

Exploring errors in paleoclimate proxy reconstructions

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Exploring errors in paleoclimate proxy reconstructions using Monte Carlo simulations: paleotemperature from mollusk and coral geochemistry

M. Carré¹, J. P. Sachs², J. M. Wallace³, and C. Favier¹

¹Institut des Sciences de l'Evolution, CNRS-UM2-IRD, UMR5554, Université Montpellier 2, Pl. Eugène Bataillon, 34095 Montpellier, France

²University of Washington, School of Oceanography, Box 355351, Seattle, WA 98195, USA

³University of Washington, Department of Atmospheric Sciences, Box 351640, Seattle, WA 98195, USA

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Correspondence to: M. Carré (matthieu.carre@univ-montp2.fr)

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Abstract

Reconstructions of the past climate from proxy records involve a wide range of uncertainties at every step of the process. These uncertainties and the subsequent error bar in the reconstruction of a paleoclimatic variable need to be understood and quantified in order to properly interpret the reconstructed variability and to perform meaningful comparisons with climate model outputs. Classic proxy calibration-validation techniques are not well-suited for identifying the causes of reconstruction errors, estimating their relative contribution, or understanding how errors accumulate from a multitude of sources. In this study, we focus on high resolution proxy records based on calcium carbonate geochemistry of sessile organisms such as mollusks, corals, or sclerosponges, and propose an approach based on Monte Carlo simulations with simple numerical surrogate proxies. A freely available algorithm (MoCo, <http://www.isem.cnrs.fr/spip.php?rubrique472>) is provided for estimating systematic and standard errors of mean temperature, seasonality and variance reconstructed from marine accretionary archive geochemistry. This algorithm is then used for sensitivity experiments in a case study to characterize and quantitatively evaluate the sensitivity of systematic and standard errors to sampling randomness, stochastic uncertainty sources and systematic proxy limitations. The results of the experiments yield an illustrative example of the range of variations that climate reconstruction errors may undergo, and bring to light their complexity. One of the main improvements of this method is the identification and estimation of systematic bias that would not otherwise be detected. It thus offers the possibility of correcting the proxy-based climate from these biases for a more accurate reconstruction. Beyond the findings of error sources for coral and mollusk-based reconstructions, our study demonstrates that numerical simulations based on Monte Carlo analyses are a simple and powerful approach to improve the proxy calibration process. A thorough understanding of the proxy record errors is essential for the interpretation of paleoclimate records from proxies derived from accretionary skeleton geochemistry. The error estimates provided by MoCo are

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much more comprehensive and therefore closer to reality than error estimates provided by typical calibration studies.

1 Introduction

Reconstructions of the past climate from proxy records involve a wide range of uncertainties at every step of the process. These uncertainties and the subsequent error bar in the reconstruction of a paleoclimatic variable need to be understood and quantified in order to properly interpret the reconstructed variability and to perform meaningful comparisons with climate model outputs. In a recent overview of methods used in high resolution paleoclimatology, Hughes and Ammann (2009) concluded that “*the study of the processes by which climate proxy records are formed [. . .] should be accorded high priority*”. Highly complex methods based on Bayesian statistics and involving biological models have been developed for pollen assemblages that provide a probability distribution of the paleoclimate reconstruction (Guiot et al., 2009). Considerable effort has also been devoted to statistically estimate the sensitivity of climate field reconstructions from tree rings to proxy uncertainties, the proxy network, and the calculation methods (Mann et al., 2005, 2007; Lee et al., 2008; Riedwyl et al., 2009). For many other proxies, and especially in paleo-oceanography, the climate proxy development work has been concentrated on the calculation of empirical regression models (or transfer functions) linking the proxies to the environmental variables. Then, in most studies, the uncertainty of the paleo-oceanographic variable reconstruction is estimated by the scattering of the empirical calibration dataset. Thus, in these cases, the reconstruction error bar is assumed to be identical in every application of the transfer function. We argue that, although essential, the empirical calibration-verification work only provides a first-order, generally underestimated, value of the error bar. The processes leading to a climate proxy record involve randomness and a suite of stochastic parameters operating at different scales of time and space, producing a range of potential deviation from the “true” climate that is much broader than that contained in the necessarily limited

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number of tests in a calibration-verification approach. There is growing agreement in the paleoclimate science community on the need for better methods to evaluate the uncertainties in climate proxy records (Jones et al., 2009).

In this study, we focus on high resolution proxy records based on calcium carbonate geochemistry of sessile organisms such as mollusks, corals, or sclerosponges. Short-term windows of monthly to decadal sea surface temperature (SST) can be re-constructed from these accretionary archives using paleo-temperature proxies such as Sr/Ca (Beck et al., 1992; Marshall and McCulloch, 2002; Corrège et al., 2004; Rosenheim et al, 2004) or $\delta^{18}\text{O}$ (Epstein et al., 1953; Grossman and Ku, 1986, Böhm et al., 2000; Carré et al., 2005) serially measured along the growth axis. In most works based on this technique, SSTs are calculated using an empirical regression model, verified with modern samples. The same error bar, assumed to be inherent to the proxy regression model, is ascribed to all data points. However, paleoclimatic interpretations are not based on a single data point, but rather on characteristics of the whole dataset (mean, variance, spectral power density), which is taken to be representative of the mean climate of a time period over a defined region. Even considering that the error bar was correctly estimated for single SST reconstructions, it is not readily applied to the statistical properties of the dataset. Here we develop a quantitative framework for evaluating how stochastic noise (analytic error, vital effect, weather, microenvironment heterogeneity, growth breaks . . .) and proxy-specific noise (physiological temperature tolerance, spawning growth breaks . . .) influence the statistical properties of paleoclimate data derived from mollusk, coral, and coralline sponge geochemistry.

We propose an approach based on Monte Carlo simulations with simple numerical surrogate proxies. Monte Carlo simulations have been used in previous studies (Brisquin and Harrell, 1980; Ballentine and Hall, 1999; Touchan et al., 1999; Meibom et al., 2003; Kaufman, 2003; Evans et al., 2007) to estimate the error of a paleoclimate reconstruction. The method is thus not novel but its use has been limited to the estimation of a raw uncertainty value. Here we aim to show how powerful this tool can be for performing sensitivity tests to explore the range of responses associated with a suite

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of stochastic parameters, and how it can significantly improve the understanding of the proxy signal and eventually the quality of the paleoclimate reconstruction. This technique is conceptually very simple compared to the full probabilistic modelling studies using Bayesian inferences that have been developed by statisticians for climate field reconstructions (Haslett et al., 2006; Jones et al., 2009). It is intended for use as an intermediate method, efficient enough to provide reliable assessments of paleoclimate errors, while being technically and conceptually accessible to a broad community in paleoclimate science.

Specifically, we provide a ready-to-use, parameterize-yourself, open access algorithm for estimating systematic and standard errors of mean temperature, seasonality and variance reconstructed from marine accretionary archive geochemistry (mollusks, corals, sclerosponges . . .). This algorithm is then used in a case study to characterize and quantitatively evaluate the sensitivity of systematic and standard errors to sampling randomness, stochastic uncertainty sources and systematic proxy limitations.

2 The surrogate paleoclimate proxy Monte Carlo algorithm for mollusks and corals (MoCo)

The starting hypothesis is that an empirical linear regression model, with no apparent systematic bias, is available for the calculation of a climate variable from a single geochemical proxy. This would thus apply to quaternary temperature reconstructions from Sr/Ca ratios measured in corals (Beck et al., 1992) and sclerosponges (Rosenheim et al., 2004), or to temperature reconstructions from coral $\delta^{18}\text{O}$ (Cobb et al., 2003) or mollusk shell $\delta^{18}\text{O}$ (Schöne et al., 2004) in conditions where the water isotopic composition can be constrained. As in all surrogate proxy (also referred to as “pseudo-proxy”) studies, the basic principle is to use a realistic climate time series, sample and perturb it in a way that mimics the proxy uncertainties, and compare the surrogate “reconstructed” climate with the “true” value, which is known from the original non perturbed time series (Mann and Rutherford, 2002).

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2.1 Different types of error

We explore both systematic and standard errors of statistical climate properties [annual mean T_m , variance of the annual mean $\text{var}(T_m)$, mean annual amplitude ΔT , variance of the annual amplitude $\text{var}(\Delta T)$] reconstructed from a random sample of specimens taken to be representative of a time period. T refers here to the reconstructed environmental variable, which could be temperature, salinity, pH or something else. Identifying and estimating systematic errors allows us to correct the reconstruction and improve its accuracy. A quantitative estimate of the standard deviation is also essential to determine a threshold of significance in the amplitude of the climate proxy variations.

Defining the error in a paleoclimate reconstruction from a local archive is not trivial. It may depend on the climate information sought. An ideal proxy would provide the exact temperature in a precise location and thus be considered as error-free, but if the aim is to have regional scale information, the proxy signal would still be noisy owing to micro-environment effects. Weather also contributes to the noise inherent in climate statistics. Thus some of the noise in the reconstruction is related to random sampling in time and space and is thus independent of the quality of the empirical regression model.

The formation of the proxy record involves a complex chain of physical and biological processes (for instance mechanisms of Strontium incorporation into coral aragonite) that introduce non-climate-related stochasticity and limitations in the climate-proxy relationship (Meibom et al., 2003). The scatter inherent in in situ calibration datasets partly captures this stochastic variability but does not allow the exploration of its full range nor the characterization of the error from different sources. Stochastic parameters may contribute to the standard error in the reconstruction of climate statistical properties as well as to systematic errors as we will show.

Paleoclimate reconstructions also involve systematic errors that cannot be estimated and corrected for, and could be referred to as potential systematic errors. Potential systematic errors include for instance the uncertainty of the ice volume effect when

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carbonate $\delta^{18}\text{O}$ is used as a paleotemperature proxy. They also include uncertainties in the proxy calibration model. Considering that the mechanisms behind such errors are identical for all specimens in the archive (which is generally assumed), then the model would be identically wrong for all the climate calculations. Therefore, the paleoclimate errors due to the imperfection of the model do not contribute to the standard error, but instead are more comparable to a systematic error (although its value might be linearly dependent on the proxy variable). Nevertheless, when the source of a potential systematic error can be identified, it may be possible to estimate statistically its impact on the reconstructed climate.

Owing to their different nature, and for a more complete representation of error, the standard error and the potential systematic error should be represented separately in paleoclimate results (Carré et al., 2011). Systematic errors that can be estimated should be corrected for. The MoCo algorithm yields estimates of the standard error, systematic error, and potential systematic error.

2.2 The Monte Carlo simulation

Monte Carlo techniques are useful for the analysis of complex stochastic systems (Metropolis and Ullam, 1949; Hastings, 1970). In our study, surrogate proxy records are produced by perturbing a known climate time series with a suite of random noise. Each surrogate proxy record is only of realization of the infinite number of values and combinations that noise can take. In the Monte Carlo simulation, this process is repeated many times (5000 iterations in the experiments presented here) in order to have a representative sample of the range of responses, and therefore of the probability distribution of the error (Fig. 1). The average value of the error population calculated in a Monte Carlo simulation represents the systematic error. If the reconstruction method is not biased, the mean value of the error population should be zero. If this is not the case, then a systematic bias has been identified and may be corrected for. The standard deviation of all the possible errors is by definition the standard error.

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2.3 Using the MoCo.m application

MoCo.m is freely available and can be downloaded at <http://www.isem.cnrs.fr/spip.php?rubrique472>, along with the MoCo_readme.txt file which contains step by step instructions for users. The program is designed to work with the Matlab software. The algorithm is parameterized by the user according to the specifics of the study. These input parameters are listed in table 1 and described in the next section.

3 Inputs to the algorithm

3.1 A target time series

When using the MoCo algorithm, a climate time series is first chosen that will be used as the “target climate”. As will be shown later, the characteristics of the target time series have a large influence on the reconstruction error. It is therefore important to use a realistic time series with a variability that is as far as possible similar to the paleoclimate that the proxy is being used to study. The length of the time series should be much longer than the typical proxy record length to allow adequate random sampling in time. For instance, if 50-yr long coral records are being used to study early Holocene climate, a time series of at least 1000 yr should be used as a target in the Monte Carlo simulation. Such a long time series can only be provided by climate models. Instrumental time series may be used for short-lived proxy archives such as one-year long mollusk shells. The target time series for proxies with sub-annual resolution should be monthly, starting in January, and include full years without missing data.

3.2 Random sampling of target time series

Once the target time series is identified, N time windows of N_y years are randomly extracted from it. N represents the sample size, or the number of specimens that were analyzed to study the paleoclimate. N_y is the typical duration (number of years) of the

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proxy records. Two approximations are made in this process: (1) the proxy record time resolution is assumed to be monthly and constant, (2) all specimens are assumed to have the same duration equal to N_y years.

3.3 Signal perturbation

5 In this step, the random sample of N climate time windows is perturbed by stochastic noise and by archive-related limitations.

3.3.1 Spatial heterogeneity

10 Corals, mollusks and sclerosponges, as sessile organisms, record only a very local environmental variability that may differ from the regional environmental variability. This effect is especially significant in coastal environments where large spatial heterogeneity can occur. Several specimens should thus be analyzed to average out this heterogeneity effect. In MoCo, this stochastic noise is represented by a random parameter with a normal distribution $N(0, \sigma_s)$. A random value is drawn for every specimen and added uniformly to the climate variable over the whole time window.

15 3.3.2 Monthly noise

20 MoCo provides for three additional sources of month-to-month noise: (1) the proxy analytical error, (2) the weather scale variability, (3) biogenic carbonate heterogeneity at the μm scale of microsampling owing to vital effects and diagenesis. These three types of noise follow the normal distributions $N(0, \sigma_a)$, $N(0, \sigma_w)$, $N(0, \sigma_c)$ respectively, where the standard deviation are expressed in the proxy unit (e.g. mmol/mol for coral Sr/Ca). These three independent sources of uncertainty add in quadrature and are converted to the climate unit to yield a month-to-month noise with normal distribution $N(0, \sigma_m)$ ($\sigma_m^2 = \sigma_a^2 + \sigma_w^2 + \sigma_c^2$). A random value is drawn for every monthly value of every time window. All the stochastic noise sources are here considered to be

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normally distributed because they are expected to have symmetric distributions, and each is comprised of a large number of stochastic processes.

3.3.3 Limitations of the biological archives

The archives considered in this study, corals, mollusks, sclerosponges, coralline algae, are living organisms. Their biology constrains their growth and thus the way in which they record the environment. Every species is defined by a range of physico-chemical tolerances beyond which they stop precipitating new carbonate skeletal material. If it is possible that the reconstructed variable may represent a growth limitation (like temperature or salinity) the effect of these limits should be explored and quantified. Upper and lower biological limits (Tls , Tli) for the variable T are thus considered in MoCo.

Some species systematically stop growing at a precise period of the year because their resources are exclusively dedicated to reproduction. This implies a systematic gap in the record that may affect the final calculated averages or variance. Parameters gb1 to gb12 define the typical monthly growth pattern of the species (Table 1).

Finally, growth breaks may occur randomly because of storms, predation, or sickness. The MoCo program allows the choice of occurrence of zero to 12 random growth breaks per year.

3.4 Proxy model calibration dataset

Here we only consider linear regression models between the reconstructed variable T and the proxy P : $T = \alpha.P + \beta$, which is the most common case for proxies used on biocarbonate accretionary skeletons. The calculation of the potential systematic errors related to the uncertainty of the regression model is based on the 95 % confidence interval of parameters α and β :

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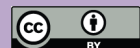
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$$I(\text{alpha}) = \pm t \cdot \frac{\sigma_T}{\sigma_P} \cdot \sqrt{\frac{(1-R^2)}{Nc-2}} \quad , \quad I(\text{beta}) = \pm t \cdot \sigma_T \cdot \sqrt{\frac{(1-R^2)}{Nc-2}} \quad (1)$$

Where Nc is the number of data points in the calibration dataset, σ_T and σ_P the standard deviations of T and P respectively in the calibration dataset, R is the Pearson's correlation coefficient, and t is the value of the Student variable at the 0.05 confidence level and $Nc-2$ degrees of freedom.

4 Sensitivity experiments

Five sensitivity experiments were performed using the MoCo algorithm to explore the influence of (1) the random sampling (exp. 1 and 2), (2) stochastic perturbations (exp. 1, 2, and 3), (3) the biological limitations of the archive (exp. 4 and 5), and (4) the target time series (exp. 3, 4, and 5) on the systematic and standard errors when reconstructing the statistical characteristics of the target time series (T_m , $\text{var}(T_m)$, ΔT , $\text{var}(\Delta T)$). To perform these experiments we chose the illustrative case study of temperature reconstructions in the eastern Pacific from mollusk shell oxygen isotopes. We used the empirical proxy model established by Grossmann and Ku (1986) for biogenic aragonite (Eq. 2), which is often considered as the definition of isotopic equilibrium for biogenic aragonite and has been widely used for paleoclimate studies from aragonitic mollusk shells:

$$T(^{\circ}\text{C}) = 19.73 - 4.34(\delta^{18}\text{O}_{\text{arag.}} - \delta^{18}\text{O}_w) \quad (2)$$

$\delta^{18}\text{O}_{\text{arag.}}$ and $\delta^{18}\text{O}_w$ are expressed in ‰ versus the V-PDB and V-SMOW standards respectively. This proxy model is used only for the case study. Any other proxy model could be used with MoCo. The biological characteristics of the species (growth breaks, temperature tolerance range, length of record ...) are varied in the experiments to evaluate their influence on the reconstruction climate parameter.

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Three sea surface temperature (SST) time series were used as “target” climatology: (1) the 1925–2002 monthly in situ instrumental record from Puerto Chicama, Peru (measured by IMARPE), (2) the 1950–2009 monthly SST time series of the Niño1+2 area (both time series are available at http://jisao.washington.edu/data_sets/#time_series), and (3) the 1000-yr long monthly SST time series of the Niño1+2 area from the preindustrial control simulation of the IPSL_CM4v2 coupled ocean atmosphere general circulation model (GCM) (for details about the simulation, see Servonnat et al., 2010). The target time series are presented in Table 2. The first 2 time series were used in all experiments except for the experiment 2 in which the GCM time series was used (Table 3). The parameterization of the sensitivity experiments are summarized in Table 3.

4.1 Experiment 1: Influence of random sampling and stochastic noise

The first experiment was designed to test the effect of sampling on the standard and systematic errors and compare it to the effect of three stochastic noises that were turned off or on. Realistic values were assigned to σ_s (spatial heterogeneity) and σ_m (month-to-month noise) based on field measurements on the Peruvian coast. In this experiment, shell records span one year and no biological limitations were included.

4.2 Experiment 2: Influence of the record length

Experiment 2 was designed to explore the effect of the record length on the skill of the reconstructions considering the existence of realistic stochastic perturbations of the proxy signal. No biological limitations were included. The record length N_y ranged from 1 to 200 yr as would be expected for coral-based records, and the total number of years $N*N_y$ recorded by the sample was held constant at 200 yr. No instrumental record was long enough for this experiment so a 1000 yr long pre-industrial OA-GCM simulation of the Niño1+2 SSTs was used as a monthly target time series.

4.3 Experiment 3: Influence of month-to-month noise

Experiment 3 explored further the effect of the individual data point quality degraded by the monthly noise, characterized by σm , which includes the analytical error, weather scale noise, and skeletal carbonate heterogeneity. Here, all perturbations were turned off and all parameters were fixed except for σm which varied from 0 (ideal proxy) to 0.5%. Simulations were performed with samples of 20 one-year long shells, and two different target time series.

4.4 Experiment 4: Influence of a growth break

Experiment 4 was designed to test the effect of yearly growth breaks (such as spawning growth breaks) on reconstruction errors. All other perturbations were turned off and all parameters except gbi were fixed. We only considered the case of a single one-month growth break per year, and compared the effect of varying its month of occurrence. Simulations were performed with samples of 20 one-year long shells, and with two different target time series.

4.5 Experiment 5: influence of temperature tolerance range

In experiment 5, we explored the effect of temperature limits on skeletal growth for the reconstruction of two target time series. Obviously, the reconstruction would not be affected if the biological temperature limits are outside the temperature range of the time series. Therefore, in this experiment, the upper (lower) temperature limit ranged from the maximum (minimum) temperature $T_{\max}(T_{\min})$ of the target time series to $T_{\max} - 10^{\circ}\text{C}$ ($T_{\min} + 10^{\circ}\text{C}$). All other perturbations were turned off and all parameters except Tls and Tli were fixed. Simulations were performed with samples of 20 one-year long shells.

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5 Results

5.1 Potential systematic error

The MoCo program calculates the potential systematic error due to errors in the linear proxy model calibration. This error not only depends on the proxy model but also on the target climate. When calculating the mean temperature for instance, the error increases with the difference between the reconstructed conditions and the calibration dataset mean value. The mean value T_0 of Grossmann and Ku's (1986) dataset was 10.5 °C. When using the Puerto Chicama time series ($T_m = 17.1$ °C), the error for T_m reconstruction due to the proxy model only is ± 2.1 °C (95 % confidence level). This error increases to ± 3.9 °C with the Niño1+2 time series ($T_m = 23.0$ °C). These uncertainties are so large because the target temperature range is far from the temperature calibration range. If the mean value of the target time series was 11 °C, the uncertainty at 95 % confidence level would only be ± 0.4 °C. The error for the mean seasonal amplitude (ΔT) was also significant for Puerto Chicama (± 1.4 °C) and for Niño1+2 (± 1.9 °C) time series. This confirms the importance of local specific calibration works to minimize this type of errors.

5.2 Random sampling (Exp. 1 and 2)

In experiment 1, the effect of random sampling is quantitatively estimated and compared to the stochastic proxy uncertainties (Fig. 2). The effect of sampling only is represented in Fig. 2 by the "ideal proxy" curves. It appears that random sampling is one of the main sources of the standard error. This error decreases rapidly with the sample size and becomes relatively insignificant for T_m and ΔT when N reaches 20. On the other hand, the standard error for $\text{var}(T_m)$ and $\text{var}(\Delta T)$ due to sampling remains relatively significant up to $N = 30$.

In experiment 2, we test whether reconstructions from long proxy records are more reliable than reconstructions obtained from short proxy records. The total number of

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years recorded ($N \cdot N_y$) is kept constant and equal to 200 in order to test only the influence of the record length. For regional mean temperature (T_m) reconstructions, it appears that a large sample set of short records provides a more precise estimate than a few long records. This result is due to the influence of local spatial temperature heterogeneity which is averaged with large sample sets but represents a significant error when determined from a single record. In a similar way, the spatial variance tends to overwhelm the climatic variability $\text{var}(T_m)$ when the sample is small, unless it is calculated from a single record (Fig. 3, $N = 1$, $N_y = 200$). Systematic errors are only affected by record length in the case of $\text{var}(T_m)$. While the annual temperature variance is overestimated with short records because of the additional spatial variance, this effect decreases when the record lengthens. Finally it appears that intermediate values of N and N_y (here 20 10-yr old shells) would yield the best compromise for accuracy and precision in the reconstruction of T_m and $\text{var}(T_m)$. The reconstruction skills for ΔT , and $\text{var}(\Delta T)$ are not significantly affected by the record length in our experiment.

5.3 Effects of stochastic noise (Exp. 1, 2, and 3)

Three kinds of stochastic perturbations (see Sect. 2.3.3.) are applied to the climate signal in experiments 1, 2, and 3. In the first experiment, their influence is observed separately and compared to ideal proxy reconstruction errors. As expected, spatial variability greatly affects the standard error of the T_m reconstruction (Fig. 2) and this effect increases with the record length (Fig. 3). It also induces a systematic positive bias for the $\text{var}(T_m)$ reconstruction which decreases with record length (Fig. 3). The monthly variability in experiment 1 does not significantly affect the T_m and $\text{var}(T_m)$ reconstructions but it induces an unexpected overestimation of the annual amplitude ΔT and of its variance (Fig. 2). This latter effect does not depend significantly on the record length (Fig. 3). Random growth breaks have no significant impact on the standard error (Fig. 2). They induce a slight positive bias in $\text{var}(T_m)$ and a slight negative bias in ΔT . These bias are due to the time series properties since they are not observed when using the Puerto Chicama time series (not shown).

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In our case study, the stochastic perturbation at the data point level characterized by σm involves monthly water $\delta^{18}\text{O}$ variability, carbonate $\delta^{18}\text{O}$ analytic error, and shell carbonate heterogeneity. Its effect on ΔT and $\text{var}(\Delta T)$ reconstructions is further explored in experiment 3 (Fig. 4) using two different target SST time series. In our experiment, the maximum value of σm is 0.5‰ (or 2.2°C on the temperature scale) which represents an extremely noisy proxy record. The systematic positive bias on ΔT estimate is $\sim 1^\circ\text{C}$ when $\sigma m = 0.1\%$ and increases to 3°C when $\sigma m = 0.4\%$. For other parameters, the response depends on the target time series. For $\sigma m = 0.2\%$, the systematic error for $\text{var}(\Delta T)$ is about 100% for the Niño1+2 time series while it is almost null for the Puerto Chicama time series. Standard errors for Niño1+2 SSTs are more sensitive to the monthly noise than those for Puerto Chicama SSTs. This can be explained by the higher variability of Puerto Chicama (Table 2), which makes the noise-related variability relatively smaller.

5.4 Effects of biological limitations (Exp. 4 and 5)

Growth hiatuses may occur every year at approximately the same date for breeding or other reasons (Sato et al., 1999). In experiment 4 (Fig. 5), we showed that the date of the growth break has little impact on the paleoclimate reconstruction standard error but may produce systematic errors. As expected, the mean annual temperature would be underestimated (overestimated) if the growth breaks occur in the warmest (coldest) period. Here, the maximum systematic error for Tm was -0.3°C . The annual amplitude may be largely underestimated if the growth hiatuses occur during seasonal extrema. In our experiment the systematic bias for ΔT reached -0.4°C with a systematic growth break in March for the Niño1+2 SST time series. Proxy reconstructions of variances were affected by growth hiatuses in a much less predictable way. For Puerto Chicama SSTs, maximum systematic errors reached about 8% for $\text{var}(Tm)$ when growth breaks occurred in September and 8% for $\text{var}(\Delta T)$ if they occurred in December. Again, the error was strongly dependent on the target time series.

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Temperature tolerance for skeletal growth is an especially important biological limitation that may induce significant systematic biases in paleoclimate reconstructions. These biases were explored with 2 different time series in experiment 5 (Fig. 6). While it is obvious that upper (lower) temperature limits cause underestimation (overestimation) of the mean temperature T_m , and that ΔT is in both cases underestimated, our experiment permits calculation of a quantitative estimate of this error. In experiment 5, the systematic error responses to lower and upper limits were not symmetrical. For Niño1+2, the effect of the lower temperature limit began to be significant when it reached $\sim 1.5^\circ\text{C}$ above the minimum temperature, whereas the effect of the upper limit began to be significant when it reached $\sim 3^\circ\text{C}$ under the maximum temperature. The systematic biases produced for $\text{var}(T_m)$ and $\text{var}(\Delta T)$ reconstructions rapidly became significant and had unpredictable profiles, switching from positive to negative values (Fig. 6), especially for the lower temperature limit.

5.5 Importance of the target time series (exp 3, 4, and 5)

The results of experiments 3, 4, and 5 showed that the error strongly depends on the climate time series used as a target in the experiment because it depends on the probability density function of the temperature. The Puerto Chicama time series has a much wider distribution than the Niño1+2 time series (Table 2) so that standard error due to random sampling is much larger for Puerto Chicama (Fig. 4 ($\sigma_m = 0$); Fig. 5). Target temperature distributions are also differently affected by proxy uncertainties, which generates different error responses (Figs. 4, 5, 6). In the three experiments, the error responses to proxy uncertainties were strongly modulated by the characteristics of the target time series. The same proxy perturbation may induce strong errors with one time series and be insignificant with another. For instance, the upper growth temperature limit had no significant effect on the reconstruction of T_m and ΔT until it reached $\sim 6^\circ\text{C}$ under the maximum value of the Puerto Chicama SST (Fig. 6) because of the highly asymmetric distribution of temperature due to El Niño phenomenon at this

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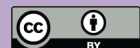
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location. These results show that the choice of the target time series when using MoCo to estimate paleoclimate reconstruction errors is a critical step.

6 Discussion

6.1 Implications for paleoclimate error representation

5 Three types of errors have been distinguished in this study that should all be treated and represented explicitly. Standard error is the classic error bar. However, while the error bar is generally represented for individual data points (σm in our case study), it is generally not even mentioned for variables calculated from the whole dataset (Tm , $\text{var}(Tm)$, ΔT , and $\text{var}(\Delta T)$), as if it was implicitly considered to be the same as for individual data points. Our experiments show how the standard error for statistical characteristics (Tm , $\text{var}(Tm)$, ΔT , and $\text{var}(\Delta T)$) is related to σm (Fig. 4), but they also show how distinct and how much more complex it is. Monte Carlo simulations are reliable and simple tools to explore issues with this level of stochasticity and complexity.

15 Systematic errors are meant to be corrected for when detected and quantified, and thus are not supposed to be represented. Systematic errors whose probability distributions only can be estimated, referred to here as potential systematic errors, should be represented separately from the standard error. In our case study, they include the error due to flaws in the proxy model and uncertainty about the regional ice volume effect on sea water $\delta^{18}\text{O}$.

20 6.2 Understanding the proxy

In many paleoceanographic studies, a precision value is attributed to the paleoclimate proxy estimates similar to that for instrumental data. Our numerical experiments simulating the process of paleoclimate reconstruction from coral or mollusk shell geochemistry show that the error cannot be considered a constant value characteristic of

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the proxy. Stochastic uncertainties and biological limitations significantly affect the resulting climate reconstruction, in different manners depending on the location and the climate parameter. Errors are affected by proxy uncertainties in a way that is so sensitive to the parameterization and to the target time series that no general relationships between errors and signal perturbations should be concluded from these experiments.

The results of the experiments, however, yield an illustrative example of the range of variations that climate reconstruction errors may undergo, and bring to light their complexity. Classic calibration-validation techniques are not well-suited for identifying the causes of reconstruction errors, estimating their relative contribution, or understanding how errors accumulate from a multitude of sources.

While the influences of several sources of error were qualitatively predictable, some perturbations produced significant unpredictable systematic bias (Figs. 4, 5, 6). Beyond the findings of error sources for coral and mollusk-based reconstructions, our study demonstrates that numerical simulations based on Monte Carlo analyses are a simple and powerful approach to improve the proxy calibration process. A thorough understanding of the proxy record errors is essential for the interpretation of paleoclimate records from proxies derived from accretionary skeleton geochemistry.

6.3 Quantifying errors

Quantifying errors in paleoclimate reconstructions is essential for accurate and meaningful proxy-proxy and proxy-model comparisons. The MoCo algorithm was designed to provide quantitative estimates of the three kinds of errors identified in Sect. 2.1 for coral and mollusk based climate reconstructions. It implies that the linear proxy model has been previously validated. The accuracy of the error quantification using MoCo may be limited in three ways:

the model for the paleoclimate reconstruction process implies simplifications including: (1) proxy records in a sample are considered of equal duration and of constant monthly resolution, (2) stochastic noise was represented by stationary normal distributions.

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The full parameterization of MoCo by the user requires field measurements and knowledge of the organism ecology and growth. Uncertainties in σ_s , σ_m , T_{li} or T_{ls} estimates may affect the quantification of errors.

By definition in paleoclimatology, the true target climate is unknown, and therefore different from the target time series used in the MoCo simulation. The errors calculated by the simulation are therefore not true errors but only estimates whose accuracy depends on the similarity between the true past climate and the target time series. In the selection process for the simulation target time series, it is recommended to seek high temporal variability so that errors will not be underestimated. Despite these caveats, and even if the user-defined inputs are imperfect, the error estimates provided by MoCo are much more comprehensive and therefore closer to reality than error estimates provided by typical calibration studies. One of the main improvements of this method is the identification and estimation of systematic bias that would not otherwise be detected. It thus offers the possibility of correcting the proxy-based climate from these biases for a more accurate reconstruction.

6.4 Extending applications

Sensitivity experiments were based on an illustrative case study of SST reconstruction from mollusk or coral $\delta^{18}\text{O}$ in an environment where water $\delta^{18}\text{O}$ is reasonably constrained. The same kind of experiment would improve the understanding of other proxies including temperature reconstructions from Sr/Ca ratios in corals (Beck et al., 1992; De Villiers et al., 1994; Marshall and McCulloch, 2002) and sclerosponges (Swart et al., 2002; Rosenheim et al., 2004), Mg/Ca ratios in coralline algae (Kamenos et al., 2008), and pH from coral $\delta^{11}\text{B}$ (Rollion-Bard et al., 2011).

In many environments, biocarbonate $\delta^{18}\text{O}$ variations yield a mixed signal between water temperature and water $\delta^{18}\text{O}$ variations related to freshwater input. Under such conditions, proxy uncertainties should be evaluated in the space of the proxy variable ($\delta^{18}\text{O}_{\text{carb}}$) using an adapted version of the Monte Carlo simulation in the MoCo algorithm. This requires a target time series of $\delta^{18}\text{O}_{\text{carb}}$ calculated from temperature and

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water $\delta^{18}\text{O}$ time series. This approach, referred to as forward modelling, has been applied to a variety of proxies, such as planktonic foraminifera $\delta^{18}\text{O}$ (Schmidt, 1999), or stalagmite $\delta^{18}\text{O}$ (Baker and Bradley, 2010). The strength of forward modeling that incorporates Monte Carlo analyses for paleoclimate proxy calibration was showed by Evans (2007) through a case study with wood cellulose $\delta^{18}\text{O}$. To our knowledge it has never been applied to corals or mollusks. MoCo-type algorithms would be especially useful for exploring the error of salinity or water $\delta^{18}\text{O}$ reconstructions based on the combination of coral $\delta^{18}\text{O}$ and Sr/Ca ratios, since both proxies add and propagate in an unpredictable way.

7 Conclusions

We demonstrated that proxy climate reconstructions from biocarbonate accretionary skeleton geochemistry involve errors that are much more complex and potentially larger than those estimated from empirical calibration scatter. We showed in an illustrative case study that surrogate proxy techniques associated with Monte Carlo analyses are powerful tools to improve the understanding and calibration of proxy records. Sensitivity experiments showed the significant and often unpredictable influence of random sampling, stochastic proxy perturbations, archive biological limitations, and the climate characteristics. These numerical experiments are a fast and efficient technique for a qualitative assessment of these influences and provide a first-order quantitative approximation of the reconstruction errors. We provided an open access Matlab algorithm, MoCo.m, available at <http://www.isem.cnrs.fr/spip.php?rubrique472>, for quantitatively estimating the error related to the proxy linear model, systematic biases, and the standard errors for proxy-based climate reconstructions. Although the algorithm is a very simple model of the climate reconstruction process, it allows significant improvement in the evaluation of the reconstruction uncertainties. Its conceptual simplicity should allow it to be used and adapted for a wide range of applications in paleoclimate research involving, among other archives, corals, mollusks, sclerosponges and coralline algae.

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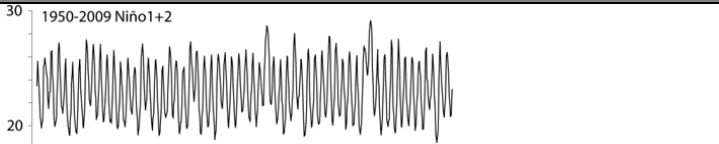
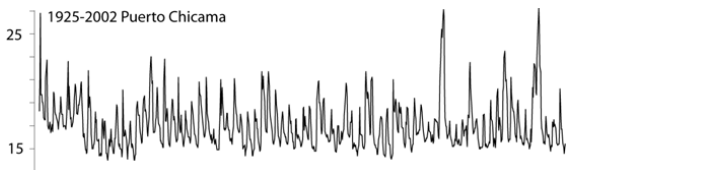
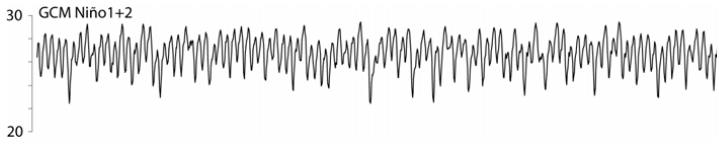
**Table 1.** MoCo input parameters.

Parameters	Description	Type
<i>Monte Carlo analysis</i>		
N	Number of specimen per sample	Integer
N_y	Number of years spanned by individual records	Integer
Tls	Biological superior limit for skeletal growth	Real (T unit)
Tli	Biological inferior limit for skeletal growth	Real (T unit)
$gbi, i=1$ to 12	Does skeletal growth occur during month i ?	0/1
gap	How many random 1-month growth gaps per year ?	0/1
σ_s	Standard deviation of spatial T variations	Real (T unit)
σ_w	standard deviation of weather monthly noise	Real (P unit)
σ_c	standard deviation of carbonate micro-heterogeneity	Real (P unit)
σ_a	Analytical error (1σ)	Real (P unit)
$Niter$	Number of iteration of the Monte Carlo analysis	Integer
<i>Proxy model calibration</i>		
α	Slope of the linear proxy model	Real (T/P unit)
β	Intercept of the linear proxy model	Real (T unit)
σ_T	Standard deviation of T in calibration dataset	Real (T unit)
σ_P	Standard deviation of P in calibration dataset	Real (P unit)
R	Pearson's correlation coefficient in calibration dataset	Real in $[0, 1]$
N_c	Number of datapoints in calibration dataset	Integer
T_0	Average value of T in calibration dataset	Real (T unit)

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Table 2. Characteristics of monthly SST time series used as target in sensitivity experiments. Only the first 100 yr of the GCM Niño1+2 SST time series are shown.

Monthly SST target time series	T_m	$\text{var}(T_m)$	ΔT	$\text{var}(\Delta T)$
 <p>1950-2009 Niño1+2</p>	23.0	0.8	6.2	0.8
 <p>1925-2002 Puerto Chicama</p>	17.1	1.6	4.5	4.3
 <p>GCM Niño1+2</p>	26.8	0.3	3.4	0.8

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Table 3. Parameter setting in sensitivity experiments 1 to 5. Gray cells indicate varying parameters.

Parameters	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 5
<i>Parameters of Monte Carlo analyses</i>					
<i>N</i>	1 to 30	1 to 200 ^b	20	20	20
<i>N_y</i>	1	1 to 200	1	1	1
<i>T_ls</i>	100	100	100	100	$T_{\max} - 10$ to T_{\max}^c
<i>T_li</i>	0	0	0	0	T_{\min} to $T_{\min} + 10$ ^c
<i>g_bi, i=1 to 12</i>	1	1	1	0/1	1
<i>gap</i>	0/1	1	0	0	0
<i>σ_s</i>	0/1.5	1.5	0	0	0
<i>σ_m^a</i>	0/0.14	0.17	0 to 0.5	0	0
<i>N_{iter}</i>	5000	5000	5000	5000	5000
<i>Target SST time series</i>					
1950–2009 Niño1+2	x		x	x	x
1950–2002 Puerto Chicama	x		x	x	x
GCM Niño 1+2		x			

^a $\sigma_m^2 = \sigma_a^2 + \sigma_w^2 + \sigma_c^2$.

^b $N \cdot N_y = 200$.

^c T_{\max} and T_{\min} are the maximum and minimum temperature values of the SST time series used as a “target”.

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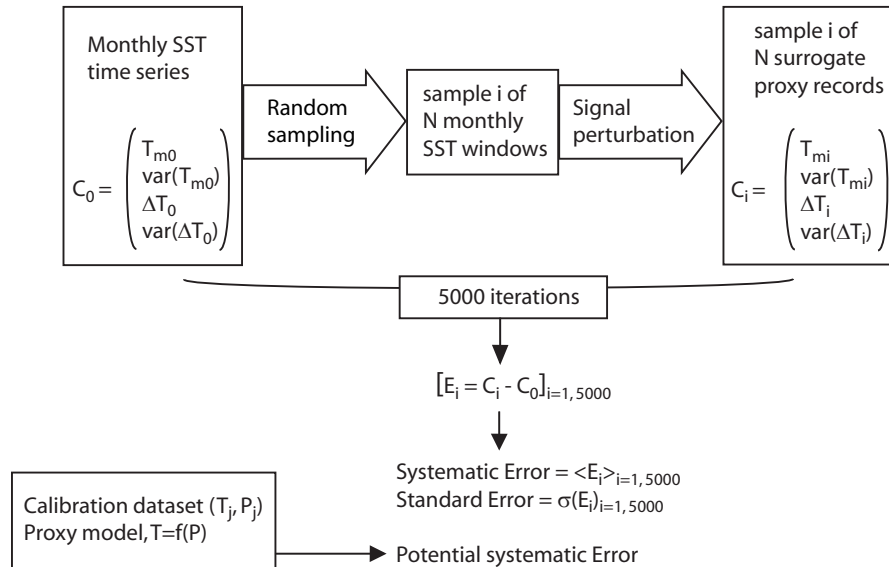


Fig. 1. Conceptual representation of the calculation of reconstruction errors in the MoCo algorithm.

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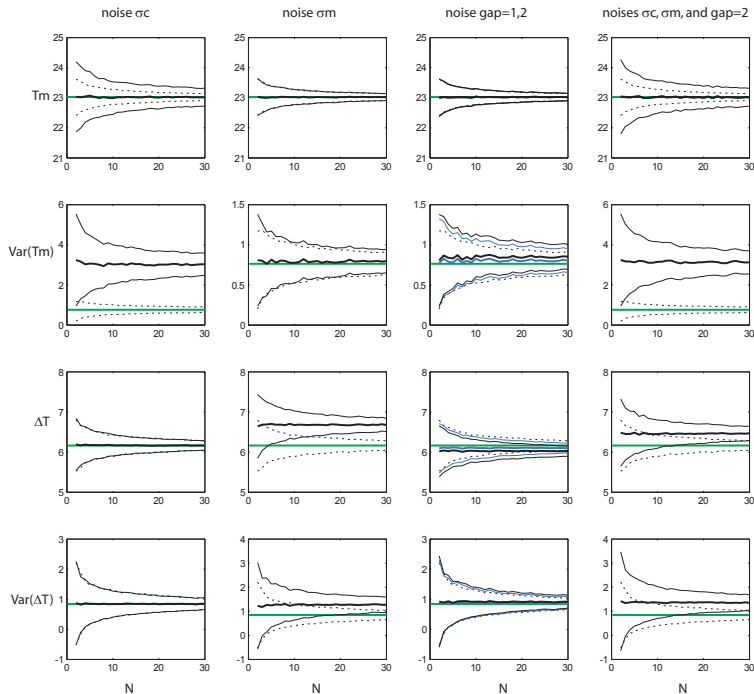


Fig. 2. Results of experiment 1 with the 1950–2009 Niño1+2 SST time series. Mean values of T_m , $\text{var}(T_m)$, ΔT , and $\text{var}(\Delta T)$ (black bold lines) calculated from 5000 iterations of surrogate proxy simulations (MoCo algorithm), and compared to the expected values (green) of the target time series, versus the sample size (e.g. number of shells). Systematic errors are indicated by the difference between the mean calculated value and the expected value. Dotted lines show the standard error interval ($\pm 1\sigma$) for an ideal proxy (no signal perturbation) versus the sample size. Thin black lines show the standard error interval ($\pm 1\sigma$) for surrogate proxies with stochastic noise. In the first three columns, the effects of spatial variability (σ_s), monthly variability (σ_m), and the occurrence of random growth breaks (blue: 1 per year, black: 2 per year) are investigated separately. Their effects are combined in the fourth column.

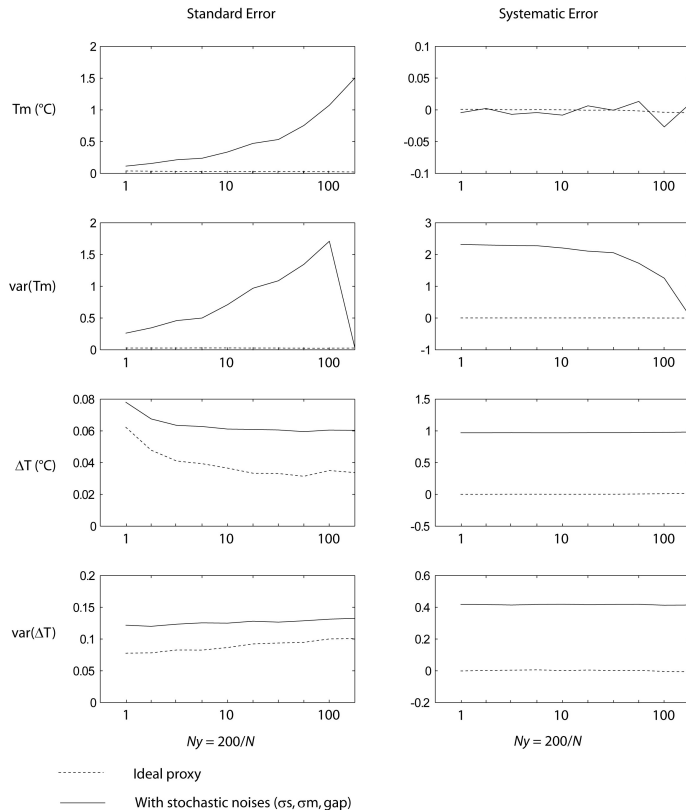


Fig. 3. Results of experiment 2 with the 1950–2009 Niño1+2 SST time series. Standard error (left) and systematic error (right) obtained for the reconstruction of T_m , $\text{var}(T_m)$, ΔT , and $\text{var}(\Delta T)$ using the MoCo algorithm, versus the length (number of years) of the proxy record, considering a constant number of 200 recorded years (from 200 one-year old shells to one 200-years old shell). Results using an ideal proxy (dotted line) were compared to results involving stochastic noise (black line).

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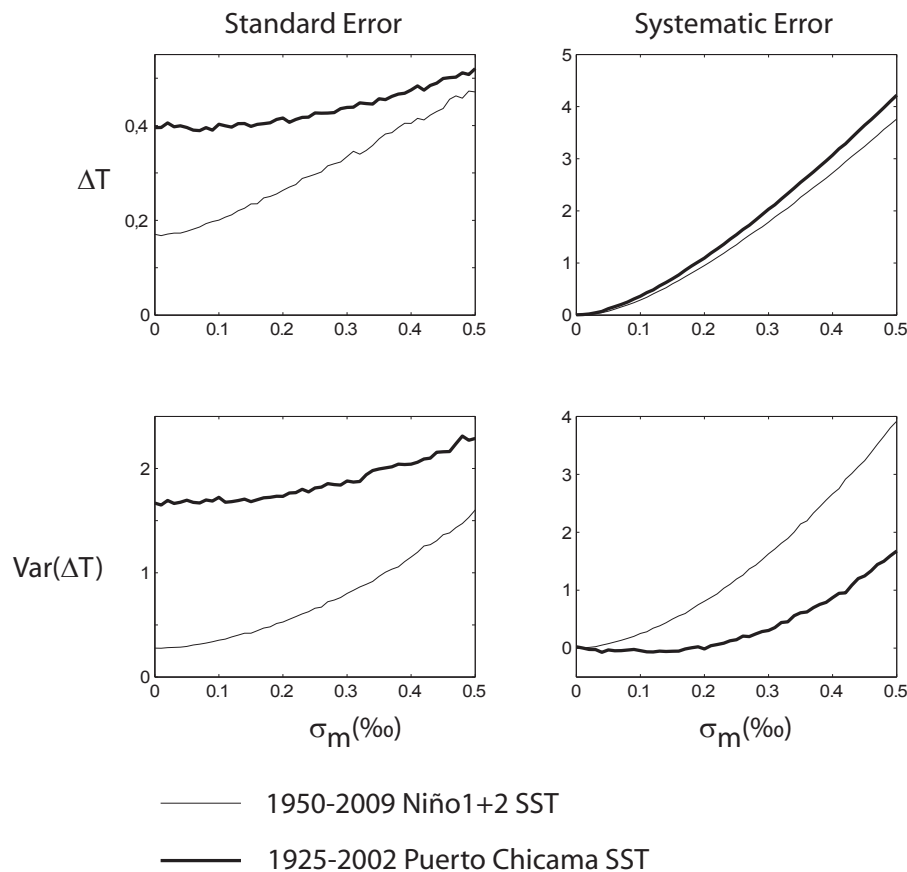


Fig. 4. Results of experiment 3. Standard error and systematic error for ΔT and $\text{var}(\Delta T)$ versus the standard deviation of the monthly stochastic perturbation. The effect was investigated using the 1950–2009 Niño1+2 (thin line) and the 1925–2002 Puerto Chicama (bold line) time series.

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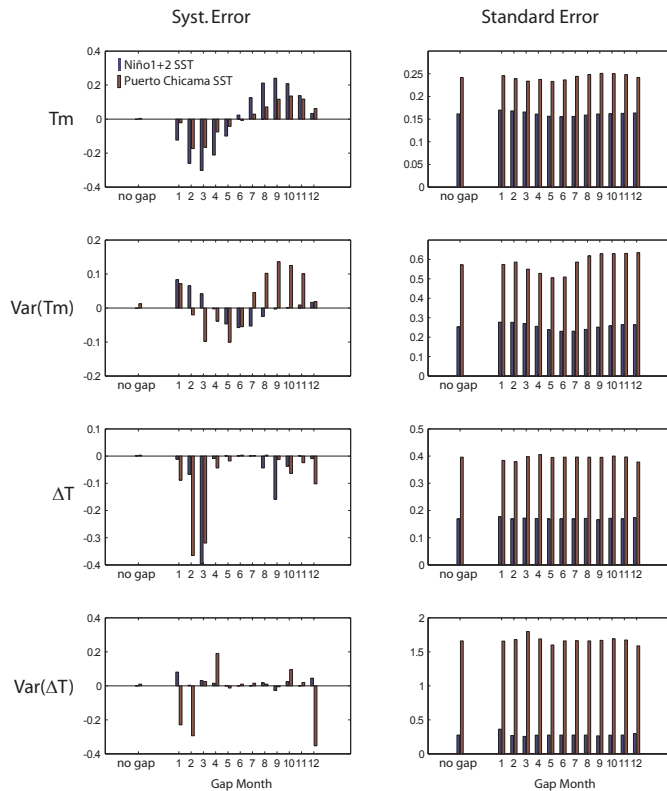


Fig. 5. Results of experiment 4. Standard and systematic errors for proxy reconstruction of T_m , $\text{var}(T_m)$, ΔT , and $\text{var}(\Delta T)$ of Niño1+2 SSTs (blue) and Puerto Chicama SSTs (red), versus the month of systematic growth hiatuses.

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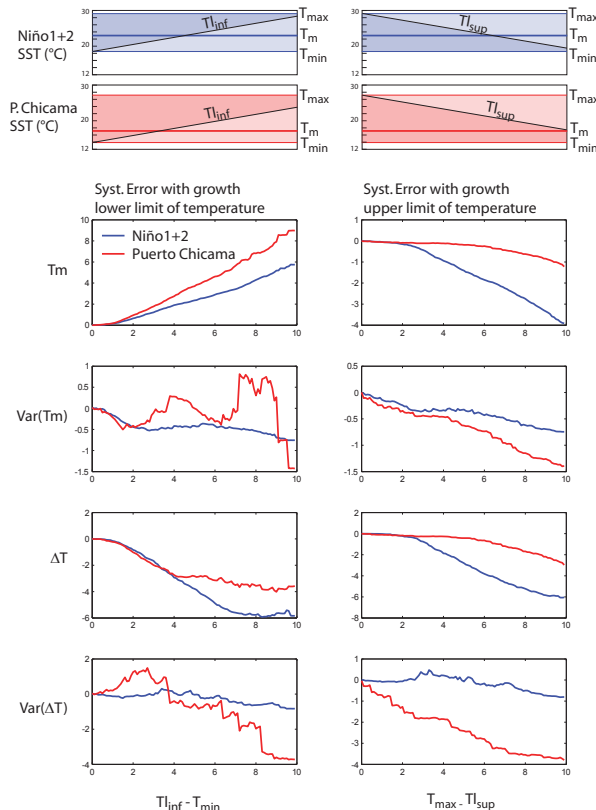


Fig. 6. Results of experiment 5. Systematic errors for T_m , $\text{var}(T_m)$, ΔT , and $\text{var}(\Delta T)$ due to growth temperature limits. The effects of inferior (superior) temperature limits are shown on the left (right). In the upper panels are indicated the temperature ranges of Niño1+2 SSTs (blue) and Puerto Chicama SSTs (red). The darker intervals show the range of temperature recorded by the archive limited by T_{li} (left) and T_{ls} (right).

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