

Dynamic Bayesian networks for evaluation of Granger causal relationships in climate reanalyses

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Key Points:

- Bayesian structure learning provides a principled approach to quantifying uncertainty in estimated network structures for relationships between teleconnections
- Dynamic Bayesian networks estimated from NCEP/NCAR and JRA-55 reanalysis data show broad overall consistency
- Structural differences in high posterior credibility associations may be indicative of biases relevant for subsequent model evaluation

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Abstract

We apply a Bayesian structure learning approach to study interactions between global teleconnection modes, illustrating its use as a framework for developing process-based diagnostics with which to evaluate climate models. Homogeneous dynamic Bayesian network models are constructed for time series of empirical indices diagnosing the activity of major tropical, Northern and Southern Hemisphere modes in the NCEP/NCAR and JRA-55 reanalyses. The resulting probabilistic graphical models are comparable to Granger causal analyses that have recently been advocated. Reversible jump Markov Chain Monte Carlo is employed to provide a quantification of the uncertainty associated with the selection of a single network structure. In general, the models fitted from the NCEP/NCAR reanalysis and the JRA-55 reanalysis are found to exhibit broad agreement in terms of associations for which there is high posterior confidence. Differences between the two reanalyses are found that involve modes for which known biases are present or that may be attributed to seasonal effects, as well as for features that, while present in point estimates, have low overall posterior mass. We argue that the ability to incorporate such measures of confidence in structural features is a significant advantage provided by the Bayesian approach, as point estimates alone may understate the relevant uncertainties and yield less informative measures of differences between products when network-based approaches are used for model evaluation.

Plain Language Summary

To produce reliable forecasts and projections, climate models should accurately reproduce the observed behavior of different processes that play a role in Earth's climate, including the relationships between them. Statistical methods can be used to describe these interactions in models and in observations, which can then be compared to evaluate how well a given model captures the observed relationships. However, networks obtained from estimates of the true historical state of the climate, known as reanalyses, will also be affected by the properties of the systems used to create these estimates, as well as random variability, and hence may have significant uncertainties. Using what are known as Bayesian statistical methods, we estimate the uncertainties associated with particular interactions in two widely used reanalyses. Interactions that are found to be very likely to be present in one reanalysis but not the other are suggested to be due to systematic differences in the two reanalysis systems and need to be kept in mind when these state

estimates are used to evaluate climate models. Therefore, it is important to account for the uncertainty associated with each relationship when analyzing state estimates and further employing them to evaluate climate models.

1 Introduction

The behavior of the Earth’s climate system, from day-to-day changes in weather to longer-term variations in climate, arises as a result of the interactions of diverse processes within the coupled land-ocean-atmosphere-cryosphere system over a vast range of spatiotemporal scales (see, e.g., Ghil and Lucarini (2020) for a recent review). Developing an accurate understanding of the underlying processes, including their response to external forcing and the interactions between different components, is an important first step in the development of realistic numerical forecasting models. Inevitably, even with a good understanding of the main processes being simulated, any given model will still be limited in its ability to represent the climate system, e.g., due to deficiencies in the parameterization of unresolved processes. These limitations manifest as systematic biases in the output of the model compared to observations. By comparing the representation of a particular component in the model with its observed counterpart, shortcomings in the model implementation can be identified for improvement, at least subject to the severe limitation that the globally contiguous observational record of the climate system, and in particular the subsurface ocean, extends only over a few decades.

This process-oriented approach, in which attention is focused on a comparatively small set of physical processes, has been widely applied in the climate science community. On the one hand, the complexity of the full coupled climate system means that it is typically only feasible to focus on specific subsystems in any given analysis, or otherwise necessitates some form of dimension reduction. For instance, specific targeted process-oriented diagnostics (Maloney et al., 2019) permit the representation of these processes in models to be evaluated against observations in order to drive model development (Eyring et al., 2019). At the same time, the existence of distinct teleconnections, i.e., recurrent large-scale modes of variability, has long been recognized (Ångström, 1935), motivating simplified models of the climate in terms of a small number of interacting modes. For example, atmospheric teleconnection patterns such as the Arctic Oscillation (AO) (Thompson & Wallace, 1998), the North Atlantic Oscillation (NAO) (Walker, 1923; van Loon & Rogers, 1978), the Pacific North American (PNA) (Wallace & Gutzler, 1981; Horel & Wallace,

1981; Barnston & Livezey, 1987) and Pacific South American patterns (PSA) (Mo & Ghil, 1987; Lau et al., 1994; O’Kane et al., 2017), and the Southern Annular Mode (SAM) (Rogers & van Loon, 1982; Thompson & Wallace, 2000) constitute important sources of low-frequency variability (Hannachi et al., 2017) and are associated with wide-ranging impacts (see, e.g., Leathers et al., 1991; Thompson & Wallace, 1998; Mo & Paegle, 2001; Hurrell et al., 2003; Gillett et al., 2006). On interannual time-scales, modes that express in the tropical oceans such as the El Niño Southern Oscillation (ENSO) (Walker, 1924; Bjerknes, 1969) and the Indian Ocean Dipole (IOD) (Saji et al., 1999) emerge as dominant sources of variability, with important implications for global weather and climate (see, e.g., Schott et al., 2009; McPhaden et al., 2021). As these large-scale modes tend to be relatively persistent, understanding their evolution and dynamics may enable more skillful forecasting over longer time-scales (Goddard et al., 2001; A. G. Marshall et al., 2014; Hannachi et al., 2017). Thus, beyond simply being convenient for reducing the dimension of the problem in model evaluation studies, simplified models based on these physically observed modes provide an approach for better understanding the properties and interactions of key sources of climate variability.

Even when focusing on only a few individual processes, it is generally difficult to directly attribute model biases to problems in the representation of a single process (Eyring et al., 2019), or to understand the behavior of an individual teleconnection mode in isolation from other processes. To capture the intrinsically coupled nature of the system in simplified models, network based approaches have become increasingly popular (Tsonis & Roebber, 2004; Tsonis et al., 2006; Donges et al., 2009b; Steinhäuser et al., 2011). In this framework, the climate system is represented in terms of a set of nodes, corresponding to appropriately defined subsystems or processes of interest, and edges describing the interactions between these nodes. The subsystems, for example, may be identified with one or more spatial gridpoints (Bello et al., 2015; Fountalis et al., 2018), or pre-defined modes characterized by empirical indices (Tsonis et al., 2007). In either case, the full climate system is then modeled in terms of a collection of individual, non-linear dynamical systems interacting with their neighbors in the constructed network. Such networks have variously been applied to study synchronization and climate shifts (Tsonis et al., 2007; G. Wang et al., 2009), to investigating the collective spatial structure of the statistical relationships between fields and changes over time (Tsonis & Swanson, 2008; Tsonis et al., 2008; Gozolchiani et al., 2008; Yamasaki et al., 2008; Donges et al., 2011;

109 Gozolchiani et al., 2011; Berezin et al., 2012; Guez et al., 2012; Steinhäuser et al., 2012;
110 Radebach et al., 2013; Y. Wang et al., 2013) and as tools for automatic mode identifi-
111 cation (Bello et al., 2015) or dimension reduction (Fountalis et al., 2018; Falasca et al.,
112 2019) via community detection methods.

113 When attempting to build a network representation of the climate, the structure
114 of the network is generally not known beforehand and must be inferred by some means.
115 A typical approach is to add or remove edges from the network on the basis of the level
116 of statistical interdependence of pairs of nodes, quantified by, e.g., the correlation (Tsonis
117 & Roebber, 2004) or mutual information (Donges et al., 2009a) between time series as-
118 sociated with each node. As these measures of association will almost always be non-
119 zero in finite samples, some level of thresholding or pruning must also be applied in or-
120 der to exclude edges corresponding to weak or spurious associations. In the simplest case,
121 the result is an undirected network; that is, the presence of an edge between two nodes
122 indicates some level of mutual association, but does not provide information on any pos-
123 sible directionality in the relationship.

124 Networks constructed in this way have proven to be very useful but do have some
125 important limitations. In particular, while correlation graphs allow for comparisons be-
126 tween modeled and observed associations (Falasca et al., 2019), often it is of interest whether
127 a particular set of variables is causally related to another set. If there is a causal mech-
128 anism, we may also wish to quantify the magnitude of the effects of those causal factors;
129 commonly, climate networks based on the above approaches do not provide direct ac-
130 cess to measures of effect. In practice, to answer these sorts of questions it is necessary
131 to imbue the networks with additional structure. This can be naturally achieved by iden-
132 tifying the original graph with an underlying statistical model, that is, by working in the
133 context of a (probabilistic) graphical model (Koller & Friedman, 2009). In a graphical
134 model, the graph encodes, in a well-defined way, the set of qualitative independence re-
135 lationships between the random variables, corresponding to nodes, in the model (Jordan,
136 2004). Given a particular functional form for the interactions between variables in terms
137 of the joint probability density function (PDF), quantitative questions can also be for-
138 mulated and addressed using standard algorithms (Pearl, 1982, 1988; Dechter, 1999; Koller
139 & Friedman, 2009).

140 Graphical models may utilize undirected or directed edges, or even a mixture of
141 both, corresponding to different ways of constructing the joint PDF of the model. Mod-
142 els based on directed acyclic graphs (DAGs), in which all edges also have an associated
143 direction and the graph does not contain any directed closed loops, provide an intuitive
144 representation of complex systems in terms of conditional independence relationships be-
145 tween quantities (Pearl, 1988; Spiegelhalter et al., 1993; Jordan, 2004). Compared to undi-
146 rected networks, directed graphs have the advantage that edges in the graph can often
147 be interpreted causally. As a result, they provide a powerful tool for studying causal re-
148 lationships (Pearl, 1995), and form a useful basis for other forms of causal inference (Greenland
149 & Brumback, 2002). Bayesian, or belief, networks (BNs), as such models are usually called,
150 have therefore received increasing attention from the climate science community (Ebert-
151 Uphoff & Deng, 2012a), having variously been used for forecasting and risk assessment
152 based on expert systems (e.g., Abramson et al., 1996; Catenacci & Giupponi, 2009; Pe-
153 ter et al., 2009; Catenacci & Giupponi, 2013; Leonard et al., 2014; Boneh et al., 2015),
154 for learning independence relationships and possible causal interactions in observations
155 (Ebert-Uphoff & Deng, 2012b; Runge et al., 2014; Runge, 2015; Runge et al., 2015; Kretschmer
156 et al., 2016, 2017; Horenko et al., 2017; Li et al., 2018; Runge, 2018a, 2018b; Runge, Nowack,
157 et al., 2019; Runge, Bathiany, et al., 2019; Samarasinghe et al., 2019, 2020; Saggioro et
158 al., 2020; Pfeiderer et al., 2020; Di Capua et al., 2020) and models (Deng & Ebert-Uphoff,
159 2014; Ebert-Uphoff & Deng, 2017), and, most recently, for model evaluation (Vázquez-
160 Patiño et al., 2020; Nowack et al., 2020).

161 One approach for using BNs as tools for model evaluation is to learn the network
162 structure in a model and in observations and assess the agreement between the two. Learn-
163 ing the structure of climate networks, in the absence of expert knowledge, has primar-
164 ily been achieved by utilizing constraint-based algorithms (Spirtes & Glymour, 1991; Colombo
165 & Maathuis, 2014) in which the set of edges is determined starting from a series of con-
166 ditional independence tests (Ebert-Uphoff & Deng, 2012a; Runge, Bathiany, et al., 2019).
167 Constraint-based methods can flexibly incorporate linear or non-linear conditional in-
168 dependence tests (Hlinka et al., 2013) together with predefined constraints, allowing for
169 non-linear dependence structures to be estimated from data. However, the inclusion of
170 edges on the basis of an (initially arbitrary) significance level together with multiple test-
171 ing adjustments makes assessing the level of confidence in the inferred networks difficult.

172 Usually, sensitivity analyses are necessary to get some handle on the robustness of the
173 resulting networks.

174 Ideally though, to apply BNs as tools for model evaluation we would not only iden-
175 tify differences between modeled and observed networks, but also assess whether any mis-
176 match is likely due to a model bias or simply sampling variability. In other words, an
177 additional level of uncertainty quantification is required. While a great deal of insight
178 can be derived from the structure of the estimated networks, quantifying both the sign
179 and magnitude of the interaction between nodes has generally been achieved by perform-
180 ing a second stage of fitting a parametric model, conditional on the inferred structure.
181 This, again, leads to complications in determining the uncertainties in the estimated in-
182 teraction strengths, which (depending on the approach used) may be insufficiently con-
183 servative (Draper, 1995). For the purposes of model evaluation, it is usually of interest
184 whether a model captures both the existence of a link and with the correct strength. Un-
185 reliable estimates for the uncertainty in fitted interaction strengths may result in an in-
186 ability to determine if an interaction is present but differs significantly in the model com-
187 pared to observations. On top of this, the additional complexity involved in implement-
188 ing such two-stage fitting procedures appears to have discouraged their use (McGraw &
189 Barnes, 2018) compared to simpler model-based analyses framed in terms of Granger causal-
190 ity (Granger, 1969).

191 In this article, we investigate possible solutions to the above limitations through
192 the use of Bayesian methods (Uusitalo, 2007). In the Bayesian framework for learning
193 the structure and effect measures (Spiegelhalter & Lauritzen, 1990; Dawid & Lauritzen,
194 1993; Madigan et al., 1995), it is natural to use the posterior probability of a given net-
195 work and its associated parameters as a score to measure model fitness (Buntine, 1991;
196 Cooper & Herskovits, 1992; Geiger & Heckerman, 1994; Heckerman et al., 1995). Ex-
197 isting knowledge and constraints may be incorporated through the use of suitable prior
198 distributions, although in practice this must be balanced against computational feasi-
199 bility. Bootstrap (Friedman et al., 1999) or sampling-based (Madigan & Raftery, 1994;
200 Madigan et al., 1995; Godsill, 2001) methods provide some measure of the uncertainties
201 in model selection, as well as allowing the predictions of multiple models to be combined
202 via model averaging (Madigan & Raftery, 1994). Consequently, the Bayesian approach
203 provides a principled quantification of the uncertainties associated with estimation of the
204 network structure and parameters. Models typically used for testing for Granger causal

relationships, that is, linear autoregressive models, can be straightforwardly expressed in graphical terms (Arnold et al., 2007; Lèbre, 2009), and, at least under a choice of conjugate priors, analyzed efficiently using closed-form expressions for the desired posterior densities (Geiger & Heckerman, 1994). In this sense, the model specification is largely familiar, reducing the barriers to use in climate applications. While there is additional complexity associated with the inference scheme, we believe that this is justified by the need for some level of uncertainty quantification.

To illustrate the utility of Bayesian methods for structure learning, we consider the application of fitting BNs to a set of teleconnection indices derived from two reanalysis datasets. Our purpose in doing so is two-fold. Firstly, as the score-based approach has not been widely used in analyses of this type, we wish to investigate the suitability of the method for networks of the size encountered in realistic data. Our second, and more important, aim is to perform a comparison of different reanalysis products on the basis of the fitted networks. In addition to allowing for possible biases and differences in the reanalyses at the level of interactions between modes to be studied, differences in the networks from different reanalyses give some additional indication of uncertainties in the observed networks that model runs are evaluated against. This, in turn, must be taken into account when deciding what level of disagreement between models and observations can be taken to indicate clear model biases.

The remainder of this paper is structured as follows. In the next section we provide a brief review of Bayesian network models and the inference methods used to fit such models. In Section 3 we describe the datasets and diagnostics that we study, together with our choice of prior distributions. In Section 4 we present the results of fitting the network models. Finally, we summarize our findings and discuss their implications for follow-up comparisons in Section 5.

2 Dynamic Bayesian networks

2.1 Structure learning

As noted above, a graphical model is simply a statistical model that has associated with it a graph encoding the relationships between the variables in the model. Each random variable in the model is represented by a node in the graph, with the allowed conditional dependence relationships between variables indicated by edges between nodes.

236 Under suitable assumptions (see, e.g., Koller and Friedman (2009) for a review), trans-
 237 lating between graphs and joint PDFs that constitute a model can be achieved using a
 238 prescribed set of rules.

239 For BNs and other graphical models based on DAGs, the graph structure implies
 240 a factorization of the joint PDF into conditional density functions. Given a set of ran-
 241 dom variables Y^1, \dots, Y^n and a DAG G , we denote by $\text{pa}_G(Y^i)$ the set of nodes in G
 242 that have a directed edge connecting to Y^i ,

$$243 \quad \text{pa}_G(Y^i) = \{Y^j | G \text{ contains an edge from } Y^j \text{ to } Y^i\}. \quad (1)$$

244 The graph G then provides a representation of the joint PDF $P(Y^1, \dots, Y^n)$ if the PDF
 245 admits a factorization of the form

$$246 \quad P(Y^1, \dots, Y^n) = \prod_{i=1}^n P(Y^i | \text{pa}_G(Y^i), \theta_i), \quad (2)$$

247 where θ_i denotes any parameters required to characterize the conditional density. For
 248 example, when all of the variables in $\{Y^i\} \cup \text{pa}_G(Y^i)$ are discrete, the conditional den-
 249 sity $P(Y^i | \text{pa}_G(Y^i), \theta_i)$ is the conditional probability table (CPT) summarizing the prob-
 250 ability of observing each level of Y^i for each combination of values of the parents $\text{pa}_G(Y^i)$;
 251 the θ_i are simply the values of each probability in the table. For continuous variables,
 252 the θ_i are any parameters required to fully specify the corresponding continuous PDF.

253 Generally in geophysical applications, the random variables of interest exhibit non-
 254 trivial spatial and temporal correlations. In our case, these variables are a collection of
 255 (continuous) teleconnection indices, some of which (e.g., ENSO) show substantial au-
 256 tocorrelation. Feedback loops or temporal dependence of this form cannot be represented
 257 in a BN with a single node for each index Y^i , due to the requirement for the graph G
 258 to be acyclic (Uusitalo, 2007). To handle this, the set of nodes is expanded to consist
 259 of the values of the random variables Y^i at the current time t , Y_t^i , as well as the values
 260 of the variables $Y_{t-\tau}^i$ at previous times $t-\tau$ (Kjærulff, 1995; Friedman et al., 1998; K. Mur-
 261 phy & Mian, 1999; K. P. Murphy & Russell, 2002), up to some maximum lag τ_{\max} . Tem-
 262 poral dependencies are described by edges between the nodes corresponding to, say, Y_t^i
 263 and $Y_{t-\tau}^i$, and a full time series of observations is described by a graph at each point in
 264 time relating the values of the variables at that time point to those in the previous time-
 265 slices. Similar graphical models for multivariate time series have also been introduced
 266 as time series graphs (Eichler, 2012). The resulting model is referred to as a dynamic
 267 Bayesian network (DBN).

268 In the simplest case, the structure of the graph and the associated parameters re-
 269 mains the same across all time-slices, so that the full time series is modeled by repeat-
 270 ing the graph at each time t . The corresponding DBN is said to be (time-)homogeneous
 271 (K. P. Murphy & Russell, 2002). The assumption of homogeneity is often violated in geo-
 272 physical applications, however. Interactions between spatially separated processes, for
 273 example, may be seasonally dependent, while on longer time-scales the possibility of cli-
 274 mate regime changes, e.g., in association with tipping points (Lenton et al., 2008), in re-
 275 sponse to anthropogenic forcing has recently become a key concern. Non-homogeneous
 276 DBNs, in which either the graph structure, parameters or both simultaneously, are al-
 277 lowed to change over time, admit the possibility of modeling features such as secular trends
 278 and regime changes (Wu et al., 2018), at the cost of a significant increase in complex-
 279 ity in terms of model specification and inference. Here we focus on the simpler case of
 280 homogeneous models for the purposes of investigating the usefulness of Bayesian meth-
 281 ods for assessing model uncertainty; the more complicated case of non-homogeneous mod-
 282 els will be described in a separate study.

283 Fitting a homogeneous DBN to an observed time series $D = \{\mathbf{y}_1, \dots, \mathbf{y}_T\}$, where
 284 \mathbf{y}_t denotes the values of the random variables $\mathbf{Y}_t = (Y_t^1, \dots, Y_t^n)^T$ at time t , requires
 285 learning (in general) both the structure of the graph G and the values of the correspond-
 286 ing parameters. Since

$$287 \quad P(\theta, G|D) = P(\theta|G, D)P(G|D), \quad (3)$$

288 where θ denotes the collection of all parameters for the conditional PDFs, the learning
 289 process can be conveniently divided into two steps. In the first, structure learning stage,
 290 the structure of the graph G is sought, independent of specific values of the parameters.
 291 Structure learning methods for BNs can be roughly categorized as constraint-based or
 292 score-based. The former set of methods attempt to reconstruct the graph structure on
 293 the basis of conditional independence tests and available prior knowledge and constraints,
 294 using, e.g., the PC-algorithm (Spirtes & Glymour, 1991) and its extensions (e.g., Colombo
 295 & Maathuis, 2014; Runge, 2018a; Runge, Nowack, et al., 2019). As discussed in Section 1,
 296 most recent examples in climate science have made use of constraint-based algorithms
 297 to learn an initial structure, followed in some cases by a separate parameter learning step.
 298 In contrast, in score-based approaches the graph G is estimated based on maximizing
 299 a suitable score function (Cooper & Herskovits, 1992; Geiger & Heckerman, 1994; Heck-
 300 erman et al., 1995), such as the marginal likelihood $P(D|G)$ or an information criterion.

301 However, when there may be significant uncertainty associated with the selection of a
 302 single model, rather than finding a single optimal model, it may be preferable to attempt
 303 to account for this model uncertainty by sampling from the full posterior distribution
 304 of possible graphs $P(G|D)$ (Madigan et al., 1995). Estimates for derived quantities of
 305 interest Δ may then be computed by averaging over the posterior distribution (Madigan
 306 & Raftery, 1994; Draper, 1995),

$$307 \quad \Pr(\Delta|D) = \sum_{G \in \mathcal{G}} \Pr(\Delta|G, D)P(G|D) \approx \frac{1}{S} \sum_{s=1}^S \Pr(\Delta|G^{(s)}, D), \quad (4)$$

308 where \mathcal{G} is the space of allowed structures and $\{G^{(s)}\}_{s=1}^S$ is a sample of size S from the
 309 posterior distribution $P(G|D)$. In particular, structural uncertainties may be quantified
 310 by taking Δ to be an indicator function for the presence of a given edge, with Eq. (4)
 311 quantifying the posterior probability of the existence of that edge, given the chosen model
 312 class and observed data.

313 Directly sampling the posterior $P(G|D)$ can be achieved in the case that the marginal
 314 likelihood

$$315 \quad P(D|G) = \int d\theta P(D|G, \theta)P(\theta|G) \quad (5)$$

316 can be evaluated, where $P(\theta|G)$ denotes a set of priors for the full set of node PDF pa-
 317 rameters θ conditional on the structure of the graph, and we have used the shorthand
 318 $\int d\theta$ to denote marginalization. The factor $P(D|G, \theta)$ is simply the likelihood under the
 319 model,

$$320 \quad P(D|G, \theta) = \prod_{t=1}^T \prod_{i=1}^n P(Y_t^i | \text{pa}_G(Y_t^i), \theta_i); \quad (6)$$

321 note that the inner multiplication follows from the assumption that the joint PDF can
 322 be factored according to G , and the outer multiplication from the assumption of homo-
 323 geneity. For simplicity, we work with the conditional likelihood assuming a sufficiently
 324 large set of pre-sample values are available to condition on. We restrict our attention to
 325 structures in which the parent set of a variable Y_t^i is not allowed to contain variables at
 326 the same time t , that is, we do not allow contemporaneous dependencies among variables.
 327 Excluding models with instantaneous links ensures that the structures we allow natu-
 328 rally satisfy structural modularity, such that the parent set of a variable Y_t^i may be cho-
 329 sen independently of the parent set for any other variable (Friedman & Koller, 2003).
 330 However, it should be kept in mind that doing so prevents any interactions that occur
 331 on time-scales that are shorter than the data sampling frequency from being directly han-
 332 dled, as these would manifest as instantaneous dependencies or feedback loops at $\tau =$

333 0. Assuming that the priors $P(\theta|G)$ satisfy the properties of parameter independence (Heckerman
 334 et al., 1995),

$$335 \quad P(\theta|G) = \prod_{i=1}^n P(\theta_i|G), \quad (7)$$

336 and modularity (that is, for any two graphs G and G' , if Y_t^i has the same parent set in
 337 G and G' , then $P(\theta_i|G) = P(\theta_i|G')$), the marginal likelihood may be written as the prod-
 338 uct of local marginal likelihoods $\Psi_i(D, G)$ (Grzegorzczuk & Husmeier, 2011):

$$339 \quad P(D|G) = \prod_{i=1}^n \int d\theta_i \prod_{t=1}^T P(Y_t^i | \text{pa}_G(Y_t^i), \theta_i) P(\theta_i|G) \equiv \prod_{i=1}^n \Psi_i(D; G). \quad (8)$$

340 For structurally modular priors of the form

$$341 \quad P(G) = \prod_{i=1}^n P(\text{pa}_G(Y_t^i)) \quad (9)$$

342 the posterior over graphs also factorizes,

$$343 \quad P(G|D) = \frac{P(D|G)P(G)}{P(D)} = \frac{1}{P(D)} \prod_{i=1}^n \Psi_i(D; G) P(\text{pa}_G(Y_t^i)), \quad (10)$$

344 so that each factor can be computed independently, up to an overall normalization.

345 2.2 Choice of conditional densities

346 The conditional densities $P(Y^i | \text{pa}_G(Y^i), \theta_i)$ can, in principle, be chosen to model
 347 arbitrary relationships between the random variables in the graph, consistent with the
 348 independence assumptions embodied by the graph structure. In practice, this prevents
 349 marginalizing out the graph parameters (i.e., evaluating $\Psi_i(D; G)$ analytically) to sam-
 350 ple from the marginal posterior distribution $P(G|D)$ directly. It is then necessary to con-
 351 struct a Markov Chain Monte Carlo (MCMC) sampler that samples from the joint pos-
 352 terior $P(\theta, G|D)$ using, e.g., reversible jump MCMC (RJMCMC) (Green, 1995) or re-
 353 lated methods (Carlin & Chib, 1995; Godsill, 2001). A summary of samplers that we use
 354 is given in Appendix A.

355 In special cases, the necessary integrals can be evaluated in closed form, allowing
 356 for the posterior $P(G|D)$ to be efficiently sampled after marginalizing out the conditional
 357 PDF parameters. For continuous data, a widely used example for which this is possi-
 358 ble is the linear Gaussian regression model (Punskaya et al., 2002; Lèbre et al., 2010).
 359 In this model, which can be regarded as a specialization of the BGe model for contin-
 360 uous data (Geiger & Heckerman, 1994), each Y_t^i is assumed to be conditionally Gaus-

361 sian distributed,

$$\begin{aligned}
 & Y_t^i | \text{pa}_G(Y_t^i), \tau_i^2 \sim N(\mu_t^i, \tau_i^{-2}), \\
 & \mu_t^i = \beta_0^i + \sum_{j=1}^{p_i} \beta_{(k_j, \tau_j)}^i Y_{t-\tau_j}^{k_j}
 \end{aligned}
 \tag{11}$$

363 with mean $\mu_t^i = E[Y_t^i | \text{pa}_G(Y_t^i)]$ given by a linear function of the parent variables $\text{pa}_G(Y_t^i) =$
 364 $\{Y_{t-\tau_j}^{k_j} | j = 1, \dots, p_i\}$. The local marginal likelihoods $\Psi_i(D; G)$ and posterior distribu-
 365 tions for the parameters of a given graph can be analytically evaluated provided that con-
 366 jugate normal-gamma priors are assumed for the conditional precision τ_i^2 and coefficients
 367 $\beta_{(k_j, \tau_j)}^i$,

$$\begin{aligned}
 & \tau_i^2 \sim \text{Gamma}(a_\tau, b_\tau), \\
 & \beta_{(k_j, \tau_j)}^i | \tau_i^2, \text{pa}_G(Y_t^i) \sim N\left(0, \frac{\nu_i^2}{\tau_i^2}\right), \quad j = 1, \dots, p_i,
 \end{aligned}
 \tag{12}$$

369 where a_τ , b_τ , and ν_i^2 are prior hyperparameters. Similar linear models have previously
 370 been applied (Kretschmer et al., 2016, 2017; Saggiaro et al., 2020; Di Capua et al., 2020)
 371 to perform estimation of the interaction strengths after an initial stage of constraint-based
 372 structure learning. Using the underlying generative model, Eq. (11), posterior estimates
 373 for both the structural features and model parameters can be obtained within a single
 374 sampling scheme. Appropriate choices for the hyperparameters a_τ , b_τ , and ν_i^2 allow vary-
 375 ing levels of regularization to be imposed so as to yield more reliable, if more conserva-
 376 tive, estimates given relatively short and noisy time series. Alternatively, they may be
 377 allowed to vary and another level of priors specified for the unknown hyperparameters.

378 In the presence of significant non-linearity, linear models of this form may no longer
 379 be appropriate. In this case, one strategy to capturing the underlying non-linear rela-
 380 tionship is to first discretize the original data and employ models for discrete data, e.g.,
 381 the analytically tractable BDe model (Buntine, 1991; Cooper & Herskovits, 1992; Heck-
 382 erman et al., 1995). However, this comes at the cost of necessarily losing some informa-
 383 tion, generally yielding only a coarse approximation of the original continuous distribu-
 384 tion (Friedman & Goldszmidt, 1996). Additionally, choosing an appropriate discretiza-
 385 tion scheme is in general difficult, as there is an inevitable trade-off between having suf-
 386 ficient resolution to describe the data versus the exponential growth in the number of
 387 parameters that are required to specify the CPT of each variable. Hence, in the follow-
 388 ing we focus on the case of continuous data.

389 For a given choice of model, after performing any initial pre-processing, fitting the
 390 homogeneous DBN model to the observed indices data then consists of sampling from

391 the posterior distribution $P(G|D)$ using the known marginal likelihood $P(D|G)$ in or-
 392 der to derive a set of candidate networks. For a given graph drawn from $P(G|D)$, the
 393 posterior distribution for the parameters, and hence summary statistics and credible in-
 394 tervals, can be computed analytically or obtained via standard within-model MCMC meth-
 395 ods.

396 2.3 Toy model example

397 To make the above discussion more concrete, it is helpful to consider a simple toy
 398 example. A standard problem in climate studies is to determine the direction of the re-
 399 lationships, if any, between some set of variables. For example, during the positive (El
 400 Niño) phase of ENSO, anomalously warm Pacific sea surface temperatures (SSTs) drive
 401 elevated mean surface temperatures over North and South America (McGraw & Barnes,
 402 2018). As a simplified example of this sort of driver-response relationship, McGraw and
 403 Barnes (2018) considered a two-dimensional system consisting of two observables D_t and
 404 R_t that evolve according to

$$405 \begin{aligned} D_t &= \alpha D_{t-1} + \sqrt{1 - \alpha^2} \epsilon_t^D, \\ R_t &= D_{t-\tau} + \gamma \epsilon_t^R. \end{aligned} \quad (13)$$

406 The innovations ϵ_t^D and ϵ_t^R are taken to be independent Gaussian noise drawn from a
 407 standard normal distribution. Typically in climate analyses, the relationships between
 408 the system variables would be studied by regressing the postulated response (e.g., sur-
 409 face temperature anomalies or R_t) on lagged values of the driver (SST anomalies or D_t),

$$410 R_t = c_0 + \sum_{j=1}^k c_j D_{t-j}, \quad (14)$$

411 and vice versa to test for the possibility of the reversed relationship. However, this ap-
 412 proach is susceptible to detecting spurious relationships when one or both processes ex-
 413 hibit substantial autocorrelation. As noted above, this often occurs in climate applica-
 414 tions, where, e.g., the driver may correspond to relatively slowly varying boundary con-
 415 ditions such as SST driving an atmospheric response, as in the ENSO-surface temper-
 416 ature example. To account for this, autoregressive models of the form

$$417 R_t = a_0 + \sum_{j=1}^k a_j R_{t-j} + \sum_{j=1}^k b_j D_{t-j}, \quad (15)$$

418 (and similarly for the dependence of D_t on R_t), may be used instead to test for the pres-
 419 ence of Granger causal links between processes.

420 Depending on the system, however, there can be considerable uncertainty associ-
 421 ated with selecting one of these models over the other. We can apply the sampling based
 422 approach described in the previous sections to better quantify this. The two models, Eq. (14)
 423 and Eq. (15), correspond to particular choices of parent set under the linear Gaussian
 424 regression model. Thus, to illustrate the method we consider the results of learning the
 425 structure of a DBN describing the system Eq. (13) under a linear Gaussian model. For
 426 given values of the system parameters, we generate a random realization of the system
 427 and fit a DBN after standardizing the input data to zero mean and unit variance. For
 428 the prior hyperparameters, we take, for example, $a_\tau = 1.5$, $b_\tau = 10$, and $\nu^2 \approx 43.3$,
 429 yielding a weakly informative t prior with 3 degrees of freedom for each coefficient, with
 430 90% prior credible intervals of $-4 \leq \beta \leq 4$. The prior 1% and 99% percentiles for the
 431 conditional precision (variance) are 0.57 (0.02) and 56.7 (1.74), respectively. Alternative
 432 choices with a heavier tailed distribution for the coefficients and much broader priors for
 433 the conditional precision, e.g., $a_\tau = 0.5$, $b_\tau = 10$, and $\nu^2 \approx 2$, tend to yield similar
 434 parameter estimates but less sparse models. The set of models considered includes all
 435 lags of up to 6 time steps and at most 4 parent nodes for each variable. Posterior sam-
 436 ples are obtained using the MC³ algorithm described in Appendix A, with the choices
 437 for the structure priors and proposal densities as described in Section 3.3.

438 Graphical summaries of the results of fitting this Gaussian DBN to realizations of
 439 the system Eq. (13) for $(\alpha, \gamma, \tau) = (0.2, 1, 2)$, $(0.5, 10, 2)$, and $(0.9, 4, 2)$ are shown in Fig-
 440 ure 1. The true system, Eq. (13), corresponds to the graph given in Figure 1(a), with
 441 the edges labeled by the values of the standardized regression coefficients. The remain-
 442 ing panels show the estimated posterior probabilities $\hat{\pi}$ for each edge, computed as in
 443 Eq. (4), for each realization of the system; for clarity, only edges for which $\hat{\pi} > 0.5$ are
 444 shown. Where an edge also appears in the maximum a posteriori (MAP) estimate for
 445 the structure, the posterior 95% highest density interval (HDI) is also shown for the cor-
 446 responding coefficient.

447 For low levels of autocorrelation and noise, the model recovers the correct edges
 448 with virtual certainty; in this case, the MAP structure consists of the (true) parent sets
 449 $\text{pa}(D_t) = \{D_{t-1}\}$ and $\text{pa}(R_t) = \{D_{t-2}\}$. Recovery of the true dependence structure
 450 is more difficult in the presence of large amounts of noise (e.g., $\gamma = 10$) or high auto-
 451 correlation (e.g., $\alpha = 0.9$). McGraw and Barnes (2018) note that, in the latter case,
 452 a bivariate Granger causality analysis exhibits reduced power for detecting the $D_{t-\tau} \rightarrow$

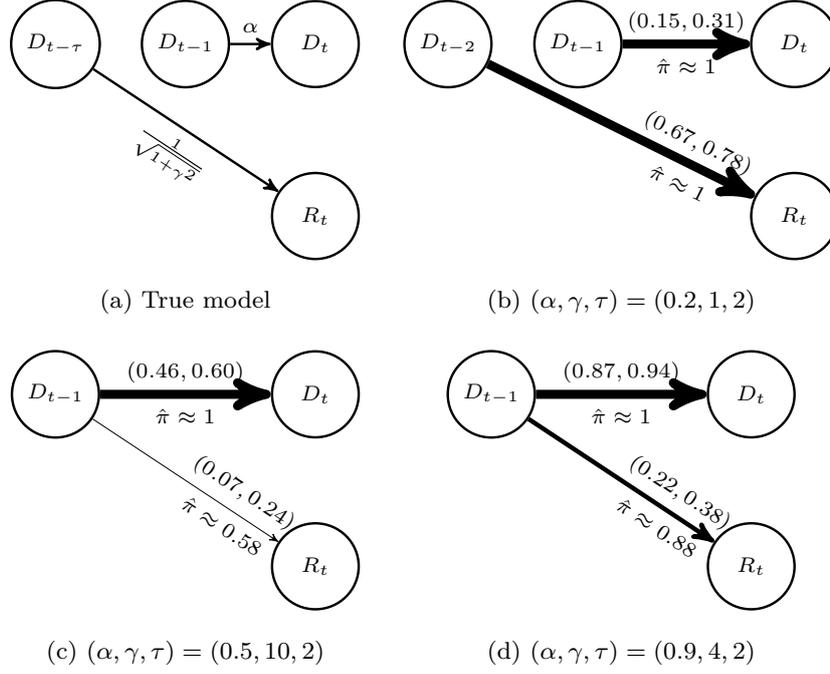


Figure 1. DBNs corresponding to (a) the true model given by Eq. (13), and network structures inferred using a linear Gaussian model for a single realization of the process with (b) $\alpha = 0.2, \gamma = 1, \tau = 2$; (c) $\alpha = 0.5, \gamma = 10, \tau = 2$; and (d) $\alpha = 0.9, \gamma = 4, \tau = 2$. For each of the fitted networks, all edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown, with thickness indicating the value of $\hat{\pi}$. Where an edge also occurs in the MAP model, the approximate posterior 95% HDI for the corresponding coefficient is also shown.

453 R_t edge while lagged regressions tend to too frequently identify spurious wrong-way re-
 454 lationships in which R drives D . For high levels of noise, both methods show reduced
 455 power for detecting the driver-response relationship, although accounting for autocor-
 456 relation successfully controls the false-positive rate for the reversed relationship. This
 457 difficulty in identifying the true underlying model is clearly evident in the lower panels
 458 of Figure 1 from the reduced estimated posterior probability of a dependence of R_t on
 459 D_t . In both cases, although the MAP structure suggests that R_t depends on lagged val-
 460 ues of D_t , the lag at which this occurs is misidentified, with $\text{pa}(R_t) = \{D_{t-1}\}$. Across
 461 all sampled models, the estimated posterior probability for lagged values of D_t to R_t re-
 462 flects greater uncertainty in the model structure, and hence in the selection of a single
 463 optimal model. For instance, while the MAP parent set for R_t when $\alpha = 0.5, \gamma = 10$
 464 is found to contain only D_{t-1} , the next most likely parent sets (for this particular sam-

465 ple, $\text{pa}(R_t) = \emptyset$ and $\text{pa}(R_t) = \{D_{t-2}\}$ also have non-negligible posterior probabili-
 466 ties, so that in practice it may be important to take this model uncertainty into account.
 467 A similar uncertainty measure is considerably more difficult to construct and interpret
 468 in the testing based approach of McGraw and Barnes (2018). As time series with long
 469 memory or large noise levels are frequently encountered in the climate analyses that we
 470 are interested in, the ability to provide some formal estimate of model uncertainty is an
 471 important advantage of the approach adopted here.

472 **3 Data and methods**

473 We now describe an application of the above methods to sets of reanalysis-derived
 474 teleconnection indices. In addition to uncertainties due to model and parameter selec-
 475 tion, in practice the reanalysis datasets that we use have associated uncertainties as well.
 476 Comparison of the networks derived from different products over a common timespan
 477 allows the role of these differences to be investigated and provides a baseline against which
 478 free-running model simulations can be compared.

479 **3.1 Data**

480 The data that we analyze are obtained from the Japanese 55-year Reanalysis (JRA-
 481 55) and the National Centers for Environmental Prediction/National Center for Atmo-
 482 spheric Research (NCEP/NCAR) Reanalysis 1 (NNR1).

483 The NCEP/NCAR Reanalysis 1 (Kalnay et al., 1996) is an atmospheric reanaly-
 484 sis covering the years 1948 to present. The data assimilation system employs a global
 485 spectral model with a T62 resolution on 28 vertical levels, and assimilates surface and
 486 atmospheric observational data. While a fixed analysis and forecast system is used for
 487 the duration of the reanalysis, changes in observing systems still have an impact and,
 488 consequently, the reanalysis is less reliable in the first decade than at later times (Kistler
 489 et al., 2001). NNR1 represents a first generation reanalysis providing a multidecadal record
 490 of the atmospheric state, albeit with several known errors (Kistler et al., 2001) and bi-
 491 ases, particularly in data-sparse regions in the high latitudes and the Southern Hemi-
 492 sphere (SH) (see, e.g., Hines et al., 2000; G. J. Marshall & Harangozo, 2000; G. J. Mar-
 493 shall, 2002; Bromwich & Fogt, 2004; Greatbatch & Rong, 2006; Hertzog et al., 2006; Bromwich
 494 et al., 2007; Lindsay et al., 2014). For the purposes of our analysis, global fields of daily

495 mean 500 hPa geopotential height ($Z_{g500 \text{ hPa}}$), zonal winds at 850 hPa and 200 hPa ($u_{850 \text{ hPa}}$
 496 and $u_{200 \text{ hPa}}$), mean sea level pressure (MSLP), and surface zonal and meridional winds
 497 (u_{sfc} and v_{sfc}) are obtained on the provided $2.5^\circ \times 2.5^\circ$ latitude-longitude grid. Daily
 498 mean top-of-atmosphere outgoing longwave radiation (OLR) fields are provided on a T62
 499 Gaussian grid and are subsequently regrided to a $2.5^\circ \times 2.5^\circ$ latitude-longitude grid
 500 using a bilinear interpolation scheme. To compute indices of tropical variability based
 501 on SST data for NNR1, we use version 1.1 of the HadISST SST dataset (Rayner et al.,
 502 2003), which provides monthly global SST on a $1^\circ \times 1^\circ$ latitude-longitude grid from 1870
 503 to present.

504 The JRA-55 reanalysis (Kobayashi et al., 2015), covering the period from 1958 to
 505 present, is a more recent atmospheric reanalysis product that aims to correct issues found
 506 in previous reanalyses. As for the NNR1 reanalysis, a frozen analysis system is employed
 507 and atmospheric and surface observations are assimilated. The assimilation system used
 508 for JRA-55 employs a TL319 resolution operational system with 60 vertical levels. The
 509 representation of the atmospheric circulation has been found to be greatly improved com-
 510 pared to previous generation reanalyses, although there remain known biases (Harada
 511 et al., 2016). Daily mean $Z_{g500 \text{ hPa}}$, $u_{850 \text{ hPa}}$, $u_{250 \text{ hPa}}$, u_{sfc} , v_{sfc} , MSLP, and OLR fields
 512 are obtained on a $1.25^\circ \times 1.25^\circ$ latitude-longitude grid. For SST fields, the model sur-
 513 face brightness temperature provided on a $1.25^\circ \times 1.25^\circ$ latitude-longitude grid is used.
 514 Where required by the definition of the index as noted below, we regrid the initial fields
 515 to a $2.5^\circ \times 2.5^\circ$ latitude-longitude grid using a bilinear interpolation method.

516 **3.2 Indices**

517 From the full gridded fields we compute a set of indices diagnosing the activity of
 518 a selection of major global teleconnections, which will form the nodes in the fitted graph-
 519 ical models. In a fully data-driven approach, the definitions of such indices might be au-
 520 tomatically determined by using community detection methods (Steinhaeuser et al., 2011;
 521 Bello et al., 2015). This has the advantage of accounting for differences between datasets
 522 or models in the representation of particular modes, e.g., due to shifts in the geographic
 523 centers of action. While these approaches have been employed in studies of causal effect
 524 networks (Kretschmer et al., 2017), here we use a set of fixed, empirical definitions for
 525 the teleconnection indices. We do so for two reasons. Firstly, this allows for a simpler
 526 evaluation of the performance of the models defined in Section 2, as the features in the

527 fitted networks can be directly compared to well-studied relationships between traditional
528 indices. Such a comparison would be more difficult to perform when using automatically
529 extracted indices, as some differences might arise solely from the definition of the index.
530 Additionally, positional shifts and other differences in the expression of particular modes
531 with respect to a predefined diagnostic are themselves of interest from the point of view
532 of comparing and evaluating models, and so we prefer to use a single set of reference def-
533 initions.

534 We choose a set of indices that provides reasonably comprehensive coverage of the
535 dominant teleconnection processes active on intraseasonal through to interannual time-
536 scales. Where anomalies are required in the definition of an index, for consistency across
537 the different datasets we compute all anomalies as differences from the daily or monthly
538 climatology calculated with respect to the reference period 1 January 1979 to 30 Decem-
539 ber 2001.

540 As measures of tropical variability, we include an updated version (Zhang et al.,
541 2019) of the multivariate ENSO index (MEI) (Wolter & Timlin, 1993, 1998, 2011), the
542 dipole mode index (DMI) to characterize IOD activity (Saji et al., 1999), and the Wheeler-
543 Hendon Madden-Julian oscillation (MJO) index (Wheeler & Hendon, 2004), denoted be-
544 low as RMM1 and RMM2. For both the MEI and the RMM1 and RMM2 indices, all
545 of the input fields are evaluated on a common $2.5^\circ \times 2.5^\circ$ latitude-longitude grid. Where
546 required, monthly MJO indices are defined as the monthly mean of the corresponding
547 daily index.

548 In the extratropical atmosphere, we include indices of the AO, the SAM, the PNA,
549 the PSA1 and PSA2 modes, and a set of modes associated with blocking in the North
550 Atlantic and western Europe. We define the AO and SAM as the leading empirical or-
551 thogonal functions (EOFs) (Lorenz, 1956) of anomalies of monthly mean Z_{g500} hPa pole-
552 ward of 20°N and 20°S , respectively. All anomalies are weighted by the square root of
553 the cosine of the gridpoint latitude when computing the EOFs. Corresponding AO and
554 SAM indices are calculated by projecting the (area-weighted) daily or monthly anoma-
555 lies onto the leading EOF and normalizing by the standard deviation of the monthly lead-
556 ing principal component (PC).

557 The PNA pattern is taken to be the leading mode obtained after performing a VARI-
558 MAX rotation (Kaiser, 1958) of the first 10 EOF modes of monthly-standardized anoma-

559 lies of monthly mean $Z_{g500 \text{ hPa}}$ polewards of 20°N during boreal winter, taken to be De-
 560 cember, January and February (DJF). The PNA index is then the projection of the stan-
 561 dardized height anomalies onto the resulting pattern, standardized by the monthly mean
 562 and standard deviation within the climatology reference period. The analogous modes
 563 in the SH, PSA1 and PSA2, are defined as the second and third modes in an EOF anal-
 564 ysis of year-round anomalies of daily mean $Z_{g500 \text{ hPa}}$ polewards of 20°S , projecting onto
 565 each mode and normalizing by the standard deviation of the corresponding PC over the
 566 reference period to obtain associated indices.

567 Following the method presented in Straus et al. (2017), we define a set of Euro-Atlantic
 568 circulation regimes via a k -means clustering analysis of the leading 24 PCs of boreal win-
 569 ter anomalies in daily mean $Z_{g500 \text{ hPa}}$ in the sector $20^\circ\text{N} - 80^\circ\text{N}$, $90^\circ\text{W} - 30^\circ\text{E}$, after ap-
 570 plying a 10 day running mean smoothing. This method has the advantage of better cap-
 571 turing spatial asymmetries present in opposing phases of the NAO. Using $k = 4$ clus-
 572 ters, we obtain a set of patterns that correspond to the positive and negative NAO phases,
 573 NAO^+ and NAO^- , as well as two clusters associated with blocking events in the Atlantic
 574 and western Europe, denoted AR and SCAND, respectively. Indices for each of the 4 clus-
 575 ters are obtained by projecting daily or monthly height anomalies onto the composites
 576 associated with each cluster and standardizing by the monthly mean and standard de-
 577 viations of the monthly index over the reference period.

578 For both reanalyses, monthly time series of the chosen indices are computed for the
 579 period 1 January 1960 to 30 November 2005, and this full time period is used for fitting
 580 DBNs. As some indices (e.g., SAM) exhibit significant trends over this period, we es-
 581 timate and remove a linear trend for every index beforehand. Each index time series is
 582 then standardized to have zero mean and unit variance over the fitting period.

583 3.3 Priors and sampler settings

584 As noted in Section 2, when excluding the possibility of contemporaneous edges,
 585 it is natural to choose structurally modular priors for the parent sets $\text{pa}_G(Y_t^i)$, such that
 586 the prior for a graph G decomposes into independent priors for the parent sets $\text{pa}_G(Y_t^i)$
 587 of each of the n indices included in the model. We fix a maximum allowed lag τ_{\max} , such
 588 that the $n(\tau_{\max} + 1)$ nodes in the network at a given time are $\cup_{i=1}^n \{Y_t^i, \dots, Y_{t-\tau_{\max}}^i\}$.
 589 For networks based on monthly indices, we take $\tau_{\max} = 6$ months, corresponding to the

590 approximate e -folding time of the MEI. To enforce some degree of sparsity in the net-
 591 works, we also impose a constraint on the maximum parent set size for each index, $|\text{pa}_G(Y_t^i)| \leq$
 592 $p_{\max} = 10$. Subject to these constraints, in the absence of additional information we
 593 adopt uniform priors over the set of possible parent sets for each index, i.e.,

$$594 \quad P(\text{pa}_G(Y_t^i)) = \begin{cases} \left[\sum_{j=0}^{p_{\max}} \binom{n\tau_{\max}}{j} \right]^{-1}, & |\text{pa}_G(Y_t^i)| \leq p_{\max}, \\ 0, & \text{otherwise.} \end{cases} \quad (16)$$

595 The MCMC sampling schemes described in Appendix A also require an appropri-
 596 ate proposal density for proposing updates to the structure of the model. We choose to
 597 adopt a uniform proposal density on graphs G' in the neighborhood of the current graph
 598 G ,

$$599 \quad q_G(G'; G) = \begin{cases} \frac{1}{|\text{nhd}(G)|}, & G' \in \text{nhd}(G), \\ 0, & \text{otherwise.} \end{cases}$$

600 The neighborhood $\text{nhd}(G)$ of a graph G is defined as the set of graphs that can be reached
 601 from that structure by a single move in a predefined move set. Note that, when an ex-
 602 plicit distinction is made between structure and parameter updates, as in the basic RJM-
 603 CMC scheme in Appendix A, we do not include the current graph itself in the neighbor-
 604 hood. We take the set of possible moves to consist of addition of a single edge, deletion
 605 of a single edge, or an exchange of two edges (Grzegorzczuk & Husmeier, 2011). The neigh-
 606 borhood of a graph contains those graphs that can be reached from it by performing one
 607 of these three moves, subject to the imposed condition on the maximum parent set size.
 608 A structure update move thus consists of determining the neighborhood of the current
 609 graph based on the available moves before selecting with equal probability one graph from
 610 this set. As the models considered here allow for the node parameters to be marginal-
 611 ized out, we use the MC³ sampling algorithm (Algorithm 2 in Appendix A) with the above
 612 proposal for fitting the model. For each index, posterior samples were obtained by run-
 613 ning 8 chains of length 10×10^6 samples. The number of samples to be retained for anal-
 614 ysis was chosen based on the estimated convergence rate from short initial runs follow-
 615 ing Brooks et al. (2003), where we required the thinning to be such that the resulting
 616 dependence between samples was reduced by a factor of 100 compared to the dependence
 617 between successive samples. To provide some assessment of chain convergence, homo-
 618 geneity of the distribution of parent sets within chains was monitored using χ^2 and Kolmogorov-
 619 Smirnov tests (Brooks et al., 2003) for each index, although we note that, as always, these
 620 tests are not sufficient alone to determine approximate convergence (Sisson, 2005). In

621 the following, both the posterior distribution over possible models and for individual fea-
 622 tures is of interest. Thus, in addition to applying these tests to the distribution of over-
 623 all model indicators, we also monitored the results for the case when each model was la-
 624 belled by a binary indicator for the presence of each possible edge, so as to check if in-
 625 ferences for the individual posterior edge probabilities were homogeneous across chains.
 626 Where required, samples for the node parameters were drawn from the conditional pos-
 627 terior distributions by Gibbs sampling.

628 The associations between the continuous valued indices are modeled using the lin-
 629 ear Gaussian conditional density, Eq. (11). For each index, we take the hyperparame-
 630 ter values $a_\tau = 1.5$, $b_\tau = 20$, and $\nu_i^2 = 3$, for $i = 1, \dots, n$. This corresponds to inde-
 631 pendent t_3 marginal priors for the regression coefficients, with 95% prior HDI $-1 \leq \beta \leq$
 632 1. The 1% and 99% percentiles for the conditional precision are respectively 1.1 and 113.4.
 633 Prior simulations suggest that this choice of priors yields a reasonable scale for the prior
 634 predictive distribution for the 1-step ahead forecast values, while not being so heavily
 635 regularized that relatively large values of the coefficients and indices are excluded. Sim-
 636 ilarly, the conditional precision hyperparameters are chosen to yield typical monthly in-
 637 novation variances of order 1 or less. As these choices lead to somewhat informative pri-
 638 ors, to assess the sensitivity of the results to the hyperparameter values we also perform
 639 fits with the much more weakly informative choices of $a_\tau = 0.5$, $b_\tau = 10$, $\nu_i^2 \approx 2$ (cor-
 640 responding to a 90% prior HDI of $-4 \leq \beta \leq 4$ and prior 1% and 99% percentiles for
 641 τ^2 of 7.6×10^{-4} and 33.2, respectively), which we find lead to qualitatively similar re-
 642 sults (see supporting information).

643 4 Results

644 4.1 Full year networks for monthly indices

645 We first consider the results of applying the above methods to year-round monthly
 646 indices for the two reanalyses. To better display the spatial structure of interactions, we
 647 separate the full network into subgraphs consisting of those indices corresponding to North-
 648 ern Hemisphere (NH) extratropical, tropical, and SH extratropical modes, together with
 649 their inferred parent sets. From the posterior samples over possible parent sets for each
 650 index, approximate posterior probabilities $\hat{\pi}$ for the presence of each edge in the network
 651 are computed as the sample average, Eq. (4), of the corresponding indicator function.

652 The results are summarized in Figure 2 and Figure 3 for the possible parent sets of trop-
 653 ical indices, in Figure 4 for the NH extratropical indices, and in Figure 5 for the SH ex-
 654 tratropical indices. For each subset, edges are shown with weights corresponding to their
 655 estimated posterior probability; for clarity, only those edges for which this value is at least
 656 0.5 are shown. Overall, the learned structures for the two reanalyses are similar. In par-
 657 ticular, there is broad agreement in terms of those edges for which the estimated pos-
 658 terior probability is high. These edges largely correspond, as is expected, to relationships
 659 in which there is a strong association between the parent and child node, either through
 660 strong autocorrelation or Granger causal links.

661 Strong evidence of long-range dependence on lagged values, reflecting the expected
 662 high levels of autocorrelation, is apparent for indices representing ENSO and the MJO,
 663 with the fitted models for both products featuring posterior probabilities near one for
 664 dependence of the MEI and both RMM indices on lags of up to four months (Figure 2
 665 and Figure 3). In both cases, the preferred lags are consistent with the expected time-
 666 scales for these modes, noting that a maximum lag of 6 months is imposed when fitting
 667 the model. Purely atmospheric modes, on the other hand, exhibit little memory beyond
 668 time horizons of several weeks to a month. This is apparent in the fitted networks for
 669 both models in the absence of strong evidence for dependence of the NH extratropical
 670 (Figure 4) and SH extratropical indices (Figure 5) on lagged values of themselves beyond
 671 lags of one month. For instance, in both NNR1 and JRA-55 there is found to be little,
 672 or at most relatively weak, evidence for serial dependence on monthly time-scales for the
 673 AR and SCAND indices, which respectively represent blocking in the Atlantic and Scan-
 674 dinavia with a characteristic time-scale of 7 - 10 days. Although the DMI diagnoses In-
 675 dian Ocean SST variability, the partial autocorrelation structure of the monthly mean
 676 DMI is consistent with an AR(1) process, and hence only the edge $DMI_{t-1} \rightarrow DMI_t$
 677 is found to have appreciable posterior mass.

678 Where a high posterior probability edge is inferred between distinct indices, the
 679 edge generally matches with well-known associations or teleconnections among the modes
 680 included in the fit. This is highlighted, for example, in Figure 6, where the posterior prob-
 681 abilities for edges entering the AO, NAO^+ , and NAO^- nodes in both reanalyses are shown.
 682 The close association between the AO and NAO is clearly evident in both reanalyses,
 683 and the estimated dependence relationships involving just these two indices are in es-
 684 sentially exact agreement. For both NNR1 and JRA-55, the presence of an edge in the

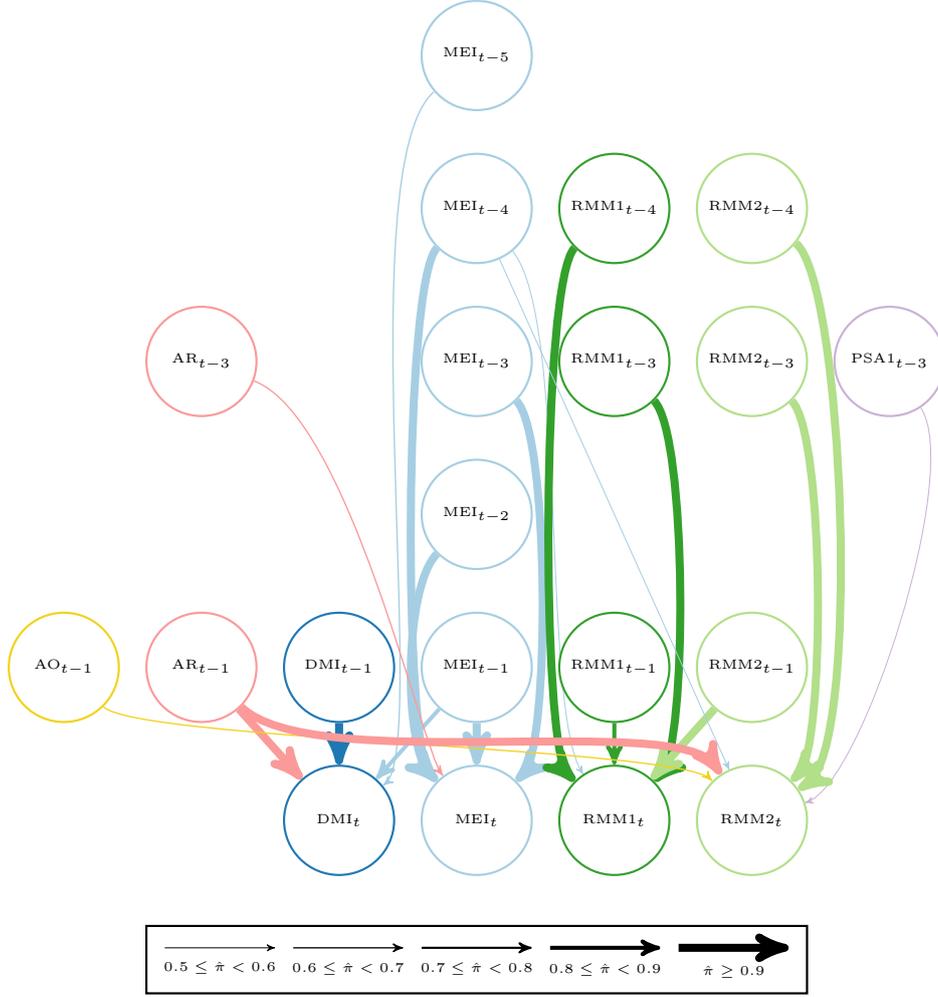


Figure 2. Subgraphs corresponding to the fitted parent sets of the tropical indices in NNR1 based on full-year data for $a_r = 1.5$, $b_r = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

685 network from the AO at lag 1 to each of the child nodes AO_t , NAO_t^+ , and NAO_t^- is in-
 686 ferred with very high confidence. The same is true for the edges $NAO_{t-1}^- \rightarrow AO_t$ and
 687 $NAO_{t-1}^- \rightarrow NAO_t^+$. This clear interdependence of the AO and NAO is, of course, very
 688 well established, to the extent that the existence of the former as a distinct physical mode
 689 has been debated (Deser, 2000; Ambaum et al., 2001). The appearance of this relation-
 690 ship in the learned structures does, however, provide a useful check that the method re-
 691 covers the expected relationships among particular modes. That these features agree be-
 692 tween the two reanalyses also suggests that the relationships between these modes are
 693 consistent in the separate datasets.

694 Similarly, the fitted parent sets for the monthly PNA index in NNR1 and JRA-55,
 695 shown in Figure 7, both include with posterior probability greater than 0.5 dependence
 696 on the value of the PNA index at a lag of one month ($\hat{\pi} \approx 0.95$ and $\hat{\pi} \approx 0.91$ in NNR1
 697 and JRA-55, respectively) and on the MEI at lag one ($\hat{\pi} \approx 0.71$ and $\hat{\pi} \approx 0.59$ for NNR1
 698 and JRA-55, respectively). In this case, the results of the fit indicate that in both re-
 699 analyses there is reasonable evidence that the PNA is associated with tropical forcing,
 700 here captured by the lagged value of the MEI, consistent with previous observational and
 701 modeling studies (e.g., Hoskins & Ambrizzi, 1993; Trenberth et al., 1998; Franzke et al.,
 702 2011). The posterior mass for this edge is similar in NNR1 and JRA-55, suggesting that,
 703 as for the AO and NAO, this relationship is also consistent in the two products, in the
 704 sense that there is comparable evidence for the association across the two datasets.

705 Although the structures estimated from the NNR1 and JRA-55 datasets agree well
 706 in the above examples, there are notable differences in the estimated edge probabilities
 707 as well. Moreover, several of these differences involve features that are assigned appre-
 708 ciable posterior probability (i.e., $\hat{\pi} \geq 0.5$) based on the data from one reanalysis and
 709 not the other. That is, the differences are not limited only to associations that are weakly
 710 supported in both datasets. For example, in Figure 7, the estimated structure for NNR1
 711 contains an edge from the lag one monthly mean RMM1 index to the monthly PNA in-
 712 dex at lag 0 with high posterior probability. The same feature in JRA-55 is found to have
 713 a posterior probability $\hat{\pi} \approx 0.38$ that is less than 40% of that found for NNR1. Given
 714 the observed evidence for interactions between tropical convection and extratropical modes
 715 such as the PNA on intraseasonal time-scales (Lau & Phillips, 1986), in this case the weaker
 716 evidence for an MJO-PNA relationship in the JRA-55 data may arise due to the sup-
 717 pressed MJO observed in the JRA-55 reanalysis (Harada et al., 2016). It should be noted,
 718 however, that directly attributing the difference to this bias is not straightforward; for
 719 example, other known associations between the MJO and other modes of variability are
 720 identified in the JRA-55 fits, discussed below. Confirming whether there is a difference
 721 in this particular feature, and the underlying source of the difference, would require a
 722 closer examination of the representation of the two processes in the reanalysis, which is
 723 left for further studies. Nevertheless, this does highlight that comparison of the learned
 724 parent sets between the two reanalyses allows differences in the captured interactions be-
 725 tween modes to be identified, particularly when we may have confidence that such a dif-
 726 ference is in fact present. By adopting a Bayesian approach to structure learning, the

727 level of confidence in this difference can be estimated: while the edge $\text{RMM1}_{t-1} \rightarrow \text{PNA}_t$
 728 may be found in individual models for the time-evolution of the PNA index in both re-
 729 analyses, the existence of this feature is approximately 2.5 times more likely in NNR1
 730 than in JRA-55 given the class of models and possible parent nodes that we consider.
 731 The presence of this edge with reasonable confidence in one product and not the other
 732 is suggestive of an underlying bias in one reanalysis, rather than simply being due to sam-
 733 pling variability.

734 Other differences in edges with large posterior mass, however, do not have quite
 735 as clear possible sources in specific underlying biases. In both reanalyses, the parent set
 736 of the NAO_t^+ node is estimated to contain the monthly PSA2 index at lag one, but with
 737 a posterior probability that is approximately 1.8 times larger in NNR1 ($\hat{\pi} \approx 0.89$ com-
 738 pared to $\hat{\pi} \approx 0.50$, see Figure 6). Similarly, the posterior probability for the edge $\text{PSA2}_{t-1} \rightarrow$
 739 NAO_t^- is ≈ 4.7 times larger in NNR1, but in this case for both NNR1 and JRA-55 the
 740 estimated probability is less than 0.5, while an edge $\text{PSA1}_{t-1} \rightarrow \text{AR}_t$ is also present in
 741 both reanalyses. O’Kane et al. (2016) and O’Kane et al. (2017) concluded that the PSA
 742 modes predominantly reflect dynamics localized to within the SH waveguide, such that
 743 a direct physical interaction between the PSA2 mode and the NAO is unlikely. Thus,
 744 in contrast to the $\text{RMM1}_{t-1} \rightarrow \text{PNA}_t$ feature, one might expect that the differing level
 745 of confidence in this edge between the two reanalyses may be due to differences in rel-
 746 evant factors that are omitted from this simple analysis. In particular, as the fit shown
 747 in Figure 6 is based on data from all seasons, the presence of such a feature may reflect
 748 seasonal covariations in the extratropical circulation in both hemispheres that is other-
 749 wise unaccounted for here. While we consider the effects of seasonality in Section 4.2 be-
 750 low, ultimately direct determination of the root of these differences must be based on
 751 detailed evaluation of the two products. Here we seek only to highlight the use of the
 752 fitted networks for learning possible dependence relationships and hence their utility for
 753 guiding comparative analyses on the basis of identifying relationships that can be inferred
 754 to be present or absent with reasonable confidence.

755 Features for which there is lower confidence tend to differ more between the two
 756 reanalyses, although in these cases it becomes less clear as to whether they indicate sub-
 757 stantive differences. This is most evident in the subgraphs corresponding to the parent
 758 sets for the SH extratropical indices in Figure 5. While there is agreement between the
 759 models fitted to NNR1 and JRA-55 in features such as the one month memory in the

760 SAM and the presence of an association (even if not a direct interaction) between the
 761 PSA1 and tropical forcing captured by the MEI, a larger number of features with pos-
 762 terior mass $\hat{\pi} > 0.5$ are found using the NNR1 data, involving a larger set of indices
 763 as parents. This greater disagreement between reanalyses, and overall lower confidence
 764 in the inferred non-independence relationships, may in part be due to the disparate res-
 765 olutions and configurations of the respective atmospheric models in combination with
 766 relatively sparse observations in the SH prior to the satellite period. Spurious associa-
 767 tions may also arise as a result of omitted factors, such as seasonal changes in the cir-
 768 culation, and low signal-to-noise ratios outside of the SH winter. For instance, the pos-
 769 terior distributions over parent nodes for the SAM index in the two reanalyses are sum-
 770 marized in Figure 8. In both NNR1 and JRA-55, non-zero associations are found with
 771 the MEI at lags of 4 and 6 months, albeit with somewhat higher posterior probabilities
 772 in JRA-55, and in NNR1 an edge from $AR_{t-5} \rightarrow SAM_t$ is identified with $\hat{\pi} \approx 0.52$.
 773 The same edge in JRA-55 is found to have $\hat{\pi} \approx 0.42$. Noting that a similar, compar-
 774 atively low confidence relationship is found between NAO^+ and the PSA1 at a lag of four
 775 months in NNR1, and absent a mechanism for such interactions, it appears likely that
 776 in this case the association is an artifact arising from the use of year-round data; we con-
 777 firm that this is the case in the following section. It is worth noting, however, that the
 778 fact that there is overall low posterior weight for these edges in both reanalyses allows
 779 identifying them as lacking robustness. This in turn is of use for the purposes of guid-
 780 ing model evaluation, where differences to observations in low probability relationships
 781 are of potentially less relevance.

782 It is important to bear in mind that the structures discussed above summarize the
 783 marginal posterior probability for the presence or absence of each individual edge over
 784 all possible models, rather than the presence or strength of an association between two
 785 indices within a single model. In addition to inspecting the estimated marginal distri-
 786 butions for each feature, given a sample from the approximate posterior distribution it
 787 may also be of interest to consider aspects of the sample that involve either the joint oc-
 788 currence of one or more edges, as well as the posterior distribution over complete mod-
 789 els. In particular, point-estimates for the parent set, analogous to those obtained using
 790 constraint-based approaches, can be obtained as the MAP estimate with the largest pos-
 791 terior probability. As all parent sets are assigned equal prior probability, this structure
 792 is simply the one that maximizes the marginal log-likelihood. Conditional on a partic-

793 ular MAP structure, estimates for the parameters under the model may be simply ob-
 794 tained by sampling from the conditional distributions $P(\theta|G, D)$, which in the case of
 795 the linear Gaussian model can be evaluated in closed form. Thus, in the sampling-based
 796 approach we may also obtain estimates of the strength of an association, conditioned on
 797 a particular model, in addition to the above estimates for the probability of the presence
 798 of the corresponding edge in the structure.

799 For example, the MAP parent sets for the NH extratropical modes in each reanal-
 800 ysis are summarized in Table 1, where we show both the estimated posterior probabil-
 801 ity for each edge in the parent set, as well as the posterior mean and 95% HDI for the
 corresponding coefficient in Eq. (11). In general, edges present in the MAP parent sets

Table 1. MAP parent sets for monthly NH extratropical teleconnection indices across all sea-
 sons for NNR1 and JRA-55 for fits with $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$, showing the estimated
 posterior probability $\hat{\pi}$ of the edge, the mean parameter value $\hat{\beta}$ conditional on the MAP struc-
 ture, and the 95% posterior HDI. Dashes indicate a node that is not in the MAP parent set for a
 given reanalysis.

Parent node	JRA-55			NNR1		
	$\hat{\pi}$	$\hat{\beta}$	95% HDI	$\hat{\pi}$	$\hat{\beta}$	95% HDI
AO_t						
AO _{t-1}	1.00	0.45	(0.35, 0.56)	1.00	0.46	(0.35, 0.57)
NAO _{t-1}	0.99	0.24	(0.13, 0.35)	0.99	0.25	(0.13, 0.36)
AR_t						
NAO _{t-6} ⁺	0.44	0.12	(0.03, 0.19)	0.32	0.12	(0.04, 0.20)
PNA _{t-1}	0.58	0.14	(0.06, 0.22)	0.36	0.14	(0.06, 0.22)
PSA1 _{t-1}	0.97	-0.17	(-0.25, -0.09)	0.67	-0.14	(-0.22, -0.06)
RMM2 _{t-5}	0.11	-	-	0.43	-0.12	(-0.20, -0.04)
NAO_t⁺						
AO _{t-1}	1.00	0.35	(0.23, 0.46)	1.00	0.37	(0.24, 0.48)
NAO _{t-1} ⁺	0.66	0.17	(0.05, 0.29)	0.69	0.17	(0.06, 0.29)
NAO _{t-1} ⁻	0.98	0.31	(0.19, 0.43)	1.00	0.34	(0.22, 0.46)
PSA2 _{t-1}	0.50	-0.11	(-0.19, -0.03)	0.89	-0.14	(-0.22, -0.06)
NAO_t⁻						
AO _{t-1}	1.00	-0.52	(-0.65, -0.39)	1.00	-0.52	(-0.65, -0.39)
NAO _{t-1} ⁻	0.78	-0.22	(-0.34, -0.10)	0.70	-0.23	(-0.35, -0.11)
PNA _{t-1}	0.73	-0.17	(-0.26, -0.07)	0.55	-0.15	(-0.24, -0.06)
PSA2 _{t-1}	0.10	-	-	0.47	0.12	(0.04, 0.20)
PNA_t						
MEI _{t-1}	0.58	0.21	(0.12, 0.29)	0.71	0.21	(0.12, 0.29)
PNA _{t-1}	0.91	0.15	(0.07, 0.24)	0.95	0.16	(0.08, 0.24)
RMM1 _{t-1}	0.38	-	-	0.99	0.17	(0.09, 0.25)
SCAND_t						
MEI _{t-6}	0.34	-0.13	(-0.21, -0.05)	0.28	-	-
SCAND _{t-1}	0.53	0.13	(0.04, 0.21)	0.31	-	-
MEI _{t-5}	0.23	-	-	0.45	-0.13	(-0.22, -0.05)
AR _{t-1}	0.28	-	-	0.53	-0.13	(-0.21, -0.05)

802

803 tend to have at least moderately high posterior probabilities, that is, they correspond

804 to non-independence relationships that are also present in a large fraction of the sam-
 805 pled models. Edges found in the MAP parent set are not necessarily found in the ma-
 806 jority of possible models, however, with several edges having posterior probabilities of
 807 order ~ 0.3 in Table 1. For these edges, while their inclusion leads to a good fit for this
 808 particular sample, the data do not provide especially strong evidence for their presence
 809 compared to other edges in the MAP structure, given the set of all other possible pre-
 810 dictors. To some extent this also reflects the fact that multiple models with parent sets
 811 that do not include these edges may still provide a reasonable fit to the observed data,
 812 despite not maximizing the marginal likelihood, and hence can account for non-negligible
 813 posterior mass. Considering only the single most probable structure may therefore fail
 814 to take into account relevant model uncertainty. Notably, differences between the MAP
 815 structures for the two reanalyses are again not only restricted to edges with low poste-
 816 rior mass, suggesting that at least some differences may be due to systematic effects rather
 817 than as a result of minor differences in the two samples. For example, the absence of the
 818 edge $\text{RMM}_{t-1} \rightarrow \text{PNA}_t$ in the MAP parent set from JRA-55 indicates that not only is
 819 there weak evidence for this relationship in the dataset, but that it is also not required
 820 in order to produce a good fit to the observed time series. Where an edge is present in
 821 the MAP parent set for both reanalyses, there is good agreement between the two prod-
 822 ucts in terms of the estimated coefficient. For the NH modes, the two reanalyses yield
 823 very similar estimates for the strength of each association, while there are somewhat larger
 824 differences for the tropical and SH extratropical modes (see supporting information).

825 **4.2 Seasonal networks for monthly indices**

826 Overall, the fitted networks based on full year data show good agreement between
 827 the two reanalyses. Some of the differences noted in the previous section may arise due
 828 to confounding or spurious associations generated by, among other things, the omission
 829 of relevant variables in the fit (i.e., failure of causal sufficiency, in the case that the mod-
 830 els are interpreted as being causal). An obvious possible factor is the seasonal variation
 831 in relationships between nodes that arises as a result of seasonal changes in the back-
 832 ground flow and hence in the available pathways for propagation of disturbances (e.g.,
 833 Hoskins & Ambrizzi, 1993; Ambrizzi et al., 1995). To account for this seasonal depen-
 834 dence, one possibility would be to include a seasonal indicator as a node within the graph
 835 itself. For simplicity, however, to investigate the impact of seasonal variation we consider

836 the results of repeating the above analysis restricted to data in the three month winter
 837 season for each hemisphere. Note that, as lags of up to six months are still allowed, ob-
 838 servations entering into these fits also include lagged values of the indices during the pre-
 839 vious season. For brevity, we restrict our attention to only a subset of the major tele-
 840 connections within each hemisphere.

841 In Figure 9, the estimated posterior probabilities for the parent sets of the NAO^+
 842 and NAO^- indices during DJF are shown. As for the full year fits, in both reanalyses
 843 there is strong evidence for an association between the AO and the two phases of the NAO,
 844 with approximately equal posterior mass assigned to each edge in NNR1 and JRA-55.
 845 Compared to the full year networks, the edge from $\text{PSA2}_{t-1} \rightarrow \text{NAO}_t^+$ is no longer found
 846 to have appreciable posterior mass ($\hat{\pi} < 0.1$ in both reanalyses), consistent with this
 847 edge arising as a result of the use of full-year data. In both NNR1 and JRA-55, a rela-
 848 tionship between the MJO, via the value of the RMM1 index at a lag of two months, with
 849 the positive phase of the NAO is found in a large fraction of sampled models ($\hat{\pi} \approx 0.67$
 850 in NNR1 and $\hat{\pi} \approx 0.83$ in JRA-55). Interactions between the MJO and the NAO have
 851 previously been reported in winter season observations (e.g., Lin et al., 2009) arising from
 852 known dynamical mechanisms (e.g., Frederiksen & Frederiksen, 1993). The inferred pres-
 853 ence of this relation, with moderately high confidence, indicates that both products are
 854 consistent in capturing this association, although it should be noted that monthly mean
 855 data is being used here in contrast to the more usual daily or pentad data. In both NNR1
 856 and JRA-55, additional edges are also found with somewhat lower posterior probabili-
 857 ties, including the edges $\text{NAO}_{t-5}^+ \rightarrow \text{NAO}_t^-$, $\text{PSA1}_{t-5} \rightarrow \text{NAO}_t^-$, and $\text{PNA}_{t-3} \rightarrow \text{NAO}_t^+$
 858 with estimated probabilities $\hat{\pi} \approx 0.55, 0.51$, and 0.54 in JRA-55, respectively, and $\hat{\pi} \approx$
 859 $0.49, 0.43$, and 0.45 in NNR1. As these features are present in both reanalyses with rel-
 860 atively similar posterior weights, this suggests that there is some, if comparatively weak,
 861 evidence for these associations from both products, and the two reanalyses appear to thus
 862 be consistent. More notably, the feature $\text{DMI}_{t-6} \rightarrow \text{NAO}_t^-$ is estimated to have a pos-
 863 terior probability of $\hat{\pi} \approx 0.52$ based on the indices computed using NNR1 and HadISST
 864 data, while when fitted to JRA-55 the same feature is assigned a posterior mass of only
 865 $\hat{\pi} \approx 0.09$, implying substantially weaker evidence is found for the presence of this edge
 866 in the JRA-55 data.

867 For fits based on austral winter (June-July-August, JJA) data, similar results are
 868 found in that several apparently spurious associations cease to be present in a large frac-

869 tion of the sampled structures. In Figure 10, the estimated posterior probabilities for par-
 870 ent nodes of the PSA1 index during JJA are shown for the two reanalyses. Compared
 871 to the previous, full-year fits in Figure 5, the set of edges with high posterior mass from
 872 NNR1 data no longer includes long-range dependence on the positive phase of the NAO,
 873 or on the PSA2 index. Instead, an edge $\text{RMM1}_{t-5} \rightarrow \text{PSA1}_t$ is found with posterior prob-
 874 ability $\hat{\pi} \approx 0.60$, with the same feature being obtained from the JRA-55 data with $\hat{\pi} \approx$
 875 0.77 . The JRA-55 fit also contains an edge $\text{RMM2}_{t-6} \rightarrow \text{PSA1}_t$ with estimated poste-
 876 rior probability $\hat{\pi} \approx 0.94$; in NNR1, the corresponding feature is found to have $\hat{\pi} \approx$
 877 0.42 . Associations between the MJO and the PSA modes on intraseasonal time-scales
 878 during winter have previously been noted (Mo & Paegle, 2001), although the fitted mod-
 879 els here assign greater posterior weight to dependence at longer lags. While the poste-
 880 rior probability for the presence of RMM1 as a predictor of the monthly mean PSA1 is
 881 roughly consistent between NNR1 and JRA-55, the approximate factor of two difference
 882 in the value of the sampled posterior probability for the RMM2 edge is more sizable and
 883 may provide weak evidence of a difference between the two reanalyses in terms of this
 884 relationship. A similar statement may be made for the $\text{MEI}_{t-1} \rightarrow \text{PSA1}_t$ edge, for which
 885 the fitted posterior probabilities are $\hat{\pi} \approx 0.59$ in JRA-55 and $\hat{\pi} \approx 0.22$ in NNR1. In-
 886 terestingly, approximately half ($\hat{\pi} \approx 0.49$) of the sampled structures in NNR1 instead
 887 contain an edge $\text{PNA}_{t-1} \rightarrow \text{PSA1}_t$, which may reflect the effects of a common depen-
 888 dence on tropical forcing. Overall, there are a larger number of features with high pos-
 889 terior mass in the JRA-55 fits. As usual, the precise underlying reasons for these differ-
 890 ences are not determined by the fits alone. Possible biases, such as a poorer represen-
 891 tation of the wintertime SH circulation in one product compared to the other, would re-
 892 quire further detailed follow-up. Our purpose here has been to highlight the use of Bayesian
 893 structure learning as a tool to identify possible differences, and to estimate the level of
 894 uncertainty associated with each.

895 5 Summary

896 Probabilistic graphical models provide a natural and intuitive framework with which
 897 to describe the complicated interactions between climate processes. As a result, they are
 898 increasingly being applied for the purposes of studying potential causal relationships and
 899 for model evaluation (Vázquez-Patiño et al., 2020; Nowack et al., 2020). In this latter
 900 application, models are generally evaluated on the basis of structural comparisons be-

901 tween graph structures inferred from observations and from model runs. Additionally,
902 the strength of associations may be compared by performing a second stage of model fit-
903 ting, conditional on the inferred structure. As is, this constitutes a powerful lens for ex-
904 amining differences between models and observations.

905 That being said, existing approaches still have some important limitations when
906 used as tools for model evaluation. In particular, the most widely used strategy of first
907 learning a suitable structure using a constraint-based learning algorithm, followed op-
908 tionally by fitting a regression model conditioned on this structure, does not lend itself
909 to easily estimating the level of confidence in the obtained model. While sensitivity anal-
910 yses enable some determination of the robustness of particular features, in general the
911 sampling properties associated with this procedure are difficult to assess (Madigan & Raftery,
912 1994; Draper, 1995). This can present a challenge for using learned structures as tools
913 for model evaluation, where some measure of significance of observed differences is usu-
914 ally desirable so as to assess whether they are due to model biases or sampling variabil-
915 ity.

916 This limitation can in principle be overcome by employing a Bayesian approach to
917 structure learning. By learning a posterior distribution over possible structures, rather
918 than selecting a single graph, overall model uncertainty can be quantified and accounted
919 for. This can be particularly important where multiple different structures may all be
920 nearly equally well supported by the data, in which case selection of a single model may
921 overestimate the confidence warranted in particular features. Given a sample from the
922 model posterior distribution, by averaging over the set of possible models the posterior
923 credibility of given features may instead be estimated in the Bayesian approach to iden-
924 tify edges that are well supported by the data. Subsequent estimation of the model pa-
925 rameters conditional on a given structure is straightforward, and provides a basis for com-
926 paring the magnitude of relationships between different processes.

927 The result of the sampling-based structure learning algorithms is a sample from
928 the set of possible models, from which posterior probabilities for particular features can
929 be derived. In this way, robust features for which there is high confidence may be iden-
930 tified, and the set of such edges may in turn form the focus of model comparisons. To
931 illustrate this approach, we have applied an MCMC based approach to learn DBNs de-
932 scribing associations between teleconnections in two different reanalyses, with the goals

933 of identifying the robust structural differences between the two products and to estab-
934 lish a set of baseline estimates for subsequent model evaluation studies.

935 In general, features in the networks derived from NNR1 and JRA-55 data that have
936 high estimated posterior probabilities agree reasonably well. While not surprising, as both
937 reanalyses attempt to provide an estimate of the same climate state, this provides some
938 reassurance that consistent results are obtained using a sampling algorithm, and that
939 the expected associations and dependence structures, such as long memory in oceanic
940 modes and close correspondence between the AO and NAO, are recovered with reason-
941 able levels of certainty. Differences between the models estimated from the two reanal-
942 yses are not only limited to edges with low posterior mass, however. In some cases, these
943 differences involve modes for which there are known biases in one reanalysis or the other;
944 the lack of evidence for a dependence of the PNA on the MJO in JRA-55 is one such ex-
945 ample. In other cases, these features may arise as a result of the effects of omitted con-
946 founding effects, such as seasonal cycles and other common drivers, that nevertheless dif-
947 fer between the two reanalyses. Some evidence for this is found by considering networks
948 fitted from data restricted to only the winter season in each hemisphere. In these fits,
949 apparently spurious cross-equatorial dependence present in fits to year-round data are
950 no longer found to have strong evidence to support their presence. A greater number of
951 differences between the networks derived from the two reanalyses are found for edges that
952 have lower posterior probabilities, with this being particularly noticeable for the SH modes.
953 This may in part be due to greater differences in the representation of these modes, as
954 well as lower signal-to-noise ratios, at least outside of the austral winter.

955 It is important to note that in this study our aim has not been to perform a de-
956 tailed evaluation of the differences between the two reanalysis products. Extensive char-
957 acterization of the performance and biases of both NNR1 and JRA-55 has been done in
958 the past, and further investigations of the differences found here would require additional
959 detailed study of the involved processes in each product. Rather, our purpose has been
960 to demonstrate the applicability of the Bayesian approach to structure learning in de-
961 riving graphical models suitable for use as tools for process-based model evaluation. We
962 argue that an important aspect of this application is the need to account for inevitable
963 model uncertainty in order to identify differences that are likely to be robust and hence
964 represent genuine model biases. Independent of the context of the analysis, this can be
965 naturally achieved in the Bayesian approach. By considering a relatively straightforward

966 initial application to reanalysis data, for which there exists (at least some) consensus on
967 the interactions between modes, we have shown that a score-based sampling approach
968 recovers the expected relationships, while also providing additional benefits over constraint-
969 based approaches in the form of estimates for the posterior distribution over models and
970 features.

971 Given this, we have primarily focused on a single analysis of year-round monthly
972 mean data, or data within a single season. While sufficient to illustrate the relevant fea-
973 tures of the results, in order to utilize this approach in the context of causal discovery
974 it would be necessary to further extend the analysis presented here. In addition to care-
975 ful selection of the relevant variables, time periods, and temporal resolution, further con-
976 sideration should be given to the form of the likelihood and priors used in defining the
977 model. In this work, the simplest case of a linear model with conjugate priors on the pa-
978 rameters defining the conditional PDFs has been used, together with priors on the struc-
979 tures to ensure structural modularity. No prior restriction has been enforced to ensure
980 stationarity of the resulting autoregressive model. Additionally, no attempt has been made
981 to incorporate pre-existing or expert knowledge into the definition of the chosen priors.
982 More complex forms for the conditional PDF, as well as the use of non-conjugate pri-
983 ors and inclusion of additional constraints, may be directly handled using a generic re-
984 versible jump MCMC instead of the more specialized MC³ used here.

985 Whether or not the resulting model has analytic structure, care must be taken in
986 the design of the sampler and in assessing the approximate convergence of the simula-
987 tion to the target posterior distribution. For the results presented here, the non-parametric
988 convergence diagnostics of Brooks et al. (2003) have been used to monitor (non-)convergence,
989 but in general assessing convergence for trans-dimensional MCMC remains challenging
990 (Sisson, 2005). In our case, trace plots and convergence diagnostics applied to individ-
991 ual edge indicators suggested that (model-averaged) estimates derived from individual
992 chains were consistent and stable, but there was evidence for non-homogeneity in the pos-
993 terior distribution over structures across chains based on 10×10^6 samples. For this rea-
994 son, we have avoided making definitive statements with respect to Bayes factors and other
995 model-specific quantities, recognizing that further sampling would be required for these
996 to be reliably determined. Poor mixing and multi-modal posterior distributions over mod-
997 els may also be problematic, with the sampled chains remaining trapped in the vicin-
998 ity of a single mode. Given the large model space considered here, this is a concern as

1099 ensuring the chains have adequately explored the full posterior distribution is unlikely
1000 to be feasible, raising the possibility that the fits have converged to a local mode in the
1001 model space. For generating causal hypotheses, it may be more suitable to restrict at-
1002 tention to smaller systems of variables. On the other hand, the relatively close agree-
1003 ment between the fits for the two reanalyses shown here suggests that the simulations
1004 explore sufficiently similar regions of the model space for useful qualitative comparisons
1005 to still be performed. As in this paper only two datasets were compared, direct inspec-
1006 tion of the individual fitted networks, amounting to visual inspection of the sampled pos-
1007 terior distributions, was sufficient. In more extensive evaluation studies, this may be ex-
1008 tended by the use of appropriate summary measures computed on the fits for different
1009 models.

1010 The DBN models obtained for the NNR1 and JRA-55 reanalyses form a set of ground
1011 truth results against which free-running models may be compared; we are currently per-
1012 forming such a comparison over the historical period. However, the homogeneous mod-
1013 els considered here cannot model one of the most notable features of the observed cli-
1014 mate over this period, namely, the existence of secular trends in the behavior of partic-
1015 ular modes. Key open questions remain as to whether there is evidence for accompany-
1016 ing changes in the underlying interaction structures, and whether models indicate the
1017 possibility of regime shifts under future forcing scenarios. Addressing these questions in
1018 this framework will require the use of non-homogeneous network models in which either
1019 the model parameters or structure are allowed to vary. In a forthcoming article, we per-
1020 form just such a comparison against the reanalysis-derived networks presented here for
1021 a subset of the CMIP5 ensemble, as well as relaxing the time-homogeneity assumptions
1022 discussed above to study the existence of regime transitions in projections. Assessing the
1023 evidence for, say, the existence of sudden structure changes versus slow variation in the
1024 underlying network parameters does not entail any additional conceptual changes, mak-
1025 ing the approach presented here well-suited for investigating such questions.

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1028 scribed in Rayner et al. (2003), and may be accessed at [https://www.metoffice.gov](https://www.metoffice.gov.uk/hadobs/hadisst/)
1029 [.uk/hadobs/hadisst/](https://www.metoffice.gov.uk/hadobs/hadisst/) (last access: 29 April 2019). The NCEP/NCAR reanalysis out-
1030 put used is provided by the NOAA/OAR/ESRL PSL, Boulder, Colorado, USA, described

1031 in Kalnay et al. (1996), and may be accessed at [https://psl.noaa.gov/data/reanalysis/](https://psl.noaa.gov/data/reanalysis/reanalysis.shtml)
 1032 [reanalysis.shtml](https://psl.noaa.gov/data/reanalysis/reanalysis.shtml) (last access: 10 May 2019). The JRA-55 reanalysis output used is
 1033 made available through the JRA-55 project and may be accessed following the proce-
 1034 dures and access conditions described in Kobayashi et al. (2015) and at [https://jra](https://jra.kishou.go.jp/JRA-55/index_en.html)
 1035 [.kishou.go.jp/JRA-55/index_en.html](https://jra.kishou.go.jp/JRA-55/index_en.html) (last access: 12 April 2019).

1036 Regridding of the reanalysis fields was performed using the Climate Data Oper-
 1037 ators software suite (Schulzweida, 2019), while the analysis code was implemented us-
 1038 ing the Python libraries NumPy (Oliphant, 2006; Van Der Walt et al., 2011), SciPy (Virtanen
 1039 et al., 2020), pandas (Wes McKinney, 2010), scikit-learn (Pedregosa et al., 2011), and
 1040 xarray (Hoyer & Hamman, 2017). Plots were generated using the Python package Mat-
 1041 plotlib (Hunter, 2007). All source code and the generated indices used to perform the
 1042 analyses presented in this study may be found at [https://doi.org/10.5281/zenodo](https://doi.org/10.5281/zenodo.4331149)
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1048 **Appendix A MCMC sampling methods**

1049 In this appendix we summarize the MCMC methods used for structure learning.
 1050 We employ the composite parameter space formulation described in detail in Godsill (2001).
 1051 For the models considered in the main text, in the absence of same-time edges the net-
 1052 works are structurally modular and the parent set associated with each index can be in-
 1053 ferred independently. However, in general a given structure $G \in \mathcal{G}$ will describe the joint
 1054 distribution of all of the indices simultaneously at a given time. To accommodate such
 1055 models, we keep the notation relatively general.

1056 The observed data takes the form of a time series of one or more indices $D = \{\mathbf{y}_1, \dots, \mathbf{y}_T\}$.
 1057 The allowed set of models \mathcal{G} to describe these data are taken to be specified a priori. Let
 1058 $\boldsymbol{\theta}$ denote the collection of all such parameters across all of the possible models in \mathcal{G} . For
 1059 example, for the set of all linear Gaussian models, the vector $\boldsymbol{\theta}$ would contain all of the
 1060 possible regression coefficients $\beta_{(j,\tau)}^i$ associated with the possible edges $Y_{t-\tau}^j \rightarrow Y_t^i$ as
 1061 well as the conditional precisions τ_i^2 and intercept parameters β_0^i . Any given model G

1062 will only use a small subset of all of the possible parameters. The subset of the param-
 1063 eters used by a structure G will be written $\boldsymbol{\theta}_{\mathcal{I}(G)}$; here $\mathcal{I}(G)$ is an appropriate index set
 1064 indicating which components of the complete parameter vector $\boldsymbol{\theta}$ are required by G . The
 1065 remaining parameters not used by G will be denoted by $\boldsymbol{\theta}_{-\mathcal{I}(G)}$. A particular model for
 1066 the indices $\{Y^1, \dots, Y^n\}$ is described by the pair $(G, \boldsymbol{\theta}) \in \mathcal{G} \times \Theta$, where $\mathcal{G} \times \Theta$ is the
 1067 composite model space (Godsill, 2001).

1068 To infer the network structure and parameters given data D , we aim to sample from
 1069 the posterior distribution

$$1070 \quad P(G, \boldsymbol{\theta}|D) \propto P(D|G, \boldsymbol{\theta})P(G, \boldsymbol{\theta}).$$

1071 The likelihood $P(D|G, \boldsymbol{\theta})$ is taken to depend only on the subset of parameters associ-
 1072 ated with G ,

$$1073 \quad P(D|G, \boldsymbol{\theta}) \equiv P(D|G, \boldsymbol{\theta}_{\mathcal{I}(G)}),$$

1074 while the prior distribution $P(G, \boldsymbol{\theta})$ is taken to be of the form

$$1075 \quad P(G, \boldsymbol{\theta}) = P(\boldsymbol{\theta}_{\mathcal{I}(G)}|G)P(\boldsymbol{\theta}_{-\mathcal{I}(G)}|\boldsymbol{\theta}_{\mathcal{I}(G)}, G)P(G).$$

1076 The factor $P(\boldsymbol{\theta}_{-\mathcal{I}(G)}|\boldsymbol{\theta}_{\mathcal{I}(G)}, G)$ corresponds to a set of proper pseudo-priors (Carlin &
 1077 Chib, 1995) for the parameters not used by G , and may otherwise be chosen essentially
 1078 freely. The samplers that we use correspond to Metropolis-Hastings schemes in the com-
 1079 posite model space (Godsill, 2001) with a proposal density of the form

$$1080 \quad q(G', \boldsymbol{\theta}'; G, \boldsymbol{\theta}) = q_1(G'; G)q_2(\boldsymbol{\theta}'_{\mathcal{I}(G')}; \boldsymbol{\theta}_{\mathcal{I}(G)})P(\boldsymbol{\theta}'_{-\mathcal{I}(G')}|\boldsymbol{\theta}'_{\mathcal{I}(G')}, G'), \quad (\text{A1})$$

1081 for a move from $(G, \boldsymbol{\theta})$ to $(G', \boldsymbol{\theta}')$ with corresponding acceptance probability

$$1082 \quad \alpha = \min \left\{ 1, \frac{q_1(G; G') q_2(\boldsymbol{\theta}_{\mathcal{I}(G)}; \boldsymbol{\theta}'_{\mathcal{I}(G')}) P(G', \boldsymbol{\theta}'_{\mathcal{I}(G')}|D)}{q_1(G'; G) q_2(\boldsymbol{\theta}'_{\mathcal{I}(G')}; \boldsymbol{\theta}_{\mathcal{I}(G)}) P(G, \boldsymbol{\theta}_{\mathcal{I}(G)}|D)} \right\}. \quad (\text{A2})$$

1083 When the class of models considered does not admit analytic evaluation of any of
 1084 the required integrals, we make use of the simple reversible jump MCMC scheme given
 1085 in Algorithm 1. At each iteration, either an update to the parameter associated with the
 1086 structure G is chosen, with probability $j_\theta(G, \boldsymbol{\theta}_{\mathcal{I}(G)})$, or an update to the current struc-
 1087 ture is proposed. In the case of a parameter update, the model structure is left unchanged,
 1088 $G' = G$, and a new set of parameter values $\boldsymbol{\theta}'_{\mathcal{I}(G)}$ is drawn from a proposal density $q_\theta(\boldsymbol{\theta}'_{\mathcal{I}(G)}; \boldsymbol{\theta}_{\mathcal{I}(G)})$.
 1089 The updated state $(G, \boldsymbol{\theta}'_{\mathcal{I}(G)})$ is accepted with probability

$$1090 \quad \alpha = \min \left\{ 1, \frac{j_\theta(G, \boldsymbol{\theta}'_{\mathcal{I}(G)}) q_\theta(\boldsymbol{\theta}_{\mathcal{I}(G)}; \boldsymbol{\theta}'_{\mathcal{I}(G)}) P(G, \boldsymbol{\theta}'_{\mathcal{I}(G)}|D)}{j_\theta(G, \boldsymbol{\theta}_{\mathcal{I}(G)}) q_\theta(\boldsymbol{\theta}'_{\mathcal{I}(G)}; \boldsymbol{\theta}_{\mathcal{I}(G)}) P(G, \boldsymbol{\theta}_{\mathcal{I}(G)}|D)} \right\}. \quad (\text{A3})$$

1091 Note that, when the probability of a parameter update move is the same in both states,
 1092 this is simply an ordinary Metropolis-Hastings update for a single model. If instead a
 1093 structure update move is chosen, a new structure G' is proposed according to the pro-
 1094 posal distribution $q_G(G'; G)$. Any parameters that are common to both G' and G are
 1095 held fixed at their current values, while any new parameters $\theta'_{\mathcal{I}(G') \setminus \mathcal{I}(G)}$ are sampled from
 1096 an additional proposal density $\tilde{q}_\theta(\theta'_{\mathcal{I}(G') \setminus \mathcal{I}(G)})$; if $\mathcal{I}(G') \subset \mathcal{I}(G)$ we set $\tilde{q}_\theta \rightarrow 1$. Pa-
 1097 rameters that are either present in the initial structure but not in the proposed struc-
 1098 ture, or are not used by either, are left unchanged for simplicity. The acceptance ratio
 1099 for this move is

$$1100 \quad \alpha = \min \left\{ 1, \frac{j_G(G', \theta'_{\mathcal{I}(G')}) q_G(G; G') \tilde{q}_\theta(\theta_{\mathcal{I}(G) \setminus \mathcal{I}(G')}) P(G', \theta'_{\mathcal{I}(G')} | D)}{j_G(G, \theta_{\mathcal{I}(G)}) q_G(G'; G) \tilde{q}_\theta(\theta'_{\mathcal{I}(G') \setminus \mathcal{I}(G)}) P(G, \theta_{\mathcal{I}(G)} | D)} \right\}. \quad (\text{A4})$$

1101 This structure update move is just a particular case of the general reversible jump move
 1102 (Green, 1995) with a unit Jacobian. For more general mappings from the current to pro-
 1103 posed parameters a non-trivial Jacobian factor would remain following the change of vari-
 1104 ables in the proposal density Eq. (A1).

1105 When the models considered allow for the conditional posterior distribution $P(\theta_{\mathcal{A}(G)} | \theta_{\mathcal{I}(G) \setminus \mathcal{A}(G)}, G, D)$
 1106 of some subset of the parameters $\theta_{\mathcal{A}(G)}$, $\mathcal{A}(G) \subseteq \mathcal{I}(G)$, to be evaluated given G and
 1107 any remaining parameters $\theta_{\mathcal{I}(G) \setminus \mathcal{A}(G)}$, we adopt a conditional Metropolis-Hastings scheme
 1108 that takes better advantage of this structure. For simplicity, we assume that the set of
 1109 parameters $\theta_{\mathcal{I}(G) \setminus \mathcal{A}(G)}$, if not empty, is shared across all of the possible structures. Up-
 1110 dates to the structure are proposed as before under the proposal $q_G(G'; G)$. The shared
 1111 parameters $\theta_{\mathcal{I}(G) \setminus \mathcal{A}(G)}$ are kept at their previous values, while the remaining param-
 1112 eters are drawn from the exactly known posterior distribution $P(\theta'_{\mathcal{A}(G')} | \theta'_{\mathcal{I}(G') \setminus \mathcal{A}(G')}, G', D)$.
 1113 Under this proposal, the acceptance ratio simplifies to

$$1114 \quad \alpha = \min \left\{ 1, \frac{q_G(G; G') P(G' | \theta'_{\mathcal{I}(G') \setminus \mathcal{A}(G')}, D)}{q_G(G'; G) P(G | \theta_{\mathcal{I}(G) \setminus \mathcal{A}(G)}, D)} \right\}. \quad (\text{A5})$$

1115 The parameters associated with the current structure can be updated via a standard Metropolis-
 1116 Hastings or Gibbs step, as in the parameter update move for the simple reversible jump
 1117 scheme. Parameter and structure updates can either be proposed randomly or performed
 1118 in a fixed order. For the models presented in Section 4, the conditional posterior distri-
 1119 bution for all of the parameters can be evaluated, i.e., the set $\theta_{\mathcal{I}(G) \setminus \mathcal{A}(G)}$ is empty. In
 1120 this case, the scheme reduces to the MC³ scheme of Madigan et al. (1995), with the de-
 1121 pendence on the graph parameters dropping out entirely. The acceptance ratio for a struc-

Algorithm 1 Simple RJMCMC sampler

Require: initial state $x^{(1)} \equiv (G^{(1)}, \boldsymbol{\theta}^{(1)})$, observed data D , chain length $2S$

- 1: **for** $s = 2, \dots, 2S$ **do**
 - 2: Draw $u_1, u_2 \sim \text{Uniform}(0, 1)$
 - 3: **if** $u_1 < j_{\theta}(x^{(s-1)})$ **then**
 - 4: Set $G' \leftarrow G^{(s-1)}$
 - 5: Draw new parameters $\boldsymbol{\theta}'_{\mathcal{I}(G')}$ from $q_{\theta}(\boldsymbol{\theta}'_{\mathcal{I}(G')}; \boldsymbol{\theta}_{\mathcal{I}(G^{(s-1)})}^{(s-1)})$
 - 6: Calculate α according to Eq. (A3)
 - 7: **else**
 - 8: Draw new parent set G' from $q_G(G'; G^{(s-1)})$
 - 9: Draw $\boldsymbol{\theta}'_{\mathcal{I}(G') \setminus \mathcal{I}(G^{(s-1)})}$ from $\tilde{q}_{\theta}(\boldsymbol{\theta}'_{\mathcal{I}(G') \setminus \mathcal{I}(G^{(s-1)})})$
 - 10: Calculate α according to Eq. (A4)
 - 11: **if** $u_2 < \alpha$ **then**
 - 12: $x^{(s)} \leftarrow (G', \boldsymbol{\theta}')$
 - 13: **else**
 - 14: $x^{(s)} \leftarrow (G^{(s-1)}, \boldsymbol{\theta}^{(s-1)})$
 - 15: Discard first S samples as warm-up
 - 16: **return** $\{x^{(S+1)}, \dots, x^{(2S)}\}$
-

1122 ture drawn according to $q_G(G'; G)$ is in this case

$$1123 \quad \alpha = \min \left\{ 1, \frac{q_G(G; G') \frac{P(D|G') P(G')}{q_G(G'; G) \frac{P(D|G) P(G)}} \right\}, \quad (\text{A6})$$

1124 where the likelihood can be written in terms of the local marginal likelihoods, as in Eq. (8).

1125 Particular choices of the proposal density and structure priors are described in Section 3.3.

1126 We summarize the resulting sampling scheme for the structures in Algorithm 2. For each

1127 sampling method, we run multiple chains, discarding the first half of each sample as burn-

1128 in. For the MC³ sampler, approximate convergence of the chains to the target distribu-

1129 tion is assessed using the χ^2 and Kolmogorov-Smirnov tests proposed in Brooks et al.

1130 (2003).

Algorithm 2 MC³ sampler

Require: initial state $G^{(1)}$, observed data D , chain length $2S$

- 1: **for** $s = 2, \dots, 2S$ **do**
 - 2: Draw $u \sim \text{Uniform}(0, 1)$
 - 3: Draw new parent set G' from $q_G(G'; G^{(s-1)})$
 - 4: Calculate α according to Eq. (A6)
 - 5: **if** $u < \alpha$ **then**
 - 6: $G^{(s)} \leftarrow G'$
 - 7: **else**
 - 8: $G^{(s)} \leftarrow G^{(s-1)}$
 - 9: Discard first S samples as warm-up
 - 10: **return** $\{G^{(S+1)}, \dots, G^{(2S)}\}$
-

1131 **Appendix B Expressions for marginal likelihoods**

1132 In this appendix we state the closed-form expressions for the prior and posterior
 1133 densities for the parameters of the node conditional distributions, and the resulting marginal
 1134 likelihoods or local scores, for the models used in the main text.

The linear Gaussian model given in Section 2 reads

$$\begin{aligned} \tau_i^2 &\sim \text{Gamma}(a_\tau, b_\tau), \\ \beta_0^i | \tau_i^2, \nu_i^2 &\sim N\left(0, \frac{\nu_i^2}{\tau_i^2}\right), \\ \beta_{(k_j, \tau_j)}^i | \tau_i^2, \nu_i^2, \text{pa}_G(Y_t^i) &\sim N\left(0, \frac{\nu_i^2}{\tau_i^2}\right), \quad j = 1, \dots, |\text{pa}_G(Y_t^i)|, \\ Y_t^i | \beta_0^i, \beta_{(k_j, \tau_j)}^i, \tau_i^2, \text{pa}_G(Y_T^i) &\sim N\left(\beta_0^i + \sum_{j=1}^{|\text{pa}_G(Y_t^i)|} \beta_{(k_j, \tau_j)}^i Y_{t-\tau_j}^{k_j}, \frac{1}{\tau_i^2}\right), \end{aligned}$$

1135 For the prior on the conditional precision τ_i^2 , we adopt the convention

1136
$$P(\tau_i^2 | a_\tau, b_\tau) = \frac{1}{\Gamma(a_\tau)} \frac{(\tau_i^2)^{a_\tau-1}}{b_\tau^{a_\tau}} \exp\left(-\frac{\tau_i^2}{b_\tau}\right).$$

1137 With this convention, the unconditional prior distribution for a given coefficient β is a
 1138 generalized t -distribution with scale $\hat{\sigma}^2 = \nu^2/(a_\tau b_\tau)$ and $2a_\tau$ degrees of freedom, $\beta \sim$
 1139 $T_1(0, \nu^2/(a_\tau b_\tau), 2a_\tau)$. For the models shown in Section 4, a_τ , b_τ , and ν_i^2 are taken as fixed
 1140 hyperparameters. In practice, the signal-to-noise ν_i^2 may be poorly known, in which case
 1141 it is possible to also sample it from a conjugate inverse gamma prior using the sampling

1142 schemes for models with partial analytic structure discussed in Appendix A. For a given
 1143 parent set, we write the vector of predictor variables as $(p_i = |\text{pa}_G(Y_t^i)|)$

1144
$$\mathbf{x}_t^{iT} = (1, y_{t-\tau_1}^{k_1}, \dots, y_{t-\tau_{p_i}}^{k_{p_i}}),$$

1145 at each time $t = 1, \dots, T$ and introduce the $T \times (p_i + 1)$ design matrix

1146
$$X_i = \begin{pmatrix} \mathbf{x}_1^{iT} \\ \vdots \\ \mathbf{x}_T^{iT} \end{pmatrix}.$$

1147 The likelihood for the observed values of the index Y^i then takes the simple form of a
 1148 product of normal densities, and the local marginal likelihood $\Psi_i(D; G)$ can be evalu-
 1149 ated using standard conjugacy results. The marginal joint distribution for the observed
 1150 index values $\mathbf{y}_i^T = (y_1^i, \dots, y_T^i)$ under this model is a multivariate t -distribution, giv-
 1151 ing

1152
$$\Psi_i(D; G) = \frac{\Gamma\left(\frac{T+2a_\tau}{2}\right)}{\Gamma\left(\frac{2a_\tau}{2}\right) \pi^{T/2} (2a_\tau)^{T/2}} (\det \Sigma_i)^{-1/2} \left(1 + \frac{1}{2a_\tau} \mathbf{y}_i^T \Sigma_i^{-1} \mathbf{y}_i\right)^{-\frac{T+2a_\tau}{2}}, \quad (\text{B1})$$

1153 where

1154
$$\Sigma_i = \frac{1}{a_\tau b_\tau} (I_{T \times T} + \nu_i^2 X_i X_i^T), \quad (\text{B2})$$

1155 and $I_{T \times T}$ is the $T \times T$ identity matrix. For a given parent set, the regression coefficients
 1156 and precision can be sampled from the conditional posterior distributions

1157
$$\tau_i^2 | D, G, \nu_i^2 \sim \text{Gamma}\left(\frac{T+2a_\tau}{2}, \frac{b_\tau}{1 + \frac{1}{2a_\tau} \mathbf{y}_i^T \Sigma_i^{-1} \mathbf{y}_i}\right), \quad (\text{B3})$$

1158
$$\beta_i | \tau_i^2, \nu_i^2, D, G \sim N(\tau_i^2 \Sigma_{\beta_i} X_i^T \mathbf{y}_i, \Sigma_{\beta_i}), \quad (\text{B4})$$

1160 where the posterior covariance matrix for the coefficients $\beta_i^T \equiv (\beta_0^i, \beta_{(k_1, \tau_1)}^i, \dots, \beta_{(k_{p_i}, \tau_{p_i})}^i)$
 1161 is given by

1162
$$\Sigma_{\beta_i} = \frac{\nu_i^2}{\tau_i^2} (I_{(p_i+1) \times (p_i+1)} + \nu_i^2 X_i^T X_i)^{-1}.$$

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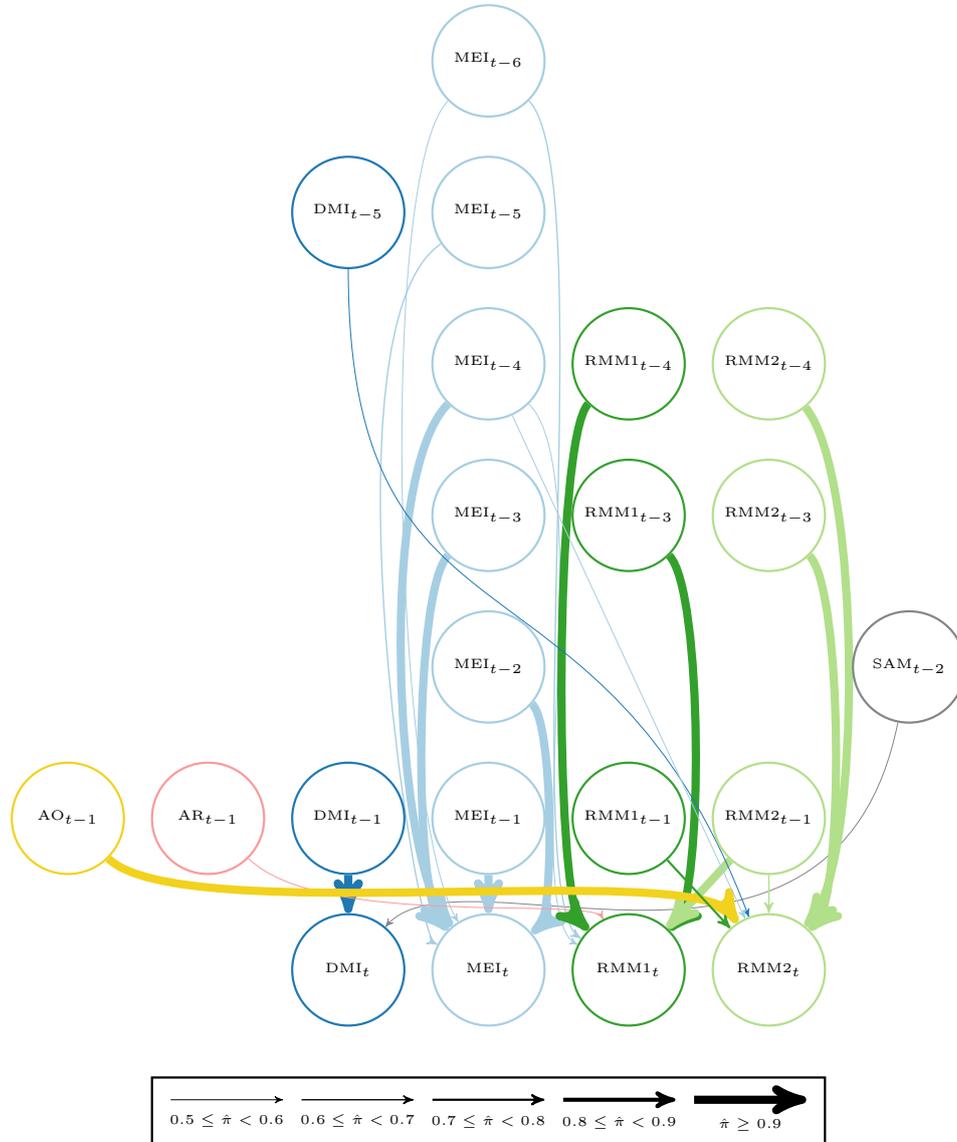


Figure 3. Subgraphs corresponding to the fitted parent sets of the tropical indices in JRA-55 based on full-year data for $a_r = 1.5$, $b_r = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

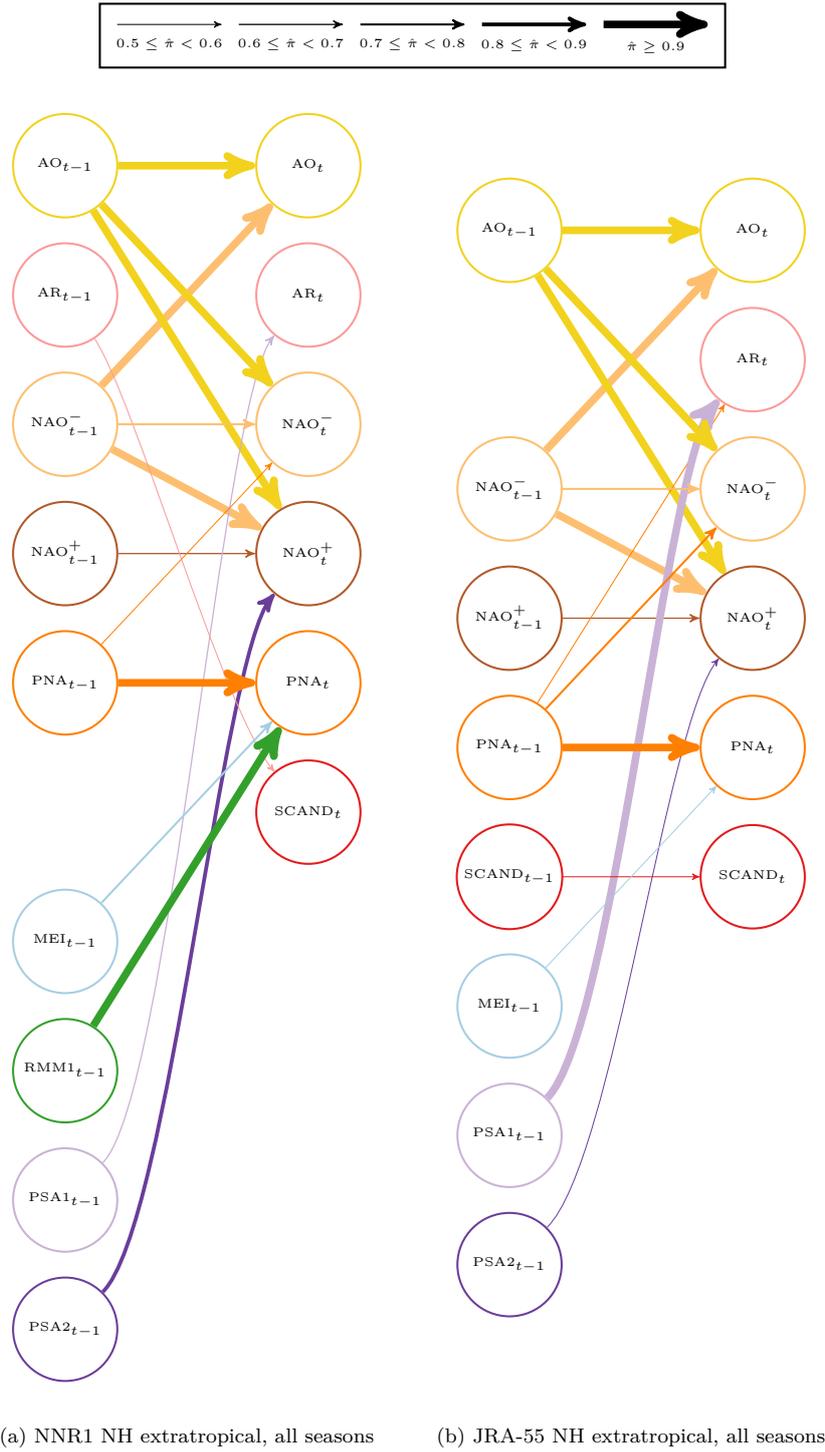


Figure 4. Subgraphs corresponding to the fitted parent sets of the NH extratropical indices in (a) NNR1 and (b) JRA-55 for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

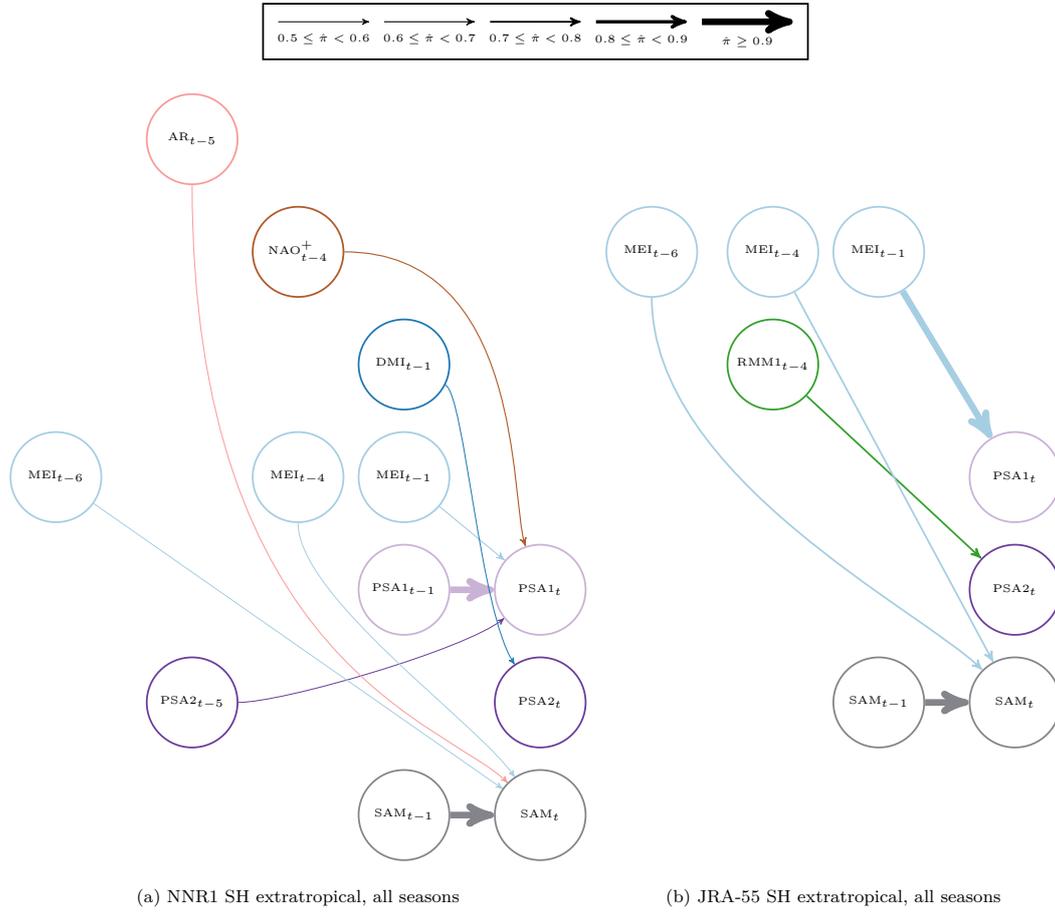


Figure 5. Subgraphs corresponding to the fitted parent sets of the SH extratropical indices in (a) NNR1 and (b) JRA-55 for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

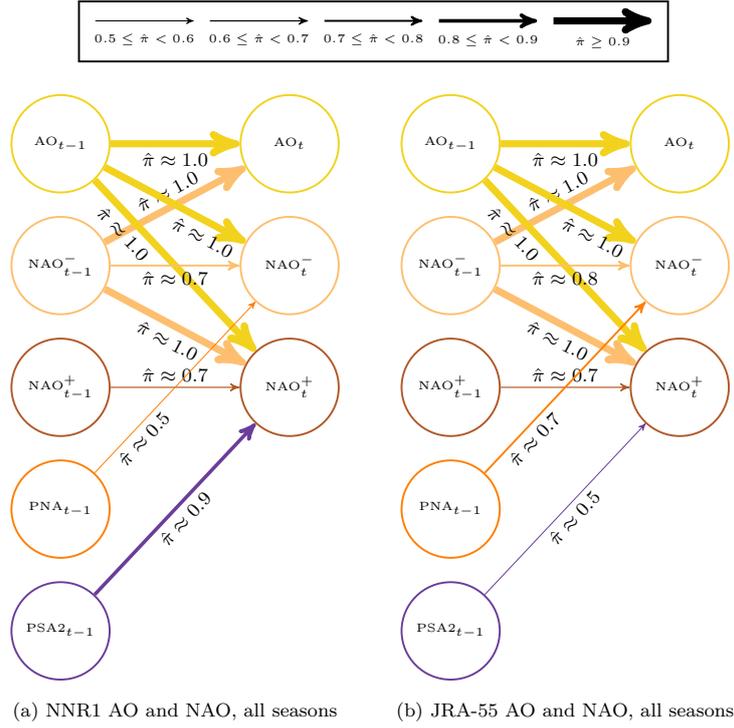


Figure 6. Subgraphs corresponding to the fitted parent set of the monthly AO and NAO indices in (a) NNR1 and (b) JRA-55, for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

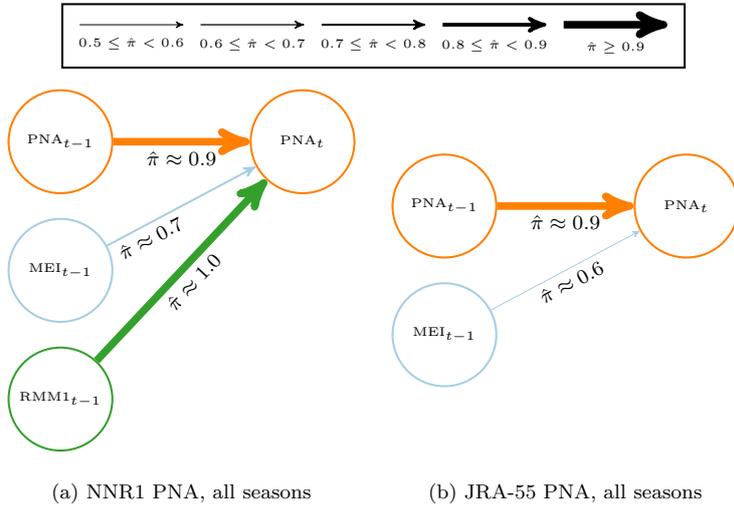


Figure 7. Subgraphs corresponding to the fitted parent set of the monthly PNA index in (a) NNR1 and (b) JRA-55, for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

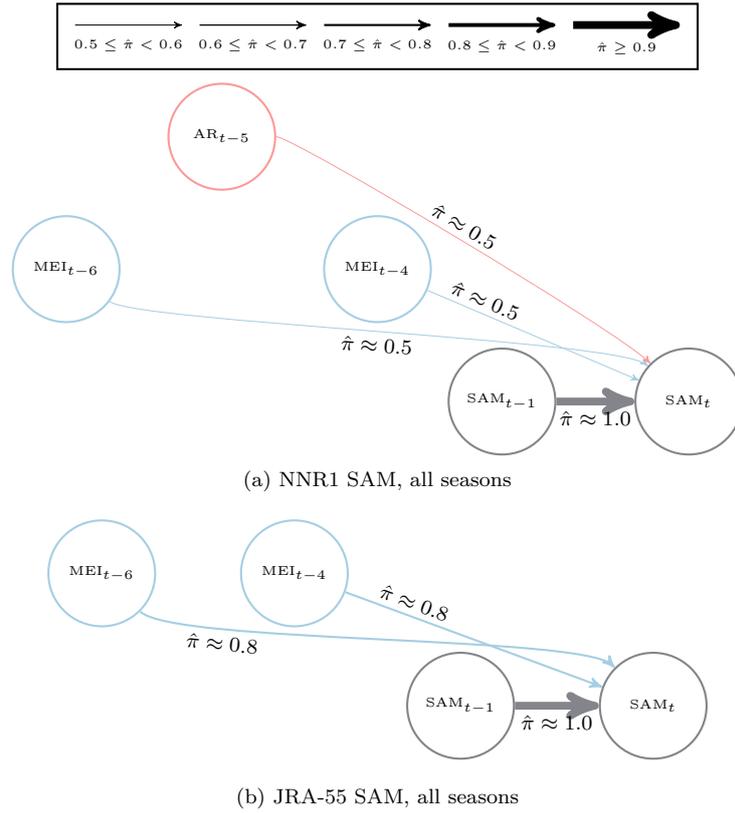


Figure 8. Subgraphs corresponding to the fitted parent set of the monthly SAM index in (a) NNR1 and (b) JRA-55, for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

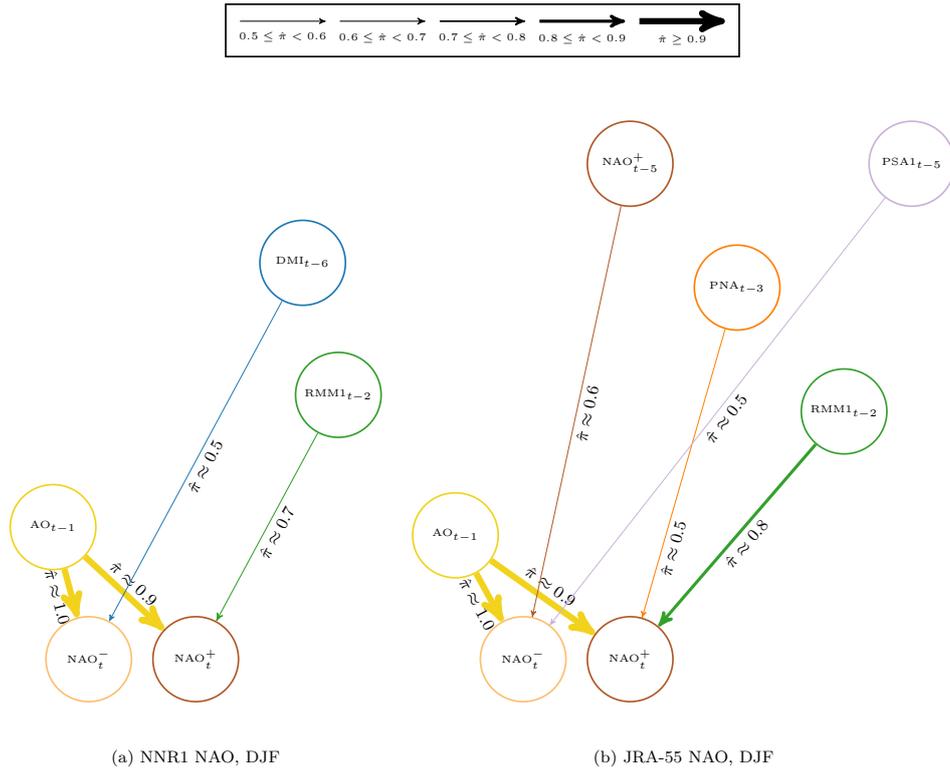


Figure 9. Subgraphs corresponding to the fitted parent set of the monthly NAO indices in (a) NNR1 and (b) JRA-55, for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$ during DJF. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

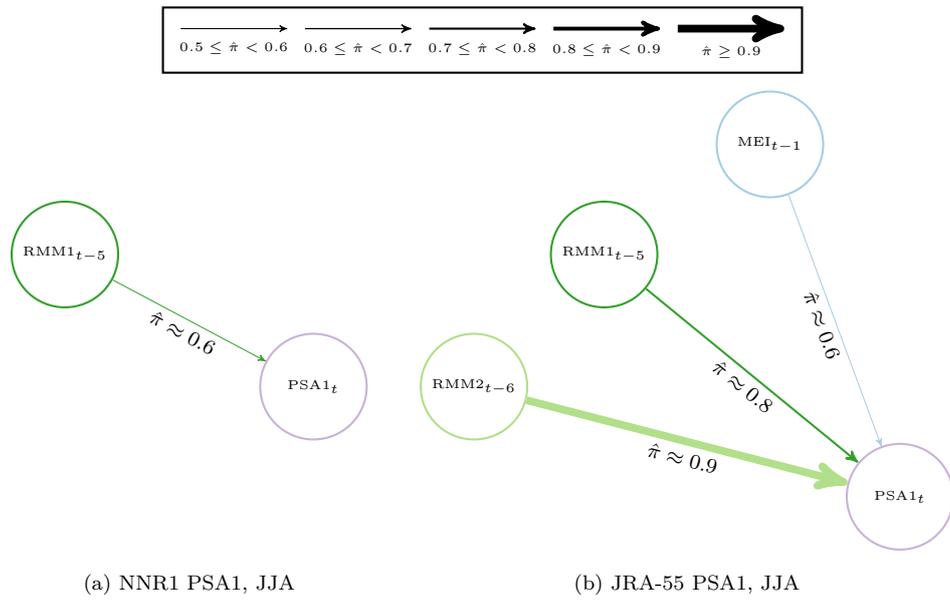


Figure 10. Subgraphs corresponding to the fitted parent set of the monthly PSA1 index in (a) NNR1 and (b) JRA-55, for $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$ during JJA. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

Supporting Information for ”Dynamic Bayesian networks for evaluation of Granger causal relationships in climate reanalyses”

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2. Tables S1 to S2

Introduction

This supporting information provides the patterns corresponding to the teleconnection indices analyzed in the main text, summaries of the edge posterior distributions for the alternative choice of hyperparameters, and summaries of the maximum a posteriori (MAP) structure estimates for the fits presented in the main text.

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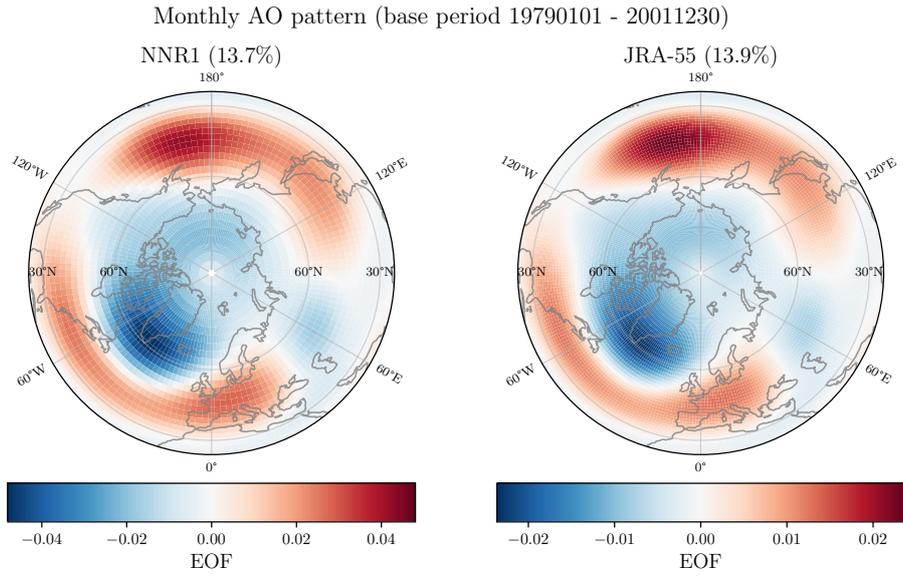


Figure S1. AO loading pattern of 500 hPa geopotential height anomalies in NNR1 (left) and JRA-55 (right).

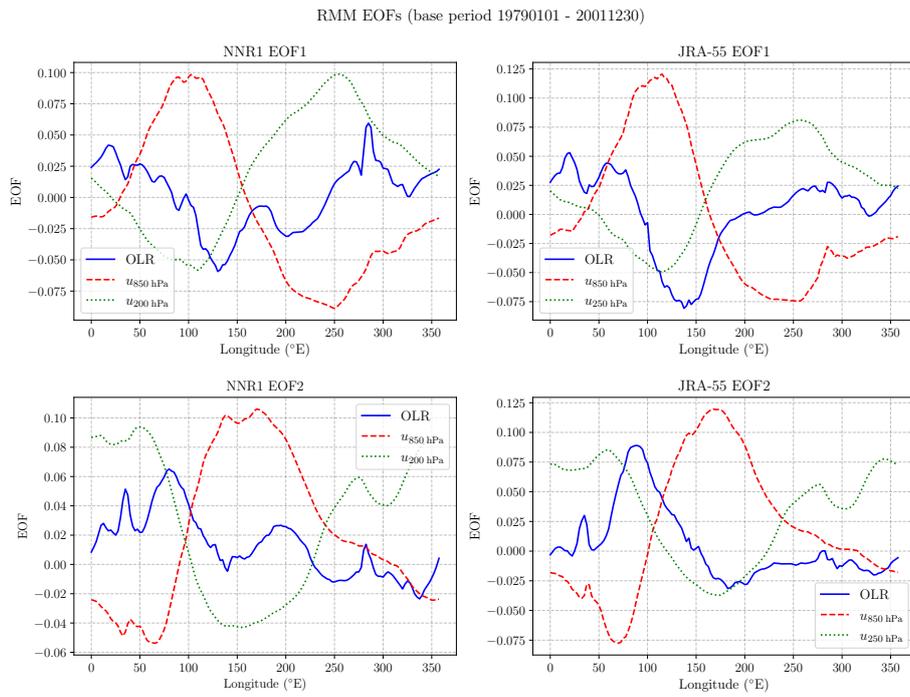


Figure S2. RMM EOFs in HadISST and NNR1 (left column) and JRA-55 (right column).

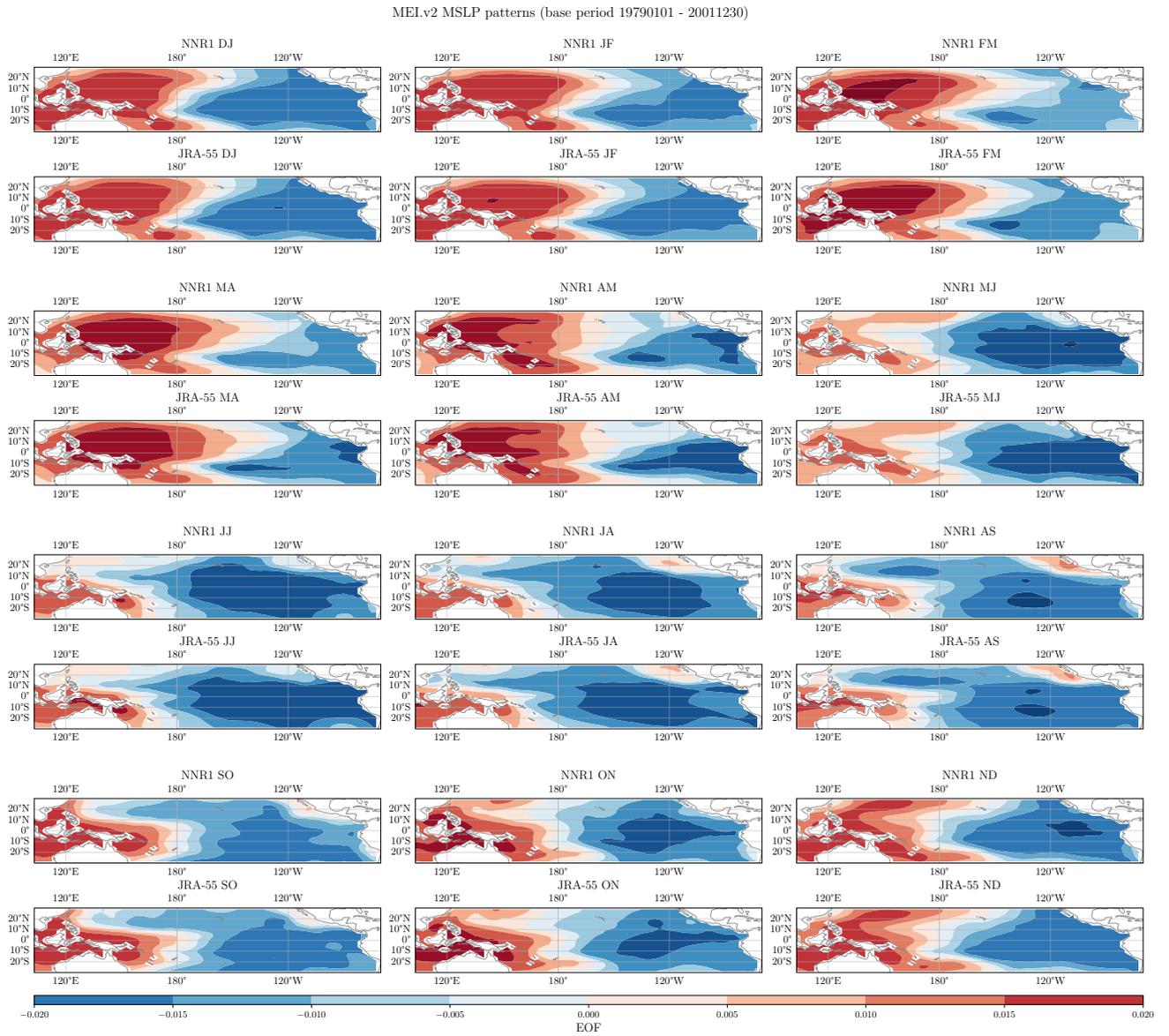


Figure S3. Seasonal MSLP anomaly patterns contributing to the MEI in HadISST and NNR1 (odd numbered rows) and JRA-55 (even numbered rows).

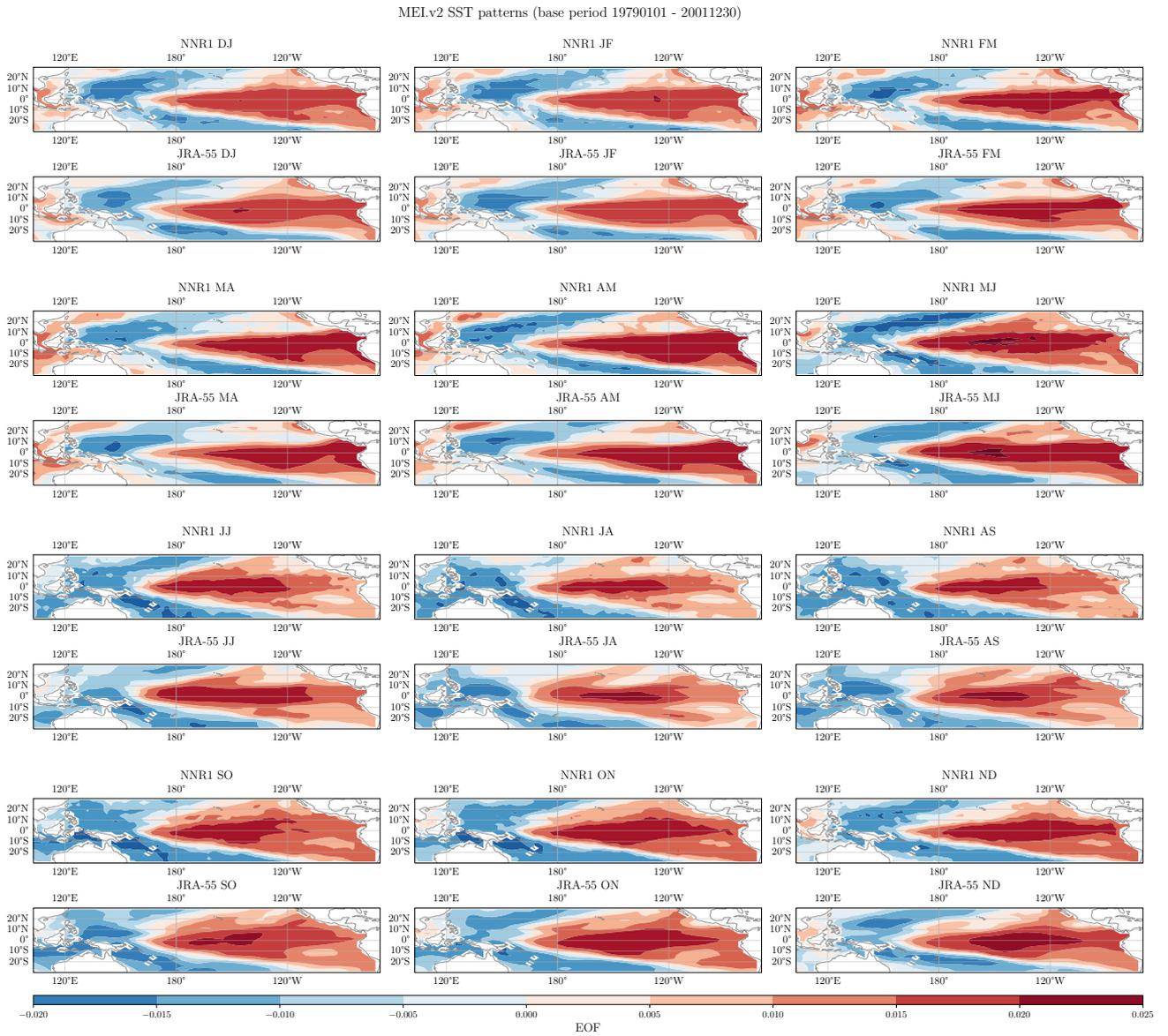


Figure S4. Seasonal SST anomaly patterns contributing to the MEI in HadISST and NNR1 (odd numbered rows) and JRA-55 (even numbered rows).

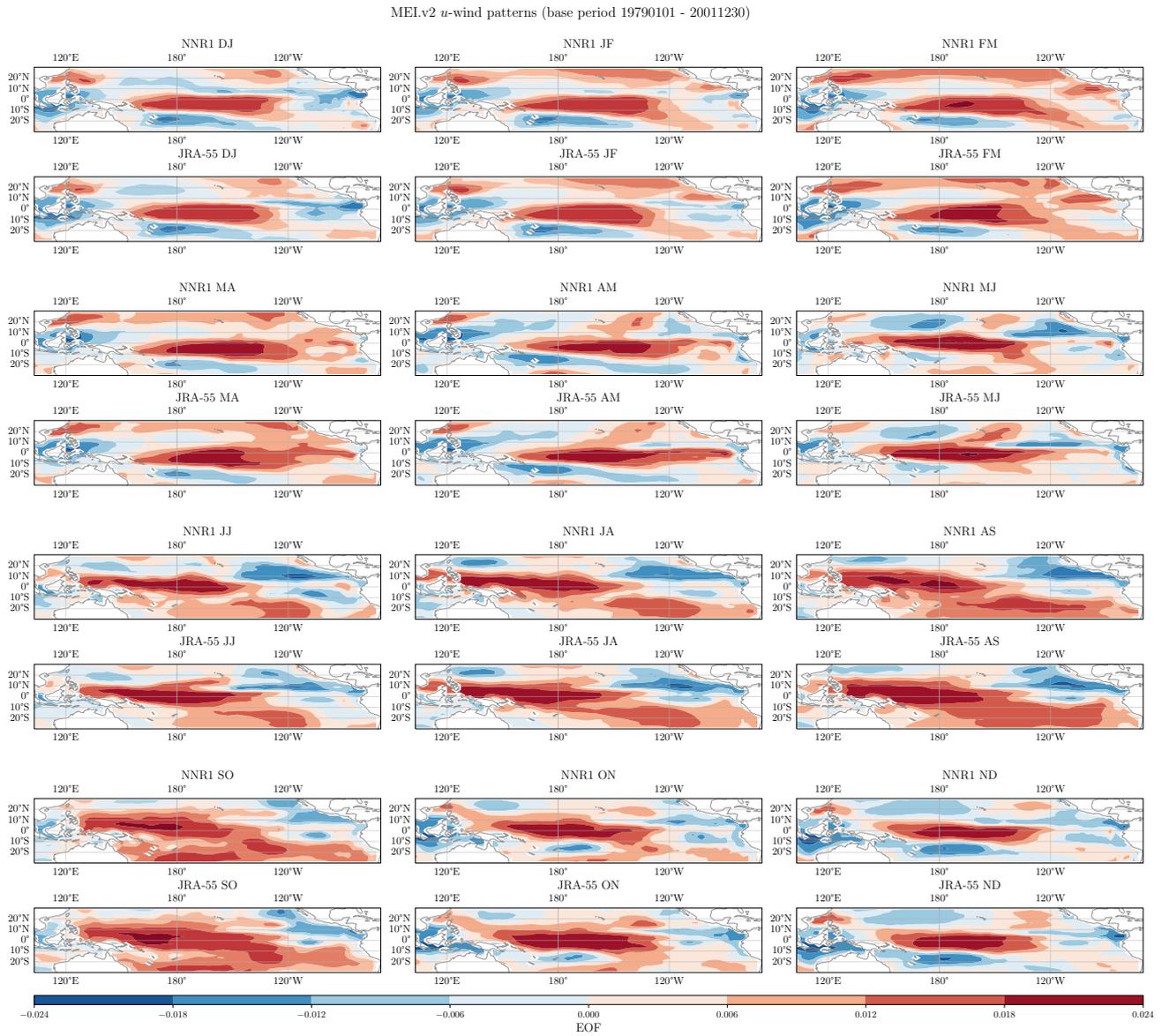


Figure S5. Seasonal zonal wind anomaly patterns contributing to the MEI in HadISST and NNR1 (odd numbered rows) and JRA-55 (even numbered rows).

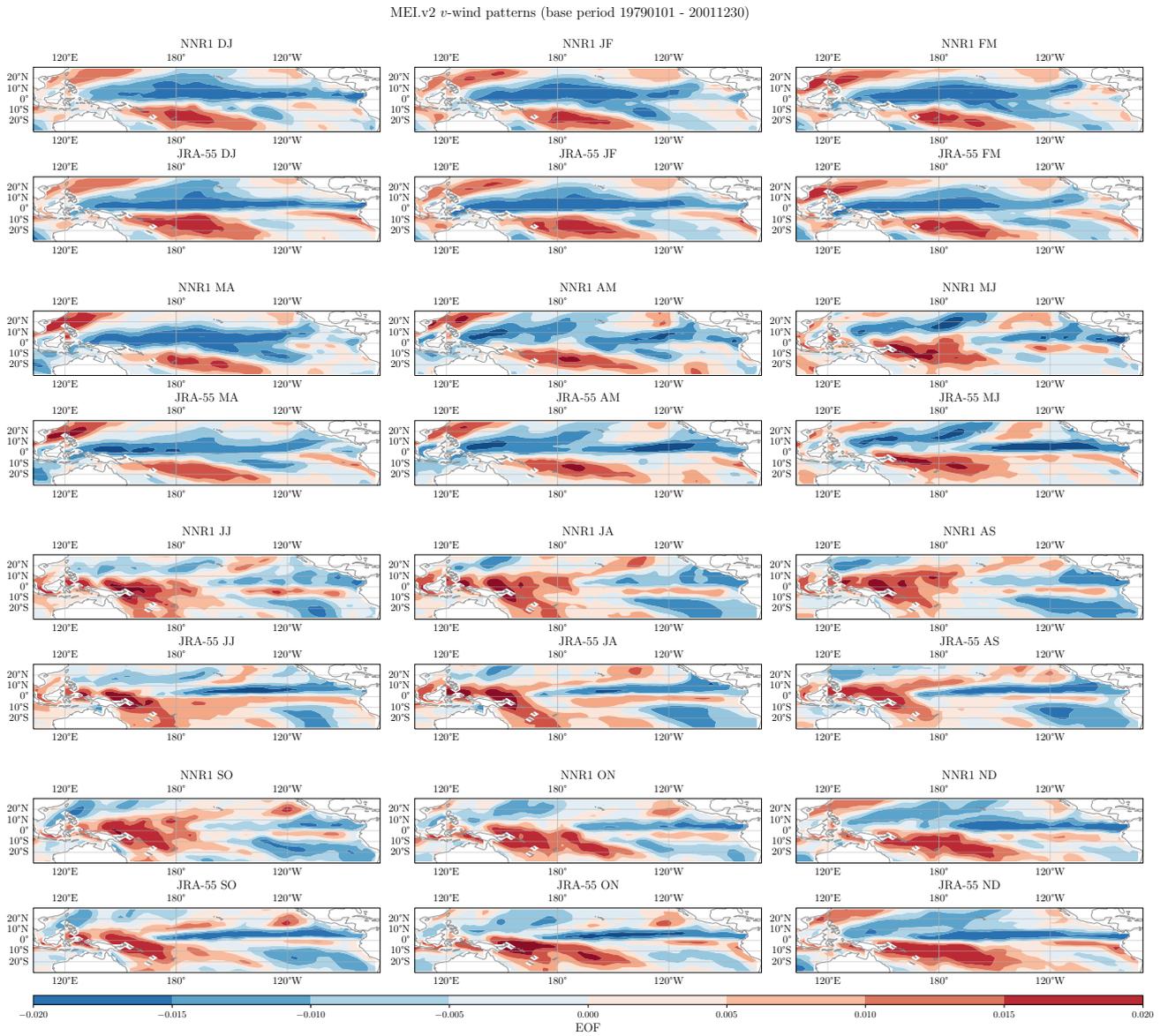


Figure S6. Seasonal meridional wind anomaly patterns contributing to the MEI in HadISST and NNR1 (odd numbered rows) and JRA-55 (even numbered rows).

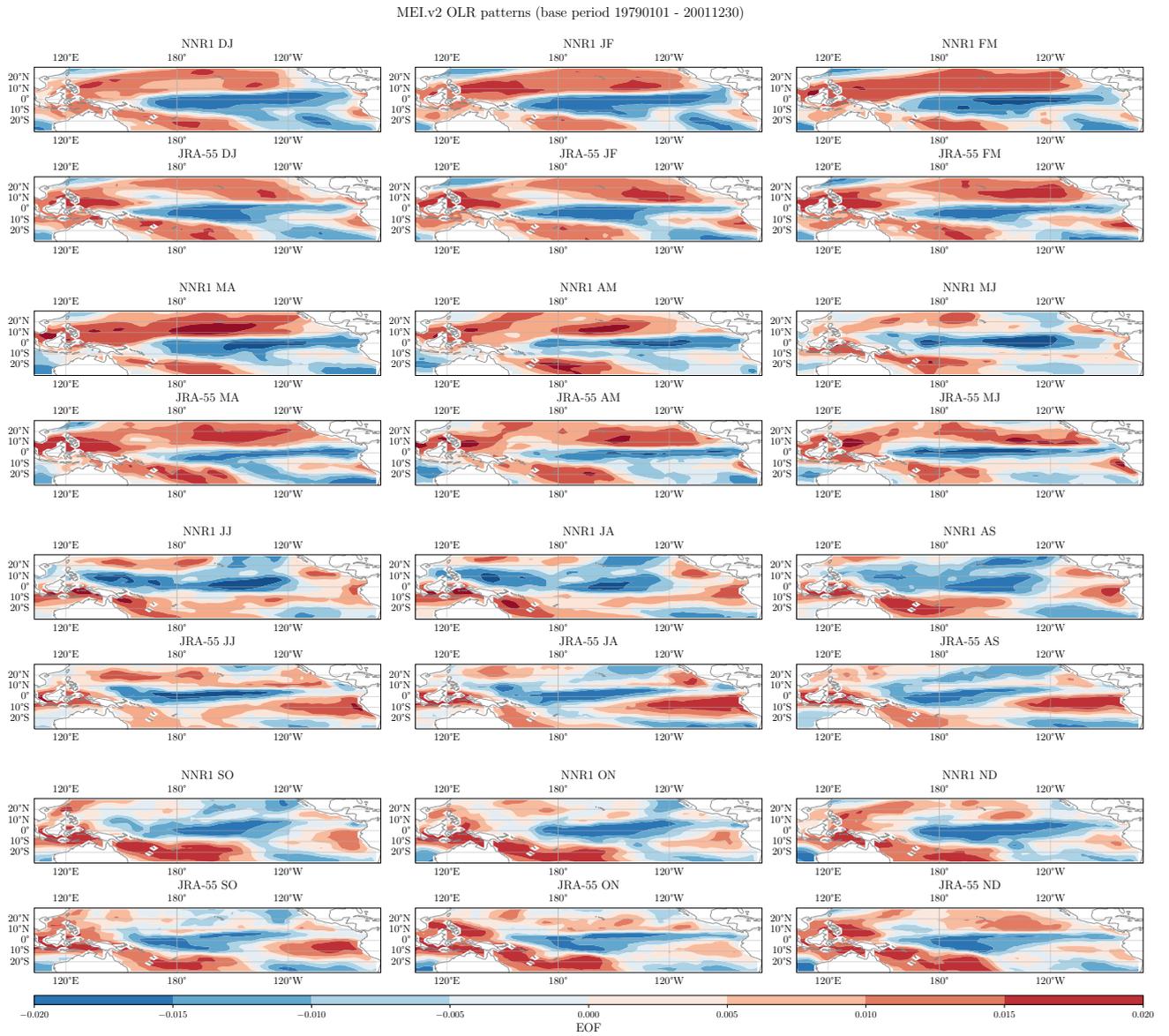
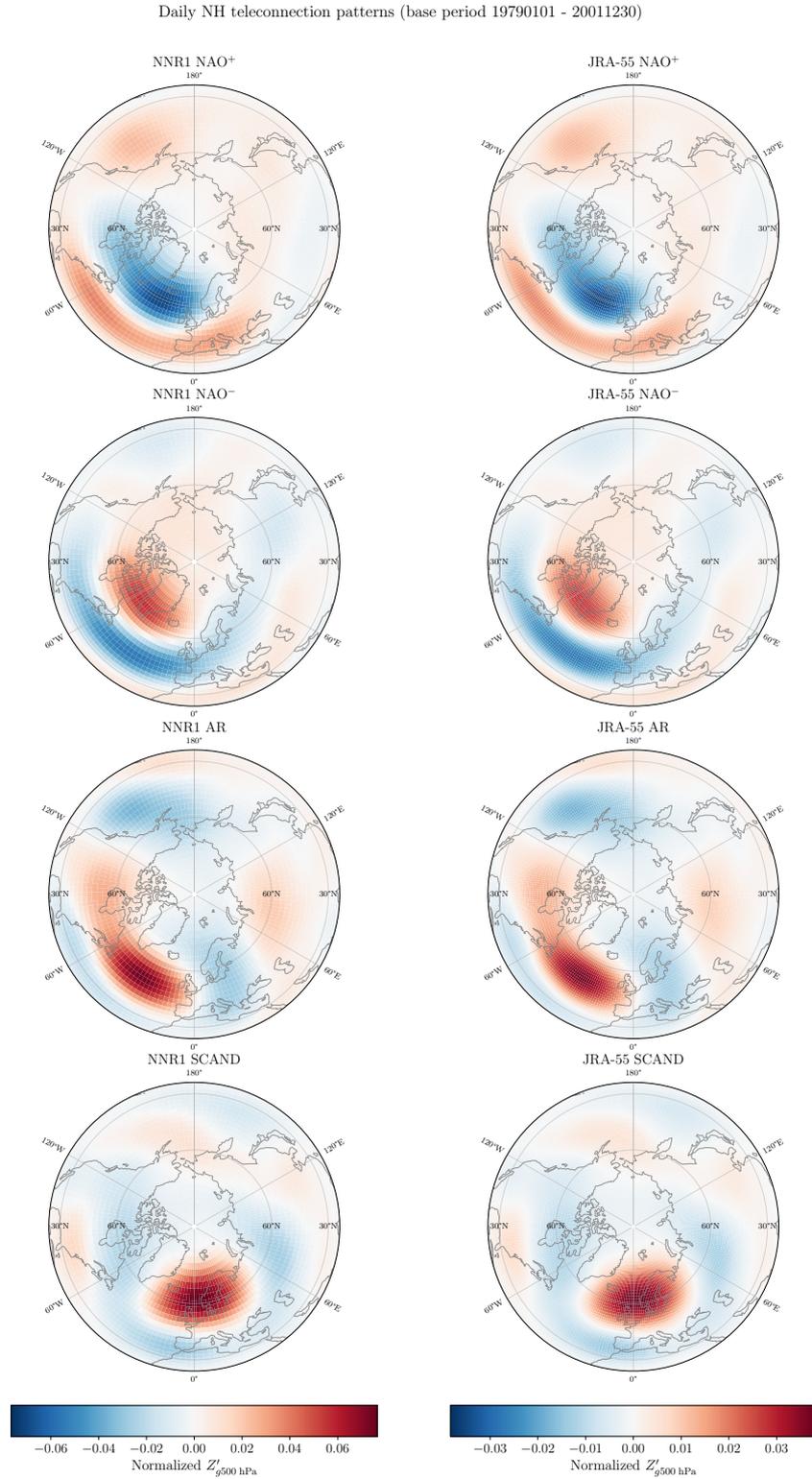


Figure S7. Seasonal OLR anomaly patterns contributing to the MEI in HadISST and NNR1 (odd numbered rows) and JRA-55 (even numbered rows).



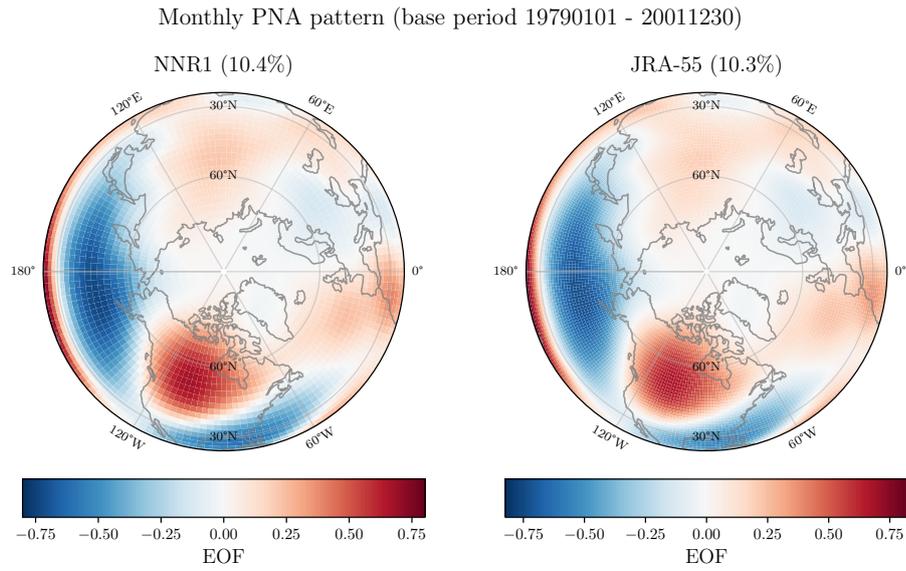


Figure S9. PNA loading pattern of 500 hPa geopotential height anomalies in NNR1 (left) and JRA-55 (right).

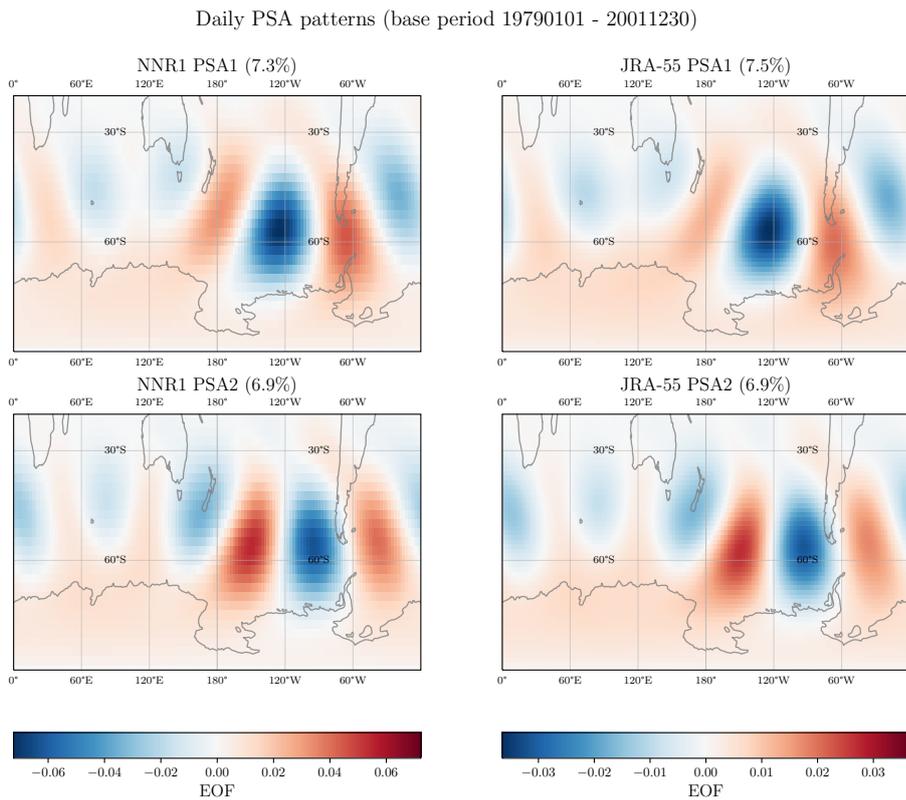


Figure S10. PSA loading patterns of 500 hPa geopotential height anomalies in NNR1 (left) and JRA-55 (right).

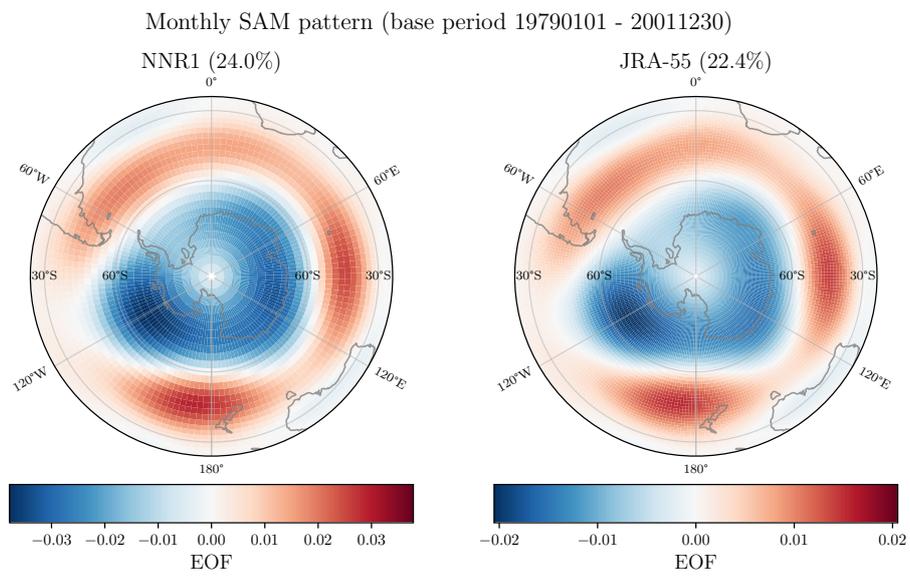


Figure S11. SAM loading pattern of 500 hPa geopotential height anomalies in NNR1 (left) and JRA-55 (right).

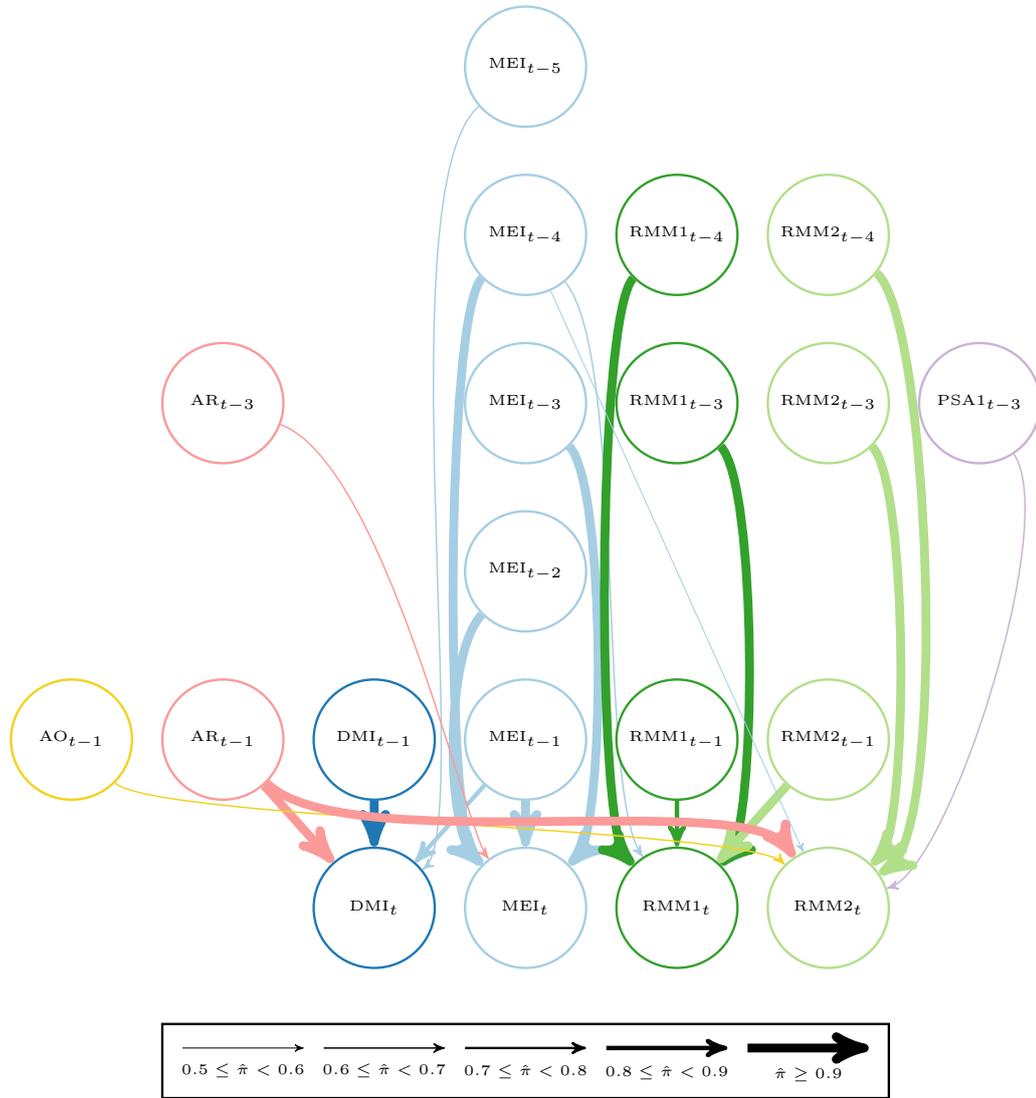


Figure S12. Subgraphs corresponding to the fitted parent sets of the tropical indices in NNR1 based on full-year data for $a_\tau = 0.5$, $b_\tau = 10$, and $\nu^2 \approx 2$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

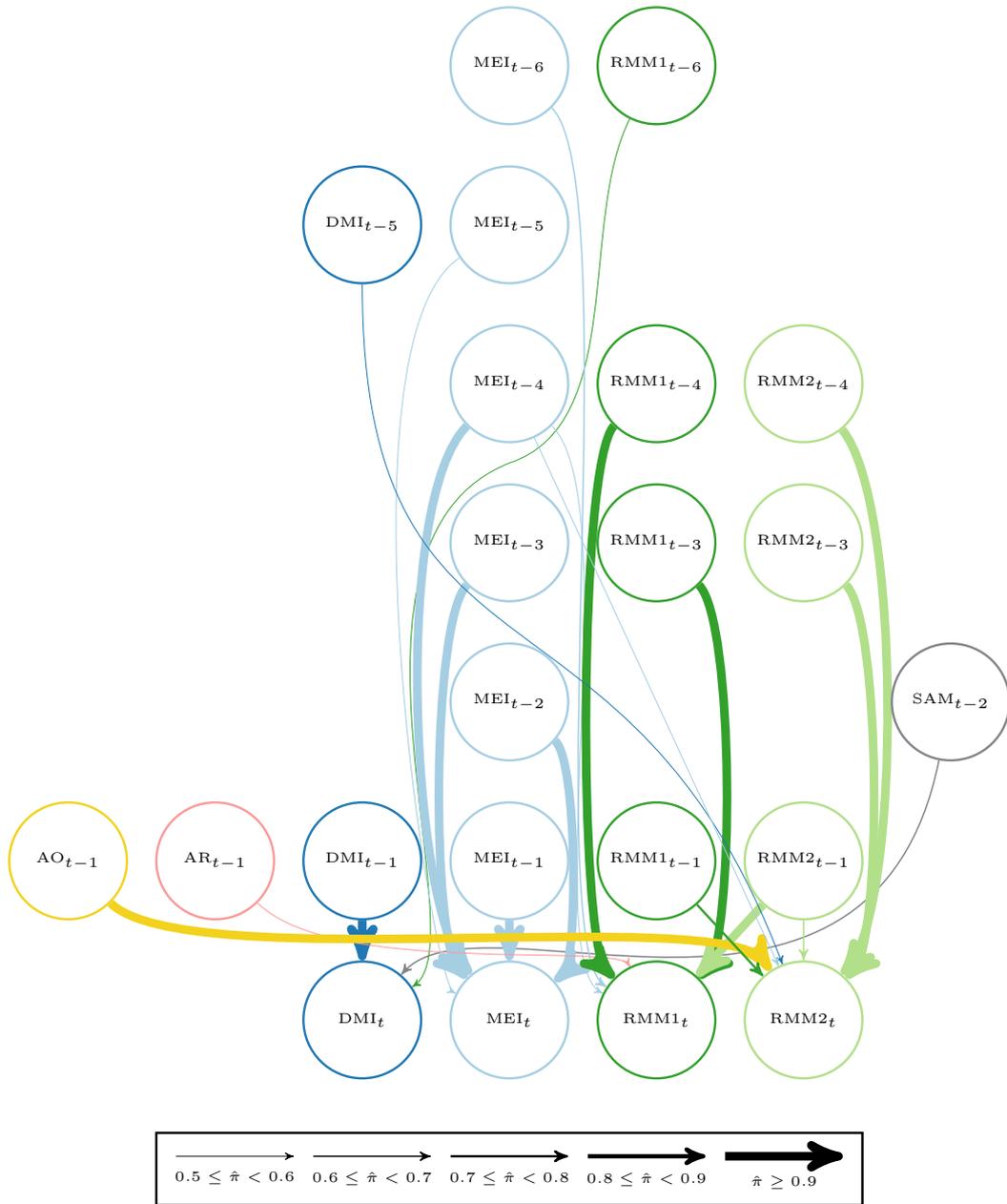


Figure S13. Subgraphs corresponding to the fitted parent sets of the tropical indices in JRA-55 based on full-year data for $a_\tau = 0.5$, $b_\tau = 10$, and $\nu^2 \approx 2$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

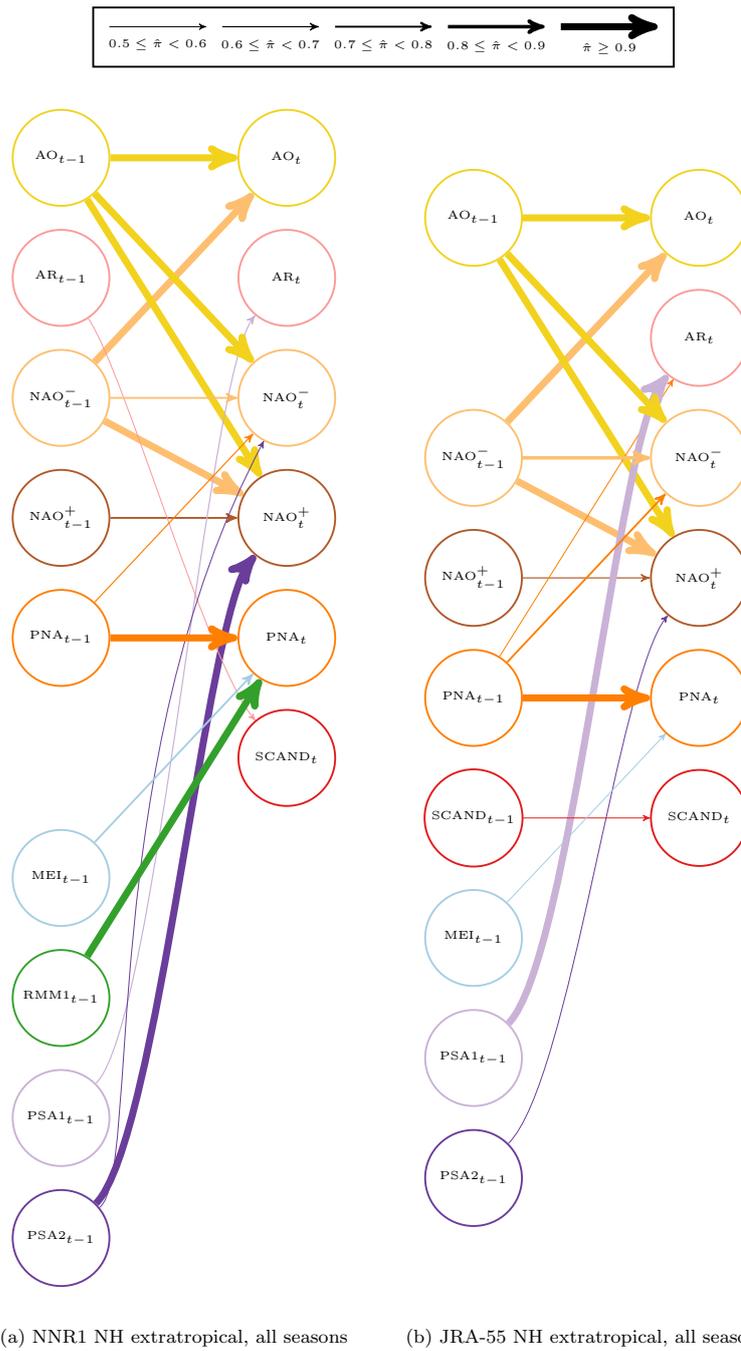


Figure S14. Subgraphs corresponding to the fitted parent sets of the NH extratropical indices in (a) NNR1 and (b) JRA-55 for $a_\tau = 0.5$, $b_\tau = 10$, and $\nu^2 \approx 2$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

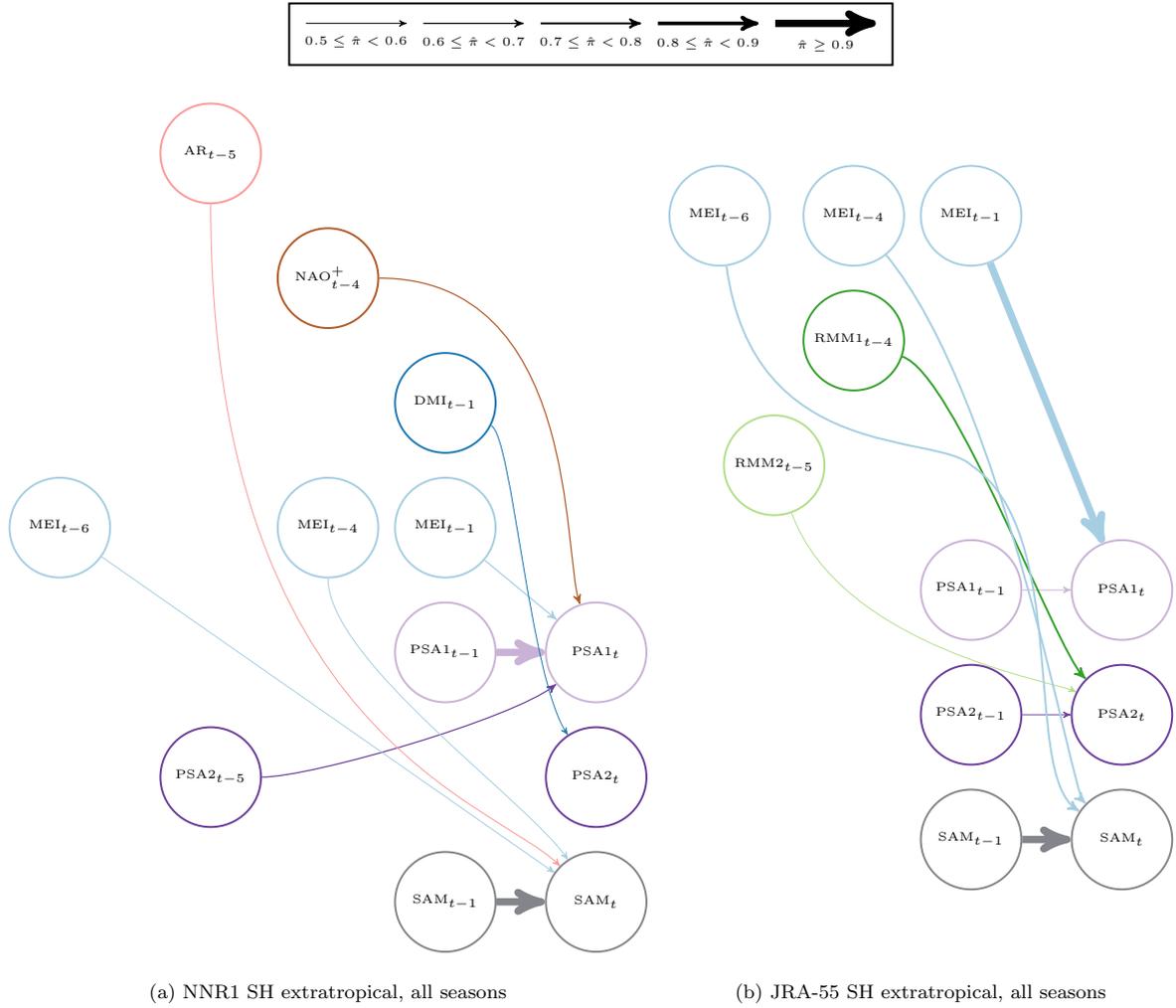


Figure S15. Subgraphs corresponding to the fitted parent sets of the SH extratropical indices in (a) NNR1 and (b) JRA-55 for $a_\tau = 0.5$, $b_\tau = 10$, and $\nu^2 \approx 2$. All edges with an estimated posterior probability $\hat{\pi}$ greater than 0.5 are shown.

Table S1. MAP parent sets for monthly tropical teleconnection indices across all seasons for NNR1 and JRA-55 for fits with $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$, showing the estimated posterior probability $\hat{\pi}$ of the edge, the mean parameter value $\hat{\beta}$ conditional on the MAP structure, and the 95% posterior HDI. Dashes indicate a node that is not in the MAP parent set for a given reanalysis.

Parent node	JRA-55			NNR1		
	$\hat{\pi}$	$\hat{\beta}$	95% HDI	$\hat{\pi}$	$\hat{\beta}$	95% HDI
DMI_t						
DMI _{t-1}	1.00	0.63	(0.56, 0.69)	1.00	0.74	(0.68, 0.79)
SAM _{t-2}	0.59	0.09	(0.03, 0.16)	0.33	—	—
MEI _{t-1}	0.22	—	—	0.80	0.13	(0.06, 0.20)
MEI _{t-5}	0.08	—	—	0.65	-0.14	(-0.21, -0.07)
AR _{t-1}	0.04	—	—	0.94	0.10	(0.05, 0.16)
MEI_t						
MEI _{t-1}	1.00	1.45	(1.37, 1.54)	1.00	1.43	(1.34, 1.51)
MEI _{t-2}	1.00	-0.85	(-1.00, -0.70)	1.00	-0.73	(-0.87, -0.59)
MEI _{t-3}	1.00	0.65	(0.49, 0.80)	1.00	0.38	(0.24, 0.52)
MEI _{t-4}	1.00	-0.48	(-0.63, -0.31)	0.98	-0.15	(-0.23, -0.07)
MEI _{t-5}	0.65	0.28	(0.13, 0.42)	0.17	—	—
MEI _{t-6}	0.57	-0.14	(-0.22, -0.06)	0.10	—	—
NAO ⁺ _{t-2}	0.38	0.04	(0.01, 0.06)	0.17	—	—
AO _{t-2}	0.06	—	—	0.46	0.05	(0.02, 0.07)
AR _{t-3}	0.05	—	—	0.66	-0.04	(-0.07, -0.02)
RMM2 _{t-3}	0.34	—	—	0.41	0.04	(0.01, 0.06)
RMM1_t						
MEI _{t-3}	0.47	-0.37	(-0.49, -0.24)	0.37	—	—
MEI _{t-6}	0.61	0.24	(0.13, 0.36)	0.33	—	—
AR _{t-1}	0.54	-0.12	(-0.20, -0.04)	0.24	—	—
PSA1 _{t-3}	0.38	-0.14	(-0.22, -0.05)	0.11	—	—
SAM _{t-3}	0.34	-0.13	(-0.20, -0.04)	0.09	—	—
RMM1 _{t-1}	0.40	-0.12	(-0.19, -0.04)	0.86	-0.14	(-0.21, -0.06)
RMM1 _{t-3}	0.99	-0.17	(-0.25, -0.09)	0.97	-0.16	(-0.24, -0.08)
RMM1 _{t-4}	1.00	-0.20	(-0.27, -0.12)	1.00	-0.19	(-0.27, -0.11)
RMM2 _{t-1}	0.99	-0.17	(-0.25, -0.09)	1.00	-0.20	(-0.27, -0.12)
MEI _{t-4}	0.58	—	—	0.59	-0.45	(-0.68, -0.22)
MEI _{t-5}	0.41	—	—	0.35	0.34	(0.11, 0.57)
RMM2_t						
AO _{t-1}	0.94	0.18	(0.10, 0.26)	0.63	0.15	(0.07, 0.23)
DMI _{t-5}	0.50	-0.12	(-0.20, -0.04)	0.06	—	—
MEI _{t-4}	0.56	-0.15	(-0.23, -0.07)	0.52	—	—
AR _{t-1}	0.44	0.13	(0.05, 0.21)	0.93	0.16	(0.08, 0.24)
RMM1 _{t-1}	0.71	0.13	(0.05, 0.21)	0.26	0.14	(0.06, 0.22)
RMM2 _{t-1}	0.61	-0.13	(-0.21, -0.05)	0.45	—	—
RMM2 _{t-3}	1.00	-0.24	(-0.32, -0.16)	0.98	-0.16	(-0.23, -0.08)
RMM2 _{t-4}	0.94	-0.17	(-0.25, -0.09)	0.94	-0.16	(-0.24, -0.09)
MEI _{t-1}	0.10	—	—	0.22	-0.18	(-0.26, -0.10)
AR _{t-6}	0.03	—	—	0.33	-0.11	(-0.19, -0.04)
PSA1 _{t-3}	0.05	—	—	0.59	-0.13	(-0.22, -0.05)
RMM1 _{t-5}	0.03	—	—	0.20	0.11	(0.03, 0.19)
RMM2 _{t-2}	0.02	—	—	0.16	0.13	(0.05, 0.20)

Table S2. MAP parent sets for monthly SH extratropical teleconnection indices across all seasons for NNR1 and JRA-55 for fits with $a_\tau = 1.5$, $b_\tau = 20$, and $\nu^2 = 3$, showing the estimated posterior probability $\hat{\pi}$ of the edge, the mean parameter value $\hat{\beta}$ conditional on the MAP structure, and the 95% posterior HDI. Dashes indicate a node that is not in the MAP parent set for a given reanalysis.

Parent node	JRA-55			NNR1		
	$\hat{\pi}$	$\hat{\beta}$	95% HDI	$\hat{\pi}$	$\hat{\beta}$	95% HDI
<u>PSA1_t</u>						
MEI _{t-1}	0.94	-0.15	(-0.23, -0.07)	0.68	-0.13	(-0.21, -0.05)
NAO ⁺ _{t-4}	0.39	-0.11	(-0.20, -0.04)	0.60	-0.13	(-0.21, -0.05)
PSA1 _{t-1}	0.49	0.12	(0.04, 0.21)	0.96	0.16	(0.08, 0.24)
PSA2 _{t-5}	0.17	-	-	0.58	-0.12	(-0.21, -0.04)
<u>PSA2_t</u>						
PSA1 _{t-4}	0.31	0.12	(0.03, 0.20)	0.30	-	-
PSA2 _{t-1}	0.49	0.12	(0.04, 0.21)	0.34	-	-
RMM1 _{t-4}	0.73	0.14	(0.05, 0.21)	0.43	-	-
RMM2 _{t-5}	0.47	0.12	(0.04, 0.20)	0.41	-	-
DMI _{t-1}	0.07	-	-	0.54	-0.14	(-0.23, -0.06)
<u>SAM_t</u>						
MEI _{t-4}	0.75	-0.30	(-0.45, -0.16)	0.51	-	-
MEI _{t-6}	0.76	0.27	(0.13, 0.42)	0.54	-	-
SAM _{t-1}	1.00	0.29	(0.21, 0.37)	1.00	0.32	(0.24, 0.40)