Manfred Mudelsee

Climate Time Series Analysis

Classical Statistical and Bootstrap Methods



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To my parents,

Anna-Luise Mudelsee, née Widmann

and

Richard Mudelsee

Preface

Climate is a paradigm of a complex system. Analysing climate data is an exciting challenge. Analysis connects the two other fields where climate scientists work, measurements and models. Climate time series analysis uses statistical methods to learn about the time evolution of climate. The most important word in this book is "estimation." We wish to know the truth about the climate evolution but have only a limited amount of data (a time series) influenced by various sources of error (noise). We cannot expect our guess (estimate), based on data, to equal the truth. However, we can determine the typical size of that deviation (error bar). Related concepts are confidence intervals or bias. Error bars help to critically assess estimation results, they prevent us from making overstatements, they guide us on our way to enhance the knowledge about the climate. Estimates without error bars are useless.

The complexity of the climate system and the nature of the measurement or modelling act may introduce (1) non-normal distributional shape, (2) serial dependence, (3) uneven spacing and (4) timescale uncertainties. These difficulties prohibit in many cases the classical statistical approach to derive error bars by means of calculating the theoretical distribution of the estimates. Therefore we turn to the bootstrap approach, which generates artificial resamples of the time series in the computer, repeats for each resample the estimation (yielding the replication) and calculates the error bars from the distribution of the replications. The typical number of replications is 2000. This computing-intensive approach yields likely more realistic error bars.

Still, there is theoretical work to be done: how to best preserve the shape and serial dependence in the bootstrap resamples, how to estimate with smallest error bars. Uneven spacing in time series analysis has not been the preferred study object of statisticians. Timescale uncertainties and their effect on error bars (widening, but how much?) is almost

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completely unexplored. This book adapts existing and introduces new bootstrap algorithms for handling such problems.

We test our methods by means of Monte Carlo experiments. When the true parameter values are known, it is possible to generate random samples and calculate bootstrap error bars and confidence intervals and check whether, for example, a 95% confidence interval for the estimated parameter does indeed contain in 95% of the Monte Carlo runs the known parameter. The number of Monte Carlo runs is typically 47,500. The computational burden increases to $2000 \times 47,500$. To create of this book required relatively powerful computers. In Chapter 9, we look on what may become possible when quantum computers exist.

Chapter 1 introduces you to climate time series and their statistical properties. Chapter 2 gives stochastic models of serial dependence or persistence, which are needed in Chapter 3, where bootstrap resampling, the determination of error bars and the construction of confidence intervals is explained. This concludes Part I on fundamental concepts. Chapters 4, 5 and 6 employ the concepts in the univariate setting (Part II), where the sample consists of only one time series. Chapters 7 and 8 deal with the bivariate setting (Part III).

Each of the chapters has a section "Background material," which contains supplementary material from statistics and climatology. You find also reported "stories"—comments, discussions and replies on certain papers in a scientific journal. Such exchanges, as also the "discussion" parts in read statistical papers, provide insight into the production of science—often more intimate than what polished journal articles reveal. The chapters have also a section entitled "Technical issues," where you find, besides information about numerical algorithms, listed software with internet links.

Intuition and creativity is needed for developing statistical estimation techniques for complex problems. Therefore I praise occasionally the artistic scientist, not at least in response to papers that make derogative remarks on that capacity. On the other hand, the artist in us must not forget to look for previous work on the same subject done in other disciplines and to scrutinize the own development by means of objective methods, such as Monte Carlo tests.

Regarding the notation, I have tried to find a route between convention on the one hand and consistency on the other. However, the most important symbols, including t for sampled time, x for a sampled climate variable, n for data size and $\{t(i), x(i)\}_{i=1}^n$ for a time series sample, possess their role throughout the book. I take this opportunity to introduce the counterpart of the time series sample, the stochastic process, $\{T(i), X(i)\}_{i=1}^n$. I hope that not only statisticians find that traditional

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distinction (Fisher 1922) between sample (i.e., numbers) and process (i.e., random variables) useful. Regarding the reference list, this notes only the first of the places of a publisher and it gives, in square brackets, additional information. This is not done consistently (e.g., the doi is given mostly to identify more recent papers published by the American Geophysical Union). The author list may be more aptly denoted as "first-author list."

The URL for this book is http://www.manfredmudelsee.com/book. It has the links to the sites of the software (including own products) and the data. It has also, inevitably, an errata section. As the person responsible for the content, I offer my apologies in advance of the discovered errors, and I thank you for informing me. My email address is mudelsee@mudelsee.com.

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Hannover, Germany December 2009

Manfred Mudelsee

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Part I

Fundamental Concepts

Chapter 1

Introduction

Superiority of quantitative methods over qualitative

-Popper

"Weather is important but hard to predict"—lay people and scientists alike will agree. The complexity of that system limits the knowledge about it and therefore its predictability even over a few days. It is complex because many variables within the Earth's atmosphere, such as temperature, barometric pressure, wind velocity, humidity, clouds and precipitation, are interacting, and they do so nonlinearly. Extending the view to longer timescales, that is, the climate system in its original sense (the World Meteorological Organization defines a timescale boundary between weather and climate of 30 years), and also to larger spatial and further processual scales considered to influence climate (Earth's surface, cryosphere, Sun, etc.), does not reduce complexity. This book loosely adopts the term "climate" to refer to this extended view, which shall also include "paleoclimate" as the climate within the geologic past.

Man observes nature and climate to learn, or extract information, and to predict. Since the climate system is complex and not all variables can be observed at arbitrary spatial and temporal range and resolution, our knowledge is, and shall be, restricted and uncertainty is introduced. In such a situation, we need the statistical language to acquire quantitative information. For that, we take the axiomatic approach by assuming that to an uncertain event ("it rains tomorrow" or "before 20,000 years the tropics were more than 5°C colder than at present") a probability (real number between 0 and 1) can be assigned (Kolmogoroff 1933). Statistics then deciphers/infers events and probabilities from data. This is an

1 Introduction

assumption like others in the business: three-dimensional space, time arrow and causality, mathematical axioms (Kant 1781; Polanyi 1958; Kandel 2006). The book also follows the optimistic path of Popper (1935): small and accurately known ranges of uncertainty about the climate system enable more precise climate hypotheses to be tested, leading to enhanced knowledge and scientific progress. Also if one shares Kuhn's (1970) view, paradigm shifts in climatology have better success chances if they are substantiated by more accurate knowledge. It is the aim of this book to provide methods for obtaining accurate information from complex time series data.

Climate evolves in time, and a stochastic process (a time-dependent random variable representing a climate variable with not exactly known value) and time series (the observed or sampled process) are central to statistical climate analysis. We shall use a wide definition of trend and decompose a stochastic process, X, as follows:

$$X(T) = X_{\text{trend}}(T) + X_{\text{out}}(T) + S(T) \cdot X_{\text{noise}}(T), \quad (1.1)$$

where T is continuous time, $X_{\text{trend}}(T)$ is the trend process, $X_{\text{out}}(T)$ is the outlier process, S(T) is a variability function scaling $X_{\text{noise}}(T)$, the noise process. The trend is seen to include all systematic or deterministic, long-term processes such as a linear increase, a step change or a seasonal signal. The trend is described by parameters, for example, the rate of an increase. Outliers are events with an extremely large absolute value and are usually rare. The noise process is assumed to be weakly stationary with zero mean and autocorrelation. Giving $X_{\text{noise}}(T)$ standard deviation unity enables introduction of S(T) to honour climate's definition as not only the mean but also the variability of the state of the atmosphere and other compartments (Brückner 1890; Hann 1901; Köppen 1923). A version of Eq. (1.1) is written for discrete time, T(i), as

$$X(i) = X_{\text{trend}}(i) + X_{\text{out}}(i) + S(i) \cdot X_{\text{noise}}(i), \qquad (1.2)$$

using the abbreviation $X(i) \equiv X(T(i))$, etc. However, for unevenly spaced T(i) this is a problematic step because of a possibly non-unique relation between $X_{\text{noise}}(T)$ and $X_{\text{noise}}(i)$, see Section 2.1.2.1. The observed, discrete time series from process X(i) is the set of size n of paired values t(i) and x(i), compactly written as $\{t(i), x(i)\}_{i=1}^{n}$. To restate, the aim of this book is to provide methods for obtaining quantitative estimates of parameters of $X_{\text{trend}}(T)$, $X_{\text{out}}(T)$, S(T) and $X_{\text{noise}}(T)$ using the observed time series data $\{t(i), x(i)\}_{i=1}^{n}$.

A problem in climate analysis is that the observation process superimposes on the climatic process. $X_{\text{noise}}(T)$ may show not only climatic

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1.1 Climate archives, variables and dating

but also measurement noise. Outliers can be produced by power loss in the recording instrument. Non-climatic trends result, for example, from changing the recording situation. An example is temperature measurements made in a town that are influenced by urbanization (meaning an increased heat-storage capacity). However, measurement noise can in principle be reduced by using better instruments, and outliers and trends owing to the observation system can be removed from the data climatologists denote such observation trend free data as homogeneous.

A further problem in real-world climatology is that also the time values have to be estimated, by dating (Section 1.1). Dating errors are expected to add to the noise and make the result more uncertain.

Consider a second climate variable, Y(T), composed as X(T) in Eq. (1.1) of trend, outliers, variability and noise. The interesting new point is the dependence between X(T) and Y(T). Take as example the relation between concentration of CO₂ in the atmosphere and the global surface temperature. In analogy to univariate X, we write $\{X(T), Y(T)\}$, $\{T(i), X(i), Y(i)\}$ and $\{t(i), x(i), y(i)\}_{i=1}^{n}$ for such bivariate processes and time series. This book describes methods only for uni- and bivariate time series. Possible extensions to higher dimensions are mentioned in Chapter 9.

 $\{t(i), x(i), y(i)\}_{i=1}^{n}$ need not result from the natural climate system but may also be the output from a mathematical climate model. Such models attempt to rebuild the climate system by connecting climate variables with governing mathematical-physical equations. Owing to the limited performance of computers and the uncertain knowledge about climatic processes, climate models are necessarily limited in spatial, processual and temporal resolution (McAvaney et al. 2001; Randall et al. 2007). On the other hand, climate models offer the possibility to perform and repeat climate experiments (say, studying the influence of doubled concentrations of CO₂ in the atmosphere on precipitation in dependence on different model implementations of the role of clouds).

1.1 Climate archives, variables and dating

Climate archives "contain" the time series. The measured variables (x(i), y(i)) either are of direct interest, as in case of precipitation and temperature, or they bear indirect information (indicator or proxy variables). The estimated times (t(i)), in geosciences often called timescale, are obtained either by direct, absolute dating methods or indirectly by comparison with another, dated time series. Table 1.1 gives an overview about climate archives and absolute dating methods. Table 1.2 informs about climate variables and their proxies studied in this book. More details are provided in Figs. 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9 and

1 Introduction

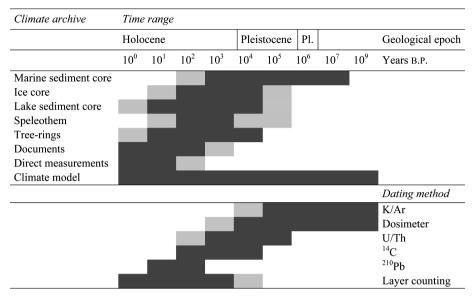


Table 1.1. Main types of climate archives, covered time ranges and absolute datingmethods.

Dark shading means "frequently used," *light shading* means "occasionally used." Pl., Pliocene; B.P., "before the present." Background material (Section 1.6) gives details and references on geological epochs (also before Pliocene), archives and dating.

1.10, where some of the time series analysed in this book are presented, and in the background material (Section 1.6).

1.2 Noise and statistical distribution

The noise, $X_{\text{noise}}(T)$, has been written in Eq. (1.1) as a zero-mean and unit-standard deviation process, leaving freedom as regards its other second and higher-order statistical moments, which define its distributional shape and also its spectral and persistence properties (next section). The probability density function (PDF), f(x), defines

$$\operatorname{prob}\left(a \le X_{\operatorname{noise}}(T) \le a + \delta\right)|_{\delta \to 0} = \int_{a}^{a+\delta} f(x)dx, \quad (1.3)$$

putting our incomplete knowledge in quantitative form.

For analysing, by means of explorative tools, the shape of f(x) using time series data $\{t(i), x(i)\}_{i=1}^{n}$, it is important to estimate and remove the trend from the data. An unremoved trend would deliver a false, broadened picture of f(x). Trend removal has been done for constructing Fig. 1.11, which shows histograms as estimates of the distributions of $X_{\text{noise}}(T)$ for various climate time series. The estimation of trends is

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1.2 Noise and statistical distribution

Climate archive Location Time Proxy variable Resolu-Climate variable range (a) tion (a) 10^{6} δ^{18} O. benthic 10^{3} Marine sediment core Eastern Ice volume. foraminifera equatorial bottom water Pacific temperature 10^{5} 10^{3} Ice core Antarctica CO₂, air bubbles CO₂, atmosphere 10^{2} δD. ice Air temperature Greenland 10^{5} SO₄ content, ice 10^{0} Volcanic activity Ca content, ice 10^{0} Aeolian dust, wind Dust content, ice 10^{0} Aeolian dust, wind 10^{0} Conductivity,^a Soluble material. ice wind Na content, ice 10^{0} Seasalt, wind Δ^{14} C, wood Tree-rings Worldwide 10^{4} 10^{0} Solar irradiance. ocean circulation 10^{3} 10^{0} Wind^b Lake sediment core Varve thickness Boston area δ^{18} O. carbonate 10^{4} 10^{1} Speleothem Southern Oman Monsoon rainfall Weikinn 10^{3} 10^{0} Floods, river Elbe Documents source texts River runoff 10^{2} 10^{0} Climate model Hadley Centre, HadCM3 10^{2} 10^{-1} Direct measurements Siberia. Surface North Atlantic temperature

Table 1.2.	Climate	archives	and	variables	studied	in	this	book	(selection)).
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Time range refers to the length of a record, resolution to the order of the average time spacing (see Section 1.4). "Proxy variable" denotes what was actually measured on which material. "Climate variable" refers to the climatic variations recorded by the variations in the proxy variable. The ability of a proxy variable to indicate a climate variable depends on the characteristic timescales (between resolution and time range). For example, δ^{18} O variations in benthic foraminifera over timescales of only a few decades do not record ice-volume variations (which are slower). The Weikinn source texts are given by Weikinn (1958, 1960, 1961, 1963, 2000, 2002).

^a Electrical conductivity of the melted water.

^b Extremely thick varves (graded beds) indicate extremely high wind speed (hurricane).

one of the primary tasks in climate time series analysis and described in Chapter 4. In Fig. 1.11, outliers, sitting at the tail of the distribution, are tentatively marked. The variability, S(T), has only been normalized in those panels in Fig. 1.11 where it is not time-constant.

As the histogram estimates of the PDFs reveal, some distributions (Fig. 1.11b, i, j) exhibit a fairly symmetrical shape, resembling a Gaussian

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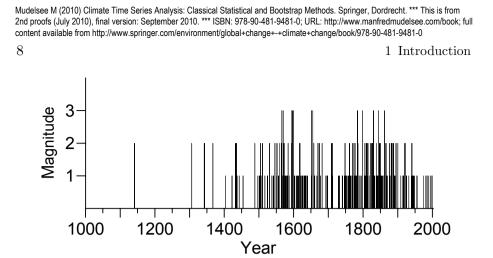


Figure 1.1. Documentary data: floods of the river Elbe during winter over the past 1000 years. x, the flood magnitude, is in three classes (1, minor; 2, strong; 3, exceptionally strong). Hydrological winter is from November to April. Data for $t \leq 1850$ were extracted from Curt Weikinn's compilation (Weikinn 1958, 1960, 1961, 1963, 2000, 2002) of source texts on hydrography in Europe; accuracy of flood dates is ~ 1 month. Data for t > 1850 were inferred from daily measurements of water stage and runoff (volume per time interval) at Elbe station Dresden (Global Runoff Data Centre, Koblenz, Germany) via a calibration of magnitude versus water stage/runoff (Mudelsee et al. 2003). Because floods can last up to several weeks, only the peaks in stage/runoff were used to ensure independence of the data. Total number of points is 211. Data sparseness for $t \leq 1500$ is likely caused by document loss (inhomogeneity). One climatological question associated with the data is whether floods occur at a constant rate or there is instead a trend. (Data from Mudelsee et al. 2003.)

(Fig. 3.1). Other PDFs (Fig. 1.11c–h, k), however, have more or less strongly right-skewed shape. Possibly Fig. 1.11d (Vostok δD) reflects a bimodal distribution.

Table 1.3 informs about the size of the variability, S(T), in relation to the uncertainty associated with the pure measurement for the time series analysed here. S(T) reflects the variability of the climate around its trend (Eq. 1.1), the limited proxy quality when no directly measured variables are available and, finally, measurement error. As is evident from the data shown, the measurement error is often comparably small in climatology. It is in many studies that use proxy variables one of the major tasks to quantify the proxy error. For example, if δ^{18} O in shells of benthic foraminifera from deep-sea sediment cores is used as proxy for global ice volume, bottom-water temperature fluctuations make up nearly 1/3 of S(T), see Table 1.3.

A relation proxy variable–climate variable established under laboratory conditions is not perfect but shows errors, quantifiable through regression (Chapter 8). Assuming that such a relation holds true also in

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1.2 Noise and statistical distribution

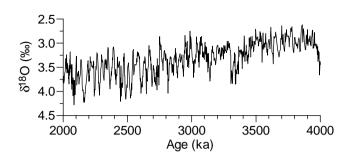


Figure 1.2. Marine sediment core data: δ^{18} O record from Ocean Drilling Program (ODP) site 846 (eastern equatorial Pacific) within 2–4 Ma. The core was drilled from a ship through ~ 3300 m water into the ocean floor, it has a length of \sim 460 m and a diameter of \sim 35 cm. The oxygen isotope record (Shackleton et al. 1995b) was measured on the calcareous shells of benthic foraminifera, mainly C. wuellerstorfi and Uvigerina spp., using a mass spectrometer. Values are given in delta notation: $\delta^{18}O = [({}^{18}O/{}^{16}O)_{\text{sample}}/({}^{18}O/{}^{16}O)_{\text{PDB}} - 1] \cdot 1000\%$, where $({}^{18}O/{}^{16}O)$ is the number ratio of oxygen isotopes ${}^{18}O$ and ${}^{16}O$ and PDB is "Pee Dee Belemnite" standard. A value of 0.64‰ was added to all δ^{18} O values from C. wuellerstorfi to correct for a species-dependent offset (Shackleton and Hall 1984). The depth scale was transformed into a timescale in several steps (Shackleton et al. 1995a). First. biostratigraphic positions, that is, core depths documenting first or last appearances of marine organisms, provided a rough time frame. (Unlike many other marine sediment cores, site ODP 846 lacks a magnetostratigraphy, that is, recorded events of reversals of the Earth's magnetic field, which might had improved the temporal accuracy at this step.) Second, a proxy record of sediment density was measured using a gammaray attenuation porosity evaluation (GRAPE) tool. Third, the ODP 846 GRAPE record was tuned (Section 1.6) to the combined GRAPE record from ODP sites 849, 850 and 851. This stacked GRAPE record had in turn been previously tuned to the time series of solar insolation at 65° N (Berger and Loutre 1991), calculated using standard procedures from astronomy. The reason behind this cross-tuning procedure is the observation (Hays et al. 1976) that Earth's climatic variations in the order of tens of thousands to several hundreds of thousands of years are influenced by solar insolation variations. Since the sedimentation rate in the geographic region of site ODP 846 varies with climate (Shackleton et al. 1995a), one cannot assume a constant accumulation of the marine archive. Hence, the dates of sediment samples between the biostratigraphic fixpoints cannot be obtained by interpolation and the GRAPE density records had to be used to obtain an absolute timescale by tuning. Note that time runs "in paleoclimatic manner" from the right to the left. In the same fashion, the δ^{18} O scale is inverted such that glacial conditions (large ice volume, low bottom water temperature or large δ^{18} O values) are indicated by the bottom part and interglacial conditions by the top part of the plot. The number of data points, n, within the shown interval is 821, the average spacing is $\sim 2.4a$. A comparison between absolutely dated and tuned magnetostratigraphic timescales for the Pliocene to early Pleistocene (Mudelsee 2005) suggests an average age deviation of ~ 25 ka; this value can also serve to indicate the magnitude of the absolute error of the ODP 846 timescale. The record indicates variations in global ice volume and regional bottom water temperature. One task is to quantify the long-term δ^{18} O increase, which reflects the glaciation of the northern hemisphere in the Pliocene.

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1 Introduction

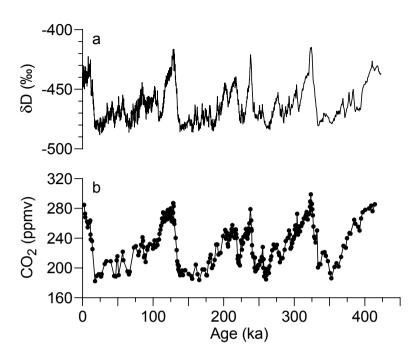


Figure 1.3. Ice core data: deuterium and CO_2 records from the Vostok station (Antarctica) over the past 420,000 years. The core was drilled into the ice (diameter: 12 cm, length: 3623 m) and recovered in segments. The deuterium record (a) was measured on ice material using a mass spectrometer. Values are given in delta notation: $\delta D = [(D/H)_{sample}/(D/H)_{SMOW} - 1] \cdot 1000\%$, where (D/H) is the number of D particles over the number of H particles and SMOW is "Standard Mean Ocean Water" standard. Total number of points, n, is 3311. The CO₂ record (**b**) was measured on air bubbles enclosed in the ice. Values are given as "parts per million by volume," n is 283. In **b**, values (*dots*) are connected by lines; in **a**, only lines are shown. The present-day CO₂ concentration (~ 389 ppmv) is not recorded in **b**. The construction of the timescale (named GT4) was achieved using a model of the ice accumulation and flow. Besides glaciological constraints, it further assumed that the points at 110 and 390 ka correspond to dated stages in the marine isotope record. Construction of the CO_2 timescale required additional modelling because in the ice core, air bubbles are younger in age than ice at the same depth. One climatological question associated with the data is whether variations in CO_2 (the values in air bubbles presenting the atmospheric value accurately) lead over or lag behind those of deuterium (which indicate temperature variations, low δD meaning low temperature). (Data from Petit et al. 1999.)

the geologic past increases the proxy error. Spatially extending the range for which a variable is thought to be representative is a further source of error. This is the case, for example, when variations in air temperature in the inversion height above Antarctic station Vostok are used to repre-

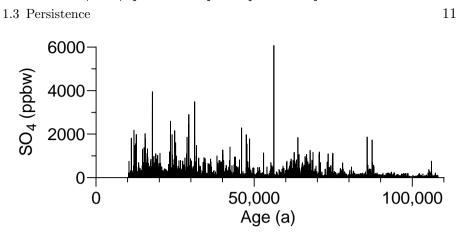


Figure 1.4. Ice core data: sulfate record from the NGRIP core (Greenland) over the interval from ~ 10 to ~ 110 ka. The sulfate content was determined by continuously melting the ice core along its axis and measuring SO_4 of the melt water by means of a photometer (continuous flow analysis, CFA; see Röthlisberger et al. (2000) and Bigler et al. (2002)); ppbw, parts per billion by weight. Meltspeed and signal dispersion limit the length resolution to ~ 1 cm over the measured record length (1530 m). In the young part of the record ($t \leq 105$ ka), the NGRIP timescale was obtained by tuning to the ss09sea timescale of the Greenland GRIP ice core (Johnsen et al. 2001) using the records of ice isotopes (North Greenland Ice Core Project members 2004), electrical conductivity and dielectric properties. In the old part, the NGRIP timescale was obtained by tuning to the GT4 timescale of the Vostok ice core (Fig. 1.3) using the records of δ^{18} O and methane concentration. (An absolutely dated alternative to the GRIP ss09sea timescale was published by Shackleton et al. (2004).) The sulfate record was finally averaged to 1-year resolution. Using the Ca and Na records, proxies for mineral dust and seasalt content, respectively, it is possible to remove peaks in the sulfate record from dust and salt input—the remaining peaks in the "excess" SO₄ record, shown here, likely reflect the input from volcanic eruptions via the atmosphere. The record therefore bears the possibility to reconstruct volcanic activity throughout the last glacial period. (Data from Bigler M 2004, personal communication.)

sent those of the total southern hemisphere. However, such uncertainties are often unavoidable when general statements about the climate system are sought. All individual noise influences on a climate variable (natural variability, proxy and measurement noise) seem to produce a process $X_{\text{noise}}(T)$ with a PDF that is better described by a product than a sum of individual PDFs and that likely has a right-skewed shape, such as the lognormal distribution (Aitchison and Brown 1957).

1.3 Persistence

The other property of $X_{\text{noise}}(T)$ besides distributional shape regards serial dependence. The autocovariance, $E[X_{\text{noise}}(T_1) \cdot X_{\text{noise}}(T_2)]$ for

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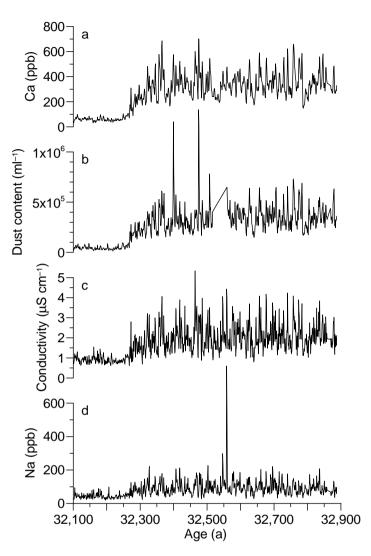


Figure 1.5. Ice core data: Ca concentration (**a**), dust content (**b**), electrical conductivity (**c**) and Na concentration (**d**) from the NGRIP core (Greenland) during the onset of Dansgaard–Oeschger (D–O) event 5. The four variables were measured using CFA on the melted water (Fig. 1.4). ppb, parts per billion; ml^{-1} , number of particles per ml; Sm^{-1} , SI unit for electrical conductivity. A data gap (hiatus) exists at around 32,550 a in the dust-content record. Records were "downsampled" to annual resolution. The Ca record indicates variations of mineral dust transported to the atmosphere over Greenland, the dust content indicates atmospheric dust load, electrical conductivity is a proxy for input of soluble material (integrating various environmental signals) and Na is a proxy for seasalt. One climatological question is whether the changes in all four variables happened simultaneously at the onset of D–O event 5. D–O events are short-term warmings during the last glacial period. (Data from Röthlisberger R 2004, personal communication.)

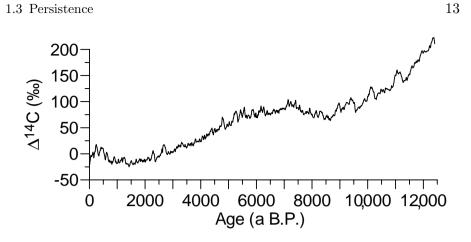


Figure 1.6. Tree-ring data: record of atmospheric radiocarbon content over the past 12,410 years. The tree-ring radiocarbon equilibrates with atmospheric radiocarbon via the photosynthetic cycle. The ¹⁴C radioactivity was measured by counting the β particles on CO₂ produced by combusting the wood material. Original sampling resolution was yearly (individual tree-rings) and lower; data shown are 5-year averages (n = 2483). The values are presented in delta notation (Fig. 1.3) with the oxalic acid standard of the National Bureau of Standards, for conventional reasons " Δ " is used instead of " δ ." The timescale (given as years before present (B.P.) where "present" is, as in "radiocarbon terminology," the year 1950) is based on a counted tree-ring chronology, established by matching radiocarbon patterns from individual trees. Since the age spans of the trees overlap, it is possible to go back in time as far as shown (and beyond). Since the radiocarbon data act as a proxy for solar activity (high Δ^{14} C means low solar irradiance), it is possible to analyse Sun-climate connections by studying correlations between Δ^{14} C and climate proxy records. (Data from Reimer et al. 2004.)

 $T_1 \neq T_2$, is here of interest; higher-order moments are neglected. Lag-1 scatterplots (x(i-1) versus x(i)) of the climate time series, using detrended $\{t(i), x(i)\}_{i=1}^n$ as realizations of the noise process, explore the autocovariance structure (Fig. 1.12). It is evident that all examples exhibit a more or less pronounced orientation of the points along the 1:1 line. This indicates positive serial dependence, or "memory," also called persistence in the atmospheric sciences. The reason for that memory effect is twofold. First, it is characteristic for many types of climatic fluctuations (Wilks 1995). Second, it can be induced by the sampling of the data. A record sampled at high resolution has often stronger persistence than when sampled at low resolution (see next section).

The lag-1 scatterplots (Fig. 1.12) reflect also the right-skewed shape of many of the distributions (more spreading towards right-up) and let some outliers appear.

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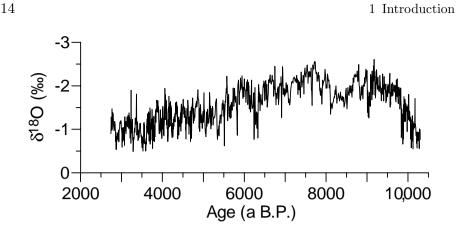
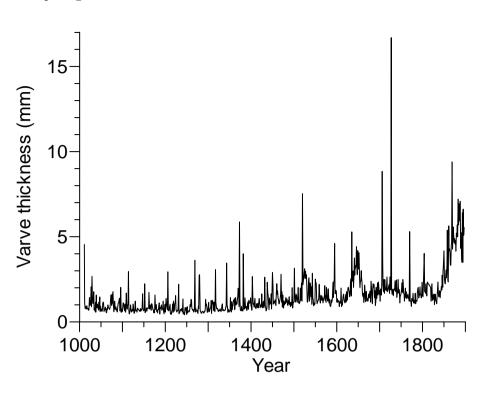


Figure 1.7. Speleothem data: oxygen isotope record from stalagmite Q5 from southern Oman over the past 10,300 years. Along the growth axis of the nearly 1 m long stalagmite, every ~ 0.7 mm about 5 mg material (CaCO₃) was drilled, yielding n = 1345samples. The carbonate powder was analysed with an automatic preparation system linked to a mass spectrometer to determine the δ^{18} O values. (The (18 O/ 16 O) ratio is given relative to the Vienna Pee Dee Belemnite (VPDB) standard analogously to the description in Fig. 1.3.) The timescale (years before 1950) is based on 18 U/Th mass-spectrometric ages, obtained on separated and purified material. Dates for samples between absolutely dated positions were obtained by linear interpolation. Time runs from right to left. The δ^{18} O scale is inverted "in paleoclimatic manner" so that the transition from the last glacial to the present Holocene interglacial at around 10 ka is "upwards." Note that growth of stalagmite Q5 ceased at ~ 2740 a B.P. Climatological questions associated with the data are whether the transition to the Holocene occurred synchronously with climatic transitions in other locations and whether there exist solar influences on the variations in monsoon rainfall (indicated by δ^{18} O variations, low δ^{18} O reflecting strong monsoon). (Data from Fleitmann et al. 2003.)

1.4 Spacing

Archives other than documentary collections or climate models require measurements on the archive material. Material-size requirements lead in many cases to a constant length interval, L(i), from which material for one measurement is taken, and also the length spacing, l(i), between the measurement mid-points on the length axis is often constant (Fig. 1.13). Dating transfers from length into the time domain with the "sample duration," D(i), and the temporal spacing, d(i) = t(i) - t(i-1), here in this book briefly denoted as "spacing." The spacing is frequently nonconstant: archives normally accumulate not at a constant rate. They might also be subject to postdepositional length distortions such as compressing in the case of ice cores. Archives that allow pre-sampling (visual)





Lake sediment core data: varve thickness record from Lower Mystic Lake Figure 1.8. (Boston area) over the past 1000 years. Multiple overlapping cores were retrieved from the lake, split and photographed in the laboratory. The sediments consist of varves of alternating siliciclastic (bright) and biogenic (dark) layers. The total combined length of the records is about 2 m. Sediment blocks extracted from cores were embedded in epoxy resin to produce petrographic thin sections and X-ray densitometry slabs. A master, composite sequence of stratigraphy was constructed from high-resolution imagery of observations made via petrographic microscopy, back scattered electron microscopy and X-ray densitometry (Besonen 2006). Age control from varve counting was confirmed by means of radiocarbon dating on terrestrial macrofossils. In addition to varve thickness, Besonen (2006) determined the dates of graded beds based on visual examination of the petrographic thin sections and X-ray imagery. A thick varve and a graded bed can be jointly used as a proxy for hurricane activity in the area of the lake. Hurricane-strength precipitation saturates the watershed, results in erosive overland flow that entrains sediment and carries it into the lake where it is deposited as a graded bed. This is enhanced by hurricane-strength winds that disturb vegetation and uproot trees, exposing loose sediment (Besonen 2006). The proxy information was verified by means of pollen data and documentary information (available from about 1630 to the present). The time series (n = 877) covers the interval from A.D. 1011 to 1897, minor hiatuses are present (1720–1721, 1803, 1812–1818), also a major above the depth corresponding to 1897. The record bears information on hurricane activity in the Boston area over the past 1000 years. (Data from Besonen et al. 2008.)



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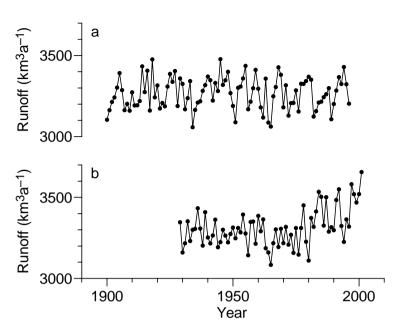


Figure 1.9. Climate model data: runoff from Arctic rivers. a Natural forcing only; b combined anthropogenic and natural forcing. In a climate model, the physical equations for energy, momentum and mass conservation are numerically solved in time steps over a spatial grid. HadCM3 (Gordon et al. 2000) is a coupled Atmosphere-Ocean General Circulation Model (AOGCM) for the global domain, run by the Hadley Centre for Climate Prediction and Research, Bracknell, United Kingdom. The atmospheric component has a horizontal grid spacing of 2.5° in latitude by 3.75° in longitude and 19 vertical levels. The oceanic component has 20 vertical levels on a 1.25° by 1.25° grid. The time step used for integrating the differential equations representing the atmospheric component was 30 min, for the oceanic component one hour. The total interval simulated (~ 140 years) was longer than the data shown (**a** 1900–1996; **b** 1929–2001). Plotted are annual-mean ensemble averages, for which the model year starts on 1 December. The averages were constructed from four ensemble runs, that is, runs with identical forcings but different initial conditions. The initial conditions used were taken from states separated by 100 years in a HadCM3 run, in which external forcings where set to have no year-to-year variations ("control run"). Unlike previous models, HadCM3 does not require flux adjustments of heat and water at the air-sea interface to maintain a stable climate without drift behaviour (Johns et al. 1997; Stott et al. 2000). This makes the results obtained with HadCM3 more reliable than previous results. The natural forcing included changes in the amount of stratospheric aerosols stemming from volcanic eruptions and variations in solar irradiation. The anthropogenic forcing included changes in atmospheric concentrations of CO₂, methane, sulfate aerosols and ozone. The river runoff records were generated (Wu et al. 2005) by summing the precipitation contributions from affected grid cells north of 65°N. Model simulations can be used to analyse past and forecast future climate changes. Questions associated with the data are those after the size and the timing of changes in runoff as a result of an intensified hydrological cycle caused by anthropogenically induced warming. (Data from Wu et al. 2005.)

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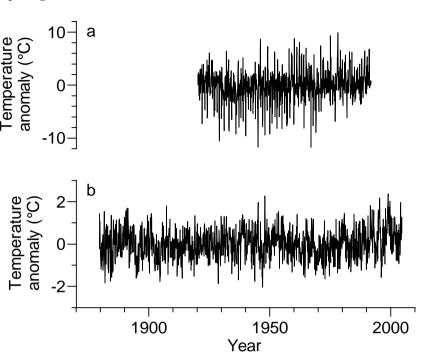


Figure 1.10. Measured data: surface air temperature records from Siberia (**a**) and North Atlantic (**b**). Data are monthly temperature anomalies with respect to the 1961–1990 means from a gridded, global set. Siberia is presented by the grid cell 50–55°N, 90–95°E, effectively reflecting station Krasnojarsk; the North Atlantic by 35–40°N, 25–30°W. Shown are the gap-free time intervals (**a** May 1920 to November 1991, n = 859; **b** July 1879 to July 2004, n = 1501). The annual cycles were removed by subtracting the monthly averages. (Raw data from Jones and Moberg 2003.)

detection of time-equidistant sampling points, such as tree-rings, varves (that is, annually laminated sediments) or speleothems (Fig. 1.14), appear to be the exception rather than the rule. That mixture of deterministic and stochastic influences on the spacing, is pictured in Fig. 1.15. The Elbe floods (Fig. 1.1) are an example where d(i) (or equivalently t(i)) is the major research object, not x(i), see Chapter 6.

The nonzero sample duration, D(i), imposed by material requirements, can be subject to extension to D'(i) by diffusion-like processes in the archive (Fig. 1.13). Besides physical diffusion of material, for example in ice cores, bioturbation in sedimentary archives (mixing by activities of worms and other animals in the upper (young) layer) can play a role. The other data archives studied here (Table 1.1) likely have no diffusion effects.

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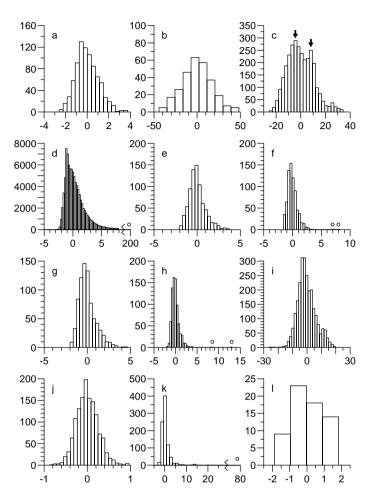


Figure 1.11. Statistical noise distributions of selected climate time series. a ODP 846 δ^{18} O; **b** Vostok CO₂; **c** Vostok δ D; **d** NGRIP SO₄; **e** NGRIP Ca; **f** NGRIP dust content; **g** NGRIP electrical conductivity; **h** NGRIP Na; **i** tree-ring Δ^{14} C; **j** Q5 δ^{18} O; **k** Lower Mystic Lake varve thickness; **I** HadCM3 runoff. The distributions are estimated with histograms. Data and units are given in Figs. 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8 and 1.9. In **a** and **e**-**h**, the trend component was estimated (and removed prior to histogram calculation) using a ramp regression model (Figs. 4.6 and 4.7); in **b** and **c** using a harmonic filter (Section 5.2.4.3); in **d** and **k** using the running median (Figs. 4.16 and 4.17); in **i** using nonparametric regression (Fig. 4.14); in **j** using a combination of a ramp model in the early and a sinusoidal in the late part (Fig. 4.18); and in I using the break regression model (Fig. 4.12). Outliers are tentatively marked with open circles (note broken axes in \mathbf{d}, \mathbf{k}). In \mathbf{c} , the modes of the suspected bimodal distribution are marked with arrows. In **a**, **e**-**h** and **j**, time-dependent variability, S(T), was estimated using a ramp regression model (Chapter 4); in **d** and **k** using the running MAD (Figs. 4.16 and 4.17); and in I using a linear model. Normalizing (dividing by S(T)) for those time series was carried out prior to histogram calculation. The other time series assume constant S(T), values are given in Table 1.3.

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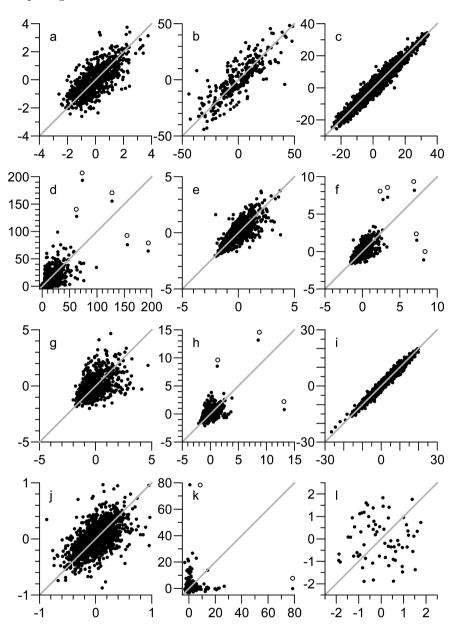


Figure 1.12. Persistence of noise in selected climate time series. **a** ODP 846 δ^{18} O; **b** Vostok CO₂; **c** Vostok δ D; **d** NGRIP SO₄; **e** NGRIP Ca; **f** NGRIP dust content; **g** NGRIP electrical conductivity; **h** NGRIP Na; **i** tree-ring Δ^{14} C; **j** Q5 δ^{18} O; **k** Lower Mystic Lake varve thickness; **l** HadCM3 runoff. Noise data are shown as lag-1 scatterplots (in each panel, x(i-1) is plotted on the ordinate against x(i) on the abscissa as *points*), together with 1:1 lines (*grey*). Data and units are given in Figs. 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8 and 1.9. Detrending and S(T) normalization prior to analysis was carried out as in Fig. 1.11. Note that in **d**, all points are shown (unlike as in Fig. 1.11d). Outliers are tentatively marked with *open circles*.

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Archive	Variable	Error range		
		Total, S(T)	Measurement	Proxy
Marine core	δ^{18} O	$0.2 - 0.3\%^{a}$	$0.06\%^{ m b}$	$\sim 1/3^{\rm c}$
Ice core	CO_2 content	17.5 ppmv^{a}	$2–3 \text{ ppmv}^{d}$	$\operatorname{Small}^{\mathrm{e}}$
	$\delta \mathrm{D}$	$10.5\%^{\mathrm{a}}$	$\leq 1\%^{\rm d}$	$7\%^{\mathrm{f}}$
	SO_4 content	$40.5 \text{ ppbw}^{\text{g}}$	$10\%^{\rm h}$	Unknown ⁱ
	Ca content	43 ppb^{j}	$10\%^{\rm h}$	$\mathrm{Unknown}^{\mathrm{i}}$
	Dust content	$0.56 \cdot 10^5 \ {\rm ml}^{-1 {\rm j}}$	$10\%^{ m h}$	Unknown ⁱ
	Conductivity	$0.37 \mu \mathrm{S cm^{-1 j}}$	$10\%^{ m h}$	Unknown ⁱ
	Na	$28 \text{ ppb}^{\text{j}}$	$10\%^{\rm h}$	Unknown ⁱ
Tree-rings	$\Delta^{14}C$	$6.2\%^{\mathrm{a}}$	$\sim 2\%^{\rm k}$	$\mathrm{Small}^{\mathrm{l}}$
Speleothem	$\delta^{18}O$	$0.25\%^{\mathrm{a}}$	0.08% ^m	$\mathrm{Unknown}^{\mathrm{n}}$
Lake core	Varve thickness	$0.33 \mathrm{~mm^g}$	0.1 mm°	NA^{p}
Climate model	River runoff	$93 \text{ km}^3 \text{a}^{-1 \text{ q}}$	0	NA
Direct measure-	Temperature	$0.69^{\circ}\mathrm{C^{r}}$	$0.03^{\circ} C^{s}$	0
ment		$2.97^{\circ}C^{t}$	$0.03^{\circ} C^{s}$	0

Table 1.3. Measurement and proxy errors in selected climate time series (Table 1.2).

Measurement errors were usually determined using repeated measurements. Proxy errors refer to the climate variables in Table 1.2 unless otherwise noted. NA, not applicable. ^a Standard deviation of detrended $\{t(i), x(i)\}_{i=1}^{n}$ (Fig. 1.11).

^b Shackleton et al. (1995b).

^c As ice-volume indicator, relative error. This error comes from other variations than of ice volume: mainly of bottom water temperature and to a lesser degree of salinity (Mudelsee and Raymo 2005).

^d Petit et al. (1999).

^e Raynaud et al. (1993).

^f As air-temperature indicator; own determination of $MS_E^{1/2}$ (Eq. 4.8) after Jouzel et al. (2007: Fig. S4 therein).

^g Average MAD value (Figs. 4.16 and 4.17), divided by 0.6745 (a standard normal distribution has an MAD of ~ 0.6745).

^h Relative error (Röthlisberger et al. 2000).

ⁱ Trace substances are part of a complex system, involving variations at the source, during transport (wind) and at deposition; they represent a more local or regional climate signal. ^j Time-average of $\widehat{S}(i)$ (Fig. 4.7).

^k Reimer et al. (2004).

 $^1\,\Delta^{14}{\rm C}$ in tree-rings on yearly to decadal resolution has a (small) proxy error as atmospheric Δ^{14} C indicator because the wood formation is not constant (the major portion is formed in spring and early summer) and because tree-ring thickness varies (Stuiver et al. 1998). $\Delta^{14}C$ variations are a good proxy of solar activity variations because other influences (variations in ocean circulation, changes in the intensity of the Earth's magnetic field) are weak on Holocene timescales (Solanki et al. 2004).

^m Fleitmann et al. (2003).

ⁿ Unknown on longer timescales (Table 1.2) because observed monsoon rainfall time series (Parthasarathy et al. 1994) are too short (150 a) to permit comparison.

^o Time-average; depends on varve distinctiveness and human component (Besonen MR 2010, personal communication).

^p Only information about hurricane existence sought, not about hurricane strength.

^q Time-average of $\widehat{S}(i)$ (Fig. 4.12).

^r North Atlantic, time-average.

- ^s Upper limit (Tetzlaff G 2006, personal communication).
- ^t Siberia, time-average.

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1.4 Spacing

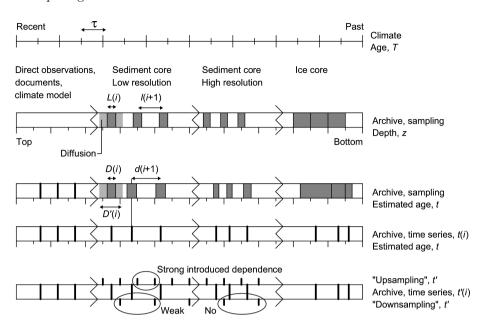


Figure 1.13. Sampling of time series from climate archives. The archive, documenting climate over a time span, is sampled (depth domain), dated (time domain) and possibly interpolated to an evenly spaced time grid. τ denotes a typical timescale of climatic fluctuations, $X_{\text{noise}}(T)$. L(i), length over which material is sampled (dark shading); l(i), length spacing between mid-points of L(i); D(i), time-domain analogue of L(i); d(i), time-domain analogue of l(i), denoted as "spacing." Light shading indicates effects of a diffusion-like process, that is, extension of D(i) to D'(i). Diffusion need not act symmetrically. Thick vertical lines indicate t(i). Terms "sediment core", "ice core", etc. denote here the sampling type rather than a specific archive (for example, a speleothem is often sampled like a "sediment core"). In case of ice cores, t(i) often is not the average time but the time at the upper end of the sample. Real ice cores contain two sub-archives, ice material and enclosed air bubbles, with different age-depth relations (Chapter 8). Interpolation to a fine grid ("upsampling") introduces a strong additional dependence in addition to climatic dependence; "downsampling" introduces weak or no additional dependence. High-resolution time series (d(i) small) have the advantage that this effect is weaker than for low-resolution records. (Note that our usage of "grid" is not restricted to two dimensions.)

The sampled time series $\{t(i), x(i)\}_{i=1}^{n}$ carries information about observed climatic variations up to an upper bound equal to the record length and down to a lower bound of

$$\max\left(\tau, D'(i), \bar{d}\right),\tag{1.4}$$

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where \bar{d} is the average of d(i). Whereas the upper bound is obvious, the lower bound is explained as follows. The "persistence time," τ , of the climatic noise measures the decay of the autocorrelation function ("memory loss") of $X_{\text{noise}}(T)$, see Chapter 2. Deterministic influences acting on shorter timescales are by definition (Eq. 1.1) not part of the description. Information within interval D'(i) is lost by the sampling process and eventual diffusion. Information theory shows that for evenly spaced time series (d(i) = d = const.) the lower limit is 2 d (or one over Nyquist frequency). The factor 2 is omitted in Eq. (1.4) because for uneven spacing the bound may be lower than for even spacing (Chapter 5).

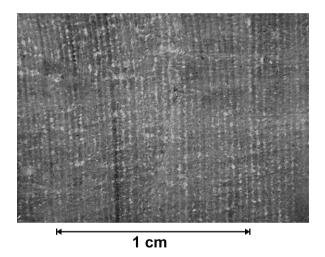


Figure 1.14. Plain-light photomicrograph from a polished section of stalagmite S3 from southern Oman. U/Th dating of samples and the seasonally varying monsoon precipitation pattern in the geographic region suggest that the laminae are annual. Dark (bright) layers reflect a higher (lower) density of pores and fluid inclusions (Fleitmann 2001). The stalagmite covers the period from approximately A.D. 1215 to 1996. Annual layer thickness and oxygen isotopic (δ^{18} O) composition, measured on the stalagmite, record variations in the intensity of Indian monsoonal rainfall. (From Burns et al. (2002), with permission from the publisher).

Interpolation of the unevenly spaced time series $\{t(i), x(i)\}_{i=1}^{n}$ is in climatology usually done to obtain an evenly spaced series $\{t'(i), x'(i)\}_{i=1}^{n'}$. This series can then be analysed with sophisticated statistical methods for which currently only implementations exist that require even spacing. This advantage, however, is accompanied by following disadvantages. First, additional serial dependence can be introduced, depending mainly on n'. If n' > n ("upsampling"), that effect is strong (Fig. 1.13).

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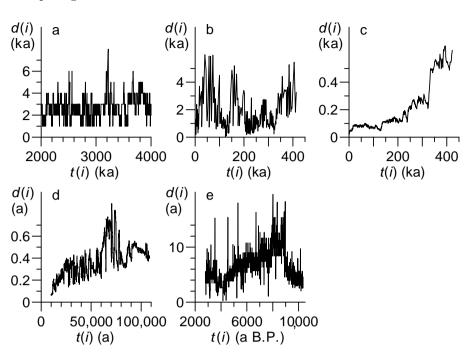


Figure 1.15. Spacing of selected climate time series. **a** ODP 846 δ^{18} O; **b** Vostok CO₂: **c** Vostok δD ; **d** NGRIP SO₄; **e** Q5 δ^{18} O. Data are given in Figs. 1.2, 1.3, 1.4 and 1.7. In **d**, d(i) is shown for the D(i) = 0.5 cm data; the time series with t(i) = 1 a (Fig. 1.4) is obtained from the 0.5-cm data using "downsampling." The ice core data (**b-d**) reflect to some degree the effects of ice compaction, that means, d(i) increases with t(i). The Q5 speleothem spacing time series (e) suggests visually a strong negative correlation with the speleothem δ^{18} O series (Fig. 1.7). This is explained as follows. Low (high) δ^{18} O means strong (weak) Indian monsoonal rainfall, this in turn faster (slower) movement of the rainwater through the soil, weaker (stronger) uptake of soil-CO₂, lower (higher) pH of the water, reduced (enhanced) solution of soil-carbonate, less (more) material for calcite precipitation, small (large) annual stalagmite layers and, finally, a higher (lower) temporal spacing because the depth spacing is nearly constant (Fig. 1.7). Note that at places with other soil properties, the relation $\delta^{18}O$ spacing may be different (Burns et al. 2002). The values of the average spacing, \bar{d} , and the coefficient of variation of spacing, CV_d , which is defined as the standard deviation of the spacing divided by \bar{d} , are as follows. **a** $\bar{d} = 2.40$ a, $CV_d = 0.41$; **b** $\bar{d} = 1.46$ a, $CV_d = 0.82$; **c** $\bar{d} = 0.13$ a, $CV_d = 0.85$; **d** $\bar{d} = 0.32$ a, $CV_d = 0.47$; **e** $\bar{d} = 5.62$ a, $CV_d = 0.49.$

If $n' \approx n$ it is weaker, and only for n' < n ("downsampling") it may be absent. That means, interpolation does not allow to go in resolution below the limit set by Eq. (1.4). Second, depending on the type of in-

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terpolation method (linear, cubic spline, etc.), x'(i) may show serious deviations from x(i) in terms of variability or noise properties. That is, interpolation takes us a step further away from the observed process.

Achieving insight into shorter-term climatic processes through sampling an archive is best done by increasing the resolution. Reducing d(i)might require reducing D(i) by employing a measurement method that consumes less material. However, the restriction imposed by diffusion processes and climatic persistence still applies (Eq. 1.4). "Overlapped sampling," d(i) < D(i), is no means to obtain higher resolved information than with $d(i) \ge D(i)$.

1.5 Aim and structure of this book

We have certain hypotheses about time-dependent climate processes, about $X_{\text{trend}}(T)$, $X_{\text{out}}(T)$, S(T) and $X_{\text{noise}}(T)$, which we would like to test. Alternatively, we wish to estimate parameters of climate processes. For that purpose, we use certain methods that take uncertainty into account, that means, statistical methods. Smaller error bars or narrower confidence intervals for the results obtained with the methods, guarantee better testability or more accurate knowledge. To construct confidence intervals, in principle, two approaches exist: classical and bootstrap. The classical approach makes substantial assumptions, such as normally distributed data, no serial dependence, and, often, even time spacing, whereas the bootstrap approach does not make such. Since the preceding sections showed that the assumptions made by the classical approach may be violated when applied to climate time series analysis, the bootstrap may yield more reliable results.

That does not imply that all results obtained on climate time series using classical methods are invalid. However, caution as regards their statistical accuracy is appropriate. The reasons why the classical approach was used are obvious. First, the bootstrap was invented late (Efron 1979), but it soon became accepted in the statistical community and recognized/accepted in the natural sciences (Casella 2003). Bootstrap methods for time series (serially dependence) lag one decade behind in their development. Second, there has been an increase in computing power, which made bootstrap calculations feasible.

This book presents the bootstrap approach adapted to a number of statistical analysis methods that have been found useful for analysing climate time series at least by the author. Linear and nonlinear regression (Chapter 4), spectral analysis (Chapter 5) and extreme value time series analysis (Chapter 6) are explained in case of univariate climate time series analysis (Part II). Correlation (Chapter 7) as well as lagged and other variants of regression (Chapter 8) come from the field of bivari-

1.5 Aim and structure of this book

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ate time series (Part III). Application of each method is illustrated with one or more climate time series, several of which already presented. A section ("Background material") reports alternative techniques and provides a look at the literature that is intended to serve climatologists who wish to learn about the statistical basics of the method, as well as statisticians who wish to learn about the relevant climatology encountered. While both lists cannot be exhaustive, this is more the aim for the also given literature where the bootstrap approach to a statistical method has been used in climatology and related fields as, for example, ecology. A further section ("Technical issues") informs about details such as numerical accuracy and software implementations, it gives also internet references where the computer programs implementing the method can be obtained.

Some topics are not covered in this book. Extension to tri- and higher dimensional multivariate time series seems to be straightforward. Methods from dynamical systems theory, attempting to describe climate as a low-dimensional chaotic system, are likely too demanding in terms of data size (Section 1.6). Also other methods that require even spacing are not dealt with but briefly reviewed in Section 1.6.

However, before starting with adaptions of the bootstrap approach to statistical methods in climatology we need to review bootstrap methodology for time series in some detail, which is done in Chapter 3. Necessary statistical concepts such as confidence intervals or standard errors are also explained. One bootstrap variant ("parametric bootstrap") employed in this book assumes a statistical model of the climatological persistence (Chapter 2). These chapters complete Part I.

Sceptics among the readers may ask whether or not the bootstrap approach brings indeed more reliable results than the classical approach. Therefore you will find throughout the book comparisons between both approaches. These are based on Monte Carlo simulations, that means, artificial time series with pre-defined attributes, for which the true result is known a priori. In the same way, different bootstrap variants are also compared with each other. Finally, the (adverse) effects of interpolation are also explored by means of Monte Carlo simulations.

The final part (IV) of the book is an outlook on future directions in climate time series analysis with the bootstrap. Chapter 9 outlines climate archive modelling to take into account timescale uncertainties and includes "normal" extensions to novel estimation problems and higher dimensions. We also look on paradigm changes that may result from a strong increase in computing power in the future and influence the way how we model the climate and analyse climate time series.

1 Introduction

1.6 Background material

The **prologue** is a translation from Popper (1935: p. 78 therein). Other relevant books on quantification and philosophy of science are predominantly written by physicists: Einstein (1949), Heisenberg (1969), Lakatos and Musgrave (1970), von Weizsäcker (1985) and Sokal and Bricmont (1998).

As statistics texts, accessible to non-statisticians, describing the various roads to probability and estimation, may serve Priestlev (1981: Chapters 1-3 therein), Fine (1983), Davison (2003) and Wasserman (2004). The Bayesian road (Lindley 1965; Spall 1988; Bernardo and Smith 1994; Bernardo et al. 2003) seems not to be so well followed in geosciences, but this may change in future. Davis (1986) is a text book written by a geologist; Wilks (2006) and von Storch and Zwiers (1999) were written by climatologists. The latter three contain parts on time series analysis. As text books on time series analysis, accessible to nonstatisticians, the following can be used: Priestlev (1981), Diggle (1990), Brockwell and Davis (1996) and Shumway and Stoffer (2006); the latter work includes software examples in the R computing environment. A further book on time series analysis is by Anderson (1971). The only book devoted to time series analysis of unevenly spaced data seems to be Parzen (1984); an early review is by Marquardt and Acuff (1982); there is a thesis (Martin 1998) from the field of signal processing. We finally mention the Encyclopedia of statistical sciences (Kotz et al. 1982a,b, 1983a, b, 1985a, b, 1986, 1988a, b, 1989, 1997, 1998, 1999).

Climatology text books: The reports by Working Group I of the Intergovernmental Panel on Climate Change (IPCC–WG I) (Houghton et al. 2001; Solomon et al. 2007) are useful on weather (that is, meteorology) and short-term climate. Paleoclimate, covering longer-term processes in, say, the Holocene (last $\sim 10,000$ years) and before, is described by Crowley and North (1991), Bradley (1999) and Cronin (2010). We finally mention the Encyclopedia of Atmospheric Sciences (Holton et al. 2003), the Encyclopedia of Earth System Science (Nierenberg 1992), the Encyclopedia of Geology (Selley et al. 2005), the Glossary of Geology (Neuendorf et al. 2005), the Handbook of Hydrology (Maidment 1993) and the Encyclopedia of Ocean Sciences (Steele et al. 2001).

The form of **decomposition** in Eq. (1.1) of a process into trend, outliers, variability and noise is non-standard. Outliers are often considered as gross errors in the data that only have to be removed. However, in climatology, outliers may bear information on extreme events and can also be the object of analysis (Chapter 6). The notion of systematic behaviour of a trend leaves space for interpretation of what can be included. Certainly worth so are nonlinear trends to account for climatic

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changes (Chapter 4). Also incorporated are harmonic signals like the daily or annual cycle, which can be recorded in climate archives. Since the focus here in this book is on longer-term processes, we omit to write an own seasonal signal into Eq. (1.1); such an approach is common in econometrics (Box et al. 1994). Other, longer-term cyclic influences on climate are also astronomical in origin, such as variations in solar activity or Milankovitch variations in Earth orbital parameters. However, since their imprint in the climate system as regards amplitude, phase and frequency, is not precisely known (and also sometimes debated), these signals are investigated in this book by analysing the spectral properties of the noise process (Chapter 5).

Detailed accounts of **climate archives** give the following. Usage of marine sediment cores is a standard method (has been applied over decades), see Kennett (1982), Seibold and Berger (1993) and the series of reports on and results of scientific drilling into the ocean floor (Deep Sea Drilling Project 1969–1986; Ocean Drilling Program 1986–2004, 1988– 2007). Ice cores (Oeschger and Langway 1989; Hammer et al. 1997) and lake sediment cores (Negendank and Zolitschka 1993; Zolitschka 1999) are likewise regularly employed. Usefulness of speleothems (Baker et al. 1993; Gillieson 1996; Daoxian and Cheng 2002; Fairchild et al. 2007) is recognized since the 1990s. Dendroclimatology has a long tradition (Douglass 1919, 1928, 1936; Schweingruber 1988). Analysis of documentary climate data is described by Pfister (1999), Brázdil et al. (2005) and Glaser (2001). Construction and use of climate models is a growing field, see McGuffie and Henderson-Sellers (1997) or Randall et al. (2007). From this book's data analysis view, climate modelling is similar to probing and measuring a natural climate archive.

An upper limit to the **time range** over which climate can be studied is set by the age of Earth (~ 4.6 Ga). The course of the evolution of Earth, including its climate, division and subdivision into different geological epochs, is described by Stanley (1989). A geological timescale refers to a chronology of events (first or last appearance of species, reversals of Earth's magnetic field, climatic, etc.) which is updated as new data and new datings become available. Currently used are: Gradstein et al. (2004) covering the whole time range, Cande and Kent (1992, 1995) going back before the Cenozoic (last ~ 65 Ma) into the late Cretaceous, Berggren et al. (1995b) for the Cenozoic and Berggren et al. (1995a) for the last 6 Ma. (Note the various meanings of "timescale" in geosciences.)

Absolute dating methods almost entirely use one of the many clocks provided by natural radioactive elements. A comprehensive treatise is Geyh and Schleicher (1990), see also Walker (2005). K/Ar dating (Dalrymple and Lanphere 1969) utilizes the decay of 40 K. The potas-

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sium isotope has a half-life, $T_{1/2}$, of 1.266 Ga (Section 8.7), it decays into 40 Ar with a chance of ~ 11% and 40 Ca (~ 89%). One measures 40 K and also the amount of ⁴⁰Ar that accumulated in a sample since argon was removed by a process whose age is to be determined. Such a zeroing process can be a volcanic eruption, which produced the rock sample. The natural decay chains in uranium and thorium provide a wealth of clocks, running on a wide range of timescales (Ivanovich and Harmon 1992). U/Th dating utilizes the decays of 234 U to 230 Th ($T_{1/2} \approx 245$ ka) and ²³⁰Th to ²²⁶Ra ($T_{1/2} \approx 76$ ka). Since speleothems contain essentially no thorium at the time of formation, dating means measuring the amount of accumulated thorium since that time. ²¹⁰Pb dating (Appleby and Oldfield 1992) takes the decay chain of 210 Pb $(T_{1/2} \approx 22.3 a)$ to $^{206}\mathrm{Pb.}\,$ Radiocarbon dating (Taylor 1987) employs the decay of $^{14}\mathrm{C}$ to ¹⁴N ($T_{1/2} \approx 5730$ a). $T_{1/2}$ determines the limits for a reliable age determination. For ages below, say, $\sim 0.1 \cdot T_{1/2}$ and above $\sim 10 \cdot T_{1/2}$, the uncertainties introduced at the determination of the amounts of parent or daughter products become likely too large. Using modern mass spectrometers, this range can be somewhat widened. Besides measurement uncertainties and those owing to imperfectly known half-lifes, another error source is bias that occurs when assumptions, such as complete zeroing or absent sample contamination, are violated. In fact, eliminating measurement bias is often the major task in absolute dating. Using an archive as a dosimeter for dating (Table 1.1) means to measure the dose (effect) a sample has received over time exposed to a dose-rate (effect per time interval). One example is electron-spin-resonance dating, where the effect consists in the number of trapped electrons (for example in carbonate material in a sediment core) and the dose-rate is from natural radioactivity (Grün 1989); the other is cosmic-ray-exposure dating, where one of the effects used regards the number of ¹⁰Be atoms transported to an archive from the atmosphere, where cosmic rays had produced them (Gosse and Phillips 2001). Another absolute dating method is counting of yearly layers, either of tree-rings or growth layers in a stalagmite (Fig. 1.14). The assumption that layers present a constant time interval is crucial. Documentary data contain together with the variable usually also the date (which is susceptible to reporting errors).

Relative dating methods rely on an assumed relation between the measured series in the depth domain, $\{z(i), x(i)\}_{i=1}^{n_X}$, and another, dated time series, $\{t_Y(j), y(j)\}_{j=1}^{n_Y}$. If the relation between X and Y is simple (linear, no lag), $t_Y(j)$ can be projected onto $t_X(i)$ rather easily. If it is more complex, a mathematical model may have to be used. Climatologists denote that procedure as correlation or "tuning." As illustration

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we note that besides the GT4 timescale for the Vostok ice core (Fig. 1.3), two tuned timescales exist. One uses as x(i) Vostok δ^{18} O in air bubbles and as y(i) the precession of Earth's orbit (Shackleton 2000); the other uses as x(i) Vostok methane content in air and as y(i) mid-July insolation at 30°N (Ruddiman and Raymo 2003). One critical point with relative dating is how well the assumed relation holds. Bayesian approaches to timescale construction were developed by Agrinier et al. (1999) for a geomagnetic polarity record from the Cretaceous–Cenozoic and by Blaauw and Christen (2005) for a Holocene archive in form of a peat-bog core. Section 4.4 gives more details and references on the approaches.

Most before mentioned textbooks on climate and climate archives contain also information on **proxy variables** and how well those indicate climate. Other sources are Broecker and Peng (1982) and Henderson (2002). δ^{18} O in shells of marine living foraminifera (Fig. 1.2) was in the beginning seen as a "paleothermometer" (Emiliani 1955) until Shackleton (1967) showed that the major recorded climate variable is global ice volume, although he partly withdraw later from this position (Shackleton 2000). The main idea is that polar ice is isotopically light (low δ^{18} O) and that during an interglacial (warm) more of that is as water in the ocean, where for a build their calcareous, δ^{18} O-light shells. Stacks of ice volume records, such as that from the "Spectral Analysis, Mapping, and Prediction" (SPECMAP) project (Imbrie et al. 1984), going back nearly 800 ka, and that of Shackleton et al. (1995b), extending into the Miocene (before ~ 5.2 Ma), were produced and a nomenclature (Prell et al. 1986) of marine isotope stages (MISs) erected. A recently constructed Plio- to Pleistocene δ^{18} O stack is by Lisiecki and Raymo (2005). Atmospheric CO_2 is rather accurately reflected by CO_2 in air bubbles from Antarctic ice cores (Fig. 1.3), mainly because CO_2 mixes well in the atmosphere (Raynaud et al. 1993). The currently longest record comes from the European Project for Ice Coring in Antarctica (EPICA), Dome C site, the core covering the past ~ 800 ka (Section 8.6.1). For earlier times, other proxies for atmospheric CO_2 have to be used, such as the size and spatial density of stomata in fossil leaves (Kürschner et al. 1996), resulting in significantly larger proxy errors. δD variations in polar ice (Fig. 1.3) reflect variations in air temperature as this variable determines how enriched the precipitation becomes during its net transport from the mid-latitudes to the poles (Rayleigh destillation) (Dansgaard and Oeschger 1989). As regards the various proxy variables from the NGRIP ice core (Figs. 1.4 and 1.5), see the captions and references given therein. Radiocarbon (Fig. 1.6) is produced in the upper atmosphere via reactions with cosmogenic neutrons; the cosmic-ray flux is

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modulated by the Sun's activity through the solar wind. Another influence that can be seen using Δ^{14} C is variations in the exchange between the oceanic carbon storage and the atmosphere, see Beer et al. (1994) and Cini Castagnoli and Provenzale (1997). Pollen records and their proxy quality are explained by Moore et al. (1991) and Traverse (2007). The proxy quality of δ^{18} O in speleothems from the Arabian peninsula as indicator of monsoon rainfall is largely based on Rayleigh destillation processes (Fleitmann et al. 2004, 2007a).

Ergodicity. Detrended and normalized x(i) were used for analysing the distributional shape for the process $X_{\text{noise}}(T)$ (Fig. 1.11). That is, instead of an ensemble of different realizations at a particular time, one realization was taken at different times. A process for which this replacement gives same results is called ergodic. Since in climatological practice no repeated experiment can be carried out, except with climate models, ergodicity has to be added to the set of made assumptions in this book.

Density estimation. The histograms in Fig. 1.11 were constructed using a bin width equal to $3.49 s_{n-1} n^{-1/3}$ (Scott 1979), where s_{n-1} is the sample standard deviation. More elaborated approaches to density estimations use kernel functions (Silverman 1986; Simonoff 1996; Wasserman 2006). Applications of density estimation to climatology have been made occasional. They include analyses of the Pleistocene ice age (Matteucci 1990; Mudelsee and Stattegger 1997) and of the recent planetary-scale atmospheric circulation (Hansen and Sutera 1986). Standard references on statistical properties of distributions are Johnson et al. (1994, 1995) on continuous univariate and Kotz et al. (2000) on continuous multivariate distributions. Random variables that are composed of products or ratios of other random variables have since long successfully defied analytical derivation of their PDF. Only very simple forms, like $Z = X^2 + Y^2$ with Gaussian X and Y, which has a chisquared density (right-skewed), can be solved. See Haldane (1942) or Lomnicki (1967) for other cases.

Bioturbation in deep-sea sediments acts as a low-pass filter (Eq. 1.4) (Goreau 1980; Dalfes et al. 1984; Pestiaux and Berger 1984). However, since the accumulated sediment passes the bioturbation zone (the upper few tens of cm of sediment) unidirectionally, signal processing techniques, termed "deconvolution," have been successfully developed to use that information to improve the construction of the timescale (Schiffelbein 1984, 1985; Trauth 1998). An example demonstrating what effects have to anticipated when sampling natural climate archives such as sediment cores is given by Thomson et al. (1995), who found offsets of ~ 1.1 ka between ages of large (> 150 µm diameter) foraminifera and fine bulk

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carbonate at same depth in a core. The most likely explanation is a size-dependent bioturbation that preferentially transports fine material downwards because that is cheaper in terms of energy.

Inhomogeneities in time series owing to systematic changes in the observation system (i.e., the archive) may arise in manifold ways. It is evidently of importance to detect and correct for these effects. A simple case is a sudden change, such as when the time at which daily temperature is recorded, is shifted. This type can be detected using methods (Basseville and Nikiforov 1993) that search for an abrupt change in the mean, $X_{\text{trend}}(T)$. Inhomogeneities in the form of gradual changes in mean, or variability, may be analysed using regression techniques (Chapter 4). Quality assessment of climate data deals predominantly with types and sizes of inhomogeneities (Peterson et al. 1998a,b). Inhomogeneities in the form of periodic changes of the observation system can influence the estimated spectral properties (Chapter 5).

Physics' nonlinear dynamical systems theory has developed time series analysis techniques (Abarbanel et al. 1993; Kantz and Schreiber 1997; Diks 1999; Chan and Tong 2001; Tsonis and Elsner 2007; Donner and Barbosa 2008) that can be applied to study, for example, the question whether the climatic variability sampled by $\{t(i), x(i)\}_{i=1}^{n}$ is the product of low-dimensional chaos. A positive answer would have serious consequences for the construction of climate models because only a handful of independent climate variables had to be incorporated; and also the degree of climate predictability would be precisely known (Lyapunov exponents). Although it was meteorology that boosted development of dynamical systems theory by constructing a simplified atmosphere model (Lorenz 1963), we will not pursue related time series analysis methods for two reasons. First, for most applications in climatology the data sizes are not sufficient to allow reasonably accurate conclusions. For example, Nicolis and Nicolis (1984) analysed one late Pleistocene (last ~ 900 ka) δ^{18} O time series (cf. Fig. 1.2) and found a "climatic attractor" with dimensionality ~ 3.1 , meaning that four variables could explain the ice age. Grassberger (1986), and later Ruelle (1990), convincingly refuted that claim, which was based on a data size of a few hundred instead of several thousand necessary (Eckmann and Ruelle 1992). Later, Mudelsee and Stattegger (1994) analysed the longest Plio-/Pleistocene $\delta^{18} {\rm O}$ records then available. They found no low-dimensional attractor and could only conclude that at least five variables are acting. Since one assumption for such analyses is that the proxy quality of the measured variable (δ^{18} O, indicating ice volume) holds over all timescales sampled, the limits owing to the sampling process (Eq. 1.4) and the proxy quality (Table 1.2) effectively prohibit exploration of low-dimensional climatic

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chaos—not to mention the amount of measurements required. Lorenz (1991) considered that decoupled climatic subsystems with low dimensionality could be found. Second, nonlinear dynamical systems methods reconstruct the physical phase space by the method of delay-time coordinates (Packard et al. 1980). Instead of using multivariate time series $\{t(i), x(i), y(i), z(i), \ldots\}_{i=1}^{n}$ (forming the data matrix), this method takes $\{t(i), x(i), x(i+L), x(i+2L), \ldots\}_{i=1}^{n'}$, with n' < n and L (integer) appropriately selected. The delay-time method requires equidistance. For many climate time series encountered in practice, this would mean interpolation, which this book does not advocate (Section 1.4).

Even time spacing is also required for current implementations of two other analysis techniques. The first, Singular Spectrum Analysis or SSA (Broomhead and King 1986), also uses delay-time coordinates explained in the preceding paragraph to reconstruct the data matrix from one univariate time series. The eigenvectors associated with the largest eigenvalues yield the SSA decomposition of the time series into trend and other more variable portions. There exists a successful approach based on computer simulations to assess the significance of eigenvalues in the presence of persistence, which has been applied to observed equidistant temperature time series (Allen and Smith 1994). Again, because for many real-world paleoclimatic time series interpolation would have to be performed, we do not include SSA here. Note that similar to SSA is Principal Component Analysis (PCA), also termed Empirical Orthogonal Function (EOF) analysis, which does the same as SSA on multivariate time series. PCA is a standard method to search for patterns in high-dimensional meteorological time series such as pressure and temperature fields (Preisendorfer 1988; von Storch and Zwiers 1999). The second time series analysis method that requires even spacing and is often applied in climatology, is wavelet analysis, which composes a time series using "wave packets," localized in time and frequency. Percival and Walden (2000) is a textbook accessible to non-statisticians. Applications to climatology include Fligge et al. (1999), who analyse sunspot time series (Fig. 2.12), and Torrence and Compo (1998), who analyse time series of the El Niño-Southern Oscillation (ENSO) climatic mode. (El Niño is defined by sea-surface temperature anomalies in the eastern tropical Pacific, while the Southern Oscillation Index is a measure of the atmospheric circulation response in the Pacific–Indian Ocean region.) It might well be possible to develop adaptions of phase-space reconstruction and nonlinear dynamical systems analysis, SSA, PCA and wavelet analysis to explore unevenly spaced time series directly, circumventing adverse effects of interpolation-at the moment, such adaptions seem not to be available (but see Section 5.3 as regards wavelets).

Chapter 2

Persistence Models

Climatic noise often exhibits persistence (Section 1.3). Chapter 3 presents bootstrap methods as resampling techniques aimed at providing realistic confidence intervals or error bars for the various estimation problems treated in the subsequent chapters. The bootstrap works with artificially produced (by means of a random number generator) resamples of the noise process. Accurate bootstrap results need therefore the resamples to preserve the persistence of $X_{\text{noise}}(i)$. To achieve this requires a model of the noise process or a quantification of the size of the dependence. Model fits to the noise data inform about the "memory" of the climate fluctuations, the span of the persistence. The fitted models and their estimated parameters can then be directly used for the bootstrap resampling procedure.

It turns out that for climate time series with discrete times and uneven spacing, the class of persistence models with a unique correspondence to continuous-time models is rather limited. This "embedding" is necessary because it guarantees that our persistence description has a foundation on physics. The first-order autoregressive or AR(1) process has this desirable property.

2.1 First-order autoregressive model

The AR(1) process is a simple persistence model, where a realization of the noise process, $X_{\text{noise}}(i)$, depends on just the value at one time step earlier, $X_{\text{noise}}(i-1)$. We analyse even and uneven spacing separately.

2 Persistence Models

2.1.1 Even spacing

In Eq. (1.2) we let the time increase with constant spacing d(i) = d > 0 and write the discrete-time Gaussian AR(1) noise model,

$$X_{\text{noise}}(1) = \mathcal{E}_{N(0, 1)}(1),$$

$$X_{\text{noise}}(i) = a \cdot X_{\text{noise}}(i-1) + \mathcal{E}_{N(0, 1-a^2)}(i), \qquad i = 2, \dots, n.$$
(2.1)

Herein, -1 < a < 1 is a constant and $\mathcal{E}_{N(\mu, \sigma^2)}(\cdot)$ is a Gaussian random process with mean μ , variance σ^2 and no serial dependence, that means, $E\left[\mathcal{E}_{N(\mu, \sigma^2)}(i) \cdot \mathcal{E}_{N(\mu, \sigma^2)}(j)\right] = 0$ for $i \neq j$. It readily follows that $X_{noise}(i)$ has zero mean and unity variance, as assumed in our decomposition (Eq. 1.2). Figure 2.1 shows a realization of an AR(1) process.

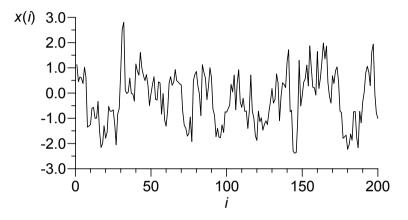


Figure 2.1. Realization of an AR(1) process (Eq. 2.1); n = 200 and a = 0.7.

The autocorrelation function,

$$\rho(h) = \frac{E\left[\left\{X_{\text{noise}}(i+h) - E\left[X_{\text{noise}}(i+h)\right]\right\} \cdot \left\{X_{\text{noise}}(i) - E\left[X_{\text{noise}}(i)\right]\right\}\right]}{\left\{VAR\left[X_{\text{noise}}(i+h)\right] \cdot VAR\left[X_{\text{noise}}(i)\right]\right\}^{1/2}}$$
$$= E\left[X_{\text{noise}}(i+h) \cdot X_{\text{noise}}(i)\right],$$
(2.2)

where h is the time lag, E is the expectation operator and VAR is the variance operator, is given by (Priestley 1981: Section 3.5 therein)

$$\rho(h) = a^{|h|}, \qquad h = 0, \pm 1, \pm 2, \dots$$
(2.3)

For a > 0, this behaviour may be referred to as "exponentially decreasing memory" (Fig. 2.2).

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2.1 First-order autoregressive model

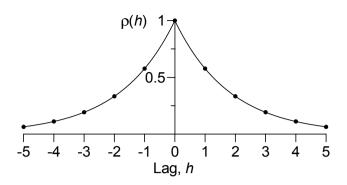


Figure 2.2. Autocorrelation function of the AR(1) process, a > 0. In the case of even spacing (Section 2.1.1) $\rho(h)$ is given by $a^{|h|} = \exp[-|h| \cdot d/\tau]$, in the case of uneven spacing (Section 2.1.2) by $\exp[-|T(i+h) - T(i)|/\tau]$. In both cases, the decrease is exponential with decay constant τ .

Note that the assumptions in Eq. (1.2), namely $E[X_{\text{noise}}(i)] = 0$ and $VAR[X_{\text{noise}}(i)] = 1$, required the formulation of the AR(1) model as in Eq. (2.1), which is non-standard. See Section 2.6 for the standard formulation.

Persistence estimation for the AR(1) model means estimation of the autocorrelation parameter, a. To illustrate autocorrelation estimation, assume that from the time series data, $\{x(i)\}_{i=1}^{n}$, the outliers have been removed and the trend and variability properties (Eq. 1.2) determined and used (as in Fig. 1.11) to extract $\{x_{\text{noise}}(i)\}_{i=1}^{n}$, realizations of the noise process. An estimator of the autocorrelation parameter, that means, a recipe how to calculate a from $\{x_{\text{noise}}(i)\}_{i=1}^{n}$, is given by

$$\widehat{a} = \sum_{i=2}^{n} x_{\text{noise}}(i) \cdot x_{\text{noise}}(i-1) \left/ \sum_{i=2}^{n} x_{\text{noise}}(i)^{2} \right.$$
(2.4)

(Chapter 3 introduces estimators and the "hat notation.") Note that estimator \hat{a} is biased, that means, if $\{X_{\text{noise}}(i)\}$ is an AR(1) process with parameter a, then $E(\hat{a}) \neq a$. Only approximation formulas exist for the bias in general autocorrelation estimation. Such formulas can be used for bias correction. Similarly, also the estimation variance, $VAR(\hat{a})$, is only approximately known. In general, bias and variance decrease with n. The background material (Section 2.6) gives various bias and variance formulas, informs about bias correction and lists other autocorrelation estimators.

Chapter 3

Bootstrap Confidence Intervals

In statistical analysis of climate time series, our aim (Chapter 1) is to estimate parameters of $X_{\text{trend}}(T)$, $X_{\text{out}}(T)$, S(T) and $X_{\text{noise}}(T)$. Denote in general such a parameter as θ . An estimator, $\hat{\theta}$, is a recipe how to calculate θ from a set of data. The data, discretely sampled time series $\{t(i), x(i)\}_{i=1}^{n}$, are influenced by measurement and proxy errors of x(i), outliers, dating errors of t(i) and climatic noise. Therefore, $\hat{\theta}$ cannot be expected to equal θ . The accuracy of $\hat{\theta}$, how close it comes to θ , is described by statistical terms such as standard error, bias, mean squared error and confidence interval (CI). These are introduced in Section 3.1.

With the exploration of new archives or innovations in proxy, measurement and dating techniques, new $\hat{\theta}$ values, denoted as estimates, become available and eventually join or replace previous estimates. A telling example from geochronology is where θ is the time before present when the Earth's magnetic field changed from reversed polarity during the Matuyama epoch to normal polarity during the Brunhes epoch, at the beginning of the late Pleistocene. Estimates published over the past decades include 690 ka (Cox 1969) and 730 ka (Mankinen and Dalrymple 1979), both based on K/Ar dating; and 790 ka (Johnson 1982) and 780 ka (Shackleton et al. 1990), both based on astronomical tuning. The currently accepted value is 779 ka with a standard error of 2 ka (Singer and Pringle 1996), written as 779 ± 2 ka, based on 40 Ar/ 39 Ar dating (a high-precision variant of K/Ar dating). An example with a much greater uncertainty regards the case where θ is the radiative forcing (change in net vertical irradiance at the tropopause) of changes in atmospheric concentrations of mineral dust, where even the sign of θ is uncertain (Penner et al. 2001; Forster et al. 2007). It is evident that the

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3 Bootstrap Confidence Intervals

growth of climatological knowledge depends critically on estimates of θ that are accompanied by error bars or other measures of their accuracy.

Bootstrap resampling (Sections 3.2 and 3.3) is an approach to construct error bars and CIs. The idea is to draw random resamples from the data and calculate error bars and CIs from repeated estimations on the resamples. For climate time series, the bootstrap is potentially superior to the classical approach, which relies partly on unrealistic assumptions regarding distributional shape, persistence and spacing (Chapter 1). However, the bootstrap, developed originally for data without serial dependence, has to be adapted before applying it to time series. Two classes of adaptions exist for taking persistence into account. First, nonparametric bootstrap methods resample sequences, or blocks, of the data. They preserve the dependence structure over the length of a block. Second, the parametric bootstrap adopts a dependence model. As such, the AR(1) model (Chapter 2) is our favorite.

It turns out that both bootstrap resampling types have the potential to yield acceptably accurate CIs for estimated climate parameters. A problem for the block bootstrap arises from uneven time spacing. Another difficult point is to find optimal block lengths. This could make the parametric bootstrap superior within the context of this book, especially for small data sizes (less than, say, 50). The block bootstrap, however, is important when the deviations from AR(1) persistence seem to be strong. Various CI types are investigated. We prefer a version (so-called BCa interval) that automatically corrects for estimation bias and scale effects. Computing-intensive calibration techniques can further increase the accuracy.

3.1 Error bars and confidence intervals

Let θ be the parameter of interest of the climatic process $\{X(T)\}$ and $\hat{\theta}$ be the estimator. Extension to a set of parameters is straightforward. Any meaningful construction lets the estimator be a function of the process, $\hat{\theta} = g(\{X(T)\})$. That means, $\hat{\theta}$ is a random variable with statistical properties. The standard deviation of $\hat{\theta}$, denoted as standard error, is

$$\operatorname{se}_{\widehat{\theta}} = \left[VAR\left(\widehat{\theta}\right) \right]^{1/2}.$$
 (3.1)

The bias of $\hat{\theta}$ is

$$\operatorname{bias}_{\widehat{\theta}} = E\left(\widehat{\theta}\right) - \theta.$$
 (3.2)

 $\operatorname{bias}_{\widehat{\theta}} > 0$ ($\operatorname{bias}_{\widehat{\theta}} < 0$) means a systematic overestimation (underestimation). $\operatorname{se}_{\widehat{\theta}}$ and $\operatorname{bias}_{\widehat{\theta}}$ are illustrated in Fig. 3.1. Desirable estimators have small $\operatorname{se}_{\widehat{\theta}}$ and small $\operatorname{bias}_{\widehat{\theta}}$. In many estimations, a trade-off problem

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3.1 Error bars and confidence intervals

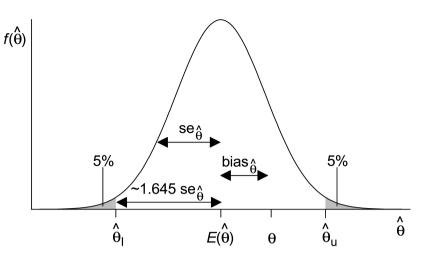


Figure 3.1. Standard error $(se_{\hat{\theta}})$, bias $(bias_{\hat{\theta}})$ and equi-tailed confidence interval $(CI_{\hat{\theta},1-2\alpha} = [\hat{\theta}_{l};\hat{\theta}_{u}])$ for a Gaussian distributed estimator, $\hat{\theta}$. The true parameter value is θ ; the confidence level is $1 - 2\alpha = 90\%$.

between $\mathrm{se}_{\widehat{\theta}}$ and $\mathrm{bias}_{\widehat{\theta}}$ occurs. A convenient measure is the root mean squared error,

$$\operatorname{RMSE}_{\widehat{\theta}} = \left\{ E\left[\left(\widehat{\theta} - \theta \right)^2 \right] \right\}^{1/2}$$

= $\left(\operatorname{se}_{\widehat{\theta}}^2 + \operatorname{bias}_{\widehat{\theta}}^2 \right)^{1/2}.$ (3.3)

The coefficient of variation is

$$CV_{\widehat{\theta}} = se_{\widehat{\theta}} / \left| E\left(\widehat{\theta}\right) \right|.$$
(3.4)

While $\hat{\theta}$ is a best guess of θ or a point estimate, a CI is an interval estimate that informs how good a guess is (Fig. 3.1). The CI for θ is

$$\operatorname{CI}_{\widehat{\theta},1-2\alpha} = \left[\widehat{\theta}_{l};\widehat{\theta}_{u}\right],$$
(3.5)

where $0 \leq 1 - 2\alpha \leq 1$ is a prescribed value, denoted as confidence level. The practical examples in his book consider 90% ($\alpha = 0.05$) or 95% ($\alpha = 0.025$) CIs, which are reasonable choices for climatological problems. $\hat{\theta}_{l}$ is the lower, $\hat{\theta}_{u}$ the upper endpoint of the CI. $\hat{\theta}_{l}$ and $\hat{\theta}_{u}$ are random variables and have statistical properties such as standard error

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3 Bootstrap Confidence Intervals

or bias. The properties of interest for CIs are the coverages,

$$\gamma_{\rm l} = \operatorname{prob}\left(\theta \le \widehat{\theta}_{\rm l}\right),$$
(3.6)

$$\gamma_{\rm u} = \operatorname{prob}\left(\theta \ge \widehat{\theta}_{\rm u}\right)$$
(3.7)

and

$$\gamma = \operatorname{prob}\left(\widehat{\theta}_{l} < \theta < \widehat{\theta}_{u}\right) = 1 - \gamma_{l} - \gamma_{u}.$$
(3.8)

Exact CIs have coverages, γ , equal to the nominal value $1 - 2\alpha$. Construction of exact CIs requires knowledge of the distribution of $\hat{\theta}$, which can be achieved only for simple problems. In more complex situations, only approximate CIs can be constructed (Section 3.1.3). As regards the division of the nominal coverage between the CI endpoints, this book adopts a practical approach and considers only equi-tailed CIs, where nominally $\gamma_{\rm l} = \gamma_{\rm u} = \alpha$. As a second CI property besides coverage, we consider interval length, $\hat{\theta}_{\rm u} - \hat{\theta}_{\rm l}$, which is ideally small.

Preceding paragraphs considered estimators on the process level. In practice, on the sample level, we plug in the data $\{t(i), x(i)\}_{i=1}^{n}$ for $\{T(i), X(i)\}_{i=1}^{n}$. Following the usual convention, we denote also the estimator on the sample level as $\hat{\theta}$. An example is the autocorrelation estimator (Eq. 2.4).

3.1.1 Theoretical example: mean estimation of Gaussian white noise

Let the process $\{X(i)\}_{i=1}^n$ be given by

$$X(i) = \mathcal{E}_{\mathcal{N}(\mu, \sigma^2)}(i), \qquad i = 1, \dots, n,$$
(3.9)

which is called a Gaussian purely random process or Gaussian white noise. There is no serial dependence, and the times T(i) are not of interest. Consider as estimator $\hat{\theta}$ of the mean, μ , the sample mean, written on process level as

$$\hat{\mu} = \bar{X} = \sum_{i=1}^{n} X(i)/n.$$
 (3.10)

Let also σ be unknown and estimated by the sample standard deviation, $\hat{\sigma} = S_{n-1}$, given in the next example (Eq. 3.19). The properties of \bar{X} readily follow as

$$\operatorname{se}_{\bar{X}} = \sigma \cdot n^{-1/2}, \tag{3.11}$$

$$\operatorname{bias}_{\bar{X}} = 0, \tag{3.12}$$

$$RMSE_{\bar{X}} = se_{\bar{X}} \tag{3.13}$$

3.1 Error bars and confidence intervals

and

$$\operatorname{CV}_{\bar{X}} = \sigma \cdot n^{-1/2} \cdot \mu^{-1}. \tag{3.14}$$

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An exact CI of level $1 - 2\alpha$ can be constructed by means of the Student's t distribution of \bar{X} (von Storch and Zwiers 1999):

$$\operatorname{CI}_{\bar{X},1-2\alpha} = \left[\bar{X} + t_{n-1}(\alpha) \cdot S_{n-1} \cdot n^{-1/2}; \bar{X} + t_{n-1}(1-\alpha) \cdot S_{n-1} \cdot n^{-1/2}\right]$$
(3.15)

 $t_{\nu}(\beta)$ is the percentage point at β of the *t* distribution function with ν degrees of freedom (Section 3.9).

On the sample level, we write the estimated sample mean,

$$\hat{\mu} = \bar{x} = \sum_{i=1}^{n} x(i)/n,$$
(3.16)

the estimated standard error,

$$\widehat{\operatorname{se}}_{\bar{x}} = \left\{ \sum_{i=1}^{n} \left[x(i) - \bar{x} \right]^2 / n^2 \right\}^{1/2}, \qquad (3.17)$$

and the confidence interval,

$$\operatorname{CI}_{\bar{x},1-2\alpha} = \left[\bar{x} + t_{n-1}(\alpha) \cdot s_{n-1} \cdot n^{-1/2}; \bar{x} + t_{n-1}(1-\alpha) \cdot s_{n-1} \cdot n^{-1/2}\right],$$
(3.18)

where s_{n-1} is given by Eq. (3.25).

The performance of the CI in Eq. (3.18) for Gaussian white noise is analysed by means of a Monte Carlo simulation experiment. The CI performs excellent in coverage (Table 3.1), as expected from its exactness. The second CI property, length, decreases with data size. It can be further compared with CI lengths for other location measures.

3.1.2 Theoretical example: standard deviation estimation of Gaussian white noise

Consider the Gaussian white-noise process (Eq. 3.9) with unknown mean, and as estimator of σ the sample standard deviation, written on process level as

$$\widehat{\sigma} = S_{n-1} = \left\{ \sum_{i=1}^{n} \left[X(i) - \bar{X} \right]^2 / (n-1) \right\}^{1/2}.$$
(3.19)

Part II

Univariate Time Series

Chapter 4

Regression I

Regression is a method to estimate the trend in the climate equation (Eq. 1.1). Assume that outlier data do not exist or have already been removed by the assistance of an extreme value analysis (Chapter 6). Then the climate equation is a regression equation,

$$X(T) = X_{\text{trend}}(T) + S(T) \cdot X_{\text{noise}}(T).$$
(4.1)

One choice is to write $X_{\text{trend}}(T)$ as a function with parameters to be estimated. A simple example is the linear function (Section 4.1), which has two parameters, intercept and slope. A second example is the nonlinear regression model (Section 4.2). The other choice is to estimate $X_{\text{trend}}(T)$ nonparametrically, without reference to a specific model. Nonparametric regression (Section 4.3) is also called smoothing.

Trend is a property of genuine interest in climatology, it describes the mean state. This chapter deals also with quantifying S(T), the variability around the trend, as second property of climate. Regression methods can be used to measure climate changes: their size and timing. For that aim, the ramp regression (Section 4.2.1) constitutes a useful parametric model of climate changes.

We compare the bootstrap with the classical approach to determine error bars and CIs for estimated regression parameters. The difficulties imposed by the data are non-Gaussian distributions, persistence and uneven spacing. We meet another difficulty, uncertain timescales. This leads to adaptions of the bootstrap (Section 4.1.7), where the resampling procedure is extended to include also the time values, t(i).

The present chapter studies regression as a tool for quantifying the time-dependence of $X_{\text{trend}}(T)$, the relation between trend and time in univariate time series. A later chapter (Regression II) uses regression to

4 Regression I

analyse the relation in bivariate time series, between one time-dependent climate variable, X(T), and another, Y(T).

4.1 Linear regression

The linear regression uses a straight-line model,

$$X_{\text{trend}}(T) = \beta_0 + \beta_1 T. \tag{4.2}$$

The climate equation without outlier component is then written in discrete time as a linear regression equation,

$$X(i) = \beta_0 + \beta_1 T(i) + S(i) \cdot X_{\text{noise}}(i).$$

$$(4.3)$$

T is called the predictor or regressor variable, X the response variable, β_0 and β_1 the regression parameters.

4.1.1 Weighted least-squares and ordinary least-squares estimation

In a simple, theoretical setting, where the variability S(i) is known and $X_{\text{noise}}(i)$ has no serial dependence, the linear regression model can be fitted to data $\{t(i), x(i)\}_{i=1}^{n}$ by minimizing the weighted sum of squares,

$$SSQW(\beta_0, \beta_1) = \sum_{i=1}^{n} \left[x(i) - \beta_0 - \beta_1 t(i) \right]^2 / S(i)^2 , \qquad (4.4)$$

yielding the weighted least-squares (WLS) estimators

$$\widehat{\beta}_{0} = \left[\sum_{i=1}^{n} x(i)/S(i)^{2} - \widehat{\beta}_{1} \sum_{i=1}^{n} t(i)/S(i)^{2}\right] / W,$$
(4.5)

$$\widehat{\beta}_{1} = \left\{ \left[\sum_{i=1}^{n} t(i) / S(i)^{2} \right] \left[\sum_{i=1}^{n} x(i) / S(i)^{2} \right] / W - \sum_{i=1}^{n} t(i) x(i) / S(i)^{2} \right\} \times \left\{ \left[\sum_{i=1}^{n} t(i) / S(i)^{2} \right]^{2} / W - \sum_{i=1}^{n} t(i)^{2} / S(i)^{2} \right\}^{-1}, \quad (4.6)$$

where

$$W = \sum_{i=1}^{n} 1/S(i)^2.$$
(4.7)

4.1 Linear regression

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In a practical setting, S(i) is often not known and has to be replaced by $\widehat{S}(i)$. If prior knowledge indicates that S(i) is constant, then one may take as estimator the square root of the residual mean square MS_E (Montgomery and Peck 1992),

$$\widehat{S}(i) = \widehat{S} = \left\{ \sum_{i=1}^{n} \left[x(i) - \widehat{\beta}_0 - \widehat{\beta}_1 t(i) \right]^2 / (n-2) \right\}^{1/2} = M S_E^{1/2}.$$
 (4.8)

If S(i) is unknown and possibly time-dependent, the following iterative estimation algorithm can be applied (Algorithm 4.1). As long as S(i) is required only for weighting, this produces the correct estimators also if only the relative changes of S(i), instead of the absolute values, are estimated. Analogously, if S(i) is required only for weighting and known to be constant, then Eqs. (4.5) and (4.6) can be used with S(i) = 1, i = 1, ..., n and W = n. This estimation without weighting is called ordinary least squares (OLS). For the construction of classical CIs (Section 4.1.4), however, an estimate of S(i) has to be available.

Step 1	Make an initial guess, $\widehat{S}^{(0)}(i)$, of the variability.
Step 2	Estimate the regression parameters, $\widehat{\beta}_{0}^{(0)}$ and $\widehat{\beta}_{1}^{(0)}$, with the guessed variability used instead of $S(i)$ in Eqs. (4.5), (4.6) and (4.7).
Step 3	Calculate $e(i) = x(i) - \hat{\beta}_0 - \hat{\beta}_1 t(i), i = 1,, n$. The $e(i)$ are called the unweighted regression residuals.
Step 4	Obtain a new variability estimate, $\widehat{S}^{(1)}(i)$ from the residuals. This can be done either nonparametrically by smoothing (e.g., running standard deviation of $e(i)$) or fitting a parametric model of $S(i)$ to $e(i)$.
Step 5	Go to Step 2 with the new, improved variability estimate until regression estimates converge.

Algorithm 4.1. Linear weighted least-squares regression, unknown variability.

4.1.1.1 Example: Arctic river runoff

The climate model run with natural forcing only (Fig. 4.1a) does not exhibit a slope significantly different from zero. (See Section 4.1.4 for the determination of regression standard errors.) The run with combined anthropogenic and natural forcing (Fig. 4.1b) displays significant upwards trends in runoff. Wu et al. (2005) conjecture that there might be a change-point at around 1965, when the slope changed.



4 Regression I

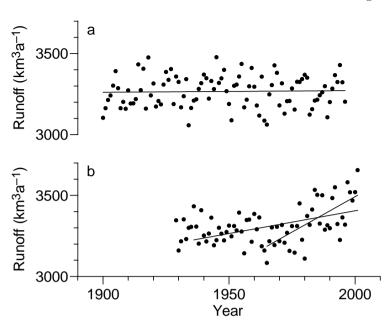


Figure 4.1. Linear regression models fitted to modelled Arctic river runoff (Fig. 1.9). **a** Natural forcing only; **b** combined anthropogenic and natural forcing. Following Wu et al. (2005), the fits (*solid lines*) were obtained by OLS regression using the data from (**a**) the whole interval 1900–1996 and (**b**) from two intervals, 1936–2001 and 1965–2001. The estimated regression parameters (Eqs. 4.5 and 4.6) and their standard errors (Eqs. 4.24 and 4.25) are as follows. **a** $\hat{\beta}_0 = 3068 \pm 694 \text{ km}^3 \text{a}^{-1}$, $\hat{\beta}_1 = 0.102 \pm 0.356 \text{ km}^3 \text{a}^{-2}$; **b** 1936–2001, $\hat{\beta}_0 = -2210 \pm 1375 \text{ km}^3 \text{a}^{-1}$, $\hat{\beta}_1 = 2.807 \pm 0.698 \text{ km}^3 \text{a}^{-2}$; **b** 1965–2001, $\hat{\beta}_0 = -13,977 \pm 3226 \text{ km}^3 \text{a}^{-1}$, $\hat{\beta}_1 = 8.734 \pm 1.627 \text{ km}^3 \text{a}^{-2}$.

4.1.2 Generalized least-squares estimation

In a practical climatological setting, $X_{\text{noise}}(i)$ often exhibits persistence. This means more structure or information content than a purely random process has. This knowledge can be used to apply the generalized least-squares (GLS) estimation, where the following sum of squares is minimized:

$$SSQG(\boldsymbol{\beta}) = (\mathbf{x} - \mathbf{T}\boldsymbol{\beta})' \mathbf{V}^{-1} (\mathbf{x} - \mathbf{T}\boldsymbol{\beta}).$$
(4.9)

Herein,

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \text{ (parameter vector)}, \tag{4.10}$$

4.1 Linear regression

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$$\mathbf{x} = \begin{bmatrix} x(1) \\ \vdots \\ x(n) \end{bmatrix}$$
(data vector), (4.11)

$$\mathbf{T} = \begin{bmatrix} 1 & t(1) \\ \vdots & \vdots \\ 1 & t(n) \end{bmatrix}$$
(time matrix) (4.12)

and ${\bf V}$ is an $n~\times~n$ matrix, the covariance matrix. The solution is the GLS estimator,

$$\widehat{\boldsymbol{\beta}} = \left(\mathbf{T}'\mathbf{V}^{-1}\mathbf{T}\right)^{-1}\mathbf{T}'\mathbf{V}^{-1}\mathbf{x}.$$
(4.13)

GLS has the advantage of providing smaller standard errors of regression estimators than WLS in the presence of persistence. Analogously, in the case of time-dependent S(i), the WLS estimation is preferable (Sen and Srivastava 1990) to OLS estimation. The covariance matrix has the elements

$$V(i_1, i_2) = S(i_1) \cdot S(i_2) \cdot E[X_{\text{noise}}(i_1) \cdot X_{\text{noise}}(i_2)], \qquad (4.14)$$

 $i_1, i_2 = 1, \ldots, n$. Climatological practice normally requires to estimate besides the variability also the persistence (Chapter 2) to obtain the **V** matrix. In the case of the AR(1) persistence model for uneven spacing (Eq. 2.9), the only unknown besides S(i) required for calculating **V** is the persistence time, τ . The estimated **V** matrix has then the elements

$$\widehat{V}(i_1, i_2) = \widehat{S}(i_1) \cdot \widehat{S}(i_2) \cdot \exp\left[-|t(i_1) - t(i_2)|/\widehat{\tau}'\right], \quad (4.15)$$

 $i_1, i_2 = 1, \ldots, n$, where $\hat{\tau}'$ is the estimated, bias-corrected persistence time (Section 2.6). For even spacing, replace the exponential expression by $(\hat{a}')^{|i_1-i_2|}$. (In the case of persistence models more complex than AR(1), **V** is calculable and, hence, GLS applicable only for evenly spaced time series.) The autocorrelation or persistence time estimation formulas (Eqs. 2.4 and 2.11) are applied to the weighted WLS regression residuals,

$$r(i) = \left[x(i) - \widehat{\beta}_0 - \widehat{\beta}_1 t(i) \right] / \widehat{S}(i), \qquad (4.16)$$

 $i = 1, \ldots, n$. Detrending by a linear regression is not the same as mean subtraction, and the bias of those autocorrelation and persistence time estimators need not follow the approximations given for mean subtraction (Section 2.6), but are unknown. However, the deviations are likely negligible compared with the other uncertainties. Also in the case of unknown persistence, an iterative procedure similar to that for WLS can

4 Regression I

be applied, which is called estimated generalized least squares (EGLS) (Sen and Srivastava 1990: Section 7.3 therein). Section 4.1.4.1 gives an EGLS procedure for the case of AR(1) persistence.

4.1.3 Other estimation types

Least squares (OLS, WLS, GLS) is one type of fit criterion. Another is maximum likelihood (Section 2.6, p. 58). Further criteria result from further preferences in the regression procedure. A notable choice is robustness against the influence of outlier data, $X_{out}(i)$. This can be achieved by minimizing instead of the sum of squares (Eq. 4.4), the median of squares,

$$\widehat{m}\left\{\left[x(i) - \beta_0 - \beta_1 t(i)\right]^2 / S(i)^2\right\}_{i=1}^n.$$
(4.17)

Preferably (background material) is to minimize the trimmed sum of squares,

$$SSQT(\beta_0, \beta_1) = \sum_{i=j+1}^{n-j} \left[x'(i) - \beta_0 - \beta_1 t'(i) \right] / S'(i)^2 , \qquad (4.18)$$

where $j = INT(\delta n)$, $INT(\cdot)$ is the integer function, $0 < \delta < 0.5$, x'(i) is size-sorted x(i), and t'(i) and S'(i) are the "slaves," correspondingly rearranged. Trimming excludes the 2j most extreme terms from contributing to the estimation. Also by the minimization of the sum of absolute deviations,

$$SSQA(\beta_0, \beta_1) = \sum_{i=1}^{n} |x(i) - \beta_0 - \beta_1 t(i)| / S(i) , \qquad (4.19)$$

outlier values (if not already excluded by means of a prior analysis) can be given less influence on regression estimates than in least-squares minimization. Such criteria could also be preferable (in terms of, say, standard errors of estimates) to least squares when instead of $X_{out}(i)$ we considered heavy-tailed or skewed $X_{noise}(i)$ distributions.

The various criteria introduced so far and the related minimization techniques represent the computational aspect of the regression estimation problem. The second and perhaps more relevant aspect is suitability of the linear regression model. In climatology this means whether a linear increase or decrease is not too simple for describing $X_{\text{trend}}(T)$. Model suitability can be evaluated graphically via various types of plots of the regression residuals (Eq. 4.16). These realizations of the noise process should nominally not exhibit more structure than the assumed persistence model.

Chapter 5

Spectral Analysis

Spectral analysis investigates the noise component in the climate equation (Eq. 1.2). A Fourier transformation into the frequency domain makes it possible to separate short-term from long-term variations and to distinguish between cyclical forcing mechanisms of the climate system and broad-band resonances. Spectral analysis allows to learn about the climate physics.

The task is to estimate the spectral density function, and to test for harmonic (cyclical) signals. This poses more difficulties than, for example, linear regression because now we estimate a function and not just two parameters. Spectral smoothing becomes therefore necessary, and this brings a trade-off between estimation variance and frequency resolution.

The multitaper smoothing method achieves the optimal trade-off for evenly spaced time series. The method of choice for unevenly spaced records is Lomb–Scargle, which estimates in the time domain and avoids distortions caused by interpolation.

Bootstrap resampling enhances multitaper and Lomb–Scargle methods by providing a bias correction and CIs. It supplies also a detection test for a spectral peak against realistic noise alternatives in form of an AR(1) process ("red noise"). Section 5.2.8 introduces bootstrap adaptions to take into account the effects of timescale uncertainties on detectability and frequency resolution.

5.1 Spectrum

Let us assume in this chapter that the climate process in continuous time, X(T), has no trend and no outlier components and a constant

5 Spectral Analysis

variability, S,

$$X(T) = X_{\text{trend}}(T) + X_{\text{out}}(T) + S(T) \cdot X_{\text{noise}}(T)$$

= $S \cdot X_{\text{noise}}(T).$ (5.1)

Such a process could be derived from a "real" climate process, that is, with trend and so forth, by subtracting the trend and outlier components and normalizing (standard deviation). Techniques for quantifying trend and variability and detecting outliers are presented in Chapter 4.

It is then straightforward (Priestley 1981) to define a truncated process,

$$X_{T'}(T) = \begin{cases} X(T) & \text{for } -T' \le T \le T', \\ 0 & \text{elsewhere,} \end{cases}$$
(5.2)

and express it as a Fourier integral,

$$X_{T'}(T) = (2\pi)^{1/2} \int_{-\infty}^{\infty} G_{T'}(f) e^{2\pi i f T} df, \qquad (5.3)$$

where

$$G_{T'}(f) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} X_{T'}(T) e^{-2\pi i f T} dT$$
$$= (2\pi)^{-1/2} \int_{-T'}^{T'} X(T) e^{-2\pi i f T} dT.$$
(5.4)

This introduces the frequency, f. (The symbol *i* in the exponent denotes $\sqrt{-1}$.) This is a useful quantity for describing phenomena that exhibit a periodic behaviour in time. The period (time units) is given by $T_{\text{period}} = 1/f$. If one associates X(T) with movement and kinetic energy, then $2\pi |G_{T'}(f)^2| df$ can be seen as the energy contribution of components with frequencies within the (arbitrarily small) interval [f; f + df]. Regarding the truncation, because with $T' \to \infty$ also the energy goes to infinity, one defines the power, $\pi |G_{T'}(f)^2|/T'$. Because the previous formulas in this section apply to a time series rather than a stochastic process, one uses the expectation operator to define

$$h(f) = \lim_{T' \to \infty} \left\{ E\left[2\pi \left| G_{T'}(f)^2 \right| / T' \right] \right\}.$$
 (5.5)

5.1 Spectrum

The function h(f) is called one-sided non-normalized power spectral density function of the process X(T), often denoted just as (non-normalized) spectrum. It is the average (over all realizations) of the contribution to the total power from components in X(T) with frequencies within the interval [f; f + df]. h(f) is defined for $f \ge 0$ and integrates to S^2 . A closely related function is

$$g(f) = h(f) / S^2,$$
 (5.6)

the one-sided normalized power spectral density function, which integrates to unity. A two-sided version of the spectrum, symmetric about f = 0, is also used (Bendat and Piersol 1986).

The functions h(f) and g(f) are the Fourier transforms of the autocovariance and autocorrelation functions, $R(\tau)$ and $\rho(\tau)$, respectively, provided they exist (Priestley 1981: Section 4.8 therein):

$$h(f) = \pi^{-1} \int_{-\infty}^{\infty} R(\tau) e^{-2\pi i f \tau} d\tau, \qquad (5.7)$$

$$g(f) = \pi^{-1} \int_{-\infty}^{\infty} \rho(\tau) e^{-2\pi i f \tau} d\tau.$$
(5.8)

Herein,

$$R(\tau) = E\left[X(T) \cdot X(T+\tau)\right],\tag{5.9}$$

$$\rho(\tau) = R(\tau) / R(0) \tag{5.10}$$

and the symbol τ is used to denote a lag in continuous time. The caveat refers to the fact that not all processes X(T) have a spectral representation; however, the existence of the Fourier transform of the autocovariance function $R(\tau)$ of X(T) is a sufficient condition.

Turning to the discrete-time version of the climate process, X(i), we assume also here absent trend, absent outliers and constant variability and find

$$X(i) = S \cdot X_{\text{noise}}(i). \tag{5.11}$$

The spectral theory is in this case similar to the continuous-time case (Priestley 1981: Section 4.8.3 therein), except that the frequency range is now restricted in both directions and the discrete Fourier transform is invoked to calculate the power spectral density functions. For example, with even time spacing, d(i) = d > 0,

$$g(f) = (d/\pi) \sum_{l=-\infty}^{\infty} \rho(l) e^{-2\pi i f l} dl, \qquad 0 \le f \le 1/(2d).$$
(5.12)

5 Spectral Analysis

Herein, l denotes a lag in discrete time. The frequency $f_{Ny} = (2d)^{-1}$ is denoted as Nyquist frequency; it sets the upper frequency bound.

5.1.1 Example: AR(1) process, discrete time

Consider the discrete-time AR(1) process (Section 2.1.1) with an autocorrelation parameter a on an evenly spaced timescale, d(i) = d > 0, with $n = \infty$ points. Then (Priestley 1981: Section 4.10 therein),

$$g(f) = 2d(1-a^2) \left/ \left[1 - 2a\cos(2\pi f d) + a^2 \right], \qquad 0 \le f \le 1/(2d).$$
(5.13)

Plots of the AR(1) spectrum (Fig. 5.1) show higher power at lower frequencies for a > 0; such a spectrum is, hence, called "red."

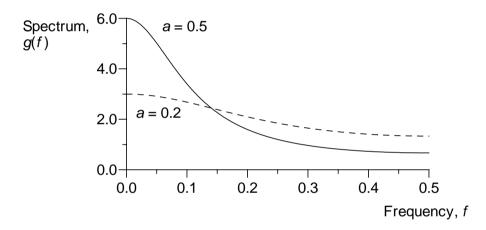


Figure 5.1. Spectrum of the AR(1) process (Eq. 5.13). Two parameter settings are shown; d = 1 and $f_{Ny} = 0.5$.

5.1.2 Example: AR(2) process, discrete time

Consider the discrete-time AR(2) process (Section 2.2) with parameters a_1 and a_2 on an evenly spaced timescale with d > 0 and $n = \infty$. Then (Priestley 1981: Section 4.10 therein),

$$g(f) = 2d(1+a_2)(1-a_2)^{-1} \left[(1-a_2)^2 - a_1^2 \right] \left[(1+a_2)^2 (5.14) + a_1^2 - 2a_1(1-a_2)\cos(2\pi f d) - 4a_2\cos(2\pi f d)^2 \right]^{-1},$$

with $0 \le f \le 1/(2d)$. Plots of the AR(2) spectrum (Fig. 5.2) reveal that besides redness such spectra may exhibit quasi-cyclical behaviour (Eq. 2.15).

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5.1 Spectrum

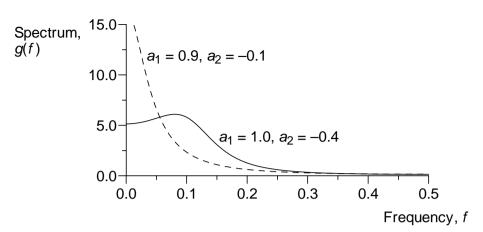


Figure 5.2. Spectrum of the AR(2) process (Eq. 5.14). Two parameter settings are shown; d = 1 and $f_{Ny} = 0.5$.

5.1.3 Physical meaning

The importance of the power spectral density functions h(f) and g(f) lies in the possibility of decomposing a process into contributions from different frequency intervals. That allows to separate short-term from long-term variations and also to distinguish between cyclical forcing mechanisms of the climate system and broad-band resonances. This means that spectral analysis permits to learn about the physics of the sampled climate system. As always when having instead of a perfect knowledge only a handful of data contaminated with measurement and, perhaps, proxy errors, the task is to *estimate*, namely the spectrum. The following sections explain methods to infer h(f) or g(f) from $\{t(i), x(i)\}_{i=1}^{n}$.

We expect the climate spectrum either as continuous (Fig. 5.3b), reflecting a random process, or as a mixture of continuous and line components (Fig. 5.3c), the latter representing a deterministic, periodic influence. Note that estimating a spectrum is estimating a function from a finite data set. This means we can expect more difficulties and a higher susceptibility to the validness of made assumptions than for easier tasks, where only few parameters have to estimated, such as in linear regression.

A word on the notation: The literature has developed a rich variety of different notations (factors 2π , frequency versus angular velocity, etc.),

Chapter 6

Extreme Value Time Series

Extreme value time series refer to the outlier component in the climate equation (Eq. 1.2). Quantifying the tail probability of the PDF of a climate variable—the risk of climate extremes—is of high socioeconomical relevance. In the context of climate change, it is important to move from stationary to nonstationary (time-dependent) models: with climate changes also risk changes may be associated.

Traditionally, extreme value data are evaluated in two forms: first, block extremes such as annual maxima, and second, exceedances of a high threshold. A stationary model of great flexibility for the first and the second form is the Generalized Extreme Value distribution and the generalized Pareto distribution, respectively. Classical estimation techniques based on maximum likelihood exist for both distributions.

Nonstationary models can be constructed parametrically, by writing the extreme value models with time-dependent parameters. Maximum likelihood estimation may impose numerical difficulties here. The inhomogeneous Poisson process constitutes an interesting nonparametric model of the time-dependence of the occurrence of an extreme. Here, bootstrap confidence bands can be constructed and hypothesis tests performed to assess the significance of trends in climate risk. A recent development is a hybrid, which estimates the time-dependence nonparametrically and, conditional on the occurrence of an extreme, models the extreme value parametrically.

6.1 Data types

We distinguish among several types of extreme value data. One guide for doing so is the accuracy of $X_{out}(i)$, the outlier or extreme component in the climate equation (Eq. 1.2). Even data with a very low accuracy

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6 Extreme Value Time Series

can be analysed, for example, cases where only the time an extreme occurred is known. A related guide comes from considering how the extreme data were obtained. An example is outlier detection by imposing a threshold (Section 4.3.3).

6.1.1 Event times

In the low-accuracy case it is just known about an event that it did occur, that means, $X_{\text{out}}(i) \neq 0$. The time points of the events recorded by a time series are

$$\left\{T_{\text{out}}(j)\right\}_{j=1}^{m} = \left\{T(i) \middle| X_{\text{out}}(i) \neq 0\right\}_{i=1}^{n}.$$
(6.1)

On the sample level, the set of time points inferred from analysing $\{t(i), x(i)\}_{i=1}^{n}$ is written as $\{t_{out}(j)\}_{j=1}^{m}$. The number of extreme events is m; it is $m \leq n$.

A second constraint imposed on $X_{out}(i)$, besides being unequal to zero, is independence. The observed extreme should have occurred because a climate process generated it and not because there had previously been another, interfering event.

6.1.1.1 Example: Elbe winter floods

The winter floods of the river Elbe (Fig. 1.1) were recorded with a slightly higher accuracy $(x'_{out}(j) = 1, 2 \text{ or } 3)$. For the documentary period (up to 1850), independence of events was achieved by studying the historical sources (Mudelsee et al. 2003). Consider the ice flood in 1784, for which Weikinn (2000) gives 32 source texts that report about the breaking ice cover in the last week of February, the rising water levels, the considerable damages this and the moving ice floes caused and, finally, the decreasing water levels in the first week of March 1784. Mudelsee et al. (2003) considered this as one single event ($t_{out}(j) = 1784.167$) and not two (February, March).

The question after the flood risk, whether winter floods occur at a constant rate or there exist instead changes, is analysed by means of occurrence rate estimation (Section 6.3.2).

6.1.2 Peaks over threshold

If X(i) is known with higher accuracy, a threshold criterion may be applied to detect extremes.

$$\left\{T_{\text{out}}(j), X'_{\text{out}}(j)\right\}_{j=1}^{m} = \left\{T(i), X(i) \middle| X(i) > u\right\}_{i=1}^{n}$$
(6.2)

is a rule for detecting maxima with a constant threshold, u. The extension to detecting minima is straightforward.

6.1 Data types

The peaks-over-threshold (POT) data can be analysed in two ways. Occurrence rate estimation (Section 6.3.2) uses the sample $\{t_{out}(j)\}_{j=1}^{m}$ to infer trends in the occurrence of extremes. Fitting a generalized Pareto distribution (Section 6.2.2) to $\{x'_{out}(j)\}_{j=1}^{m}$ is helpful for studying the risk of an event of pre-defined size, $\operatorname{prob}(X(i) > u + v)$ with v > 0.

In climatology it is also useful to consider a time-dependent threshold to take into account effects of trends in mean, $X_{\text{trend}}(T)$, and variability, S(T). To fulfill the assumption of mutual independence of the POT data, imposing further criteria than passing the threshold may be necessary.

6.1.2.1 Example: volcanic peaks in the NGRIP sulfate record (continued)

Outlier/extremes detection in the NGRIP sulfate record (Fig. 4.16) employed a time-dependent threshold, $X_{\text{trend}}(i) + z \cdot S(i)$, and robust estimates of trend ("background") and variability, to take into account variable oceanic input. A second criterion was the absence of contemporaneous Ca and Na peaks to extract the extremes caused by volcanic eruptions (Fig. 1.4). To satisfy the independence assumption, further threshold exceedances closely neighboured in time were discarded (third criterion). In general, the size of such a neighbourhood can be estimated using persistence models (Chapter 2). Instead of taking $\{X'_{\text{out}}(j)\}_{j=1}^m$ from $\{[X(i) - X_{\text{trend}}(i)]/S(i)\}_{i=1}^n$. Scaling is one form of taking nonstationarity into account (Section 6.3).

6.1.3 Block extremes

It may sometimes be that climate or weather data are in the form of extremes over a certain time period. An example of such a block extreme is the annual maximum,

$$X'_{\text{out}}(j) = \max\Big(\big\{X(i)\big\}_{T(i) \text{ within } j\text{th year of time series}}\Big), \quad (6.3)$$
$$T_{\text{out}}(j) = i\text{th year of time series}, \quad (6.4)$$

The block extremes $X'_{out}(j)$ are the input for fitting a Generalized Extreme Value distribution (Section 6.2.1). The estimation result sheds light on the risk at which an extreme of a pre-defined size and at a pre-defined block length occurs.

Risk estimation (Section 6.2.1) assumes that an extreme is taken from a block with a large number k (at least, say, 100) of independent observations. This can be done explicitly, by segmenting or "blocking" an original series $\{X(i)\}_{i=1}^{n}$. Alternatively, the blocking may have already been done implicitly. An example is documentary data in form of max-

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imum annual water stage in a river, where original daily observations have not been preserved or have simply not been made. Another possibility, theoretically also conceivable, are proxy measurements with a machine that records not the mean value (e.g., of a concentration) but the extreme value. In any case, the independence assumption should be approximately fulfilled if the block length (time units) is large compared with $\max(\tau, D'(i))$ (Fig. 1.13). For practical applications, τ and D(i)have to be estimated.

6.1.4 Remarks on data selection

The rules for selecting $\{X'_{out}(j)\}_{j=1}^m$ from $\{X(i)\}_{i=1}^n$ are not uniquely determined. This allows the analyst to explore various climate system properties regarding extremes.

One area is threshold selection in the POT approach. Besides allowing time-dependence, the size can be adjusted. A high (low) threshold size for maxima detection leads evidently to fewer (more) cases and, hence, to more conservative (liberal) results but likely also to wider (narrower) CIs. Furthermore, a too low threshold may lead to violations of the conditions of convergence to an extreme value distribution. Data in form of event times have implicitly also undergone a threshold selection. The documentary data about Elbe floods, for example, were critically screened (Mudelsee et al. 2003) whether there is enough evidence that merits inclusion into the flood record or there had instead been just an elevated water level noticed by a hypercritical observer.

For block extremes, the adjustable parameter is the block length. In the case of original data X(i) with even spacing, this corresponds to a fixed number, k, of X(i) values per block. In the case of uneven spacing, besides leaving the block length constant, one may also fix k. The connection to nonparametric regression and the smoothing problem (Section 4.3) is evident.

Henceforth we omit for convenience the prime and write $\{X_{\text{out}}(j)\}_{j=1}^{m}$ on the process and $\{x_{\text{out}}(j)\}_{j=1}^{m}$ on the sample level.

6.2 Stationary models

In stationary models, the distribution parameters and related quantities, such as risk, do not change over time.

6.2.1 Generalized Extreme Value distribution

The Generalized Extreme Value (GEV) distribution is suitable for analysing block extremes. Our treatment follows closely that of Coles (2001b: Chapter 3 therein).

6.2 Stationary models

6.2.1.1 Model

The GEV distribution function is given by

$$F_{\rm GEV}(x_{\rm out}) = \begin{cases} \exp\{-\left[1 + \xi \left(x_{\rm out} - \mu\right) / \sigma\right]^{-1/\xi}\} & (\xi \neq 0), \\ \exp\{-\exp\left[-\left(x_{\rm out} - \mu\right) / \sigma\right]\} & (\xi = 0), \end{cases}$$
(6.5)

where $1 + \xi (x_{\text{out}} - \mu) / \sigma > 0$, $-\infty < \mu < \infty$, $\sigma > 0$ and $-\infty < \xi < \infty$. The parameters μ and σ identify location and scale, respectively, while the shape parameter, ξ , determines the tail behaviour of $F_{\text{GEV}}(x_{\text{out}})$.

The importance of the GEV distribution lies in the fact that it is the limiting distribution of the block maximum (for k large). Under mild conditions, nearly irrespective of what the common, but generally unknown distributional shape of the individual variables X(i) is, the distribution of $X_{out}(j)$ approaches the GEV (Fig. 6.1). This is in essence the extreme value analogue of the central limit theorem (Coles 2001b).

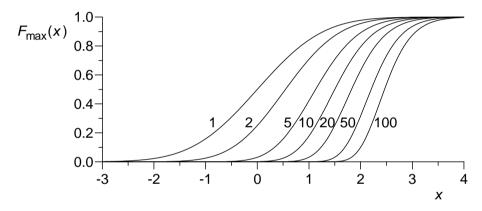


Figure 6.1. Distribution of the maximum of k independent standard normal variates. The plotted distribution functions, $F_{\max}(x)$, are labelled with k. For k = 1, the symmetric form of the standard normal distribution, $F_N(x)$ (Eq. 3.49), appears. In general, $F_{\max}(x) = [F_N(x)]^k$. Letting k increase has three effects: the location (average) is shifted to the right, the scale (standard deviation) is decreased and the right-skewness (shape parameter) is increased. With increasing k, $F_{\max}(x)$ approaches $F_{\text{GEV}}(x)$. This is a theoretical example, with prescribed $F_N(x)$ and exactly determined $F_{\max}(x)$. In a practical setting, with distribution and parameters of the independent variables unknown, $F_{\max}(x)$ can still be approximated by $F_{\text{GEV}}(x)$.

6.2.1.2 Maximum likelihood estimation

Assume that the approximation is perfect and the block maxima $\{x_{\text{out}}(j)\}_{j=1}^{m}$ do come from a GEV distribution (Eq. 6.5). Assume further that $\xi \neq 0$. Adopting the maximum likelihood principle (Section 2.6,

Part III

Bivariate Time Series

Chapter 7

Correlation

The correlation measures how strong a coupling is between the noise components of two processes, $X_{\text{noise}}(i)$ and $Y_{\text{noise}}(i)$. Using a bivariate time series sample, $\{t(i), x(i), y(i)\}_{i=1}^{n}$, this measure allows to study the relationship between two climate variables, each described by its own climate equation (Eq. 1.2).

Pearson's correlation coefficient (Section 7.1) estimates the degree of the *linear* relationship. It is one of the most widely used statistical quantities in all branches of the natural sciences. Spearman's correlation coefficient (Section 7.2) estimates the degree of the *monotonic* relationship. Although clearly less often used, it offers robustness against violations of the Gaussian assumption, as also the Monte Carlo experiments (Section 7.3) show.

Explorative climate data analyses should strongly benefit from correlation estimates that are supported by a CI and not only a P-value of a test of the null hypothesis of no correlation. It is then possible to take several pairs of variables and rank the associations. One finding may be, for example, that global temperature changes are stronger associated to variations of CO₂ than to those of solar activity (background material). The challenge of providing accurate CIs is met by pairwise bootstrap resampling (MBB or ARB), which takes into account the serial dependence structures of both climate processes.

A second, rarely mentioned challenge appears when the processes differ in their sampling times (Section 7.5). This book introduces two novel estimators, denoted as binned and synchrony correlation, respectively. These are able (and outperform interpolation) to recover correlation information under the conditions of (1) persistence in the system, which is realistic for climate, and (2) not too large spacings of the time series.

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7 Correlation

7.1 Pearson's correlation coefficient

Let us assume in this chapter, for simplicity of exposition, that the climate process, X(i), has a constant trend function at level μ_X , a constant variability, S_X , and no outlier component. In discrete time,

$$X(i) = X_{\text{trend}}(i) + X_{\text{out}}(i) + S(i) \cdot X_{\text{noise}}(i)$$

= $\mu_X + S_X \cdot X_{\text{noise}}(i).$ (7.1)

Assume analogously for the second climate process, Y(i), which is on the same time points, T(i), as the first climate process,

$$Y(i) = \mu_Y + S_Y \cdot Y_{\text{noise}}(i). \tag{7.2}$$

The correlation coefficient is then defined as

$$\rho_{XY} = \frac{E\left[\{X(i) - \mu_X\} \cdot \{Y(i) - \mu_Y\}\right]}{S_X \cdot S_Y}.$$
(7.3)

The correlation measures the degree of the linear relationship between the variables X and Y; ρ_{XY} is between -1 ("anti-correlation") and 1.

For convenience of presentation we introduce here the correlation operator,

$$CORR[X(i), Y(i)] = \frac{COV[X(i), Y(i)]}{\{VAR[X(i)] \cdot VAR[Y(i)]\}^{1/2}}.$$
 (7.4)

The definition of the correlation coefficient is thus based on the assumption of time-constancy of $CORR[X(i), Y(i)] = \rho_{XY}$.

Let $\{X(i), Y(i)\}_{i=1}^{n}$ be a bivariate sample (process level). Pearson's (1896) estimator of ρ_{XY} is

$$r_{XY} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{X(i) - \bar{X}}{S_{n,X}} \right) \cdot \left(\frac{Y(i) - \bar{Y}}{S_{n,Y}} \right),$$
(7.5)

where

$$\bar{X} = \sum_{i=1}^{n} X(i) / n$$
 (7.6)

and

$$\bar{Y} = \sum_{i=1}^{n} Y(i) / n \tag{7.7}$$

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are the sample means and

$$S_{n,X} = \left\{ \sum_{i=1}^{n} \left[X(i) - \bar{X} \right]^2 / n \right\}^{1/2}$$
(7.8)

and

$$S_{n,Y} = \left\{ \sum_{i=1}^{n} \left[Y(i) - \bar{Y} \right]^2 / n \right\}^{1/2}$$
(7.9)

are the sample standard deviations calculated with the denominator n (instead of n-1). On the sample level, given a bivariate sample $\{x(i), y(i)\}_{i=1}^{n}$, plug in those values for X(i) and Y(i) in Eqs. (7.5), (7.6), (7.7), (7.8) and (7.9). The estimator r_{XY} is called Pearson's correlation coefficient. Also r_{XY} is between -1 and 1.

7.1.1 Remark: alternative correlation measures

It is of course possible to employ other estimators. For example, S_{n-1} (Eq. 3.19) may replace S_n for estimating S_X or S_Y , leading to an (unfortunate) correlation estimator that can have values $\langle -1 \text{ or } \rangle 1$. Another option may be to subtract the sample medians (Galton 1888) and not the sample means (Eqs. 7.6 and 7.7). More complex examples arise when time-dependent trend functions are subtracted or time-dependent variability functions used for normalization. Such cases may be relevant for climate time series analysis. All those examples lead to other correlation measures than ρ_{XY} and other correlation estimators than r_{XY} . Their properties and CI performance can in principle be studied in the same manner with Monte Carlo methods. Here we focus on r_{XY} , stationary trends and variabilities. Another measure (Spearman's) is analysed in Section 7.2.

7.1.2 Classical confidence intervals, non-persistent processes

Let X(i) and Y(i) both be a stochastic process without persistence or "memory." Let further X(i) and Y(i) both have a Gaussian distributional shape; their joint distribution is then denoted as bivariate normal or binormal distribution (Section 7.1.3.1). The PDF of Pearson's corre-

7 Correlation

lation coefficient is then (Fisher 1915):

$$f(r_{XY}) = \frac{\left(1 - \rho_{XY}^2\right)^{(n-1)/2} \left(1 - r_{XY}^2\right)^{(n-4)/2}}{\sqrt{\pi} \, \Gamma[(n-1)/2] \, \Gamma[(n-2)/2]} \\ \times \sum_{j=0}^{\infty} \frac{\{\Gamma[(n-1+j)/2]\}^2}{j!} \, (2 \, \rho_{XY} \, r_{XY})^j \,. \tag{7.10}$$

Numerous discussions on, and much work in the implementation of, this celebrated formula exist in statistical science. Hotelling (1953) gave approximations for the moments of r_{XY} . In particular,

$$bias_{r_{XY}} = \left(1 - \rho_{XY}^2\right) \left[-\frac{\rho_{XY}}{2n} + \frac{\rho_{XY} - 9\rho_{XY}^3}{8n^2} + \frac{\rho_{XY} + 42\rho_{XY}^3 - 75\rho_{XY}^5}{16n^3} + \mathcal{O}\left(n^{-4}\right) \right]$$
(7.11)

and

$$se_{r_{XY}} = \left(1 - \rho_{XY}^2\right) \left[\frac{1}{n^{1/2}} + \frac{11\rho_{XY}^2}{4n^{3/2}} - \frac{192\rho_{XY}^2 - 479\rho_{XY}^4}{32n^{5/2}} + \mathcal{O}\left(n^{-7/2}\right)\right].$$
(7.12)

Regarding the focus of this chapter, CI construction, it is common practice to employ Fisher's (1921) transformation. The quantity

$$z = \tanh^{-1}\left(r_{XY}\right) \tag{7.13}$$

approaches with increasing n a normal distributional shape considerably faster than r_{XY} , particularly when $\rho_{XY} \neq 0$. Fisher's z has for large n the following properties (Rodriguez 1982):

$$E[z] \approx \tanh^{-1}\left(\rho_{XY}\right) \tag{7.14}$$

and

$$se_z \approx (n-3)^{-1/2}$$
. (7.15)

This leads to the approximate classical CI for r_{XY} ,

$$\operatorname{CI}_{r_{XY},1-2\alpha} = \left[\tanh\left[z+z(\alpha)\cdot\operatorname{se}_{z}\right]; \tanh\left[z-z(\alpha)\cdot\operatorname{se}_{z}\right] \right], \quad (7.16)$$

7.1 Pearson's correlation coefficient

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where $z(\alpha)$ is the percentage point of the normal distribution (Section 3.9).

If we keep the assumption of absence of persistence for processes X(i)and Y(i), but drop the Gaussian assumption, less is known, and no exact formula for the distribution of r_{XY} has been found. One recipe is then to work with higher-moment properties of the distributions and approximate solutions (Section 7.6). The alternative recipe is to use still the formulas for the Gaussian case (Eqs. 7.13, 7.14, 7.15 and 7.16) and assume robustness of this method. Johnson et al. (1995: Chapter 32 therein) give an account of the bewildering diversity of opinions in the research literature on the suitability of this approach.

7.1.3 Bivariate time series models

A bivariate model describes not only the distributional and persistence properties of two processes, X(i) and Y(i), but also the correlation between them. The bivariate white-noise model characterizes persistence-free processes and serves to build bivariate autoregressive and higher-order processes.

7.1.3.1 Bivariate white noise

The bivariate Gaussian white noise model is given by

$$X(i) = \mathcal{E}_{N(0,1)}^{X}(i), \qquad i = 1, \dots, n,$$

$$Y(i) = \mathcal{E}_{N(0,1)}^{Y}(i), \qquad i = 1, \dots, n.$$
(7.17)

The Gaussian random processes $\mathcal{E}_{N(0,1)}^X(\cdot)$ and $\mathcal{E}_{N(0,1)}^Y(\cdot)$ are indexed. The correlation coefficient between them is denoted as $\rho_{\mathcal{E}}$.

The moments of this special case of the bivariate Gaussian white noise model are by definition

$$E[X(i)] = E[Y(i)] = 0,$$
 (7.18)

$$VAR[X(i)] = VAR[Y(i)] = 1$$
(7.19)

and

$$CORR\left[X(i), Y(i)\right] = \rho_{XY} = \rho_{\mathcal{E}}.$$
(7.20)

In the general case, X(i) has mean μ_X and variance S_X^2 , and Y(i) has mean μ_Y and variance S_Y^2 . The binormal PDF of X(i) and Y(i) (Section 7.6) is uniquely determined by the means, variances and correlation.

Chapter 8

Regression II

Regression serves in this chapter to relate two climate variables, X(i) and Y(i). This is a standard tool for formulating a quantitative "climate theory" based on equations. Owing to the complexity of the climate system, such a theory can never be derived alone from the pure laws of physics—it requires to establish empirical relations between observed climate processes.

Since not only Y(i) but also X(i) are observed with error, the relation has to be formulated as an errors-in-variables model, and the estimation has to be carried out using adaptions of the OLS technique. This chapter focuses on the linear model and studies three estimation techniques (denoted as OLSBC, WLSXY and Wald–Bartlett procedure). It presents a novel bivariate resampling approach (pairwise-MBBres), which enhances the coverage performance of bootstrap CIs for the estimated regression parameters.

Monte Carlo simulations allow to assess the role of various aspects of the estimation. First, prior knowledge about the size of the measurement errors is indispensable to yield a consistent estimation. If this knowledge is not exact, which is typical for a situation in the climatological practice, it contributes to the estimation error of the slope (RMSE and CI length). This contribution persists even when the data size goes to infinity; the RMSE does then not approach zero. Second, autocorrelation has to be taken into account to prevent estimation errors unrealistically small and CIs too narrow.

This chapter studies two extensions of high relevance for climatological applications: linear prediction and lagged regression.

Regression as a method to estimate the trend in the climate equation (Eq. 1.2) is presented in Chapter 4.

8 Regression II

8.1 Linear regression

To make a regression of the predictor variable, X, on the response variable, Y, we re-apply the errors-in-variables model (Section 4.1.7),

$$Y(i) = \beta_0 + \beta_1 [X(i) - S_X(i) \cdot X_{\text{noise}}(i)] + S_Y(i) \cdot Y_{\text{noise}}(i), \quad (8.1)$$

i = 1, ..., n. The variability of process X(i) and Y(i) is denoted as $S_X(i)$ and $S_Y(i)$, respectively; the noise component, $X_{\text{noise}}(i)$ and $Y_{\text{noise}}(i)$, is of assumed AR(1) type with persistence time τ_X and τ_Y , respectively. One task is to estimate the regression parameters, β_0 and β_1 , given a bivariate sample, $\{t(i), x(i), y(i)\}_{i=1}^n$. Another, related task is to make a prediction of an unknown Y for a given value of X.

The errors-in-variables model (Eq. 8.1) differs from the simple model (Eq. 4.3) in its nonzero noise component of the predictor. Several estimators for the errors-in-variables model have been developed to deal with this more complex situation.

8.1.1 Ordinary least-squares estimation

The simple OLS estimation minimizes the unweighted sum of squares,

$$SSQ(\beta_0, \beta_1) = \sum_{i=1}^{n} \left[y(i) - \beta_0 - \beta_1 x(i) \right]^2.$$
(8.2)

This yields the estimators

$$\widehat{\beta}_0 = \left[\sum_{i=1}^n y(i) - \widehat{\beta}_1 \sum_{i=1}^n x(i)\right] / n \tag{8.3}$$

and

$$\widehat{\beta}_{1} = \left\{ \left[\sum_{i=1}^{n} x(i) \right] \left[\sum_{i=1}^{n} y(i) \right] / n - \sum_{i=1}^{n} x(i) y(i) \right\} \\ \times \left\{ \left[\sum_{i=1}^{n} x(i) \right]^{2} / n - \sum_{i=1}^{n} x(i)^{2} \right\}^{-1}.$$
(8.4)

Using OLS means ignoring heteroscedasticity, persistence and errors in the predictor variable, X. However, heteroscedasticity and persistence can successfully be taken into account by employing WLS and GLS estimation, respectively. The success of ignoring errors in X depends on how large these are relative to the spread of the "true" X values (Eq.

8.1 Linear regression

4.34), which are given by $X_{\text{true}}(i) = X(i) - S_X(i) \cdot X_{\text{noise}}(i)$. If $S_X(i) = S_X$ is constant and $S_X^2 \ll VAR[X_{\text{true}}(i)]$, the estimation bias should be negligible. If $S_X(i)$ is not constant, one may expect a similar condition to the average of $S_X(i)$. The decisive quantity is $VAR[X_{\text{true}}(i)]$, which may be difficult to control for an experimenter prior to sampling the process.

If $X_{\text{noise}}(i)$ and $Y_{\text{noise}}(i)$ are independent, the estimator $\widehat{\beta}_1$ is biased downwards (Section 4.1.7) as $E\left(\widehat{\beta}_1\right) = \kappa \cdot \beta_1$, where $\kappa \leq 1$ is the attenuation factor or reliability ratio,

$$\kappa = \left(1 + S_X^2 / VAR\left[X_{\text{true}}(i)\right]\right)^{-1}.$$
(8.5)

The intuitive reason of the bias downwards is that "smearing" the "true" predictor variable, $X_{\text{true}}(i)$, leads to a situation where the "cheapest fit solution" in terms of SSQ is a line that is horizontally tilted (Fig. 8.1).

8.1.1.1 Bias correction

Eq. (8.5) points to a bias-corrected slope estimation. Let $S_X(i) = S_X$ be constant and known, and let the variance of the "true" predictor values be given by $VAR[X_{true}(i)] = VAR[X(i)] - S_X^2$. This leads to

$$\widehat{\beta}_{1} = \widehat{\beta}_{1,\text{OLS}} / \left\{ 1 - S_{X}^{2} / VAR\left[X(i)\right] \right\},$$
(8.6)

where $\hat{\beta}_{1,\text{OLS}}$ is the simple OLS slope estimator (Eq. 8.4). We denote this estimation method (Eq. 8.6) as ordinary least squares with bias correction (OLSBC). The OLSBC intercept estimator equals the OLS intercept estimator (Eq. 8.3). In practice (sample level), plug in x(i) for X(i).

8.1.1.2 Prior knowledge about standard deviations

Assume homoscedastic noise components, $S_Y(i) = S_Y$ and $S_X(i) = S_X$, and denote their squared ratio as

$$\lambda = S_Y^2 \left/ S_X^2 \right. \tag{8.7}$$

Knowledge prior to the estimation about S_X , S_Y or λ can increase the estimation accuracy.

If S_X is known, then OLSBC can be readily performed (Eq. 8.6). Such prior knowledge may be acquired, for example, by repeating measurements. Or there may exist theoretical information about the measuring device and, hence, S_X .

If S_X is only known within bounds, OLSBC estimation can still be applied. CI construction has then to take into account the limited prior



8 Regression II

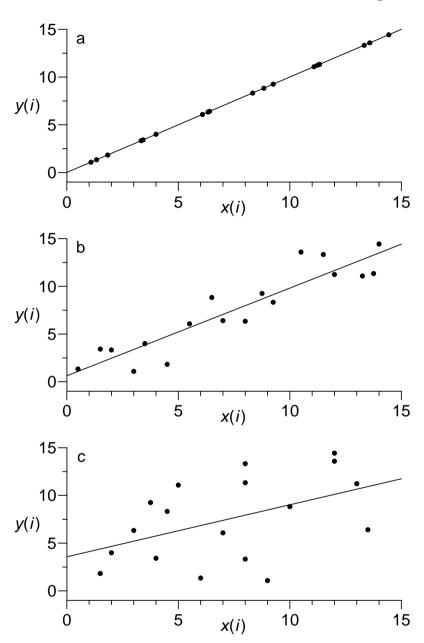


Figure 8.1. Linear errors-in-variables regression model, OLS estimation. The $\{y(i)\}_{i=1}^{n}$ are identical in panels **a–c**; the data size is n = 18; and the $\{x(i)\}_{i=1}^{n}$ are realizations of a predictor variable, X(i), with constant zero (**a**), small (**b**) and large (**c**) noise components, $S_X(i) \cdot X_{\text{noise}}(i)$. The true slope is $\beta_1 = 1.0$ (**a**). The OLS fits (*solid lines*) exhibit slope estimates that are unbiased (**a** $\hat{\beta}_1 = 1.0$) or biased (**b** $\hat{\beta}_1 = 0.92$; **c** $\hat{\beta}_1 = 0.55$).

Part IV

Outlook

Chapter 9

Future Directions

What changes may bring the future to climate time series analysis? First we outline (Sections 9.1, 9.2 and 9.3) more short-term objectives of "normal science" (Kuhn 1970), extensions of previous material (Chapters 1, 2, 3, 4, 5, 6, 7 and 8). Then we take a chance (Sections 9.4 and 9.5) and look on paradigm changes in climate data analysis that may be effected by virtue of strongly increased computing power (and storage capacity). Whether this technological achievement comes in the form of grid computing (Allen 1999; Allen et al. 2000; Stainforth et al. 2007) or quantum computing (Nielsen and Chuang 2000; DiCarlo et al. 2009; Lanyon et al. 2009)—the assumption here is the availability of machines that are faster by a factor of ten to the power of, say, twelve, by a mid-term period of, say, less than a few decades.

9.1 Timescale modelling

Climate time series consist not only of measured values of a climate variable, but also of observed time values. Often the latter are not evenly spaced and also influenced by dating uncertainties. Conventional time series analysis largely ignored uneven and uncertain timescales, climate time series analysis has to take them into account.

The process that generated the times, $\{t_X(i)\}\$ for univariate and also $\{t_Y(j)\}\$ for bivariate series, depends on the climate archive. We have studied linear and piecewise linear processes for speleothem or sedimentary archives (Section 4.1.7) and nonparametric models for ice cores (Section 8.6.1). Such types of models are the basis for including uncertain timescales in the error determination by means of bootstrap resampling $(\{t_X^*(i)\}\)$ and also $\{t_Y^*(j)\}\)$. In bivariate and higher dimensional estimation problems, also the joint distributions of the timescale processes are

9 Future Directions

important. See the example of the Vostok ice core (Section 8.6.1) with the coupled timescales for the ice and the gas.

Climate archive modelling should be enhanced in the future to provide accurate descriptions of uncertain timescales. Archive models should evidently include the physics of the accumulation of the archive. One may even think of physiological models describing the performance of humans in layer counting of regular sequences such as varves (Table 1.3). A second ingredient of climate archive modelling are statistical constraints, for example, a strictly monotonically increasing age-depth curve in a speleothem archive or an absolutely dated fixpoint in a marine sediment core. An exemplary paper (Parrenin et al. 2007) of climate archive modelling studies the accumulation and flow in an ice sheet, into which a core is drilled. The Bayesian approach may be suitable for combining the inputs from physics and statistical constraints (Buck and Millard 2004).

9.2 Novel estimation problems

Chapters 2, 3, 4, 5 and 6 presented stochastic processes and estimation algorithms for inferring the fundamental properties of univariate climate processes in the climate equation (Eq. 1.2): trend, variability, persistence, spectrum and extremes. Chapters 7 and 8 studied bivariate processes: correlation and the regression relation between two univariate processes. We believe to have covered with these chapters the vast majority of application fields for the climate sciences.

However, in science there is always room for asking more questions, that means in a quantitative approach, for attempting to estimate different climate parameters in the uni- or bivariate setting.

An obvious example of such a novel estimation problem is SSA, mentioned in the background material of Chapter 1. This decomposition method has been formulated so far only for evenly spaced, discrete time series. Interpolation to equidistance is obsolete because it biases the objectives of the decomposition (estimates of trend, variability, etc.). SSA formulations applicable to unevenly spaced records should therefore be developed.

Other novel estimation approaches are expected to come from the array of nonlinear dynamical systems theory (Section 1.6). This field has a focus more on application data from controlled measurements or computer experiments and less on unevenly spaced, short paleoclimatic time series. A breakthrough, also with respect to SSA, may come from techniques of reconstructing the phase space at irregular points.

9.3 Higher dimensions

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9.3 Higher dimensions

Climate is a complex, high-dimensional system, comprising many variables. Therefore it makes sense to study not only univariate processes (Part II), X, or bivariate processes (Part III), X and Y, but also trivariate processes, X and Y and Z, and so forth. A simple estimation problem for such high-dimensional processes is the multivariate regression, mentioned occasionally in previous chapters (Sections 4.2 and 8.7),

$$Y(i) = \theta_0 + \theta_1 X(i) + \theta_2 Z(i) + \dots + S_Y(i) \cdot Y_{\text{noise}}(i).$$
(9.1)

The higher number of dimensions may also result from describing the climate evolution in the spatial domain (e.g., X is temperature in the northern, Y in the southern hemisphere). There is a variety of high-dimensional, spatial estimation problems: multivariate regression, PCA and many more (von Storch and Zwiers 1999: Part V therein).

As regards the bootstrap method, there is no principle obstacle to perform resampling in higher dimensions. An important point is that resampling the marginal distributions, of X and Y and Z separately, is not sufficient; the joint distribution of (X, Y, Z), including dependences among variables, has to be resampled to preserve the original covariance structure. This requires adaptions of the block bootstrap (MBB) approach. A further point, which may considerably exacerbate the estimation as well as the bootstrap implementation, is unequal observation times. The sets

$$\{t_X(i)\}_{i=1}^{n_X}, \ \{t_Y(j)\}_{j=1}^{n_Y}, \ \{t_Z(k)\}_{k=1}^{n_Z}$$
(9.2)

need not be identical. Depending on the estimation problem and the properties of the joint climate data generating process (e.g., persistence times), the algorithm for determining $\theta_0, \theta_1, \theta_2$, and so forth, has to be adapted. This is a step into new territory. An example from the bivariate setting is the "synchrony correlation coefficient" (Section 7.5.2). A final point of complication from the move into higher dimensions is dependence among the timescale variables. Since this type of complication can occur already in two-dimensional problems (Section 8.6.1), we expect it in higher dimensions as well. This challenge must be met by means of timescale modelling (Section 9.1).

9.4 Climate models

Computer models render the climate system in the form of mathematical equations. The currently most sophisticated types, AOGCMs (Fig. 1.9), require the most powerful computers. Nevertheless, the rendered spatial and temporal scales are bounded by finite resolutions and finite domain sizes. Also the number of simulated climate processes is limited.

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