Supporting Information for "Quantifying Dynamical Proxy Potential through Oceanic Teleconnections in the North Atlantic"

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Uncertainty quantification in ocean state estimation. Ocean state estimation optimally 'fits' an ocean general circulation model to the available ocean observations, by adjusting a set of uncertain control variables, consisting of initial conditions, atmospheric forcing, and model parameters (green box in Fig. 1(c)). For the sake of a simpler notation, the control variables $F_m(x_i, y_j, t_k)$ inside the green box in Fig. 1(c) are flattened into a control vector $\mathbf{x} = (x_1, \dots, x_N)$, with each of the small green boxes illustrating one control variable x_i. The goal is to optimize $\mathbf{x} = (x_1, \dots, x_N)$ such as to minimize a least-squares cost function J (Wunsch, 1996; Tarantola, 2005). For the simple case of a single available observation, J takes the form

$$J(\mathbf{x}) = \frac{1}{2}\left(\frac{y - \mathrm{Obs}(\mathbf{x})}{\varepsilon}\right)^2 + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T\,\mathbf{B}\,(\mathbf{x} - \mathbf{x}_0). \tag{S.1}$$

The first term in eq. (S.1) measures the misfit between the observation y and the the observation counterpart, $\mathrm{Obs}(\mathbf{x})$, simulated by the model. The second term penalizes deviations from a first-guess $\mathbf{x}_0$. Observational noise and prior uncertainties are assumed to be Gaussian, with distributions $\mathcal{N}(0,\varepsilon^2)$ and $\mathcal{N}(\mathbf{x}_0,\mathbf{B})$.

The solution of the inverse problem is the minimizer of the cost function (S.1), $\mathbf{x}_{\min} = \min_{\mathbf{x}} J$. The posterior uncertainty in $\mathbf{x}_{\min}$ can be approximated by the Gaussian covariance matrix (Thacker, 1989; Bui-Thanh et al., 2012)

$$\mathbf{P} = \left(\varepsilon^{-2}\,(\nabla_{\mathbf{x}}\mathrm{Obs})\,(\nabla_{\mathbf{x}}\mathrm{Obs})^T + \mathbf{B}^{-1}\right)^{-1}, \tag{S.2}$$

with $\nabla_{\mathbf{x}}\mathrm{Obs} := \left[\frac{\partial\mathrm{Obs}}{\partial\mathbf{x}}_{|\mathbf{x}_{\min}}\right]^T$. The matrix $\mathbf{P}$ in eq. (S.2) is the inverse of the linearized Hessian matrix of J at $\mathbf{x}_{\min}$, which describes the curvature of the cost function (S.1). By means of the matrix inversion lemma, eq. (S.2) can be rewritten as

$$\mathbf{P} = \mathbf{B} - \left(\varepsilon^2 + \sigma^2_{\mathrm{Obs}}\right)^{-1}(\mathbf{B}\,\nabla_{\mathbf{x}}\mathrm{Obs})\,(\mathbf{B}\,\nabla_{\mathbf{x}}\mathrm{Obs})^T, \tag{S.3}$$

with $\sigma^2_{\mathrm{Obs}} = (\nabla_{\mathbf{x}}\mathrm{Obs})^T\,\mathbf{B}\,(\nabla_{\mathbf{x}}\mathrm{Obs})$. Eq. (S.3) describes uncertainty reduction in all control variables $\mathbf{x}$, which is achieved by the uncertainty propagation via the first two black arrows in Fig. 1(c), from the pink box to the green box. Eq. (S.3) phrases the posterior uncertainty $\mathbf{P}$ as the prior uncertainty $\mathbf{B}$, less any information obtained from the observation.

To assess uncertainty reduction in a QoI, the uncertainty propagation along the first two black arrows in Fig. 1(c) has to be followed by a subsequent uncertainty propagation along the last two black arrows, from the green box to the purple box. The subsequent propagation is achieved by projecting the prior and posterior error covariance matrices $\mathbf{B}$ and $\mathbf{P}$ onto the QoI, resulting in the prior variance $\sigma_{\mathrm{QoI}}^2 = (\nabla_{\mathbf{x}}\mathrm{QoI})^T\,\mathbf{B}\,(\nabla_{\mathbf{x}}\mathrm{QoI})$ and posterior variance $(\sigma_{\mathrm{QoI}}^{\mathbf{P}})^2 = (\nabla_{\mathbf{x}}\mathrm{QoI})^T\,\mathbf{P}\,(\nabla_{\mathbf{x}}\mathrm{QoI})$. The relative uncertainty reduction is given by

$$\tilde{\Delta}\sigma_{\mathrm{QoI}}^2 := \frac{\sigma_{\mathrm{QoI}}^2 - (\sigma_{\mathrm{QoI}}^{\mathbf{P}})^2}{\sigma_{\mathrm{QoI}}^2} \in [0,1]. \tag{S.4}$$

Due to the observational information that is propagated through the model dynamics, $(\sigma_{\mathrm{QoI}}^{\mathbf{P}})^2$ is smaller than σ_{QoI}^2, i.e., uncertainty gets reduced. $\tilde{\Delta}\sigma_{\mathrm{QoI}}^2 = 0$ represents the case $(\sigma_{\mathrm{QoI}}^{\mathbf{P}})^2 = \sigma_{\mathrm{QoI}}^2$, when the observation does not add any information for the QoI. The other extreme is $\tilde{\Delta}\sigma_{\mathrm{QoI}}^2 = 1$, which corresponds to $\sigma_{\mathrm{QoI}}^{\mathbf{P}} = 0$, i.e., a perfectly constrained QoI by the observation. By means of identity (S.3), relative uncertainty reduction in eq. (S.4) can be re-written as

$$\tilde{\Delta}\sigma_{\mathrm{QoI}}^2 = \left(\sigma_{\mathrm{QoI}}^2 \cdot (\varepsilon^2 + \sigma_{\mathrm{Obs}}^2)\right)^{-1} \left(\mathbf{B}^{1/2}\nabla_{\mathbf{x}}\mathrm{QoI} \bullet \mathbf{B}^{1/2}\nabla_{\mathbf{x}}\mathrm{Obs}\right)^2, \tag{S.5}$$

where $\mathbf{B}^{1/2}$ is the square root of the matrix $\mathbf{B}$, and $\bullet$ denotes the dot product of two vectors in $\mathbb{R}^N$. In the limit of vanishing observational noise $\varepsilon^2 \searrow 0$, the expression in eq. (S.5) converges to

$$\tilde{\Delta}\sigma_{\mathrm{QoI}}^2 \nearrow \left(\left[\sigma_{\mathrm{QoI}}^{-1}\,\mathbf{B}^{1/2}\nabla_{\mathbf{x}}\mathrm{QoI}\right] \bullet \left[\sigma_{\mathrm{Obs}}^{-1}\,\mathbf{B}^{1/2}\nabla_{\mathbf{x}}\mathrm{Obs}\right]\right)^2. \tag{S.6}$$

The limit in eq. (S.6) is equal to the definition of dynamical proxy potential (eq. (4)), if the prior covariance matrix $\mathbf{B}$ is diagonal.

References

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