Supporting Information for "Quantifying Dynamical Proxy Potential through Shared Adjustment Physics in the North Atlantic"

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Contents of this file

Additional Supporting Information (Files uploaded separately)

1. Captions for Movies S1 to S9

Text S1. Uncertainty Quantification in Ocean State Estimation. In ocean state estimation, one optimizes a vector of control variables, $\mathbf{x} = (x_1, \ldots, x_N)$, such as to minimize a least-squares cost function J (Tarantola, 2005; Wunsch, 1996). For the simple case of a single available observation, J takes the form

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

The first term in eq. (S.1), $J_{\text{misfit}}(\mathbf{x})$, measures the misfit between the observation y and the observation counterpart, $\text{Obs}(\mathbf{x})$, simulated by the model. The second term, $J_{\text{prior}}(\mathbf{x})$, 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), $\mathbf{x}_{\text{min}} = \min_{\mathbf{x}} J$. The posterior uncertainty in $\mathbf{x}_{\text{min}}$ can be approximated by the Gaussian covariance matrix (Bui-Thanh et al., 2012; Thacker, 1989),

$$\mathbf{P} = \Big(\underbrace{\varepsilon^{-2} \, (\nabla_{\mathbf{x}}\text{Obs}) \, (\nabla_{\mathbf{x}}\text{Obs})^T}_{=\mathbf{H}_{\text{misfit}}} + \mathbf{B}^{-1} \Big)^{-1}, \tag{S.2}$$

with $\nabla_{\mathbf{x}}\text{Obs} = [(\partial(\text{Obs})/\partial x_1)_{|\mathbf{x}_{\text{min}}}, \ldots, (\partial(\text{Obs})/\partial x_N)_{|\mathbf{x}_{\text{min}}}]^T$. The matrix $\mathbf{P}$ in eq. (S.2) is equal to $\mathbf{H}_J^{-1}$, the inverse of the linearized Hessian matrix of J at $\mathbf{x}_{\text{min}}$. The linearized Hessian $\mathbf{H}_J$, in turn, is the sum of two matrices: first, the misfit Hessian, $\mathbf{H}_{\text{misfit}}$, which as the linearized Hessian of the model-data misfit term J_{misfit} (eq. (S.1)) characterizes the observational constraints on the control variables; and second, $\mathbf{B}^{-1}$, which is the Hessian of the regularization term J_{prior} (eq. (S.1)).

By means of the matrix inversion lemma (e.g., Section 2.7.3 in Press et al., 2007), eq. (S.2) can be rewritten as

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

with $\sigma^2_{\text{Obs}} = (\nabla_{\mathbf{x}}\text{Obs})^T \, \mathbf{B} \, (\nabla_{\mathbf{x}}\text{Obs})$. 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 $\sigma^2_{\mathrm{QoI}} = (\nabla_{\mathbf{x}}\mathrm{QoI})^T \mathbf{B}\,(\nabla_{\mathbf{x}}\mathrm{QoI})$ and posterior variance $(\sigma^{\mathbf{P}}_{\mathrm{QoI}})^2 = (\nabla_{\mathbf{x}}\mathrm{QoI})^T \mathbf{P}\,(\nabla_{\mathbf{x}}\mathrm{QoI})$. The relative uncertainty reduction is given by

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

Due to the observational information that is propagated through the model dynamics, $(\sigma^{\mathbf{P}}_{\mathrm{QoI}})^2$ is smaller than σ^2_{QoI}, i.e., uncertainty gets reduced. $\tilde{\Delta}\sigma^2_{\mathrm{QoI}} = 0$ represents the case $(\sigma^{\mathbf{P}}_{\mathrm{QoI}})^2 = \sigma^2_{\mathrm{QoI}}$, when the observation does not add any information for the QoI. The other extreme is $\tilde{\Delta}\sigma^2_{\mathrm{QoI}} = 1$, which corresponds to $\sigma^{\mathbf{P}}_{\mathrm{QoI}} = 0$, 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

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

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, $\varepsilon^2 \searrow 0$, relative uncertainty reduction (i.e., the expression in eq. (S.5)) converges to

$$\tilde{\Delta}\sigma^2_{\mathrm{QoI}} \nearrow \Big(\underbrace{\left[\sigma^{-1}_{\mathrm{QoI}} \cdot \mathbf{B}^{1/2}\nabla_{\mathbf{x}}\mathrm{QoI}\right]}_{\mathbf{q}} \bullet \underbrace{\left[\sigma^{-1}_{\mathrm{Obs}} \cdot \mathbf{B}^{1/2}\nabla_{\mathbf{x}}\mathrm{Obs}\right]}_{\mathbf{v}}\Big)^2. \tag{S.6}$$

The limit in eq. (S.6) is equal to the definition of dynamical proxy potential (eq. (4)).

In the limit of vanishing observational noise, relative uncertainty reduction, $\tilde{\Delta}\sigma^2_{\mathrm{QoI}}$, is solely determined by the vectors $\mathbf{q}$ and $\mathbf{v}$ (eq. (S.6)). $\mathbf{q}$ is the direction of interest within the control space, i.e., the *information required* to recover the QoI. On the other hand, $\mathbf{v}$ is the eigenvector of the non-dimensionalized misfit Hessian, $\mathbf{B}^{1/2}\,\mathbf{H}_{\mathrm{misfit}}\,\mathbf{B}^{1/2}$ (cf. eq. (S.2)), and fully characterizes the *information captured* by the observation. (Note that in the case of only one observation, the misfit Hessian and the non-dimensionalized misfit Hessian are matrices of rank one.)

Movie S1. Time-evolving monthly mean anomaly in North Atlantic bottom pressure (normalized by density, p/ρ) in response to a positive northward wind stress anomaly of amplitude $0.05\,\mathrm{N/m^2}$ along the western African coast. The final five years of the ECCOv4r2 solution serve as our control simulation. The wind stress perturbation is imposed inside the green contour, and maintained over the full five-year time period. As for the time label, $t = 0$ corresponds to the (simultaneous) start of the simulation and perturbation. The black lines mark the contours of the 500 m, 1000 m, 1500 m, 2000 m, 3500 m, 4000 m, 4500 m, and 5000 m isobaths. Time averaging of the monthly mean anomalies shown in this movie (over the full five-year time period) generates Fig. 5(a).

Movie S2. As Movie S1, but anomaly in the barotropic stream function. Negative values indicate anomalous counterclockwise rotation.

Movie S3. As Movie S1, but anomaly in North Atlantic potential temperature at 300 m depth. The black line marks the 300 m depth contour. Time averaging of the monthly mean anomalies shown in this movie generates Fig. 5(c).

Movie S4. As Movie S3, but anomaly in potential temperature along the trans-Atlantic section at 41 °N, in longitude-depth space. The green circle marks the location of θ^B. Baroclinic Rossby waves propagate a positive temperature anomaly from the eastern boundary westward.

Movie S5. As Movie S4, but anomaly in vertical velocity along the trans-Atlantic section at 15 °N. The green bar marks the longitudinal extent (20 °W - 17 °W) of the imposed northward wind stress anomaly (whose latitudinal extent is 10 °N - 20 °N). Ekman convergence/pumping occurs to the east of the wind stress anomaly, and Ekman divergence/suction to the west of the wind stress anomaly. Maintenance of the wind stress anomaly locks this vertical velocity dipole in place.

Movie S6. As Movie S5, but anomaly in potential temperature. Ekman pumping to the east of the wind stress anomaly (Movie S5) creates warming, while Ekman suction to the west (Movie S5) creates cooling. The negative thickness anomaly associated with shoaling of the thermocline (and cooling) to the west is propagated into the interior by baroclinic Rossby waves. Note that the positive thickness anomaly associated with deepening of the thermocline (and warming) to the east propagates northward along the North Atlantic boundary and then into the interior, once it is past the latitude band in which the wind anomaly is applied (Movies S3 and S4).

Movie S7. As Movie S1, but anomaly in response to a positive northward wind stress anomaly along the western Icelandic coast, imposed inside the green contour. Time averaging of the monthly mean anomalies shown in this movie generates Fig. 5(b).

Movie S8. As Movie S2, but anomaly in response to a positive northward wind stress anomaly along the western Icelandic coast, imposed inside the green contour.

Movie S9. As Movie S3, but anomaly in response to a positive northward wind stress anomaly along the western Icelandic coast, imposed inside the green contour. Time averaging of the monthly mean anomalies shown in this movie generates Fig. 5(d).

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