

1 **A pseudoproxy evaluation of the CCA and RegEM methods for reconstructing climate fields of**  
2 **the last millennium**

3

4 Jason E. Smerdon and Alexey Kaplan

5 *Lamont-Doherty Earth Observatory of Columbia University, Palisades, NY*

6

7 Diana Chang

8 *Tri-Institutional Training Program in Computational Biology and Medicine, Cornell University,*

9 *Ithaca, NY*

10

11 Michael N. Evans

12 *Department of Geology and Earth Systems Science Interdisciplinary Center, University of Maryland,*

13 *College Park, MD*

14 **Abstract**

15 Canonical correlation analysis (CCA) is evaluated for paleoclimate field reconstructions in the context  
16 of pseudoproxy experiments assembled from the millennial integration (850-1999 C.E.) of the National  
17 Center for Atmospheric Research Climate System Model 1.4. A parsimonious method for selecting  
18 the order of the CCA model is presented. Results suggest that the method is capable of resolving  
19 approximately 3-18 climatic patterns given the estimated proxy observational network and the amount  
20 of observational uncertainty. CCA reconstructions are compared to those derived from the regularized  
21 expectation maximization method using ridge regression regularization (RegEM-Ridge). CCA and  
22 RegEM-Ridge yield similar skill patterns that are characterized by high correlation regions collocated  
23 with dense pseudoproxy sampling areas in North America and Europe. Both methods also produce  
24 reconstructions characterized by spatially variable warm biases and variance losses, particularly at high  
25 pseudoproxy noise levels. RegEM-Ridge in particular is subject to significantly larger variance losses  
26 than CCA, even though the spatial correlation patterns of the two methods are comparable. Results  
27 collectively indicate the importance of evaluating the field performance of methods that target spatial  
28 climate patterns during the last several millennia, and indicate that the results of currently available  
29 climate field reconstructions should be interpreted carefully.

## 30 **1. Introduction**

31 A concerted research effort over the last decade has focused on reconstructing global or hemispheric  
32 climate during the last millennium using networks of climate proxies (e.g. Folland et al. 2001; Jansen et  
33 al. 2007, North et al. 2006, Jones and Mann 2004; Jones et al. 2009). These efforts are in many ways an  
34 outgrowth of earlier studies that developed reconstructions on regional scales, particularly pioneering  
35 work in dendroclimatology that extends back to the 1960s and 70s (e.g. Fritts et al. 1971). Recent  
36 efforts have employed single-proxy (e.g. Cook et al. 1994, 2004; Briffa 2000; Briffa et al. 2001; Esper  
37 et al. 2002; Evans et al. 2002; D'Arrigo et al. 2006, 2009) or multi-proxy statistical approaches (Mann  
38 et al., 1998, 1999, 2005, 2007, 2008; Jones et al., 1998; Crowley and Lowery 2000; Rutherford et al.  
39 2005; Moberg et al. 2005; Hegerl et al. 2007) to calibrate proxy records on observational data during  
40 their period of overlap and subsequently to reconstruct past climate variability using derived climate-  
41 proxy relationships. Various efforts have demonstrated the promise of these approaches (e.g. Cook et  
42 al. 1994, 2004; Mann et al. 1998, 1999; Evans et al. 2002; Luterbacher et al. 1999, 2004; Rutherford  
43 et al. 2005; Casty et al. 2005; Pauling et al. 2006), but in some cases results and methodologies  
44 have been vigorously debated (Broecker 2001; Huang et al. 2000; Harris and Chapman 2001; Esper  
45 et al. 2002; Beltrami 2002; González-Rouco et al. 2003, 2006; von Storch et al. 2004, 2006; Pollack  
46 and Smerdon 2004; Rutherford and Mann 2004; McIntyre and McKittrick 2005; Xoplaki et al. 2005;  
47 von Storch and Zorita 2005; Bürger and Cubasch 2005; Huybers 2005; Wahl et al. 2006; Bürger et  
48 al. 2006; Zorita et al. 2007; Lee et al. 2007; Smerdon and Kaplan 2007, Smerdon et al. 2008a;  
49 Wahl and Ammann 2007; Ammann and Wahl 2007; Mann et al. 2003, 2005, 2007a, b, c, 2008;  
50 Moberg et al. 2005, 2008; Hegerl et al. 2007; Küttel et al. 2007; Christiansen et al. 2009). One  
51 of the principal issues of this debate surrounds the magnitude of reconstructed temperature variability

52 during the last millennium on decadal and longer time scales, particularly as it relates to the magnitude,  
53 phasing and ubiquity of the putative Medieval Climatic Anomaly and Little Ice Age (e.g. Hughes and  
54 Diaz 1994; Broecker 2001; Mann 2002; Bradely et al. 2003; Mann et al. 2003, 2005, 2007a, b, c).  
55 Although a great deal of progress has been made to understand how various reconstructions may or may  
56 not accurately represent the characteristics of these past epochs, there remain important unanswered  
57 questions about reconstruction uncertainties. These questions are tied to understanding, for example,  
58 the impact of proxy distributions and abundance, the connections between climate and proxy responses  
59 across different spectral domains, the response of proxies to multiple environmental variables, and the  
60 role of teleconnections and noise in the calibration data - questions that are ultimately fundamental to  
61 the success of efforts to reconstruct past climatic variability (e.g. North et al. 2006; Jansen et al. 2007).

62 An additional element of uncertainty in climate reconstructions that has recently gained more at-  
63 tention is the degree to which specific reconstruction methodologies impose their own error and biases  
64 on derived reconstructions. Here we focus specifically on the uncertainties in hemispheric-scale tem-  
65 perature reconstructions of the past millennium that arise principally from the applied methodology.  
66 Reconstruction methods for this purpose generally can be divided into two groups, one in which indi-  
67 vidual indices are targeted (see discussion in Mann et al. 2005) and climate field reconstruction (CFR)  
68 methods (Evans et al. 2001). Index methods target mean hemispheric or global temperature time series  
69 as predictand, therefore yielding reconstructions of only these individual indices (e.g. Groveman and  
70 Landsberg 1979, Esper et al. 2002, 2005, Crowley and Lowery 2000, Moberg et al. 2005, Hegerl et  
71 al. 2007, D'Arrigo et al. 2006; Mann et al. 2007, 2008). Although index methods have the disad-  
72 vantage of offering no spatial information, they have the benefit of being more straightforward, robust  
73 and likely require no more than a few tens of predictors for skillful reconstructions of hemispheric

74 or global temperature variability (e.g. Crowley and Lowery 2000; Hegerl et al. 2007). In contrast  
75 to index approaches, CFR methods attempt to reconstruct spatial patterns of temperature variability,  
76 which is the fundamental promise of these methods (e.g. Cook et al. 1994, Mann et al. 1998, 1999,  
77 2005, 2007a, Rutherford et al. 2005, Evans et al. 2002; Luterbacher et al. 2004, Xoplaki et al. 2005).  
78 CFR methods can be complicated, however, by the ill-conditioned nature of the problem, are more  
79 dependent on the stability of climate-proxy connections and climate teleconnections, and require more  
80 extensive distributions of proxies than index reconstructions.

81 In spite of the differences between index and CFR methods, the debate surrounding temperature  
82 reconstructions of the last millennium has almost exclusively been limited to comparisons between  
83 mean NH or global time series (e.g. Briffa and Osborn 2002; Jones and Mann 2004; North et al. 2006;  
84 Folland et al. 2001; Jansen et al. 2007); in the case of CFRs, these mean time series are computed from  
85 the underlying reconstructed fields. Consequently, there have been few assessments of the robustness  
86 of spatial patterns in the collection of available CFRs. Some field comparisons of CFRs have been done  
87 on regional scales. Cook et al. (1994) compared two CFR techniques applied to dendroclimatic series  
88 in western Europe and eastern North America and found them to produce similar results. Similarly,  
89 Zhang et al. (2004) investigated two methods for drought reconstructions over the continental United  
90 States and also found their performance comparable. A more recent study has compared the field skill  
91 of two temperature field reconstruction methods over the North Atlantic and the European continent  
92 (Riedwyl et al. 2008). At global and hemispheric scales, however, proxy distributions are more diffuse,  
93 predictor networks comprise multiple proxies, and teleconnection patterns are likely more essential to  
94 the skill of the reconstruction. It therefore is crucial to evaluate not only the mean global or hemispheric  
95 characteristics of CFRs, but also the spatial skill of the fields derived from these methods.

96 A significant challenge for CFR comparisons is the fact that researchers must use proxy networks  
97 of opportunity and thus of variable composition in proxy type, location and temporal extent. Uncer-  
98 tainty in any given reconstruction is therefore the combination of uncertainties in the method used, the  
99 spatial sampling of the proxy network, and the actual climate-proxy connection of each of the proxy  
100 series used in the network. If the objective is to isolate the impact of one of these factors, it is difficult  
101 to do so from comparisons between these real-world CFR results. The advent of pseudoproxy experi-  
102 ments (Mann and Rutherford 2002) has circumvented some of these challenges, however, by granting  
103 a consistent test bed on which to test reconstruction methodologies (González-Rouco et al. 2006; von  
104 Storch et al. 2004, 2006; Mann et al. 2005, 2007a; Hegerl et al. 2007; Smerdon and Kaplan 2007;  
105 Smerdon et al. 2008a; Lee et al. 2007; Küttel et al. 2007; Riedwyl et al. 2008; Christiansen et al.  
106 2009).

107 Pseudoproxy experiments have typically employed millennial integrations from General Circula-  
108 tion Models (GCMs) that only recently have become available (González-Rouco et al. 2003, 2006;  
109 Ammann 2007). These experiments are generally performed in the following steps: (1) the complete  
110 GCM field is subsampled to mimic the availability of instrumental and proxy information in real-world  
111 climate reconstructions of the last millennium; (2) the time series that represent proxy information  
112 are perturbed to simulate the spatial and temporal noise characteristics present in real-world proxies;  
113 (3) reconstruction algorithms are applied to the model-sampled pseudo “instrumental data” and pseu-  
114 doproxy series to derive a reconstruction of the climate simulated by the GCM; and (4) the derived  
115 reconstruction is compared to the known model target. There are indeed some open questions asso-  
116 ciated with these experiments, such as whether or not the adopted noise models in the pseudoproxy  
117 network are realistic and how well the model statistics represent real-world climate characteristics that

118 affect reconstruction skill (e.g. teleconnections). Nevertheless, the utility of pseudoproxy experiments  
119 lies in their ability to provide an objective dataset on which to test reconstruction methods. While fu-  
120 ture improvements in the implementation of pseudoproxy tests will undoubtedly be made, much insight  
121 into the performance of multiple reconstruction methods has already been gained from this approach  
122 (von Storch et al. 2004, 2006; Mann et al. 2005, 2007a; Smerdon and Kaplan 2007; Lee et al. 2007;  
123 Küttel et al. 2007; Hegerl et al. 2007; Riedwyl et al. 2008; Moberg et al. 2008; Smerdon et al. 2008a;  
124 Christiansen et al. 2009).

125 Here we investigate skill and uncertainty in CFRs arising from application of a reconstruction  
126 algorithm using canonical correlation analysis (CCA). CCA is a well-established method within the  
127 climate sciences (e.g. Anderson 1984; Barnett and Preisendorfer 1987; Bretherton et al. 1992; Cook  
128 et al. 1994; Wilks 1995; von Storch and Zwiers 2000; Luterbacher et al. 2000; Tippett et al. 2003,  
129 2008), but has not been widely applied for the purpose of deriving large-scale temperature CFRs (CCA  
130 is mentioned briefly in Mann et al. (1998) as being unsuitable for their purposes and has more re-  
131 cently been applied by Christiansen et al. (2009) as one of a number of methods tested in the context  
132 of reconstructed NH means). Our purposes herein are to evaluate in detail the application of CCA  
133 for reconstructing NH temperatures during the last millennium and to specifically focus on the field  
134 characteristics of the derived CFRs.

135 In addition to investigating the performance of CCA, we compare CCA-derived results to those  
136 obtained using the regularized expectation maximization (RegEM) method (Schneider 2001). RegEM  
137 is a recently favored method for NH temperature reconstructions (e.g. Rutherford et al. 2005; Mann  
138 et al. 2005, 2007a, 2008), but pseudoproxy experiments also have shown some implementations of  
139 RegEM to be susceptible to warm biases and variance losses (Smerdon and Kaplan 2007; Smerdon et

140 al. 2008a; Riedwyl et al. 2008; Christiansen et al. 2009). These findings are consistent with previ-  
141 ous pseudoproxy experiments that have demonstrated similar behavior associated with the Mann et al.  
142 (1998, 1999) CFR method (von Storch et al. 2004, 2006). Since application of CCA requires selection  
143 of only three model dimensions, with reconstruction based on the minimum of these, it is straightfor-  
144 ward to assess skill of the method and computationally cheap to construct all possible models. This  
145 characteristic is in contrast to the more complicated structure of the iterative and more computationally  
146 expensive RegEM algorithm. Hence comparison of the two methods can help elucidate the strengths  
147 and weaknesses of each.

148

## 149 **2. Data**

150 We use pseudoproxies derived from the millennial simulation (850-1999 C.E.) of the National Center  
151 for Atmospheric Research (NCAR) Climate System Model (CSM) 1.4, a coupled atmosphere-ocean  
152 GCM that has been driven with natural and anthropogenic forcings (Ammann et al. 2007). The simu-  
153 lated model fields of annual surface temperature means have been interpolated to a  $5^\circ$  longitude-latitude  
154 grid (Smerdon et al. 2008b; Rutherford et al. 2008). For consistency in latter comparisons to RegEM-  
155 derived results, we use the same realizations of CSM pseudoproxies employed by Mann et al. (2005)  
156 with locations shown in Figure 1 (publicly available at <http://fox.rwu.edu/rutherfordo/supplements/Pseudoproxy05/>).  
157 These pseudoproxies were sampled from the  $5^\circ$  grid-box locations that approximate the actual proxy  
158 locations of the Mann et al. (1998) multiproxy network, totaling 104 sampled grid cells. Pseudoproxies  
159 at these selected locations contain white noise at four different levels to produce signal-to-noise ratios  
160 (SNRs), by standard deviation, of infinity (noise free), 1.0, 0.5 and 0.25.

161 To further facilitate comparisons with previous pseudoproxy work, we also use the same subsam-



162 pled CSM field used by Mann et al. (2005, 2007) to approximate the availability of the instrumental  
 163 temperature data. Grid points missing more than 30% of the annual data between 1856-1998 C.E. in  
 164 the Jones et al. (1999) dataset were excluded from use as target data (Mann and Rutherford 2002).  
 165 This restriction limits the total number of grid cells to 669 in the Eq-70° N region (the target region).  
 166 Also in keeping with Mann et al. (2005, 2007a), the subsampled instrumental (calibration) data are  
 167 constrained to 1856-1980 C.E.; all annual temperature values within this period are retained for each  
 168 targeted temperature grid.

169

### 170 **3. Methods**

#### 171 **3.1 Least-Squares CFRs as Multivariate Linear Regression**

172 Multivariate linear regression is the underlying formalism of most CFR methods used to date. The  
 173 fundamental approach relates a matrix of climate proxies to a matrix of climate data during a common  
 174 time interval (generally termed the calibration interval) using a linear model. For instance, let  $P$  be an  
 175  $m \times n$  matrix of proxy values and  $T$  be an  $r \times n$  matrix of instrumental temperature records where  
 176  $m$  is the number of proxies,  $r$  is the number of spatial locations in the instrumental field, and  $n$  is the  
 177 temporal dimension corresponding to the period of overlap between the proxy and instrumental data.  
 178 We write the regression of  $T$  columns on  $P$  columns for time-standardized matrices ( $T'$  and  $P'$ ) with  
 179 rows that have means of zero and standard deviations of one:

$$T = M_t + S_t T', \quad P = M_p + S_p P',$$

180 where  $M_t$  is a matrix of identical columns equal to the average of all columns of the matrix  $T$ , and  $S_t$   
 181 is a diagonal matrix with elements that are the standard deviations of the rows of matrix  $T$ ;  $M_p$  and  $S_p$

182 are similarly defined for matrix  $P$ . In these terms,

$$T' = BP' + \varepsilon, \quad (1)$$

183 where  $B$  is a matrix of regression coefficients with dimensions  $r \times m$ , and  $\varepsilon$  is the residual error. The  
184 error variances of all the elements of  $\varepsilon$  in (1) are simultaneously minimized if  $B$  is chosen as:

$$B = (T'P'^T)(P'P'^T)^{-1}, \quad (2)$$

185 where the superscript  $T$  denotes the matrix transpose. Temperature thus can be predicted, or “recon-  
186 structed”, using this regression matrix during periods in which proxy data are available:

$$\hat{T} = M_t + S_tBS_p^{-1}(P - M_p), \quad (3)$$

187 where  $\hat{T}$  denotes a matrix of reconstructed temperature values.

188 While the above formalism is straightforward, it works best when the system is overdetermined;  
189 that is, the time dimension  $n$  is much larger than the spatial dimension  $m$ , because the covariances are  
190 more reliably estimated. The challenge for CFR methods involves the manner in which  $B$  is estimated  
191 in practical situations when this condition is not met. It is often the case in climate applications that  
192 the number of target variables exceeds the time dimension, yielding a rank-deficient problem. For  
193 instance, in most global or NH CFRs, the number of grid cells in the climate field is typically on  
194 the order of many hundreds or a few thousands, while the observational record usually contains 150  
195 annual fields or less. The number of proxies is typically on the order of a few tens to hundreds, which  
196 may exceed or at least be comparable to the time dimension. In such cases, the covariance matrices  
197  $\langle T'P'^T \rangle$  and  $\langle P'P'^T \rangle$  cannot be well estimated. The inversion in (2) therefore requires some form of

198 regularization. Published linear methods for global temperature CFRs vary primarily in the form of  
199 this regularization. In the following subsections we discuss CCA and RegEM as the two regularization  
200 approaches considered in this manuscript.

201

### 202 **3.2. Canonical Correlation Analysis**

203 For the purposes described herein, we outline the Barnett and Preisendorfer (1987) version of CCA  
204 formalism as presented by Tippett et al. (2003, 2008). This formalism as applied to the CFR problem  
205 is presented in detail in Appendix A and summarized below. Two elements of the CCA application  
206 involve the eigenvalue decomposition and subsequent truncation of the proxy and temperature matrices.  
207 Both of these reductions are helpful in real-world applications where the temperature and proxy fields  
208 each contain noise. Retaining a subset of EOFs in both fields can therefore guard against the possibility  
209 of calibrating modes dominated by noise (e.g. Barnett and Preisendorfer 1987; Barnett et al. 1992).  
210 With regard to the reduction of the temperature field specifically, there are examples in the literature of  
211 CFR approaches that choose to either neglect or adopt a reduction of the field (e.g. Luterbacher et al.  
212 2004, Mann et al. 2007). Although we build the potential for reduction of the temperature field into the  
213 CCA formalism, the degree of reduction is determined from a cross-validation scheme that does not a  
214 priori require truncation. This scheme is discussed later in the manuscript and provides an objective  
215 means of determining whether or not reduction is warranted and by how much.

216 Decomposition of the standardized proxy matrix  $P'$  during the calibration interval using Singular  
217 Value Decomposition (SVD; Golub and Van Loan, 1996) is written:

$$P' = U_p \Sigma_p V_p^T. \quad (4)$$

218 where the columns of  $U_p$  represent spatial patterns (empirical orthogonal functions or EOFs) and the

219 principal components (PCs),  $\Sigma_p V_p$ , are orthonormal time series that combine with the EOF patterns to  
 220 produce the original data set. The diagonal matrix  $\Sigma_p$  contains the non-negative singular values, with  
 221 squares proportional to the variance captured by the corresponding EOF-PC pairs. If the diagonal ele-  
 222 ments of  $\Sigma_p$  decrease quickly, as is often the case in climatological data where leading climate patterns  
 223 dominate over many more weakly expressed local patterns or noise, a reduced-rank representation of  
 224  $P'$  using only a few leading EOF-PC pairs is typically a good approximation of the full-rank version.  
 225 Thus we employ a reduced rank representation of  $P'$  such that  $d_p$  EOF-PC pairs are retained:

$$P^r = U_p^r \Sigma_p^r V_p^{r T}. \quad (5)$$

226 Here  $P^r$  denotes the reduced-rank representation of  $P'$ , and matrices with the superscript  $r$  are the  
 227 truncated versions of the SVD factors corresponding to the retained number of  $d_p$  singular values.  
 228 Similarly, the reduced-rank version of  $T'$  is written:

$$T^r = U_t^r \Sigma_t^r V_t^{r T}, \quad (6)$$

229 where  $T^r$  only uses  $d_t$  singular values and the corresponding number of singular vectors. Note that  
 230  $\text{rank}(P^r) = d_p$  and  $\text{rank}(T^r) = d_t$ , while  $\text{rank}(P') = \min(m, n - 1)$  and  $\text{rank}(T') = \min(r, n - 1)$ .

231 The above decompositions can be substituted into (2) and the corresponding matrix of regression  
 232 coefficients written as

$$B_{cca} = U_t^r \Sigma_t^r V_t^{r T} V_p^r (\Sigma_p^r)^{-1} U_p^{r T} = U_t^r \Sigma_t^r O_t^r \Sigma_{cca}^r O_p^{r T} (\Sigma_p^r)^{-1} U_p^{r T},$$

233 where  $O_t^r \Sigma_{cca}^r O_p^{r T}$  is the truncated SVD of the covariance matrix  $V_t^{r T} V_p^r$  in which  $d_{cca}$  leading canon-  
 234 ical coefficients have been retained. From the formal derivation in Appendix A, the above expression  
 235 for  $B_{cca}$ , takes a simple form:

$$B_{cca} = C_t \Sigma_{cca}^r W_p^T, \quad (7)$$

236 where  $C_t = U_t^r \Sigma_t^r O_t^r$  has the CCA temperature patterns in its columns and  $W_p = U_p^r (\Sigma_p^r)^{-1} O_p^r$  is the  
 237 CCA proxy weighting matrix.

238 Applying  $B_{cca}$  to  $P'$  in order to reconstruct  $T'$  is therefore equivalent to a three-step procedure:

239 (i) use the weighting patterns  $W_p$  to convert  $P'$  into the CCA time series

$$Q_p^T = W_p^T P',$$

240 (ii) scale these time series by the canonical correlations, i.e. the diagonal element of  $\Sigma_{cca}^r$ , to produce  
 241 the CCA timeseries for temperature:

$$\hat{Q}_t^T = \Sigma_{cca}^r Q_p^T,$$

242 (iii) and use the  $C_t$  patterns to reconstruct a standardized version of the temperature fields:

$$\hat{T}' = C_t \hat{Q}_t^T.$$

243 Note that in our formulated pseudoproxy experiments the actual CCA temperature time series,

$$Q_t^T = W_t^T T',$$

244 during the reconstruction period can be directly compared with their prediction on the basis of the  
 245 proxies in item (ii) above. The use of these statistics are illustrated further in Section 4.2.1.

246 For the non-standardized version of temperature fields and proxies given in (3), the CCA tempera-  
 247 ture CFR becomes

$$\hat{T} = M_t + S_t B_{cca} S_p^{-1} (P - M_p). \quad (8)$$

248 Performing this reconstruction thus requires the determination of five matrices: two in which all  
249 columns contain the mean vectors for the temperature field and the proxies,  $M_t$  and  $M_p$ ; the two  
250 diagonal matrices of the temperature and proxy standard deviations,  $S_t$  and  $S_p$ , and the CCA low-rank  
251 regression matrix  $B_{cca}$ . Under the assumption of stationarity between the mutual proxy and climate  
252 statistics, (8) can be used to reconstruct temperatures in any temporal interval, including those outside  
253 of the calibration period. The only formal change is in the number of columns in matrices  $M_t$  and  $M_p$ ,  
254 which of course change to match the length of the given reconstruction period.

255 The operator  $B_{cca}$  is a reduced-rank ( $\text{rank}(B_{cca}) = d_{cca}$ ) representation of the standard multivariate  
256 regression operator. Given calibration interval data sets  $T$  and  $P$ , the matrix  $B_{cca}$  is completely deter-  
257 mined upon the selection of three parameters for truncated ranks,  $d_{cca}$ ,  $d_p$ , and  $d_t$ . Note that traditional  
258 applications of CCA did not involve rank reductions of the predictor and predictand matrices, and thus  
259 only depended on  $d_{cca}$  (see the discussion in Bretherton et al. 1992). Steps for reducing these matrix  
260 ranks by selecting  $d_p$  and  $d_t$  parameters prior to estimating the CCA time series and maps were added  
261 by Barnett and Preisendorfer (1987) (termed the BP method by Bretherton et al. 1992). Tippett et al.  
262 (2003) and Christiansen et al. (2009) used and referred to this latter BP version as CCA, as do we here-  
263 inafter. The canonical formalism also reduces to other special forms of multivariate regression under  
264 specific assumptions. Cogent discussions about the connection between CCA and other multivariate  
265 regression methods can be found in Barnett and Preisendorfer (1987), Barnett et al. (1992), von Storch  
266 and Zwiers (2002) and Tippett et al. (2008).

267

### 268 **3.3. CCA Model-Dimension Selection**

269 Appropriate selections of the  $d_{cca}$ ,  $d_p$ , and  $d_t$  dimensions are crucial for the application of the CCA

270 method. Previous CCA applications have proposed various forms of model selection. Christiansen et  
271 al. (2009) set  $d_p$  and  $d_t$  by maintaining a specific level of retained variance in  $T$  and  $P$  and imposing  
272 the additional constraint that  $d_{cca}$  be equal the minimum of  $d_p$  and  $d_t$ . Barnett and Preisendorfer (1987)  
273 used principal component truncation rules to determine  $d_p$  and  $d_t$  as proposed by Preisendorfer et  
274 al. (1981). The number of canonical coefficients ( $d_{cca}$ ) was then estimated using jackknife cross-  
275 validation statistics computed for a set of withheld single time samples (“leave-one-out”). Tippett et  
276 al. (2003) employed a similar approach, but used a jackknife cross-validation scheme to optimize all  
277 three truncation dimensions. Our approach is similar to the latter application except we use a much  
278 cheaper “leave-half-out” approach to cross-validation to reduce computational costs. This procedure  
279 produces cross-validation statistics by calibrating independently on either the first or second halves of  
280 the target data and using the left-out half for validation. In an application using proxy data series with  
281 annual resolution, this approach is also more conservative with respect to validation of the reconstructed  
282 decadal-centennial timescale variations.

283 To perform the leave-half-out cross-validation procedure, the instrumental period is split into two  
284 temporal halves: 1856-1917 and 1918-1980 C.E. We generate two sets of reconstructions using (8)  
285 and calibrate using each half of the target data to estimate the  $B_{cca}$  matrix, as well as the means and  
286 standard deviation fields for the proxy and temperature data ( $M_p$ ,  $S_p$ ,  $M_t$ ,  $S_t$ ). The reconstructions are  
287 verified on the left-out halves of the instrumental data. Two cross-validation statistics are used: (1) the  
288 area-weighted Root Mean Square Error (RMSE) of the reconstructed field relative to the target; and (2)  
289 the correlation between the reconstructed and target area-weighted mean NH time series (hereinafter  
290 termed NH mean correlation (NHMC)). These validation statistics from both experiments are combined  
291 to determine the statistics for the entire instrumental data interval from 1856-1980 C.E.

292 Using the above cross-validation scheme we compute the RMSE and NHMC for a range of  $d_{cca}$ ,  $d_p$   
 293 and  $d_t$  combinations. The optimal selection of  $d_{cca}$ ,  $d_p$  and  $d_t$  is based on the cross-validated reconstruc-  
 294 tion skill in terms of either small RMSE or large NHMC. After this selection, all the matrix parameters  
 295 of (8) are computed for the entire calibration interval (1856-1980 C.E.) and used for reconstructions in  
 296 the preinstrumental period. Using the definitions

$$B_f = S_t B_{cca} S_p^{-1}, \quad M_f = M_t - B_f M_p, \quad (9)$$

297 the reconstruction in (8) can be rewritten in the final form of a linear transform with a constant:

$$\hat{T} = M_f + B_f P. \quad (10)$$

298 All columns of the matrix  $M_f$  are identical and specify offsets for all  $r$  locations of the predicted  
 299 temperature fields, therefore  $M_f$  contains  $r$  independent parameters. The linear-transform matrix  $B_f$   
 300 has the dimensions  $r \times m$  and thus contains  $rm = 669 \cdot 104 = 69,576$  elements. This number is about  
 301 one third smaller than the number of elements in the target temperature data during the calibration  
 302 period ( $rn = 669 \cdot 125 = 96,625$ ) from which the elements of  $B_f$  must be determined. Fortunately,  
 303 not all elements in  $B_f$  are independent parameters because of the CCA rank reduction. Since  $B_{cca}$  has  
 304 rank  $d_{cca}$ , and  $B_f$  is obtained in (9) by multiplying  $B_{cca}$  by non-singular diagonal matrices,  $B_f$  has the  
 305 same size ( $r \times m$ ) and rank ( $d_{cca}$ ) as  $B_{cca}$ . Such a matrix has  $d_{cca}$  non-zero singular values and as many  
 306 left and right singular vectors corresponding to these values. Using the non-zero singular values of  $B_f$   
 307 in non-increasing order to form a diagonal matrix  $\Sigma$  and arranging the corresponding singular vectors  
 308 as the columns of matrices  $U$  and  $V$ , we can uniquely (up to the reordering of the columns in  $U$  and  $V$   
 309 corresponding to identical singular values) present  $B_f$  as

$$B_f = U \Sigma V^T. \quad (11)$$



310 The first column of  $U$ , as a unit vector in the  $r$ -dimensional space, has  $r - 1$  degrees of freedom. The  
 311 second column, subject to an additional constraint of orthogonality to the first column has  $r - 2$  degrees  
 312 of freedom, etc. Therefore the entire matrix  $U$ , consisting of  $d_{cca}$  orthonormal vectors has

$$N(U) = \sum_{i=1}^{d_{cca}} (r - i) = rd_{cca} - \frac{d_{cca}(d_{cca} + 1)}{2} = d_{cca} \left( r - \frac{d_{cca} + 1}{2} \right).$$

313 Similarly, the number of independent parameters in  $V$  is

$$N(V) = d_{cca} \left( m - \frac{d_{cca} + 1}{2} \right),$$

314 and  $N(\Sigma) = d_{cca}$ . In the general case, non-zero singular values of a matrix  $B_f$  are different, the  
 315 decomposition (11) is unique and, therefore,

$$N(B_f) = N(U) + N(\Sigma) + N(V) = d_{cca}(r + m - d_{cca}).$$

316 Together with the constant offset parameters, the number of independent parameters that have to be  
 317 determined in order to produce the reconstruction formula (10) is

$$N_{\text{tot}} = N(B_f) + N(M_f) = d_{cca}(r + m - d_{cca}) + r. \quad (12)$$

318 Substituting the values of  $r$  and  $m$  specific to the present pseudoproxy scenario ( $r = 669$  and  $m = 104$ ),  
 319 the number of independent parameters in the CCA temperature field reconstructions are

$$N_{\text{tot}} = 669 + 773d_{cca} - d_{cca}^2. \quad (13)$$

320 The number of independent parameters in the CCA reconstructions therefore depends only on  $d_{cca}$ , the  
 321 number of CCA modes retained. The number does not depend on  $d_p$  and  $d_t$ , i.e. the numbers of retained  
 322 EOF modes for the proxy and temperature data, respectively. The actual values of  $B_f$  and  $M_f$  in (10)

323 of course do depend on the  $d_p$  and  $d_t$  choices, but the underlying number of parameters that need to be  
 324 specified in order to determine these values does not. Furthermore, when  $d_{cca} \ll r + m = 773$ , the  
 325  $d_{cca}^2$  term in (12) and (13) is negligible compared to  $(r + m)d_{cca} = 773d_{cca}$ . Analyses we will present  
 326 suggest that reasonable values of  $d_{cca}$  are well below 50. Therefore,  $N_{tot}$  grows nearly linearly with  
 327  $d_{cca}$ , and 773 additional parameters need to be specified in the coefficients of (10) when  $d_{cca}$  increments  
 328 by 1. Considering the relative shortness of the data set available for calibration and cross-validation,  
 329 choosing a reconstruction model that requires a smaller, rather than larger number of free parameters  
 330 (i.e. value of  $d_{cca}$ ) becomes especially important. In Section 4.1 we demonstrate a practical means  
 331 of selecting the smallest  $d_{cca}$  that produces a reconstruction with cross-validated RMSE practically  
 332 indistinguishable from the absolute minimum of RMSE over all combinations of  $d_{cca}$ ,  $d_p$ , and  $d_t$ .  
 333 Thus the above arguments underlie the dimensional selection strategy that we employ throughout the  
 334 remainder of the manuscript.

335

### 336 3.4. RegEM

337 Application of the RegEM method to the problem of NH CFRs has been discussed in detail within  
 338 the literature (Schneider 2001; Rutherford et al. 2005; Mann et al. 2005, 2007a,c, 2008; Smerdon and  
 339 Kaplan 2007; Lee et al. 2007; Smerdon et al. 2008a; Christiansen et al. 2009; Riedwyl et al. 2008).  
 340 While RegEM is an iterative method, the underlying formalism is based on a linear regression model  
 341 that reconstructs missing data  $X_m$  from available data  $X_a$  and can be written as

$$X_m = M_m + S_m B S_a^{-1} (X_a - M_a). \quad (14)$$

342 The notation here is analogous to (3), except the subindices  $a$  and  $m$  denote available and missing data,

343 respectively, and are consistent with the notation adopted by Schneider (2001).

344 For the conventional expectation maximization (EM) algorithm, in which regularization is not em-  
345 ployed, the estimate of the regression matrix  $B$  is given, in full analogy to (2), by the standard multi-  
346 variate regression formula for standardized data sets  $X'_m$  and  $X'_a$ :

$$B = (X'_m X'_a{}^T)(X'_a X'_a{}^T)^{-1}. \quad (15)$$

347 Similar to CCA, however, regularization is required for application to CFRs of the last millennium.  
348 Multiple regularization approaches for the expectation maximization algorithm have been discussed  
349 (Schneider 2001; Rutherford et al. 2005; Mann et al. 2005, 2007a,c; Smerdon and Kaplan 2007;  
350 Christiansen et al. 2009), but the differences between reconstructions derived from these approaches  
351 has not been sufficiently explored (Smerdon et al. 2008a). For our purposes herein we employ the  
352 more widely applied ridge regression regularization in which the inverse covariance matrix in (15) is  
353 replaced by

$$(X'_a X'_a{}^T)^{-1} \longrightarrow (X'_a X'_a{}^T + h^2 I)^{-1} \quad (16)$$

354 where  $h$  is a positive number called the ridge parameter (see Schneider (2001) for a detailed derivation  
355 and discussion of these equations). In keeping with the reconstructions performed by Rutherford et al.  
356 (2005) and Mann et al. (2005),  $h$  is chosen herein by minimization of the generalized cross validation  
357 (GCV) function. Although the further details of the RegEM method are extensive, it is important to  
358 note that even though the *calculation* of the RegEM regression-coefficient matrix is non-linear, the  
359 final RegEM reconstruction in this millennial CFR context is derived from a set of linear operators  
360 acting on the proxy matrix (Smerdon et al. 2008a), i.e. it takes the form of (14) for a specific choice  
361 of  $M_a$ ,  $S_a$ ,  $M_m$ ,  $S_m$ , and  $B$ . If the proxy data in  $P$  are substituted for the “available” data  $X_a$ , and the

362 “missing” data  $X_m$  are taken to be temperature  $T$  during the reconstruction interval, then the RegEM  
363 reconstruction in (14) essentially becomes (3) and is comparable to the same form given for the CCA  
364 reconstruction in (8). In fact, both of these reconstruction formulas can be brought to the form in (10)  
365 using one offset and one linear transformation.

366 The main difference between (8) and (14-16) is of course the form of regularization used for the  
367 regression matrix  $B$ , and the iteratively computed estimates of RegEM. Several relative advantages of  
368 the RegEM-Ridge method have been noted (Schneider 2001). In typical climatological applications  
369 where only a few principal components are retained based on often weak separations of the leading  
370 elements in the eigenvalue spectrum, the continuous filtering of the spectrum in ridge regression may  
371 provide advantages over regularizations, like CCA, that use finite eigenvalue truncation. The iterative  
372 EM procedure also allows the use of all data in the data matrix, as opposed to only the predictand  
373 and predictor data during their period of overlap in the calibration interval. In the specific type of  
374 paleoclimatic application considered herein, however, this advantage is limited principally to the pre-  
375 calibration period of the proxy matrix because the target data are completely missing prior to the  
376 mid-19th century (cf. Smerdon et al. 2008).

377

## 378 **4. Reconstruction Results**

### 379 **4.1 Selected model dimensions**

380 We select  $d_{cca}$ ,  $d_p$ , and  $d_t$  values for the collection of CCA reconstructions that calibrate the 104  
381 pseudoproxies on the instrumental period from 1856-1980 C.E. and compute CFRs during the interval  
382 850-1855 C.E. These are the same experiments performed by Mann et al. (2005, 2007a) to test the  
383 RegEM method using white-noise pseudoproxies. In all cases,  $P$  and  $T$  are standardized over the

384 calibration period prior to estimating the regression matrix  $B_{cca}$  using equation (7); reconstructions  
385 during the validation period are performed using (8).

386 Following the approach described in Section 3.3, CCA was calibrated on each half of the the in-  
387 strumental data and tested on the other half using all combinations of  $d_{cca}$ ,  $d_p$  and  $d_t$  between 1 and 50  
388 modes such that  $d_{cca} \leq \min(d_p, d_t)$  (yielding  $d_{cca}^2$  triplets  $(d_{cca}, d_p, d_t)$  for each  $d_{cca}$  value between 1  
389 and 50 and thus a total of  $1^2 + 2^2 + \dots + 50^2 = 50 \cdot (50 + 1) \cdot (2 \cdot 50 + 1)/6 = 42,925$  reconstruction  
390 models). The cross-validation statistics for early and late-calibration halves are given in Table 1. These  
391 results for both halves of the instrumental period were combined to produce cross-validation statistics  
392 for the entire interval and a given set of dimensions. RMSE values were combined as the square root  
393 of the mean residual sum of squares in the two intervals and NHMCs were calculated as the average  
394 correlation coefficients for the two intervals weighted by the number of years in each interval.

395 Table 2 gives the minimum RMSE and maximum NHMC values among all  $d_{cca}$ ,  $d_p$ , and  $d_t$  combi-  
396 nations used, as well as the dimensional combinations that achieve these extrema. Results are tabulated  
397 for each pseudoproxy noise level. While the two statistics are optimized at somewhat similar dimen-  
398 sional combinations, the results are not identical; the alternative statistic for each optimization is also  
399 provided in Table 2.

400 The RMSE and the NHMC statistics are plotted in Figure 2 for an SNR of 0.5, showing that the  
401 former generally decreases as the latter increases. More importantly, the range of possible NHMCs de-  
402 creases as the RMSE becomes smaller. The reciprocal constraint, however, is much weaker: increases  
403 in NHMCs are not accompanied by nearly as large a decrease in the range of RMSE. For instance,  
404 when confined to a range of RMSE values within 1% of the minimum, the range of possible NHMCs  
405 spans 12% their total range. By contrast, if confined to the range of NHMCs that are within 1% of the

406 maximum, the range of possible RMSE values spans 34% of the total RMSE range. These observations  
407 suggest that RMSE is a more robust statistic for optimizing the CCA reconstructions than the NHMC.  
408 Furthermore, the colors of the circles in Figure 2 denote the values of  $d_{cca}$ , that is correspond to the  
409 number of independent parameters in the reconstruction model that is being validated. While particu-  
410 larly small  $d_{cca}$  (less than 10) correspond to reconstructions that are both poor in RMSE and NHMC  
411 performance, high  $d_{cca}$  (larger than 30) correspond to high NHMC but the full range of RMSE values.  
412 RMSE performance is especially poor for reconstructions with the largest  $d_{cca}$  values. We therefore use  
413 RMSE as the principal basis for our selection criterion in subsequent dimensional selections. There are  
414 of course alternative cross-validation statistics that could be adopted. The coefficient of efficiency (CE)  
415 and reduction of error (RE) statistics are often used in paleoclimate literature as statistical validation  
416 measures. Advocates of these statistics point out that RE and CE measure the robustness of both the  
417 resolved variance and reconstructed mean in derived reconstructions (e.g. Wahl and Ammann 2007).  
418 This advantage is shared by the RMSE statistic adopted in this study, indicating that all three skill  
419 measures would be expected to produce similar results. Nevertheless, we adopt RMSE in the present  
420 application given its readily interpretable characteristics.

421 As mentioned earlier, the total number of combinations used to determine the optimized dimensions  
422 given in Table 2 is 42,925. This collection of models was tested for their cross-validated performance  
423 on only 125 annual fields of target data, thus some combinations might correspond to low RMSE simply  
424 by chance and yield optimal reconstructions impacted by artificial skill. To guard against this likeli-  
425 hood we adopt a conservative selection strategy that seeks to find the most parsimonious of acceptable  
426 models by minimizing the number of free parameters in the final reconstruction model, which is equiv-  
427 alent to minimizing  $d_{cca}$  without deviating significantly from the absolute minimum RMSE. Figure 3

428 plots RMSE versus  $d_{cca}$  for all tested combinations of the CCA dimensions at each pseudoproxy noise  
 429 level; the black dashed line connects the RMSE minima for each value of  $d_{cca}$ :

$$\text{RMSE}^*(d_{cca}) = \min_{d_p, d_t} \text{RMSE}(d_{cca}, d_p, d_t).$$

430 If  $d_p^*(d_{cca})$  and  $d_t^*(d_{cca})$  are the values of  $d_p$  and  $d_t$  that respectively minimize  $\text{RMSE}(d_{cca}, d_p, d_t)$  for  
 431 a given  $d_{cca}$ , then the triplet  $(d_{cca}, d_p^*(d_{cca}), d_t^*(d_{cca}))$  defines the optimal (by the cross-validated RMSE  
 432 criterion) CCA reconstruction among all models with a fixed number of independent parameters. Fig-  
 433 ure 3 demonstrates that  $\text{RMSE}^*(d_{cca})$  decreases steeply for all noise levels at small values of  $d_{cca}$ .  
 434 Beginning at a given  $d_{cca}$  value, however, this drop is replaced by a rather flat plateau. For all noise  
 435 levels except the highest one, the absolute minimum (identified by the closed circle) is rather far from  
 436 the beginning of this plateau. Alternatively, using the  $d_{cca}$  value corresponding to the beginning of the  
 437 plateau yields a solution with an RMSE performance that is similar to the absolute RMSE minimum  
 438 but corresponds to a model with a much smaller number of independent parameters.

439 We identify the beginning of the plateau by selecting the minimum  $d_{cca}$  at which an increase by one  
 440 does not reduce  $\text{RMSE}^*(d_{cca})$ :

$$d_{cca}^* = \min\{d_{cca} : \text{RMSE}^*(d_{cca}) \leq \text{RMSE}^*(d_{cca} + 1)\}.$$

441 Optimal solutions  $(d_{cca}^*, d_p^*(d_{cca}^*), d_t^*(d_{cca}^*))$  are identified by stars in the panels of Figure 3 and are  
 442 listed in Table 3 along with the corresponding values of RMSE and NHMC cross-validation statistics.  
 443 At any noise level,  $\text{RMSE}^*(d_{cca}^*)$  does not exceed  $\min_{d_{cca}}(\text{RMSE}^*)$  by even 0.5%. In subsequent  
 444 presentations herein, we use these “beginning of the plateau” solutions  $(d_{cca}^*, d_p^*(d_{cca}^*), d_t^*(d_{cca}^*))$  as our  
 445 preferred choices of the CCA dimensions (termed the preferred solutions hereinafter).

446 Note that in the preferred solutions, the values of  $d_p$  and  $d_t$  are chosen as those corresponding to the  
 447 absolute minimum of RMSE for the preselected value of  $d_{cca}$ . Relatively fluid color transitions in the  
 448 panels of Figure 3 suggest smooth but significant dependence of RMSE on  $d_p$ . This impression is borne  
 449 out in a more detailed illustration of the RMSE dependence on the CCA parameters ( $d_{cca}, d_p, d_t$ ): Fig-  
 450 ure 4 presents two-dimensional fields of the RMSE minima with respect to the individual dimensions.  
 451 The area of the RMSE minimum is quite wide, therefore changes in  $d_p$  or  $d_t$  by a few units should  
 452 not affect the reconstruction quality very much. The dependence of RMSE on  $d_t$  is particularly poorly  
 453 constrained by the data: for all  $d_{cca}$  in the range between 5 and 30, a value of  $d_p$  could be selected so  
 454 that RMSE is quite close to the absolute minimum for any value of  $d_t$  exceeding  $d_{cca}$ . Nevertheless,  
 455 reductions in the dimensions of the temperature field are warranted. The yellow lines in Figure 3 plot  
 456 the minimum RMSE values in the subset of solutions when  $d_t$  is held constant at 50 (close to 62 or  
 457 63, the full-rank of the temperature field in the two halves of the instrumental period). Particularly at  
 458 higher noise levels, the preferred solutions display significantly reduced RMSE when the dimension of  
 459 the temperature field is truncated.

460

## 461 **4.2 CCA Reconstructions**

### 462 **4.2.1 Assembly of the CCA Reconstructions**

463 To demonstrate the individual elements of the CCA reconstruction we plot in Figure 5 the homogeneous  
 464 covariance maps ( $C_t$  and  $C_p$ ) and the associated time series ( $Q_t$ ) for the first three canonical patterns  
 465 of the no-noise reconstruction (see Section 3.2 and Appendix A). In the case of  $Q_t$ , we plot both the  
 466 true time series from the target data, as well as the estimated time series from the pseudoproxy matrix  
 467  $(\sum_{cca} Q_p^T)$ .



468 The three temperature covariance maps plotted in Figure 5 take on dynamically interpretable char-  
469 acteristics, although the patterns are rotated from the original model EOFs. The three plotted maps  
470 combine features of global-warming, El Nino/Southern Oscillation, and North Atlantic Oscillation like  
471 patterns. This demonstration illustrates the physical interpretability of the derived covariance maps,  
472 which ultimately can be evaluated in terms of the reconstructive skill associated with individual dy-  
473 namical patterns in the field.

474 As demonstrated in step (ii) of the three-step procedure in Section 3.2, the time series of the temper-  
475 ature covariance maps are estimated during the reconstruction interval by the product of the canonical  
476 coefficients and the time series of the proxy covariance maps. These time series are plotted in Figure 5  
477 and compare closely to the true time series of the temperature covariance maps. Correlations between  
478 the true and estimated time series for these first three patterns are all above 0.99 in the calibration in-  
479 terval and above 0.98 in the reconstruction interval (see Table 4 for these statistics at all noise levels).  
480 As dictated by the CCA formulation, correlations within the calibration interval progressively decrease  
481 from the maximum of the first pattern for all noise levels (Table 4). This is interestingly not the case in  
482 the reconstruction interval when some of the correlations for higher-order patterns exceed those of the  
483 lower-order patterns.

484 Figure 5 also plots the relative values of the proxy covariance maps for the first three canonical  
485 patterns. These maps scale location markers for the 104 pseudoproxies by their relative loadings and  
486 also designate where the loadings are positive or negative using the color of the markers. Upon in-  
487 specting the two sets of temperature and pseudoproxy covariance maps one can see that the proxy  
488 maps effectively reflect local sampling from the temperature maps. For instance, the leading canonical  
489 pattern associated with predominant warming is reflected in the proxy map that contains universally

490 positive loadings. In the other two patterns, the positive and negative loadings are roughly collocated  
491 with the areas of positive and negative temperatures in the temperature covariance maps. These maps  
492 also indicate relatively balanced loadings of the pseudoproxies in which no single record is weighted  
493 heavily in a given pattern. Equivalent maps in real-world CFR applications would similarly be useful  
494 for evaluating the impact of specific proxies in the derived reconstructions.

495

#### 496 **4.2.2 Northern Hemisphere Means**

497 The temperature covariance maps and proxy-estimated time series presented in Figure 5 are combined  
498 to yield a complete field reconstruction for each of the investigated noise levels. The total number of  
499 combined patterns is of course dictated by the number of retained  $d_{cca}$  values, which were determined  
500 for the preferred solutions in Section 4.1 to range from 18 in the no-noise case to 3 at an SNR of  
501 0.25 (see Table 3). Complete CCA reconstructions are assembled from these collections of patterns  
502 and time series. We first plot the area-weighted mean NH time series associated with these complete  
503 reconstructions in Figure 6a.

504 The correlations between the reconstructed mean NH time series and the model target are all signif-  
505 icant, even though they reduce with increasing noise levels (Table 5). These correlations are interest-  
506 ingly less than those determined for the first three canonical patterns at all noise levels given in Table  
507 4. This is indicative of the fact that the leading individual patterns are reconstructed more skillfully  
508 than the mean of the combined field containing the full range of scaled canonical patterns.

509 Although the determined correlations are all significant, the time series in Figure 6a suffer from  
510 warm biases and variance losses during the reconstruction interval, both of which increase with higher  
511 noise levels. This behavior is not associated with the difference between the dimensions chosen for

512 the preferred solutions in Section 4.1 and those for the absolute minimum RMSE: Figure 6b plots the  
513 mean time series from the reconstructions using the latter-derived dimensions and the results still suffer  
514 from the observed effects. These absolute-minimum time series correlate with the preferred-solution  
515 reconstructions at levels of  $r = 0.97$  or better. In fact, it is virtually impossible to discern the differences  
516 between Figures 6a and 6b, pointing to the robustness of the achieved results and the prevalence of the  
517 observed warm biases and variance losses in the NH means. Local correlations also reflect a strong  
518 consistency between the absolute minimum and preferred reconstructions: the area-weighted mean  
519 field correlations from 850-1855 C.E. between the two reconstructions are 0.97, 0.95, and 0.89 for  
520 SNR = infinity, 1.0, and 0.5, respectively (note that the dimensional selections for the SNR = 0.25 case  
521 were the same for both the absolute minimum and preferred solutions, thus no correlation statistics  
522 are necessary for that noise level). These comparisons demonstrate a spatial consistency between the  
523 two dimensional choices and suggest that the large-scale features are well captured for different sets of  
524 CCA dimensions (assuming the RMSE is held close to the absolute minimum).

525 The box plots in Figures 6c and 6d are calculated from the distribution of the individual annual  
526 means in each NH time series during the reconstruction interval. The plots further demonstrate the  
527 warm biases and variance losses in the reconstructed NH time series, as well as the reduced number  
528 of extreme events in the reconstructed time series relative to the known model target. These extrema  
529 are typically associated with volcanic events in the model simulated NH mean, and are manifest as  
530 cold outliers in both the model target and the reconstructed time series. The number and extent of the  
531 outliers is diminished in the reconstructed time series, however, and indicates that the reconstructions  
532 have the potential to miss the characterization of these important annual events in the model simulated  
533 climate.

534

### 535 **4.2.3 Reconstructed Fields**

536 Figure 7 shows the spatial distributions of validation statistics for the preferred CCA reconstruc-  
537 tions at SNRs of 1.0 and 0.5; statistics are computed during the reconstruction interval and summary  
538 statistics for all noise levels are given in Table 5. Field correlations of course reduce with increased  
539 noise, but Figure 7 illustrates the spatial variability of the local correlation coefficient. In all reconstruc-  
540 tions, regions containing the largest correlations are over North America and Europe. These regions  
541 correspond to the areas with the largest density of pseudoproxies (see Figure 1), i.e. the reconstruc-  
542 tions perform best where the field is sampled the most. Similarly, regions that are not sampled in the  
543 pseudoproxy network have comparatively low verification correlations. Correlations fall to particularly  
544 low values over some important regions (e.g. subtropical and mid-latitude ocean basins or the Asian  
545 continent) at high-noise levels.

546 The warm biases and variance losses observed in the mean NH time series (Figure 6) are also mani-  
547 fest in the reconstructed fields, but their spatial patterns show important regional distinctions (Figure 7).  
548 Standard deviation ratios (sample standard deviation of the reconstruction divided by the correspond-  
549 ing model value) indicate that variance is most strongly preserved in areas where field correlations are  
550 high, whereas variance losses are largest over the ocean basins where the lowest field correlations are  
551 observed (see Smerdon et al. (2008) for a discussion on the use of this metric for the purpose of evalu-  
552 ating field skill). Overall, significant variance losses are observed for all noise levels: the area-weighted  
553 mean standard deviation ratio is respectively 0.58 and 0.44 for the SNR cases of 1.0 and 0.5 shown in  
554 Figure 7, while the ratio drops to 0.37 at a SNR of 0.25 (Table 5). Additionally, large variance losses  
555 can accompany reconstructions with relatively high correlations in the field: standard deviation ratios

556 drop below 0.5 in many regions of the reconstruction for an SNR of 1.0 (Figure 7).

557 Mean biases also display regional variations, although they appear more spatially uniform than ob-  
558 served for the local correlations or standard deviation ratios. While most regions of the reconstructions  
559 are warmer than the actual model field, means are colder in a few areas (e.g. North America and the  
560 North Atlantic). The proportion of colder to warmer regions is reduced with increasing noise levels and  
561 is reflected in the average mean biases calculated for the fields (see Table 5); high-noise reconstructions  
562 therefore are dominated by warm-biased regions.

563 The bottom panels in Figure 7 show the RMSE of the fields, which combine errors associated  
564 with variance losses and mean biases. The RMSE patterns follow most closely the patterns in the  
565 mean biases, indicating that the error is dominated by differences between the reconstructed and actual  
566 means. Contrary to the correlation patterns, it is also important to note that the RMSE is in some cases  
567 largest over regions where the pseudoproxy network is densest. Mean biases, and therefore RMSE, do  
568 not appear to be as strongly tied to the distribution of the pseudoproxy network as the correlation and  
569 standard deviation ratios.

570

### 571 **4.3. Comparison of CCA and RegEM Reconstructions**

572 We have used the same pseudoproxies from the CCA experiments above to compute corresponding  
573 non-hybrid (Rutherford et al. 2005) RegEM-Ridge reconstructions. The derived reconstructions are  
574 the same reconstructions presented by Smerdon et al. (2008a) and employ a standardization scheme  
575 realistically confined to the calibration interval (Smerdon and Kaplan 2007) during which no detrending  
576 has been applied; all reconstructions have used a stagnation tolerance of  $1 \times 10^{-4}$ . Figures 8a and 8b  
577 compare the mean NH time series computed from the CCA and RegEM-Ridge reconstructed fields at

578 SNRs of 1.0 and 0.5. The time series at all noise levels compare very closely: correlations between  
579 the CCA and RegEM-Ridge time series are 0.96, 0.97, 0.96, and 0.89 for SNR=infinity, 1.0, 0.5, 0.25,  
580 respectively. The reconstructed NH means also correlate with the true model mean at comparable levels  
581 (Table 5). There is, however, an indication that the RegEM-Ridge method performs slightly better at  
582 higher noise levels given that the correlations increase by a few hundredths above those observed for  
583 CCA. The mean biases and variance losses are larger in the RegEM-Ridge reconstructions, however,  
584 and can be clearly seen in the box plots in Figures 8c and 8d. The failure to reconstruct extreme events  
585 is also most strongly associated with the RegEM-Ridge reconstructions as illustrated in these latter  
586 panels of Figure 8.

587 The correlation fields between the CFRs derived from the two methods are plotted in Figure 9,  
588 again showing results for SNRs of 1.0 and 0.5. Correlations between the two reconstructions depend  
589 on location, but overall the area-weighted mean field correlations are 0.89, 0.92, 0.85, and 0.65 for  
590 SNR=infinity, 1.0, 0.5, 0.25, respectively. As discussed in Section 3, CCA and RegEM-Ridge select  
591 regression coefficients in two distinctly different ways, but the widespread high field correlations be-  
592 tween the results from both methods indicate that they reconstruct similar patterns of variability in the  
593 target field (note that the exact same pseudoproxies have been used for each of these experiments).

594 Validation fields for the RegEM-Ridge reconstructions are shown in Figure 10. These are directly  
595 comparable to the CCA-validation fields shown in Figure 7. The close correspondence between the  
596 two figures further attests to the similarities between the results derived from both methods. Summary  
597 statistics for the RegEM-Ridge field correlations, standard deviation ratios, mean biases, and RMSE  
598 are given in Table 5. The mean field correlations associated with the two methods are very similar, yet  
599 indicate RegEM-Ridge to have slightly more correlation skill at increased noise levels. The RegEM-

600 Ridge mean biases also have spatial patterns very similar to CCA, but indicate that RegEM-Ridge  
601 produces larger biases at increased noise levels. The most notable difference between the two methods  
602 is associated with their standard deviation ratios. RegEM-Ridge standard deviation ratios have patterns  
603 similar to the CCA reconstructions and also maintain the most variance where the field correlations  
604 are highest. The variance loss in RegEM-Ridge, however, is much more pronounced than in the CCA  
605 reconstructions: mean standard deviation ratios are only 62% of those achieved for the CCA recon-  
606 structions at a SNR of infinity and fall to almost 40% of the CCA counterpart at a SNR of 0.25. These  
607 variance losses are manifest in the higher RMSE values associated with the RegEM-Ridge fields, but  
608 result in only modest increases in the mean field errors (Table 5) relative to CCA. Two factors con-  
609 tribute to the similar RMSE fields in spite of the larger variance losses in the RegEM-Ridge CFRs:  
610 (1) the mean biases dominate the error fields, which are not significantly different in the reconstruc-  
611 tions from the two methods; and (2) the slightly higher correlations associated with the RegEM-Ridge  
612 reconstructions offset the errors associated with variance losses.

613

## 614 **5. Discussion**

615 Comparisons between CCA and RegEM-Ridge show that the methods produce very similar results,  
616 with the exception of the larger variance losses observed in the RegEM-Ridge reconstructions. The  
617 source of variance losses is likely associated with the manner in which the eigenvalue spectra are  
618 truncated in the two methods. Ridge regression filters the eigenvalue spectrum using a continuous  
619 filter function, i.e. there is no abrupt eigenvalue truncation like that used in CCA where modes that  
620 cannot be reliably calibrated are simply set to zero. This was indeed one reason why RegEM-Ridge  
621 was originally proposed as a potentially advantageous method in CFR contexts (Schneider 2001). A

622 consequence of the continuous filtering function, however, is the fact that leading modes may be overly  
623 dampened if only a small number of them carry a large percentage of the total variance, as in the case  
624 of the CFR application presently considered. By contrast, the finite truncation of the CCA method  
625 yields leading modes that are unaffected by the truncation. To demonstrate this fact, Figure 11 plots  
626 the eigenspectra for the true model field and for the RegEM-Ridge and CCA CFRs at SNR levels of  
627 1.0 and 0.5. The magnitudes of the RegEM-Ridge eigenvalues are strikingly reduced in comparison to  
628 those of CCA. Apart from their scaling, however, Figure 9 and the similarity of the correlation statistics  
629 for both methods shown in Figures 7 and 10 indicate that the two methods are reconstructing similar  
630 patterns, and differ primarily by the dampened variability of the leading modes in the RegEM-Ridge  
631 spectrum.

632 The above discussion is relevant to the important and yet-to-be-explained difference between pseu-  
633 doproxy CFRs derived using RegEM-Ridge and RegEM using truncated total least squares (hereinafter  
634 RegEM-TTLS; Mann et al. 2007). This latter method has been shown to perform well in one pseudo-  
635 proxy context (Mann et al. 2007a), particularly in terms of its ability to reproduce the NH mean index,  
636 while the former has not (Smerdon and Kaplan 2007). The original explanation for the differences  
637 between the performance of RegEM-Ridge and RegEM-TTLS was tied to the selection of the ridge  
638 parameter by means of generalized cross validation (GCV) in RegEM-Ridge (Mann et al. 2007a,c).  
639 Because GCV was not used within RegEM-TTLS, Mann et al. (2007a,c) concluded that the problem  
640 was specific to RegEM-Ridge. Smerdon et al. (2008a), however, demonstrated that the mean biases  
641 and variance losses in RegEM-Ridge were not associated with the GCV selection of the ridge param-  
642 eter, making the Mann et al. (2007a,c) explanation implausible. The similarity between the CCA and  
643 RegEM-Ridge results presented herein further indicate that mean biases and variance losses in cur-



644 rently employed CFR methods are not tied to a specific methodological choice. Moreover, the similar  
645 shortcomings observed for the Mann et al. (1998) CFR method noted by von Storch et al. (2004,  
646 2006) supports the idea that the effects cannot be connected to something specific in RegEM-Ridge. It  
647 therefore is unlikely that differences in the reported performance of multiple CFRs can be specifically  
648 associated with the method of eigenvalue truncation or filtration, pointing to the need for an improved  
649 understanding of why the differences exist.

650 Comparisons of the field performances of the different methods will ultimately help explain some  
651 of the above inconsistencies. While a complete investigation of the differences between the two RegEM  
652 methods is outside the scope of this paper, some preliminary observations are possible. Mann et al.  
653 (2007a) provide validation statistics for RegEM-TTLS using a pseudoproxy experiment identical to  
654 the configuration used herein, and compute the mean  $r^2$  values for the NH field (labeled Multivari-  
655 ate  $r^2$  in Table 2 of Mann et al. (2007a)). Their experiments d, e, f, and h correspond to the same  
656 white-noise pseudoproxy experiments performed herein for SNRs of infinity, 1.0, 0.5 and 0.25, re-  
657 spectively (although these pseudoproxies involve different noise realizations). The principal difference  
658 between these experiments is that Mann et al. (2007a) performed hybrid reconstructions that calibrate  
659 separately in high- and low-frequency domains (split at the 20-year period) before combining the two  
660 reconstructed domains in a final CFR; the authors report there to be little difference between hybrid  
661 and non-hybrid results.

662 The  $r^2$  values reported in Mann et al. (2007a) for RegEM-TTLS are 0.30, 0.23, 0.19 and 0.06,  
663 for SNRs of infinity, 1.0, 0.5 and 0.25, respectively. These values are equivalently 0.51, 0.36, 0.20,  
664 and 0.05 for CCA, and 0.48, 0.37, 0.23, and 0.07 for RegEM-Ridge. Except for the highest noise  
665 level, for which all methods perform similarly poorly (and are likely within uncertainties imposed by

666 different pseudoproxy noise realizations), these validation statistics indicate that CCA and RegEM-  
667 Ridge produce CFRs with more field skill than RegEM-TTLS. Mann et al. (2007a) also provide the  $r^2$   
668 values between the target and reconstructed NH means: 0.87, 0.86, 0.83, and 0.34 for SNRs of infinity,  
669 1.0, 0.5 and 0.25, respectively, as compared to 0.86, 0.74, 0.52 and 0.17 for CCA and 0.83, 0.73, 0.55,  
670 and 0.24 for RegEM-Ridge. RegEM-TTLS thus appears to produce more skillful mean NH time series  
671 than CCA and RegEM-Ridge, whereas the latter two methods resolve more variance in the field. An  
672 understanding of the differences between these various methods must therefore account for the origin  
673 of the disparity between these two skill performances.

674 It is also important to highlight the observed concentration of the highest field correlations (and  
675 preserved variance) in areas with high pseudoproxy concentrations, a feature of both the CCA and  
676 RegEM-Ridge CFRs. Although this result may seem intuitive, it is not necessarily an expected charac-  
677 teristic of either the CCA or RegEM-Ridge methods. Both of these techniques attempt to reconstruct  
678 large-scale climate patterns by discarding smaller-scale modes of variability and noise. Despite this  
679 emphasis on large-scale patterns, the observed correlation distributions demonstrate that the meth-  
680 ods perform best where dense sampling exists, indicating that low-noise proxies outside of the highly  
681 sampled regions is an important means of improving CFR field skill. Nevertheless, it is important to  
682 understand better the origin of the observed skill concentrations and their dependence on the underly-  
683 ing character of the target field. In the case of the reported pseudoproxy experiments, the skill patterns  
684 are dependent on the internal statistics of the model-simulated climate. Previous experiments have in-  
685 dicated that methodological performance is not strongly dependent on the employed model simulation.  
686 Integrations from two different GCMs were used by von Storch et al. (2004, 2006) to test the Mann et  
687 al. (1998) method and results were consistent across the simulations in terms of the NH means. The

688 authors also reported no significant dependence on the sampling distribution. Similarly, Mann et al.  
689 (2007a) indicated no significant sensitivity to the two GCM integrations or sampling distribution used  
690 to test RegEM-TTLS. Christiansen et al. (2009) used yet another model integration and method for  
691 generating ensemble statistics and observed mean biases and variance losses in NH means derived from  
692 multiple methods. It therefore is unlikely that differences in model integrations will affect the gross per-  
693 formance of reconstruction methods already reported. Nevertheless, the underlying field performance  
694 of CFRs is likely more sensitive to the spatial statistics of the model simulations and should be tested  
695 on multiple model integrations. More experiments using observational data (e.g. Evans et al. 2001,  
696 2002) are also needed in order to determine whether the skill patterns of pseudoproxy experiments are  
697 similar to those estimated from real-world data sets.

698 The use of pseudoproxy experiments as a research tool has proceeded under the assumption that  
699 modeled climates and pseudoproxies approximate well the conditions in real-world reconstruction  
700 problems. This assumption may require the most caution, however, when interpreting results depen-  
701 dent on the underlying spatial statistics of the field and the associated teleconnections. Furthermore,  
702 noise structures in real-world proxies are undoubtedly more complicated than the white noise models  
703 used in this study. While it is appropriate to approach the results contained herein as a best-case sce-  
704 nario, further work is necessary to more faithfully capture the nonlinear, multivariate and nonstationary  
705 noise characteristics that are likely present in many proxy series (e.g. North et al. 2006). For instance,  
706 tree-ring models have been developed to simulate dendroclimatic series with notable success (Evans  
707 et al. 2006; Anchukaitis et al. 2006) and can be used to simulate synthetic tree-ring chronologies for  
708 use in pseudoproxy studies. The seasonal dependencies of proxy records should also be considered  
709 in future work. Significant variations in field skill have been observed for multiproxy networks that

710 target individual seasons (e.g. Pauling et al. 2003) and suggest that the annual pseudoproxy records  
711 used in most studies to date is another important idealization. Incorporating these more complicated  
712 noise characteristics in pseudoproxy studies will provide more realistic evaluations of CFR methods.  
713 Recent work also has shown the importance of evaluating ensembles of reconstructions generated from  
714 multiple noise realizations in both the proxy and target datasets (Christiansen et al. 2009). Not all dif-  
715 ferences between methods tested on individual noise realizations may be statistically significant when  
716 uncertainties due to random errors are incorporated. Christiansen et al. (2009) have shown this is the  
717 case for NH mean estimates; such ensemble work has not been done in the context of reconstruction  
718 performance in the field. Future work to evaluate field skill in ensembles of CFRs is therefore highly  
719 warranted.

720

## 721 **6. Conclusions**

722 Successful application of the CCA method to the problem of reconstructing NH temperature fields  
723 during the last millennium has been demonstrated and evaluated using pseudoproxies. An element of  
724 this application involved the development of a selection procedure for the three CCA dimensions. We  
725 have demonstrated a “leave-half-out” cross-validation procedure that selects robust and parsimonious  
726 dimensional combinations while guarding against artificial skill in the reconstruction. Our experiments  
727 demonstrate that the CCA method faithfully reconstructs between 3 and 18 climatic patterns given a  
728 proxy distribution approximating the Mann et al. (1998) proxy network and a range of observational  
729 uncertainties from no noise to an SNR of 0.25 (the exact number of resolved patterns will of course vary  
730 with different noise realizations at a given SNR value and is idealized in the pseudoproxy framework).  
731 Subsequent application of the CCA method to real-world climate proxies is thus easily attainable in

732 future work. The transparency of the CCA method and its well-developed theoretical basis in the  
733 literature is a strong motivation for its application. These characteristics provide straightforward eval-  
734 uations of the CCA model selection and the source of skill in derived reconstructions. The results of  
735 our pseudoproxy experiments, however, suggest that CFRs derived using CCA, just like those derived  
736 from RegEM-Ridge, should be interpreted carefully when applied to the problem of reconstructing  
737 large-scale climate patterns during the last several millennia. We note in particular that CCA CFRs  
738 have the potential to suffer from significant mean biases and variance losses across a range of noise  
739 levels spanning those of real-world proxies.

740 Field correlations were also shown to diminish significantly with increasing noise, particularly in  
741 regions with few or no pseudoproxies. Given that SNRs in real proxy records are estimated to be  
742 on the order of 0.4 (e.g. Mann et al. 2007a) and typically characterized by more complicated au-  
743 toregressive and moving average structures than the white-noise models adopted herein, the observed  
744 skill reductions should be considered a best-case scenario. In real-world CFRs derived with CCA, the  
745 spatial patterns of field errors will depend on at least five factors: (1) the spatial distribution of the  
746 proxies; (2) the magnitude and character of noise in the proxy network; (3) the spatial coherence of  
747 the target field, i.e. the strength and character of its teleconnections; (4) the true historical variability  
748 of the climate during the reconstruction interval; and (5) the length of the calibration period used for  
749 estimating proxy-climate correlations. The dependence of the spatial skill associated with the CCA  
750 method to these factors requires further testing. Evaluation of the method using additional millennial  
751 simulations from AOGCMs or observational fields should be pursued to determine the robustness of the  
752 spatial skill dependencies that we have identified. More realistic pseudoproxy networks should also be  
753 considered that incorporate seasonal dependencies, multivariate climate responses and autoregressive

754 noise structures. The impact of these more complicated pseudoproxy characteristics should be consid-  
755 ered specifically with regard to the field characteristics as we have outlined in the present manuscript,  
756 as opposed to the more widely evaluated performance of the NH mean. Their impact within different  
757 calibration scenarios is also important, particularly with regard to the length of the calibration interval  
758 and the range of climate variability represented in the calibration interval relative to the reconstruction  
759 interval (e.g. Jones et al. 2009).

760 Comparisons between reconstructions derived from CCA and RegEM-Ridge demonstrate strong  
761 similarities between the two methods, both in terms of the derived mean NH temperatures and the  
762 spatial characteristics of the reconstructed fields. These similarities are encouraging regarding the  
763 consistency of the two linear methods, but are also an indication that there may be problems endemic  
764 to the present generation of CFR methods used to reconstruct large-scale temperature patterns during  
765 the last millennium. More research therefore is needed to characterize the performance of multiple  
766 CFR methods in terms of their field performance and to draw distinct conclusions about the similarities  
767 and differences. These studies are particularly needed in the context of CFRs derived from real-world  
768 proxies as a means of deriving a better description of the uncertainties in present estimates of late-  
769 Holocene temperature variability.

770 The similarity between the CCA and RegEM-Ridge results further points to the need to understand  
771 the differences in the performance of the RegEM-Ridge and RegEM-TTLS methods. Initial compar-  
772 isons explored herein indicate that RegEM-TTLS may produce more skillful NH mean indices, while  
773 yielding CFRs that are less skillful than those produced by either CCA or RegEM-Ridge. Resolving  
774 the origin of these differences is not only important for studies that have attempted to reconstruct tem-  
775 peratures over the last millennium (Rutherford et al. 2005, Mann et al. 2005, 2007a, 2008), but also

776 for efforts that have applied RegEM in other contexts (e.g. Zhang et al. 2004; Steig et al. 2009). This  
777 necessity is further supported by the fact that pseudoproxy experiments have demonstrated differences  
778 between the performance of the two RegEM approaches, while real-world reconstructions of late-  
779 Holocene temperatures derived from the two methods have not been notably different - at least in their  
780 representation of the NH mean (Mann et al. 2007a). Each of these observations indicates that the focus  
781 within the literature on only NH means is insufficient for evaluating CFR methods and their derived  
782 results. Furthermore, explaining the performance differences between various CFR methods remains  
783 an open research question, but the persistence of similar problems in now multiple linear reconstruc-  
784 tion methods suggests that caution must be exercised in the interpretation of published real-world CFR  
785 results.

786

## 787 **Acknowledgments**

788 This research was supported in part by the National Science Foundation by grants ATM04-07909 to  
789 AK and ATM-0902436 to JES, AK and MNE and by the National Oceanic and Atmospheric Admin-  
790 istration, U.S. Department of Commerce, by grant NA07OAR4310060 to JES, AK and MNE and by  
791 grant NAOAR4320912 to JES and AK under the Cooperative Institute for Climate Applications Re-  
792 search (CICAR). Part of this research was completed while DC was supported by a research internship  
793 from the Hughes Science Pipeline Project and JES was supported by a Mellon Postdoctoral Fellowship,  
794 both through the Department of Environmental Science at Barnard College. The statements, findings,  
795 conclusions, and recommendations are those of the authors and do not necessarily reflect the views of  
796 the any of the above organizations or agencies. LDEO contribution XXXX.

797

798

## APPENDIX A

799

### Application of CCA to the Climate Field Reconstruction Problem

800 Beginning with the SVDs of the proxy and temperature matrices written in Section 3.2, we use

801 multivariate linear regression with a matrix  $B'$

$$V_t^{rT} = B'V_p^{rT} + \varepsilon_v$$

802 ( $\varepsilon_v$  is the residual error) to predict the prewhitened PCs of temperature using the prewhitened proxy

803 PCs:

$$\hat{V}_t^{rT} = B'V_p^{rT}.$$

804 Because the prewhitened PCs are orthonormal,  $V_p^{rT}V_p^r = I$  (i.e. the identity matrix), the expression

805 for  $B'$  simplifies:

$$B' = (V_t^{rT}V_p^r)(V_p^{rT}V_p^r)^{-1} = V_t^{rT}V_p^r.$$

806 The last expression for  $B'$  can be decomposed using SVD:

$$B' = V_t^{rT}V_p^r = O_t\Sigma_{cca}O_p^T. \tag{A-1}$$

807 and can then be truncated by retaining only  $d_{cca} \leq \min(d_p, d_t)$  leading singular values and correspond-

808 ing patterns:

$$B^r = O_t^r\Sigma_{cca}^rO_p^{rT}. \tag{A-2}$$

809 Prediction of the prewhitened temperature PCs using  $B^r$  instead of  $B'$ , i.e.,



$$\hat{V}_t^{r T} = O_t^r \Sigma_{cca}^r O_p^r T V_p^r T$$

810 transforms into a simple form

$$\hat{Q}_t^T = \Sigma_{cca}^r Q_p^T \quad (\text{A-3})$$

811 if written in terms of the CCA time series; these are projections of the vectors  $V_t^r$  and  $V_p^r$  onto the sets  
812 of patterns  $O_t^r$  and  $O_p^r$ , respectively:

$$Q_t = V_t^r O_t^r, \quad Q_p = V_p^r O_p^r. \quad (\text{A-4})$$

813 Similarly, the predicted  $\hat{Q}_t$  corresponds to the predicted prewhitened temperature PCs  $\hat{V}_t^r$ :

$$\hat{Q}_t = \hat{V}_t^r O_t^r.$$

814 To obtain the CCA timeseries,  $Q_t$  and  $Q_p$ , directly from the standardized data sets, it is convenient  
815 to define the weight matrices,

$$W_t = U_t^r (\Sigma_t^r)^{-1} O_t^r, \quad W_p = U_p^r (\Sigma_p^r)^{-1} O_p^r, \quad (\text{A-5})$$

816 so that

$$Q_t^T = W_t^T T', \quad Q_p^T = W_p^T P', \quad (\text{A-6})$$

817 where Eqs. (5) and (6) and the orthonormality of the truncated EOF sets of  $U_t^r$  and  $U_p^r$ , i.e. columns,  
818 were used.

819 It follows from (A-4) that the columns of  $Q_t$  and  $Q_p$  are orthonormal sets. Moreover, inserting  
820 (A-4) into (A-1) yeilds,

$$Q_t^T Q_p = \Sigma_{cca}^r,$$

821 hence the columns of  $Q_t$  and  $Q_p$  with different ordering are orthogonal, while those with the same  
822 ordering are positively correlated. The correlation coefficients of these latter columns are equal to the  
823 diagonal elements of  $\Sigma_{cca}^r$ , and are called canonical correlations. Because of the SVD decomposition in  
824 (A-1), these are maximized in the following sense: the correlation coefficient between the first columns  
825 of  $Q_t$  and  $Q_p$  is the largest among the projections of  $V_t^r$  and  $V_p^r$  on any unit length vectors (patterns);  
826 these maximizing patterns are the first columns of  $O_t^r$  and  $O_p^r$ , respectively. The remaining correlation  
827 coefficients are arranged in descending order, i.e. the coefficient between the second columns of  $Q_t$   
828 and  $Q_p$  is the largest among projections of  $V_t^r$  and  $V_p^r$  on unit length vectors orthogonal to the first  
829 columns of  $O_t^r$  and  $O_p^r$ , respectively, and the patterns that achieve the latter correlation are the second  
830 columns of  $O_t^r$  and  $O_p^r$ ; the correlation coefficient between the third columns of  $Q_t$  and  $Q_p$  is the largest  
831 among projections of  $V_t^r$  and  $V_p^r$  on unit length vectors orthogonal to the first and second columns of  
832  $O_t^r$  and  $O_p^r$ , and so on.

833 The predictions of the CCA temperature time series by (A-3) amount to a simple multiplication of  
834 the CCA time series of the proxies by the diagonal elements of  $\Sigma_{cca}^r$ . To perform these predictions for  
835 the fields of temperature on the basis of the original proxy data, however, we require the spatial patterns  
836 of their regression on the CCA timeseries:

$$T' = C_t Q_t^T + \varepsilon_t, \quad P' = C_p Q_p^T + \varepsilon_p.$$

837 To determine  $C_p$  and  $C_t$  (the CCA patterns) or the CCA homogeneous covariance maps, we use the  
838 orthonormality of the CCA timeseries and the decomposition in (4):

$$C_p = (P' Q_p)(Q_p^T Q_p)^{-1} = P' Q_p = U_p \Sigma_p V_p^T V_p^r O_p^r = U_p^r \Sigma_p^r O_p^r \quad (\text{A-7})$$

839 and similarly,

$$C_t = T' Q_t = U_t^r \Sigma_t^r O_t^r. \quad (\text{A-8})$$

840 Thus the use of the low-rank CCA approximations in (5), (6), and (A-2) in the regression matrix  
 841 formula given in (2) results in

$$B_{cca} = U_t^r \Sigma_t^r V_t^{r T} V_p^r (\Sigma_p^r)^{-1} U_p^{r T} = U_t^r \Sigma_t^r O_t^r \Sigma_{cca}^r O_p^{r T} (\Sigma_p^r)^{-1} U_p^{r T},$$

if the inverse of the proxy covariance matrix is replaced by the pseudo-inverse (Golub and Van Loan, 1996):

$$(P' P'^T)^{-1} \longrightarrow (P' P'^T)^+ = (P^r P^{r T})^+ = U_p^r (\Sigma_p^r)^{-2} U_p^{r T}.$$

842 Given the definitions in Eqs. (A-5) and (A-8),  $B_{cca}$ , takes a simple form:

$$B_{cca} = C_t \Sigma_{cca}^r W_p^T. \tag{A-9}$$

843 **References**

844 Ammann, C. M., F. Joos, D. S. Schimel, B. L. Otto-Bliesner, and R. A. Tomas, 2007: Solar influence  
845 on climate during the past millennium: Results from transient simulations with the NCAR Climate  
846 System Model. *Proc. Nat. Acad. Sci. USA*, **104**, 3713-3718, doi:10.1073-pnas.0605064.103.

847

848 Ammann, C. and E. Wahl, 2007: The Importance of the Geophysical Context in Statistical Evaluations  
849 of Climate Reconstruction Procedures, *Climatic Change*, 85, 71-88, doi:10.1007/s10584-007-9276-x.

850

851 Anchukaitis, K. J., M. N. Evans, A. Kaplan, E. A. Vaganov, M. K. Hughes, H. D. Grissino-Mayer, and  
852 M. A. Cane, 2006: Forward modeling of regional scale tree-ring patterns in the southeastern United  
853 States and the recent influence of summer drought. *Geophys. Res. Lett.*, **33**, L04705, doi:10.1029/2005GL025050.

854

855 Anderson, T.W., 1984: *An Introduction to Multivariate Statistical Analysis*. 2nd ed. Wiley-Interscience,  
856 704 pp.

857

858 Barnett, T., and R. Preisendorfer, 1987: Origins and levels of monthly and seasonal forecast skill for  
859 United States surface air temperature determined by canonical correlation analysis. *Monthly Weather  
860 Review*, **115**, 1825-1850.

861

862 Bradley, R. S., M. K. Hughes and H. F. Diaz, 2003: Climate in Medieval Time, *Science*, **302**, 5644,  
863 404-405

864

865 Bretherton, C., C. Smith, and J.M. Wallace, 1992: An intercomparison of methods for finding coupled  
866 patterns in climate data. *J. Climate*, **5**, 541-560.

867

868 Beltrami, H., 2002: Climate from borehole data: Energy fluxes and temperatures since 1500. *Geophys.*  
869 *Res. Lett.*, **29**, doi:10.1029/2002GL015702.

870

871 Briffa, K. R., 2000: Annual climate variability in the Holocene: interpreting the message of ancient  
872 trees. *Quat. Sci. Rev.*, **19**, 87-105.

873

874 Briffa, K. R., and T. J. Osborn, 2002: Blowing hot and cold. *Science*, **295**, 2227-2228.

875

876 Briffa, K. R., T.J. Osborn, F.H. Schweingruber, I.C. Harris, P.D. Jones, S.G. Shiyatov, S.G. and E.A.  
877 Vagano, 2001: Low-frequency temperature variations from a northern tree ring density network. *J.*  
878 *Geophys. Res.*, **106**, 2929-2941.

879

880 Broecker, W.S., 2001: Paleoclimate - Was the medieval warm period global? *Science*, **291**, 5508,  
881 1497-1499.

882

883 Bürger, G., and U. Cubasch, 2005: Are multiproxy climate reconstructions robust? *Geophys. Res.*  
884 *Lett.*, **32**, L23711, doi:10.1029/2005GL024155.

885

886 Bürger, G., I. Fast, and U. Cubasch, 2006: Climate reconstruction by regression. *Tellus, Ser. A*, **58**,

887 227235.

888

889 Casty, C., D. Handorf, and M. Sempf, 2005: Combined winter climate regimes over the North At-  
890 lantic/European sector 1766-2000. *Geophys. Res. Lett.*, **32**, L13801, doi:10.1029/2005GL022431.

891

892 Christiansen, B. T. Schmith, and P. Thejll, 2009: A surrogate ensemble study of climate reconstruction  
893 methods: Stochasticity and robustness, *J. Climate*, **22**(4), 951-976, DOI:10.1175/2008JCLI2301.1.

894

895 Cook, E. R., K. R. Briffa, and P. D. Jones, 1994: Spatial regression methods in dendroclimatology: A  
896 review and comparison of two techniques. *Int. J. Climatol.*, **14**, 379-402.

897

898 Cook, E., J. Esper, and R. D'Arrigo, 2004: Extra-tropical Northern Hemisphere land temperature  
899 variability over the past 1000 years. *Quat. Sci. Rev.*, **23**, 2063-2074.

900

901 Crowley, T. J., and T. S. Lowery, 2000: How warm was the Medieval Warm Period? *Ambio*, **29**, 5154.

902

903 D'Arrigo, R., R. Wilson, and G. Jacoby, 2006: On the long-term context for late twentieth century  
904 warming. *J. Geophys. Res.*, **111**, D03103, doi:10.1029/2005JD006352.

905

906 D'Arrigo, R., R. Wilson, and A. Tudhope, 2009: The impact of volcanic forcing on tropical tempera-  
907 tures during the past four centuries. *Nature Geosci.*, **2**, 51-56.

908

909 Esper, J., E. R. Cook, and F. H. Schweingruber, 2002: Low-frequency signals in long tree-ring chronolo-  
910 gies for reconstructing past temperature variability. *Science*, **295**, 2250-2253.

911

912 Esper, J., D. C. Frank, R. J. S. Wilson, and K. R. Briffa, 2005: Effect of scaling and regression  
913 on reconstructed temperature amplitude for the past millennium, *Geophys. Res. Lett.*, **32**, L07711,  
914 doi:10.1029/2004GL021236.

915 Evans M.N., A. Kaplan, M.A. Cane, and R. Villalba, 2001: Globality and optimality in climate field  
916 reconstructions from proxy data, in V. Markgraf (ed.) *Present and Past Inter-Hemispheric Linkages in*  
917 *the Americas and Their Societal Effects*, Cambridge University Press, p. 53-72.

918

919 Evans, M. N., A. Kaplan, and M. A. Cane, 2002: Pacific sea surface temperature field reconstruc-  
920 tion from coral  $\delta^{18}\text{O}$  data using reduced space objective analysis. *Paleoceanography*, **17**(1), 1007,  
921 doi:10.1029/2000PA000590.

922

923 Evans, M.N., B.K. Reichert, A. Kaplan, K.J. Anchukaitis, E.A. Vaganov, M.K. Hughes and M.A. Cane,  
924 2006: A forward modeling approach to paleoclimatic interpretation of tree-ring data. *J. Geophys. Res.*,  
925 **111**, G03008, doi:10.1029/2006JG000166

926

927 Folland, C.K., T.R. Karl, J.R. Christy, R.A. Clarke, G.V. Gruza, J. Jouzel, M.E. Mann, J. Oerlemans,  
928 M.J. Salinger, and S.-W. Wang, 2001: Observed Climate Variability and Change. pp. 99-181 In:  
929 *Climate Change 2001: The Scientific Basis*. Contribution of Working Group I to the Third Assessment  
930 Report of the Intergovernmental Panel on Climate Change (Houghton, J.T., Ding, Y., Griggs, D.J.,

931 Noguera, M., van der Linden, P.J., Dai, X., Maskell, K. and Johnson, C.A. Eds.). Cambridge University  
932 Press, Cambridge, UK, 881 pp.

933

934 Fritts, H. C., T. J. Blasing, B. P. Hayden, and J. E. Kutzbach, 1971: Multivariate techniques for speci-  
935 fying tree-growth and climate relationships and for reconstructing anomalies in paleoclimate. *J. Appl.*  
936 *Meteorol.*, **10**, 845-864

937

938 González-Rouco, F., H. von Storch, and E. Zorita, 2003: Deep soil temperature as proxy for surface  
939 air-temperature in a coupled model simulation of the last thousand years. *Geophys. Res. Lett.*, **30**(21),  
940 2116, doi:10.1029/2003GL018264.

941

942 González-Rouco, J. F., H. Beltrami, E. Zorita, and H. von Storch, 2006: Simulation and inversion of  
943 borehole temperature profiles in surrogate climates: Spatial distribution and surface coupling. *Geo-*  
944 *phys. Res. Lett.*, **33**, L01,703,doi:10.1029/2005GL024,693.

945

946 Groveman, B. S., and H. E. Landsberg, 1979: Simulated northern hemisphere temperature departures  
947 1579-1880. *Geophys. Res. Lett.* , **6**, 767-770.

948

949 Golub, G. H. and C. F. Van Loan, 1996: *Matrix Computations*, Johns Hopkins University Press, 3rd  
950 Ed.

951

952 Harris, R.N., and D.S. Chapman, 2001: Mid-latitude (30°N – 60°N) climatic warming inferred by



953 combining borehole temperatures with surface air temperatures. *Geophys. Res. Lett.*, **28**, 747-750.

954

955 Hegerl, G. C., T. Crowley, M. Allen, W. T. Hyde, H. Pollack, J. Smerdon, and E. Zorita, 2007:

956 Detection of human influence on a new 1500 yr climate reconstruction. *J. Climate*, **20**, 650-666,

957 DOI:10.1175/JCLI4011.1.

958

959 Huang, S., H.N. Pollack, and P.Y. Shen, 2000: Temperature trends over the last five centuries recon-

960 structed from borehole temperatures. *Nature*, **403**, 756-758.

961

962 Hughes, M.K. and H.F. Diaz, 1994: Was there a medieval warm period, and if so, where and when?

963 *Clim. Ch.*, **26**, 2-3, 109-142.

964

965 Huybers, P., 2005: Comment on “Hockey sticks, principal components, and spurious significance” by

966 S. McIntyre and R. McKittrick. *Geophys. Res. Lett.*, **32**, L20705, doi:10.1029/2005GL023395.

967

968 Jansen, E., J. Overpeck, K.R. Briffa, J.-C. Duplessy, F. Joos, V. Masson-Delmotte, D. Olago, B. Otto-

969 Bliesner, W.R. Peltier, S. Rahmstorf, R. Ramesh, D. Raynaud, D. Rind, O. Solomina, R. Villalba and D.

970 Zhang, 2007: Palaeoclimate. In: *Climate Change 2007: The Physical Science Basis*. Contribution of

971 Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change

972 (Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M. Tignor and H.L. Miller

973 (eds.)). Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.

974

975 Jones, P.D., K.R. Briffa, T.J. Osborn, J.M. Lough, T.D. van Ommen, B.M. Vinther, J. Luterbacher, E.R.  
976 Wahl, F.W. Zwiers, M.E. Mann, G.A. Schmidt, C.M. Ammann, B.M. Buckley, K.M. Cobb, J. Esper,  
977 H. Goosse, N. Graham, E. Jansen, T. Kiefer, C. Kull, M. Küttel, E. Mosely-Thompson, J.T. Overpeck,  
978 N. Riedwyl, M. Schulz, A.W. Tudhope, R. Villalba, H. Wanner, E. Wolff, E. Xoplaki, 2009: High-  
979 resolution paleoclimatology of the last millennium: a review of current status and future prospects,  
980 *Holocene*, **19**, 3-49.

981

982 Jones, P. D., and M. E. Mann, 2004: Climate over past millennia. *Rev. Geophys.*, **42**, RG2002,  
983 doi:10.1029/2003RG000143.

984

985 Jones, P. D., M. New, D. E. Parker, S. Martin, and J. G. Rigor, 1999: Surface Air Temperature and its  
986 Changes over the Past 150 Years. *Rev. Geophys.*, **37**, 173-199.

987

988 Jones P.D., K.R. Briffa, T.P. Barnett, and S.F.B. Tett, 1998: High-resolution palaeoclimatic records for  
989 the last millennium: Interpretation, integration and comparison with general circulation model control-  
990 run temperatures. *Holocene*, **8**, 455-471.

991

992 Küttel, M., J. Luterbacher, E. Zorita, E. Xoplaki, N. Riedwyl, and H. Wanner, 2007: Testing a European  
993 winter surface temperature reconstruction in a surrogate climate. *Geophys. Res. Lett.*, **34**, L07710,  
994 doi:10.1029/2006GL027907.

995

996 Lee, T.C.K, F.W. Zwiers, and M. Tsao, 2007: Evaluation of proxy-based millennial reconstruction

997 methods. *Clim. Dyn.*, DOI 10.1007/s00382-007-0351-9

998

999 Luterbacher, J., C. Schmutz, D. Gyalistras, E. Xoplaki, and H. Wanner, 1999: Reconstruction of  
1000 monthly NAO and EU indices back to AD 1675. *Geophys. Res. Lett.*, **26**, 2745-2748.

1001

1002 Luterbacher, J., D. Dietrich, E. Xoplaki, M. Grosjean, and H. Wanner, 2004: European seasonal and  
1003 annual temperature variability, trends, and extremes since 1500. *Science*, **303**, 149-1503.

1004

1005 Luterbacher, J., R. Rickli, C. Tinguely, E. Xoplaki, E. Schüpbach, D. Dietrich, J. Hsler, M. Ambhl, C.  
1006 Pfister, P. Beeli, U. Dietrich, A. Dannecker, T. D. Davies, P. D. Jones, V. Slonosky, A. E. J. Ogilvie, P.  
1007 Maheras, F. Kolyva-Machera, J. Martin-Vide, M. Barriendos, M. J. Alcoforado, F. Nunez, T. Jónsson,  
1008 R. Glaser, J. Jacobeit, C. Beck, A. Philipp, U. Beyer, E. Kaas, T. Schmith, L. Barring, P. Jönsson, L.  
1009 Racz, L. and H. Wanner, 2000: Reconstruction of monthly mean sea level pressure over Europe for the  
1010 Late Maunder Minimum period (1675-1715). *Int. J. Climatol.*, **20**, 1049-1066.

1011

1012 Mann, M.E., Ammann, C.M., Bradley, R.S., Briffa, K.R., Crowley, T.J., Hughes, M.K., Jones, P.D.,  
1013 Oppenheimer, M., Osborn, T.J., Overpeck, J.T., Rutherford, S., Trenberth, K.E., Wigley, T.M.L., 2003:  
1014 On past temperatures and anomalous late 20th-century warmth. *Eos*, **84**, 256-258.

1015

1016 Mann, M.E., 2002: The Value of Multiple Proxies. *Science*, **297**, 1481-1482.

1017

1018 Mann, M. E., and S. Rutherford, 2002: Climate reconstruction using pseudoproxies. *Geophys. Res.*

1019 *Let.*, **29**(10), 1501, doi:10.1029/2001GL014554.

1020

1021 Mann, M. E., R. S. Bradley, and M. K. Hughes, 1998: Global-scale temperature patterns and climate  
1022 forcing over the past six centuries. *Nature*, **392**, 779-787.

1023

1024 Mann, M. E., R. S. Bradley, and M. K. Hughes, 1999: Northern Hemisphere temperatures during the  
1025 past millennium: Inferences, uncertainties, and limitations. *Geophys. Res. Lett.*, **26**, 759-762.

1026

1027 Mann, M. E., S. Rutherford, E. Wahl, and C. Ammann, 2005: Testing the fidelity of methods used in  
1028 proxy-based reconstructions of past climate. *J. Climate*, **18**, 4097-4107.

1029

1030 Mann, M. E., S. Rutherford, E. Wahl, and C. Ammann, 2007a: Robustness of proxy-based climate  
1031 field reconstruction methods. *J. Geophys. Res.*, **112**, D12109, doi:10.1029/2006JD008272.

1032

1033 Mann, M.E., S. Rutherford, E. Wahl, C. Ammann, 2007b: Reply to Comments on “Testing the Fidelity  
1034 of Methods Used on Proxy-based Reconstructions of Past Climate” by Zorita et al. *J. Climate*, **20**,  
1035 3699-3703.

1036

1037 Mann, M.E., Rutherford, S., Wahl, E., Ammann, C., 2007c: Reply to Comments on “Testing the  
1038 Fidelity of Methods Used on Proxy-based Reconstructions of Past Climate” by Smerdon and Kaplan.  
1039 *J. Climate*, **20**, 5671-5674.

1040

1041 Mann, M. E., Z. Zhang, M. K. Hughes, R. S. Bradley, S. K. Miller, S. Rutherford, and F. Ni, 2008:  
1042 Proxy-based reconstructions of hemispheric and global surface temperature variations over the past  
1043 two millennia. *Proc. Nat. Acad. Sci. USA*, **105**, 36, 13252-13257.

1044

1045 McIntyre, S., and R. McKittrick, 2005: Hockey sticks, principal components, and spurious significance.  
1046 *Geophys. Res. Lett.*, **32**, L03710, doi:10.1029/2004GL021750.

1047

1048 Moberg, A., R. Mohammad, and T. Mauritsen, 2008: Analysis of the Moberg et al. (2005) hemispheric  
1049 temperature reconstruction. *Clim. Dyn.*, **31**, 957-971, doi: 10.1007/s00382-008-0392-8.

1050

1051 Moberg, A, D.M. Sonechkin, K. Holmgren, N.M Datsenko, W. Karlen, 2005: Highly variable Northern  
1052 Hemisphere temperature reconstructed from low- and high-resolution proxy data. *Nature*, **433**, 7026,  
1053 613-617.

1054

1055 North, G.R. et al., 2006: *Surface Temperature Reconstructions for the Last 2,000 Years*, The National  
1056 Academies Press, Washington D.C., 196 pp.

1057

1058 Pauling, A., J. Luterbacher, and H. Wanner, 2003: Evaluation of proxies for European and North At-  
1059 lantic temperature field reconstructions, *Geophys. Res. Lett.*, **30**(15), 1787, doi:10.1029/2003GL017589.

1060

1061 Pauling, A., J. Luterbacher, C. Casty, and H. Wanner, 2006: 500 years of gridded high-resolution  
1062 precipitation reconstructions over Europe and the connection to large-scale circulation. *Clim. Dyn.*,

1063 **26**, 387-405.

1064

1065 Pollack, H. N., and J. E. Smerdon, 2004: Borehole climate reconstructions: Spatial structure and  
1066 hemispheric averages. *J. Geophys. Res.*, **109**, D11106, doi:10.1029/2003JD004163.

1067

1068 Preisendorfer, R., F. Zwiers and T.P. Barnett, 1981: Foundations of principal component selection  
1069 rules, SIO Ref. Ser. 81-4.

1070

1071 Riedwyl, N., M. Küttel, J. Luterbacher, H. and Wanner, 2009: Comparison of climate field reconstruc-  
1072 tion techniques: Application to Europe. *Clim. Dynam.*, **32**, 381-395

1073

1074 Rutherford, S., and M. E. Mann, 2004: Correction to Optimal surface temperature reconstructions us-  
1075 ing terrestrial borehole data by Mann et al. *J. Geophys. Res.*, **109**, D11107, doi:10.1029/2003JD004290.

1076

1077 Rutherford, S., M. E. Mann, T. J. Osborn, R. S. Bradley, K. R. Briffa, M. K. Hughes, and P. D.  
1078 Jones, 2005: Proxy-based Northern Hemisphere surface temperature reconstructions: Sensitivity to  
1079 methodology, predictor network, target season and target domain. *J. Climate*, **18**, 2308-2329.

1080

1081 Rutherford, S., Mann, M.E., Wahl, E., Ammann, C., 2008: Reply to comment by Jason E. Smerdon  
1082 et al. on “Robustness of proxy-based climate field reconstruction methods.” *J. Geophys. Res.*, **113**,  
1083 D18107, doi:10.1029/2008JD009964.

1084

1085 Schneider, T., 2001: Analysis of incomplete climate data: Estimation of mean values and covariance  
1086 matrices and imputation of missing values. *J. Climate*, **14**, 853-887.

1087

1088 Smerdon, J.E., and A. Kaplan, 2007: Comments on “Testing the fidelity of methods used in proxy-  
1089 based reconstructions of past climate”: The role of the standardization interval. *J. Climate*, **20**, 22,  
1090 5666-5670.

1091

1092 Smerdon, J.E., A. Kaplan, and D. Chang 2008a: On the standardization sensitivity of RegEM climate  
1093 field reconstructions, *J. Climate*, **21**(24), 6710-6723.

1094

1095 Smerdon, J.E., J.F. González-Rouco, and E. Zorita, 2008b: Comment on “Robustness of proxy-based  
1096 climate field reconstruction methods” by Michael E. Mann et al. *J. Geophys. Res.*, **113**, D18106,  
1097 doi:10.1029/2007JD009542.

1098

1099 Steig, E.J., D.P. Schneider, S.D. Rutherford, M.E. Mann, J.C. Comiso, D.T. Shindell, 2009: Warming  
1100 of the Antarctic ice sheet surface since the 1957 International Geophysical Year. *Nature*, **1457**, 459-  
1101 463.

1102

1103 Tippett, M. K., M. Barlow, and B. Lyon, 2003: Statistical correction of Central Southwest Asia winter  
1104 precipitation simulations. *Int. J. Climatol.*, **23**, 1421-1433.

1105

1106 Tippett, M. K., T. DelSole, S. J. Mason, and A. G. Barnston, 2008: Regression-Based Methods for

1107 Finding Coupled Patterns. *J. Climate*, **21**(17), 4384-4398.

1108

1109 von Storch, H., and F.W. Zwiers, 2000: *Statistical Analysis in Climate Research*, Cambridge University  
1110 Press, Cambridge, United Kingdom, 484 pp.

1111

1112 von Storch, H., and E. Zorita, 2005: Comment on “Hockey sticks, principal components, and spurious  
1113 significance” by S. McIntyre and R. McKittrick. *Geophys. Res. Lett.*, **32**, L20701, doi:10.1029/2005GL022753.

1114

1115 von Storch, H., E. Zorita, J. M. Jones, Y. Dimitriev, F. González-Rouco, and S. F. B. Tett, 2004:  
1116 Reconstructing past climate from noisy data. *Science*, **306**, 679-682.

1117

1118 von Storch, H., E. Zorita, J. M. Jones, F. González-Rouco, and S. F. B. Tett, 2006: Response to  
1119 comment on “Reconstructing past climate from noisy data.” *Science*, **312**, 529c.

1120

1121 Wahl, E. R., and C. M. Ammann, 2007: Robustness of the Mann, Bradley, Hughes reconstruction of  
1122 surface temperatures: Examination of criticisms based on the nature and processing of proxy climate  
1123 evidence. *Clim. Ch.*, **85**, 1-2, 33-69.

1124

1125 Wahl, E. R., D. M. Ritson, and C. M. Ammann, 2006: Comment on “Reconstructing past climate from  
1126 noisy data.” *Science*, **312**, 529b.

1127

1128 Wilks, D. S., 1995: *Statistical Methods in the Atmospheric Sciences*. Academic Press: New York., 467



1129 pp.

1130

1131 Xoplaki, E., J. Luterbacher, H. Paeth, D. Dietrich, N. Steiner, M. Grosjean, and H. Wanner (2005), Eu-  
1132 ropean spring and autumn temperature variability and change of extremes over the last half millennium.  
1133 *Geophys. Res. Lett.*, **32**, L15713, doi:10.1029/2005GL023424.

1134

1135 Zhang, Z., M.E. Mann, E.R. Cook, 2004: Alternative methods of proxy-based climate field recon-  
1136 struction: application to summer drought over the conterminous United States back to AD 1700 from  
1137 tree-ring data. *Holocene*, **14**, 502-516.

1138

1139 Zorita, E., J. F. González-Rouco, and H. von Storch, 2007: Comment on “Testing the fidelity of meth-  
1140 ods used in proxy-based reconstructions of past climate” by Mann et al. *J. Climate*, **20**, 14, 2693-3698.

1141 **Figure 1.** Map of grid-cell locations for the pseudoproxy network chosen to approximate the Mann et  
1142 al. (1998) proxy locations.

1143

1144 **Figure 2.** Cross-validation statistics during the calibration interval (1856-1980 C.E.) for the ensemble  
1145 of CCA reconstructions at an SNR of 0.5. Colors in the figure indicate the value of  $d_{cca}$ , which ranges  
1146 from 1-50. The symbols in the figure correspond to the following CCA solutions: the absolute mini-  
1147 mum RMSE (black dot), the maximum NHMC (black square), and preferred solution based on RMSE  
1148 (black star).

1149

1150 **Figure 3.** RMSE as a function of  $d_{cca}$  for all reconstructions spanning the collection of dimensional  
1151 combinations between 1 and 50. Colors in the figure indicate the value of  $d_p$  chosen for the derived  
1152 RMSE value. Yellow lines in each of the RMSE plots indicate the minimum RMSE achieve when  $d_t$  is  
1153 held constant at 50. Black dots correspond to the absolute minimum RMSE and the values of  $d_{cca}$ ,  $d_p$ ,  
1154 and  $d_t$  are given in the parenthesis next to each dot. The locations of the preferred solutions based on  
1155 RMSE are also shown in each panel with a black star; the dimensional combinations for these values  
1156 are also given in parenthesis.

1157

1158 **Figure 4.** Minimum RMSE values for each pairing of the  $d_{cca}$ ,  $d_p$  and  $d_t$  dimensions. The absolute  
1159 minimum RMSE value is plotted as a white dot; the preferred solution value is plotted as a white star.

1160

1161 **Figure 5.** Temperature homogeneous covariance maps ( $C_t$ ; left column), target and predicted time  
1162 series of the temperature maps ( $Q_t$  and  $\Sigma_{cca}Q_p^t$ ; middle column) and proxy homogeneous covariance

1163 maps ( $C_p$ ; right column) for the first three canonical patterns of the no-noise reconstructions (rank  
1164 increases from the top panels to the bottom). The markers in the proxy covariance maps reflect the  
1165 loadings for each pattern, where blue and red markers are positive and negative loadings, respectively,  
1166 and the size of the markers scale according to the size of the loadings. All elements are estimated over  
1167 the calibration interval, but the time series are extended into the reconstruction interval by projecting the  
1168 covariance maps onto the temperature and proxy matrices over the full temporal period. Correlations  
1169 between the target and predicted time series during the calibration and reconstruction intervals are given  
1170 in the middle column of panels. The percentage of variance explained in the target field during the  
1171 calibration interval are 10.5, 6.6 and 6.3% by the first, second and third covariance maps, respectively.

1172

1173 **Figure 6.** Area-weighted NH time series for the CCA reconstructions using  $d_{cca}$ ,  $d_p$ , and  $d_t$  values  
1174 associated with: (a) the preferred solution (Table 3); and (b) the absolute minimum RMSE values  
1175 (Table 2). Time series have been smoothed using a decadal low-pass filter. Also shown in (c) and (d)  
1176 are the box plots associated with the two combinations of the of  $d_{cca}$ ,  $d_p$ , and  $d_t$  values. These plots  
1177 were calculated from the distribution of the individual annual means in each NH time series during the  
1178 reconstruction interval.

1179

1180 **Figure 7.** Field comparisons between derived CCA reconstructions (using the preferred-solution values  
1181 of  $d_{cca}$ ,  $d_p$ , and  $d_t$ ) and the known CSM model fields: correlation (top row), standard deviation ratios  
1182 (second row), mean biases (third row) and RMSE (last row). Standard deviation ratios are computed  
1183 between the reconstruction and model and mean biases are computed as reconstruction minus model,  
1184 i.e. negative (positive) biases indicate a colder (warmer) reconstruction mean. Results are shown for

1185 SNRs of 1.0 (left panels) and 0.5 (right panels); summary statistics for all noise levels are given in  
1186 Table 4. All statistics are computed over the reconstruction interval (850-1855 C.E.).

1187

1188 **Figure 8.** Same as in Figure 6, but for comparisons between the area-weighted NH time series for CCA  
1189 and RegEM-Ridge reconstructions. Results are shown for SNRs of 1.0 and 0.5; summary statistics for  
1190 all noise levels are given in Table 5.

1191

1192 **Figure 9.** Correlation fields between the CCA and RegEM-Ridge reconstructions. Results are shown  
1193 for SNRs of 1.0 (left panel) and 0.5 (right panel) and are computed over the reconstruction interval  
1194 (850-1855 C.E.).

1195

1196 **Figure 10.** Same as in Figure 7, but for the RegEM-Ridge reconstructions.

1197

1198 **Figure 11.** Eigenspectra computed from the true model temperature field and the CCA and RegEM-  
1199 Ridge reconstructed temperature fields during the reconstructed interval (850-1855 C.E.). The CCA  
1200 spectra have the characteristic truncation to zero at the selected rank, while the RegEM-Ridge spectra  
1201 reflect the continuous filtration constraint applied in ridge regression.

SNR	<u>Early-Half Calibration</u>					<u>Late-Half Calibration</u>				
	RMSE	$d_{cca}$	$d_p$	$d_t$	NHMC	RMSE	$d_{cca}$	$d_p$	$d_t$	NHMC
Inf.	0.46	21	26	27	0.84	0.49	19	28	37	0.84
1.0	0.55	16	26	25	0.75	0.57	23	27	41	0.71
0.5	0.64	14	25	46	0.66	0.65	7	28	12	0.61
0.25	0.69	2	40	4	0.31	0.72	3	44	4	0.24

Table 1: Early (1856-1916 C.E.) and late-half (1917-1980 C.E.) cross-validation statistics for CCA; all statistics and dimensions represent those achieved for the minimum RMSE in the two respective cross-validation periods.

SNR	<u>Absolute minimum RMSE</u>					<u>Absolute maximum NHMC</u>				
	RMSE	$d_{cca}$	$d_p$	$d_t$	NHMC	RMSE	$d_{cca}$	$d_p$	$d_t$	NHMC
Inf.	0.48	21	26	50	0.82	0.52	21	41	35	0.87
1.0	0.56	24	27	45	0.72	0.57	20	27	35	0.74
0.5	0.65	15	25	47	0.63	0.67	25	34	32	0.69
0.25	0.71	3	44	4	0.28	0.73	4	12	44	0.44

Table 2: CCA reconstruction statistics using the absolute minimum RMSE or maximum NHMC criteria during the calibration interval (1856-1980 C.E.).

Preferred Solutions

SNR	RMSE	$d_{cca}$	$d_p$	$d_t$	NHMC
Inf.	0.48	18	25	36	0.84
1.0	0.56	13	27	21	0.70
0.5	0.66	7	28	12	0.62
0.25	0.71	3	44	4	0.28

Table 3: CCA reconstruction statistics for the preferred solutions in which parsimonious dimensional combinations have been chosen as the first local minimum of the RMSE statistic.

CCA Rank	<u>SNR Infinity</u>		<u>SNR 1.0</u>		<u>SNR 0.5</u>		<u>SNR 0.25</u>	
	Cal.	Recon.	Cal.	Recon.	Cal.	Recon.	Cal.	Recon.
1	0.999	0.991	0.975	0.916	0.920	0.734	0.876	0.397
2	0.997	0.990	0.969	0.875	0.895	0.653	0.792	0.454
3	0.996	0.987	0.958	0.853	0.876	0.528	0.719	0.252
4	0.994	0.969	0.936	0.839	0.817	0.700	---	---
5	0.989	0.965	0.928	0.810	0.785	0.671	---	---
6	0.984	0.950	0.905	0.671	0.694	0.252	---	---
7	0.983	0.951	0.869	0.652	0.658	0.333	---	---
8	0.975	0.899	0.820	0.638	---	---	---	---
9	0.971	0.916	0.803	0.553	---	---	---	---
10	0.964	0.889	0.764	0.422	---	---	---	---
11	0.956	0.861	0.757	0.586	---	---	---	---
12	0.950	0.875	0.625	0.364	---	---	---	---
13	0.913	0.700	0.592	0.279	---	---	---	---
14	0.912	0.815	---	---	---	---	---	---
15	0.887	0.752	---	---	---	---	---	---
16	0.879	0.800	---	---	---	---	---	---
17	0.820	0.548	---	---	---	---	---	---
18	0.747	0.644	---	---	---	---	---	---

Table 4: Correlation statistics between the true canonical temperature time series,  $Q_t$ , and those predicted by the proxy PCs, i.e.  $\Sigma_{cca}Q_p^T$ . Statistics are shown for both the reconstruction and calibration intervals.



CCA

SNR	NHMC	Mean of Field Correlations	Mean STD Ratio	Mean Bias (K)	Local RMSE Mean (K)
Inf.	0.93	0.69	0.76	0.04	0.37
1.0	0.86	0.58	0.58	0.09	0.45
0.5	0.72	0.43	0.44	0.17	0.53
0.25	0.41	0.22	0.37	0.23	0.61

RegEM-Ridge

SNR	NHMC	Mean of Field Correlations	Mean STD Ratio	Mean Bias (K)	Local RMSE Mean (K)
Inf.	0.91	0.68	0.47	0.01	0.42
1.0	0.86	0.60	0.37	0.11	0.47
0.5	0.74	0.46	0.23	0.20	0.55
0.25	0.49	0.24	0.15	0.26	0.61

Table 5: Validation statistics computed during the reconstruction interval (850-1855 C.E.) for the CCA and RegEM-Ridge reconstructions. Reconstructions from each method were derived with the same set of pseudoproxies at all noise levels. All field statistics were weighted by the cosine of the mid-latitude for each grid cell.

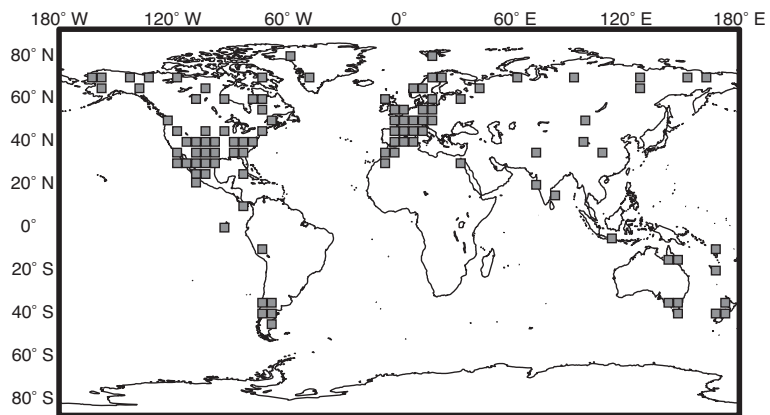


Figure 1: Map of grid-cell locations for the pseudoproxy network chosen to approximate the Mann et al. (1998) proxy locations.

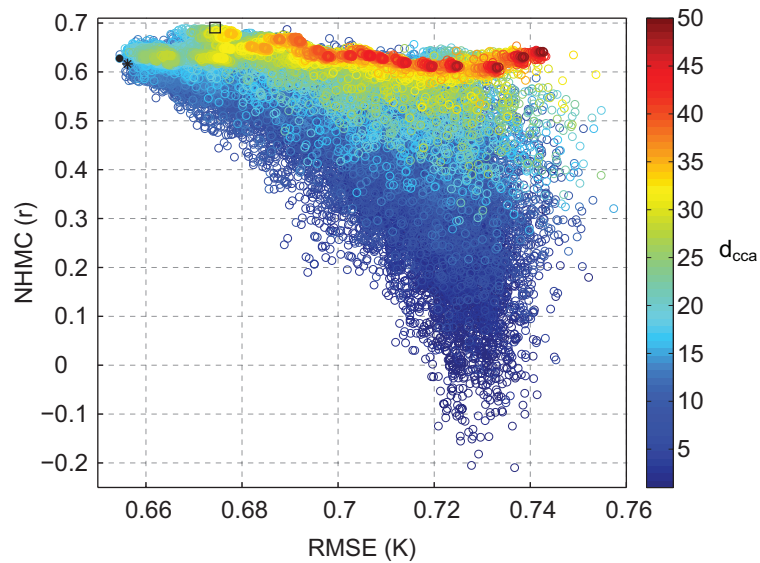


Figure 2: Cross-validation statistics during the calibration interval (1856-1980 C.E.) for the ensemble of CCA reconstructions at an SNR of 0.5. Colors in the figure indicate the value of  $d_{cca}$ , which ranges from 1-50. The symbols in the figure correspond to the following CCA solutions: the absolute minimum RMSE (black dot), the maximum NHMC (black square), and preferred solution based on RMSE (black star).

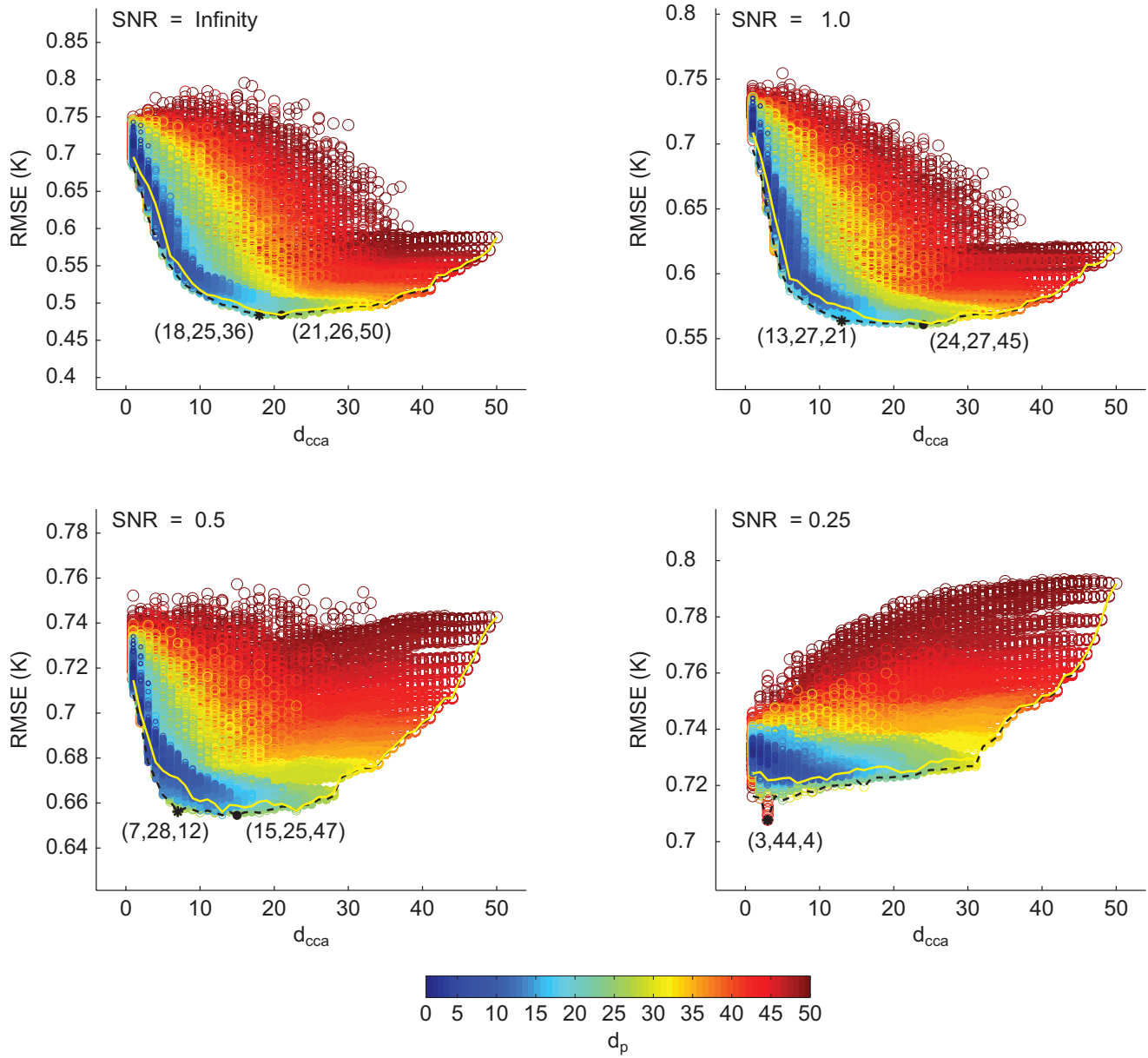


Figure 3: RMSE as a function of  $d_{cca}$  for all reconstructions spanning the collection of dimensional combinations between 1 and 50. Colors in the figure indicate the value of  $d_p$  chosen for the derived RMSE value. Yellow lines in each of the RMSE plots indicate the minimum RMSE achieved when  $d_t$  is held constant at 50. Black dots correspond to the absolute minimum RMSE and the values of  $d_{cca}$ ,  $d_p$ , and  $d_t$  are given in the parenthesis next to each dot. The locations of the preferred solutions based on RMSE are also shown in each panel with a black star; the dimensional combinations for these values are also given in parenthesis.

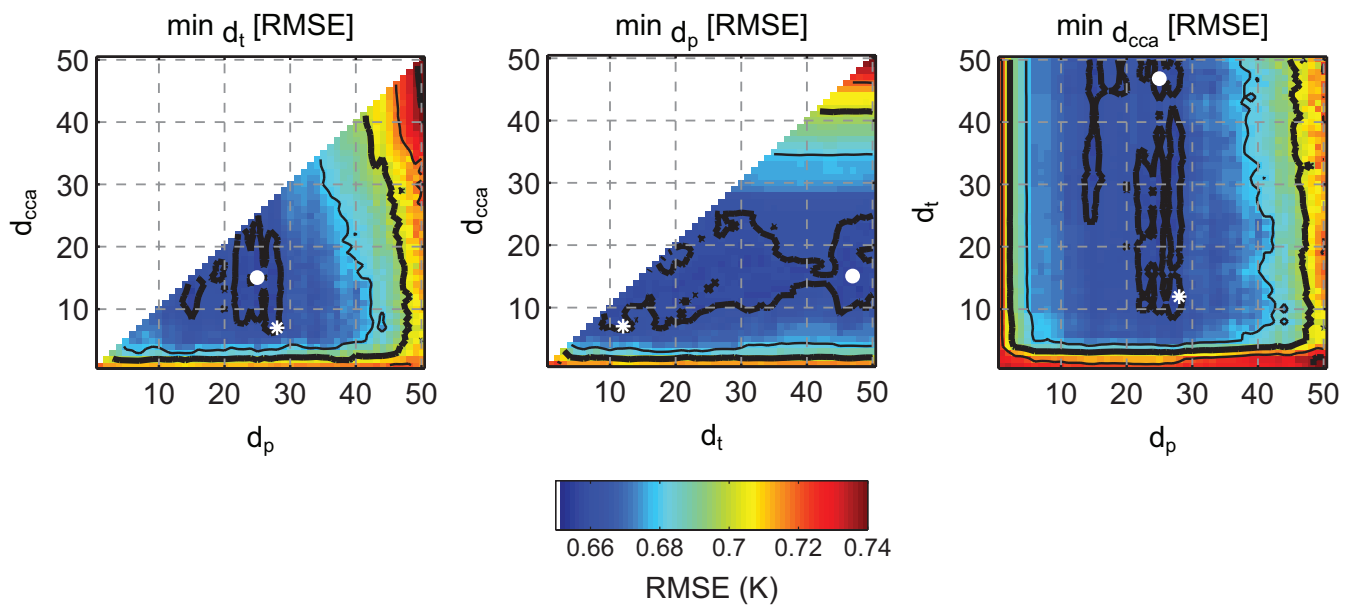


Figure 4: Minimum RMSE values for each pairing of the  $d_{cca}$ ,  $d_p$  and  $d_t$  dimensions. The absolute minimum RMSE value is plotted as a white dot; the preferred solution value is plotted as a white star.

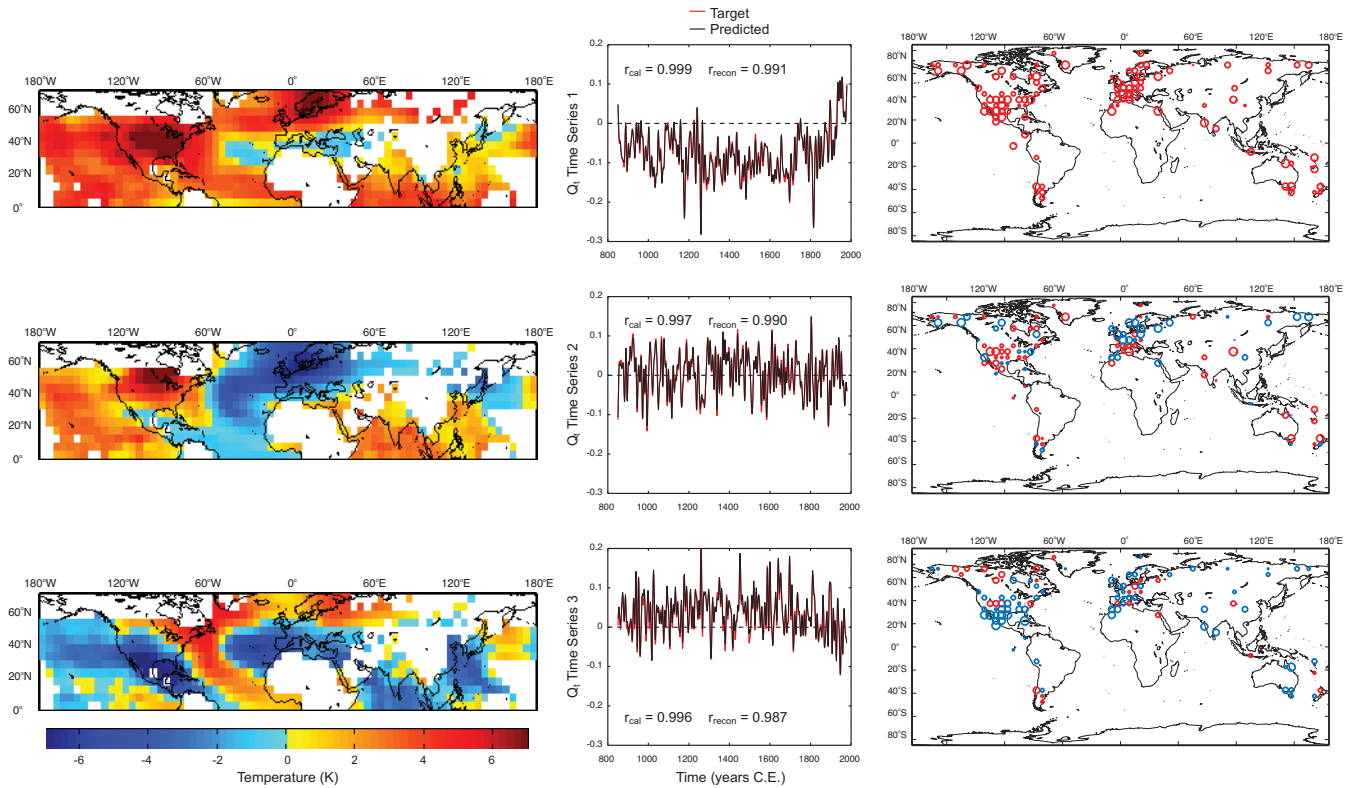


Figure 5: Temperature homogeneous covariance maps ( $C_t$ ; left column), target and predicted time series of the temperature maps ( $Q_t$  and  $\Sigma_{cca}Q_p^t$ ; middle column) and proxy homogeneous covariance maps ( $C_p$ ; right column) for the first three canonical patterns of the no-noise reconstructions (rank increases from the top panels to the bottom). The markers in the proxy covariance maps reflect the loadings for each pattern, where blue and red markers are positive and negative loadings, respectively, and the size of the markers scale according to the size of the loadings. All elements are estimated over the calibration interval, but the time series are extended into the reconstruction interval by projecting the covariance maps onto the temperature and proxy matrices over the full temporal period. Correlations between the target and predicted time series during the calibration and reconstruction intervals are given in the middle column of panels. The percentage of variance explained in the target field during the calibration interval are 10.5, 6.6 and 6.3% by the first, second and third covariance maps, respectively.

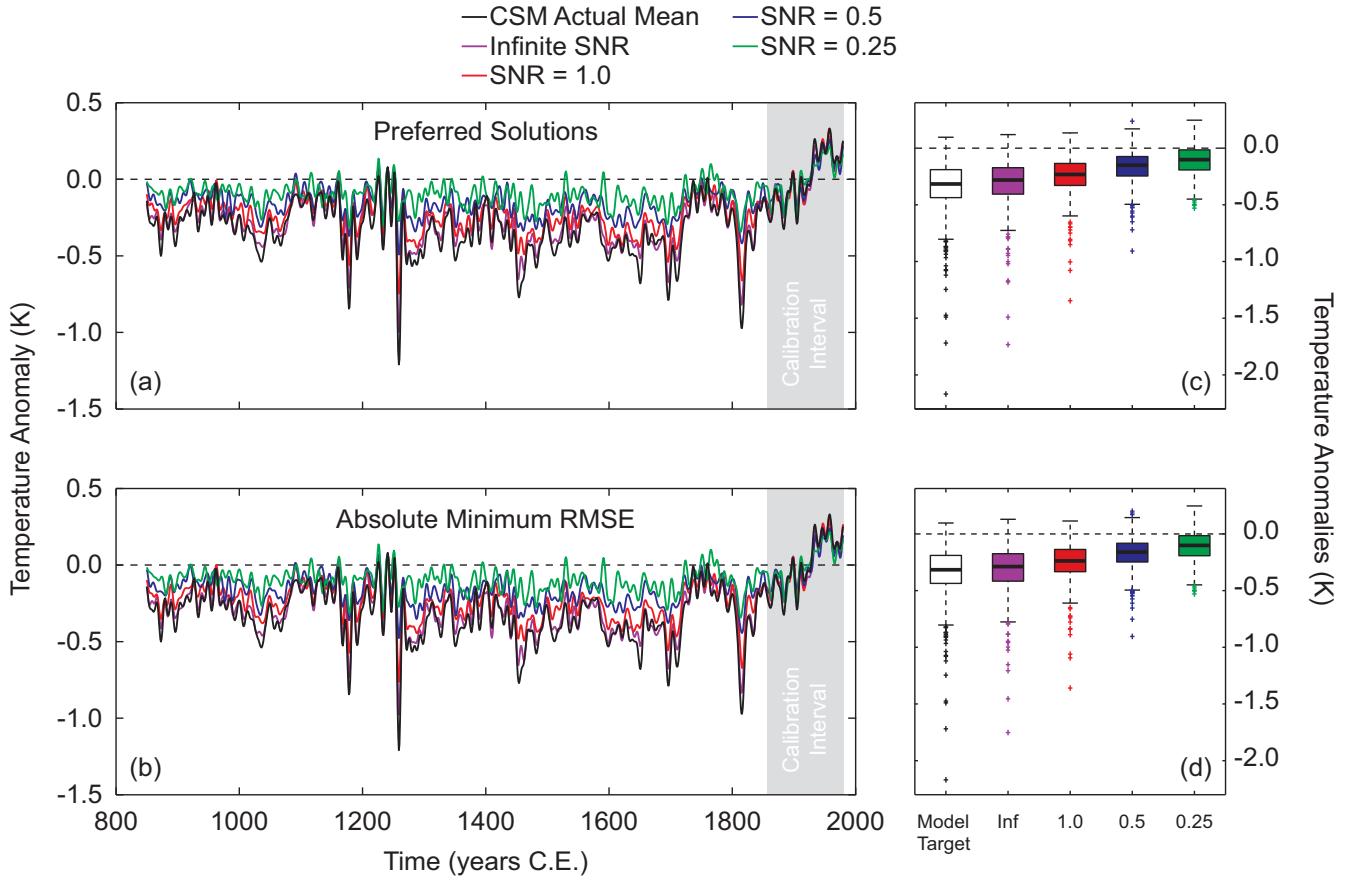


Figure 6: Area-weighted NH time series for the CCA reconstructions using  $d_{cca}$ ,  $d_p$ , and  $d_t$  values associated with: (a) the preferred solution (Table 3); and (b) the absolute minimum RMSE values (Table 2). Time series have been smoothed using a decadal low-pass filter. Also shown in (c) and (d) are the box plots associated with the two combinations of the of  $d_{cca}$ ,  $d_p$ , and  $d_t$  values. These plots were calculated from the distribution of the individual annual means in each NH time series during the reconstruction interval.

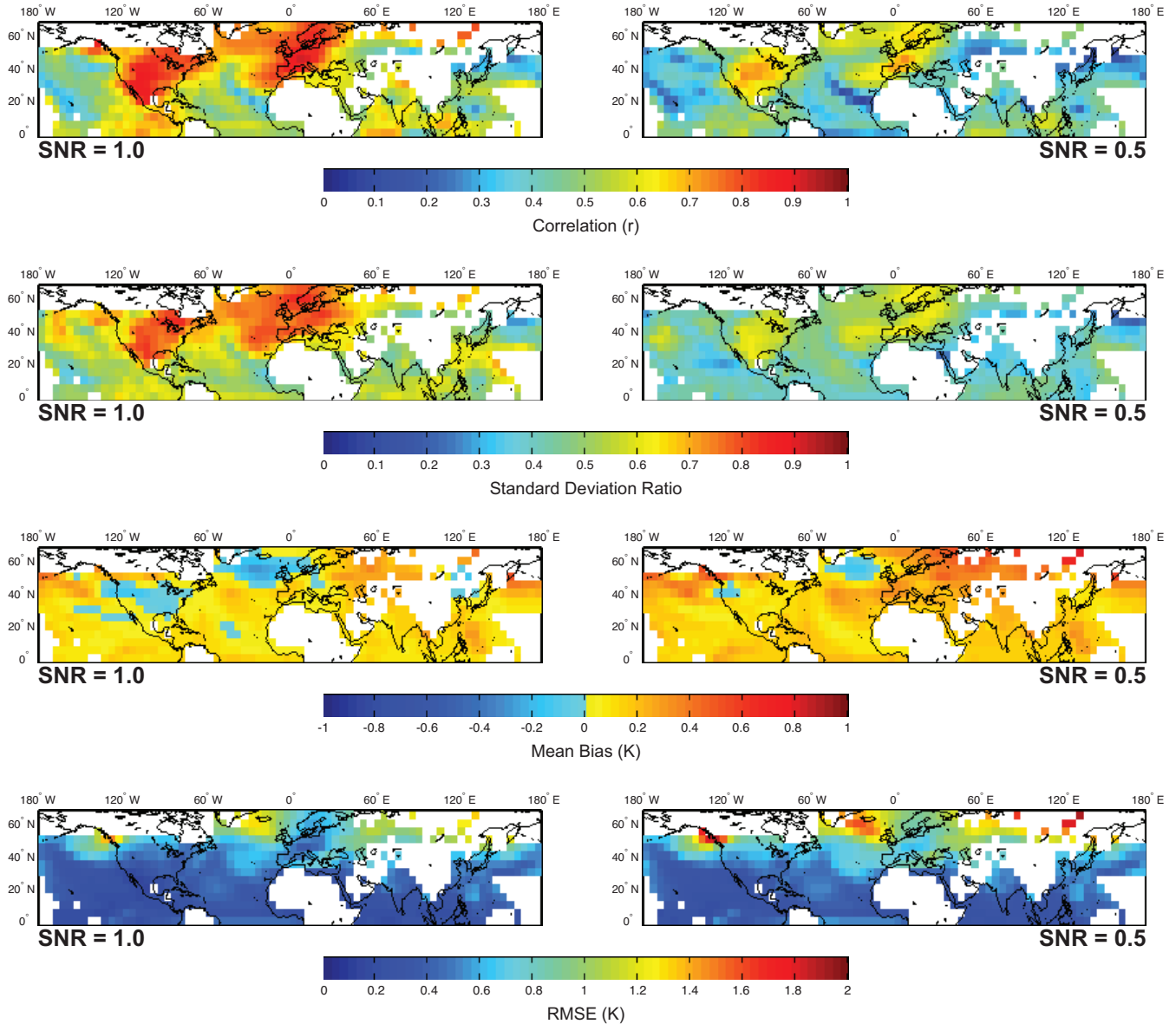


Figure 7: Field comparisons between derived CCA reconstructions (using the preferred-solution values of  $d_{cca}$ ,  $d_p$ , and  $d_t$ ) and the known CSM model fields: correlation (top row), standard deviation ratios (second row), mean biases (third row) and RMSE (last row). Standard deviation ratios are computed between the reconstruction and model and mean biases are computed as reconstruction minus model, i.e. negative (positive) biases indicate a colder (warmer) reconstruction mean. Results are shown for SNRs of 1.0 (left panels) and 0.5 (right panels); summary statistics for all noise levels are given in Table 4. All statistics are computed over the reconstruction interval (850-1855 C.E.).



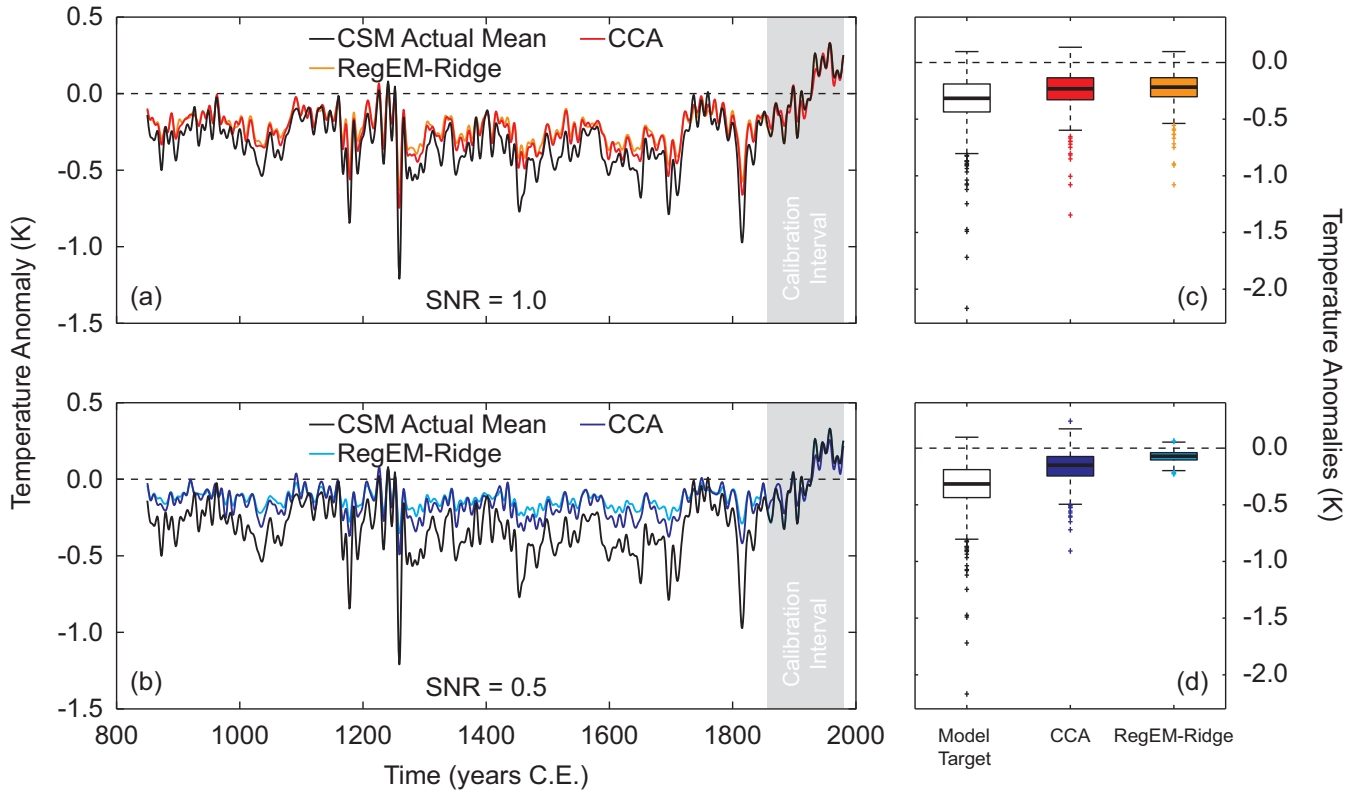


Figure 8: Same as in Figure 6, but for comparisons between the area-weighted NH time series for CCA and RegEM-Ridge reconstructions. Results are shown for SNRs of 1.0 and 0.5; summary statistics for all noise levels are given in Table 5.

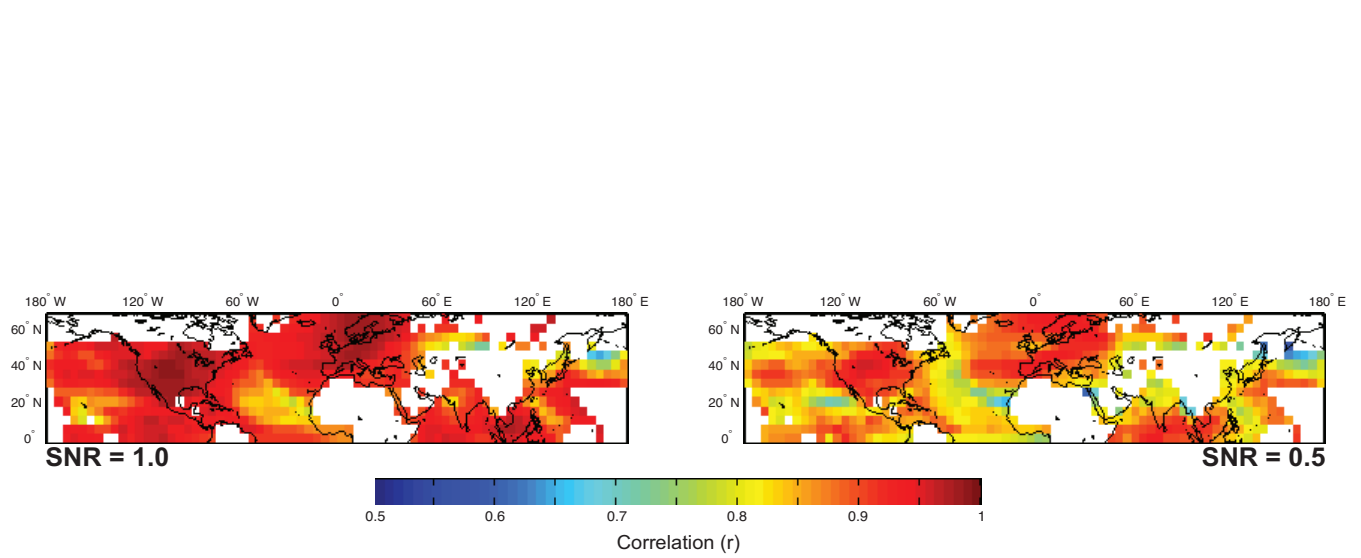


Figure 9: Correlation fields between the CCA and RegEM-Ridge reconstructions. Results are shown for SNRs of 1.0 (left panel) and 0.5 (right panel) and are computed over the reconstruction interval (850-1855 C.E.).

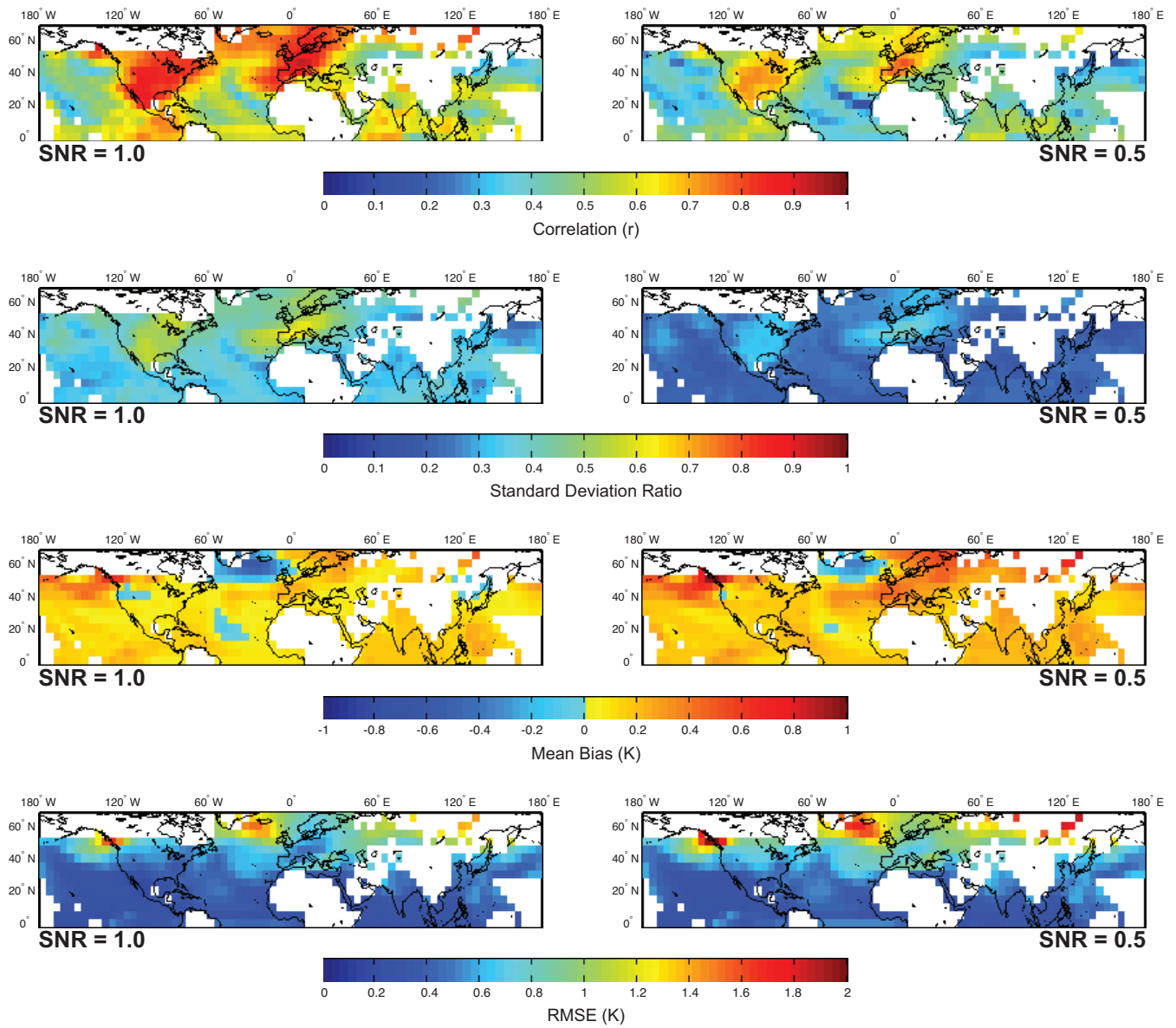


Figure 10: Same as in Figure 7, but for the RegEM-Ridge reconstructions.

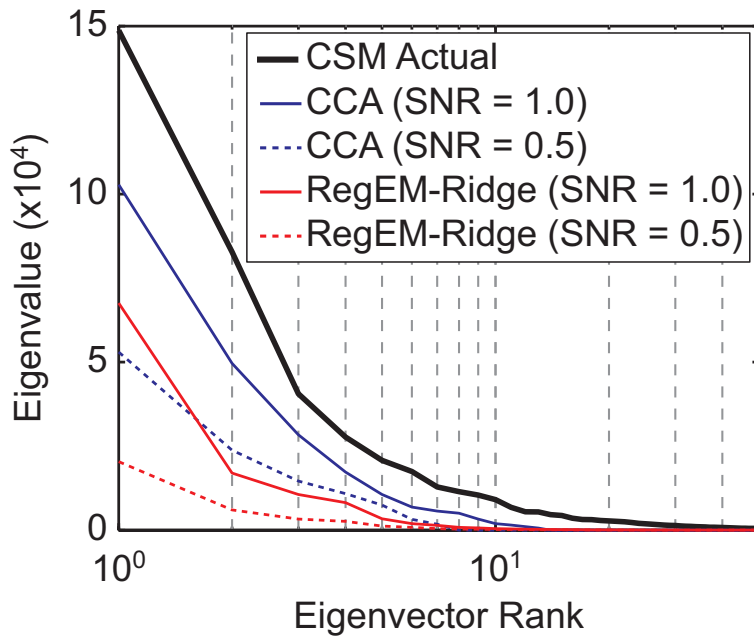


Figure 11: Eigenspectra computed from the true model temperature field and the CCA and RegEM-Ridge reconstructed temperature fields during the reconstructed interval (850-1855 C.E.). The CCA spectra have the characteristic truncation to zero at the selected rank, while the RegEM-Ridge spectra reflect the continuous filtration constraint applied in ridge regression.