LOCALIZATION OF THE ENSEMBLE COVARIANCES USING THE DIFFUSION OPERATOR APPROACH

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MOTIVATION

1. **Schur product of the ensemble covariance with heuristic localization functions**
   + computaionally cheap
   - flow dependnce, positive definiteness

2. **Enriching the ensemble with Schur cross-products of the ensemble members (Bishop and Hodyss, 2007)**
   - computationally expensive
   + flow dependence, positive definiteness

3. **Approximating the ensemble covariance with a positive function of the diffusion operator**
   computationally inexpensive
   flow dependence, positive definiteness

OBJECTIVE: explore (3) and compare it with (1-2) in terms of accuracy/computational cost in a realistic setting

OUTLINE

1. The diffusion operator technique
   a. Gaussian and spline models
   b. Differential method
   c. Integral method

2. Experimental setting and comparison with adaptive and non-adaptive methods
   a. Diffusion tensor model
   b. Ensemble generation and error metrics
   c. Accuracy
   d. Computational efficiency

3. Summary

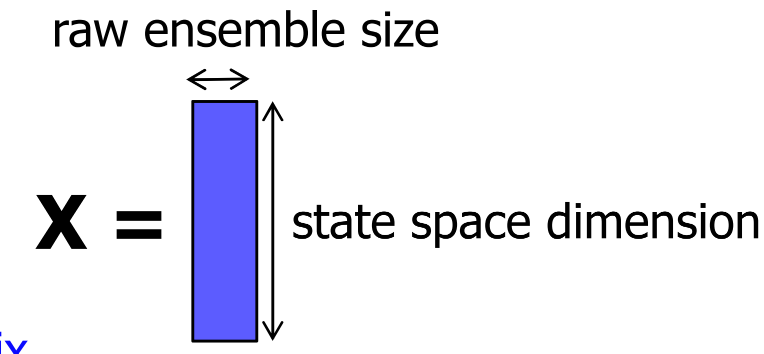
Localization methods (1)

$$\mathbf{B} \equiv \mathrm{cov}\{\mathbf{x}_k\} = \mathbf{X}\mathbf{X}^{\mathsf{T}}$$

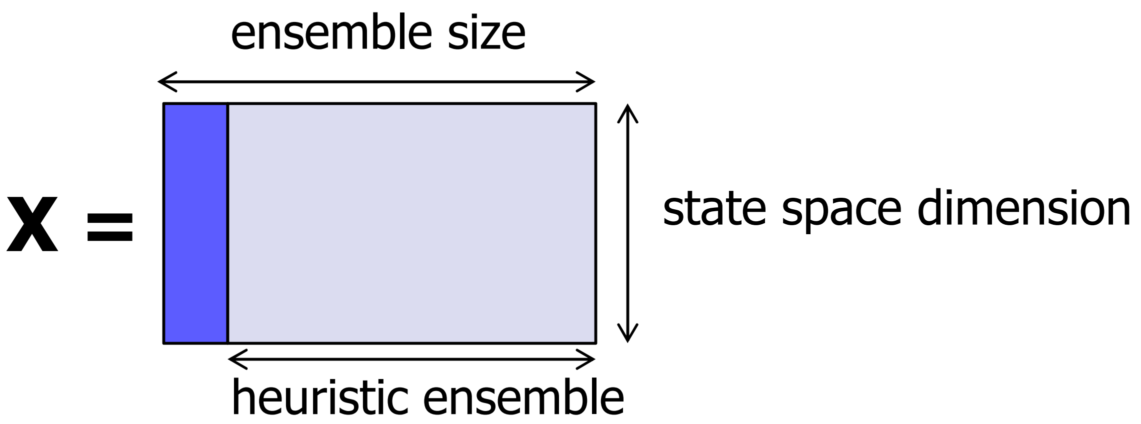
$$\mathbf{B}_\ell = \mathbf{B} \circ \mathbf{W}_d$$

localization matrix

$$\mathbf{B}_\ell = \mathbf{V}\mathbf{C}_\ell\mathbf{V}$$



adaptive



Diffusion operator (DO) approach

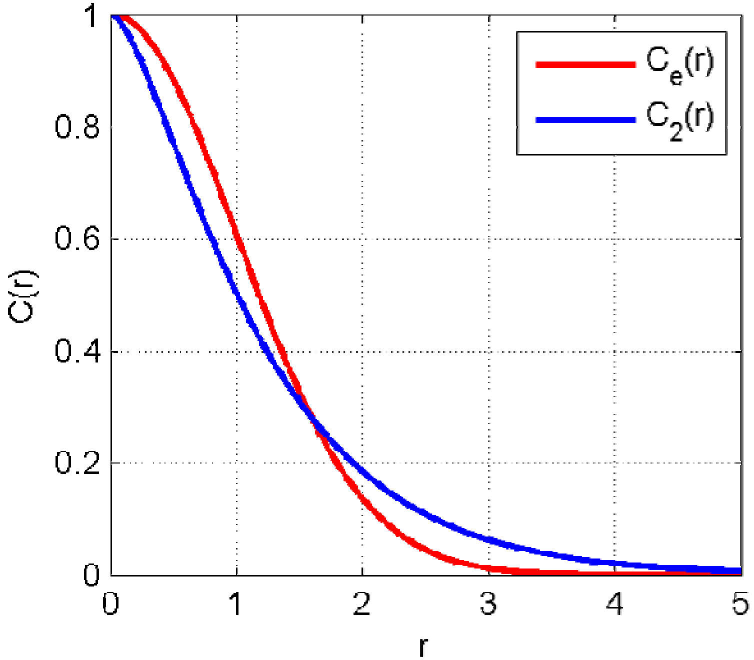
$$\mathbf{B}_\ell = \mathbf{V}\boxed{\mathbf{C}_\ell \circ \mathbf{W}_d}\mathbf{V}$$

$$\mathbf{D} = -\nabla_\alpha D^{\alpha\beta}\nabla_\beta$$

Gauss: $F_e\{\mathbf{D}\} \;=\; \exp(-\frac{\mathbf{D}}{2})$ $\quad\rightarrow\quad$ $\mathbf{C}^e_\ell(\boldsymbol{r}) \;=\; \exp\left(-\frac{r^2}{2}\right)$

Spline: $F_n\{\mathbf{D}\} \;=\; (\mathbf{I} + \frac{\mathbf{D}}{2n})^{-n}$ $\quad\rightarrow\quad$ $\mathbf{C}^n_\ell(\boldsymbol{r}) \;=\; \frac{(\sqrt{2n}r)^{n-1}\mathcal{K}_{n-1}(\sqrt{2n}r)}{2^{n-2}(n-2)!}$

$$\boldsymbol{r}^2 = r^\alpha D^{-1}_{\alpha\beta} r^\beta; \quad \boldsymbol{r} = \boldsymbol{x} - \boldsymbol{y}$$



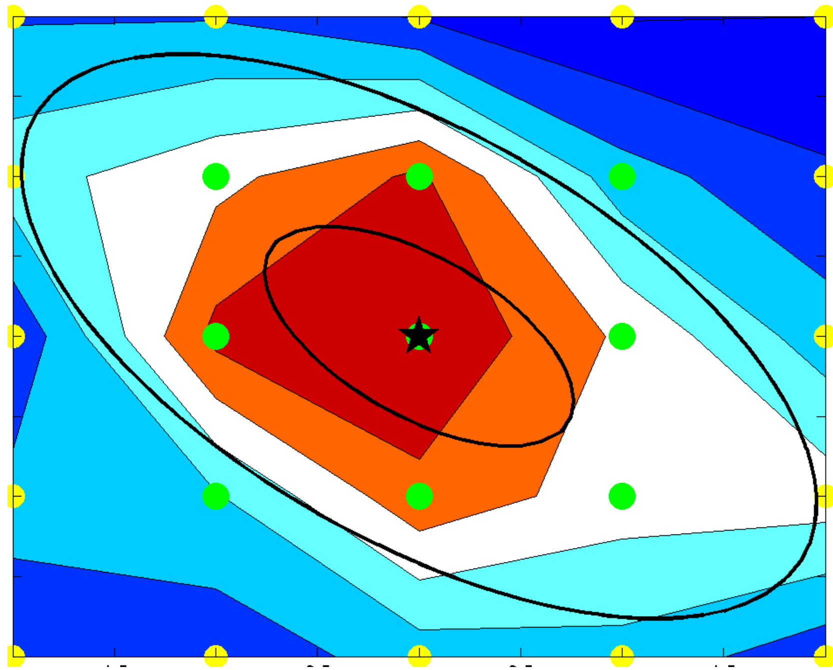
DO approach: differential method

$$D_{\alpha\beta}^{-1} = -\frac{1}{a}\nabla_\alpha \nabla_\beta C(r) \qquad a = \lim_{r\to 0} \frac{1}{r}\frac{\partial C}{\partial r}$$

$$a^e = 1 \qquad a^n = 1 - \frac{2}{n}$$

$$[\nabla_\alpha \nabla_\beta \mathbf{C}] = \frac{\langle (\nabla_\alpha \mathbf{x}) \circ (\nabla_\beta \mathbf{x}) \rangle - (\nabla_\alpha \mathbf{v}) \circ (\nabla_\beta \mathbf{v})}{\mathbf{v} \circ \mathbf{v}}$$

Estimate the inverse of D from the curvature of the sample correlation matrix at the diagonal



DO approach: integral method

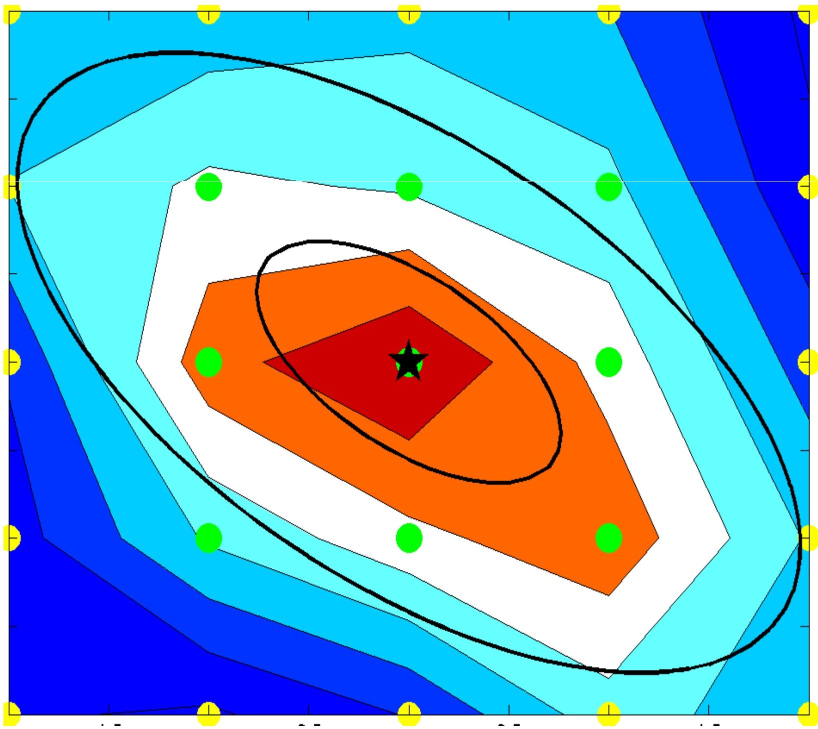
$$\boxed{J(\boldsymbol{x}) = \int\limits_{\omega} \left(\mathbf{C}_\ell(\boldsymbol{x}-\boldsymbol{y}) - \tilde{\mathbf{C}}(\boldsymbol{x},\boldsymbol{y}) \right)^2 d\boldsymbol{y} \to \min_{\boldsymbol{D}(\boldsymbol{x})}}$$

$$\mathbf{C}_\ell^e(\boldsymbol{r}) = \exp\left(-\frac{r^2}{2}\right)$$

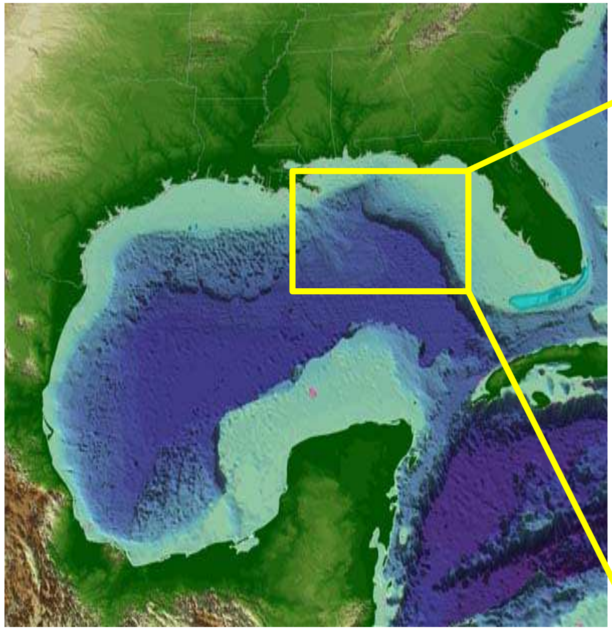
$$\mathbf{C}_\ell^n(\boldsymbol{r}) = \frac{(\sqrt{2n}r)^{n-1}\mathcal{K}_{n-1}(\sqrt{2n}r)}{2^{n-2}(n-2)!}$$

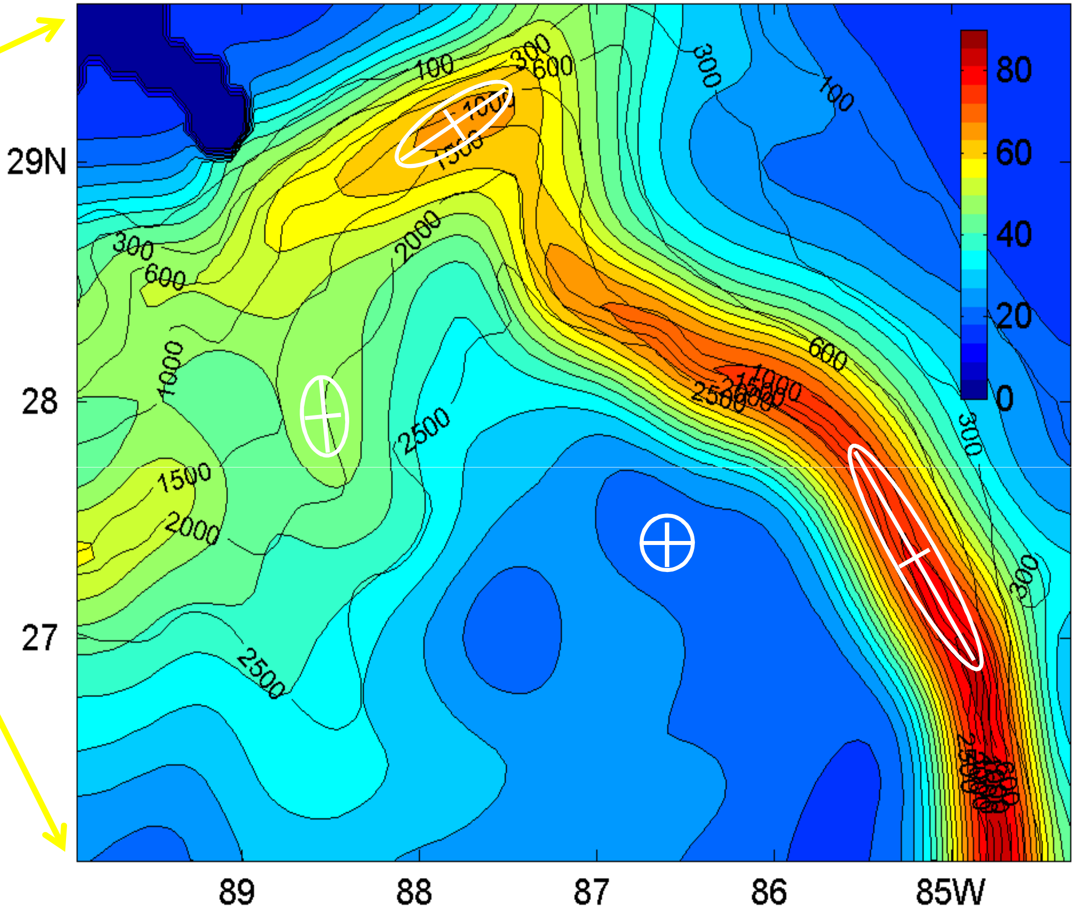
$$\boldsymbol{r}^2 = r^\alpha D^{-1}_{\alpha\beta} r^\beta; \quad \boldsymbol{r} = \boldsymbol{x} - \boldsymbol{y}$$

Estimate D by minimizing the misfit between the sample correlation matrix and its analytic approximation in the given vicinity ω of the diagonal



Diffusion tensor model



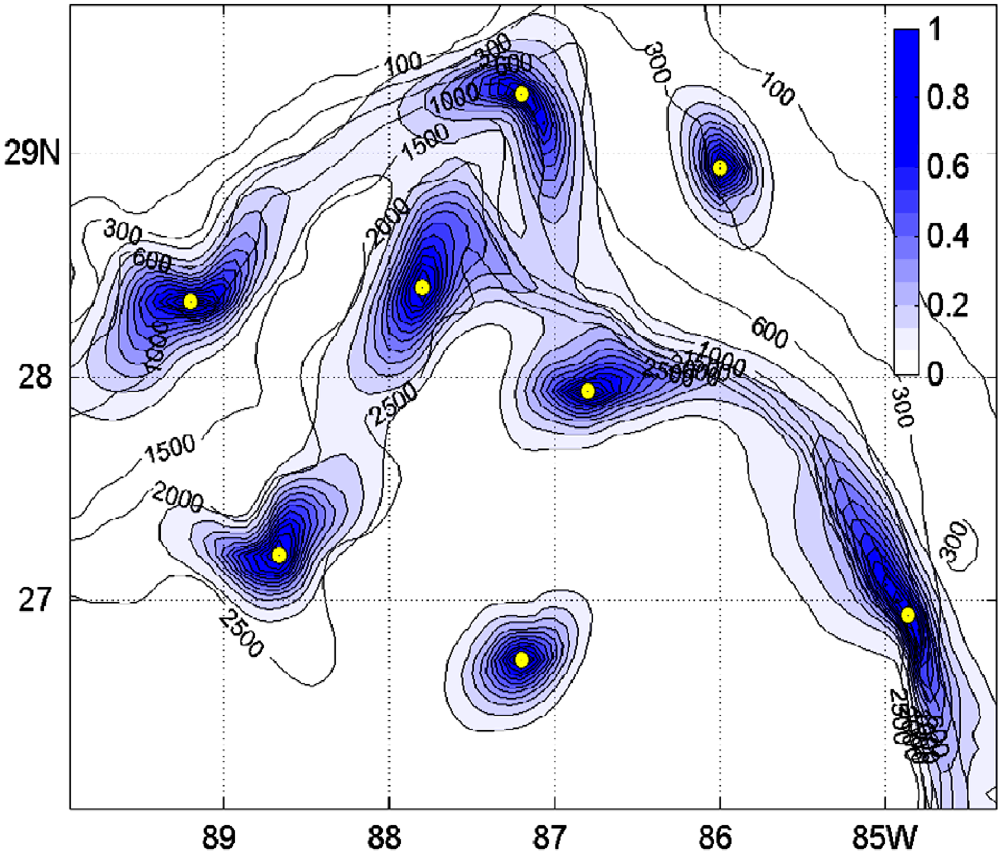


$$\mathbf{D} = \nabla_\alpha D^{\alpha\beta} \nabla_\beta \qquad D = K^{\mathsf{T}} K$$

$$K = \rho_b \begin{pmatrix} \xi & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{pmatrix}$$

$$\xi = \max(1, \sqrt{|\mathbf{u}\tau| / \rho_b}) \qquad \tan\gamma = \frac{v}{u}\,\theta(|\mathbf{u}\tau| - \rho_b)$$

Ensemble generation



true correlation (spline model)

$$\exp(-\frac{\mathbf{D}}{2})\mathbf{x} \simeq \left(\mathbf{I} - \frac{\mathbf{D}}{2n}\right)^n \mathbf{x}$$

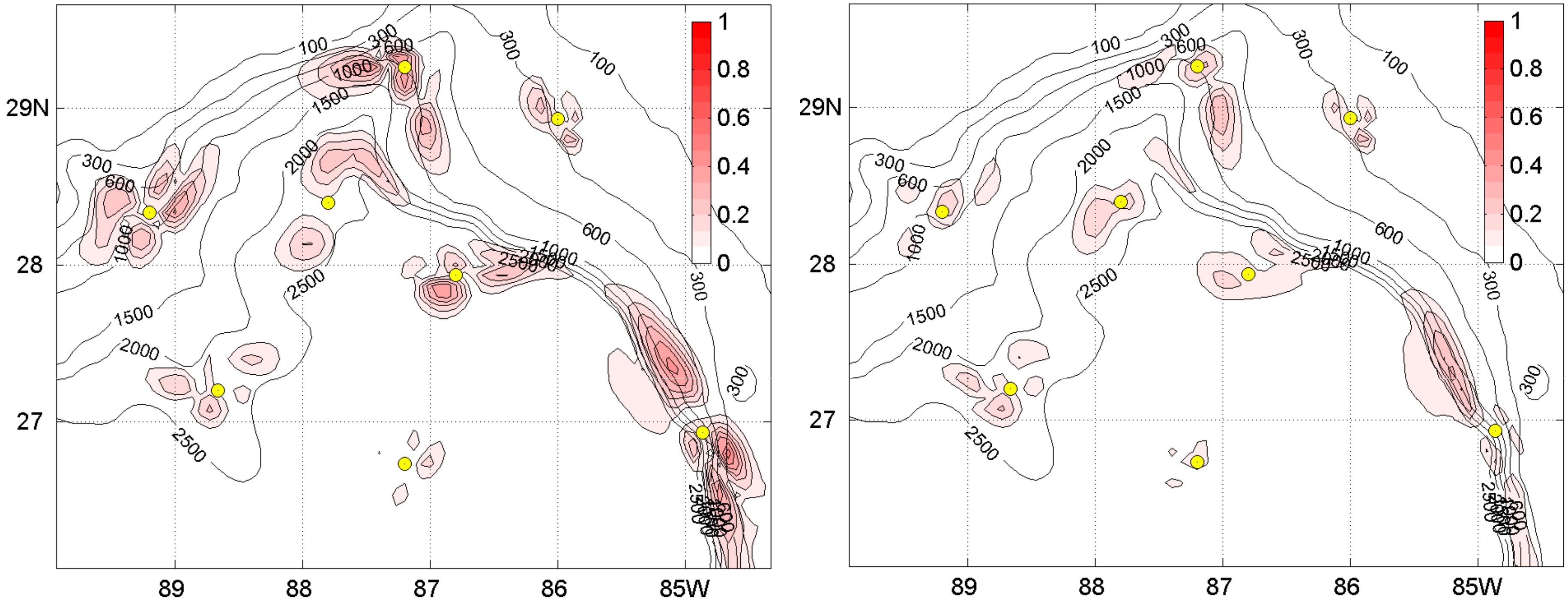
$$\mathbf{C}_\ell^e = (\mathrm{diag}\,\mathbf{c})^{-1/2} \exp((-\frac{1}{2}\mathbf{D})(\mathrm{diag}\,\mathbf{c})^{-1/2}$$

$$\mathbf{c} = (2\pi)^{-1} \exp(-\frac{1}{6}\mathbf{D})(\det \boldsymbol{D})^{-1/2}$$

$$\mathbf{X}_e = \mathbf{V}\mathbf{C}_e^{1/2}\mathbf{R}$$

X = (20,000 × 4,603)

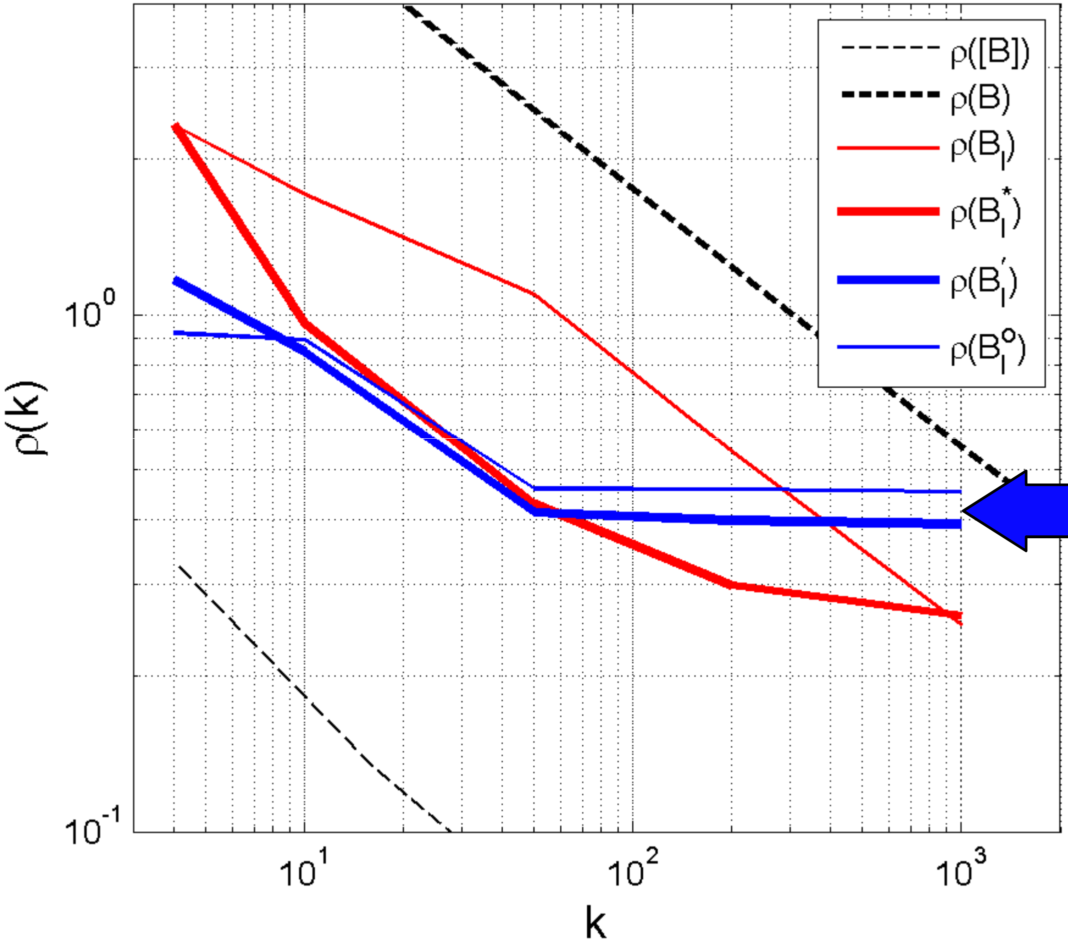
Error mertrics



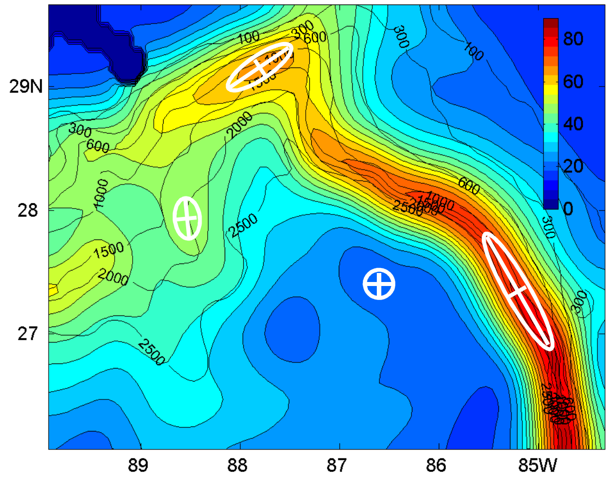
differential method **integral method**

$$\rho(\mathbf{B}_\ell, \mathbf{B}) = \sqrt{\frac{|\mathbf{B}_\ell - \mathbf{B}|}{|\mathbf{B}|}}$$

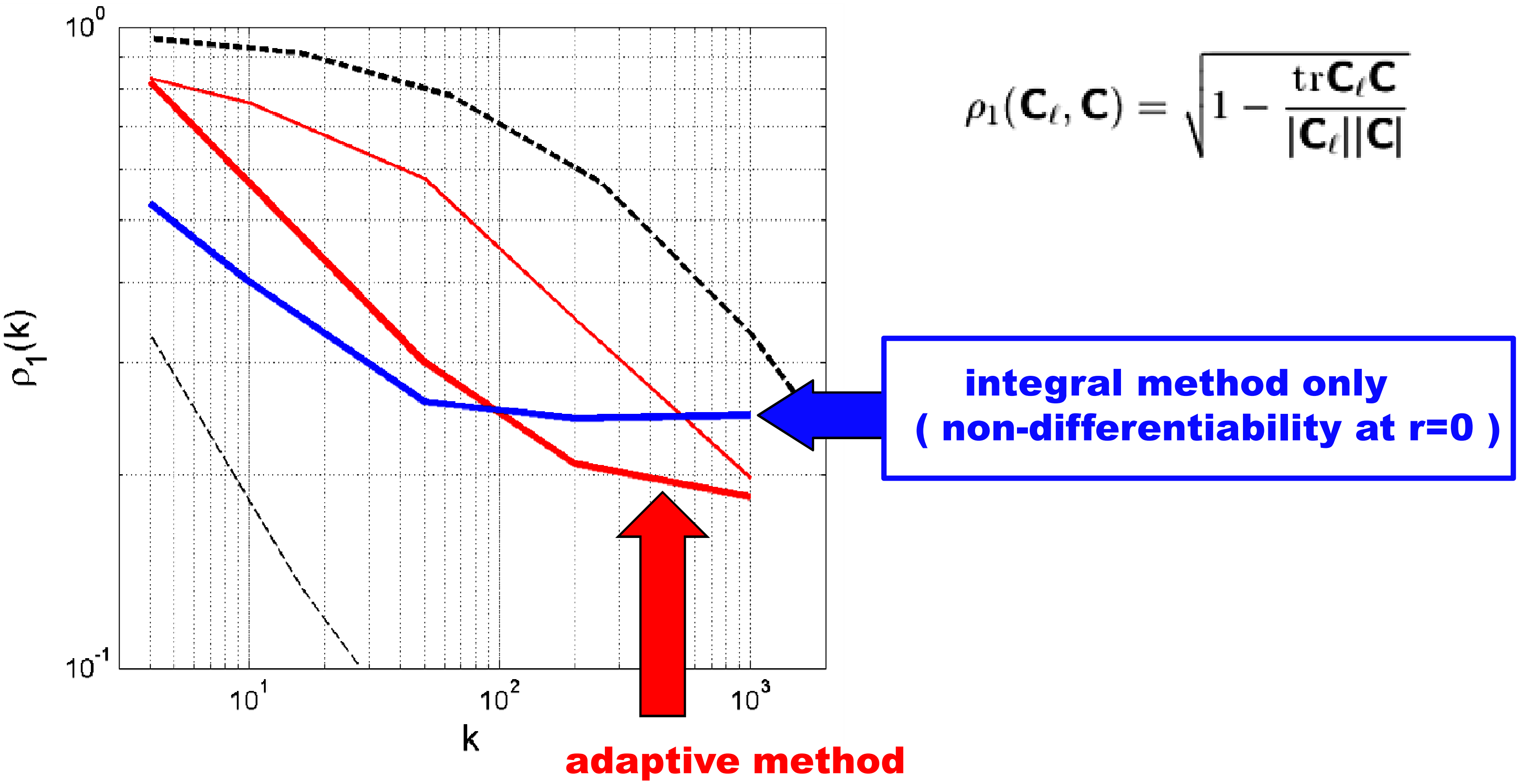
Accuracy: Gaussian model



saturation imposed by violation of local homogeneity

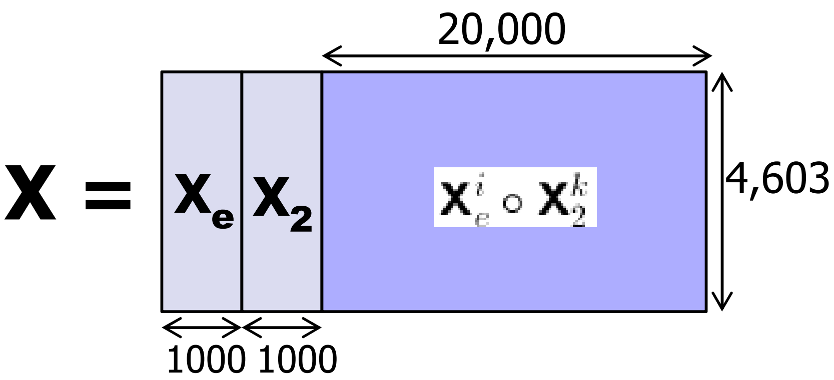


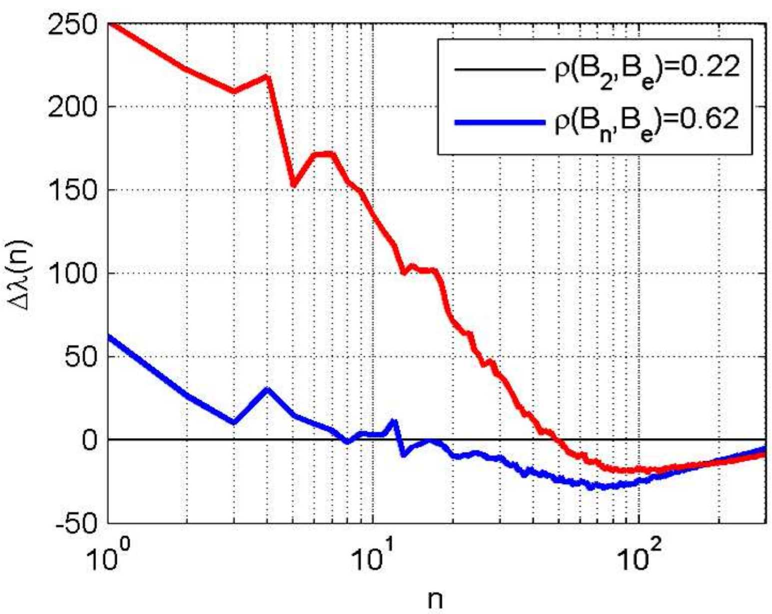
Accuracy: spline model

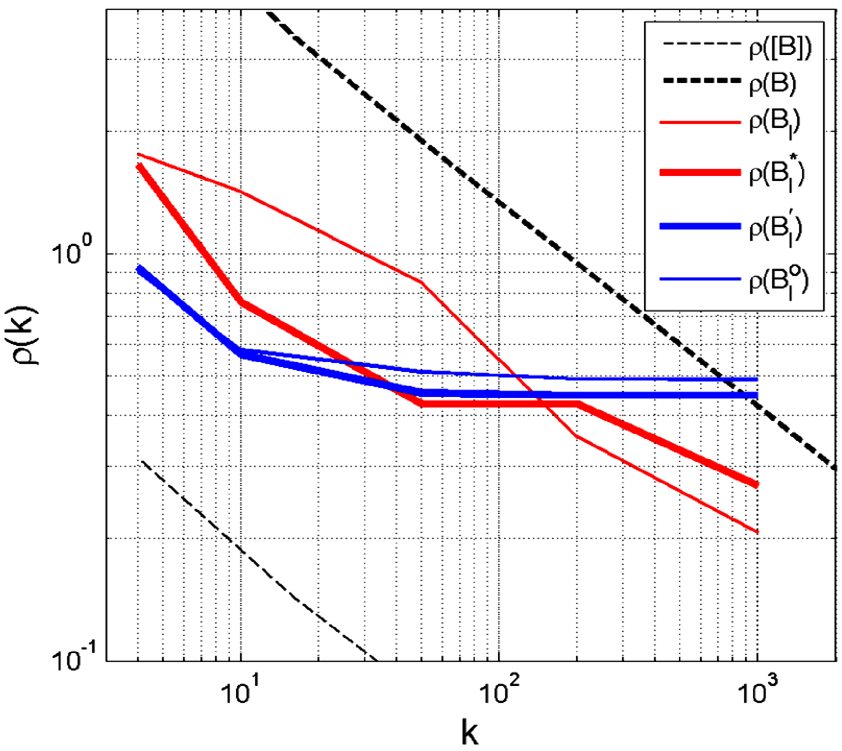


$$\rho_1(\mathbf{C}_\ell, \mathbf{C}) = \sqrt{1 - \frac{\mathrm{tr}\,\mathbf{C}_\ell \mathbf{C}}{|\mathbf{C}_\ell||\mathbf{C}|}}$$

Accuracy: synthetic model







Computational cost

$$M \simeq n_s k N$$

$$M^* \simeq n_s k N J$$

$$M' \simeq n_s k N (0.2 + \frac{1}{k} + \frac{m}{5k})$$

$$M^\circ \simeq n_s k N (0.5 + \frac{2}{k} + \frac{m}{5k})$$

$m \sim 10^2 - 10^3$ **B-iterations (DO methods)**

$k \sim 10^2$ **ensemble size**

$N \sim 10^6 - 10^7$ **state space dimension**

$n_s \sim 50$ **correlation stencil size**

cost relative to the non-adaptive scheme

$$\boxed{M^*/M = J \qquad M'/M = 0.2(1+\frac{m}{k}) \qquad M^\circ/M = 0.5(2.5+\frac{m}{k})}$$

Summary

Accuracy and computational cost of the DO-based covariance localization methods have been tested

1. **An integral DO method has been proposed**
2. **DO methods demonstrate better accuracy at ensemble sizes less than one hundred.**
3. **At larger ensemble sizes the accuracy of DO methods is limited by the violation of the local homogeneity assumption in realistic applications.**
4. **Integral method is more accurate, but 1.5-3 times more computationally expensive than the differential method.**
5. **DO localization methods are more computationally efficient than the adaptive method while providing similar accuracies at $K < 100$.**

These features indicate that DO localization methods could be tested with larger problems emerging in real applications

Appendix

$$\boxed{R_{ik} = -\left(\frac{1}{r}\frac{\partial C}{\partial r}\right)^{-1}_{r=0} \nabla_i \nabla_k C}$$

$$r^2 := x^i R_{ik} x^k$$

$$\nabla_i \nabla_k C = \frac{C_r}{r} R_{ik} + \left(C_{rr} - \frac{C_r}{r}\right) \frac{1}{r^2} R_{ij} x^j R_{km} x^m$$

$$C(r) = (2\pi)^{-n} \int_{\mathrm{R}^n} C(\boldsymbol{k}) \exp(-i\boldsymbol{k}\boldsymbol{x}) d\boldsymbol{k} \simeq \int_0^\infty C(k) k^{n/2} \frac{J_{n/2-1}(kr)}{r^{n/2-1}} dk$$

$$\left[\frac{\partial^2 C}{\partial r^2} - \frac{1}{r}\frac{\partial C}{\partial r}\right]_{r=0} = 0$$