

Optimal multiproxy reconstruction of sea surface temperature from corals

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[1] Past sea surface temperatures have been reconstructed using coral measurements of single geochemical proxies. There is some interest in improving reconstruction by combining results from different proxies. The construction of the optimal multiproxy reconstruction is described. The approach is illustrated using some data from New Caledonia. *INDEX TERMS*: 1050 Geochemistry: Marine geochemistry (4835, 4850); 4221 Oceanography: General: Dendrochronology; 4267 Oceanography: General: Paleooceanography; *KEYWORDS*: multiproxy, sea surface temperature

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1. Introduction

[2] A variety of geochemical measurements in coral skeletons have been used to reconstruct past sea surface temperatures [Beck *et al.*, 1992; Fairbanks *et al.*, 1997; Gagan *et al.*, 2000]. Although most studies use a single geochemical proxy, there is some interest in combining the results from different proxies to improve SST reconstruction. In a recent paper, Quinn and Sampson [2002] found that simply averaging the results for different proxies did not improve SST reconstruction, in the sense that this average performed worse than the best single-proxy reconstruction.

[3] In general, simple averaging is not the best way to combine single-proxy SST reconstructions. The purpose of this note is to outline the optimal multiproxy reconstruction. The optimal multiproxy reconstruction performs at least as well as the best single-proxy reconstruction. We illustrate the method using the data from Quinn and Sampson [2002].

2. Optimal Multiproxy Reconstruction

[4] Suppose that there are n proxies and let Y_j denote the measured value of proxy j . These proxies are assumed to be related to the corresponding SST through the linear regression models:

$$Y_j = \alpha_j + \beta_j \text{SST} + \varepsilon_j \quad j = 1, \dots, n, \quad (1)$$

where α_j and β_j are regression parameters and ε_j is a random error with mean 0 and variance σ_j^2 . The error ε_j includes both measurement error and natural variability in Y_j unrelated to variations in SST. As the source of this natural variability may affect more than one proxy, the errors in different proxies may not be independent. To account for this possibility, let ρ_{jk} be the correlation between ε_j and ε_k . Note that this is not the direct correlation between proxies j and k , but the correlation between the variations in these proxies once the SST effect on each has been removed.

[5] Suppose now that measurements of the n proxies are made at the same location in the coral skeleton. Let Y_j^o denote the measurement of proxy j at this location. Interest centers on using these measurements to reconstruct the corresponding sea surface temperature SST^o . The reconstruction based on proxy j alone is given by:

$$\hat{\text{SST}}_j^o = \frac{Y_j^o - \alpha_j}{\beta_j} \cong \text{SST}^o + \frac{\varepsilon_j^o}{\beta_j}, \quad (2)$$

where ε_j^o is the (unobserved) error in Y_j^o . This reconstruction is approximately unbiased and has approximate variance:

$$\text{Var}(\hat{\text{SST}}_j^o) \cong \sigma_j^2 / \beta_j^2. \quad (3)$$

Furthermore, the covariance between $\hat{\text{SST}}_j^o$ and $\hat{\text{SST}}_k^o$ is approximately:

$$\text{Cov}(\hat{\text{SST}}_j^o, \hat{\text{SST}}_k^o) \cong \rho_{jk} \sigma_j \sigma_k / \beta_j \beta_k. \quad (4)$$

[6] Consider now a multiproxy reconstruction of SST^o formed by a linear combination of the single-proxy reconstructions:

$$\hat{\text{SST}}_{\text{multi}}^o = \sum_{j=1}^n w_j \hat{\text{SST}}_j^o, \quad (5)$$

Table 1. Standard Deviations of SST Reconstruction Errors ($^{\circ}\text{C}$)

| Parameter | Value |
|-----------|-------|
| U/Ca | 2.17 |
| Mg/Ca | 1.49 |
| Sr/Ca | 0.93 |
| Average | 1.23 |
| Optimal | 0.89 |

Table 2. Estimates of Error Correlations ρ_{jk}

| | Mg/Ca | Sr/Ca |
|-------|-------|-------|
| U/Ca | -0.56 | 0.38 |
| Mg/Ca | | -0.41 |

where w_j is the weight applied to the reconstruction based on proxy j . For $\hat{SST}_{\text{multi}}^0$ to be unbiased, it is necessary that the weights have unit sum:

$$\sum_{j=1}^n w_j = 1. \quad (6)$$

The variance of $\hat{SST}_{\text{multi}}^0$ is given by:

$$\text{Var}(\hat{SST}_{\text{multi}}^0) = \sum_{j=1}^n \sum_{k=1}^n w_j w_k \text{Cov}(\hat{SST}_j^0, \hat{SST}_k^0). \quad (7)$$

[7] The vector $w = (w_1 w_2 \dots w_n)^t$ of weights in equation (5) that minimizes the variance (equation (7)) subject to the nonbias condition (equation (6)) is:

$$w_{\text{opt}} = \frac{\Sigma^{-1} e}{e^t \Sigma^{-1} e}, \quad (8)$$

where the superscript t denotes the transpose, e is a vector of 1s, and Σ is the n -by- n variance-covariance matrix of the single-proxy reconstructions [e.g., Wunsch, 1996]. That is, the diagonal elements of Σ are the variances in equation (3) and the off-diagonal elements are the covariances in equation (4). For this choice of weight vector, the variance of $\hat{SST}_{\text{multi}}^0$ is $(e^t \Sigma^{-1} e)^{-1}$. All other choices of weight vector that satisfy the nonbias condition lead to larger values of this variance.

[8] In practice, the parameter values needed to construct w_{opt} are unknown. However, it is straightforward to estimate them from a calibration sample of matched measurements of the proxies and SST. These estimates can then be used in place of the true values in forming w_{opt} . The resulting reconstruction should be viewed as an approximation to the true optimal reconstruction.

3. Illustration

[9] In this section, the optimal multiproxy reconstruction of SST is constructed for some data from Amédée Island (22°29'S, 166°28'E) in New Caledonia. These data were

kindly provided by Terrence Quinn and are described in detail in the work of Quinn and Sampson [2002] [see also Quinn *et al.*, 1996, 1998]. The data consist of matched monthly measurements of $n = 3$ proxies (U/Ca, Mg/Ca, and Sr/Ca) from a *Porites lutea* coral and the corresponding local SST measurements. This order of the proxies, U/Ca, Mg/Ca, Sr/Ca, will be maintained below. The results from the calibration regressions are reported in the work of Quinn and Sampson [2002, Table 3], with the estimates of σ_j reported as SE ratio.

[10] Because of suspected analytical problems, the periods covered by the time series for the 3 proxies varied somewhat. The standard deviations of the single-proxy reconstruction errors for the period of overlap are reported in Table 1. These are in close agreement with the theoretical values given in equation (3). The best single proxy is Sr/Ca with reconstruction error standard deviation of 0.93°C. As reported in Table 1, when the 3 reconstructions are simply averaged, the reconstruction error standard deviation is 1.23°C. Turning to the optimal multiproxy reconstruction, the correlations ρ_{jk} estimated from calibration regression residuals for the period of overlap are reported in Table 2. The vector of optimal weights from equation (8) is $w_{\text{opt}} = (-0.03 \ 0.17 \ 0.86)^t$. The error standard deviation for the optimal multiproxy reconstruction, which is also reported in Table 1, is 0.89°C. This value, which is also in close agreement with its theoretical value, is only a modest 5% improvement over the best single-proxy reconstruction.

4. Discussion

[11] The multiproxy SST reconstruction formed by simply averaging single-proxy reconstructions is not guaranteed to perform better than the best single-proxy reconstruction. However, the optimal multiproxy reconstruction cannot (in theory) be worse than the best single-proxy reconstruction. In the illustration presented in the previous section, the multiproxy reconstruction outperformed the best single-proxy reconstruction by around 5%. In experimenting with other published data sets, we have found similar results, suggesting that great gains may not be possible even when single-proxy SST reconstructions are combined optimally.

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