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Julian Austin

Department of Mathematics, Statistics and Physics.
Newcastle University

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Dedication will be here.

Declaration

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Julian Austin
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Abstract

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Nomenclature

Roman Symbols

J_i Number of temporal observations for i^{th} functional observation.

N Number of spatial observations.

$\mathscr{S}$ Spatial Domain.

$\mathscr{T}$ Temporal Domain.

t Temporal dimension.

$\mathscr{X}$ Functional random variable.

y_{ij} Observed response at time t_j for i^{th} functional observation. See Equation 1.2.

Y Observed data set. See Equation 1.1.

Greek Symbols

χ Functional data (observation of $\mathscr{X}$).

ε_{ij} Noise process at time t_j for i^{th} functional observation. See Equation 1.2.

Subscripts

i Spatial index.

j Temporal index.

Acronyms / Abbreviations

CESM Community Earth System Model.

EO Earth Observation.

FDA Functional Data Analysis.

NCAR National Centre for Atmospheric Research.

SAR Synthetic Aperture Radar.

Chapter 1

Introduction

1.1 Earth observation

Many area of science produce data on both a spatial and temporal scale. Take for example, the production of Earth observation data. Earth Observation (EO) is the collection of information on the state of a physical, chemical or biological system of the planet. Typically EO data is acquired through some form of remote sensing in addition to perhaps some in-situ measurements. Typically EO data is acquired to study a process either over a large area of land, a large time horizon, or both. For example such EO studies include; land usage change in wetland environments in southern Spain, [21], crop production in the Netherlands, [16], and land deformation of the Tuscany region over a two year time period, [23]. In each case there is significant spatial and temporal dependency that is to be considered in the observed processes. For example Raspini et al. use the temporal dependency in ground deformation signals to highlight areas of significant change in movement, [23]. They combine this with spatial maps to provide a monitoring bulletin for their area of interest. Of course to provide actionable insights from EO data requires an understanding of both the spatial and temporal dependency and as such models that can handle both forms of dependency whilst maintaining parsimony are desired in the EO community.

The three studies highlighted above all use space borne remote sensing to observe their process of interest. Space borne remote sensing, typically achieved through the use of satellite based sensors, is becoming more prominent as a source of EO data. This is largely due too the increase in satellites launched which have been designed to capture various processes of the earth. Figure 1.1 highlights the rise in availability of a single type of remote sensing satellite. One particularly prominent remote sensing system is the European Space Agency's Sentinel Constellation, [1]. The Sentinel constellation of satellites provides a wide range of remote sensing sensors which are easily accessible. The constellation provides capabilities capturing various EO processes through various forms of sensors such as Synthetic Aperture Radar (SAR), optical and multispectral sensors. As such the Sentinel constellation has been widely used in EO studies. For example the three studies above, [21, 16, 23] all utilise the Sentinel 1 SAR sensors for their observation source.

A prominent focus of the Sentinel satellite constellation is their ability to provide repeated observations at relatively high frequency, [1]. This is in response to the rising demand for

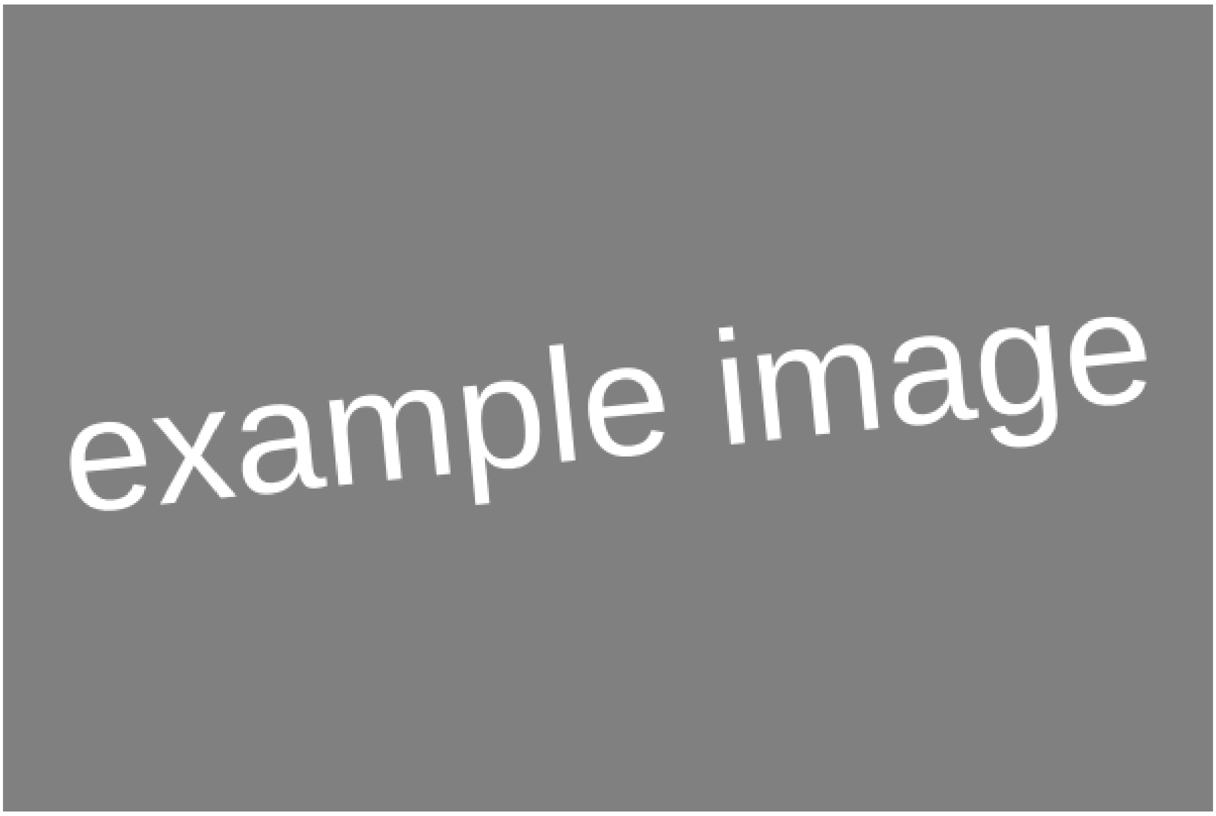

Fig. 1.1 A timeline of major satellite launches and operating periods for EO missions using SAR based sensors.

monitoring EO processes over time. This has been made possible by the development of remote sensing technologies which makes the revisit time possible. For example the Sentinel 1 satellite constellation can provide revisit times of approximately five days for areas of Europe. Such short revisit times are advantageous as they give higher temporal resolution and thus models can incorporate this additional information. For example, Raspini et al. utilise this in their study of land deformation change to identify anomalous regions. Figure 1.2 gives an example of EO data taken from the Sentinel 1 satellite of the Sentinel constellation. The figure gives an idea about the spatial and temporal resolution available using such a data source. The increasing availability of high temporal frequency EO data such as those provided by the Sentinel satellite constellation thus drives a demand for statistical models which can handle high resolution spatial and high resolution temporal dependency.

Another area where EO data is prominent is climatology. In this setting the focus, rather than in the geological studies in [21, 16, 23], is on the study of the atmosphere and weather over the globe. In this case spatial and temporal dependency in the EO data used in various climatology studied is obvious. For example, consider the Community Earth System Model (CESM), [15], produced by the National Centre for Atmospheric Research (NCAR). Such a model provides simulations of various aspects of the Earth's climates for past, present and future time points. The data derived through the CESM shares various aspects with typical remotely sensed EO data such as the Sentinel data.

In particular, both sources of data share an inherent spatial and temporal dependency. That is to say the underlying process driving both remotely sensed observations of the Earth and the

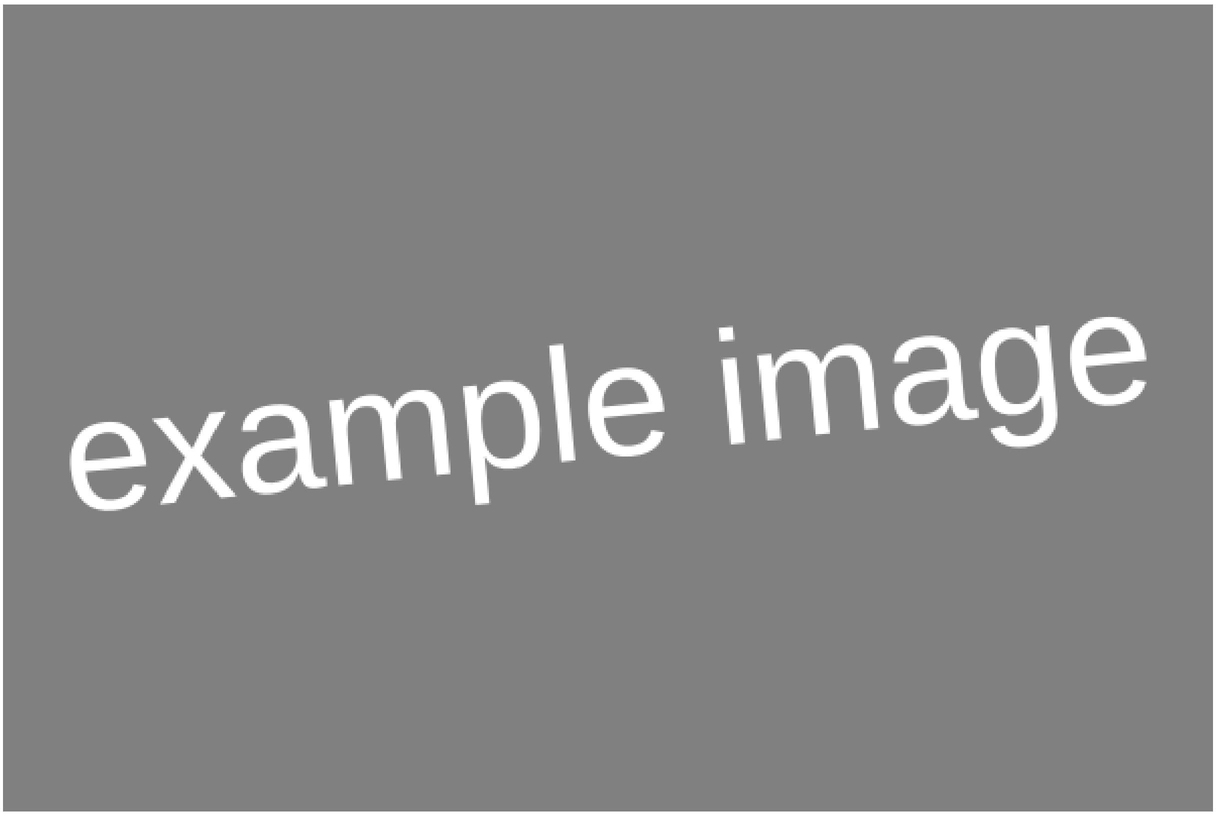

Fig. 1.2 An collection of Sentinel 1 SAR images over Newcastle, UK for the period between January 2019 and January 2021. This example of Earth observation data exhibits spatial and temporal dependencies. Contains modified Copernicus data.

CESM simulations will vary over the globe and also will be driven by the state of the system at a prior time points. That is not to say the process is the same for both but rather that there is a commonality in that they could both be considered spatio-temporal processes. In addition there are more concrete similarities in the data. Typically, both data sources are described on a lattice of points over space which is usually regular. Such a lattice is usually represented through a geodetic coordinate system which grounds an datum to a real world location. Finally, both sets have repeated observations through time over the same space. Due to the cross over in properties of both data sources typically we observe similar statistical techniques being used for both.

The description of such spatio-temporal processes is well studied in statistics and a large amount of effort has been used to develop various models to suit them. A well known monograph which deals with such processes is that written by Cressie and Wikle, [5]. The monographs details various forms of spatio-temporal processes and typically focuses on the extension of spatial method to incorporate the additional temporal dimension. We discuss these methods in more detail in Section 1.3. Of particular importance is that temporal and spatial dimensions are distinct as they are inherently different in the physical process. For example one could consider a spatial point influencing its neighbours in all directions however a temporal point reasonably shouldn't influence its past. As such there is often a distinction in the method used to model the temporal and spatial aspects of the physical process.

Another area of statistics which is often used to model data with temporal dependency is Functional Data Analysis (FDA). FDA is typically applied to analyse data which vary over a continuum. Time is one such continuum. EO data with high frequency temporal observations are therefore suitable candidates for FDA models. FDA is a relatively new branch of statistics and as such few studies have been presented which use FDA techniques on EO data. Liu et al. considers FDA techniques on periodic EO data, [18] and similarly Hooker et al. considers FDA techniques to model the Harvard modified vegetation index sourced from EO data. In both the above studies they consider EO data as a collection of functional observations which each observation representing the trajectory of response over time. The monograph of Ramsay and Silverman provides a comprehensive introduction to the themes of FDA, [22]. FDA are often intuitive since viewing responses as being discretely sampled from an unknown smooth random function in some contexts closely matches the actual data generating process compared to a multivariate analysis. Therefore the use of such techniques could be helpful in modelling such high frequency ST data in conjunction with the multivariate methods discussed by Cressie and Wikle in [5]. However, focus in the FDA literature to date has primarily revolved around independently observed functional data. This is typically not the case in our motivating case of Earth observation data where there is often obvious spatial dependency. Thus there is a need to describe functional data models which incorporate dependency among observations. In this work we consider developing such models for dependent functional data with a focus on application to Earth observation data. We consider adapting well studied FDA methodologies and borrow techniques from spatio-temporal statistics to allow for spatially dependent observations. In Section 1.2 we make concrete our definition of functional data.

1.2 Functional representation

As mentioned in 1.1 EO data can be viewed as a collection of functional data. However there is a choice about how we interpret observations in this conversion. We may consider the data as a collection of functional observations with time being our functional dimension and space our collection dimension. Or we may consider the functional observations having a spatial domain and the collection dimension being time. The canonical presentation of functional data in FDA is to use time as the functional dimension, [22] and thus we use the below definition of functional data from this point of view.

1.2.1 Functional data

Multivariate data analysis usually revolves around the study of observations which are finite dimensional and is well studied. Modern data collection techniques can now create data which are extremely numerous and thus can often be viewed as functions and in some sense infinite dimensional.

For example, Ferraty and Vieu consider the case where we can observe a random variable at several times between some minimum and maximum time, $(t_{\min}, t_{\max})$. A single observation can then be considered as the collection $\{X(t_j); j = 1, 2, \ldots, J\}$ where J is the total number of temporal sample points and $X(t)$ is the response variable at time t. Unlike multivariate data we consider the case that the separation between observations becomes minimal. That is we consider the data as an observation from the continuous random process $\mathscr{X} = \{X(t); t \in (t_{\min}, t_{\max})\}$. We therefore propose as in [7] and [27] the following definition of a *functional variable*.

Definition 1.1 (Functional Variable)**.** *A random variable $\mathscr{X}$ is called a functional variable if it takes values in an infinite dimensional space (or functional space). An observation χ of $\mathscr{X}$ is called a functional data.*

Further to this, suppose we observe a collection of functional data (realisations of $\mathscr{X}$). Then we will denote this collection by the term *functional dataset*.

Definition 1.2 (Functional Dataset)**.** *A functional dataset, $\chi_1, \chi_2, \cdots, \chi_N$ is the collection of N realisations of functional variables $\mathscr{X}_1, \cdots, \mathscr{X}_N$ identically distributed to $\mathscr{X}$.*

The canonical way to present functional data and the subsequent methods is to use time as the continuous variable, [22, 7, 27], as described above. However, there is no such restrictions in either Definition 1.1 or Definition 1.2. In fact, another case is to consider the functional domain of the variables to be space. In our proposed methodologies we present when possible with respect to time due to the simplification it brings in notation. We will make explicit reference to when we change the domain of our functional data, for example if we consider space as our continuous domain.

We introduce the following notation for use in the remainder of this work. We consider our EO data set to be observed in some spatial domain which we denote by $\mathscr{S} \subset \mathbb{R}^2$ and temporal domain donated by $\mathscr{T} \subset \mathbb{R}$. Any observed dataset we can enumerate with one index over the spatial location and the other indexing the temporal locations. For completeness we introduce two separate notations, one for the case when we wish to treat time as our domain for the functional variable and the other for treating space as the domain for the functional variable.

We assume our dataset is comprised of N spatial locations and let $s_i \in \mathscr{S}$ be the spatial location of the i^{th} observed functional variable. At each spatial location we suppose we observe J_i temporal observations and denote by $t_{ij} \in \mathscr{T}$ the j^{th} temporal observation of the i^{th} functional variable. Then our dataset can be summarised by Y where:

$$Y = \{y_{ij}; i = 1, 2, \cdots, N, j = 1, 2, \cdots, J_i\} \tag{1.1}$$

where y_{ij} is the response value of the i^{th} functional variable at time t_{ij} observed with error. That is we consider for each spatial location the discrete temporal observations being a sample from a realisation of a functional variable observed with error. That is:

$$y_{ij} = \chi_i\left(t_{ij}\right) + \varepsilon_{ij} \tag{1.2}$$

where as in Definition 1.2 χ_i is a realisation of functional variable $\mathscr{X}_i$ for $i = 1, 2, \cdots, N$. We consider each functional variable as being identically distributed as $\mathscr{X}$. As is common in most observation models we assume we observe data with error, typically one assumes that the error process $\{\varepsilon_{ij}; i = 1, 2, \cdots, N, j = 1, 2, \cdots, J_i\}$ is a white noise process with variance σ_ε^2.

In this case one considers the modelling of the EO dataset by ensuring smoothness of some kind over the temporal domain via its functional data representation. We can then consider building in spatial dependency by assuming a sampling correlation in our N functional data. An area where such spatial dependency has been long studied is multivariate spatio-temporal methods we discuss the common method in the following section.

1.3 Spatio-Temporal methods,

In the statistical literature spatial and spatio-temporal models have been extremely well studied, especially due to the prevalence of geo-statistical applications. In the following we briefly review some of the most commonly observed spatial and ST statistical models in the multivariate analysis literature.

The monograph of [4] and references within provide a succinct summary of traditional methodologies in spatial statistics, many of which are applicable to remotely sensed data. Generally speaking spatial data can be split into one of three categories; geo-statistical, area and point process data. In this work the EO data described in Section 1.1 are most suitably modelled using geo-statistical models. The canonical model used in geo-statistical setting is the Kriging model. The Kriging model is well described in [28]. Such models treat spatial data as samples from a random spatial process and that predictions for unknown values can be calculated from a weighted combination of known values in a neighbourhood of our unknown location utilising the correlation among neighbouring points. A prime example of the spatial Kriging model in use for remote sensing data is given in [24]. Extensions to the basic Kriging technique have also been employed across a number of geo-statistical settings, including Co-Kriging involving extra covariate information for reconstruction, [29]. Kriging is well known in many fields through various names, in the FDA literature it is most often referred to as Gaussian Processes Regression. Shi and Choi describes in detail the concept of Gaussian processes in the context of functional regression.

As is detailed in [4] an key aspect to geo-statistical modelling is the specification of spatial dependency in the observed data. A common way for such specification is through parametric covariance or kernel functions. [4] details the traditional stationary parametric functions such as the Matèrn covariance. These commonly rely on the assumption of isotropy and stationarity in modelling which rarely holds in practice. Further literature has considered extensions of these and is in fact an active area of research. Schmidt and Guttorp compares a variety of methods for producing non stationary and heterogeneous covariance structures for the goal of spatial interpolation, [26]. They group the various methods of creating such structures into four categories; deformation, convolution, covariate and stochastic partial differential equations. The deformation approach proposed by Sampson and Guttorp extends the anisotropic stationary covariances such as though describe in [4] by allowing for a non linear transformation to the space which creates a latent space where isotropy holds, [25]. The convolution approach proposed by Higdon uses a specific form of the covariance kernel which can be represented as a convolution between a convolution kernel and a white noise process. We discuss such an approach more in Chapter 5. The covariate based non stationary kernels tends to be constructed using an adaption to the convolution or deformation approaches with specific covariates. Finally the stochastic partial differential equation method proposed by Lindgren et al. construct non stationary covariances as the resultant Gaussian process is the solution of a stochastic partial differential equation and allowing the parameters of the equation to vary over space, [17].

A natural extension to purely spatial modelling of spatio-temporal data is to include the temporal domain that is often present, such models are known as spatio-temporal models. spatio-temporal models are well discussed the monograph [5]. In addition spatio-temporal Kriging models are well suited to our data however such models are relatively scarce in the literature. [19] considers the application of such modelling in the satellite remote sensing literature and reasons the lack of such modelling is primarily due to the added complexity such models produce in specifying valid and appropriate space-time covariance functions. As such one particular direction spatio-temporal modelling has considers is the creation of spatio-temporal covariance functions. [3, 10, 14] consider the construction of non separable covariance functions in the early literature. Separability between spatial and temporal correlations is often a key assumption in some methods due to the ease on computations involved in such models, as such [20, 8, 2] considers tests for when such assumptions hold. In particular for EO data, [9] consider such selection of separable covariances and [6] consider such models for air pollution data.

1.4 Summary of Research

The motivation of this work is to provide a model designed for EO data which provides an explanation of both the spatial and temporal process in a parsimonious way. We present a novel method named Correlated Principal Analysis through Conditional Expectation (CPACE), that is designed for modelling EO data. The model builds upon existing FDA techniques to extend modelling from independently observed functional data to functional data which exhibits spatial correlation. The emphasis in the work is to utilise the FDA paradigm over the temporal domain to aid in the decomposition of the data, with the understanding that our data generating process is smooth across the temporal domain. Such a decomposition gives a parsimonious description of the data over the temporal domain into its principal modes of variation. We then estimate a spatial correlation structure for each component using well known spatial statistical methods. The combination of the resulting estimated spatial covariance structures with the principal directions aims to capture the majority of temporal and spatial dependency observed in the data. We can then utilise the CPACE model to help predict response at unseen spatial and temporal locations, which is a keen area of interest in EO studies. We asses our model using various simulated data both with known correct data generating distribution and to simulations drawn from an incorrect data generating procedure. We apply our CPACE model to the select atmospheric variables from the CESM data set as an example application of the model to EO data.

In particular the work is structured as follows. In Chapter 2 we describe our example data sets which we use to illustrate the performance of the model. In Chapter3 we present the methodologies underpinning the CPACE models, these are typically well known FDA and ST statistical methods. We also present the smoothing methodologies used to estimate the mean and covariance surfaces of our random functional variables. In Chapter 4 we present an interim model built on the combination of two well known existing methodologies in the FDA literature with a focus on application to an Earth observation data set. Such a model proposes an novel approach to modelling Earth observation data but helps to highlight the need of including both spatial and temporal effects in modelling such data. In addition the proposed model in Chapter 4 provides an opportunity to explore EO data where the functional domain is space rather than time. We present the benefits and limitations of such an approach in practice in this chapter also. In Chapter 5 we introduce the main contribution of this work which is the CPACE model for correlated functional data. We describe the model in details as well as provide asymptotic results for the model. In Chapter 6 we apply the CPACE model to simulated and real world data sets. Simulation results are presented with comparisons to various existing models with a focus on comparative ability to recover known data generating parameters. Applied results to real world data sets are included with comparisons to existing techniques with a focus on interpolation and forecasting abilities of the model. In Chapter 7 we highlight the practical difficulties in implementing the model with discussion on various techniques which are used to overcome the high dimensionality which is typical in the EO data. Finally, in Chapter 8 we draw the conclusions of the work and present area of further work.

Chapter 2

Data sets

In the following chapter we describe in detail our data which we will use as a source for assessing the performance of the models described within. We use a publicly available set of climate model simulations known as the CESM Large Ensemble (CESM-LE) data set, [15]. The CESM-LE data set provides a good example of EO data that is discussed in Section 1.1. This data set will be used throughout this body of work as a intriguing example of the abilities of the discussed methodology.

2.1 Community Earth System Model - Large Ensemble, [15]

The CESM-LE data set is an extremely popular and significant data set in the climate research community. It was developed to enable the assessment of recent past and near future climate change in the presence of internal climate variability, [15]. It does so by providing 40 simulations of a complex climate model where each simulation is subject to the same radiative forcing scenario but begin a slightly perturbed atmospheric state. As such the forty resultant simulations present the various trajectories the model might take due to internal climate variability of the model.

The model used to run the forty member ensemble is the Community System Earth Model version 1, [13], with the Community Atmosphere model version 5, [13], as the atmospheric component. The model is a fully coupled climate model which consists of a model for each the Land, Ocean, Atmosphere and Sea Ice components of the climate. These are brought together with a coupler model. Figure 2.1 provides a simple overview as to how CESM model couples the various components. Such a model is capable of simulating various Land, Ocean, Atmosphere and Sea Ice variables of the climate, such as the wind speed, temperature or pressure. The CESM-LE produces simulations of such variables on the nominal 1 deg horizontal separation across the globe which induces our spatial resolution of the data. The ensemble produces results at varying levels of temporal resolution between the years 1920 and 2100 for non-control simulations. The temporal resolution varies by variable of interest between 6-hourly, Daily, and Monthly frequency of observations.

For this body of work we use the CESM-LE data by considering the forty members as separate simulations. Each simulation giving us a realisation of the various climate variables

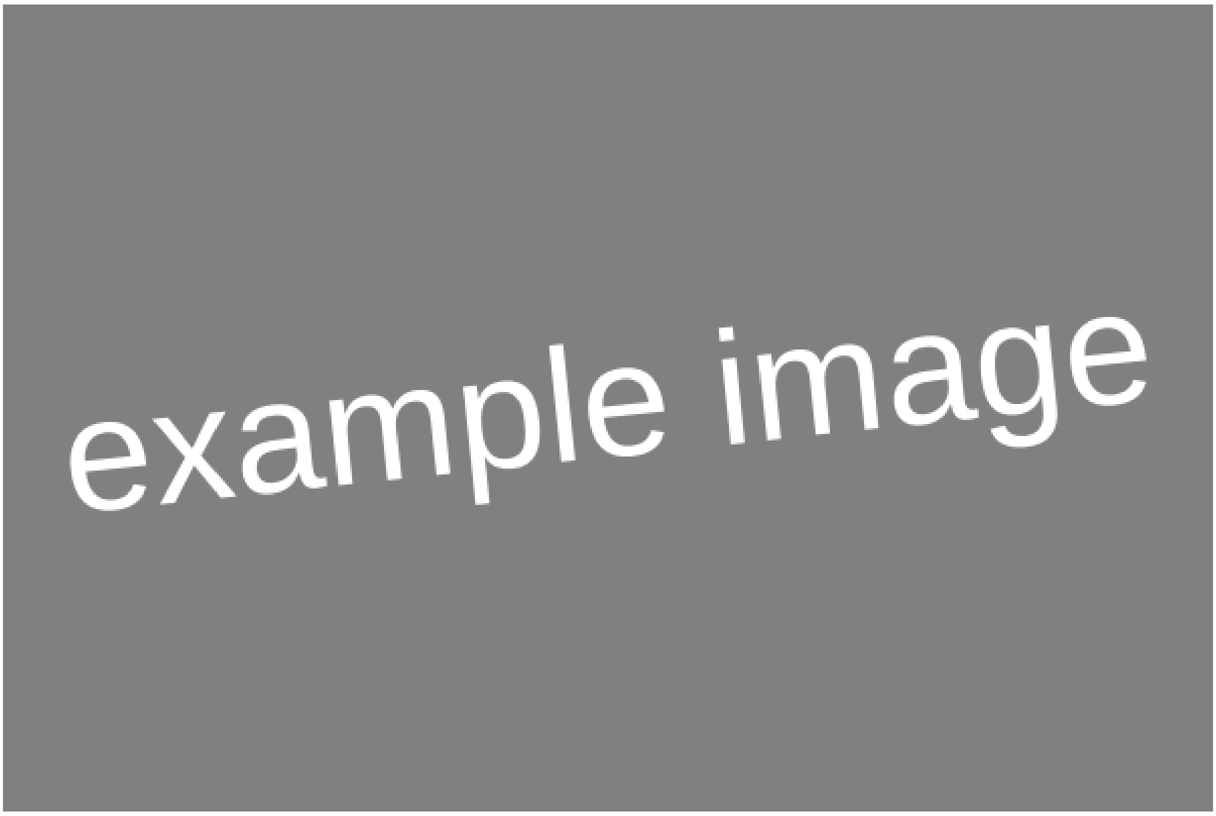

Fig. 2.1 The component models for the full CESM model, [15].

generated by the process described in [15]. Further we only consider modelling the time between December 2020 and January 2025. These time points were chosen such that the length of time gave reasonable ability to capture periodic elements but that the size of the data did not become too large. Additional to reduce the size of the data we resample the model simulations to a smaller spatial grid. Figure 2.2 shows the resampled spatial observation grid over the globe that we use.

In the following work we focus on four atmospheric model variables from the CESM-LE simulations. These are; pressure (see Section 2.1.2), Temperature (see Section 2.1.3), Precipitation (see Section 2.1.1), and Wind (see Section 2.1.4). We describe each component in detail in their respective section and throughout this work we consider each as a separate EO data set.

2.1.1 Precipitation

The total (vertically integrated) precipitable water component abbreviated as TMQ in the model descriptions is an atmospheric component output of the CESM-LE. The component is given units of $\mathrm{kg\,m^{-2}}$ and is available monthly on the full spatial grid with monthly precipitation being average over time from the model 6 hourly output.

We can see clearly the spatial variability of the precipitation over the globe by considering the heat map of June 2021 monthly precipitation for a single simulation which is shown in Figure 2.3. As one would expect there is clear spatial correlation as for example the tropics observe large amounts of precipitation whereas desert regions observe little.

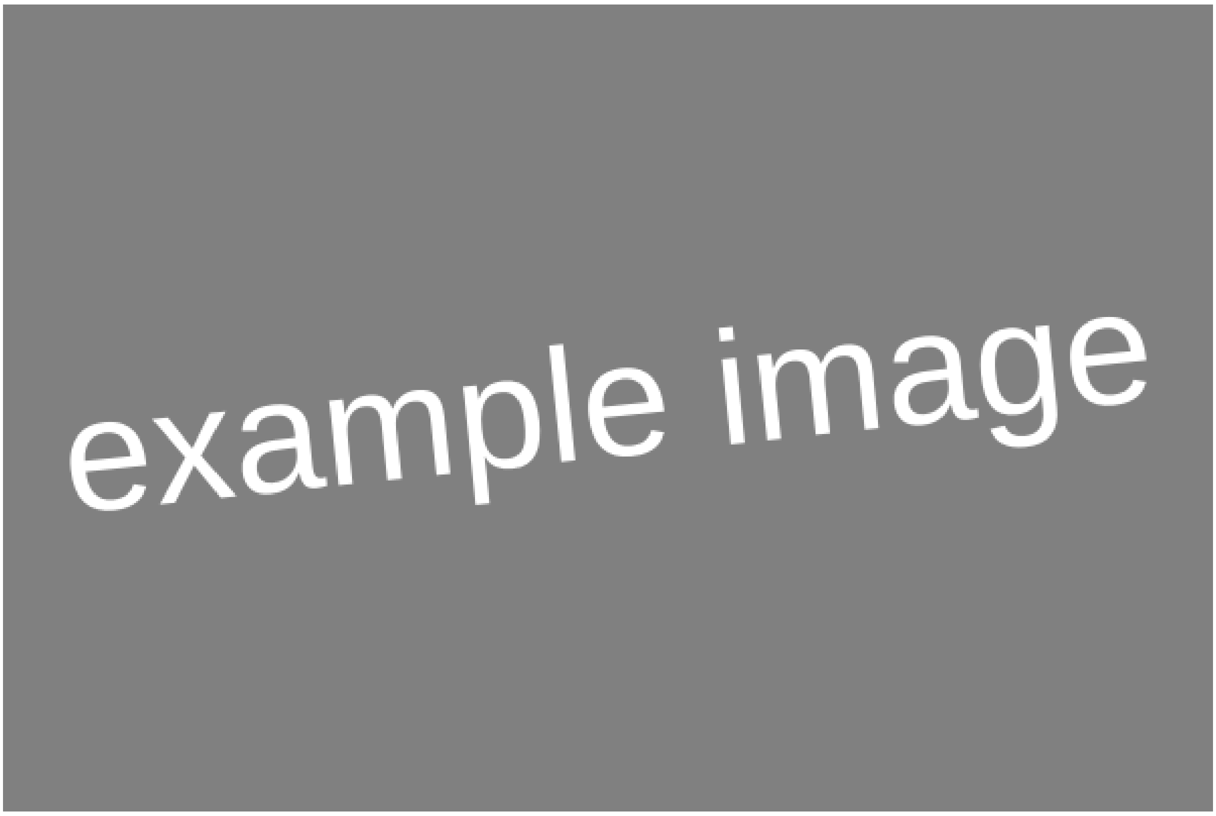

Fig. 2.2 The resampled spatial grid of observation measurements across the globe.

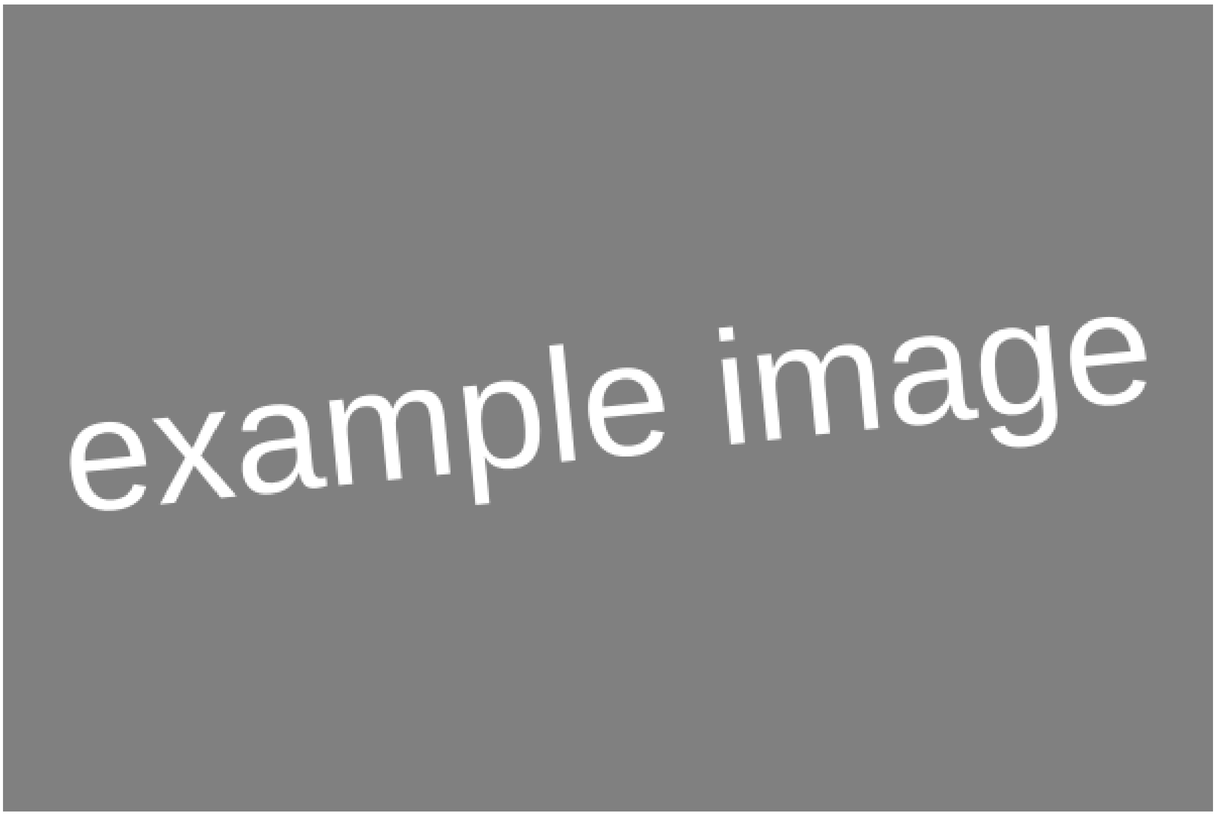

Fig. 2.3 The simulated average monthly precipitation across the globe for June 2021 from ensemble member 1 of the CESM-LE data.

We can similarly observe clear temporal correlations in the precipitation variable of the CESM model. In particular Figure 2.4 shows the time series of two locations on the globe. Each exhibit clear periodic signals as wet seasons and dry seasons repeat each year. Additional we see clearly that there is in sense a smooth transition from one month to the next in terms of precipitation value which suggest a FDA approach as discussed in Chapter 1 may be relevant.

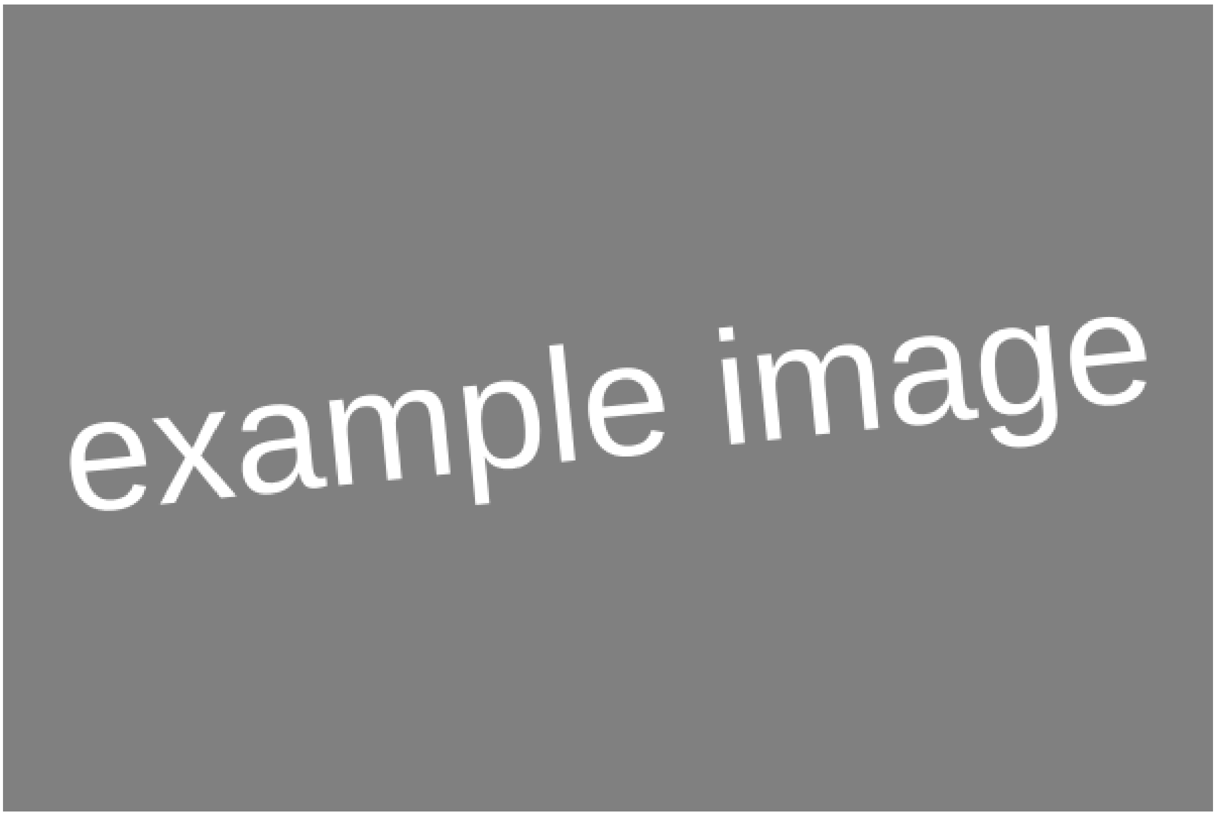

Fig. 2.4 The simulated average monthly precipitation at two points on the globe from ensemble member 1 of the CESM-LE data over five years between December 2020 and January 2025.

2.1.2 Pressure

The surface pressure component abbreviated as PS in the model descriptions is an atmospheric component output of the CESM-LE. The component is given in units of Pa and is available monthly on the full spatial grid with monthly pressure being averaged over time from the model 6 hourly outputs.

2.1.3 Temperature

The temperature model component abbreviated to TREFHT in the model description is an atmospheric component output of the CESM-LE. The component refers to the average temperature in K at the model reference height which is wm above sea level. The average is available monthly with the average being that of the model 6 hourly output for the month. Such a response variable is again available on the full spatial grid of the model.

2.1.4 Wind

The wind model component abbreviated to U10 in the model description is an atmospheric component output of the CESM-LE. The component refers to the average wind speed in $\mathrm{m\,s^{-1}}$ at a height of 10m. Again the component is available on the full spatial grid and is available as a monthly average over time.

Chapter 3

Background Methodologies

Chapter 4

Dynamic functional time series modelling

Chapter 5

Correlated principal analysis through conditional expectation

Chapter 6

Application of CPACE model

Chapter 7

Implementation of CPACE model

Chapter 8

Conclusions and further work

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