS signals [Loiselet et al., 2000; Luntama, 2006; Luntama et al., 2008]. The GRAS instrument has the characteristics of wide antenna coverage, a high signal-to-noise ratio and an ultra-stable clock reference [Bonnedal et al., 2010]. It tracks GPS signals in a closed loop mode in atmospheric regions when the signal-to-noise ratio is high and track signals in an open-loop mode where the signal-to-noise ratio is low. Due to the robustness of the GRAS instrument and also the setup of the MetOp satellites, atmospheric profiles are found of high quality and accuracy based on the study of MetOp-A satellite data [von Engeln et al., 2011; von Engeln et al., 2009]. The number of MetOp occultation events is almost twice that of a single COSMIC satellite. Figure 2.6 shows the distribution of MetOp-A satellite on 15 July, 2008.

![Figure 2.6 The distribution of occultation events from MetOp-A satellites on 15 July, 2008](image)

In addition to the currently available GPS RO missions, there are many other planned missions. The COSMIC-2 mission will launch six satellites into low-inclination orbits in 2016 and six satellites into high inclination orbits in 2018. These satellites will carry advanced radio receivers named TGRS for TriG (Tri-GNSS) GNSS Radio-occultation system, developed by the Jet Propulsion Laboratory (JPL). This new payload will be able to track up to 12,000 high-quality profiles per day once all the 12 satellites are in orbit.

All these current and future RO missions provide us a great opportunity to study the climate of the Earth with long-term data records. Table 2.3 lists most of the past, current and planned RO missions.
Table 2-3 A list of the past, current and planned RO missions

<table>
<thead>
<tr>
<th>RO mission</th>
<th>Launched time</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Microlab-1/GPS/MET</td>
<td>April, 1995</td>
<td>Decommissioned</td>
</tr>
<tr>
<td>Ørsted</td>
<td>Feb, 1999</td>
<td>Decommissioned</td>
</tr>
<tr>
<td>SUNSET</td>
<td>Feb, 1999</td>
<td>Decommissioned</td>
</tr>
<tr>
<td>CHAMP</td>
<td>July, 2000</td>
<td>Decommissioned</td>
</tr>
<tr>
<td>FedSat</td>
<td>December, 2002</td>
<td>Decommissioned</td>
</tr>
<tr>
<td>SAC-C</td>
<td>November, 2000</td>
<td>Operational</td>
</tr>
<tr>
<td>GRACE</td>
<td>March, 2002</td>
<td>Operational</td>
</tr>
<tr>
<td>COSMIC</td>
<td>April, 2006</td>
<td>Operational</td>
</tr>
<tr>
<td>MetOp-A</td>
<td>October, 2006</td>
<td>Operational</td>
</tr>
<tr>
<td>TerraSAR-X</td>
<td>June, 2007</td>
<td>Operational</td>
</tr>
<tr>
<td>Oceansat-2</td>
<td>Sep, 2009</td>
<td>Operational</td>
</tr>
<tr>
<td>MetOp-B</td>
<td>Sep, 2012</td>
<td>Operational</td>
</tr>
<tr>
<td>FY-3</td>
<td>2013</td>
<td>To be launched</td>
</tr>
<tr>
<td>MetOp-C</td>
<td>2016</td>
<td>To be launched</td>
</tr>
<tr>
<td>COSMIC-2</td>
<td>2016, 2018</td>
<td>To be launched</td>
</tr>
</tbody>
</table>

The key characteristics of the GNSS RO technique are summarised as follows:

**Vertical and horizontal resolution** The RO data are of high vertical resolution and low horizontal resolution. The vertical resolution ranges from about 1.4 km in the middle atmosphere to about 0.5 km in the lower troposphere and this is a much better vertical resolution than that of AMSU data. The horizontal resolution is about 300 km which is rather low. The reason to that is the RO measurement is an integrated effect over the entire ray path from GPS to LEO satellites, thus, the horizontal resolution is determined by the distance traversed by the radio path as it enters and exits an atmospheric layer within a certain vertical resolution; since the ray path is generally rather large, the resultant horizontal resolution is also large [Kirchengast, 2004; Kursinski et al., 1997; Syndergaard, 1999].

**Self-calibration** In GPS RO technique, the atmospheric profiles are not derived from absolute phase delays, but from Doppler shifts (phase changes) which is un-attenuated and rather stable during the short RO measurement time (1~2 minutes). Therefore, RO measurements are long-term stable and can be combined together without the need of inter-calibration if the same data processing system is used [Ho et al., 2009; von-Engeln, 2006]. The RO derived climatologies from multiple satellites are consistent with each other [Foelsche et al., 2009; Foelsche et al., 2011].

**Geographical coverage** The number and geographic distribution of the measured RO events within a given time period, e.g., per day, depends on the number and positions of satellites and
receiver sensors involved in an occultation observing system. So far, the global coverage of RO events has been achieved by all the past and existing events and the global coverage will still be ensured with the future RO missions.

**Accuracy** The RO atmospheric retrievals are most accurate in the UTLS regions, where temperature is within 1K. At higher altitudes, the accuracy of the atmospheric retrievals is degraded by residual ionospheric effects and other observational errors. At lower altitudes, the accuracy of the retrievals is degraded by multipath effects which are mainly caused by water vapour.

The GPS RO technique has distinctive advantages of high vertical resolution and accuracy, self-calibration and global coverage. These characteristics make the RO data suitable for atmosphere study. However, the disadvantages of the RO data are also obvious. Firstly, refractivity suffers from a water vapour ambiguity, the retrieval of atmospheric variables always needs priori information. Secondly, only limited atmospheric parameters can be retrieved, i.e., temperature, pressure, density and humidity. Therefore, the GPS RO technique is complemented by its generalization which is discussed in Section 2.3.4.

### 2.3.4 Advancement of the GPS RO technique - LMIO

The LMIO (Figure 2.7), which is the combination of the LEO-LEO microwave occultation (LMO) and the LEO-LEO infrared-laser (LIO) techniques, utilises signals between two LEO satellites to retrieve atmospheric profiles [Kirchengast and Schweitzer, 2011]. The LMO technique uses microwave signals of centimetre- and millimetre-wavelength between LEO satellites to exploit atmospheric profiles, such as refractivity, temperature and humidity [Herman et al., 2004; Kirchengast and Hoeg, 2004; Kursinski et al., 2004; Kursinski et al., 2002; Schweitzer et al., 2011b]. Different to the GPS RO technique which needs auxiliary data to retrieve atmospheric profiles in moist regions, the LMO technique requires no auxiliary data. The reason is that the LMO exploits frequencies (22 GHz and 183 GHz) at the wings and near the line centre of absorption lines of water vapour [Schweitzer et al., 2011b]. Therefore, the signals are sensitive to both refraction and absorption, while the signals from GPS RO, which is in L-band (19.0 cm and 24.4 cm) are only sensitive to refraction (except signals in the lower troposphere). Using the observed amplitude attenuation of each transmitted signal during an occultation event, the absorption coefficient profile can be derived which provide accurate constrain on the water vapour. The water vapour, together with the measured atmospheric refractivity (derived from refraction) allows the calculation of temperature, pressure and humidity.

The LIO technique uses infrared-laser signals with 2 to 2.5 μm wavelength to sense atmosphere and retrieve greenhouse gases (e.g., CO₂, CH₄) and line-of sight wind profiling [Kirchengast and
Schweitzer, 2011; Proschek et al., 2011; Schweitzer et al., 2011a]. Frequency channels for different greenhouse-gases are also different [Kirchengast and Schweitzer, 2011].

Figure 2.7 The concept of LMIO technique (from Kirchengast and Schweitzer, 2011)

According to simulated results, the accuracies of the retrieved temperature, pressure and humidity profiles from LMO are < 0.5 K, < 0.2% and < 10% root-mean-square (R.M.S), respectively [Schweitzer et al., 2011b]. The results of greenhouse gases from LIO are <1% to 3% R.M.S error [Kirchengast and Schweitzer, 2011; Proschek et al., 2011]. These encouraging results indicate that the LMIO method has potential for benchmarking climate monitoring. Although by the early 2013 there is none LMO mission in operation, from current simulated study, the LMO technique is believed to be of great importance for climate study. The LIO experiment has been prepared based on two ground stations. It is expected that a real LMIO satellite mission could be carried out in 2016.

Both the LMO and the LIO are advancements on the current GPS RO technique and share the same characteristics with the GPS RO technique. These two techniques complement the GPS RO technique by allowing accurate retrieval of atmospheric profiles (refractivity, temperature and humidity) in the moist lower troposphere and retrieval of greenhouse gases profiles.

2.4 Atmospheric data assimilation and ECMWF products

The atmospheric data assimilation combines observation data with short period forecast data (typically 6 hours) to give an optimal estimate of the state of the atmosphere (e.g., temperature,
pressure) called analysis fields. Analysis products that are most often used by researchers are those from European Centre for Medium-Range Weather Forecasts (ECMWF) [Uppala et al., 2005] and National Centers for Environmental Prediction (NCEP) [Kalnay et al., 1996]. Observations that are used for data assimilation include data from radiosonde stations, ships, buoys, weather satellites, etc. Since 2006, RO measurements have been integrated into the ECMWF four-dimensional variational assimilation system [Healy and Thépaut, 2006] and RO measurements have also been used in the data assimilation system at the NCEP [Cucurull and Derber, 2008]. In the data assimilation, different types of observations as well as the forecast data have different accuracies, thus their weights are assigned differently in the optimal estimation, depending on their errors (or uncertainties). The obtained analysis data are then used in NWP system to produce forecast data for a period, e.g. for a medium range forecast of 3-6 days. The forecast data are then updated and combined with the observation data in the same period to produce the analysis data for the period. Due to variables from the analysis fields are rather accurate and are global distributed, they are often used as the references of other observation data.

In this thesis, analysis and forecast data from ECMWF will be used as references of RO retrieved atmospheric profiles and background information for the RO data processing, respectively. Currently, the highest horizontal resolution of ECMWF products is T1279 (spectral representation with triangular truncation at wave number 1279), which is about 0.125° in latitude. Data records with other horizontal resolutions are also available, such as the T42 data used in this thesis. The horizontal resolution of T42 data is about 2.5° in degree and about 300 km in distance. The main reason for the ECMWF T42 data is used in this thesis is that their horizontal resolution is close to that of RO data. The finest vertical resolution of ECMWF data is 91 levels from the surface to about 80 km [Untch et al., 2006]. The vertical levels above 60 km, especially above 70 km are rather sparse, while the levels in the lower troposphere are denser. Data of other vertical levels are also available, e.g., 60 levels, however, the 91 levels data are used in this thesis to capture more accurate vertical atmospheric information.

The ECMWF analysis fields are usually generated at 00, 06, 12 and 18 UTC (Universal Time Coordinated). The forecast data used is 24-hour forecast data and they are generated at 00 and 12 UTC time.

It should be noted that, the reason that using forecast data to provide background information in the RO data processing rather than using analysis data are the RO data has been assimilated into the analysis fields since 2006. Although, the forecast data are produced based on the analysis data, they are believed to be less correlated with the RO data and can be used as background.
2.5 Summary

This chapter introduces two of the most commonly used atmospheric methods radiosonde and weather satellite. The measurements from radiosonde are rather accurate and also of high vertical resolution. However, due to the considerable cost of radiosonde launches and also geographical accessibility, the data are rather sparse and can only be used for regional climate and weather study. Weather satellites have been a major advancement in the history of atmospheric observations. They can observe the Earth’s atmosphere on a global-scale. Weather satellites carry many different types of instruments to sense the atmosphere. The most commonly used instrument is the MSU/AMSU. However, data from MSU/AMSU are of low vertical resolution which can not capture important features of the vertical atmospheric structure.

Since the 1990s, the GPS has been used in the study of meteorology. According to the location of GPS receivers, the GPS meteorology could be divided into ground-based GPS meteorology, and space-based GPS RO technique. The ground based-GPS meteorology has been proved to be robust in the study of water vapour distribution. The GPS RO exploits the atmospheric refractions of the GPS signals to provide accurate atmospheric profiles, refractivity, temperature, density and pressure. Due to the properties of high-vertical resolution, self-calibrating and global coverage, the GPS RO data has been widely used in atmosphere study. The GPS RO technique is more robust in the dry air condition (above 8 km at the polar regions and above 14 km at the tropics). In moist atmospheric regions, it could be complemented by the LMIO technique which is an atmospheric sounding method between two LEO satellites. The LMIO includes the LMO and LIO. The LMO occultation utilizes microwave signals to sense temperature, pressure and humidity without the need of “a priori” information. The LIO occultation utilizes infrared-laser signals to sense greenhouse gases. Currently, there are no satellite missions for the LMIO technique, but this kind of missions attracts much attention.

To conclude, the RO technique has demonstrated a great potential in climate monitoring, numerical weather prediction and space weather research. Therefore, it is selected as the research topic of this thesis. Next chapter will discuss the detail of the RO data processing.
Chapter 3. GPS RO Technique for Atmospheric Retrievals

This chapter presents the GPS RO algorithms for retrieving atmospheric profiles. The propagation of GPS signals through the atmosphere obeys Maxwell’s equations in which the propagation medium is characterised by a three-dimensional spatial distribution of a complex and dispersive refractive index [Melbourne et al., 1994]. For GPS signals, it is reasonable to assume that the refractive index has zero absorption and the signals are monochromatic. In addition, for most of the atmospheric regions, the wavelengths of GPS signals are much smaller than the scale of atmospheric structure. Due to these reasons, for most part of the atmosphere, it is reasonable to invert atmospheric profiles based on the Geometric Optics (GO) approximation in which GPS signals are approximated as rays passing through the atmosphere and are refracted according to Snell’s law.

However, in the lower troposphere where significant amount of water vapour exists, the approximation of GO is not reasonable anymore. In this case, the Wave Optics (WO) method is often used to retrieve atmospheric profiles. WO methods that have been proposed include the back-propagation [Gorbunov and Gurvich, 1998], radio-optics [Sokolovskiy, 2001], Fresnel diffraction theory [Mortensen and Høeg, 1998], Canonical transform [Gorbunov, 2002], and Full Spectrum Inversion methods [Jensen et al., 2003], and eikonal acceleration technique [Pavelyev, 2009] etc.

This thesis focuses on the retrievals of atmospheric profiles in the height regions above 20 km where there is not much water vapour. Therefore, it is reasonable to use some formulas which are found based on GO approximations, such as Snell’s law, Bouguer’s rule and Fermat’s principle, to accurately retrieve atmospheric profiles. Section 3.1 introduces the measurement principle of the GPS RO technique; Section 3.2 to Section 3.8 introduce the retrieving algorithms using the principle of GO, and retrieved profiles from an example RO event are used to illustrate the properties of the RO profiles. The software used to retrieve the example COSMIC events is the EGOPSv2951 (End-to-End Generic Occultation Performance Simulation and Processing System version 2951) software package developed by WEGC of University of GRAZ. A summary is given in Section 3.9.

3.1 Measurement principle of the GPS RO technique

The RO technique sets specially designed GPS receivers onboard LEO satellites to receive GPS signals. These receivers usually collect GPS signals at a 50 Hz sampling rate. According to the
direction of the relative motion between the GPS and LEO satellites, the atmosphere is scanned either from top downwards (setting RO event) or from bottom upwards (rising RO event). The instantaneous geometry of the RO technique at each sampling time could be approximated as a single ray passing through the atmosphere from the transmitter to the receiver. Figure 3.1 illustrates the geometry of an occultation event.

![Figure 3.1 The geometry of an occultation event](image)

In this figure, only three example rays from the transmitter to the receiver are shown. An occultation event usually lasts about 1–2 minutes, therefore there are a large number of rays (e.g., more than 2000 rays) for an occultation event. When a GPS ray passes through the atmosphere, it is refracted due to the gradient of the refractive index in the atmosphere. The overall effects of the atmosphere on a ray could be subjected to a small total bending angle $\alpha$, as shown in Figure 3.1. The refraction also causes a delay in the arrival time of the ray at the receiver, compared to the arrival time in a vacuum. In Figure 3.1, $L$ represents the real path of a GPS ray in the atmosphere, $\rho$ represents the geometric distance between the GPS and LEO satellites. Using $L$ and $\rho$, the excess phase $\Delta L$ could be calculated:

$$\Delta L = L - \rho$$ (3.1)

The excess phase together with the orbits of both GPS and LEO satellites allows the calculation of the ray’s bending angle $\alpha$ based on the principle of Geometric Optics (GO). The derived bending angle for all the rays of an occultation event yields a set of bending angles at different heights of the atmosphere which form a near vertical profile. The bending angle profile can then be used to calculate
refractivity profile which could be then used for the calculation of atmospheric profiles, such as temperature, atmospheric density and pressure. The following sections will elaborate the algorithms of retrieving these atmospheric profiles step by step.

### 3.2 Derivation of GPS RO excess phase

The first step of the RO data processing is to derive the excess phase shown in Eq. (3.1), in which \( \rho \) can be easily calculated via:

\[
\rho = \sqrt{(X_{GPS} - X_{LEO})^2 + (Y_{GPS} - Y_{LEO})^2 + (Z_{GPS} - Z_{LEO})^2}
\] (3.2)

where \( X_{GPS}, Y_{GPS}, Z_{GPS} \) are the coordinates of GPS satellites and \( X_{LEO}, Y_{LEO}, Z_{LEO} \) are the coordinates of LEO satellites. The coordinates of the GPS satellites can be obtained from satellites’ orbit/ephemeris. The coordinates of the LEO satellites can be obtained from Precise Orbit Determination (POD).

The range \( L \) (L1 or L2) can be calculated using either phase pseudoranges or code pseudoranges. However, since the phase pseudorange (see Section 2.3.1) has a much higher accuracy, it is therefore used in the RO technique to determine the \( L \).

\[
L = \lambda \cdot \Phi
\] (3.3)

The phase range \( L \) contains the effects of the neutral atmosphere, the ionosphere and observational errors, and could be modelled as [Hofmann-Wellenhof et al., 2008; Pirscher, 2010]:

\[
L = \rho + d\rho + c\delta_{LEO} + c\delta_{LEO,sys} + c\delta_{GPS} + c\delta_{GPS,sys} + \\
\lambda N + \varepsilon_{antenna} + \varepsilon_{multi} + \varepsilon_{rel} + \varepsilon_{cycleslips} + \lambda \Phi_{neutral} + \lambda \Phi_{iono} + \varepsilon
\] (3.4)

where \( d\rho \) are the orbit errors of both GPS and LEO satellites; \( \delta_{LEO} \) and \( \delta_{GPS} \) are the clock errors of the GPS and LEO satellites respectively; \( \delta_{LEO,sys} \) and \( \delta_{GPS,sys} \) are the systematic errors of the receiver and transmitter respectively; \( N \) is the unknown initial integer number of phase cycles between the satellite and the receiver, and is called phase ambiguity; \( \Phi_{neutral} \) and \( \Phi_{iono} \) are signal delays induced by the neutral atmosphere and the ionosphere respectively; \( \varepsilon_{antenna} \) is the error caused by the LEO satellite’ antenna phase centre offset and variation; \( \varepsilon_{multi} \) represents the error caused by multiple paths of the GPS signal; \( \varepsilon_{rel} \) is the relativistic effect, \( \varepsilon_{cycleslips} \) is the cycle slip of the GPS signal and \( \varepsilon \) denotes the residual errors.

Moving the term \( \rho \) to the left-hand side of Eq. (3.4) yields the excess phase:

\[
\Delta L = L - \rho = d\rho + c\delta_{LEO} + c\delta_{LEO,sys} + c\delta_{GPS} + c\delta_{GPS,sys} + \\
\lambda N + \varepsilon_{antenna} + \varepsilon_{multi} + \varepsilon_{rel} + \varepsilon_{cycleslips} + \lambda \Phi_{neutral} + \lambda \Phi_{iono} + \varepsilon
\] (3.5)

As can be seen from Eq. (3.5), the excess phase is also affected by error sources which are brought in by the phase pseudorange observation. For the RO technique, only the part of the excess phase that is induced by the neutral atmosphere \( \lambda \Phi_{neutral} \) is used to derive atmospheric variables, hence all the other
terms on the right-hand side of Eq. (3.5) needed to be corrected or mitigated as much as possible. The methods for correcting each of these error terms are discussed below.

**Orbit Error.** The orbit error includes both position error and velocity error. The position errors of GPS and LEO satellites are usually in metre and several centimetre levels respectively. Simulation study shows that the position error of up to 50 cm has no significant effects on the retrieved atmospheric profiles [Kirchengast, 1998]. The velocity errors of GPS and LEO satellites are within 0.05 mm/s and 0.02 mm/s [Schreiner et al., 2010] respectively. Simulation study also shows that a 0.05 mm/s velocity error only introduces very small errors in RO retrievals. Although the orbit error has no significant impact on RO retrievals, it is still needed to use accurate ephemerides of GPS satellites and accurately determined orbit of LEO satellites to process RO observations.

**Clock Error.** Due to the instability and drifts of the frequency oscillators in both LEO and GPS satellites, the clocks of the receiver and the transmitter are not synchronized and thus result in errors in the calculated phase range. The clock errors can be eliminated by double-differencing, single-differencing or zero-differencing techniques.

The double-differencing technique [Hajj et al., 2002; Schreiner et al., 2010] makes use of not only the occulting GPS and LEO satellites, but also another GPS satellite (reference GPS satellite) and another ground GPS station (reference station). The first step of this approach is differencing the two phase observations at the LEO satellite from the occulting GPS satellite and the observations at the reference GPS satellite. This step is called single-differencing at the LEO satellite. The clock error of the LEO satellite is cancelled out in the single-differenced phase observations. Similarly, another single-differenced phase observation received at the ground/reference GPS station from the same occulting GPS satellite and the reference GPS satellite can be obtained. The resultant single-differenced phase observation removes the clock error of the ground/reference station receiver. Finally, the double-differencing is the differencing of the above two single-differenced phase observations, in which the clock errors of both the occulting GPS satellite and the reference GPS satellite are cancelled out. The three steps cancel out all the clock errors associated with occulting GPS and LEO satellites and also the reference GPS satellite and the reference GPS ground station. However, the main weakness of the double-differencing method is that it introduces new errors from the ground GPS station’s observations, such as multipath, residual atmospheric and ionospheric biases, thermal noise etc. [Schreiner et al., 2010]. The effects of these errors on the excess phase cannot be neglected.

To avoid the errors introduced by the ground GPS reference station, the single-differencing approach is preferred by many scientists [Wickert et al., 2002]. In this case, only the clock error of the LEO satellite is cancelled out. The clock errors of the two GPS satellites are corrected by other means, e.g., obtaining the corrections from a 5 minutes clock solution from GPS orbit determination for the
LEO satellite [König et al., 2002]. Although the single-differencing approach does not use the ground station to avoid introducing new errors, it requires extra data management and calculation for the GPS clocks at a high rate, and both tasks are complicated.

An alternative method called zero-difference is introduced by scientists [Beyerle et al., 2005]. This approach can potentially produce lower noise excess phase data than single- and double-differencing by using estimated LEO and GPS clocks. However, this approach requires the receiver on a LEO satellite to have an ultra-stable oscillator [Beyerle et al., 2005]. The GRACE and MetOp are examples where zero-differencing is possible.

**Systematic errors of transmitter and receiver.** The systematic errors refer to errors caused by the hardware of the transmitter and/or receiver, e.g. cables and electronics. Since these two errors are constants for a phase range observation, they will be omitted in the subsequent step when calculating excess Doppler, which is the time derivative of the excess phase.

**Phase ambiguity and cycle slip.** In GPS phase observations, the difference between the received and the transmitted phases, i.e. $\varphi_r - \varphi_t$ (Eq. (3.3)), is called beat phase. The beat phase consists of a fractional part which is less than 2π and an initial integer counter $N$ which is incremented by one cycle whenever the fractional phase changes from 2π to 0. Since this $N$ cannot be directly obtained from the phase observation, it is called phase ambiguity. If no loss of signal tracking occurs, the value of $N$ remains the same integer number during the measurement. In high accuracy positioning, $N$ needs to be estimated and fixed. However, in RO, which favours the knowledge of the excess Doppler, the integer phase ambiguity will be omitted.

In ionospheric region where there are large vertical electron density gradients and in lower troposphere where there are large atmospheric refractive gradients, GPS receivers may lose track of signals for a short time. In this case, the integer counter $N$ is reinitialised and results in a sudden jump in the instantaneous accumulated phase by an integer number of cycles. The sudden jump in the phase observation is called cycle slip. Cycle slips can be detected by subtracting a predicted value of atmospheric Doppler shifts from the measured one and examine the residuals [Hajj et al., 2002]. If large cycle slips are detected, the corresponding ray is discarded.

**Antenna phase centre offset and variations.** When determining the orbit of a LEO satellite, the centre of mass of the satellite is used as the point for determination. However, the observing point is the GPS receiver antenna’s phase centre. The two points are in different places and the difference is called phase centre offset. In addition, the phase centre varies with elevation, azimuth, intensity of the satellite signals, therefore, each signal received has a unique antenna phase centre. The antenna phase centre offset and variations can be corrected using the coordinates of the satellites and the position of the receiver.

**Multipath error.** Multipath includes local multipath and atmospheric multipath. The atmospheric multipath occurs when GPS signals scatter off from the small-scale atmospheric structures in the...
vicinity of the receiver antenna and results in multiple signals arriving at the receiver. The local multipath creates a slowly varying phase error which further introduces significant errors in atmospheric retrievals [Kursinski et al., 1997]. The local multipath can be mitigated using more directional antennas. The atmospheric multipath, which occurs in the lower troposphere where signals are scattering off from the large refractive gradient, is caused by the existence of water vapour. WO methods are used to retrieve atmospheric profiles in the lower troposphere which mitigate the multipath error in the atmospheric profiles.

**Relativistic effects.** The relativistic effects include both general and special relativity effects. The general relativity effect results from the clocks used by the transmitter and the clock as well as the clock defined in the GPS system operating at places with different gravitational potential. The special relativity effect results from the clocks moving with different velocities. These two effects contribute a frequency shift between the transmitter clock and the receiver clock. If the double-differencing approach is used to eliminate the clock errors, the relativistic effects can be also eliminated. If single-differencing or zero-differencing is applied, then the relativistic effects need to be removed using other approaches. The relativistic effects can be mitigated by empirical models. For example, the periodic relativistic effect between the GPS/LEO satellite clock and proper time can be modelled using GPS/LEO satellite earth-centred inertial position and velocity vectors at signal transmitting time. The gravitational delay can be modelled using the satellite and receiver radial positions at signal transmitting and receiving times, the geometric distance between the GPS and LEO satellites and other constants [Ashby, 2003; Zhang et al., 2006].

**Ionospheric effects.** The first-order ionospheric effect can be eliminated by the following ionosphere-free linear combination of phase ranges observed from L1 and L2 signals at the same sampling time $t$ [Syndergaard, 1999]:

$$L_c(t) = \frac{f_1^2 L_1(t) - f_2^2 L_2(t)}{f_1^2 - f_2^2}$$  \hspace{1cm} (3.6)

where $L_1$ and $L_2$ denote the phase ranges of GPS L1 and L2 signals; $f_1$ and $f_2$ are the two frequencies of GPS signals; and $L_c$ is the combined ionosphere-corrected phase range. This approach assumes that both L1 and L2 signals propagate through the same path. However, due to the dispersive nature of the ionosphere, the paths of L1 and L2 signals are different, thus, the ionosphere-corrected phase range is not optimal.

An alternative approach is to leave the ionospheric contributions in the original phase range observation and remove their effects on the bending angle level using a similar linear combination [Vorob'ev and Krasil'nikova, 1994]. This approach is commonly used to remove the ionospheric effects by most of the RO data processing centres since good results have been obtained. The detail of this approach will be elaborated in Section 3.4.
In principle, after eliminating or mitigating all the above errors (except the ionospheric error which will be corrected at the bending angle level), the excess phase obtained should then be used for the retrieval of bending angle. However, due to the reason that the observational errors can never be fully removed, the remaining errors in the excess phase make the data not plausible for retrieving bending angles. For example, in principle, the excess phase should always be positive since the geometric distance between the GPS satellite and the LEO satellite is the shortest. However, for some RO events, the excess phase may tend to be negative in the beginning of the measurement. This may results from the technical limitation of RO receivers. Therefore, before the excess phases are used for bending angle retrieval, they are applied with some quality control. Commonly used quality control mechanism include replacing negative values with a small positive value, removing outliers, smooth excess phases with regularisation method [e.g., Feng and Herman, 1999; Pirscher, 2010].

After applied with quality control, the resulting excess phase can then be used for the retrieval of bending angles. Figure 3.2 shows the excess phase of an example MetOp RO event (MTPA.2008.197.00.08.G24) after quality control is applied.

![Figure 3.2 Excess phase of an example MetOp RO event after quality control applied.](image)

The left panel shows excess phase in the time range of the whole measurement, the middle panel shows excess phase in the time range of the initial 30 seconds of the measurement, the right panel shows excess phase in the initial 2 seconds of the measurement.

It can be seen from the left panel of Figure 3.2 that this occultation event lasts about 65 seconds. Excess phases range from zero in the beginning to about 1200 m for both L1 and L2 signals. The middle panel shows that the excess phases range from zero to more than 10 m at 30 seconds, and the two excess phases reveal obvious differences in this time range. The right panel shows the excess phases range from zero to about 0.76 m at 2 s for L1 and to about 0.48 m at 2 s for L2. The differences of the two excess phases are caused by the different frequencies of L1 and L2 signals.
3.3 From excess phase to bending angle

After the excess phase is obtained, the excess Doppler $\frac{dL}{dt}$ can be derived by differentiating the excess phases of consecutive samples. For example, in EGOPSv2951 software package, the following 3-point differentiation formula is used [Pirscher, 2010]:

$$\frac{dL}{dt} = \frac{L(n+1) - L(n-1)}{t(n+1) - t(n-1)}$$  \hspace{1cm} (3.7)

where $n$ denotes the $n$th observation, and $t$ is the sampling time.

The excess Doppler can also be expressed as the multiplication of the signal’s wavelength $\lambda$ with the atmospheric Doppler shift $\Delta f$, and the atmospheric Doppler shift is related to the location and velocity of the GPS and LEO satellites. As a result, the excess Doppler can be expressed as [Melbourne et al., 1994]:

$$\frac{dL}{dt} = \lambda \Delta f = \left| \hat{R}_{\text{LEO}} \right| \cos(\varphi(a)) + \left| \hat{R}_{\text{GPS}} \right| \cos(\chi(a)) - \hat{R}_{\text{LEO-GPS}}$$  \hspace{1cm} (3.8)

where $\hat{R}_{\text{LEO}}$ and $\hat{R}_{\text{GPS}}$ are the projections of LEO and GPS velocities onto the occultation plane which is defined by the positions of the two satellites and the centre of refraction; $\varphi$ is the angle between $\hat{R}_{\text{LEO}}$ and the vector of the ray path of the LEO satellite; $\chi$ is the angle between $\hat{R}_{\text{GPS}}$ and the vector of the ray path as seen from the GPS satellite; $\hat{R}_{\text{LEO-GPS}}$ is the temporal deviation of the geometric distance between the LEO and the GPS satellites; $a$ is the impact parameter in meters which is a constant for a ray. Figure 3.3 illustrates these variables.

![Figure 3.3 Geometry of a single RO ray](image-url)
Equation (3.8) assumes that the Earth’s atmosphere is spherical symmetry. Due to the Earth’s oblateness, the centre of the earth is not the centre of symmetry. In this case, the satellites’ positions, which are determined based on the centre of the earth, need to be corrected based on the symmetry centre. The symmetrical centre is also called the centre of refraction and is usually defined as the centre of a circle that is tangent to the earth’s ellipse at the tangent point of the ray path with its radius the same as the radius of curvature of the ellipse at the same tangent point [Syndergaard, 1999]. The tangent point is defined as the point on the ray path that is closest to the earth’s surface. The detail of the correction for the satellite position can refer to other related references [Hajj et al., 2002; Pirscher, 2010; Syndergaard, 1998].

The effects of a planet’s oblateness on radio occultation observations were realised first from the observations of Jupiter’s atmosphere [Kliore et al., 1974; Kliore et al., 1975]. It was found that neglecting the oblateness of Jupiter would cause large errors in temperature observations in the deep troposphere [Eshleman, 1975]. Syndergaard [1998] analysed the error introduced in the atmospheric profiles by neglecting the Earth’s oblateness in the GPS RO technique. It is found that it may introduce a 6 K error in temperature at the surface of the Earth. This suggests that correcting the Earth’s oblateness is significant for high accuracy atmospheric retrievals.

After correcting the satellite positions based on the centre of refraction, one can retrieve the excess Doppler using Eq. (3.8) from which, together with the Snell’s law (the law of refraction) and the occultation geometry as shown in Figure 3.3, the bending angle of the ray can be derived. The Snell’s law states that a ray passing from medium-1 to medium-2 follows the following rule:

$$\frac{\sin \theta_1}{\sin \theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1}$$  \hspace{1cm} (3.9)

where $\theta_1$ is the angle of incidence and $\theta_2$ is the angle of refraction; $v_1$ and $v_2$ are velocities of the ray in medium-1 and medium-2 respectively; $n_1$ and $n_2$ are the corresponding refractive indices of the two mediums.

Under the assumption that the Earth’s atmosphere is spherical symmetry, the Bouguer’s rule which is based on Snell’s law can be used to describe the refraction of a ray [Born and Wolf, 1999]:

$$nr \sin \phi = \text{constant} \equiv a$$  \hspace{1cm} (3.10)

where $r$ is the distance from the centre of refraction to any point of the ray path, $n$ is the local refractive index at the point, $\phi$ is the angle between the ray direction and the vector form of $r$, $a$ is the above mentioned impact parameter and is a constant for a ray. As $r \to \infty$, the refractive index $n \to 1$. As a result, at the location of GPS and LEO satellites where the distance from the centre of refraction to the satellites is large, we have:
where $\phi_{\text{GPS}}$ and $\phi_{\text{LEO}}$ are the angles between the ray path and the radius of GPS and LEO satellites respectively, relative to the centre of refraction (c.f. Figure 3.3). The approximation of Eq. (3.11) only introduces a very small error in the bending angle retrievals induced by the ionosphere, and this error can be cancelled out by the linear combination of L1 and L2 bending angles [Hajj and Romans, 1998].

According to the geometry shown in Figure 3.3 and Eq. (3.11), two angles $\varphi$ and $\chi$ can be calculated by:

$$
\varphi = \zeta - \phi_{\text{LEO}} = \zeta - \arcsin \left( \frac{a}{R_{\text{LEO}}} \right)
$$

(3.12)

$$
\chi(a) = \pi - \eta - \phi_{\text{GPS}} = \pi - \eta - \arcsin \left( \frac{a}{R_{\text{GPS}}} \right)
$$

(3.13)

where $\zeta$ and $\eta$ can be calculated using the coordinates and velocities of the GPS and LEO satellites. Using Eqs. (3.8), (3.12) and (3.13), the impact parameter $a$ can be calculated through an iterative process. Then the bending angle can be calculated by:

$$
\alpha = \pi - (2\pi - \theta - \phi_{\text{GPS}} - \phi_{\text{LEO}}) = \theta - \arccos \left( \frac{a}{R_{\text{GPS}}} \right) - \arccos \left( \frac{a}{R_{\text{LEO}}} \right)
$$

(3.14)

Since the ionospheric correction is not applied at the excess phase level, the bending angle obtained from the L1 and L2 excess phases contains the contributions from both the ionosphere and the neutral atmosphere. The following section discusses the ionospheric correction for the bending angles.

### 3.4 Ionospheric correction for bending angles

The ionospheric correction for bending angles was introduced by Vorob’ev and Krasil’nikova in 1994. Similar to the ionospheric correction approach for the phase ranges, a linear combination of bending angles retrieved from L1 and L2 signals ($\alpha_1$ and $\alpha_2$) at the same impact parameter is used to obtain a ionosphere-corrected bending angle $\alpha_{\text{IC}}$ at that impact parameter:

$$
\alpha_{\text{IC}}(a) = \frac{f_1^2 \alpha_1(a) - f_2^2 \alpha_2(a)}{f_1^2 - f_2^2}
$$

(3.15)

As mentioned in Section 3.2, due to the poor quality of the L2 signal, its bending angle retrieval contains larger noises than that from L1. The noise in $\alpha_2$ is propagated into the ionosphere-corrected
bending angle. In order to reduce the contributions of the noises in $\alpha_2$ to $\alpha_{IC}$, an alternative approach is adopted by some scientists [e.g., Hajj et al., 2002]:

$$\alpha_{IC}(a) = x_4(a) + 1.54x_4(a)$$ (3.16)

where $x_4(a) = \alpha_1(a)$, and $x_4(a) = \alpha_4(a) - \alpha_3(a)$, a standard smoothing is applied for $x_4$ (e.g., a 0.5 s smoothing window, 25 points for 50 Hz sampling data) and a larger smoothing window is applied for $x_4$ (e.g., a 2 s smoothing window, 100 points for 50 Hz sampling data). This approach can provide less noisy ionosphere-corrected bending angle. There also have been some other slightly different approaches to smooth $\alpha_2$ for less noisy ionosphere-corrected bending angles [Pirscher, 2010].

The limitation of linear combination (for both bending angles and phase ranges) to reduce the ionospheric effects is that only the first-order ionospheric effects are eliminated, the high-order ionospheric effects (residual ionospheric effects) remains in the corrected bending angles. The magnitude of the residual effects varies, depending on the strength and location of the regional ionospheric irregularities. Simulation study shows that the higher-order ionospheric effects introduce an error of up to $-0.1 \mu$rad in bending angles in solar maximum conditions [Danzer et al., 2013; Liu et al., 2013; Rocken et al., 2009]. This error in the bending angle will further result in an error of about 0.2% in refractivity at 30 km altitude and 0.5 K error in temperature at the same altitude.

Apart from the residual ionospheric effects, the ionosphere-corrected bending angles are also affected by residual observational errors that have not been mitigated in the phase observations, e.g. errors introduced by the differencing technique which is for removing the clock errors, the remaining orbit error and other observational errors as described in Section 3.2.

A conventional and commonly used method to provide optimal bending angles is statistical optimisation which combines the ionosphere-corrected bending angle with background bending angle in a statistical-optimal way. The background bending angles are usually derived from a climatological model. The statistical optimisation is based on the least squares approach. The weights of the observed bending angle and the background bending angle are based on their estimated error covariance matrices.

Beyond the conventional statistical optimisation approach, many other approaches have been developed to mitigate the errors in the ionosphere-corrected bending angles. Sokolovskiy et al. [2009] suggested a method for mitigating the higher-order ionospheric effects from $\alpha_{IC}$ using an optimal smoothing window for $x_4$ in Eq. (3.16) [Sokolovskiy et al., 2009]. The optimal smoothing window is determined by minimizing the combined effects of the L2 noise and the ionospheric residuals. It was found that this approach can improve the accuracy of RO retrieved profiles in the stratosphere.

An alternative approach for removing the higher-order ionospheric effects was proposed by Danzer et al. [2013]. In her approach, the ionospheric residuals were modelled using simulated bending angle profiles and the modelled residuals were used to correct the higher-order ionospheric
effects. Preliminary results showed that this method can also improve the accuracy of atmospheric profiles.

Although these approaches have been investigated to alleviate the errors in the ionosphere-corrected bending angles, they are mainly proposed to mitigate the residual ionospheric effects. However, the residual ionospheric-effects are the main error sources in the ionosphere-corrected bending angles and the effects of observational errors cannot be neglected. Bending angles obtained from these approaches may still be contaminated by the residual observational errors and thus not to be suitable for high quality refractivity retrievals.

As a result, the conventional statistical optimisation is still a commonly used method to obtain optimal bending angles by major RO data processing centres [Ho et al., 2009]. In fact, the retrieval of refractivity, which uses the Abel integral, requires the bending angles to be available up to infinite. In practice, an upper boundary is selected, e.g., 120 km. However, the RO derived bending angles are usually only available up to 80 km. Therefore, initialisation for bending angles above the top of the observed profiles is also needed and the methods for the initialisation will be introduced in Section 3.5.

### 3.5 High altitude initialisation and statistical optimisation of bending angles

Bending angles in the height range from the top of the observed profile to the selected upper boundary are initialised by those derived from a background model. From the top of the observed profile to a lower boundary (e.g., 30 km), bending angles are initialised/optimised through the statistical optimisation. Since the statistical optimisation is the focus of this thesis, a detailed review of existing approaches is given in Chapter 4 where the new approach is also introduced. In order to show the effectiveness of the statistical optimisation, Figure 3.4 compares an ionosphere-corrected bending angle profile with its statistically-optimised profile. The bending angle profile extracted from ECMWF analysis fields is regarded as a reference. All the profiles are anchored to the mean location of the selected RO event. The mean location of an RO event is the projection of the mean tangent point of the event on the Earth’s surface. The mean tangent point can be defined as the point, where the straight line between the LEO and the GPS satellite is tangent to the Earth’s surface [Pirscher, 2010]. In the RO data processing and the evaluation of the RO retrievals where profiles from climatological models are needed, profiles are all derived from the mean location of the event. In the following description, the co-located profiles all denote profiles derived from the mean location.
Figure 3.4 Comparisons among raw, statistically-optimised and co-located ECMWF analysis bending angle profiles. The upper two panels and the left panel of the bottom two show the three types of bending angle profiles in three different height ranges, i.e., 80 km to 40 km, 40 km to 20 km, 20 km to the Earth’s surface; the bottom right panel shows the relative difference of both raw and optimised bending angles relative to the reference bending angle profile for the entire altitude range from the surface up to 80 km.

The RO event used in Figure 3.4 is the same as the one used in Figure 3.2. The statistical optimisation algorithm used is the one developed in the release of the Occultation Processing System version 5.4 software which optimises the bending angles above 30 km. It can be seen from the upper left panel and also the bottom right panel that, the statistically optimised bending angle profile is much smoother than the raw one (ionosphere-corrected bending angle profile), and the optimised one is also much closer to the reference profile. The optimised bending angles range from a rather small value at 80 km to about 38 µrad at 40 km. From the upper right panel, one can see that the optimised bending angle profile almost overlaps with the raw bending angle profile, and this is due to the reason that observed bending angles are less affected by the observational and residual ionospheric noises than higher altitudes. This panel also shows that bending angles values range from about $3.8 \times 10^{-5}$ rad at 40 km to more than $1 \times 10^{-3}$ rad at 20 km. The bottom left panel shows similar characteristics of the two types of bending angles as the upper right panel, i.e., the optimised bending angle profile almost overlap with the raw bending angle profile. This panel also shows that bending angle value range from about 0.0012 rad at 20 km to about 0.024 rad at about 2.5 km. The bottom right panel
shows that both the optimised bending angles and the raw bending angles at the height above 40 km have large deviation from the reference bending angles. The raw bending angle profile which is affected more by the remaining observational and ionospheric errors reveal larger deviations than the optimised bending angle. Below 30 km, the differences for both of the two types of bending angles are within +/- 4% for most of the altitude levels.

3.6 From bending angle to refractivity

Derivation of refractivity utilises some GO approximations, e.g., Fermat’s principle and Bouguers’s rule. Bouguers’s rule has already been introduced in Section 3.3. Fermat’s principle is also known as the principle of least time and it states that the path taken between two points by a ray of light is the path that can be traversed in the least time. Based on this principle, the phase range $L$ can be expressed by the line integral of the refractive index $n$ along the ray path between the GPS satellite and the LEO satellite:

$$L = \int_{LEO}^{GPS} n \, ds$$

(3.17)

where $ds$ is an element of length along the ray path.

Based on these GO approximations and under the assumption of spherical symmetry of the Earth’s atmosphere, the total bending angle of the ray $\alpha$ has a unique relation with the atmospheric refractive index along the ray [Fjeldbo et al., 1971]:

$$\alpha(a) = -2a \int_{r_T}^{r_C} \frac{1}{\sqrt{r^2 n^2 - a^2}} \frac{d \ln(n)}{dr} \, dr$$

(3.18)

where $r_T$ is the radial distance from the centre of refraction to the tangent point.

According to Bouguer’s rule, $r_T$ can be calculated by $r_T = a / n(r_T)$. These quantities can be seen from a simplified occultation geometry shown in Figure 3.5:

![Figure 3.5 Simplified geometry of a single RO ray.](image)
Equation (3.18) is the Abel integral (forward Abel). The inversion of the Abel integral (inverse Abel), allows the calculation of refractive index $n$ at a tangent point $n(r_{tp})$ using the obtained bending angles:

$$n(r_{tp}) = \exp\left(\frac{1}{\pi} \int_{a}^{\infty} \frac{\alpha(x)}{\sqrt{x^2 - a^2}} dx\right)$$  \hspace{1cm} (3.19)

where the impact parameter of the ray $a = n(r_{tp}) \times r_{tp}$.

Due to the non-linearity of Eq. (3.19), in data processing, the bending angle function $\alpha(x)$ are usually approximated as a known function of $y$ between successive height levels, for which an analytical solution to the Abel integral can be found [Lewis, 2008]. Equation (3.19) is then solved by summing contributions from the solutions to the known sub-integrals for each height level. The function $y$ often used includes the linear function and exponential function.

Since the refractive index in the free atmosphere is close to unity and its variations are very small, the term atmospheric refractivity, which has larger variations, is often used in atmospheric study. Refractivity is defined as:

$$N(h) = 10^6(n(h)-1)$$  \hspace{1cm} (3.20)

where $h$ is the height above the Earth’s ellipsoid, and is calculated by subtracting the local radius of curvature $R_c$ from $r_{tp}$:

$$h = r_{tp} - R_c = \frac{a}{n(r_{tp})} - R_c$$  \hspace{1cm} (3.21)

In some cases, the Mean Sea Level (MSL) altitude is preferred to show in figures for large ensemble of RO atmospheric retrievals, and the MSL altitude is the base in calculating atmospheric profiles. The MSL altitude $z$ is calculated by subtracting $h$ from local geoid undulation ($U_g$):

$$z = h - U_g = \frac{a}{n(r_{tp})} - R_c - U_g$$  \hspace{1cm} (3.22)

Figure 3.6 shows the comparison between the RO retrieved refractivity profile and the reference refractivity profile extracted at the mean RO location from the ECMWF analysis fields as a function of the MSL altitude. It can be seen that the refractivity range from a rather small value at 40 km to about 270 N at 2.5 km. The difference of RO retrieved refractivity relative to its co-located refractivity profile extracted from ECMWF analysis profile is within 4% for most of the altitude levels in the shown altitude range.
Figure 3.6 Comparison between RO retrieved and ECMWF analysis refractivity profiles. The left panel shows refractivity values and the right panel shows the difference of the RO retrieved refractivity relative to the co-located ECMWF analysis profile.

3.7 Derivation of dry density, temperature and pressure profiles

For microwave signals in the atmosphere, their refractivity can be given by [Kursinski et al., 1997; Smith and Wientraub, 1953]:

\[
N = k_1 \frac{P}{T} + k_2 \frac{P_w}{T} - C \frac{n_e}{f^2} + 1.4W
\]

(3.23)

where \(P\) is the atmospheric pressure in hPa, \(P_w\) is partial pressure of water vapour, \(n_e\) is the electron density in electrons/ m\(^3\), and \(W\) is liquid water content in grams per cubic meter. The first two terms and the fourth term on the right-hand side of Eq. (3.23) are the contributions from the neutral atmosphere. The third term is the contribution from the first-order ionospheric effects. The higher-order ionospheric effects have limited influence on the L-band frequency GPS observations [Höeg et al., 1996; Melbourne et al., 1994], thus they are not included in Eq. (3.23).

The values of \(k_1\) and \(k_2\) are empirically derived coefficients and they are slightly different from different experiments [Bevis et al., 1994; Hasegawa and Stokesberry, 1975; Healy, 2009]. Often used values for \(k_1\) and \(k_2\) are those from Smith and Weintraub [1953], where \(k_1 = 77.6\) K/hPa, \(k_2 = 3.73 \times 10^5\) [Healy, 2009] K/hPa. \(C = 40.3 \times 10^6\) and is determined based on fundamental physical constants.

Since the first-order ionospheric effect term has already been eliminated by the ionospheric correction, the effects of the third term in Eq. (3.23) can be neglected. In addition, the last term, which represents the scattering term, can also be neglected since the content of liquid water is very small compared to other terms. In atmospheric regions where moisture is negligible, which is a reasonable assumption for altitudes above 8 km at polar winter and 14 km at tropics [Foelsche et al., 2008], the contributions from the moisture atmosphere can also be neglected. As a result, the refractivity in dry atmospheric regions is only related to the dry air pressure \(P_d\):
\[ N = k \frac{P}{T} \]  

(3.24)

To calculate dry atmospheric profiles, the ideal gas law is also used:

\[ P_d = \frac{\rho_d RT}{M_d} \]  

(3.25)

where \( \rho_d \) is the density of dry atmosphere, \( R = 8314.5 \, J \, K^{-1} \, kmol^{-1} \) is the universal molar gas constant, \( M_d = 28.964 \, kg \, kmol^{-1} \) is the mean molar mass of dry air. Combining Eqs (3.24) and (3.25), dry atmospheric density can be given by:

\[ \rho_d(z) = \frac{N(z)}{k_1 R_d} \]  

(3.26)

where \( R_d \) is the dry air gas constant, and \( R_d = R / M_d = 87.06 \, J \, kg^{-1} \, K^{-1} \).

With the derived dry atmospheric density, dry atmospheric pressure could be easily calculated using the following hydrostatic equation:

\[ P_d(z) = \int_{h}^{z} g(\phi, z) \rho_d(z) dz \]  

(3.27)

where \( g(\phi, h) \) is the gravity of the Earth at the location of latitude \( \phi \) and height \( h \).

In practice, a reasonable upper boundary (e.g., 120 km) is set for Eq. (3.27). With the obtained dry air density and dry atmospheric pressure, dry temperature could be calculated by:

\[ T_d(z) = \frac{P_d(z)}{R_d \rho_d(z)} \]  

(3.28)

From Eqs. (3.27) and (3.28), it is can be seen that if bending angle errors at high altitudes are transferred downwards into refractivity, these errors will be also transferred down to pressure through the hydrostatic equation and further transferred down to temperature through Eq. (3.28). This also suggests that it is important to perform statistical optimisation at the bending angle level.

Figure 3.7 shows the comparison of RO retrieved dry profiles and their reference profiles. It can be seen that the dry density starts from a small value at 40 km and increases to about 1.2 kg/m\(^3\) at 2.5 km. The dry pressure also starts from a small value at 40 km and increases to about 880 hPa at 2.5 km. The dry temperature starts from about 236 K at 40 km and decreases to about 188 K at about 20 km and then increase to about 250 K at 2.5 km. The relative differences between the RO retrieved dry profiles with their reference profiles are all within 4% for most of the altitude levels.
3.8 Derivation of physical density, temperature, pressure and humidity profiles

In the case of moist air, the contributions from the humidity in Eq. (3.23) cannot be neglected. In this case, the atmospheric refractivity is expressed as [Healy, 2009]:

\[ N = k_1 \frac{P}{T} + k_2 \frac{P_w}{T^2} \] (3.29)

The retrieval of physical atmospheric profiles requires independent knowledge of one of the three parameters \((T, P, P_w)\) to solve for the other two. The retrieval of these parameters is an iterative process. Since this thesis only focuses on values above 20 km where the moisture in the atmosphere can be neglected, the detail of the retrieval of physical atmospheric profiles could refer to the work of other scientists [Hajj et al., 2002; Kursinski et al., 1995].

Figure 3.7 Comparisons between RO retrieved dry density, pressure, temperature profiles with their corresponding co-located ECMWF profiles
With $P$ and $P_w$, specific humidity $q$ can be calculated [Hajj et al., 2002]:

$$q = \left[ \frac{M_d}{M_w} \left( \frac{P}{P_w} - 1 \right) + 1 \right]^{-1} \approx \frac{M_w}{M_d} \frac{P_w}{P}$$ (3.30)

where $M_w = 18.0153 \text{ kg kmol}^{-1}$ is the mean molar mass of water vapour.

The above is the conventional method to retrieve physical atmospheric profiles. However, this approach is not optimal since the error of both the observation data and priori information are not accounted for, and these two types of errors will result in large errors in the retrievals.

A method for optimal physical profile retrievals is through a non-linear 1dVar processing [Healy and Eyre, 2000; Lewis, 2010; Palmer et al., 2000]. This method aims to find a maximum likelihood estimate of a vertical atmospheric profile $x$ based on a set of observations $y_0$ and some priori knowledge of the background atmospheric state $x_b$. This method is usually formulated as a minimisation problem of the cost function [Lewis, 2010]:

$$J(x) = \frac{1}{2}(x - x_b)^T B^{-1}(x - x_b) + \frac{1}{2}(y_0 - H[x])^T O^{-1}(y_0 - H[x])$$ (3.31)

where $H[x]$ denotes a forward operator from measured quantity $y_0$ to any given atmospheric state $x$; $B$ is the assumed background-error covariance matrix, $O$ is the assumed error covariance matrix for both the measurements and the forward operator. Minimising the cost function $J$ with respect to the state vector $x$ gives a solution that minimises the total deviation against the background and observational data. This approach is under the assumption that errors are normally distributed and both background and measurements are unbiased. The observations $y_0$ could be either bending angle or refractivity.

This approach has proved to be much more robust than the conventional method [Healy and Eyre, 2000; Palmer and Barnett, 2001]. Hence, it has now become a commonly used method in retrieving atmospheric profiles and been implemented by many RO data processing centres.

### 3.9 Summary

In this chapter, the measurement principle and the algorithms of retrieval of atmospheric profiles of the RO technique based on the Geometric Optics principle are discussed. The RO concept relies on setting specially-designed GPS receivers on LEO satellites to receive GPS signals. As the GPS signals propagating through the atmosphere, they are refracted due to the inhomogeneity of the atmospheric density and the consequent refractivity gradient. The instantaneous geometry of the RO technique at each sampling time could be regarded as a single ray. The total effect of the atmosphere to the ray could be subject to a total bending angle. For an occultation event, which has numerous rays (e.g., more than 2000 rays), bending angles at different heights of the atmosphere could be derived which
then forms a near vertical profile. The obtained bending angle profile is then the basis for the retrieval of atmospheric profiles.

The RO data processing starts from the derivation of excess phase. The excess phase is calculated from the GPS phase observations. After correcting the observational errors, the obtained excess phase could then be used for the calculation of bending angle together with the orbits of both GPS and LEO satellites using the assumption of spherical symmetry and some GO approximations. The bending angles obtained from GPS L1 and L2 signals are applied with a linear combination at the same impact parameter to remove the first-order ionospheric effects. The obtained bending angles are still affected by the higher-order ionospheric effects and also remaining observation errors that have not been fully corrected at the excess phase level, therefore, a statistical optimisation is usually applied to estimate optimal bending angles for the calculation of refractivity and the consequent atmospheric profiles. After the optimal bending angles are obtained, the refractivity could be calculated through Abel integral. Atmospheric profiles in dry atmospheric regions could be retrieved using Smith and Weintraub [1953] equation. Profiles in moist regions could be retrieved through a 1-dVar process.

Due to the quality of the bending angles is critical for the calculation of refractivity and the consequent atmospheric profiles, the statistical optimisation has become an important process in the RO data processing. Therefore, in chapter 4, a new statistical optimisation approach is introduced. In order to compare the existing algorithms with our new approach, the literature review of existing algorithms are also given in chapter 4.
Chapter 4. High Altitude Initialisation and Statistical Optimisation of GPS RO Bending Angles

The statistical optimisation, as briefly discussed in Chapter 3, is to combine the RO observed bending angles (ionosphere-corrected bending angle) with background bending angles to obtain statistically optimized bending angles. The background bending angles are usually forward propagated from the variables extracted from a climatological model. The statistical optimisation is critical for initialising bending angle profiles at high altitudes (e.g., > 30 km) and providing optimal bending angles for subsequent calculation of refractivity and atmospheric profiles. The most important consideration for the optimisation is the accuracy of the estimated background and observation error covariance matrices. However, it is never straightforward to obtain the error matrices, especially for background errors. Therefore, current approaches usually use empirical values and analytical functions to approximate error covariance matrices which are of low accuracy. To address this weakness, a new dynamic approach that uses large ensemble of ECMWF short-range and analysis as well as RO observed bending angle to dynamically estimate background and observation error covariance matrices is developed in this Chapter. The new approach avoids the use of empirical values to crude estimate error matrices, but realistically estimates both error covariance matrices which can reflect the true error characteristics of background and observed bending angles. It is expected that this new approach can improve the quality of the optimised bending angle and subsequently retrieved refractivity and temperature profiles.

This chapter firstly reviews existing statistical optimisation algorithms. Due to the statistical optimisation algorithm from the Occultation Processing System (OPSV5.4) is the algorithm that is used to compare with our new algorithm in this thesis, its formulations are elaborated in Section 4.2. Section 4.3 introduces an alternative algorithm of statistical optimisation that uses mean observed bending angle for preparing refractivity and atmospheric profile climatologies. Sections 4.4 to 4.7 introduce the new statistical optimisation algorithm. The procedure of the new algorithm implemented in EGOPS software is discussed in Section 4.8. A summary is given in the final section.
4.1 Existing statistical optimisation algorithms

Statistical optimisation was first introduced for RO data processing by Sokolovskiy and Hunt [1996]. This method combines observed bending angles with background bending angles to determine optimal ones, and the weights of the two types (observed and background) of bending angles are determined by their error covariance matrices or by approximations to them (e.g., from ignoring error correlations). The general picture is as follows [Gobiet et al., 2007; Healy, 2001; Rieder and Kirchengast, 2001]: At high altitudes in the mesosphere (above about 60 km), the background errors are smaller than the observation errors, thus the background bending angle contributes more to the optimised bending angle. With the decrease of altitude, the background error increases while the observation error stays roughly constant, so that the optimised bending angles smoothly transit from being more weighted toward the background to being more weighted toward the observed bending angles. In the height range below about 40 km, the observed bending angles are of higher quality, so they dominate in the optimised bending angles.

Given an unbiased background bending angle profile and observed bending angle profile \( \alpha_b \) and \( \alpha_o \), respectively, and their error covariance matrices \( C_b \) and \( C_o \), the statistically optimised bending angle profile \( \alpha_{SO} \) can be calculated by [Gobiet and Kirchengast, 2004; Healy, 2001]:

\[
\alpha_{SO} = \alpha_b + C_b (C_b + C_o)^{-1} \cdot (\alpha_o - \alpha_b).
\]  

(4.1)

This method is a generalised least squares approach [Rodgers, 1976; 2000], weighting the bending angles by their inverse covariances. As an illustrative and typical example, the background bending angles can be obtained from a climatological model such as the Mass Spectrometer and Incoherent Scatter Radar (MSIS) model [Hedin, 1991], and the background error covariance matrix by guessing a typical relative standard error of the model and a simple error correlation structure like exponential fall-off over about an atmospheric scale height [Healy, 2001] or just disregarding correlations [Hocke, 1997; Sokolovskiy and Hunt, 1996]. Similarly, the observation error covariance matrix can be formulated from estimating the observation error at mesospheric altitudes (where the signal is small as noted above) and guessing simple error correlations [Gobiet and Kirchengast, 2004; Gobiet et al., 2007] or again just ignoring the latter.

The main difficulty of effective statistical optimisation is to obtain an accurate error covariance formulation for the background bending angles since this is neither supplied together with common (climatological) models nor is its construction a straightforward task. As a result, Sokolovskiy and Hunt [1996] calculated the statistically optimised bending angles in that pioneering work by neglecting the vertical correlations among the background errors and among the observation errors. Eq. (4.1) can be expressed in this case as an equation of inverse variance weighting:
\[ \alpha_{SO,i} = \alpha_{b,i} + \frac{\sigma_{b,j}^2}{\sigma_{b,j}^2 + \sigma_{o,j}^2} (\alpha_{o,j} - \alpha_{b,j}) \] (4.2)

where \( \sigma_{b,j} \) and \( \sigma_{o,j} \) are the standard deviations of the background bending angle and the observed bending angle at the \( i \)th impact altitude level, respectively. \( \sigma_b \) is estimated as a fixed fraction of \( \alpha_b \) and \( \sigma_o \) is an empirically estimated as a constant value at mesospheric altitudes, in line with the illustrative example described above.

An alternative approach was adopted by Hocke [1997] and Steiner et al. [1999] for the purpose of down-weighting outliers and smoothing the obtained optimised bending angles at high altitudes:

\[ \alpha_{SO,i} = \alpha_{b,i} + \frac{\sigma_{b,j}}{\sigma_{b,j} + \sigma_{o,j}} (\alpha_{o,j} - \alpha_{b,j}) \] (4.3)

This was found effective for the purpose, but from the viewpoint of unbiased optimal estimation it can be argued that this approach overweighs the background bending angle if the background error is larger than the observation error, and it also overweighs the observed bending angle if the observation error dominates [Healy, 2001].

Healy [2001] and Rieder and Kirchengast [2001] were the first to suggest and demonstrate the value of using full error covariance matrices for RO statistical optimisation, considering this carefully in the framework of optimal estimation methodology [Rodgers, 2000]. The Healy [2001] formulations are described as follows. As above, the background standard deviations are assumed to be a fixed fraction of the background bending angles and the observation standard deviations are empirically estimated as a constant, however, the correlations are no longer ignored. The background error correlations were expressed by a correlation function of Gaussian shape with a correlation length of 6 km, reflecting the atmospheric scale height. The observation errors were assumed uncorrelated or correlated with a small correlation length (about 1 km, also using a Gaussian shape for the correlation functions). Adopting this, each element of the background error covariance \( C_b \) is formulated as:

\[ C_{b,ij} = \sigma_{b,i} \sigma_{b,j} \exp \left( -\frac{(a_i - a_j)^2}{L^2} \right) \] (4.4)

where \( a_i \) and \( a_j \) are the impact parameters at height indices \( i \) and \( j \), and \( L \) is the background error correlation length. The formulation of the observation error covariance matrix \( C_o \) is the same as the formulation of \( C_b \), but with \( \sigma_o \) and a shorter correlation length.

Healy [2001] demonstrated that the background error correlation is important and helpful for smoothing the optimised bending angle profile while keeping it unbiased at the same time. If the background error correlations are neglected, the optimised profile is bounded by the observed and the background profile at each single impact altitude level and takes the noisy shape of the observed profile. Regarding the shape of the correlation functions it subsequently became clear that exponential
fall-off is of numerical advantage over Gaussian shape, since the former leads to error covariance matrices that are robustly invertible while the inversion of the latter is readily unstable, except if the Gaussian is approximated by a suitable polynomial fit [Steiner and Kirchengast, 2005, section 6 therein].

Gorbunov [2002] introduced an algorithm combining ionospheric correction and statistical optimisation. Briefly, this method dynamically estimates signal and noise covariances at individual impact altitude levels; vertical error correlations are not accounted for [Gorbunov, 2002]. The signal covariance is estimated from the differences between the observed bending angle and background bending angle in a height range where the neutral atmospheric signal prevails (i.e., lower stratosphere). The noise covariance is estimated from the bending angles at the two GPS frequencies in the height range where ionospheric signals prevail (i.e., mesosphere). With the estimated signal and ionospheric observation covariances, the neutral atmospheric bending angle (statistically optimised bending angle in our context) could then be optimally estimated and used for the calculation of refractivity. The current retrieval at the RO processing centre at Danish Meteorological Institute (DMI) employs this Gorbunov [2002] approach as part of its statistical optimisation [Ho et al., 2012; Lauritsen et al., 2011].

Lohmann [2005] showed that if both observed and background errors were estimated dynamically and the vertical correlation was neglected, the two types of errors are not damped equally when using the Abel transform to calculate refractivity. To mitigate this problem, Lohmann [2005] adjusted the magnitude of the two types of errors using a scaling factor estimated from calculated error correlation lengths of the two types of errors. The current retrieval of the University Corporation for Atmospheric Research (UCAR) RO processing centre is employing this Lohmann [2005] approach as part of its statistical optimisation [Ho et al., 2012].

Gobiet and Kirchengast [2002] followed the Healy [2001] and Rieder and Kirchengast [2001] approaches of using a full error covariance matrix for the statistical optimisation [Gobiet and Kirchengast, 2002]. Instead of using a Gaussian-shape function, an exponential fall-off function was used to estimate the error correlation for both background and observed bending angles. They also used a search for that background bending angle profile in the MSIS model space that best fits the observed profile over the stratopause region. Gobiet and Kirchengast, [2004] updated this algorithm by performing an additional bias correction to the background bending angle profile before the statistical optimisation, aiming at further minimizing residual biases in the optimised bending angle profile under adverse conditions such as during high-latitude winter. Another improvement by Gobiet et al. [2007] introduced the use of background profiles from European Centre for Medium-range Weather Forecast (ECMWF) fields rather than from the MSIS model (avoiding also the additional bias correction noted above).
The Wegener Center for Climate and Global Change (WEGC) Occultation Processing System version 5.4 (OPSv5.4) [Ho et al., 2012; Pirscher, 2010; Steiner et al., 2013], which is used as reference system for this study, uses co-located bending angle profiles extracted from ECMWF short-range (24h/30h) forecast fields as background profiles. Its statistical optimisation is otherwise following Gobiet et al. [2007], as recently summarized in Ho et al. [2012]. The ECMWF forecast fields are used at horizontal resolution T42 (spectral representation with triangular truncation at wave number 42), corresponding to about 300 km, for roughly matching the horizontal resolution of RO data. This OPSv5.4 algorithm is used as the evaluation reference for the new approach, since it is amongst the major RO processing centres currently the only one employing statistical optimisation with full covariance matrices [cf. algorithm descriptions in Ho et al., 2012] and since recent intercomparison results indicate that this is a performance advantage above about 20 km [Ho et al., 2012; Steiner et al., 2013]. It is therefore considered that a best available current state-of-the-art algorithm is compared so that any evidence of further improvement that we may find is expected to improve also over any less advanced of the existing algorithms. Since the OPSv5.4 algorithm is the algorithm that is used for the comparison of the new approach of this thesis, the detail formulations of this algorithm are elaborated in Section 4.2 to help us better understand the differences between this existing algorithm and our new algorithm.

### 4.2 OPSv5.4 statistical optimisation algorithm

As briefly mentioned above, the OPSv5.4 algorithm exploits the full covariance matrix for both background and observation error covariance matrices. For the convenience of description, we use a superscript OPSv5.4 for the notations of background and observation error matrices, i.e., $C_{b}^{\text{OPSv5.4}}$ and $C_{o}^{\text{OPSv5.4}}$. Both of the matrices are estimated using exponential functions as described in the following Eqs. (4.5) and (4.6):

$$C_{b;i,j}^{\text{OPSv5.4}} = \sigma_{b;i}^{\text{OPSv5.4}} \sigma_{b;j}^{\text{OPSv5.4}} \exp \left[ - \frac{d_{i} - d_{j}}{L_{b}} \right]$$  \hspace{1cm} (4.5)

$$C_{o;i,j}^{\text{OPSv5.4}} = \sigma_{o;i}^{\text{OPSv5.4}} \sigma_{o;j}^{\text{OPSv5.4}} \exp \left[ - \frac{d_{i} - d_{j}}{L_{o}} \right]$$  \hspace{1cm} (4.6)

where $L_{b}$ and $L_{o}$ are the correlation lengths for background and observation errors, respectively. In generally, the background errors are highly correlated, while the observations errors are less correlated. Therefore, $L_{b}$ is set to 10 km and $L_{o}$ is set to 2 km. $\sigma_{b}^{\text{OPSv5.4}}$ is background standard
deviation and is estimated as 15% of background bending angle; $\sigma_{o}^{OPSv5.4}$ is observation uncertainty and is defined as the average standard deviation of the observed bending angles relative to the bias-corrected MSIS bending angles at the impact height levels between 65 km and 80 km (or to top of profile if reached lower than 80 km; for details on the relevant OPSv5.4 quality control see Pirscher, 2010):

$$\sigma_{o}^{OPSv5.4} = \sqrt{\frac{1}{|k_{top} - k_{65}|} \sum_{i=k_{65}}^{k_{top}} \left[ \alpha_{RO,i} - \left( \alpha_{MSIS,i} + \beta_{o} \right) \right]^2}.$$  (4.7)

Herein, $k_{top}$ and $k_{65}$ are the impact height indices for top altitude (nominally 80 km) and 65 km, respectively; and the bending angle bias $\beta_{o}$ is estimated by averaging the differences between the RO bending angle $\alpha_{RO}$ and the MSIS-derived bending angle $\alpha_{MSIS}$ in the impact altitude range from 65 km to top (nominally 80 km):

$$\beta_{o} = \frac{1}{|k_{top} - k_{65}|+1} \sum_{i=k_{65}}^{k_{top}} \left( \alpha_{RO,i} - \alpha_{MSIS,i} \right).$$  (4.8)

It should be noted that Eq. (4.7) cannot always reflect the real quality of RO observed bending angle [Gobiet, 2005; Pirscher, 2010]. For such cases, the estimated $\sigma_{o}^{OPSv5.4}$ is modified according to some additional quality checks [Pirscher, 2010].

### 4.3 Other initialisation methods

Recently, Ao et al. [2012] and Gleisner and Healy [2013] introduced an alternative high altitude initialization method that can be used for preparing refractivity and atmospheric profile climatologies without first retrieving individual profiles that require statistical optimisation with background profiles [Ao et al., 2012; Gleisner and Healy, 2013]. This method first averages large ensembles of observed bending angle profiles to effectively mitigate random noise in the resulting climatological bending angle profiles at high altitudes, and based on the climatological bending angle profiles, climatological refractivity and atmospheric profiles can then be directly retrieved without the need for further initialization. The relative quality of these climatologies, compared to climatologies averaged from individual-profile retrievals that included initialisation by statistical optimisation, will depend on the data quality (i.e., will be different for different RO receivers such as on CHAMP, COSMIC, and MetOp-A), the suitability of the data quality-control and averaging scheme used, the space-time averaging domain trade-offs involved, and not least the quality of the background profiles and the whole statistical optimisation scheme used for the individual-profile retrievals providing the comparative results.
The new dynamic optimisation approach that introduced in this thesis does not look at these two avenues as a competition, but rather exploits their synergy and combines them: averaged-observed bending angle profiles are integral part of background bending angle estimation and their weight in resulting background profiles will depend on the uncertainties estimated for these averaged profiles relative to those estimated for co-located profiles determined from ECMWF fields. The whole new approach is described in detail in the following Sections 4.4, 4.5, 4.6 and 4.7.

4.4 The new statistical optimisation algorithm

The new dynamic approach estimates more adequate background bending angles $\alpha_b$, the background error covariance matrix $C_b$, and the observation error covariance matrix $C_o$, and used these quantities for the statistical optimisation (Eq. (4.1)). The background error covariance matrix is estimated using a large ensemble of bending angle profiles from ECMWF analysis and short-range forecast fields as well as averaged-observed bending angle profiles. The observation error covariance matrix is formulated using a large ensemble of RO ionosphere-corrected bending angles and ECMWF analysis profiles. The biases in the background profiles are also corrected.

Figure 4.1 illustrates the main algorithmic steps of the new method. The new method mainly consists of two parts, i.e., estimation of background bending angle profiles and its associated error covariance (left part of Figure 4.1) and the estimation of observation error covariance matrix (right part of Figure 4.1). For RO events of a given day, a corresponding daily background error field of the day that contains all the needed quantities for formulating the background error covariance matrix should be formulated. The estimation of background error covariance sequentially include the three major steps: 1) constructing the basic daily background fields for any day to be processed, 2) preparing the derived daily background fields with the specific statistical quantities directly needed for estimating background error covariance matrix, and 3) performing dynamic estimation of background error covariance matrix for a given RO event of the day correct the biases in background bending angle profile. These three major steps are explained in Section 4.5, and the component tasks as indicated in Figure 4.1 for these three major steps are discussed in Section 4.6. The estimation of observation error covariance matrix includes two steps (right part of Figure 4.1), 1) estimation observation error correlation uses large ensemble of RO observed data and ECMWF analysis data; 2) dynamic estimation of observation error covariance matrix in terms of estimation of observation uncertainty. These two steps are presented in Section 4.7.

After obtaining background bending angle profile and its associated error covariance matrix as well as observation errors covariance matrix, the new statistical optimisation for processing RO
events of a given day could be carried out. As can be seen from Figure 4.1, assuming $k = 1, \ldots, N_{occ}$ being sequentially numbered RO events of a day, using the estimated $\alpha^k_b$, $C^k_b$, and $C^k_o$, and the observed bending angle from the OPSv5.4 system, $\alpha^k_o$, and interpolate these variables to the required standard grids for the statistical optimisation of each occultation event $k$, the statistically optimised bending angle from the new algorithm could then be calculated via Eq. (4.9):

$$
\alpha_{SO}^k = \alpha^k_b + C^k_b \left(C^k_b + C^k_o\right)^{-1} \cdot \left(\alpha^k_o - \alpha^k_b\right).
$$

(4.9)

Figure 4.1 Flowchart of the new dynamic statistical optimisation approach
4.5 Dynamic estimation of background bending angles and error covariance matrix for the new algorithm

This section introduces the main algorithmic steps for estimating \( \alpha_b^k \) and \( C_b^k \) as shown in Figure 4.1, i.e., construction of daily background fields, preparation of derived daily background fields, and the dynamic estimation of background error covariance matrix.

4.5.1 Construction of daily background fields

In order to suitably capture the large-scale background error dynamics as a function of latitude, longitude, (impact) altitude and time, we prepare once-daily fields of all basic background variables needed globally at a 10° latitude × 20° longitude grid (centre of base cell/anchor grid point at 5°N, 10°E), at 200 representative (impact) altitude levels from 0.1 km to 80 km. This yields daily fields at a global 18 × 18 × 200 grid.

The basic statistical variables that are needed for the dynamic estimation of background error covariance matrix in form of such gridded fields—which we prepared into daily data files for easy use for processing all RO events of a day—include: (i) the mean analysis bending angle from the ensemble of analysis values for any grid point (i.e., any of the 200 levels in each of the 18 × 18 cells) \( \bar{\alpha}_a \), (ii) the analysis spread (standard deviation of the ensemble of analysis values) against this mean \( s_a \), (iii) the estimated bias (systematic uncertainty) of this mean \( b_a \), (iv) the mean forecast bending angle \( \bar{\alpha}_f \), (v) the standard deviation of the forecast values against this mean \( s_f \), (vi) the standard deviation of the forecast-minus-analysis difference profiles for any grid point \( s_{f-a} \), (vii) the number of values in the analysis and the forecast ensemble for any grid point \( N_{a,f} \), (viii) the background error correlation matrix (200 × 200 correlation values) estimated from the forecast-minus-analysis difference profiles over the entire globe \( \mathbf{R}_{f-a} \), (ix) the mean observed bending angle from the ensemble of observed values for any grid point \( \bar{\alpha}_o \), (x) the standard deviation of the observed values against this mean \( s_o \), (xi) the estimated bias (systematic uncertainty) of this mean \( b_o \), (xii) the mean co-located bending angle \( \bar{\alpha}_c \), (xiii) the standard deviation of the co-located values against this mean \( s_c \), and (xiv) the number of values in the observed and the co-located ensemble for any grid point \( N_{o,c} \).

In constructing the averaged variables on these daily 18 × 18 × 200 grid fields, we apply time-averaging over at least five days (from two days before to two days after the day of interest in this study) and horizontal-averaging over geographic domains of at least 1000 km × 1000 km size (over
10° lat × 20° lon cells out to 60°S/60°N latitude in this study, polewards over larger longitude ranges of 25° in 60°-70°, 40° in 70°-80°, 90° in 80°-90°); only the daily background error correlation matrix is constructed from horizontal-averaging over the entire globe (yielding a robust estimation of the 200 × 200 correlation values, i.e., of the 200 vertical correlation functions of all 200 altitude levels).

This construction approach, and the degree of averaging applied, was proven by extensive sensitivity tests with different time- and space averages (more and less days, larger and smaller horizontal domains, etc.) and found to be just adequate so that the variables in the resulting fields have essentially averaged-out all weather variability (at scales of up to several days and including all mesoscale-sized systems) but still neatly trace all weekly- to climate-scale variations and large-scale geographic variation patterns. The sensitivity tests also proved that the averaging is robust (sufficiently large number of ensemble members in the average) and not sensitive to the exact choices of time period and geographic size as long as at least about 5 days and 1000 km scale sizes are utilized (e.g., 5 days to 7 days and 1000 km to 2000 km horizontal scale sizes not making much difference; if options of even stronger averaging are used, like up to a month, some important weekly-scale structures, like from sudden stratospheric warming events as an arbitrary example, are no longer traced by the estimated mean fields). In other words, the averaging is decided based on the trade-off between what is considered mean-field variation, which should be dynamically traced by the background error formulation to enable to be as unbiased as possible in a statistical sense, and what is considered weather variability, the quasi-random variation of individual RO profiles in the sense of a spread or standard deviation around the mean.

In this new algorithm, ECMWF analysis fields and corresponding 24h-forecast fields at T42L91 resolution (about 2.5° lat x 2.5° lon, 91 vertical levels up to about 80 km), at 00 UTC and 12 UTC each day, are used as the basis to construct the 18 × 18 × 200 grid fields of analysis and forecast variables. On the observation side, the observed RO bending angle profiles mainly from Formosat-3/COSMIC that were obtained from Wegener Center OPSv5.4 processing on the basis of excess phase and orbit data obtained from UCAR/CDAAC are used for the calculation. These OPSv5.4 RO profiles come with co-located ECMWF analysis profiles that are also co-used here for estimating and taking into account the sampling error [Scherllin-Pirscher et al., 2011b]. The approach is generic, however, any other source of analysis and short-range forecast fields and observed bending angle profiles could be used as well. The ECMWF and WEGC-OPS are chosen for their proven track records of datasets of leading quality [Ho et al., 2012; Ho et al., 2009; Scherllin-Pirscher et al., 2011a; b; Steiner et al., 2013; Untch et al., 2006]. As an alternative to the ECMWF operational fields, the analysis and forecast fields from the ERA-Interim re-processing are also considered to be used [Dee et al., 2011; Simmons et al., 2007].

The 200 level vertical grid was defined to safely accommodate different analysis/forecast level schemes up to fine ones, such as ECMWF’s level schemes from L60 (before Feb 2006) to L137 (from
June 2013), but still keeping the level number reasonably small for the sake of efficient data storage, considering these daily grid fields will be needed over years of climate data processing. Practically, the level spacing found useful and therefore adopted is 100 m below 1 km, then linearly increasing from 100 m at 1 km to 600 m near 60 km, furthermore to 1000 m at 70 km, then kept constant at 1000 m up to 80 km.

The fundamental ensemble of bending angle profiles for statistically computing all the analysis and forecast variables for each of the $18 \times 18$ cells was extracted from the ECMWF T42L91 fields on a $2.5^\circ \times 2.5^\circ$ native grid, for the ten UTC time layers of five days, and at the 200 target levels. This yields an ensemble of many hundreds of profiles per cell (and many thousands globally for the correlation matrix), which allows robust estimates of the statistical variables. The GCM Atmosphere Model (GCMAtm) of the Wegener Center OPS software was used for this purpose, which enables extraction from native ECMWF Gridded-Binary files at arbitrary target grids, including also of derived RO variables such as the bending angle. The latter is derived in the GCMAtm by forward Abelian transformation from refractivity which in turn is derived from the variables of pressure, temperature, and humidity by Smith-Weintraub’s refractivity equation. The ensemble of observed bending angle profiles, and their co-located analysis profiles, is simply adopted to consist of all RO events that fall into each cell over the five days, which also typically leads to more than forty RO events per cell. More details of how these basic statistical variables were computed together with illustrations are separately described in Section 4.6.

### 4.5.2 Preparation and pre-processing of the derived daily background fields

Using the basic background fields—read in from the applicable daily NetCDF file before processing the RO events of a day—the next step is to prepare those specific statistical quantities on the $18 \times 18 \times 200$ grid that are directly needed in estimating the background error covariance matrix of the RO events of the day. These include the forecast-minus-analysis standard deviation $s_{f-a}$, which represents the estimated random uncertainty of the 24h-forecasts and can be adopted as is, the mean background bending angle $\overline{\alpha}_b$, which is an optimally estimated combination of $\overline{\alpha}_a$ and $\overline{\alpha}_o$, and the difference of the forecast mean to this background mean $\Delta \overline{\alpha}_{f-b}$, and the estimated combined standard uncertainty of the background mean $\sigma_b$, respectively.

The background mean $\overline{\alpha}_b$, its associated uncertainty $\sigma_b$, and the forecast-minus-background mean difference $\Delta \overline{\alpha}_{f-b}$ are computed using standard equations for variance-based uncertainty propagation and for inverse-variance weighting as follows:
\[
\bar{\alpha}_b = \frac{u_o^2}{u_o + u_a^2} \bar{\alpha}_a + \frac{u_a^2}{u_a + u_o^2} \left[ \bar{\alpha}_o - (\bar{\alpha}_c - \bar{\alpha}_a) \right],
\]
(4.10)

\[
u_b = \left[ \frac{u_a^2 u_o^2}{u_a + u_o^2} \right]^{1/2},
\]
(4.11)

\[
\Delta \bar{\alpha}_{f,b} = \bar{\alpha}_f - \bar{\alpha}_b,
\]
(4.12)

where

\[
u_a = \left[ b_a^2 + \left( s_a^2 / N_{af} \right) \right]^{1/2}
\]
(4.13)

and

\[
u_o = \left[ b_o^2 + \left( s_o^2 / N_{of} \right) + r_{resSE}^2 (\bar{\alpha}_c - \bar{\alpha}_a) \right]^{1/2}
\]
(4.14)

are the estimated combined standard uncertainties of the mean analysis bending angle and the mean observed bending angle, respectively. The third term on the right-hand-side of Eq. (4.14) is the residual sampling error estimate for the RO observations [Scherllin-Pirscher et al., 2011b], where the reduction factor \( r_{resSE} \) is set to 0.3 following the (conservative) empirical estimate by Scherllin-Pirscher et al. [2011b]. Due to the fairly high numbers of profiles per grid cell, the bias terms (\( b_a \) and \( b_o \) terms) generally dominate in Eqs. (4.13) and (4.14) so that the resulting background mean uncertainty \( u_b \) (Eq. (4.11)) represents essentially a bias-type (systematic) uncertainty. Further discussion of these estimates follows in Section 4.6 below.

Eqs. (4.10) to (4.14) are applied grid-point wise to the entire 18 \times 18 \times 200 grid so that the quantities needed for the statistical optimisation, \( \Delta \bar{\alpha}_{f,b} \),\( u_b \), and \( s_{f,a} \), are conveniently available in form of this global grid for interpolation to any RO event location occurring during the day.

Completing this once-daily preparation of variables, the error correlation matrix of the day, \( R_{f,a} \), is interpolated from its 200-level formulation to the target vertical grid of the statistical optimisation. For the latter, a 200 m equidistant grid is used, with 400 levels from 0.2 km to 80 km, so that this yields a correlation matrix with up to 400 \times 400 values (in this new approach, the statistical optimisation is applied down to 30 km, corresponding to 251 \times 251 values). The interpolation is performed linearly along the diagonal and parallels to the diagonal (at the top and bottom boundaries linearly along the boundaries) to accurately conserve the shape of the matrix. The resulting matrix
\(\mathbf{R}_{\text{occ}}^f\) is also ensured to be robustly invertible and can now be used for all RO events of the day; further details are given in Section 4.6 below.

### 4.5.3 The dynamic estimation of background error covariance matrix

For each occultation event \(k\), assuming \(k = 1 \ldots N_{\text{occ}}\) being sequentially numbered RO events of the day, the co-located profiles \(\Delta\alpha_{\text{occ}}^k\), \(u_b^k\), and \(s_{\text{occ}}^{k}\) from the respective grids \(\Delta\alpha^k\), \(u_b\), and \(s_{\text{occ}}^{k}\) are determined by bi-linear latitude/longitude interpolation to the RO event location and linear vertical interpolation to the (200 m spacing, 400 level) target grid of the statistical optimisation. The correlation matrix \(\mathbf{R}_{\text{occ}}^{k} = \mathbf{R}_{\text{a,occ}}^{k}\) is also employed for each event \(k\) of the day, to represent its background error correlations.

The co-located background bending angle (c.f. Section 4.4), \(\alpha_b^k\), is calculated by subtracting the forecast-minus-background mean difference \(\Delta\alpha_{\text{occ}}^k\) from the co-located forecast bending angle \(\alpha_f^k\) in order to effectively reduce the residual bias in \(\alpha_b^k\) to within the estimated uncertainty of the background mean \(u_b^k\) (otherwise, as in the existing OPSv5.4 scheme, potential biases in \(\alpha_f^k\) would survive):

\[
\alpha_b^k = \alpha_f^k - \Delta\alpha_{\text{occ}}^k.
\]  

(4.15)

The background error covariance matrix \(\mathbf{C}_b^k = \mathbf{C}_{b,i,j}^k\) is formulated as:

\[
\mathbf{C}_{b,i,j}^k = \mathbf{u}_{b,i,j}^{\text{occ}} \cdot \mathbf{u}_{b,i,j}^{\text{occ}} \cdot R_{\text{occ}}^{k},
\]  

(4.16)

where the combined standard uncertainty profile \(\mathbf{u}_{b}^{\text{occ}}\), determining the diagonal variances (\(\mathbf{u}_{b,i,j}^{\text{occ}} \cdot \mathbf{u}_{b,j,i}^{\text{occ}} \cdot 1\)) and the off-diagonal covariance elements of \(\mathbf{C}_b^k\), is estimated as:

\[
\mathbf{u}_{b}^{\text{occ}} = \left( \mathbf{f}_{\text{bcvg}} \cdot \mathbf{u}_b^k \right)^2 + \left( \mathbf{s}_{\text{occ}}^k \right)^2 \right)^{1/2}.
\]  

(4.17)

Herein the bias coverage factor \(\mathbf{f}_{\text{bcvg}}\) is employed to strongly penalize the estimated bias-type uncertainty \(\mathbf{u}_b^k\) (cf. Eqs. (4.11)) relative to the estimated random uncertainty \(\mathbf{s}_{\text{occ}}^k\), in order to minimize the influence from potential residual background biases on the resulting optimised profile \(\alpha_{\text{SO}}^k\) (in this study \(\mathbf{f}_{\text{bcvg}} = 5\), for more discussion see Chapter 5).
Till now, the background bending angle $\alpha_b^k$ and the error covariance matrix $C_b^k$ for a given RO event $k$ of the day has been dynamically estimated based on the location of the RO event, and they could then be used in Eq. (4.9). Taking an overall look at this new dynamic scheme of estimating the background error covariance matrix, the following summary can be made to address the key advancements of the new scheme over existing schemes: 1) we use a 3D- and time-dependent formulation of all key statistical variables needed for calculating $C_b^k$, based on reliable ensembles of atmospheric forecast and analysis profiles as well as of observed profiles, while existing formulations use globally static relative errors and either climatologies (still most common; see Section 4.1) or forecasts (OPSv5.4) or observations (climatological profile retrievals only; see Section 4.3); 2) we use a bias estimate $\Delta\alpha_{f,b}^k$, allowing to reduce bias in the co-located background profile $\alpha_b^k$, while existing schemes use no such bias mitigation measure; 3) we use estimates of background bias uncertainty $u_b^k$ and random uncertainty $s_{f,a}^k$, and penalize $u_b^k$ against $s_{f,a}^k$ to minimize bias influence on $\alpha_{SG}^k$, while existing schemes use globally static relative background errors (see Section 4.1); 4) we use daily updated realistic empirical estimates of background error correlations, $R_{f,a}^{\text{acc}}$, while existing schemes either ignore these correlations or use crude (exponential) fall-off models that not representing realistic correlation shapes.

Furthermore, Eqs. (4.11), (4.13) and (4.14) show that the dynamic method is flexible in a seamless manner to either include $(\alpha_{f,a}^k, u_b^k)$ or $(\alpha_{f,a}, u_a^k)$ or both of them in the formulation of background bias estimation $(\Delta\alpha_{f,b}^k, u_b^k)$, so that users of the method can readily decide what to include according to their context and preferences. Also, the grid definition, and the space- and time-averaging domains per grid cell, can be flexibly adjusted by users.

**Tri-linear interpolation**

Since in the beginning of this section (see also Figure 4.1), a tri-linear interpolation scheme has been used to interpolate $\Delta\alpha_{f,b}^k$, $u_b^k$, and $s_{f,a}^k$ to the corresponding latitude, longitude of a given RO location and the standard 400 altitude grids for the statistical optimisation, its scheme is presented here.

The tri-linear interpolation includes two steps. The first step is a bi-linear latitude/longitude interpolation which is to interpolate the corresponding values of the four surrounding grids of the mean location of a RO event to the mean location. The bi-linear interpolation is an extension of linear interpolation for interpolating a point on a regular 2D grid. In our case, the 2D grids denote latitude and longitude grids, and the grid points used for the interpolation are the centres of each $10^\circ \times 20^\circ$ lat/lon cell. The point to be interpolated for is the mean location of any incoming RO event, $k$. Figure
4.2 illustrates the principle of the bi-linear interpolation. The red filled circle is the mean location of a RO event; the four black points are the four grids points surrounding the mean location of the RO event. The idea of bilinear interpolation is to perform 1D linear interpolation along one direction first and then perform 1D interpolation along the second direction. In our case, the 1D interpolation along the latitudinal direction is performed first, i.e, interpolate \( Q_{11} \) and \( Q_{12} \) to obtain \( R_1 \) and interpolate \( Q_{21} \) and \( Q_{22} \) to obtain \( R_2 \), then interpolate \( R_1 \) and \( R_2 \) along the longitudinal direction to obtain the profile at the RO mean location.

![Diagram of bi-linear interpolation](image)

**Figure 4.2** Bi-linear interpolation of background quantities from the grid points to the mean location of a RO event

A special care is taken for occultation events that arrive at high altitudes (beyond \( \pm 85^\circ \)). In these areas, we cannot find four regular surrounding four grid points for the above described standard bilinear interpolation. The solution at these areas is to perform the linear interpolation along the latitude circle first and then perform the interpolation along the converge longitude that relative to the polar centre. For example, if an occultation event locates at 89° N, 25°E, so the converge longitude is 155°W. The first step is to perform the interpolation along the 85° N latitude circle to get two points with the latitude and longitude as (85° N, 25° E) and (85° N, 155° W). After that, we then interpolate the obtained two points to the mean location of the RO event.

The reason that bi-linear interpolation is applied to obtain co-located values is because it is commonly used at the ECMWF [Persson, 2011]. Since the background related variables are estimated mainly based on ECMWF fields, we would better follow the same interpolation scheme. It should be noted that although bilinear interpolation is performed along both directions, it is not linear but quadratic.
The second step of the tri-linear interpolation is to use the values at the 200 altitude levels to vertically interpolate to the 400 levels of the target grid (200 m spacing), which are used as altitude levels for all profiles or matrices in the statistical optimization. This step is a commonly used linear interpolation and it is not elaborated here. After the first and the second steps are applied, the quantities that directly needed for the statistical optimisation on the standard vertical grids and co-located with the RO event are obtained.

4.6 Estimation of intermediate variables for background error covariance matrix

This section complements the above introduction of the new method for estimating background error covariance matrix by providing more details on the computation of the key variables for constructing $C_b^K$ and $\alpha_b^K$, discussing 1) the estimation of the analysis- and forecast-related variables $\bar{\alpha}_a$, $s_a$, $\bar{\alpha}_f$, $s_f$, $s_{a-f}$, and $R_{a-f}$, 2) the estimation of the analysis bias $b_a$, and 3) the estimation of the observation-related variables $\bar{\alpha}_o$, $s_o$, $b_o$ and their associated co-located variables $\bar{\alpha}_c$ and $s_c$.

4.6.1 Estimation of analysis- and forecast-related variables

The first step is to extract the forecast bending angle and analysis bending angle profiles from the respective ECMWF T42L91 fields on a regular 2.5°×2.5° horizontal grid, which is comparable to the horizontal resolution of the ECMWF T42 fields. In order to obtain a sufficient number of bending angle profiles for statistics and also to obtain smooth profiles that filter diurnal and mesoscale weather changes, 10° latitude × 20° longitude cells (more longitude extend polewards of 60°, compensating for the meridian convergence) and five days of ECMWF data (containing ten time layers, five each 00 UTC and 12 UTC) are used, as summarized in Section 4.5.1.

As a result, in each of the 10° × 20° cells there are 320 analysis and 320 forecast profiles (more polewards of 60°) that were used to calculate the mean profiles, $\bar{\alpha}_a$ and $\bar{\alpha}_f$, and their standard deviations, $s_a$ and $s_f$, using standard estimation equations [e.g., Steiner and Kirchengast, 2004]. The calculations of $s_{a-f}$ and $R_{a-f}$ for each cell use the differences between the forecast and analysis bending angles of all the 320 pairs of profiles, also following standard estimation equations [Steiner and Kirchengast, 2004].

The global-mean correlation matrix $R_{a-f}$ is finally calculated by averaging the individual correlation matrices of all 10° × 20° cells. While the individual matrices per cell appear still noisy in shape, this global averaging effectively draws from an ensemble of more than 100,000 native profiles (320 × 18 × 18), providing a very robust estimation. Based on extensive testing, it is found that the
correlation lengths of main peaks and the shape of the correlation functions depend little on latitude and longitude, so the averaging is well justified. Although, \( \mathbf{R}_{f-a} \) (Eqs (4.16) and (4.17)) only represents the correlation of the errors expressed by \( s_{f-a}^k \), it is used as the correlation of the background uncertainty, which includes both the bias-type uncertainty \( u^k_b \) and the random uncertainty \( s_{f-a}^k \). While one could include some rough guess of long-range correlation also for the bias-type errors expressed by \( u^k_b \), which are dominated by the analysis and observation biases \( b_a \) and \( b_o \) (cf, Eqs. (4.13) and (4.14)), we considered this is not needed since these correlations are quantitatively unknown and the results are quite reasonable with just using \( \mathbf{R}_{f-a} \).

Figure 4.3 shows the variation of the relative bending angle forecast-minus-analysis standard deviations with impact altitude and latitude, 100 \( \times \) (\( s_{f-a} / \overline{u}_a \)) [%], on two example days (15 January and 15 July, 2008), which represent winter in the northern and southern hemispheres, respectively. It shows that large values of standard deviation occur in the winter hemisphere at high latitudes. In the Antarctic and Arctic winter, the relative standard deviations are larger than 10% at 80 km impact altitude, decreasing to ~5 % at 70 km, ~3 % at 50 km, and to ~1 % below 25 km. In the non-polar regions, the values amount approximately to 3 % to 4 % near 80 km and to 1 % to 2 % below. This reflects that the ECMWF 24h-forecast errors (at T42L91 resolution) are in general fairly small, much smaller than the uncertainties that typically need to be assumed for climatologies (15% to 20%).

Figure 4.3 Relative standard deviations of forecast-minus-analysis bending angle differences as a function of latitude (10˚ bins, zonal means) and impact altitude (200 level grids) on 15 January (left panel) and 15 July (right panel), 2008.

Furthermore, in course of testing, it is found that the \( s_{f-a} \) estimates consistent with flow-dependent forecast error estimates produced by ECMWF’s ensemble of data assimilations (EDA) system [M.
Bonavita, ECMWF, pers. communications, 2012; Bonavita et al., 2011; Isaksen et al., 2010]. \( s_{r,a} \) is a reasonable estimator for our purpose also in the sense that it provides a tentatively conservative estimate of random forecast errors, due to its construction from forecast and analysis differences, which include as well random analysis errors (being generally a minor contribution compared to the forecast errors, though).

Figure 4.4 illustrates exemplary error correlation functions extracted from \( R_{r,a} \), at three representative height levels (30, 50, 70 km), as well as the correlation length of the correlation functions for all the 200 altitude levels (only altitude levels within 20 km to 80 km are shown). It can be seen from the left panel that the correlation functions have a near-Gaussian shape at the main peak (confirmed by fitting tests), two somewhat asymmetric negative side peaks, two small positive side peaks, and otherwise gradually decrease to zero in the far range from the peaks. The right panel shows the variation in the error correlation length, ranging from about 0.8 km to 6 km in the impact altitude range from 20 km to 80 km. The background error correlation length assumed in the OPSv5.4 is comparatively broader [10 km throughout; e.g., Steiner et al., 2013].

![Figure 4.4](image)

**Figure 4.4** Global-mean correlation functions of background uncertainty for three representative impact altitude levels (30 km, 50 km, and 70 km; left panel) and estimated correlation length of the correlation functions at all impact altitude levels from 20 km to 80 km (right panel), for 15 July, 2008.

### 4.6.2 Systematic bias in bending angles from ECMWF analysis fields

The relative bias in the ECMWF analysis bending angles, \( 100 \times (b_a / \overline{\alpha}) \) [%], is propagated from an estimated analysis temperature bias \( b_{a,T} \). Since \( \overline{\alpha} \) is known now, \( b_a \) could be determined from the relative bias. Due to lack of robust knowledge and associated lack of robust quantification capability for the analysis bias, because the “true” state is hard to know [M. Bonavita and S.B. Healy, ECWMF,
pers. communications, 2012], $b_{a,T}$ is formulated as a simple analytical model with dependences on altitude, latitude, and season (day of year). The structure of the model largely follows the empirical-analytical error model of Scherllin-Pirscher et al. [2011b]; Eqs. (2) to (6) therein.

The selection of the model’s fitting parameters and the selected structure of the model is based on discussions with ECMWF [M. Bonavita, pers. communications, 2012] and on related ECMWF experience from intercomparison with various analysis-forecast systems from other weather centers and against non-bias-corrected reference data such as radiosondes and RO data. A particular difficulty limiting detailed knowledge on $b_{a,T}$ is that accurate reference data above about 35 km (over the upper stratosphere and mesosphere) are sparse, calling for conservative estimation.

The vertical structure of the model is slightly simplified compared to Scherllin-Pirscher et al. [2011b], Eq. (2) therein, and constructed in the following way: below the bottom of the upper stratosphere $z_{USbot}$, a small constant value of $s_0$ is set to be the bias, while above $z_{USbot}$ the bias is set to increase linearly with altitude:

$$
    b_{a,T} = \begin{cases}
    s_0 & \text{for } z_{surf} < z \leq z_{USbot} \\
    s_0 + k_0(z - z_{USbot}) & \text{for } z_{USbot} < z < z_{top}.
\end{cases}
$$

In Eq. (4.18) $z_{surf} = 0.1$ km and $z_{top} = 80$ km are the bottom and the top level altitudes of the 200 vertical levels defined in section 4.5.1; $z_{USbot}$ is set to 30 km; and $s_0$ and $k_0$ are modeled as functions of latitude and season according to Scherllin-Pirscher et al. [2011b], Eqs. (3) to (6) therein (modeling the time parameter $\tau$ in day-of-year form). The basic mean magnitude parameter $x_0$ is set to 0.5 K and 0.05 K/km for $s_0$ and $k_0$, respectively, and the maximum amplitude parameter $\Delta x$ is set to 0.6$x_0$ for both parameters. The factors $f_{\Delta x0}$ and $f_{\Delta x0}$ denote the fraction of $\Delta x$ allocated to latitudinal change and seasonal variations, respectively. These two parameters can adopt values between zero and unity and they are set to 1.0 and 0.67 in this study. The parameters $\varphi_{\Delta x0}$ and $\varphi_{\Delta xhi}$ are the lower and upper latitude boundaries for ensuring that the value of the latitude-dependence function $f(\varphi)$ is zero in the latitude range from the equator to $\varphi_{\Delta x0}$, linearly increasing from 0 to 1 in the latitude range from $\varphi_{\Delta x0}$ to $\varphi_{\Delta xhi}$, and remaining 1 from $\varphi_{\Delta xhi}$ to the poles; in this study, $\varphi_{\Delta x0}$ and $\varphi_{\Delta xhi}$ are set to 40º and 60º, respectively. All these settings ensure that $s_0$ and $k_0$ are 20% higher than their basic mean magnitude in the summer hemisphere but twice their mean magnitude in the winter hemisphere.

Figure 4.5 shows the variations of temperature systematic biases with MSL altitude and latitude in 15 January and 15 July, 2008. It can be seen from this figure that the resulting temperature biases are constant within $\pm 40^\circ$ latitude regions as designed. The biases increase with latitude and increase more in winter hemisphere.
Figure 4.5 Estimated relative biases, based on simple analytical modelling, for ECMWF analysis temperature as function of latitude and MSL altitude on 15 January (left panel) and 15 July, 2008 (right panel).

After temperature biases are obtained, the relative bending angle biases are calculated using empirically derived conversion factors from temperature to bending angle. Scherllin-Pirscher et al. [2011a] estimated the conversion factor for mapping from temperature errors to relative refractivity errors as $c_{T2N} = 0.5 \%/K$, and the conversion factor from relative refractivity to relative bending angle error as $c_{N2a} = 2.4 \%/\%$; these two factors together resulting in a conversion factor from temperature errors to relative bending angle errors of $c_{T2a} = c_{T2N} \cdot c_{N2a} = 1.2 \%/K$. Since use of these conversion factors is well sufficient for our simple model, we adopt this result and compute the relative bending angle bias in the form $100 \times (b_a / \tilde{\alpha}_a) = c_{T2a} \cdot b_a$, and in turn we invoke $\tilde{\alpha}_a$ to finally obtain the estimated bending angle bias $b_a$.

Figure 4.6 illustrates the vertical structure of $100 \times (b_a / \tilde{\alpha}_a)$ for the same two example days as used for illustrating $100 \times s_{t-a} / \tilde{\alpha}_a$ in Figure 4.3. The bending angle biases reveal a clear dependence on altitude, latitude, and season, in line with the simple model adopted. For example, at any given altitude level the bending angle biases within ±40° latitude are constant. This reflects the basic mean magnitude of the biases at each height level and it amounts approximately to 3.5 % at 80 km and decreases linearly to about 1 % at 30 km. The biases increase polewards from the 40° latitude, with a larger increase in the winter hemisphere. The largest biases are in the polar winter region where they reach roughly 4 % to 8 % in the mesosphere, reflecting that these are the most difficult conditions for the ECMWF analyses to provide accurate data.
Figure 4.6 Estimated relative biases, based on simple analytical modelling, for ECMWF analysis bending angles as function of latitude and impact altitude on 15 January 2008 (left panel) and 15 July 2008 (right panel).

4.6.3 RO observed-mean bending angle and its systematic bias

The mean observed bending angle profile for each cell is calculated using those RO measurements from COSMIC, GRACE, and MetOp-A missions that are located in the cell’s domain and that are acquired during the same five days as used for estimating the analysis- and forecast-related variables (test days from January 2008 and July 2008 used in this study; see the results in Chapter 5 below).

For all satellites, excess phase and orbit information provided by UCAR/CDAAC are used to calculate ionosphere corrected bending angles using an advanced version of OPSv5.4. Since the mean bending angle can be strongly affected by outlier profiles and since we do not apply the whole OPSv5.4 quality control mechanisms (we stop computations at bending angle level and do not check consistency of RO refractivity and temperature profiles by comparing them to reference profiles provided by ECMWF), an additional twofold quality control approach to individual bending angle profiles is applied according to Foelsche and Scherllin-Pirscher [2012]: we check individual bending angle profiles in the impact altitude range from 50 km to 80 km and exclude profiles if they have bending angles larger than 40 μrad or smaller than −40 μrad. Furthermore, all profiles that have bending angles outside of four standard deviations from the mean in the entire impact altitude range are rejected.

Regarding ensemble size, for the test days of January and July 2008 used in this study the resulting profile ensemble per cell contains about 40 profiles so that effective random error mitigation from the averaging is well possible. In general, should observed-profile ensemble sizes be considered too small during some time periods before mid-2006 where mainly the CHAMP satellite provided RO data, the averaging domain can be enlarged (primarily along longitude, secondarily in the number of days).
The mean observed bending angle profiles $\overline{\alpha}_o$ are finally calculated from averaging over all profiles that passed the quality checks; mean co-located bending angle profiles $\overline{\alpha}_c$ are obtained from averaging over the corresponding EMCFWF analysis bending angle profiles co-located to the RO events. Their associated standard deviation estimates, $s_o$ and $s_c$, are computed from the ensemble of observed and co-located profiles, respectively, by the same standard estimation equations as used for $s_a$ and $s_f$ [e.g., Steiner and Kirchengast, 2004].

The bias of the mean observed profiles, $b_o$, is set to 0.2 μrad, based on experience with analysis and inter-comparison of bending angle data at high altitudes from different RO satellites, analyses and forecasts, and climatologies. This educated-guess value of 0.2 μrad includes errors due to the incomplete removal of the ionospheric contribution to the measurement, multipath errors, errors in the satellite’s orbits and velocities, as well as clock bias estimates.

4.7 Dynamic estimation of observation error covariance matrix for the new algorithm

This section introduces the main algorithmic steps for estimating $C_o^k$ as shown in the right part of Figure 4.1, i.e., construction of observation error correlation matrix and dynamic estimation of observation error covariance matrix.

4.7.1 Construction of observation error correlation matrix

The global-mean correlation matrix of observation errors $R_o$ is estimated in a similar way as the estimation of $R_{f,a}$, but using the differences between RO observed bending angle profiles and their co-located analysis bending angle profiles. The observation data used are the same for calculating the mean observed bending angles in Section 4.6.3. The method for estimating the error correlation matrix is the same as the estimation of forecast-minus-analysis standard deviations which has been described in Section 4.6.1. For the convenient use in statistical optimisation, this global-mean correlation matrix is also pre-calculated and saved in the daily background error fields. It is the only parameter that saved in the daily background error fields but not for obtaining background information. In addition, this global-mean correlation matrix is directly calculated and saved at the (200 m spacing, 400 level) target grid of the statistical optimisation (see also Section 4.5.3). The reason that the 400 level grids is used for the observation error correlation matrix instead of the 200 altitude grids used for the background related variables is: the observed bending angles are usually on denser altitude grids than background bending angles from ECMWF fields are; using of denser altitude grids for correlation matrix of observation errors allows more vertical information to be
captured. This daily estimated global-mean correlation matrix of observation errors is also used for all the RO events of the day. For clarity, it is denoted as \( R^\text{occ} \) for the following use of constructing the observation error covariance matrix of the day.

Figure 4.7 shows correlations functions of observation errors at three representative heights of 30 km, 50 km and 70 km. It could be seen that the correlation function of observation errors has similar shape as those of background errors (see Figure 4.4), Gaussian shape at the main peak, two negative side peaks following by two positive side peaks, from which the functions gradually to zeros. From these three functions and also some other internal pictures, the correlations lengths of observation errors stay around 1 km for all of the altitude levels from 20 km to 80 km.

Figure 4.7 Global-mean correlation functions of observation errors at three representative impact altitude levels (30 km, 50 km and 70 km).

4.7.2 Dynamic estimation of observation error covariance matrix

Before estimating the observation error covariance matrix, the observation uncertainty \( u_o \) should be calculated to be used for the diagonal values of the error matrix. Different to many methods that estimate observation uncertainty as a constant value, we estimate the observation uncertainty as a function of altitude for each occultation event. The estimated bias-calibrated background bending angle profile \( \alpha_b^k \) obtained in Section 4.5.3 is regarded as the reference profile in this context (see also Figure 4.1). The procedure of the new method is described below.

The first step is to subtract \( \alpha_b^k \) from the observed bending angle profile \( \alpha_o^k \) to obtain the deviation/ fluctuation profile \( \Delta \alpha_o^k \) of the observed profile:

\[
\Delta \alpha_o^k = \alpha_o^k - \alpha_b^k, \tag{4.19}
\]

\( \Delta \alpha_o^k \) is then smoothed with a 10 km window moving average. In practice, the 10 km moving average means, for a specific level its moving average value is calculated by averaged the profile’s sample
points located between the two levels that are 5 km upwards and 5 km downwards from the specific level; for values at the topmost 5 km and bottommost 5 km where the 10 km window cannot be found, they are assigned using the value that at the height level 5 km below the top of the profile and the value at the level that 5 km above the bottom respectively. The resulting smoothed deviation profile is denoted as \( \Delta \alpha_o^k \). Figure 4.8 shows \( \Delta \alpha_o^k \) and its smoothed profile \( \Delta \alpha_o^\alpha \) for a selected sim-MetOp event. It can be seen that the smoothed deviation profile looks like an average profile of the original profile.

**Figure 4.8** Raw and smoothed deviation profiles of a sim-MetOp observed bending angle profile relative to the corresponding bias-calibrated background profile, deltaAlpha represents \( \Delta \alpha_o^k \) and deltaAlphasmoth represents \( \Delta \alpha_o^\alpha \).

The next step is to subtract the smoothed deviation profile \( \Delta \alpha_o^\alpha \) from the original deviation profile \( \Delta \alpha_o^k \) to obtain a deviation profile that contains only random errors, \( \Delta \Delta \alpha_o^k \):

\[
\Delta \Delta \alpha_o^k = \Delta \alpha_o^k - \Delta \alpha_o^\alpha.
\]  
(4.20)

The resulting \( \Delta \Delta \alpha_o^k \) is a deviation profile that contains only random errors relative to the estimated background bending angle profile \( \alpha_o^k \) due to the fact that the systematic errors have been removed through the constructions of Eqs. (4.19) and (4.20). \( \Delta \Delta \alpha_o^k \) is then used to calculate the observation uncertainty. Similarly to the above mentioned 10 km smoothing, the standard deviation of an impact altitude level \( i \) of which the corresponding impact altitude height is \( h \) can be calculated using the values of \( \Delta \Delta \alpha_o^k \) in the height range between \( h+5 \) and \( h-5 \):
\[ u_o^k = \sqrt{\frac{1}{n-1} \sum_{k=h-5}^{h+5} [\Delta \alpha_o^k]^2} \]

where \( n \) is the number of sample points between the height of \( h+5 \) and \( h-5 \), and \( k \) is the height index of a corresponding height level from \( h-5 \) to \( h+5 \). Figure 4.9 shows the new observation error profile \( u_o^k \) and its intermediate variables \( \Delta \alpha_o^k \), \( \bar{\Delta \alpha_o} \), and \( \Delta \Delta \alpha_o^k \) of the same sim-MetOp event as Figure 4.8:

**Figure 4.9** The new observation errors and their intermediate variables of the sim-MetOp RO event, deltaAlpha represents \( \Delta \alpha_o^k \), deltaAlphasmoth represents \( \bar{\Delta \alpha_o} \), deltadeltaAlpha represents \( \Delta \Delta \alpha_o^k \), and New-ObsErr represents \( u_o^k \).

Comparing the red line (\( \Delta \alpha_o^k \)) and the green line (\( \Delta \Delta \alpha_o^k \)) in Figure 4.9, we can see that the part of the red line above 50 km is slightly biased towards the positive side of the x-axis and the part below 50 km is biased towards the negative side; after Eqs. (4.19) and (4.20) are applied, the systematic biases in \( \Delta \alpha_o^k \) are removed, which leads to the green line (\( \Delta \Delta \alpha_o^k \)) to be more evenly fluctuate around zero value (of the x-axis). The new observation errors (blue line) vary a little with altitude above 50 km, while below 50 km, the new error linearly increases with the decrease of altitude and reaches about 4.7 \( \mu \)rad at 25 km and then remains at 4.7 \( \mu \)rad from 25 km down to 20 km. In fact, at altitudes below about 50 km, the increase of the observation error is not only due to the increase of the error itself, but also due to small-scale atmospheric variability. Therefore, in the real practice of statistical optimization, we adopt the error value at 50 km for errors below the altitude down to 30 km which is the lowest altitude of the new statistical optimization applied.
Using the observation uncertainty estimated from Eq. (4.21) and also the estimated correlation matrix $R^{\text{occ}}_o$, the observation error covariance matrix $C^{k}_{o}$ for the given RO event $k$ can be estimated via Eq. (4.22):

$$C^{k}_{o,i,j} = u^{k}_{o,i} \cdot u^{k}_{o,j} \cdot R^{\text{occ}}_{o,i,j}.$$ 

(4.22)

### 4.8 Implementation of the new approach into EGOPS software package

In order to evaluate the new statistical optimization approach, it is incorporated into the bending angle tool of Geometric Optics CCR Bending angle Retrieval parallel with the OPSv5.4 SO algorithm. The version of EGOPS that the new approach is incorporated into is EGOPSv2951, which is only an internally used version at the WEGC center. This version is also used in Chapter 5 for simulation and retrieval of RO events.

Before retrieving atmospheric profiles using the new statistical optimization of a given day, the background error field for that day should be prepared. In practice, the error field is saved as a NetCDF format profile under certain directory. During the RO data processing, the software will then invoke the new statistical optimization approach and read in needed quantities from the error field for statistical optimisation.

An error field file has four dimensions, lat (latitude), lon (longitude), ImpAlt (Impact-Altitude) and ImpAltgrids (Impact-Altitude grids). The lat and lon dimensions are consistent with the horizontal resolution described in Section 4.5. The ImpAlt denotes the 200 vertical levels described in Section 4.5. The ImpAltgrids represent impact altitude grids from 0.2 km to 80 km with a 0.2 km step which is the standard vertical grids for the new statistical optimization. It is only used for the global-mean correlation matrix of observation error due to the higher vertical resolution of observed bending angles.

Table 4.1 summarises the calculated variables and their dimensions included in the daily background error field. It lists both the variable names in the error field and their notations in our algorithm.

Although some variables listed in Table 4–1 are not used in the new statistical optimisation approach, they are still saved in the daily background field for other scientific purposes.
Table 4-1 Variables that included in a daily background error fields

<table>
<thead>
<tr>
<th>Name of variables (notation)</th>
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<td>lon, lat, ImpAlt</td>
</tr>
<tr>
<td>bending_angle_analysis_spread, ( $s_a$ )</td>
<td>lon, lat, ImpAlt</td>
</tr>
<tr>
<td>Bending_angle_forecast_mean, ( $\bar{\alpha}_f$ )</td>
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<tr>
<td>Bending_angle_forecast_spread, ( $s_f$ )</td>
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<tr>
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<td>lon, lat, ImpAlt</td>
</tr>
<tr>
<td>Bending_angle_analysis_mean_bias, ( $b_a$ )</td>
<td>lon, lat, ImpAlt</td>
</tr>
<tr>
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<td>ImpAlt, ImpAlt</td>
</tr>
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<td>Bending_angle_forecast_minus_analysis_errcorrlength</td>
<td>ImpAlt</td>
</tr>
<tr>
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<tr>
<td>Bending_angle_observed_spread, ( $s_o$ )</td>
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<tr>
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<td>Observed_bending_angle_errcorrmatrix, $R_o$</td>
<td>ImpAltgrids, ImpAltgrids</td>
</tr>
</tbody>
</table>

4.9 Summary

This chapter introduced a new statistical optimisation approach to dynamically estimate background bending angle profile and its associated error covariance matrix as well as observation error covariance for obtaining more reliable optimised RO bending angle profiles. This approach mainly includes two parts, i.e., 1) the estimation of background bending angle profile and its associated error covariance matrix; 2) the estimation of observation error covariance matrix. This method accounts for dependences of background variables and their uncertainties on latitude, longitude, altitude, and day of year. It uses bending angles from multiple days of ECMWF short-term forecast and analysis fields, together with mean observed bending angles, to obtain background profiles and associated error covariance matrices with geographically and vertically varying background uncertainty estimates on a daily-updated basis. This method estimate observation uncertainty uses the difference between RO observed bending angle and the estimated background bending angle, and correlation for the observation uncertainties is statistically estimated using large ensemble of RO observed bending angles and co-located ECMWF analysis bending angles.
The dynamic estimation of background error consists of three main algorithmic steps: 1) construction of basic daily background fields of key analysis-, forecast-, and observation-related variables on a global latitude-longitude-altitude grid for any day to be processed, 2) preparation of derived daily background fields with the specific statistical quantities directly needed for estimation of background error covariance matrix, and 3) performing the actual dynamic estimation of background error covariance for any RO event of a given day and correct the biases in background bending angle profile.

The key advancements of the new dynamic scheme in estimating background error covariance matrix over existing schemes could be summarized as: 1) A 3D- and time-dependent formulation is used for all key statistical variables needed in the formulation of the background error covariance matrix, these variables are calculated based on reliable ensembles of atmospheric forecast and analysis profiles as well as of observed profiles, while existing formulations use globally static relative errors and either climatologies (still most common) or forecasts (OPSv5.4) or observations (climatological profile retrievals only); 2) a background bias estimate is used to actively reduce bias in the co-located background profile, while existing schemes use no such bias mitigation measure; 3) estimates of background bias uncertainty and random uncertainty are used to formulate background errors, and the former is penalized against the latter to minimize bias influence on the resulting optimised profile, while existing schemes use globally static relative background errors; 4) a daily updated realistic background error correlation matrix is used, it is empirically estimated from forecast-minus-analysis difference profiles, while existing schemes either ignore these correlations or use crude (exponential) fall-off models not representing realistic correlation shapes.

We showed furthermore that the dynamic method is flexible in a seamless manner to either include mean-analysis or mean-observed bending angle profiles and associated uncertainties or both of them together in the formulation of mean-background profile and uncertainty estimation. Based on this versatility, users of the method can readily decide which information to include according to their context and preferences. Also, the grid definition, and the space- and time-averaging domains per grid cell, can be flexibly adjusted by users.

The dynamic estimation of observation error covariance also consists of two main steps: 1) construction of observation error correlation matrix uses multiple days of RO observed bending angle and co-located ECMWF analysis bending angle; 2) Dynamic estimation of observation error covariance matrix in terms of estimation of observation uncertainty.

The key advancements the new dynamic scheme in estimating observation error covariance matrix over many existing statistical optimisation schemes could be summarized as: 1) A altitude dependence formulation is used for estimating observation errors, while, many of the existing schemes uses an empirical constant value; 2) A daily updated realistic observation error correlation matrix is used, it is empirically estimated from observed-minus-analysis difference profiles, while existing schemes either
ignore these correlations or use crude (exponential) fall-off models not representing realistic correlation shapes.

With the dynamic construction of background error covariance matrix, the resulting background errors reveal clear variations with latitude, altitude and season, and the largest errors are found in high latitudes of the winter hemisphere. The correlation functions of background errors reveal Gaussian shape at the main peak, from which outwards, there are two negative side peaks, and the two negative peaks followed by two small positive side peaks from which the functions gradually decrease to zeros.

With the dynamic construction of the observation error covariance matrix, the observation uncertainty reveals some variations with altitude above 50 km, while below 50 km, errors increase quickly with the decrease of altitude, and these errors are believed mostly related to small scale atmospheric variability, therefore below 50 km, value at 50 km are assigned to the values below the height. The correlation functions of observation errors have similar shape to those of background errors.

Based on all these settings of advantages, it is expected that the new dynamic scheme outperforms existing schemes, and a first evaluation against the existing Wegener Center OPSv5.4 scheme, which is a leading existing scheme and therefore used as a reference. The evaluation results are presented in Chapter 5.
Chapter 5. Evaluation of the New Algorithm Using Single Days’ RO data

This chapter evaluates the performance of the new statistical optimisation described in Chapter 4 against the approach used in the Wegener Center Occultation Processing System version 5.4 (OPSw5.4) software package using single days’ RO data. Both algorithms are operated down to 30 km. Statistical errors of atmospheric profiles retrieved from the new and the existing approaches relative to their reference profiles are calculated and compared. The test data include simulated MetOp-A (sim-MetOp) occultation events on 15 July, 2008 and real RO events from CHAMP and COSMIC on 15 January and also 15 July, 2008. Due to the insufficient CHAMP measurements on these two days, for reliable statistical results, three consecutive days (14 to 16) measurements were used to calculate the statistics for the middle day, i.e., the 15th of the month.

The first part of this chapter introduces the software used for the simulation of the RO events and also for the retrieval of atmospheric profiles. After that, the new statistical optimisation algorithm is evaluated using both simulated and observed data. Since it is has been proved that background errors are usually highly correlated and background correlations are critical for smoothing bending angles at high altitudes [Healy, 2001], we first evaluate the effects of the dynamic estimated background error covariance matrix on the optimized bending angles only. To achieve this, we propose an approach called Dynamic1 SO, which uses the new background error covariance matrix described in Section 4.5 together with the observation error covariance estimated from the existing OPSv5.4, and the performance of the proposed approach is evaluated. The evaluation results are presented in Section 5.2. Then, the complete new approach, which exploits both the dynamically estimated background and observation error covariance matrices (Sections 4.5 and 4.7), is evaluated. For the convenience of description, the complete new approach is also called Dynamic2 SO hereafter. The evaluation results of Dynamic2 are presented in Section 5.3. Since the error correlations are critical for smoothing the optimised bending angles, Section 5.4 investigates the effects of different correlation matrix on RO retrievals. Finally, a summary is given to conclude the performance of the two approaches on single days RO observations.
5.1 The software and preparation of test data

5.1.1 The EGOPS software package

The End-to-End Generic Occultation Performance Simulation and Processing System (EGOPS) is a software package to provide a simulator software supporting evaluation and planning of present and future GNSS-LEO and LEO-LEO atmospheric occultation sounding activities as well as to integrate the retrieval of observed atmospheric soundings from occultation experiments [Fritzer et al., 2011; Kirchengast, 1996]. Figure 5.1 illustrates the Modular View of EGOPS.

![Figure 5.1 A modular view of EGOPS (from Fritzer et al., 2011)](image-url)
The main functionalities of the EGOPS software include two parts. The first part is for the simulation of RO events and it has three simulation tasks, i.e., Mission Analysis and Planning (MAnPI), the Forward Modelling (FoMod) and Observation System Modeling (OSMod). These three tasks mimic the RO technique and provide RO observables. The second part is Inversion and Retrieval (InRet) and it is used to retrieve atmospheric profiles for both simulated and real RO observables.

The simulation of the RO measurements starts from MAnPI. This task allows the users to plan satellite constellations, trajectory of the transmitter and receiver in the constellations, measurement time range, geographic area, antenna field-of-view and occultation tangent point height levels of interest. The inputs for this task include the orbits of the planned satellite constellation and their antenna patterns. The main outputs of this task are the geometry of RO events which are then used as the inputs for the next simulation task: FoMod.

The FoMod simulates RO observables and related required variables for atmospheric retrieval. The main observables are phase and amplitude measurements as a function of time. This task accounts for only the effects from background atmosphere (neutral atmosphere and ionosphere) on the RO observables. The outputs of FoMod are used as the inputs of OSMod where the effects of observational errors are superposed to the RO observables. Observational errors that can be modelled in OSMod include the POD error, antenna thermal noise, local multipath error, clock error, etc. The outputs from OSMod could then be used for the retrieval of atmospheric profiles in InRet.

The InRet uses the simulated or real RO observables to retrieve ionospheric profiles (ionosphere processing) and also atmospheric profiles of neutral atmosphere (atmosphere processing). The ionosphere processing is beyond the focus of this thesis. In the atmosphere processing, one can select different retrieval tools. For example, in the part of bending angle retrieval tool, one can select Geometric Optics bending angle retrieval, Wave Optics bending angle retrieval, and also geometric CCR bending angle retrieval. The statistical optimisation algorithms available include the OPSv5.4 algorithm mentioned in Section 4.2, and also some previous algorithms that use the MSIS90 model for the statistical optimisation. In this part, the co-located ECMWF analysis profiles can also be calculated and used as the references of RO retrievals.

In this thesis, the simulation of MetOp-A occultation events uses the first part of the EGOPS software and the retrieval of the atmospheric profiles uses the second part of the EGOPS software. The version used is EGOPSv2951 which is only an internally used version at the WEGC centre. It should be noted that the above mentioned OPSv5.4 statistical optimisation algorithm is the algorithm developed in the version EGOPSv5.4, and this algorithm is kept in the EGOPSv2951. For the convenience of description, we still call the OPSv5.4 algorithm for the corresponding description in this thesis.
5.1.2 Ensemble design and simulation of MetOp-A RO events

For the simulation of MetOp-A data, two simulations were performed: 1) for moderate ionospheric conditions and the level of observational noise similar to the GRAS-type receiving system [Ramsauer and Kirchengast, 2001; Steiner and Kirchengast, 2005]; 2) for perfect conditions in which the ionospheric contributions and also the observational noise to the measurements were neglected. The first stream of the data is regarded as simulated realistic observables of MetOp-A RO events. The second stream of the data is regarded as simulated ‘ideal’ observables of MetOp-A events which is only affected by the background neutral atmosphere and is regarded as the references for the first stream of data. The detail of the first simulation settings in different simulation tasks of EGOPS is explained below:

**MANpi:** The occultation simulation type selected is the GNSS-LEO occultation. Two height levels are set. The first level is for lower troposphere from 2.5 km to 15.0 km with a step of 2.5 km. The second height range is from 15 km to 85 km with 10 km as a step. The simulation accuracies for both of these height ranges are set to 0.05 km which is the highest accuracy setting in the software. If the tangent point of an occultation event passes one of the height levels defined above, the instantaneous geometry of the event is calculated and saved [Fritzer et al., 2011]. The simulated area is global and the WGS84 model is selected to describe the figure of the Earth. The SGP4 (Simplified General Perturbations version 4) orbit is used for the description of the trajectory of both GPS and MetOp-A satellite. The signal property selected is Tx-GPS-Generic.spd and the antenna pattern selected is Tx-GNSS.apd. The receiver antenna pattern selected is Rx-LEO-MetOp.apd. The receiver zenith antenna elevation limit is set to 10°.

**FoMod:** The occultation simulation type selected is space to space events – realistic geometry. Atmosphere model used is the ECMWF analysis fields of the day and the ionospheric model used is the NeUoG model which has been proved to be useful in many studies [Leitinger et al., 1996; Steiner et al., 2001]. Full-3D ray tracer is used for ray tracing computations which is the most accurate ray tracer tool in the EGOPSv2951. The ECMWF analysis fields have been introduced in Section 2.4. The NeUoG model is a global empirical solar-activity and local-time dependent 3D climatological model of the ionospheric electron density fields developed by Leitinger et al. [1996]. A moderate solar activity index F10.7 = 140 is set for the model. It should be noted that the NeUoG model does not take the small-scale ionospheric irregularities into account which should be kept in mind when analysing the simulated results.

**OSMMod:** The setting for observational error follows the GRAS receiving system performance [Ramsauer and Kirchengast, 2001; Silvestrin et al., 2000; Steiner and Kirchengast, 2005]. The settings of these errors in EGOPS have already been shown in the study of Steiner and Kirchengast,
The POD error (for both GPS and MetOp-A) are estimated based on a Kinematic POD error model. Within the error model, the radial position error for the GPS and LEO satellite is set to 0.2 m and 0.4 m, respectively, the velocity error along the GPS-to-LEO ray is set to 0.05 mm/s and the acceleration error is set to 0.05 µm/s². The receiver thermal noise error is modelled using LS-Band thermal noise model which with LEO antenna noise temperature is set to 150 K, and the loop bandwidth is set to 10Hz. The local multipath error is modelled using a sinusoidal shaped function in which the phase error period is set to 100 second, and the multipath phase error is set to 0.5 mm. The clock error is modelled based on random walk model and a ground-based single-difference correction method with the stability set to 1-sec Allan deviation of $1 \times 10^{-13}$ is used.

The above settings are for the first simulation which represents the realistic MetOp-A observables. For the second simulation, the settings of MANPI are the same as the first simulation. For the FoMod, only neutral background atmosphere is used and no ionosphere is applied. For the OSMOD, no observational errors are superposed. Therefore, the observables obtained from the second simulation are regarded as observables affected only by the neutral atmosphere, and their retrieved atmospheric profiles are considered as the reference profiles for those from the first simulation.

The number of simulated MetOp-A occultation events for the two simulations on 15 July is 723. Figure 5.2 shows the distribution of the simulated MetOp-A RO events for the test day.

Figure 5.2 The distribution of the simulated MetOp-A RO events on 15 July, 2008
5.1.3 COSMIC and CHAMP observation data

The CHAMP and COSMIC data are downloaded from CDAAC. The data type used is the atmPhs data which includes atmospheric excess phases and auxiliary data used for generating atmospheric profiles.

The total numbers of the CHAMP input data for 14 to 16 January 2008 and 14 to 16 July 2008 are 580 and 663, respectively. The total numbers of COSMIC input data for the two testing days are 2992 and 2450, respectively. For profiles retrieved from the real observed data, their co-located ECMWF analysis profiles are used as reference profiles.

5.2 Results of atmospheric profiles using only the newly estimated background error covariance matrix

This section mainly presents the results of the evaluation of Dynamic1 SO. The Dynamic1 SO uses $C_b^k$ and $\alpha_b^k$ estimated from the new approach (see Eqs. (4.16) and (4.15) in Section 4.5.3) as well as $C_o^{OPSv5.4}$ from the existing OPSv5.4 approach (see Eq. (4.6) in Section 4.2). These three terms are then used in Eq. (4.9) (replace the new $C_o^k$ with $C_o^{OPSv5.4}$) to calculate statistically optimized bending angles. For both the simulated and the observed RO data, both the Dynamic1 and the existing OPSv5.4 schemes, were applied, in order to enable inter-comparison of the result of these two data streams. The resulting retrieved profiles were compared to their co-located reference profiles, focusing on retrieval-minus-reference differences of the statistically optimised bending angle profiles $\alpha_{SO}^k$ and also inspecting the subsequently retrieved refractivity and dry temperature profiles. Relative difference profiles (retrieved-minus-reference divided by reference, units [%]) are typically produced for bending angle and refractivity, and absolute retrieved-minus-reference difference profiles for dry temperature.

These differences profiles were then used to also calculate statistics for large-scale geographic regions (global, and five latitude bands; see Section 5.2.4), where the mean systematic difference and its associated standard deviation of the difference profiles is inspected in a comparative way for the “Dynamic1 SO” and “OPSv5.4 SO” results. We now first look at individual example profiles to get some basic insight how the Dynamic1 SO works (Section 5.2.1), then turn to the statistical results (Sections 5.2.4 and 5.2.5) and finally also specifically inspect the influence of the choice of correlation matrix of background errors (Section 5.2.6). Sections 5.2.2 and 5.2.3 describe the quality control mechanisms and the method for calculating statistical errors.
5.2.1 Individual statistically optimised bending angle profiles

Figure 5.3 shows the statistically optimised bending angle profiles of three typical example events from sim-MetOp, CHAMP, and COSMIC, obtained from the Dynamic1 algorithm, the existing OPSv5.4 as well as their reference profiles; the events are from the 15th July ensemble. The profiles from the Dynamic1 SO are smoother than those from the OPSv5.4 SO and they are also closer to the reference profiles in these three cases. Although, some profiles from the OPSv5.4 SO are closer to the reference profiles than those from the Dynamic1 SO (not shown), profiles optimised by the Dynamic1 SO are generally smoother also in those cases.

**Figure 5.3** Statistically optimised bending angle profiles of three typical example events from sim-MetOp (top), CHAMP (middle), and COSMIC (bottom) on 15 July, 2008, obtained from the Dynamic1 algorithm (red) and OPSv5.4 algorithm (black), compared to their reference profile (perfect simulated profile for sim-MetOp or co-located ECMWF analysis profiles for observed CHAMP and COSMIC; cyan).
Figure 5.4 Illustration of intermediate variables contained in the formulation of Dynamic1 for the sim-MetOp (top nine panels) and COSMIC events (bottom nine panels) shown in Figure 5.3.

Figure 5.4 illustrates the results of some key intermediate variables in performing Dynamic1 for the sim-MetOp event (the upper nine panels) and the COSMIC event (the bottom nine panels) shown
in Figure 5.3. For each of the two events, the first row shows the estimated uncertainty of the mean analysis (left), mean observed (middle), and mean background (right) bending angle, respectively \( u_a \), Eq. (4.13); \( u_o \), Eq. (4.14); \( u_b \), Eq. (4.11); all interpolated to the RO event location but suppressing the upper index \( k \) index, like in \( u_{b}^{k} \), for clarity here, since these quantities do not yet occur in Eqs. (4.13), (4.14), and (4.11)). The second row shows the estimated random uncertainty of the forecast (left), combined standard uncertainty of the background (middle), and relative uncertainty of the background (right) bending angle, respectively \( s_{f-a}^{k} \), Section 4.6.1; \( u_{b}^{occ} \), Eq. (4.17); \( 100 \times (u_{b}^{occ} / \alpha_{b}^{k}) \), Eqs. (4.15) and (4.17)). The third row shows the estimated background bending angle (left), observed bending angle (middle), and relative uncertainty of the observed (right) bending angle, respectively \( \alpha_{b}^{k} \), Eq. (4.15); \( \alpha_{o}^{k} \), Eq. (4.9); \( 100 \times (\alpha_{o}^{OPSv5.4} / \alpha_{o}^{k}) \), Eqs. (4.7) and (4.9)).

For both the sim-MetOp and COSMIC events, from the first row, we can see that \( u_{a} \) is smaller than \( u_{o} \) at altitudes above about 50 km, while below 50 km \( u_{a} \) is larger than \( u_{o} \). The background bending angle uncertainty \( u_{b} \) (right), thanks to optimally combining \( u_{a} \) and \( u_{o} \) by inverse-variance weighting (Eq. (4.11)), neatly achieves the least possible uncertainty over the complete altitude range, indicating the value of this part of the new dynamic design.

From the second row, again for both the sim-MetOp and COSMIC event, it can be seen that \( s_{f-a}^{k} \) roughly has similar magnitudes as \( u_{a} \) (as also indicated by comparing Figures 4.3 and 4.6, since \( u_{a} \) essentially corresponds to \( b_{a} \)), both being very small in absolute terms above about 65 km. The combined uncertainty \( u_{b}^{occ} \), including now \( u_{b} \) (1st row, right) penalized by the bias coverage factor \( f_{bcvg} = 5 \), is still very small in absolute terms near 80 km from which it increases to within about 5 \( \mu \)rad to 10 \( \mu \)rad near 30 km; the comparison between \( s_{f-a}^{k} \) (2nd row, left) and \( u_{b}^{k} \) (1st row, right) confirms that this increase is dominated by the conservative approach that we strongly penalize the bias-type uncertainty \( u_{b}^{k} \).

This makes nicely explicit the relevance of how strongly the method’s user decides to keep bias influences into \( \alpha_{SO}^{k} \) at bay, by choosing a certain bias coverage factor (a factor of 5 to 10 appears reasonable to us; for the purpose of this introductory study \( f_{bcvg} = 5 \) is used). Furthermore, this provides a pointer to the more general discussion of the issue of how much background information the user in general wants to weigh in for support of the high altitude initialization of \( \alpha_{o}^{k} \), as a separate question from the degree of (un-)certainty that is in principle available from reliable sources of background data. This discussion is deferred as a follow-on study.
The relative background uncertainty (2nd row, right) highlights that in relative terms this uncertainty strongly increases upwards, exceeding 20% near 50 km for the sim-MetOp event and near 70 km for the COSMIC event, respectively. Such levels of difference are typical and generally driven by geographic location: in the present case the COSMIC event is located at southern mid-latitudes near 40° S, where both $u_b^k/\alpha_b^k$ and $s_{v,a}^k/\alpha_b^k$, and hence $u_b^{occ}/\alpha_b^k$ according to Eq. (4.17), are smaller than for the sim-MetOp event near 70° S (see Figures 4.3 and 4.6). Comparing these relative uncertainties to the globally static and constant relative uncertainty specifications of typically 15% to 20% in existing statistical optimisation schemes (Section 4.1), one can see that the new method in estimating the background error covariance provides the capability of significantly more realistic behaviour of the background error.

The third row of Figure 5.4, again for both the sim-MetOp and COSMIC events, confirms that $\alpha_b^k$ (left) and $\alpha_o^k$ (middle) generally go very closely together. The relative observation uncertainty $\sigma_o^{OPSv5.4}/\alpha_o^k$ (right) shows that, except typically for high altitudes in the mesosphere, its values are significantly smaller than the relative background uncertainty $u_b^{occ}/\alpha_b^k$ (2nd row, right); the “spiky” behaviour of $\sigma_o^{OPSv5.4}/\alpha_o^k$ at the high altitudes is due to $\alpha_o^k$ with its small absolute magnitude up there ($\sigma_o^{OPSv5.4}$ is a constant in the current formulation; see Section 4.2).

For each RO event, the detailed observation to background uncertainty ratio $\sigma_o^{OPSv5.4}/u_b^{occ}$ (not shown), and therefore also the transition altitude above which the observation uncertainties exceed the background uncertainties, depends on the quality of background information but more strongly on the quality of observations (e.g., CHAMP vs. COSMIC vs. sim-MetOp); both aspects are well indicated by a comparative look at the relative error panels of Figure 5.4 and well known in principle [e.g., Gobiet et al., 2007].

5.2.2 Detection of outliers for quality control of statistics

In Sections 5.2.4, 5.2.5 and 5.2.6, statistics errors of optimised bending angle profiles and atmospheric profiles retrieved from Dynamic1 and also OPSv5.4 relative to their reference profiles are calculated. In order to obtain better statistics, quality control is applied to reject outliers. In this thesis, both the EGOPS quality control and an additional control are applied. The EGOPS quality control means, in the output files of the atmospheric retrievals, a quality flag is assigned to indicate the quality of the profiles. If the flag of a profile is not equal to 0, then the profile is regarded as bad quality and should be discarded in calculating statistics. In EGOPSv2951, the bad quality of a profile is assigned if it fulfil one of the following criterions: 1) the difference between RO retrieved
refractivity with the co-located profiles is larger than 10% in the height range from 5 km to 35 km; 2) the difference between the RO retrieved dry temperature profiles with co-located profiles is larger than 20 K in the height range from 8 km to 25 km. Except the EGOPS quality control, profiles with bending angles magnitudes beyond \( \pm 40 \mu \text{rad} \) above 50 km are also rejected. After applied the above described quality control, the left profiles are used for the calculation of statistical errors.

5.2.3 Calculation of statistical error

This section introduces the method of calculating the statistical errors (i.e., systematic difference and associated standard deviation) of RO retrieved atmospheric profiles within an area. The first step for calculating the statistical errors is to calculate the absolute difference profile or relative difference profile for each retrieved atmospheric profiles within the area. For each vertical grid point, the absolute difference \( \Delta x \) is calculated by subtracting the reference value \( x_{\text{ref}} \) from the observed value \( x_{\text{RO}} \):

\[
\Delta x = x_{\text{RO}} - x_{\text{ref}}.
\] (5.1)

The relative difference \( \Delta x_{\text{rel}} \) is calculated by dividing the absolute difference with the reference value and times 100.0:

\[
\Delta x_{\text{rel}} = \frac{x_{\text{RO}} - x_{\text{ref}}}{x_{\text{ref}}} \times 100.0
\] (5.2)

The obtained ensemble of difference values allows the calculation of the mean systematic difference at that grid point and associated standard deviation. Since for both the absolute difference values and also the relative difference values, the methods of calculating the mean systematic difference and associated standard deviation are the same. the following formulations only show the estimation of statistical errors for absolute difference values. For absolute differences, the mean systematic difference value at a height level is calculated by averaging all the difference values within a given latitude and longitude area at that height level:

\[
\Delta \bar{x} = \frac{1}{n} \sum_{i=1}^{n} \Delta x_i
\] (5.3)

where \( n \) is the number of averaged profiles within the area. Using the mean systematic difference, the standard deviation of the differences could be calculated via Eq.(5.4):

\[
\sigma_x = \sqrt{ \frac{1}{n} \sum_{i=1}^{n} (\Delta x_i - \Delta \bar{x})^2 }
\] (5.4)
5.2.4 Statistical errors of the optimised bending angle profiles

Figure 5.5 shows the bending angle systematic difference and standard deviation profiles of all the sim-MetOp events on 15 July 2008 for six latitude regions: the whole globe (90°S to 90°N, Global), low latitudes (20°S to 20°N, Tropics), medium latitudes (20°S/N to 60°S/N, SHSM/NHSM = southern/northern hemisphere subtropics and mid-latitudes), and high latitudes (60°S/N to 90°S/N, SHP/NHP = southern/northern hemisphere polar). It is clear that in all these regions the bending angle standard deviation above about 40 km retrieved from the Dynamic1 is significantly smaller. The global mean standard deviation from the OPSv5.4 is larger than 6% near 60 km, which is more than twice the magnitude from the Dynamic1 SO being about 2.5% near 60 km. Also, and importantly, the bending angle systematic difference from the Dynamic1 is smoother and otherwise essentially equal or somewhat smaller. These results for the end-to-end simulated RO events, which enable to evaluate the basic potential of the Dynamic1 method since the “true” reference is closely known, are very encouraging and confirm the basic capabilities of the Dynamic1 SO.

![Graphs showing systematic differences and standard deviations of statistically optimised bending angles](image_url)

Figure 5.5 Systematic differences and standard deviations of statistically optimised bending angles, relative to the “perfect” simulated bending angles used as reference, of the ensemble of the sim-MetOp events on 15 July 2008. The statistical results are obtained from both the Dynamic1 (red) and OPSv5.4 methods (black) for six latitude regions: Global (90°S to 90°N), Tropics (20°S to 20°N), SHSM (southern hemisphere subtropics and mid-latitudes; 20°S to 60°S), NHSM (northern hemisphere subtropics and mid-latitudes; 20°N to 60°N), SHP (southern hemisphere polar latitudes; 60°S to 90°S), and NHP (northern hemisphere polar latitudes; 60°N to 90°N).
Figure 5.6 shows the bending angle statistical errors for the ensembles of CHAMP and COSMIC events available on the January and July test days. Due to the larger number of the COSMIC RO events and the better quality of the COSMIC receiver, COSMIC error profiles are less noisy compared to CHAMP’s. Inter-comparing the two methods, one can see that the bending angle standard deviation from the Dynamic1 SO is again distinctively smaller than that from the OPSv5.4 SO in all the latitude bands both in January and July.

For CHAMP data, the best improvement made by the Dynamic1 SO is found between about 35 km to 45 km with a reduction in the global-mean standard deviation to roughly half its value. Above about 45 km, the improvements made by the Dynamic1 SO decrease with height, and at 60 km both algorithms yield the same results (i.e., the background information fully dominates in both algorithms). For COSMIC data, the reduction in the standard deviation amounts to roughly one-third of the values from OPSv5.4 in the impact altitude range from about 35 km up to 60 km. At the high latitudes of the winter hemisphere (NHP in January and SHP in July), where both the background and observation errors are large, the Dynamic1 SO approach shows comparatively little improvement.

It is noted that these standard deviation results also point to the influence of the choice of bias coverage factor $f_{bcvg}$, i.e., the degree of intentionally inflating the bias-type uncertainty in Eq. (4.17) in order to safeguard $\alpha_{SO}$ from becoming biased: the standard deviation reduction is stronger if $f_{bcvg}$ is comparatively smaller (for the safeguarding argument we do not recommend a factor below 5, though, as noted in section 5.2.1). In tests that varying $f_{bcvg}$ up to a factor of 10 (not shown), it is found that the standard deviation reduction over the upper stratosphere becomes smaller; the systematic difference is essentially insensitive to this range of choices of $f_{bcvg}$, however. More discussion of potentially most adequate weightings is left to follow-on work; the current illustrative choice with $f_{bcvg} = 5$ shows what we consider like the strongest reasonable standard deviation reduction.

Furthermore, Figure 5.6 shows similar systematic differences of observed RO bending angle profiles relative to the ECMWF analysis profiles for both algorithms. The somewhat smoother systematic difference profiles resulting from Dynamic1 SO, especially for CHAMP, derive from the generally smoother individual bending angle profiles from the Dynamic1 method (cf. Figure 5.3). Despite we cannot know the “truth” from these data, it is encouraging for the Dynamic1 SO that despite its significant reductions in standard deviations, it does not show any suspicious degradation of systematic differences; this indicates that the Dynamic1 SO or the new realistically estimated background error covariance is in principle robust against “over-constraining” with background information and that the background profiles themselves, together with their uncertainty estimates, are indeed of adequate quality.
Figure 5.6 Systematic difference and standard deviations of statistically optimized bending angles, relative to co-located ECMWF analysis bending angles used as reference, of the ensembles of the CHAMP and COSMIC RO events from January (top six panels) and July, 2008 (bottom six panels). The statistical results are obtained from both the Dynamic1 (red and orange for CHAMP resp. COSMIC) and OPSv5.4 methods (black and cyan for CHAMP resp. COSMIC) for the same latitude regions as in Figure 5.5.
Figure 5.6 also reveals small “spikes” at 30 km in CHAMP’s bending angle standard deviation profiles, and the spikes are not obvious in COSMIC’s. This is because at 30 km, the signal-to-noise ratio of COSMIC profiles is significantly higher than that of CHAMP (being the “worst case” in this respect given it was a pioneering early receiver), due to the higher quality of COSMIC’s onboard receivers. In this study, the statistical optimisation was applied exactly down to 30 km (as is the setting in OPSv5.4) so that the bending angles below 30 km are purely observed bending angles. The CHAMP data quality indicates that this is a too high bottom altitude for part of the profiles, though, or alternatively more error is to be allowed [e.g., Gobiet et al., 2007].

In order to mitigate the “spikes” of CHAMP bending angle standard deviations near 30 km, we slightly amplified the background uncertainties ($\sigma_{\text{OSS}}^{\text{OPSv5.4}}$) relative to the observation uncertainties ($\sigma_{o}^{\text{OPSv5.4}}$) in the altitude range from 30 km to 40 km, so that the observed bending angles would receive more weight in the resulting $\alpha_{\text{SO}}^{\text{h}}$ in this altitude range; this adjustment made a smoother transition of the CHAMP profiles above 30 km (as shown in Figure 5.6, otherwise the “spikes” would be sharper). A more consolidated future solution may include variable bottom altitudes of the statistical optimisation and robust observation-to-background uncertainty ratio constraints enabling higher error from comparatively more noisy profiles in a controlled way.

5.2.5 Statistical errors of the refractivity and dry temperature profiles

Figure 5.7 shows the global-mean statistical errors of refractivity and temperature profiles obtained from all the three missions and the two methods. The sim-MetOp systematic differences in refractivity and their standard deviations resulting from the Dynamic1 method are slightly smaller, with the largest improvement at high altitudes but consistent small improvement overall. Slight but systematic improvement is also found for the systematic differences for sim-MetOp temperature profiles; this is again encouraging for the climatological utility of the Dynamic1 SO. Due to the downward propagation of errors by the Abelian integral and the hydrostatic integral [Gobiet and Kirchengast, 2004; Rieder and Kirchengast, 2001; Steiner and Kirchengast, 2005] clearly the absolute improvement in these retrieved variables is limited for sim-MetOp, since the OPSv5.4 SO already achieves a temperature bias of only about 1 K at 40 km for these high-quality simulated data.

The results for CHAMP and COSMIC thus look different and no conclusions can be made from these data on whether the systematic differences have been improved in the retrieval refractivities and temperatures, since there are no sufficient accurate “truth” as reference. We can therefore note at this point that the climatological performance of the Dynamic1 SO in the retrieved variables appears at least as good as from the OPSv5.4 SO; with the capability to improve upon as indicated by the sim-MetOp results. The standard deviations are clearly reduced also in refractivity and temperature, in
particular in the upper stratosphere, though the reduction is less salient than in the bending angle, again due to the downward integrations by the Abelian and hydrostatic integrals. The temperature standard deviations for CHAMP and COSMIC below 30 km are seen to be higher from Dynamic1 SO than from OPSv5.4 SO. Tests showed that this appears to be a side effect of the above discussed “spikes” in bending angles near 30 km, from the current simplified bottom altitude treatment, which tends to leave more standard deviation in retrieved temperatures. It is noted that the effect vanishes when using improved formulation of observation error correlations, as will be introduced in Dynamic2 SO, so it is do not discussed further here but in Section 5.3.

Figure 5.7 Refractivity (top) and temperature (bottom) systematic differences and standard deviations, relative to perfect simulated or co-located ECMWF analysis refractivities and temperatures used as reference, for the global ensemble of the sim-MetOp events of July 2008 (left), CHAMP and COSMIC events of January 2008 (middle), and CHAMP and COSMIC events of July 2008 (right). The statistical results are obtained from both the Dynamic1 and OPSv5.4 methods and are shown in the same layout as in Figures 5.5 and 5.6.

5.2.6 Effects of global-mean correlation matrix of background errors

This section presents the results of the investigation the differences in the RO retrievals caused by two different background error correlation matrices: 1) the empirically estimated global-mean
correlation matrix $\mathbf{R}_{f-a}$ of the background errors described in Sections 4.6.1, and 2) the simple analytical correlation matrix constructed by exponential-fall off correlation functions (i.e., the exponent term in Eq. (4.5)) with a background error correlation length of 10 km as used in the existing OPSv5.4 scheme. The Dynamic1 SO scheme is run for this specific investigation, for case 1 just as is and for case 2 with $\mathbf{R}_{f-a}$ replaced by the exponential fall-off correlation matrix but otherwise identical settings to case 1; so the only difference is the different correlation matrix.

Figure 5.8 displays the comparison of the statistically optimised bending angle, refractivity, and temperature results from sim-MetOp and COSMIC for the two different cases. It can be seen that the bending angle standard deviations, and to a smaller degree also the systematic differences, of sim-MetOp and COSMIC (left panels) are significantly reduced when using the realistic $\mathbf{R}_{f-a}$ instead of the simple exponential-falloff formulation. For example, sim-MetOp standard deviations are reduced to roughly half their values within 50 km to 60 km, and COSMIC standard deviations to roughly 80% of their values. This indicates the value of an appropriate specification of the background error correlation functions, consistent with the error characteristics of the (ECMWF) background profiles used.

It is can also be seen from Figure 5.8 that, compared to the improvements in bending angles from the realistic $\mathbf{R}_{f-a}$, the associated improvements in refractivity (middle panels) and temperature (right panels) are smaller but still clearly visible for the refractivity; while for the temperature they are very small. A closer look at the refractivity, also compared to the corresponding panels in Figure 5.7 in particular for sim-MetOp, one can see that the systematic difference benefits less than the standard deviation, since the former is more dependent on the downward propagation of bending angle errors via the Abelian integral rather than the details of the correlations (the matrix diagonal is the same in cases 1 and 2). The reason for the very small improvements in temperature standard deviations is that temperature is calculated from bending angle uses Abelian integral and hydrostatic integral, these two integrals are already able to reduce much random errors in temperature brought in by bending angles.

Overall, these effects of the correlation function formulations, realistic vs. simple exponential-falloff, clearly indicate that the use of a realistic empirically estimated background error correlation matrix as part of the new dynamic method is definitely useful.
Figure 5.8 Bending angle (left), refractivity (middle), and temperature (right) systematic difference and standard deviation, relative to their “perfect” simulated or co-located ECMWF analysis data used as reference, of the global ensemble of the sim-MetOp (top) and COSMIC (bottom) events on 15 July 2008, using either the realistic global-mean correlation matrix of background errors obtained from the new dynamic method (red; “full correlation”) or the simple exponential-falloff correlation used in the existing OPSv5.4 (black; exp falloff only).

5.3 Results of atmospheric profiles using both newly estimated background and observation error covariance matrices

This section evaluates the performance of Dynamic2 SO approach against the Dynamic1 SO and OPSv5.4 approaches. The Dynamic2 SO approach is also the complete new approach that we proposed in Chapter 4 (see Figure 4.1). It is based on Dynamic1, but adding in the realistically estimated observation error covariance matrix in Section 4.7. It uses both background and observation error covariance matrices estimated in the new approach for the statistical optimisation, i.e., uses $\mathbf{C}_b^k$, $\alpha_b^k$ and $\mathbf{C}_o^k$ (see Eqs. (4.16) and (4.15) in Section 4.5.3, and Eq. (4.22) in Section 4.7.2) for the statistical optimisation (see Eq. (4.9)). It should be noted that, this approach also uses the new background matrix estimated in Section 4.5, so the afore discussion above intermediate variables in formulating background error matrix and other related information is still valid for this approach.
5.3.1 Optimised bending angles

Figure 5.9 shows statistical errors of optimised bending angles in six latitudinal bands obtained from the three approaches: OPSv5.4 SO, Dynamic1 SO and Dynamic2 SO using sim-MetOp data of 15 July, 2008. It can be seen that bending angle standard deviations from Dynamic2 are further reduced than those from Dynamic1 in all the six latitude bands. In the global regions, the best improvements from Dynamic2 compared to Dynamic1 are about 0.7% at 60 km, and the systematic differences from Dynamic2 are similar to those from Dynamic1. These results indicate that after adding in the realistically estimated observation error covariance matrix in the statistical optimisation, the random errors of the optimised bending angles can be further reduced. These results for the end-to-end simulated RO events, which enable to evaluate the basic potential of the Dynamic2 method since the “true” reference is closely known, are very encouraging and confirm the basic capabilities of the Dynamic2 SO.

Figure 5.9 Systematic differences and standard deviations of statistically optimised bending angles, relative to “perfect” simulated bending angles used as reference, of the ensemble of the sim-MetOp events on 15 July 2008. The statistical results are obtained from the Dynamic1 (red), OPSv5.4 (black) and Dynamic2 methods (blue) for the six latitude regions.
Figure 5.10 Systematic differences and standard deviations of statistically optimised bending angles, relative to ECMWF analysis bending angles used as reference, of the ensemble of the CHAMP events on 15 January (upper six panels) and 15 July (bottom six panels), 2008. The statistical results are obtained from the Dynamic1 (red), OPSv5.4 (black) and Dynamic2 methods (blue) for the six latitude regions.
Figure 5.11 Systematic differences and standard deviations of statistically optimised bending angles, relative to ECMWF analysis bending angles used as reference, of the ensemble of COSMIC events on 15 January (upper six panels) and 15 July (bottom six panels), 2008. The statistical results are obtained from the Dynamic1 (red), OPSv5.4 (black) and Dynamic2 methods (blue) for the six latitude regions.
Figure 5.10 shows the statistical errors of the optimised bending angles in the same six latitude bands from observed CHAMP data on 14-16 January and 14-16 July, 2008. It can be seen that the standard deviations from Dynamic2 SO are larger than that from Dynamic1 SO and smaller than that from OPSv5.4 SO below about 45 km altitude in most of the latitude bands, except the two winter polar regions (SHP for July, NHP for January) in which the standard deviations from Dynamic2 SO are similar to those from OPSv5.4. Above about 45 km, the standard deviations from Dynamic2 SO are much larger than the other two approaches. The systematic differences at altitude levels below about 40 km from Dynamic2 are similar to those from Dynamic1 SO in most of the latitude bands, while at above 40 km, results from Dynamic2 SO are obviously larger than the other two approaches.

Figure 5.11 shows the same results as Figure 5.10 but for COSMIC data. Similarly to the results of CHAMP, at higher altitudes (above about 55 km), both the standard deviations and the systematic differences from Dynamic2 are much larger than those from the other two approaches in most of the latitude regions; while at lower altitudes, errors from Dynamic2 are similar to those from Dynamic1 which are smaller than those from OPSv5.4.

Comparing Figures 5.9, 5.10 and 5.11, we can see that the reductions in the bending angle standard deviation from Dynamic2 is only for sim-MetOp data, while for the observed CHAMP and COSMIC data, standard deviations from Dynamic2 are much larger than the other two approaches above 45 km for CHAMP data and above 55 km for COSMIC data. The reason that the Dynamic2 working better for sim-MetOp data is: the observation errors of simulated data are usually in a normal range, thus the estimated uncertainty values of the simulated data by Dynamic2 are in a reasonable magnitude and the weight of the observed bending angles could be accurately determined in the resulting optimised bending angles. This reason that the Dynamic2 does not work well on observed data is: the observed bending angles at high altitudes are significantly affected by higher-order ionospheric effects as well as observation errors which results the observation errors are hardly to be accurately determined. Therefore, the statistically optimized bending angles receive more weight from the noisy observed bending angles at high altitudes which therefore turns out to be nosier and result in large statistical errors at high altitudes.

The above reasons are obtained by several investigations. Firstly, we use the observation uncertainty estimated from OPSv5.4 approaches \( \sigma_o^{\text{OPSv5.4}} \) (see Eq. (4.7) in Section 4.2) together with the \( \mathbf{R}_{oo}^{\text{occ}} \) (see Section 4.7.1) to formulate the observation error covariance matrix (see Eq. (4.22), but replace \( u_o^k \) with \( \sigma_o^{\text{OPSv5.4}} \). In this case, large statistical errors of bending angles are also found at high altitudes for observed RO data. It is also found that, in this case, the statistical errors are smaller than Dynamic2 at high altitudes for CHAMP, but larger than Dynamic2 for COSMIC. This investigation proves that: 1) both the existing OPSv5.4 and the new approaches are not robust enough in estimating observation uncertainties for noisy RO events, and it is also believed that many other simple
formulations of observation errors used in existing approaches will also not help for reducing the bending angle errors at high altitudes; 2) the OPSv5.4 observation uncertainty which has some quality control to set large values for noisy events works better for CHAMP data due to the CHAMP data are usually nosier; while for COSMIC data, which are not that noisy, the observation uncertainty estimated from the new approach leads to smaller errors at high altitudes. This also indicate that quality control of observation errors can provide better results, but an advanced/sophisticated quality control should be taken in estimating observation errors for noisy RO events.

Secondly, we directly use a large value for observation uncertainty of all the RO events, e.g., 10 µrad, and then use the “Dynamic2 SO” (replace the new observation uncertainty with this large value) to calculate statistically optimized bending angles. From the results (not shown), it is found that, the bending angle random errors from this “Dynamic2 SO” approach are further reduced than the Dynamic1 SO approach for all the altitude levels. This investigation indicates that the capability of the Dynamic2 SO is limited due to the observation uncertainty that cannot be accurately estimated. However, even though, use a large value of observation uncertainty can results in good results, however, in this case, more weights are given to the background bending angles (especially at altitudes below 50 km) which may lead the optimised bending angles bias towards the background bending angle and reveal non-realistic values.

Thirdly, we apply simple quality control to estimate observation uncertainties for noisy RO events, for example, if the ratio of the observation uncertainty relative to the background uncertainty larger than 5, a large value is set to the observation uncertainty. However, these simple quality controls still leave large observation uncertainties at high altitudes for observed data. This indicates that sophisticated algorithms need to be developed to robustly and accurately estimate observation uncertainty for noisy RO events.

From the above investigations and also the results shown in Figures 5.9, 5.10 and 5.11, we can conclude that the Dynamic2 approach has the capability of further reducing the random errors in the optimised bending angles. However, its capability is limited for observed RO data due to the observation uncertainty are hardly to be accurately determined at high altitudes for noisy RO events. To robustly estimate observation errors, advanced and sophisticated quality control scheme needed to be developed, and this is left to the follow on work.

It is also noted that Dynamic1 does not generate large standard deviations for the observed data at high altitudes like Dynamic2 does. This is likely to be that Dynamic1 uses observation error covariance matrices from the existing OPSv5.4 approach which uses exponential functions for error correlation, while the Dynamic2, which uses the global-mean correlation matrix, reflects the true values and characteristics of correlations for observation errors. The true values of correlations may require the estimated observation uncertainties are also close to their true values.
It should also be noted that, the optimised bending angles from Dynamic2 SO has smaller spikes than Dynamic1 SO at 30 km. This is also due to the contributions from the realistically estimated observation error correlations.

5.3.2 Refractivity and dry temperature

Figure 5.12 shows the global-mean statistical errors of refractivity and dry temperature for the sim-MetOp RO events on 15 July, 2008. It can be seen from the left panel of this figure that the improved optimised bending angles derived from Dynamic2 result in smaller standard deviations in refractivity than Dynamic1 and OPSv5.4. The improvement is not large but still visible. The refractivity systematic differences resulting from Dynamic2 are similar to those from OPSv5.4 which are slightly larger than those from Dynamic1. The right panel of Figure 5.12 shows that the temperature standard deviations resulting from all these three approaches are rather similar. The temperature systematic differences from Dynamic2 are larger than that from Dynamic1, and both of them are smaller than those from OPSv5.4.

![Figure 5.12 Refractivity (left) and temperature (right) systematic differences and standard deviations, relative to “perfect” simulated or co-located ECMWF analysis refractivities and temperatures used as reference, for the global ensemble of the sim-MetOp events of 15 July 2008 (right). The statistical results are obtained from the Dynamic1, OPSv5.4 and Dynamic2 methods and are shown in the same layout as in Figure 5.9.](image)

Figure 5.13 shows the global mean statistical errors of refractivity and dry temperature for CHAMP RO events over the two periods of 14–16 January and 14–16 July, 2008. We can see that the quality of refractivity and dry temperature resulting from Dynamic2 are both degraded by the poor quality of their optimised bending angles at high altitudes. The upper two panels indicate that the
refractivity standard deviation from Dynamic2 are smaller than that from OPSv5.4 but larger than that from Dynamic1 below about 42 km, while above about 42 km, refractivity standard deviations from Dynamic2 are much larger than that from the other two approaches. Refractivity systematic differences from Dynamic2 are also obviously larger than that from the other two approaches above about 40 km. From the bottom two panels, we can see that, both the standard deviations and systematic differences of temperature from Dynamic2 approach are much larger than those from the other two approaches at about 30 km.

Figure 5.13 Refractivity (top) and temperature (bottom) systematic differences and standard deviations, relative to “perfect” simulated or co-located ECMWF analysis refractivities and temperatures used as reference, for the global ensemble CHAMP events of January (left) and July (right), 2008, respectively. The statistical results are obtained from are Dynamic1, OPSv5.4 and Dynamic2 methods and are shown in the same layout as in Figure 5.10.

Figure 5.14 shows the global mean statistical errors of refractivity and dry temperature for the COSMIC RO events on 15 January and 15 July, 2008. Similarly to the results shown in Figure 5.13, the refractivity standard deviations from Dynamic2 are smaller than those from the OPSv5.4 approach but larger than those from the Dynamic1 approach below about 45 km. Above about 45 km, Dynamic2 generates much larger refractivity standard deviations than the other two approaches. The
systematic differences of refractivity from Dynamic2 are also visible larger than that from the other two approaches above 40 km. From the bottom two panels, we can see that the temperature standard deviations from Dynamic2 are smaller than those from Dynamic1 and are similar to that from OPSv5.4 below 30 km. Above 30 km, the temperature standard deviations from Dynamic2 are much larger than that from the other two approaches. The temperature systematic differences from Dynamic2 are also obviously larger than the other two approaches at most of the altitude levels shown in the figure.

From this Figures 5.13 and 5.14, we also see that the phenomena that the temperature standard deviations from the Dynamic1 are larger than that from OPSv5.4 below 30 km which has also been mentioned in Section 5.2.5, is vanished by Dynamic2. This is due to the reason that the bending angles spikes at 30 km has been mitigated in Dynamic2 which does not affect the temperature standard deviations below 30 km anymore.

![Figure 5.14](image)

**Figure 5.14** Refractivity (top) and temperature (bottom) systematic differences and standard deviations, relative to the “perfect” simulated or co-located ECMWF analysis refractivities and temperatures used as reference, for the global ensemble of the COSMIC events of January (left), and of July (right), 2008. The statistical results are obtained from the Dynamic1, OPSv5.4 and Dynamic2 methods and are shown in the same layout as in Figure 5.11.
5.4 Effects of background and observation error correlation matrices

Since vertical correlations among background errors and among observation errors play a significant role in smoothing the statistically optimised bending angles, in this section, we investigate the effects of the global-mean correlation matrices of background errors and observation errors estimated in the new approach, and the correlation matrices constructed using exponentials functions (so-called exponential correlation matrices here after) used in the OPSv5.4 approach on the optimised bending angles and subsequent atmospheric profiles. Four pairs of background and observation error covariance matrices using different correlation matrices are generated: Case1) both background and observation error covariance matrices are constructed using exponential correlation matrices; Case2) the background matrix uses global-mean correlation matrix and the observation matrix uses exponential correlation matrix; 3) the background matrix uses exponential correlation matrix and the observation matrix uses global-mean correlation matrix; and Case4) both background and observation matrices use global-mean correlation matrices. In all these four cases, the diagonal elements of the background and observation error covariance matrices (i.e., background and observation uncertainties) take the values estimated from the new approach proposed in Chapter 4.

Figure 5.15 shows statistical errors of the optimised bending angle of sim-MetOp data on 15 July, 2008 from these four cases. It can be seen that, the standard deviations from Case1 (black lines) are much larger than the other three cases in all the six latitude bands. This indicates that using exponential correlation matrix for both the background and observation error covariance matrices results in larger random errors than the other approaches, cases that use at least one global-mean correlation matrix could significantly reduce random errors. Comparison among Case2, Case3 and Case4 shows that standard deviations from Case3 are slightly larger than that from Case2, and the values from Case4 are the smallest. This also indicates that using the global-mean correlation matrix for both background and observation error covariance matrices results in the smallest bending angle standard deviations. If the global-mean correlation matrix is only used for the background error matrix and the exponential correlation matrix is used for the observation error matrix, the standard deviations in the resulting optimised bending angles are slightly smaller than that of using the global-mean correlation matrix for the observation error matrix and the exponential matrix for background error matrix.

From Figure 5.15, we can also see that the systematic differences of the bending angles from Case1, Case3 and Case4 in all the six latitude bands are rather similar, and the systematic differences from Case2 are similar to the other three cases in the latitude bands of Tropics, NHSM and NHP. However, in the Global, SHSM and SHP regions, the differences from Case2 have a large deviation from the results of the other three cases. The reason for this is likely to be the new approach is still not
robust enough to accurately estimate observation uncertainty for RO events in a noisy observational environment (e.g., high latitudes of winter hemisphere), and this affects Case2 the most.

**Figure 5.15** Systematic differences and standard deviations of the optimised bending angles relative to ECMWF analysis bending angles used as reference, of the ensemble of the sim-MetOp data on 15 Jul 2008. The statistical results are obtained from four error correlation cases for the six latitude regions, the four cases are: Case1 (black) – BgrexpObsexp, i.e., both background and observation error covariance matrices use correlation matrix constructed using exponential functions, Case2 (red) – BgcorrObsexp, i.e., background uses global-mean correlation matrix, observation uses exponential correlation matrix, Case3 (cyan) – BgrexpObscorr, i.e., background uses exponential correlation matrix and observation uses global-mean correlation matrix, Case4 (orange) – BgcorrObsCorr, i.e., both background and observation error covariance matrices use global-mean correlation matrices.

Figures 5.16 and 5.17 show the statistical errors of refractivity and dry temperature profiles derived from the optimised bending angles obtained from the four cases, respectively. It can be seen from Figure 5.16 that, the standard deviations of refractivity from all the four cases are close to each other, and the results of Case4 are still slightly better than the other three cases. The standard deviations of refractivity from Case1 do not show large values (compared to other three cases) as they do for bending angles. This is because the calculation of refractivity from bending angle uses the Abel integral which work like a filter, thus the random errors in refractivity from Case1 are reduced. The
refractivity systematic differences from Case1, Case3 and Case4 are similar in all the six latitude bands, values from Case2 are only similar to the other three approaches in NHSM and NHP regions.

From Figure 5.17, we can see that the standard deviations of temperature from the four Cases are rather similar for most of the latitude bands except in Tropics where the standard deviations from Case3 and Case 4 are larger than those from Case1 and Case2 and also in SHP where the standard deviations from Case1 and Case2 are larger than that from Case3 and Case4. The phenomena in the tropics due to the reason that bending angle standard deviations from Case3 and Case4 are larger than that from Case1 and Case2 above 70 km (not shown), and these errors in bending angles are transferred downwards to temperature. The reason for the phenomena in SHP is similar. The temperature systematic differences from Case1, Case3 and Case4 are similar in all the six latitude bands. The systematic differences from Case2 deviate a lot the other three cases in SHP and SHSM. In other latitude regions, errors from Case2 are similar to that from the other three cases.

Figure 5.16 Systematic differences and standard deviations of the refractivity, relative to ECMWF analysis refractivity used as reference, of the ensemble of the sim-MetOp data on 15 Jul, 2008. The statistical errors are obtained from four error correlation cases for the six latitude regions and are shown in the same layout as Figure 5.15.
Figure 5.17 Systematic differences and standard deviations of the temperature relative to ECMWF analysis temperature used as reference, of the ensemble of the sim-MetOp data on 15 Jul, 2008. The statistical errors are obtained from four error correlation cases for the six latitude regions and are shown in the same layout as Figures 5.15 and 5.16.

5.5 Summary

In this chapter, the new approach proposed in Chapter 4 was evaluated against the existing Wegener Center Occultation Processing System version 5.4 (OPSv5.4) algorithm by inter-comparing the statistical errors of RO retrieved profiles (optimised bending angle, refractivity and dry temperature) relative to their reference profiles. The Dynamic1 SO approach, which uses only the background matrix estimated in the new approach and the observation error covariance matrix estimated in the OPSv5.4 approach (Sections 4.5 and 4.6), is evaluated first. Test data include single days’ simulated MetOp-A RO events and observed CHAMP and COSMIC data.

Findings from the evaluation of the Dynamic1 SO include: 1) the Dynamic1 method significantly reduces random uncertainties (standard deviations) in the resulting statistically optimized bending angle profiles and also leaves less or about equal residual systematic uncertainties (biases); 2) the realistic dynamic (daily) estimate of the background error correlation matrix alone already systematically improves the quality of the optimized bending angles, compared to using simply exponential-falloff correlations; 3) the subsequently retrieved refractivity profiles and atmospheric (temperature) profiles, while seeing reduced magnitude of improvement due to the filtering through
the Abelian and hydrostatic integrals, clearly benefit from the improved error characteristics of the optimized bending angles. In summary, the evidence from the first evaluation of Dynamic1 SO suggest if uses only the new background error covariance matrix in the statistical optimization, it already now outperforms the existing OPSv5.4 method.

The complete new approach Dynamic2 SO, which uses the background and observation error matrices that are both estimated by our new approach, is evaluated using the same test data as the evaluation for Dynamic1 SO. Compared with the results from Dynamic1 and OPSv5.4, the Dynamic2 approach can further reduce the standard deviations of the optimised bending angles retrieved from sim-MetOp data than Dynamic1 SO, which also results in improvement in refractivity derived from the improved optimised bending angles. However, for real observed data, Dynamic2 SO reveals its weaknesses at high altitudes (> 45 km for CHAMP data and > 55 km for COSMIC data), and the quality of its derived refractivity and dry temperature profiles are also degraded. The reason for this is likely to be that the observation errors are underestimated for noisy RO events. Use of realistic correlation matrix also require the observations errors can be realistically/accurately determined for appropriate weights given to the noisy observed bending angles at high altitudes. In summary, the Dynamic2 SO, which adding in the new realistically estimated observation error covariance (in Section 4.7) based on Dynamic1 SO, has the capability in further reducing the random errors of the optimised bending angles. However, its performance is needed to be further improved in future by developing advanced quality control for accurate estimation of observation uncertainties.

Due to the importance of the error correlation in smoothing the statistically optimised bending angles, the effects of the global-mean correlation matrix estimated by our new approach and the existing correlation matrix formulated by exponential functions on RO retrievals are investigated. It is found that, if at least one global-mean correlation matrix used in constructing the background or observation error covariance matrix, the random errors of the resulting optimised bending angles are significantly reduced than the approach that uses none global-mean correlation matrices to construct error covariance matrices. The random errors of optimised bending angles are reduced the most if both the background and observation error matrices constructed uses the new global-mean correlation matrix.

To conclude, encouraging results from this chapter suggest that, the dynamically and realistically estimated background error covariance matrix alone can already significantly reduce the random errors in optimised bending angles and benefit the subsequent refractivities and temperatures. If both realistic background and observation error matrices are used, and accurate observation uncertainties are also given, the random errors in optimised bending angle can be further mitigated.
Chapter 6. Evaluation of the New Algorithm Using Monthly RO Data

As can be seen from Chapter 5, although the Dynamic2 SO approach has better performance than Dynamic1 SO on simulated observations, it is still not robust for real observations at high altitudes. Therefore, in this chapter, we only evaluate the performance of Dynamic1 approach on monthly CHAMP and COSMIC RO events in January and July, 2008.

To retrieve atmospheric profiles for the two whole months, the daily background error fields should be prepared. In this chapter, we first investigate the characteristics of monthly background errors and their variations with day of month (DOM). Then, statistical errors of the retrieved atmospheric profiles are calculated for both January and July. The reference profiles for calculating the statistical errors are also co-located bending angle profiles forward propagated from ECMWF analysis fields.

6.1 Monthly background error fields

Before retrieving RO events, the corresponding daily error fields for the days of the two months are needed to be prepared. This section investigates the variations of background error covariance matrix with DOY. To achieve this, two typical values that formulating the background error covariance matrix, i.e, forecast-minus-analysis standard deviations ($s_{f-a}$) and correlation lengths of background errors, are selected to show their variations with DOM.

6.1.1 Forecast-minus-analysis standard deviation

Figure 6.1 shows the variations of the relative values of $s_{f-a}$ (i.e., $100.0 \cdot s_{f-a} / \bar{\alpha}$, see Section 4.6.1) with latitude and altitude in three consecutive days, 14 to 16 of January and 14 to 16 July, 2008. It can be seen from this figure that the values and characteristics of the errors of the three days in the same month are rather similar.
Figure 6.1 Relative standard deviations of forecast-minus-analysis bending angle differences as a function of latitude (10˚ bins, zonal means) and impact altitude (200 level grids) in three consecutive days of January (left panels) and July (right panels), 2008.

Figure 6.2 shows the variations of relative values of forecast-minus-analysis standard deviations with DOM and impact altitude in the three selected latitude sectors, i.e., from 0˚ N to 10˚ N, from 80˚ S to 90˚ S and from 80˚ N to 90˚ N representing the tropical, southern polar and northern polar regions respectively. From this figure, one can see that the error does not vary significantly with DOM of the month. In the tropical latitude band (first two panels), the error varies little with DOM for both January and July, the values are about 3% at about 78 km and about 2% at about 75 km. For other altitudes, the errors in both months remain around 1%. In southern polar regions (the middle two panels), the errors in July are much larger than that in January since the regions are in winter in July. In January, at above 60 km, the errors in the middle few days (e.g., 11th to 15th) of the month are
slightly smaller than those errors of other days at the same height level. The errors below 60 km remain around 1%. The errors in July reveal some variation above 40 km and the errors below 40 km stay around 1% to 2%. In the northern polar regions (the bottom two panels), the errors in January are larger than errors in July since these regions are in winter in January. The errors in January reveal clear variation with DOM. At 40 km, the errors of all the days in January are around 2%. In July, the errors only show some variations above 70 km. Below 70 km, the errors remain around 1%.

Figure 6.2 Relative standard deviations of forecast-minus-analysis bending angle differences as function of day of month and impact altitude in three latitude sectors and of January (left panels) and July (right panels), 2008

6.1.2 Correlation length of background errors

Figure 6.3 shows the correlation lengths of background errors (c.f. Section 4.5.4) for all the days in January and July. In each of the two months, the magnitudes of the correlation lengths from different
days of the same month are rather close with each other below 60 km. However, from about 60 km, the correlation lengths from different days reveal some variations. In January, their values at 80 km vary from about 4.6 km to more than 6.5 km, and in July, the values at 80 km vary from about 5.2 km to about 6.4 km. Comparison of the correlation lengths between January and July at the same impact altitude level shows similar magnitude.

**Figure 6.3** Correlation lengths of background bending angle errors of January (left panel) and July (right panel), 2008

From Figures 6.1 – 6.3, one can see that both the forecast-minus-analysis standard deviations and the correlation lengths of background errors have some variations with DOM at high altitudes. The forecast-minus-analysis standard deviations also have some variations with DOM at high latitude regions. However, generally, errors in several consecutive days are not varying significantly with DOM. The essential point is that we have relatively well behaved months here, however, in Jan 2009 – Feb 2009 where there are stratospheric warming event, the variations of background errors may be more obvious at high latitudes and high altitudes. Although, in the case we have here, we may able to use one error field for the days of the week, however, in order to obtain more accurate monthly statistical errors, the daily background error field is still used for the day of interest.

### 6.2 Monthly statistical errors

This section presents the results of the evaluation of Dynamic1 approach using RO observations from January and July. The raw RO observations (atmPhs files) are also downloaded from CDAAC. The raw observations are then processed through the EGOPSv2951 software using both OPSv5.4 and the Dynamic1 approaches to retrieve profiles. The retrieved profiles from the two months observations are applied with a similar quality control as described in Section 5.2.2, and more than 30%
of the retrieved profiles are removed. The remaining profiles of a month are then used for the calculation of statistical errors (i.e., systematic differences and standard deviations) of the month. The method of calculating the statistical errors of atmospheric profiles is the same as the method described in Section 5.2.3.

### 6.2.1 Optimised bending angle

Figure 6.4 shows statistical errors of bending angle profiles relative to profiles from ECMWF analysis fields for CHAMP and COSMIC data in January and July, 2008. Comparing it with Figure 5.6, one can see that the statistical errors from a month are rather similar to those from a single day, but with much smoother errors due to the fact that larger ensemble of data are used for the statistical calculation. Comparing the results between Dynamic1 and OPSv5.4, one can see that bending angle standard deviations from Dynamic1 is distinctively smaller than those from OPSv5.4 in all the six latitude bands for both January and July. Similarly to the single days’ results, for CHAMP data, the best improvement made by Dynamic1 is found between 35 km and 40 km, the improvements made by Dynamic1 decrease with height, and at 60 km both approaches yield the same results. For COSMIC data, the reductions in standard deviations made by Dynamic1 vary from about 1% at 35 km to about 2% at 60 km. At the high latitudes of the winter hemisphere (the NHP in January and the SHP in July), where the observation environment is noisy and both background and observation errors are large, the Dynamic1 approach only shows little improvement.

Figure 6.4 also shows systematic differences of bending angles between the two approaches. From CHAMP data, the systematic differences from Dynamic1 in the NHP in January and the NHSM as well as the NHP in July are larger than that from the OPSv5.4 approach and similar to the values from COSMIC. In the other latitude bands, the systematic differences from CHAMP data from the two approaches have similar values. For COSMIC data, the systematic differences between the two approaches are rather similar below 50 km in all the latitude bands. Above 50 km, the differences between the two methods are slightly larger than that below 50 km.
Figure 6.4 Systematic difference and standard deviations of statistically optimized bending angles, relative to co-located ECMWF analysis bending angles used as reference, of the ensembles of the CHAMP and COSMIC RO events of January (top six panels) and July (bottom six panels), 2008. The statistical results are obtained from both the Dynamic1 (red and orange for CHAMP resp. COSMIC) and OPSv5.4 methods (black and cyan for CHAMP resp. COSMIC) for the six latitude regions: the whole globe (90°S to 90°N, Global), low latitudes (20°S to 20°N, Tropics), mid latitudes (20°S/N to 60°S/N, SHSM/NHSM = southern/northern hemisphere subtropics and mid-latitudes), and high latitudes (60°S/N to 90°S/N, SHP/NHP = southern/northern hemisphere polar).
6.2.2 Refractivity and dry temperature

Figures 6.5 and 6.6 show the systematic differences and standard deviations of refractivity and dry temperature, respectively. It can be seen from Figure 6.5 that the monthly mean statistical errors are rather similar to those from single days’ (see Figure 5.7). Comparing the results of Dynamic1 with OPSv5.4, we can see that better quality CHAMP and COSMIC bending angle profiles from Dynamic1 result in better quality refractivity profiles, as expected. The largest improvement in the refractivity standard deviation from CHAMP data is at 35 km with a 1.5% reduction. The largest improvement in refractivity standard deviation from COSMIC data is in the altitude range from 35 km to 50 km with an improvement of 1% to 2%. The refractivity systematic differences from the two approaches show similar results, with slightly smaller values from OPSv5.4 for CHAMP data, and slightly larger values from Dynamic1 for COSMIC data.

From Figure 6.6, we can see that temperature standard deviations from Dynamic1 are also smaller than that from OPSv5.4 above 30 km. The largest improvement from CHAMP data is at 35 km with a 0.5K to 1K reduction in standard deviations, and the largest improvement from COSMIC data is found in the altitude range from 35 km to 50 km with a 1K reduction. Temperature systematic differences from the two methods are similar, with slightly smaller values from OPSv5.4 for CHAMP, and slightly larger values from Dynamic1 for COSMIC. Results from Figures 6.5 and 6.6 further prove the stability of the Dynamic1 approach which is not only robust on single days’ RO events, but also robust on monthly RO events.

6.3 Summary

This Chapter firstly investigate the variations of forecast-minus-analysis standard deviations and their correlation lengths with day of month. Results show that, the forecast-minus-analysis standard deviations are generally not varying significantly with DOM, and the characteristics and errors in a few neighbouring days are rather similar. However, at high altitudes of the polar regions, the errors still show some variations with DOM. Results from the correlation length of background errors also show that the values have some variations with DOM at altitudes above 60 km.

The performance of the Dynamic1 approach was then evaluated against OPSv5.4 approach using monthly CHAMP and COSMIC RO observations. The statistical errors of the retrieved optimised bending angles, refractivity and dry temperature profiles relative to ECMWF analysis profiles are then calculated. Results show that the statistical errors of RO retrieved profiles (especially bending angle) from a month are smoother than those from a single day of the same month. The values of the monthly statistical errors and daily errors are rather similar. These results further prove the stability of the Dynamic 1 approach on monthly RO observations.
Figure 6.5 Systematic difference and standard deviations of refractivity, relative to co-located ECMWF analysis refractivity used as reference, of the ensembles of CHAMP and COSMIC RO events from January 2008 (top six panels) and July 2008 (bottom six panels) in six latitude bands. The statistical results are obtained from both the Dynamic1 and OPSv5.4 methods for the same six latitude regions and are shown in the same layout as Figure 6.4.
Figure 6.6 Systematic difference and standard deviations of temperature, relative to co-located ECMWF analysis temperature used as reference, of the ensembles of CHAMP and COSMIC RO events from January 2008 (top six panels) and July 2008 (bottom six panels) in six latitude bands. The statistical results are obtained from both the Dynamic1 and OPSv5.4 methods for the same six latitude regions and are shown in the same layout as Figures 6.4 and 6.5.
Chapter 7. Summary and Recommendations

7.1 Summary

The climate change and severe weather has become a serious issue for our society. It is critical to find robust atmospheric observation methods to measure the atmosphere accurately to help for climate monitoring and weather prediction. The Global Navigation Satellite System Radio Occultation has become very useful for observing the atmosphere since it has distinctive advantages of long-term stable, high accuracy and high resolution, global coverage and self-calibrating. However, the quality of the retrieved atmospheric profiles from GNSS RO degrades above 30 km due to a low signal-to-noise ratio of GNSS signals at these high altitudes, since errors in bending angle profiles are propagated to refractivity profiles through an Abel integral and subsequently propagated to other atmospheric profiles through the hydrostatic integral. It is therefore important to carefully initialise the bending angles at high altitudes to minimise these error propagation effects and thereby provide the highest possible quality of retrieved profiles.

Statistical optimisation is a commonly used method for this purpose. This method combines the observed bending angle profile and background profile based on the estimations of their error covariance matrices, to determine “optimised” bending angle profile. The more accurate the estimated error covariance matrices, the better the quality of the obtained optimised bending angle profiles. However, the difficulty of this method is the obtaining of accurate error covariance matrices, especially for background error covariance matrix since it is neither supplied with common (climatological) models nor is its construction a straightforward task. Therefore, most statistical optimisation algorithms usually use empirical values for the background errors, ignore error correlation or use simple analytical functions for the error correlation. The same happens for the observation error matrix. These crude formulations result in the estimated background and observation error covariance matrices are inaccurate and therefore result in inaccurate optimised bending angles.

In order to address this issue, this thesis developed a new dynamic approach for statistical optimisation of GPS RO bending angles. This new approach avoids the crude formulation of both background and observation error covariance matrices and realistically estimate both of the matrices. The background bending angle profile and its associated error covariance matrix was statistically estimated using large ensemble of ECMWF short-range forecast and analysis data as well as observed RO data. The observation errors were estimated using the difference between the RO observed
bending angle profile and the estimated background bending angle profile, and the correlations of the observation errors were estimated using large ensemble of ECMWF analysis data and RO observations from COSMIC, GRACE, and MetOp-A missions. It is expected that, the quality of the statistical optimised bending angles profiles will be improved using these realistically estimated error covariance matrices. The quality of the subsequent refractivity and atmospheric profiles will also be improved which can be used for accurate climate monitoring and weather forecasting.

The estimation of background bending angle profile and its associated error covariance matrices consists of three main algorithmic steps:

1) Construction of basic daily background fields of key analysis-, forecast-, and observation-related variables on a global latitude-longitude-altitude grid for any day to be processed;
2) Preparation and pre-processing of the derived daily background fields with the specific statistical quantities directly needed for the statistical optimisation;
3) Performing the actual dynamic estimation of background error covariance for all RO events of any given day and correct the biases in background bending angle profile.

The characteristics of the new approach in estimating the background bending angle profile and its background error covariance against many of the existing schemes could be summarised as follows:

1) We use a 3D- and time-dependent formulation of all key statistical variables needed in the formulation of the background errors based on reliable ensembles of atmospheric forecast, analysis and averaged-observed profiles. This is to be considered against existing formulations which use global static relative values for background errors;
2) We use background bias estimation to actively reduce biases in the co-located background profile, while existing schemes use no such measure;
3) We use estimates of background bias uncertainty and random uncertainty, and penalise the former against the latter to minimise the bias influence on the resulting optimised profile, while existing schemes use globally static relative background errors;
4) We use a daily updated realistic background error correlation matrix, empirically estimated from forecast-minus-analysis difference profiles, while existing schemes either ignore these correlations or use crude (exponential) fall-off models not representing realistic correlation shapes.

Using this new approach, the resulting background errors reveal clear altitude, latitude and seasonal dependence (see Figures 4.3 and 4.6). The largest errors are found at the high latitudes of the
winter hemisphere. The correlation functions from the global-mean correlation matrix (see Figure 4.4) reveal a Gaussian shape at the main peak, and from the main peak outwards, there are two negative side peaks, these two negative side peaks are followed by two positive side peaks from which the values of the functions fluctuate around zeros.

In the new approach, the observation error covariance matrix was also dynamically estimated. The observation errors were calculated for each RO event using the differences between the observed bending angles and the above estimated bias-calibrated background bending angles. In order to obtain smooth observation errors, value at a specific height was calculated using values within the height range that 5 km above the height and 5 km below the height. The resulting observation errors reveal small variations at above 50 km. Below 50 km, the errors increase significantly with the decrease of altitude. However, errors below 50 km are not only related to the observations more but also related to small-scale atmospheric variability which should not be taken into account in estimating the observation errors for the statistical optimisation. Therefore, observation errors at 50 km altitude were assigned to the values below 50 km. The global-mean correlation matrix of observation errors was estimated using the differences between RO retrieved bending angles relative to their co-located analysis bending angles. Results show that the observation error correlation functions have a similar shape to that of the functions of background errors. The difference is that the correlation lengths of observation errors, which are about 1 km for all the altitude levels, are shorter than those of background errors (linearly increase from 0.8 km at 20 km altitude to about 6 km at 80 km altitude).

Since it has been proved that background errors at different height levels are usually highly correlated and background correlations are critical for smoothing bending angles at high altitudes, the background error covariance matrix estimated by the new approach was first solely used in the statistical optimisation to optimise bending angles profiles, and this approach was called Dynamic1. The Dynamic1 approach was evaluated against the existing OPSv5.4 approach by calculating statistical errors of the optimised bending angle profiles and their subsequently retrieved refractivity and dry temperature profiles relative to their reference profiles. Test data include simulated MetOp-A data and real observed CHAMP and COSMIC data from single days. The evaluation shows that:

1) The Dynamic1 approach significantly reduces random errors (standard deviations) and leaves less or about equal residual systematic errors (biases) in the optimised bending angle profiles;
2) The subsequently retrieved refractivity profiles and atmospheric (temperature) profiles benefited from the improved quality of the bending angle profiles;
3) The global-mean correlation matrix of background errors alone already improves the optimised bending angles and benefits the subsequently retrieved refractivity and dry temperature profiles;
4) These encouraging results suggest that, if uses only the new background error covariance matrix in the statistical optimization and uses the observation matrix from the existing OPSv5.4 approach, it already outperforms the OPSv5.4 approach.

Based on these encouraging results, the performance of the complete new approach that uses both the background and observation error covariance matrices estimation (Dynamic2) was evaluated. The Dynamic2 approach was evaluated against Dynamic1 and OPSv5.4 using the same test data as those for the evaluation of Dynamic1, and the following results were found:

1) The Dynamic2 approach further reduces the random errors in the optimised bending angles than Dynamic1 for sim-MetOp data;
2) The subsequent atmospheric profiles from the sim-MetOp bending angle profiles from Dynamic2 also benefit from the improved quality of the bending angles;
3) The Dynamic2 approach generates larger standard deviations of optimised bending angles than Dynamic1 but smaller than OPSv5.4 at below 45 km for CHAMP data and below about 55 km for COSMIC data, while above 45 km for CHAMP and 55 km for COSMIC, the Dynamic2 approach generates much larger standard deviations than the other two approaches;
4) The subsequent refractivity and dry temperature profiles from CHAMP and COSMIC optimised bending angles and Dynamic2 are affected by the poor quality of the bending angles and reveal larger errors than the other two approaches.

Based on the test results with the simulated MetOp data, the Dynamic2 approach has proved its capability in further reducing the random errors of the optimised bending angles than Dynamic1. The reason that Dynamic2 does not work well on real observed data is likely to be that the observation uncertainty cannot be accurately determined for noisy RO events using the method proposed in the new approach as well as the method in the existing OPSv5.4 approach, and the resulting optimised bending angle receives more weight from the noisy observed bending angle. In addition, the observation uncertainty estimated by the OPSv5.4 approach is not robust in estimating the observation uncertainty for noisy RO events. Our tests found that, after adding in the realistic correlation of observation errors, the observation uncertainty is required to be accurately and realistically estimated for all the RO events. Simple quality control cannot solve this problem, an advanced quality control scheme for accurately estimating observation uncertainties of noisy RO events needs to be developed in the future work.

In this thesis, the Dynamic1 approach was also evaluated using the two months RO observations of January and July, 2008. Before processing the two months RO data, the corresponding daily error
fields for all the days of the two months were prepared. The variations of two important variables in formulating background error covariance matrices (i.e. forecast-minus-analysis standard deviations and their correlation lengths) with DOY were evaluated. It was found that forecast-minus-analysis standard deviations did not vary significantly with DOY. However, at high altitudes of the high latitude regions, the standard deviations still reveal some variations with DOY. The correlation lengths of the forecast-minus-analysis standard deviations also reveal some variations with DOY at above 60 km. After all the daily error fields were prepared, the RO observations from the two months were processed through the EGOPSv2951 software package using both Dynamic1 and OPSv5.4 approaches. Comparison between the results of Dynamic1 and OPSv5.4 shows that the random errors of the optimised bending angles, refractivity and dry temperature profiles from Dynamic1 were distinctly smaller. The systematic differences between the two approaches are similar. The results of a month are similar to those from a day in the same month. The evaluation of Dynamic1 using monthly data proves the stability of the Dynamic1 approach.

To conclude, the encouraging results obtained in this thesis suggest that using the dynamically and realistically estimated background and observation error covariance matrices in the new statistical optimisation can significantly reduce the random errors in the statistically optimised bending angle profiles. The subsequent refractivity and dry temperature profiles benefit from the improved error characteristics of bending angle profiles. Since bending angles and refractivity are now already directly used in the data assimilation at many climatological centres, it is expected that the improved quality of bending angle and refractivity can improve the products from the assimilation system, which can further play a significant role in improving climate monitoring and weather forecasting. Based on the tests of the simulated data, the temperature systematic biases from the new approaches (Dynamic1 and Dynamic2) are also smaller than that from the OPSv5.4 approach. This indicates that the improved quality of temperature profiles can be used for more accurate climatological utilisation.

### 7.2 Recommendations

Although very encouraging results have been obtained in this thesis, several issues still need to be addressed in future to further complement the new statistical optimisation approach. First of all, to determine an optimal bias coverage factor to optimally decide how much the background information should be really weighted to support the high altitude initialisation of observed bending angles. This task could be done by comparing our estimated background errors with the errors estimated by ECMWF. The constant factor selected in this approach may need to be adjusted to vary with height.

Secondly, an advanced quality control mechanism needs to be developed to accurately determine the observation uncertainty. This task could be done based on the ratio of observation uncertainty to background uncertainty.
Thirdly, the new algorithms (Dynamic1 and more importantly the complete new algorithm Dynamic2) should be evaluated with also yearly data to further prove the stability of the new algorithm proposed in this research.

After consolidation of the new dynamic algorithm, it is intended to apply as one of the essential new algorithmic components in the next Wegener Center re-processing of the entire RO climate record, which aims at unprecedented quality of the data up into the mesosphere.
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