Chapter 9 Future Directions

Abstract What changes may the future bring to climate time series analysis? First, we outline (Sects. 9.1–9.3) more short-term objectives of "normal science" (Kuhn, The Structure of Scientific Revolutions, 2nd edn. University of Chicago Press, Chicago, 210 pp, 1970), extensions of previous material (Chaps. 1–8). Then we take a chance (Sects. 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, Nature 401(6754):642, 1999; Allen et al., Nature 407(6804):617-620, 2000; Stainforth et al., Philos Trans R Soc Lond Ser A 365(1857):2145–2161, 2007) or quantum computing (Nielsen and Chuang, Quantum Computation and Quantum Information. Cambridge University Press, Cambridge, 676pp, 2000; DiCarlo et al., Nature 460(7252):240-244, 2009; Lanyon et al., Nat Phys 5(2):134–140, 2009; Rieffel and Polak, Quantum Computing: A Gentle Introduction. MIT Press, Cambridge, MA, 372pp, 2011)-the assumption here is the availability of machines that are faster by a factor of 10 to the power of, say, 12, by a midterm period of, say, less than a few decades.

Keywords Timescale modelling • Atmosphere–ocean general circulation models • Regional climate models • Ensemble approach • Perturbed physics approach • Data assimilation • Climate forecasting uncertainty • Climate model bias correction • Optimal estimation

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 $\{t_Y(j)\}\$ for bivariate series, depends on the climate archive. We have studied linear and piecewise linear processes for speleothem or sedimentary archives (Sect. 4.1.7) and nonparametric models for ice cores (Sect. 8.6.1). Such types of models are the basis for including uncertain timescales in the error determination by means of bootstrap resampling ($\{t_X^*(i)\}\)$ and also $\{t_Y^*(j)\}\)$). In bivariate and higher-dimensional estimation problems, also the joint distributions of the timescale processes are important. See the example of the Vostok ice core (Sect. 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 1.2). A second ingredient of climate archive modelling is 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).

A recent overview is given in the background material (Sect. 9.6). It is encouraging to see that the various climate-related scientific communities (which often associate themselves with the type of archive typically employed) become active in developing methods for constructing chronologies. The degree of overlap among those methodical ideas should be kept healthily reduced if these communities manage to be active also in studying methods from other communities, especially statistical science.

9.2 Novel Estimation Problems

Chapters 2–6 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 is, 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 Chap. 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 (Sect. 1.6). This field has focus more on application data from controlled measurements or computer experiments and less on unevenly spaced, short palaeoclimatic 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

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 the previous chapters (Sects. 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

$$\{t_X(i)\}_{i=1}^{n_X}, \ \{t_Y(j)\}_{i=1}^{n_Y}, \ \{t_Z(k)\}_{k=1}^{n_Z}$$
(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 θ_0 , θ_1 , θ_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" (Sect. 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 (Sect. 8.6.1), we expect it in higher dimensions as well. This challenge must be met by means of timescale modelling (Sect. 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. 1.10), 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.

The problem of a finite spatial resolution is currently tackled by means of using an AOGCM (grid size several tens to a few hundred kilometres) for the global domain and nesting into it a regional climate model or RCM (grid size reduced by a factor ~20) for a sub-domain of interest (say, Europe). The AOGCM "forces" the RCM (Meehl et al. 2007; Christensen et al. 2007), that is, prescribes the conditions at the boundaries of the sub-domain. Sub-grid processes, not resolved even by the RCM (e.g. cloud processes) and therefore not explicitly renderable by the AOGCM–RCM combination, can be implicitly included by employing inferred parametric relations (e.g. between cloud formation and temperature). The AOGCM– RCM combination includes many variables, $(X, Y, Z, ...)' \equiv \mathbf{X}$, from the climate at grid points, and many parameters, $(\theta_0, \theta_1, \theta_2, ...)' \equiv \boldsymbol{\theta}$, from the parameterizations (Stensrud 2007) and other model equations. For convenience of presentation, we consider the climate variable vector, \mathbf{X} , and the climate model parameter vector, $\boldsymbol{\theta}$.

Our premise of a future "quantum boost" by a factor $\sim 10^{12}$ can make regionalization dispensable, and let more realistic AOGCMs (grid size several tens to a few hundred metres) become calculable with computing times reduced from, say, a year to less than a month. Regarding the sophistication of a climate model, the increased computing power can also be utilized for including processes from the fields of biology and economy, greenhouse gas emissions (Moss et al. 2010; van Vuuren et al. 2011) and "climate engineering" measures; see also Sect. 9.6. Indeed, a finer spatial grid does require more processes to be explicitly included. Regarding the temporal scale, the boost should allow to simulate much larger spans (transient palaeoclimate runs) by the means of AOGCMs and their successors.

There exists, however, another field where to invest computing power, namely, the uncertainty determination of climate model results. We sketch this area in light of the methodology presented in this book, statistical estimation and bootstrap resampling.

Physics formulates climate dynamics by means of nonlinear coupled differential equations,

$$\dot{\mathbf{X}} = f\left(\mathbf{X}, \mathbf{R}, \boldsymbol{\theta}\right),\tag{9.3}$$

where the dot denotes time derivative, f is a function, and **R** represents uncoupled, external forcing variables (e.g. solar activity). Time discretization yields

$$\mathbf{X}(i+1) = \mathbf{X}(i) + \Delta T \cdot \dot{\mathbf{X}},\tag{9.4}$$

where ΔT is a time step, in an AOGCM typically in the order of minutes to hours. From an initial climate state, **X**(1), the climate evolution is derived. This sample from the climate model "archive" is

$$\{\mathbf{x}(i)\}_{i=1}^{n}.$$
(9.5)

The climate evolution can also be observed, yielding a multivariate time series sample:

$$\{\mathbf{x}_{0}(i)\}_{i=1}^{n}$$
. (9.6)

The observations are, of course, strongly limited in the number of climate variables, geographic locations and time resolutions. There have been few observations made of, say, temperature in 1000 m height above sea level at 130°W, 30°S for the time interval from 1850 to 2010 and a spacing of $d(i) = \Delta T = 30$ min.

9.4.1 Fitting Climate Models to Observations

Let us view climate modelling as an estimation problem. The task is to estimate the model parameters, $\boldsymbol{\theta}$, given observations, $\{\mathbf{x}_{o}(i)\}_{i=1}^{n}$. This set shall include the "missing observations". The task requires to run the model and produce $\{\mathbf{x}(i)\}_{i=1}^{n}$. The less distant the model output is to the observations, the better the fit.

Let us introduce a cost function to measure the distance:

$$SSQGXYZ_{\nu}(\boldsymbol{\theta}) = g\big(\{\mathbf{x}_{o}(i)\}_{i=1}^{n}, \{\mathbf{x}(i)\}_{i=1}^{n}\big).$$

$$(9.7)$$

g may be a form of a generalized least-squares cost function that takes into account predictor uncertainty and the degrees of freedom; Sect. 9.4.3 considers the design of g in more detail. The parameter estimate minimizes the cost function:

$$\hat{\boldsymbol{\theta}} = \operatorname{argmin} \left\{ g\left(\left\{ \mathbf{x}_{o}(i) \right\}_{i=1}^{n}, \left\{ \mathbf{x}(i) \right\}_{i=1}^{n} \right) \right\}.$$
(9.8)

The parameter vector is included in the right-hand side of the equation because the model output, $\{\mathbf{x}(i)\}_{i=1}^{n}$, depends on it.

The outlined procedure is with current computing power not feasible for a full estimation of AOGCM parameters. It has been performed for a simple climate model containing only three variables (Hargreaves and Annan 2002) and an

Earth system model of intermediate complexity (Paul and Schäfer-Neth 2005). The concept of fitting climate models to data is also denoted as data assimilation or state estimation (Wunsch 2006).

Subsequent to the estimation, we should like to know the parameter uncertainties for the fitted climate model. This knowledge may be achieved by means of bootstrap methods, producing the replications:

$$\hat{\boldsymbol{\theta}}^{*} = \operatorname{argmin} \Big\{ g \big(\big\{ \mathbf{x}_{0}^{*}(i) \big\}_{i=1}^{n}, \big\{ \mathbf{x}^{*}(i) \big\}_{i=1}^{n} \big) \Big\}.$$
(9.9)

The observation resample, $\mathbf{x}_{o}^{*}(i)$, can be obtained via the surrogate data bootstrap (Sect. 3.3.3), taking into account the errors of the observation devices, the distributional shapes (which may be Gaussian or not), the covariances (which may be rather small) and the "internal climate variability" (which may have to be estimated by means of separate model experiments). The model output resample, $\mathbf{x}^{*}(i)$, incorporates a new (trial) set of parameters, $\boldsymbol{\theta}^{*}$. However, it should also be based on a random initial state, $\mathbf{x}^{*}(1)$, because the initial conditions are not exactly known. $\mathbf{x}^{*}(1)$ may be taken randomly from a set of time series values of a climate model run without changing forcing components (stationarity). This "ensemble technique" is already currently being applied to quantify the uncertainty component owing to imperfectly known initial conditions (Randall et al. 2007; van der Linden and Mitchell 2009). Also the forcing variable, $\mathbf{R}(i)$, may have to be described stochastically for being included in the surrogate data approach.

The replications, $\{\hat{\theta}^{*b}\}_{b=1}^{B}$, serve in the usual manner (Sect. 3.4) for constructing CIs. Of particular interest should be the joint PDF of the climate model parameter estimators, which may be described by means of confidence regions in the parameter hyperspace (Smith et al. 2009; Tebaldi and Sansó 2009). Realistic climate model error and CI determination do not require a handful of runs (current ensemble technique) but rather *B* runs, with *B* in the usual order of 2000 or even higher (because of the dimensionality).

9.4.2 Forecasting with Climate Models

Models are employed to forecast future climate, $\mathbf{x}(n + 1)$, at time t(n + 1). (Indeed, forecasts are made for many time steps to cover the typical range from the present to the year 2100.) This is achieved in our vision by a run of the model employing the estimated, optimal parameters, $\hat{\boldsymbol{\theta}}$. That run has to use also a guess of the future forcing, $\mathbf{R}(n + 1)$.

Of crucial importance, scientifically and socioeconomically, is to determine the size of the forecasting error. The bootstrap methodology, utilized for that purpose in the bivariate setting (Sect. 8.5), should be helpful also in the high-dimensional setting.

The recommendation is to produce forecast resamples, $\mathbf{x}^*(n+1)$, from which to calculate standard errors, CIs, confidence bands (over a time span), and so forth.

How are the $\mathbf{x}^*(n + 1)$ produced to reflect the full range of the various sources of uncertainty?

- The parameterization uncertainty can be taken into account by resampling from the set of replications, $\{\hat{\theta}^{*b}\}_{b=1}^{B}$. This preserves the covariance structure of the parameter estimates.
- The initial-condition uncertainty can be taken into account by means of the ensemble technique.
- The forcing uncertainty may be difficult to include in a quantitative manner. This step does likely necessitate the usage of separate forcing models.

9.4.3 Design of the Cost Function

Designing the cost function (Eq. 9.7) is important for achieving small standard errors and narrow CIs for the climate forecasts and the model parameter estimates. It is rather difficult to demonstrate theoretically the optimality of a certain cost function. One should perform Monte Carlo simulations to find "empirically" a suitable function. The following points may guide the design endeavour:

- A least-squares technique is mandatory. It seems impossible to write down a likelihood function (for maximization) owing to the size of the body of the climate model equations. One may wish to make the sum of squares more robust with respect to "outliers". On the other hand, one may give the "outliers" instead *more* weight in situations where the focus is on modelling the climate extremes.
- GLS, employing the covariance matrices (variability, persistence) of the many climate variables, is a possible technique to reduce the estimation standard errors. The normalization (variability) produces dimensionless *SSQG* terms for each variable, which can be processed further (e.g. summed up).
- A problem is multicollinearity (correlated predictors), stemming from spatial dependence among the climate variables (neighbouring grid points). This may indicate to reduce the number of variables in the cost function by means of spatial binning. PCA techniques should help evaluating geographically meaningful bins (regions).
- Errors in the observations $(S_X, S_Y, S_Z, ...)$ should lead researchers to consider techniques like WLSXY estimation (Sect. 8.1.2) to reduce estimation bias.
- Further weighting could be performed "in the time domain" to enforce, for example, the most recent years to be more accurately simulated.
- The degrees of freedom, v, of the observation–model combination can be taken into account (a simple division by v).
- One may put bounds to the θ hyperspace to exclude estimation results that are inconsistent with physics (hard bounds) or prior knowledge (soft bounds). Bayesian formulas may help here.

The envisaged availability of "quantum computing power" does not release us from the task of developing efficient methods to search through the hyperspace, to locate the minimum of the cost function: gradient techniques, Brent's search, hybrid procedures or Bayesian approaches (Markov chain Monte Carlo, see Hargreaves and Annan (2002) and Leith and Chandler (2010)).

9.4.4 Climate Model Bias

Climate model bias regards, generally speaking, a function of the climate variable vector:

$$\eta = h\left(\mathbf{X}\right).\tag{9.10}$$

The function, h, can be used to make η an index variable (Easterling et al. 2003) or extract a geographic region. For example, we may wish to study time-dependent, annual-mean, regional-mean, land-surface precipitation in central Europe,

$$\eta(j) = n_k^{-1} n_i^{-1} \sum_{k \in \text{region}} \sum_{T(i) \in \text{year } j} X_k(i), \qquad (9.11)$$

where $X_k(i)$ is precipitation at grid point k and time T(i), n_i is the number of time values within year j and n_k is the number of model grid points within central Europe.

Let us now view the *modelled* sequence as an estimate obtained by means of a climate model, $\hat{\eta}(j)$. Next, we consider the true sequence. Since the truth is hidden, we take instead an observed sequence, $\eta_0(j)$. This leads, in analogy to Eq. (3.2), to the climate model bias:

$$\operatorname{bias}_{\hat{\eta}}(j) = E\left[\hat{\eta}(j)\right] - \eta_{o}(j). \tag{9.12}$$

In the example of precipitation in central Europe, there are indications from a range of AOGCM–RCM combinations that $bias_{\hat{\eta}}(j) > 0$ for the time interval from 1950 to the recent past (Jacob D 2009, personal communication), that is, the climate models systematically overestimate precipitation. Similar overestimations were found for the region of Scandinavia (Goodess et al. 2009).

In the context of climate forecasting (Sect. 9.4.2), better predictions may therefore include a climate model bias correction. For example, if the model bias is simply a constant, $bias_{\hat{\eta}}$, then

$$\eta'(j_{\text{future}}) = \eta(j_{\text{future}}) - \text{bias}_{\hat{\eta}}, \qquad (9.13)$$

where j_{future} indicates future (unobserved) time and the prime denotes bias correction. Evidently, the time-dependence of the bias and also its form (additive, multiplicative) should be analysed in such situations. Further developments may employ more complex stochastic models of the climate model bias (Jun et al. 2008).

9.5 **Optimal Estimation**

Increased computer power would also allow to perform optimal estimation. We have sketched this concept in the previous parts of this book (Sect. 6.2.7 and section "Optimal Estimation" in Chap. 7). Not only climatology, other science branches as well may benefit from optimal estimation.

Central to the investigation in natural sciences, such as climatology, is to infer the truth from the data. This calls for the statistical language. In quantitative climatology, the investigative questions can be translated into a parameter, θ , which needs to be estimated using the data. The investigation cycles through loops: question, estimation, refined question based on the estimation result, new estimation, and so forth.

An estimator, $\hat{\theta}$, is a recipe on how to guess θ using the data. Since the sample size is less than infinity and the sampled climate system contains unknown influences (noise), we cannot expect that $\hat{\theta}$ equals θ . However, we can calculate the size of that error, the uncertainty. This leads to the measures se_{$\hat{\theta}$}, bias_{$\hat{\theta}$}, RMSE_{$\hat{\theta}$} and the confidence interval, CI_{$\hat{\theta},1-2\alpha$}, which is thought to include θ with probability $1 - 2\alpha$. Without having the information contained in such measures, it is difficult to assess how close $\hat{\theta}$ is to θ : estimates without error bars are useless.

For simple estimation problems (e.g. mean estimation) and simple noise properties (e.g. Gaussian distributional shape), the error measures can be analytically derived via the PDF of an estimator. However, climate is more complex—as regards the noise as well as the estimation problem. This book advocates therefore the bootstrap resampling approach, which allows to analyse complex problems for realistic (i.e. complex) properties such as non-Gaussian shape or serial dependence.

For the most part of this book, we have assumed the uncertainty to have its origin in the complex climate system and the measured variables (proxy, measurement and dating errors). We have occasionally considered (section "Monte Carlo Experiments" in Chap. 4, Sects. 4.4 and 8.3.4) another error source, a misspecified model. Statistical science refers to this error source as model uncertainty; see Chatfield (1995), Draper (1995), Candolo et al. (2003) and Chatfield (2004: Sect. 13.5 therein). By fitting a range of candidate models, it is possible to infer the range of feasible estimation outcomes. For example, one may compare the estimated 100-year return level, HQ_{100} , from a Weibull fit with the estimated HQ_{100} from a GEV fit to observed runoff data, and look whether the difference of the results is comparable to the statistical standard errors. Note that model uncertainty may regard also the assumed noise model (e.g. short versus long memory). A method



Fig. 9.1 Hyperspace of climate parameter estimation. The Monte Carlo experiment prescribes the stochastic model, parameters and other properties (shape, sample size, spacing, persistence, etc.) in a way that the problem at hand (data and estimation) is covered. The method regards estimation and CI construction. The optimal estimation is determined by using a measure

to reduce model uncertainty is to employ graphical and computational tests of model suitability. As a method to quantify model uncertainty, we may study not only the range of the estimation outcomes but impose a weighting according to the probability that a particular model is correct. The "model probability" may be based in a Bayesian approach on a prior consultation of experts (Smith et al. 2009); but see also the critical paper (in the context of emission scenarios and test significance) by von Storch and Zwiers (2013). In the example of HQ₁₀₀, there is hope that the hydrologists would put more weight on the GEV model than on the Weibull. It is principally possible to add model uncertainty as a new dimension to the hyperspace of climate estimation (Fig. 9.1).

Climate is a paradigm of a complex system that requires for its analysis the bootstrap. In addition, climate opens the new problem dimensions of unequally spaced series and timescale errors. This book has presented various bootstrap algorithms to adapt closely to the estimation problem imposed by the data: ARB, MBB, SB, surrogate data, timescale-ARB, timescale-MBB, pairwise-ARB, pairwise-MBB and pairwise-MBBres. It also described algorithms to support bootstrap resampling and CI construction: block length selection, calibration, the CI types normal, Student's t, percentile and BCa.

The critical question is: What is the best method for inferring the truth from the data? What is the optimal estimation method, and how are the most accurate CIs constructed?

Future, strongly increased computing power allows to approach that question by means of Monte Carlo experiments. We outline this optimal estimation approach (Fig. 9.1). We reiterate that optimal estimation is not limited to the field of climate sciences.

The hyperspace of climate estimation has many, but not infinite, dimensions. It consists of the three subspaces Monte Carlo design, method and measure.

The Monte Carlo design (Fig. 9.1) describes the data generating process. The design is used to generate artificial data, to which the method is applied. The design should, in some sense, cover the estimation problem (data and estimation) to be carried out. One group of dimensions is occupied by the type of estimation model and the parameters. For example, one may be interested in a linear regression model with the two parameters intercept and slope (Chaps. 4 and 8). To restate, the Monte Carlo parameters (e.g. prescribed intercept and slope) should be close to the estimated parameters (estimated intercept and slope). The other group of dimensions in the Monte Carlo subspace describe the sample size (prescribed n, which should be close to the size of the sample at hand), the spacing (again, similar to the spacing of the sample) and the noise properties (also similar). An option is to invest three dimensions to model the persistence of the noise as an ARFIMA (p, δ, q) process (which contains the simpler types such as AR(1)) and one or two to model the shape (skewness, kurtosis). Heteroscedasticity may also be modelled. The ARFIMA process contains the preferred parsimonious, embeddingproblem free AR(1) process ($p = 1, \delta = 0, q = 0$). Some dimensions have integer values (e.g. the ARFIMA parameter p), and some have real values (e.g. the slope parameter). Timescale errors may also be modelled (additional dimensions).

The method subspace (Fig. 9.1) describes the estimation and CI construction. The ticks along the estimator dimension are named least squares, maximum likelihood, and so forth. CI construction requires more dimensions: one for distinguishing between classical and bootstrap CIs and several for detailing the bootstrap methodology (block length selection for MBB, calibration, subsampling, etc.) and calculating the interval bounds from the replications. Consider, for example, the brute-force block length selector (Berkowitz and Kilian 2000): one dimension with integer values between 1 and n - 1.

The measure subspace (Fig. 9.1) describes how to detect the optimal estimation method for the Monte Carlo experiment: CI accuracy and width, RMSE, bias, robustness, and so forth. It should make sense to consider also joint measures (e.g. CI accuracy and robustness).

The hyperspace of climate parameter estimation is large. Present computing power limits our ability to explore it and find the optimal method for solving a (climate) estimation problem. This book has examined many important estimation problems (regression, spectrum, extremes and correlation) but visited only parts of the hyperspace by means of Monte Carlo experiments. For example, in linear regression (Chap. 4), we have studied the following:

- $\theta = \beta_0$ (intercept) and β_1 (slope)
- Prescribed $\beta_0 = 2, \beta_1 = 2$

- $n \in \{10, 20, 50, 100, 200, 500, 1000\}$
- Spacing: even and uneven (timescale errors)
- Shape: Gaussian and lognormal
- Persistence: AR(1), AR(2) and ARFIMA(0, 0.25, 0)
- · Estimator: least squares only
- Resampling: ARB, MBB, subsampling, timescale-ARB, timescale-MBB and pairwise-MBB
- CI type: classical and bootstrap BCa
- Confidence level: 90, 95 and 99 %
- Calibration loop: none
- Measure: RMSE, CI accuracy and CI length

We have found "acceptable" results (mainly judged via CI accuracy) from the bootstrap method applied to Monte Carlo samples generated from designed processes that are considered as close to the climate processes. These positive results have given us confidence that the results (estimate with CI) from analysing the observed, real climate time series are valid. However, we have to concede that there may exist more accurate methods, resulting in particular from (computing-intensive) CI calibration. This may be of relevance especially for small sample sizes.

The envisaged large increase in computing power may bring the following idea of optimal climate estimation into existence. Given a time series, $\{t(i), x(i)\}_{i=1}^n$, some prior information (e.g. measurement standard errors, age-depth curve) and a set of questions (parameters to be estimated), the first task is simple: perform an initial estimation on basis of existing knowledge and experience with such types of estimation problems. The second task requires the computing power: explore the hyperspace (Fig. 9.1) to find the suitable method, that is, the mode of estimation and CI construction that optimizes a selected measure for prescribed values close to the initial estimates. Also here, intelligent exploration methods (gradient, Brent, etc.) are useful. The third task is to apply the optimal estimation method to the climate time series.

9.6 Background Material

Timescale modelling has experienced a recent activation in the development of methods for constructing chronologies. The types of methods depend on the employed climate archive. As regards ice cores, Wheatley et al. (2012) presented an automated layer-counting method, which works in the presence of strong univariate signals. They tested their method on a recent instrumental record of hydrogen peroxide from Antarctica and applied it to the late Pleistocene NGRIP ice core records of ammonium and calcium from Greenland. Klauenberg et al. (2011) developed a Bayesian glaciological modelling approach, which simulates snow accumulation and ice deformation and which can take constraints into account, such as from layer counting. As regards speleothems, Scholz and Hoffmann (2011), Fohlmeister (2012) and Hercman and Pawlak (2012) presented, all in the journal Quaternary Geochronology, construction algorithms, see Sect. 4.5 for software links. Another algorithm (Hendy et al. 2012), presented for amino acid racemization dates (interconversion of amino acid types at a certain rate after death) obtained from corals, is applicable also to speleothem material. However, none of these algorithms is able to output on a routine basis, in addition to the best-fit agedepth curve, also simulated curves. Mudelsee et al. (2012) used two algorithms (Scholz and Hoffmann 2011; Fohlmeister 2012), adapted to output simulated curves, to analyse centennial-scale trends in western German climate (temperature and precipitation) over the later part of the Holocene. They utilized nonparametric kernel regression and standard-error band construction from MBB resampling with/without parametric timescale simulation to study effects of timescale errors (which were negligible). Also uncertainty in the form of the timescale model was minimal in case of the western German stalagmites (Mudelsee et al. 2012). A certain step constitutes the recent paper by Scholz et al. (2012), who compared by means of artificially generated series different algorithms of timescale construction. However, they looked only for the best algorithm in terms of an error measure. What remains to be done is a Monte Carlo comparison of algorithms in terms of coverage accuracy of the delivered confidence bands. As regards the tree-ring archive and radiocarbon dating, Blaauw (2010) and Blaauw and Heegaard (2012) review the previous papers critically, noting that (Blaauw 2010: p. 512 therein) "they are usually not explained sufficiently". Fraver et al. (2011) took into account tree growth for formulating and testing linear and nonlinear regression models on the basis of tree-ring counts.

Greenhouse gas emissions contribute a major part of the radiative forcing, $\mathbf{R}(i)$. It is difficult to quantify $\mathbf{R}(i)$ owing to the complexity of the system: components, such as carbon dioxide or methane, are part of the "nonlinear dynamical" carbon cycle, which shows threshold and feedback behaviour (Tans 2009). The carbon budget for the interval from 1959 to 2011 has been estimated and various climate forcing models assessed in their ability to reproduce the observations (Le Quéré et al. 2013). The future forcing, which depends on the modes of energy conversion ("peak oil") is considered by Murray and Hansen (2013).