Ensemble Sensitivity Analysis: Applications and Challenges

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Ensemble sensitivity analysis (ESA)

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How does the change in a set of initial state variables x_s change a forecast metric J?

$$\frac{\partial J_e}{\partial x^a}$$

- Identify dynamically relevant covariance structures in space and time
- Propose observing strategies for mesoscale, short-range forecasts in complex terrain
- Sensitivity scales (time and space) to infer predictability scales
- Predictability of specific phenomena
- Open issues:
  - Sampling error
  - Linearity assumptions in complex terrain

Ensemble Sensitivity Background

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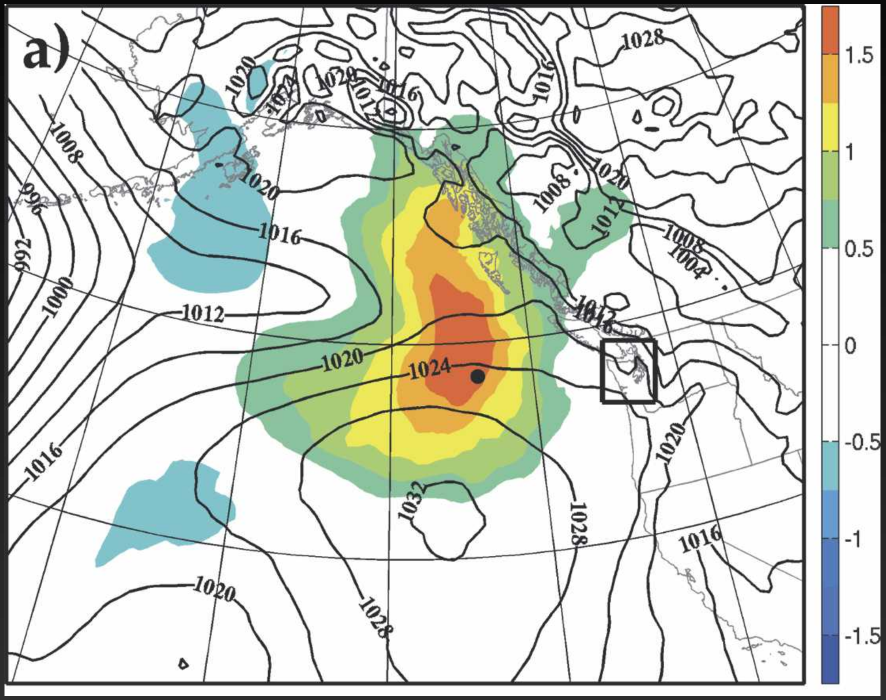
- Ancell and Hakim (2007) showed theoretical equivalence between adjoint and ensemble sensitivity for linear perturbations and Gaussian statistics
- Relies on linearization about an ensemble-mean trajectory
- Rigorous application has so far been limited to large-scale (smooth) and integrated processes where strong linear relationships are more likely

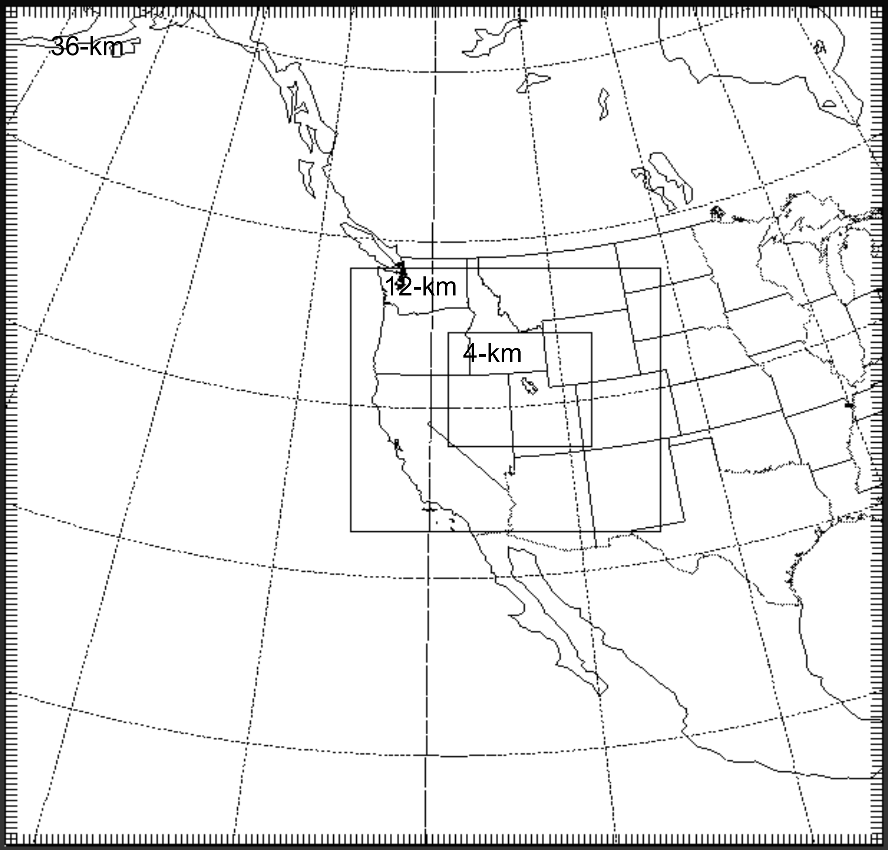
An optimal ensemble data assimilation system provides an appropriate sample



Sensitivity of 24-h sea-level pressure (SLP) over western Washington to SLP initial conditions, and ensemble-mean SLP (from Torn and Hakim 2008).

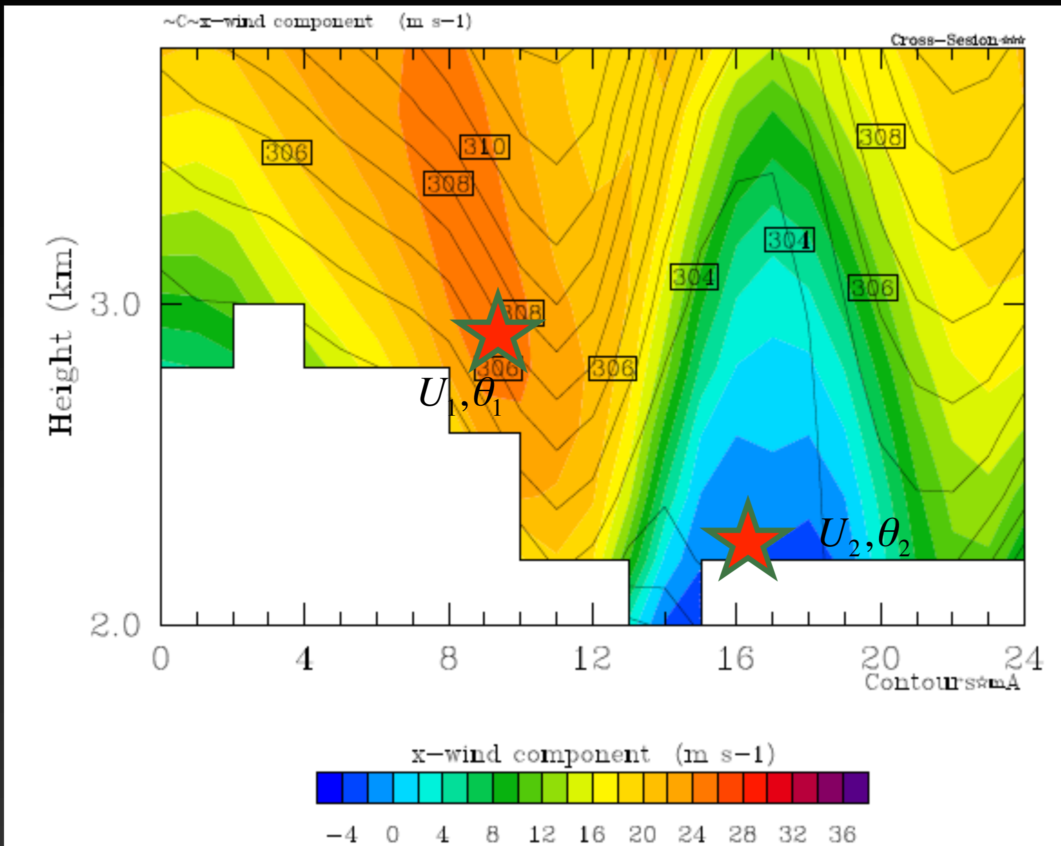
Experiment framework

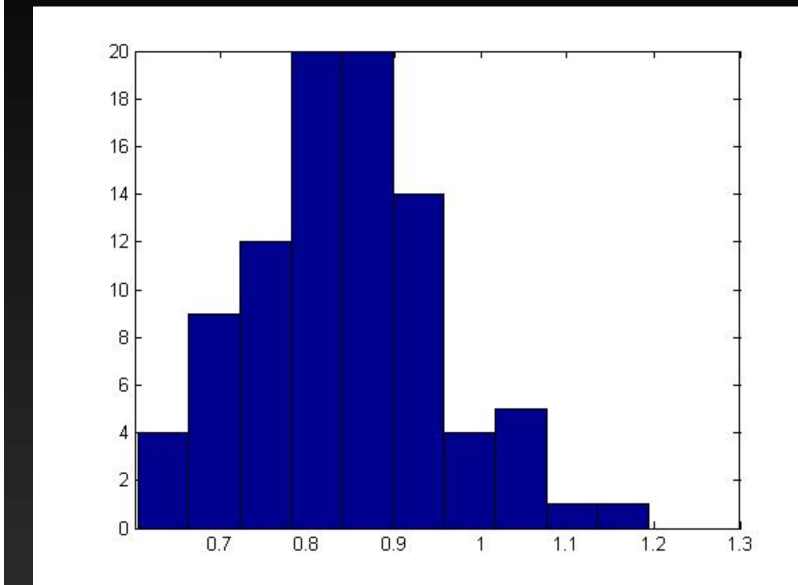
- 96-member ensemble data assimilation with the Data Assimilation Research Testbed (DART)
- Weather Research and Forecast (WRF) model
- Synthetic observations identical to rawinsonde network and surface altimeter
- 3-h cycling during Jan. 2009



Downslope winds at CO Springs

$$J_e = R_{ihB} = \frac{g}{\theta_2}\frac{(\theta_1-\theta_2)\Delta z}{(U_1-U_2)^2}$$





- Cross section looking north at U wind (shaded) and potential temperature; 3-h Ensemble mean forecast valid 30 Dec 2008 03Z
- J – analogous to the Bulk Richardson number to measures ratio of stability to shear across flow separation boundary
- Histogram of J (right) showing Gaussian distribution for metric

Predictors for wind storm

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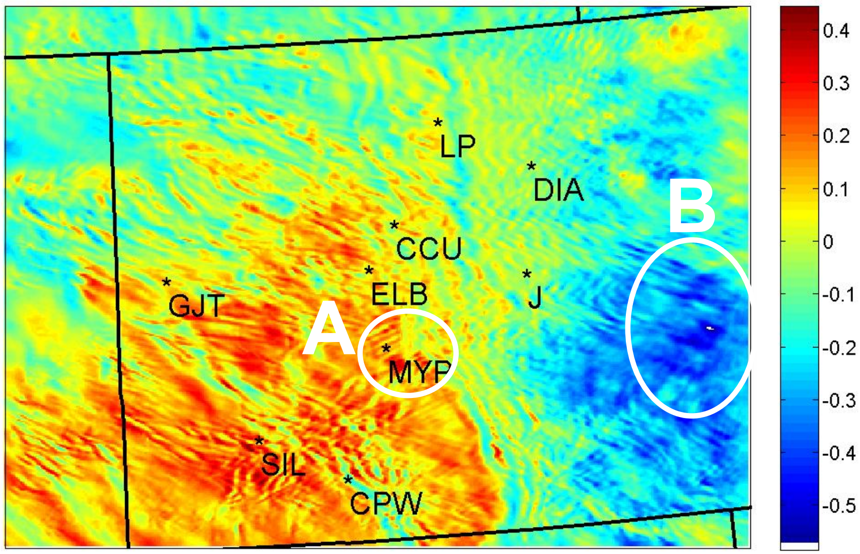
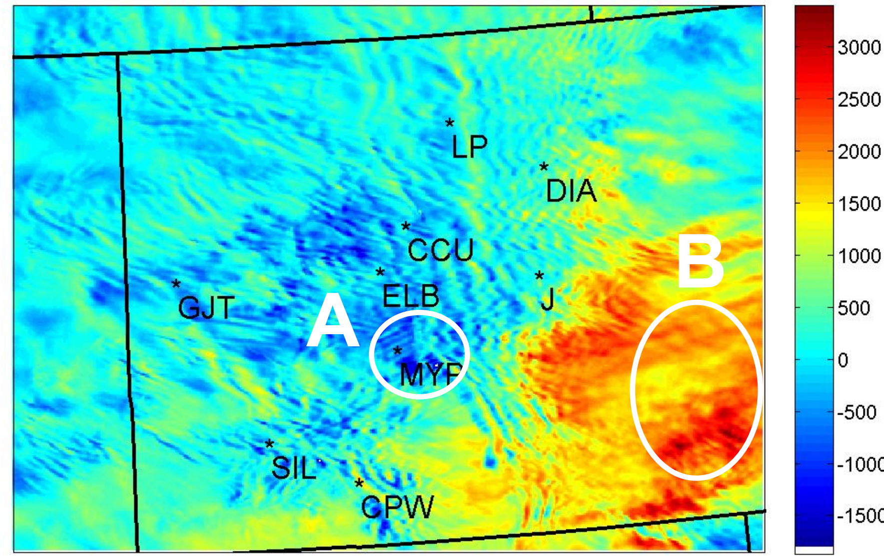


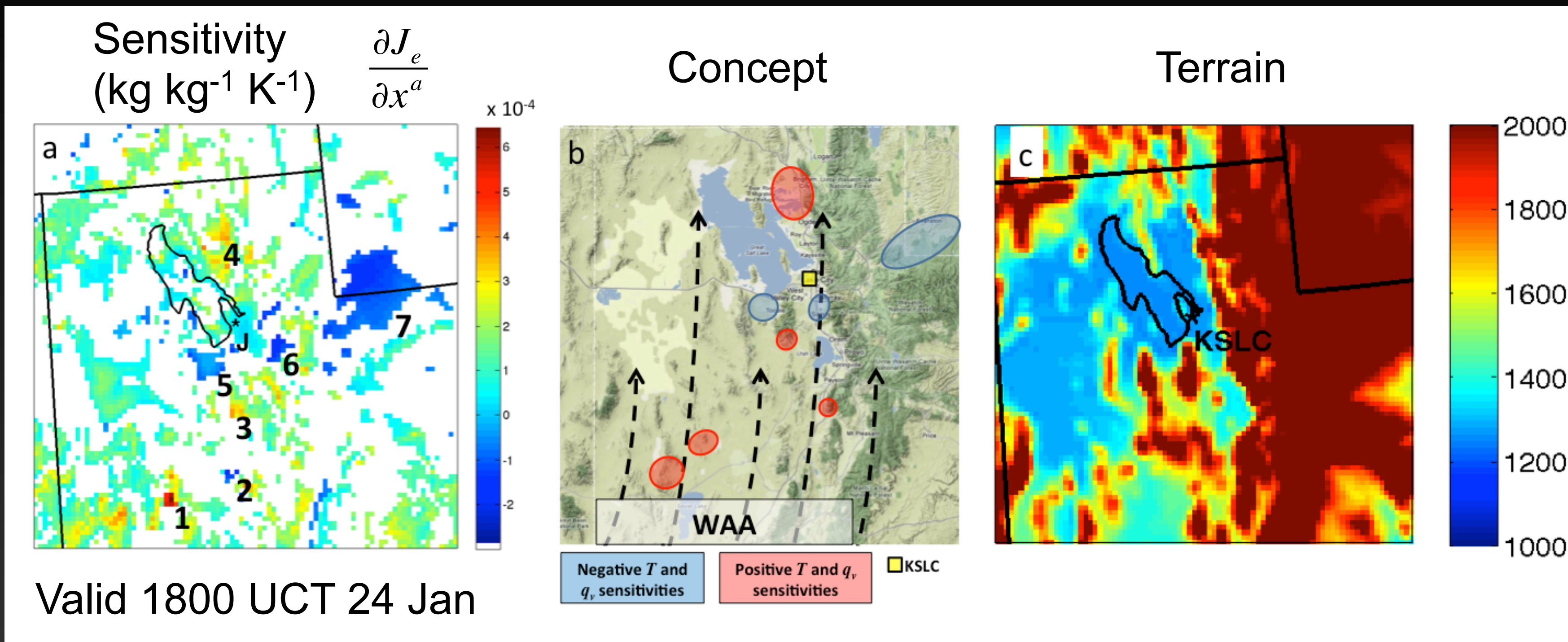
θ at model layer 14



Q_v at model layer 14

- Sensitivity of (dJ/dx) for 3-hr θ (left) and Q_v (right) at model level 14
- Strong dual sensitivities shown in both variables over plains and mountains
- Hypothesis – region A related to forcing and shear term in J, region B related to air mass characteristics over plains and stability term in J
- Good candidates for perturbations of IC for a new ensemble run

Moisture sensitivity to temperature



J = 2x2x2 box-mean water vapor mixing ratio over Salt Lake City airport

x=Potential temperature (here on model first layer)

Perturbation experiments

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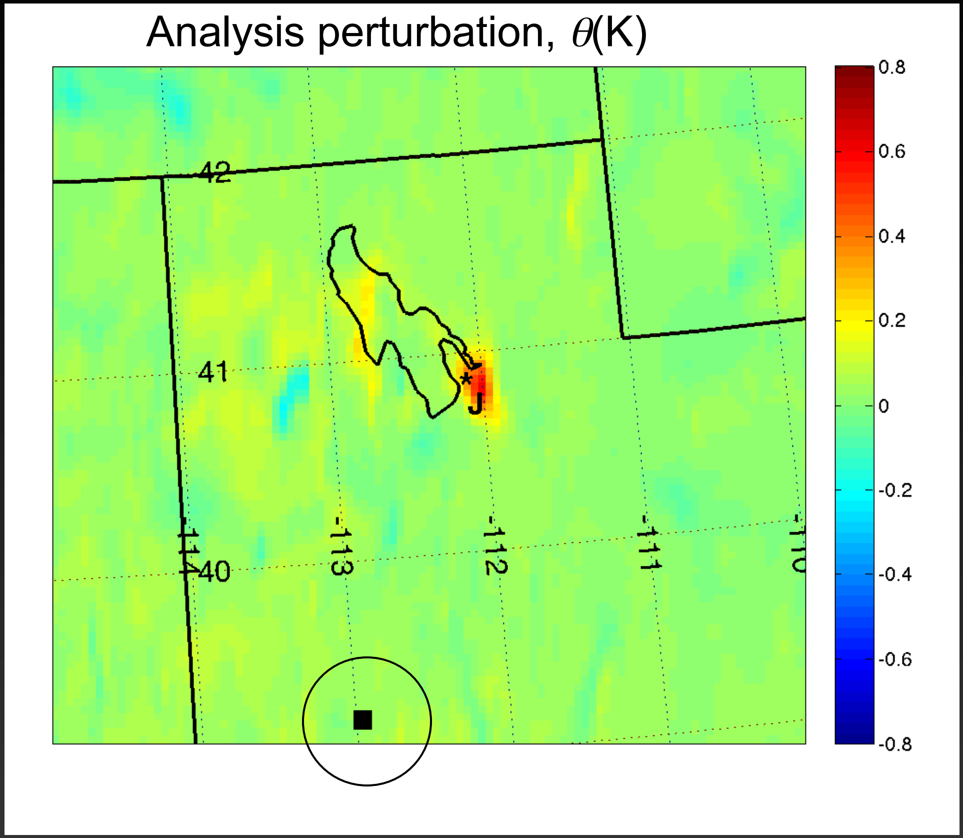

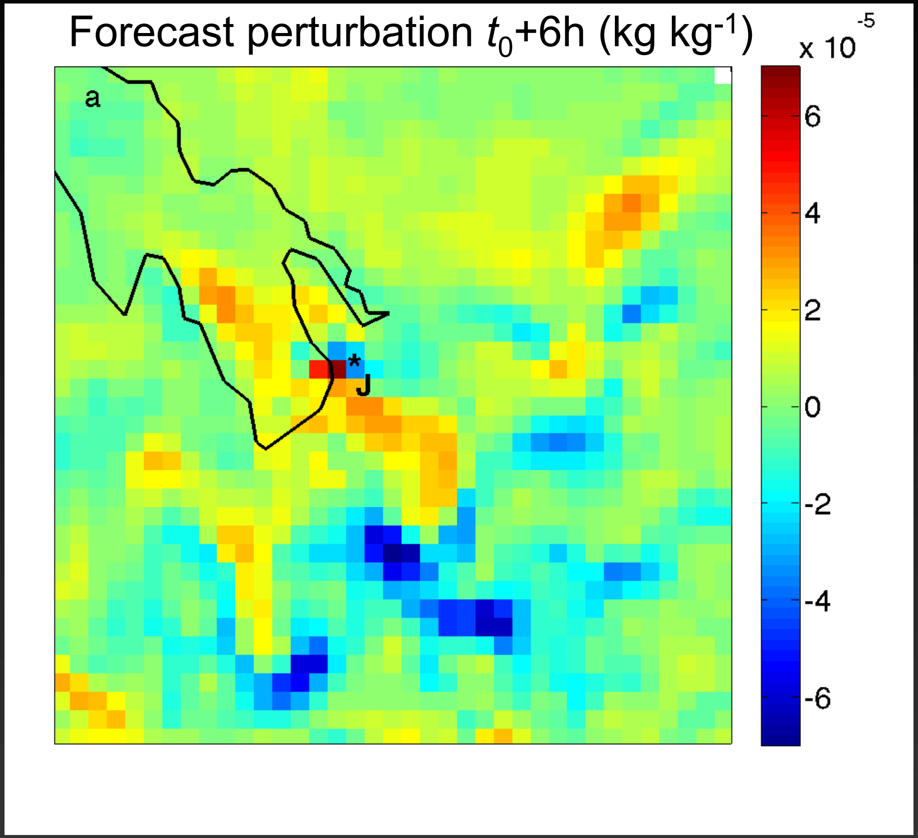

Perturbation of one analysis standard deviation in θ at the most sensitive location, *regressed* to remaining state elements.

Perturbation experiments

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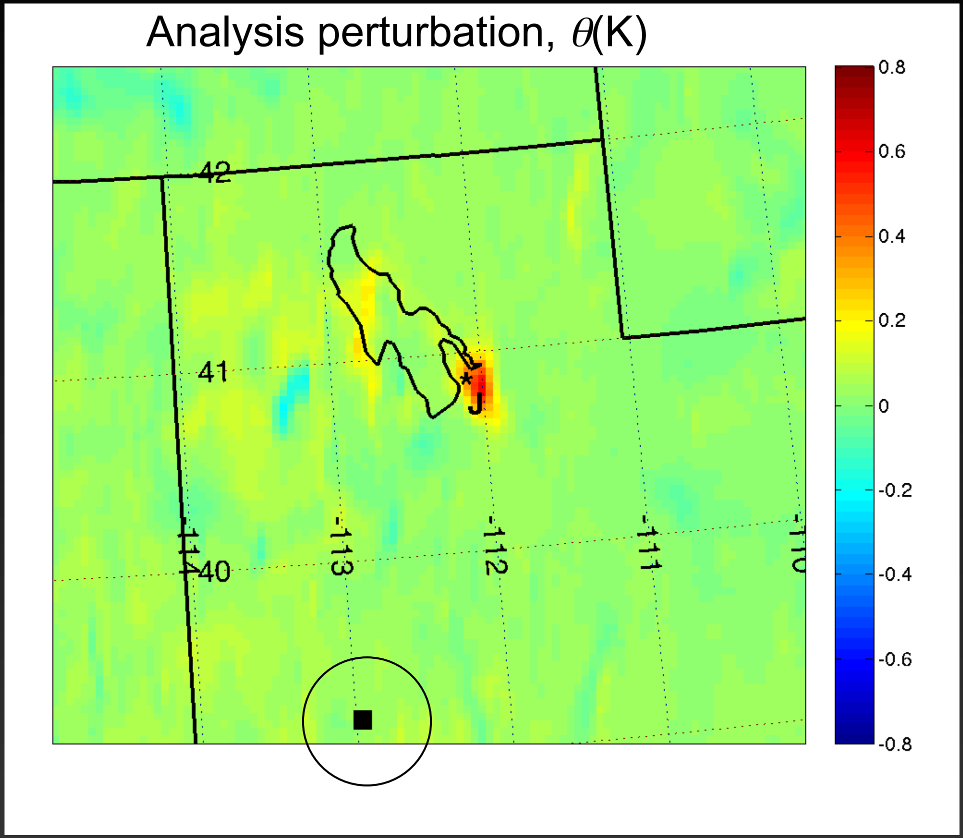

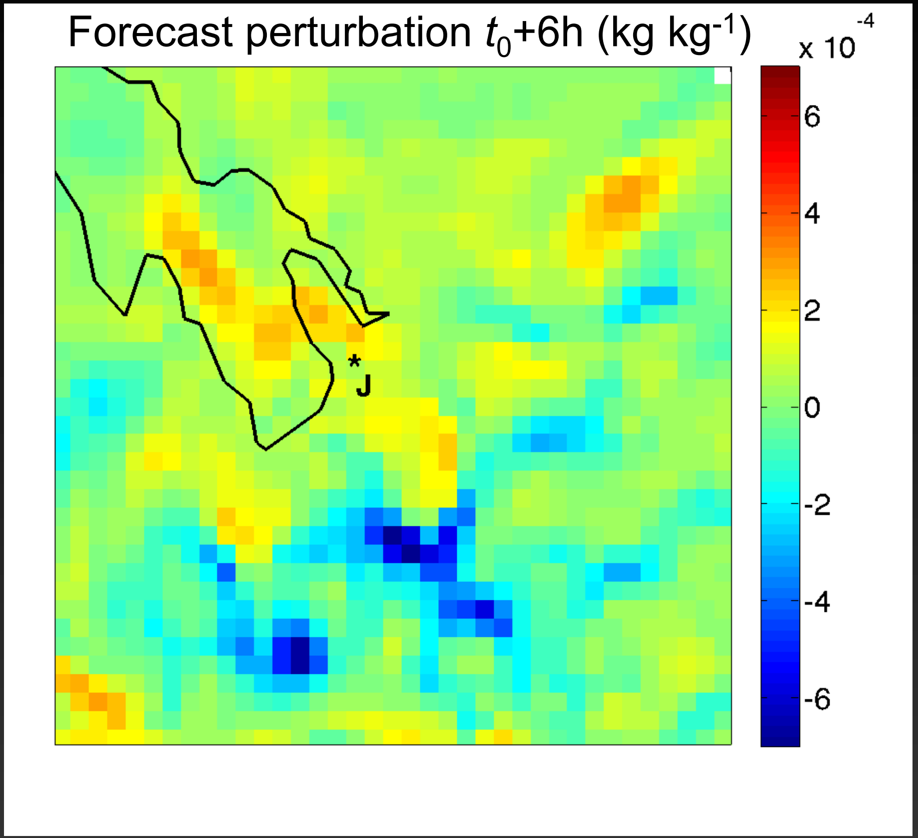

Perturbation of one analysis standard deviation in θ at the most sensitive location, *assimilated* with ensemble filter.

Effect of hypothetical θ observation

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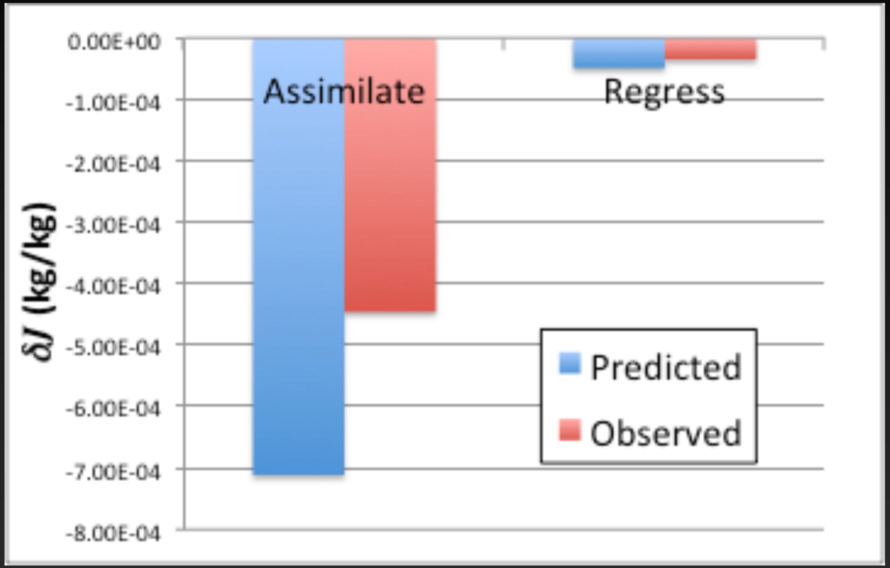
$$\delta J_e = \frac{\partial J_e}{\partial x^a}\mathbf{K}(\mathbf{y}^o - \mathbf{h}\mathbf{x}^a)$$

$$\mathbf{K} = \mathbf{P}^a\mathbf{h}^{\mathrm{T}}\left(\mathbf{h}\mathbf{P}^a\mathbf{h}^{\mathrm{T}} + \mathbf{R}\right)^{-1}$$



Can test use of sensitivities to predict the change in forecast metric resulting from a hypothetical observation. Analysis increment can come from:

- assimilating synthetic obs
- approximation with univariate linear regression

Effect of approximation

Diagonal approximation | Full covariance

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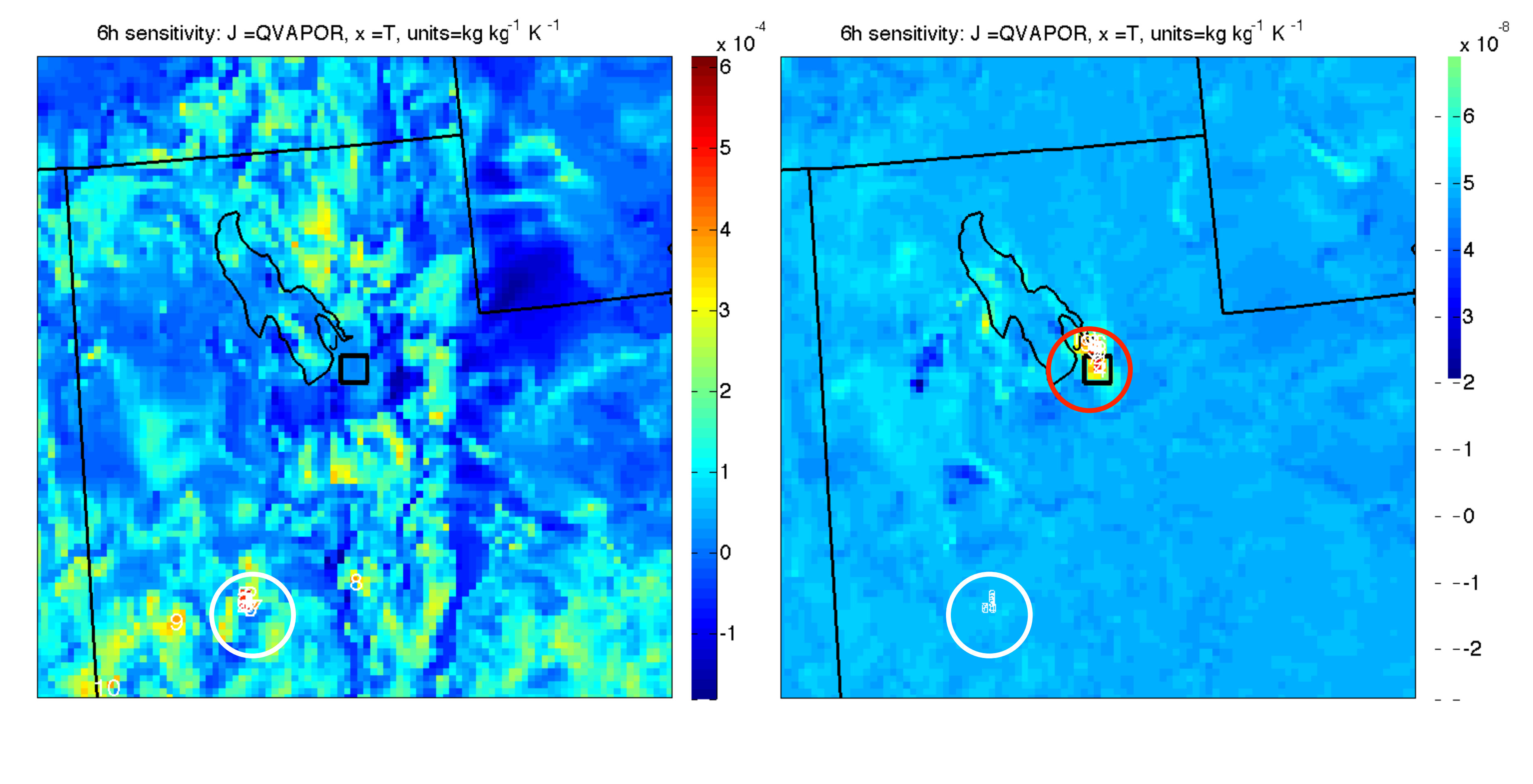

Approximation under-emphasizes sensitivities local to the response. Agreement on some sensitive points (numbered) to southwest of response.

Summary (1)

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- ESA appears promising for mesoscales and in complex terrain; hypothetical observations give qualitatively expected forecast change, but overestimated response.
- At mesoscales with weak sensitivity gradients, full covariance (and associated inversion) may be necessary.
- Linearity appears to hold for a variety of perturbations, possibly as large as 10 times the standard deviation of the analysis variable.

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Ensemble Sensitivity (1)

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$$\mathbf{J_e} = \left[\mathbf{X^a}\right]^{\mathrm{T}} \boldsymbol{\beta} + \varepsilon$$

$$\hat{\beta} = \frac{\partial J_e}{\partial \mathbf{x^a}}$$

$$\hat{\beta} = \mathbf{X^a}\left[\left(\mathbf{X^a}\right)^{\mathrm{T}} \mathbf{X^a}\right]^{-1} \mathbf{J_e} = \mathbf{QR^{-T}J_e}$$

- An ensemble sample (size K) of analysis perturbations and forecast metrics are assembled into matrix $\mathbf{X^a}$ and column vector $\mathbf{J_e}$, forming the regression equation.
- The solution, giving estimated regression coefficients, is the ensemble sensitivity defined as the gradient of the forecast metric relative to the analysis.
- Because K << N (state dimension), the system is extremely under-determined, but the minimum-norm solution is obtainable via a QR decomposition.

Ensemble Sensitivity (2)

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$$\mathbf{K}_i = \mathbf{P}_i^{\mathbf{a}} \mathbf{h}_{i+1}^{\mathbf{T}} \left(\mathbf{h}_{i+1} \mathbf{P}_i^{\mathbf{a}} \mathbf{h}_{i+1}^{\mathbf{T}} + \mathbf{R}_{i+1} \right)^{-1}$$

$$\delta J = \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}} \right)^{\mathbf{T}} \mathbf{K}_i \left(y_{i+1}^{o} - \mathbf{h}_{i+1} \mathbf{x}_i^{\mathbf{a}} \right)$$

$$= \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}} \right)^{\mathbf{T}} \delta \mathbf{x}^{\mathbf{a}}$$

$$\boxed{\mathbf{P}_i^{\mathbf{a}} = \mathbf{X}_i^{\mathbf{a}} \left(\mathbf{X}_i^{\mathbf{a}} \right)^{\mathbf{T}}}$$

$$= \mathbf{J}_{\mathbf{e}}^{\mathbf{T}} \left\{ \mathbf{X}_i^{\mathbf{a}} \left[\left(\mathbf{X}_i^{\mathbf{a}} \right)^{\mathbf{T}} \mathbf{X}_i^{\mathbf{a}} \right]^{-1} \right\}^{\mathbf{T}} \mathbf{K}_i \left(y_{i+1}^{o} - \mathbf{h}_{i+1} \mathbf{x}_i^{\mathbf{a}} \right)$$

Assimilation: a perturbation $\delta \mathbf{x}^{\mathbf{a}}$ resulting from assimilating an additional observation, multiplied by the sensitivities, gives the the expected forecast change resulting from assimilating that observation (i.e. the predicted response).

Ensemble Sensitivity (3)

$$\mathbf{K}_i = \mathbf{P}_i^{\mathbf{a}}\mathbf{h}_{i+1}^{\mathbf{T}}\left(\mathbf{h}_{i+1}\mathbf{P}_i^{\mathbf{a}}\mathbf{h}_{i+1}^{\mathbf{T}} + \mathbf{R}_{i+1}\right)^{-1}$$

$$\delta J = \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}}\right)^{\mathbf{T}} \mathbf{K}_i\left(y_{i+1}^o - \mathbf{h}_{i+1}\mathbf{x}_i^{\mathbf{a}}\right)$$

$$= \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}}\right)^{\mathbf{T}} \delta\mathbf{x}^{\mathbf{a}}$$

$$= \mathbf{J}_{\mathbf{e}}^{\mathbf{T}}\left\{\mathbf{X}_i^{\mathbf{a}}\left[\left(\mathbf{X}_i^{\mathbf{a}}\right)^{\mathbf{T}}\mathbf{X}_i^{\mathbf{a}}\right]^{-1}\right\}^{\mathbf{T}} \mathbf{K}_i\left(y_{i+1}^o - \mathbf{h}_{i+1}\mathbf{x}_i^{\mathbf{a}}\right)$$

Sampling error in ensemble data assimilation typically mitigated by reducing covariances with a function of distance; follows intuition that distant covariances must be small or zero.

Ensemble Sensitivity (4)

$$\mathbf{K}_i = \mathbf{P}_i^{\mathbf{a}} \mathbf{h}_{i+1}^{\mathbf{T}} \left(\mathbf{h}_{i+1} \mathbf{P}_i^{\mathbf{a}} \mathbf{h}_{i+1}^{\mathbf{T}} + \mathbf{R}_{i+1} \right)^{-1}$$

$$\delta J = \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}} \right)^{\mathbf{T}} \mathbf{K}_i \left(y_{i+1}^{o} - \mathbf{h}_{i+1} \mathbf{x}_i^{\mathbf{a}} \right)$$

$$= \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}} \right)^{\mathbf{T}} \delta \mathbf{x}^{\mathbf{a}}$$

$$= \mathbf{J}_{\mathbf{e}}^{\mathbf{T}} \left\{ \mathbf{X}_i^{\mathbf{a}} \left[\left(\mathbf{X}_i^{\mathbf{a}} \right)^{\mathbf{T}} \mathbf{X}_i^{\mathbf{a}} \right]^{-1} \right\}^{\mathbf{T}} \mathbf{K}_i \left(y_{i+1}^{o} - \mathbf{h}_{i+1} \mathbf{x}_i^{\mathbf{a}} \right)$$

Sampling error in sensitivities arise in spatio-temporal covariances. A few methods have been proposed in the ensemble assimilation literature. Here from a Bayesian hierarchical estimate (Anderson 2007).

Ensemble Sensitivity (5)

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$$\frac{\partial J}{\partial \mathbf{x}^{\mathbf{a}}} = \frac{\mathbf{X}^{\mathbf{a}}\mathbf{J}_{\mathbf{e}}}{\mathbf{P}^{\mathbf{f}}} \approx \frac{\mathbf{X}^{\mathbf{a}}\mathbf{J}_{\mathbf{e}}}{\mathbf{D}^{\mathbf{a}}}$$

$$\mathbf{D}^{\mathbf{a}} = \mathrm{diag}(\mathbf{P}^{\mathbf{f}})$$

Approximation: in the meteorology literature the inversion needed to solve the regression problem is always avoided by approximating the covariance with its diagonal. The result is a scalar (univariate) regression for each element in the state vector.

Ensemble sensitivity details

$$\mathbf{J}_e = \left[\mathbf{X}^a\right]^{\mathrm{T}} \boldsymbol{\beta} + \varepsilon$$

$$\hat{\boldsymbol{\beta}} = \frac{\partial J_e}{\partial \mathbf{x}^a} = \mathbf{X}^a \left(\left[\mathbf{X}^a\right]^{\mathrm{T}} \mathbf{X}^a \right)^{-1} \mathbf{J}_e = \mathbf{Q}\mathbf{R}^{-\mathrm{T}} \mathbf{J}_e$$

$\mathbf{J}_e$ are perturbations about J_e (scalars)

$\mathbf{X}^a$ are perturbations about x^a (vectors)

Sensitivity is multi-variate linear regression; coefficients can be estimated via a right pseudo-inverse.

$$\frac{\partial J_e}{\partial \mathbf{x}^a} = \left[\mathbf{P}^a\right]^{-1} \mathbf{X}^a \mathbf{J}_e \approx \left[\mathbf{D}^a\right]^{-1} \mathbf{X}^a \mathbf{J}_e$$

$$\mathbf{P}^a = \mathbf{X}^a \left[\mathbf{X}^a\right]^{\mathrm{T}}, \ \mathbf{D}^a = \mathrm{diag}\left(\mathbf{P}^a\right)$$

More common in the literature is to avoid an inversion by assuming covariances are zero, leading to a scalar problem for each state element.

Open questions

- Ensemble sensitivities in the presence of small, fast scales
  – May increase nonlinearity
  – Increases model error/inadequacy
  – Appear as noise in correlations/covariances
- Validity of diagonal approximation
- Need to account for sampling error arising from finite ensemble

Ensemble Sensitivity with Localization

$$\delta J = \alpha \circ \left\{ \mathbf{J}_{\mathbf{e}}^{\mathrm{T}} \left[\mathbf{X}_i^{\mathbf{a}} \left(\mathbf{X}_i^{\mathbf{a}\,\mathrm{T}} \mathbf{X}_i^{\mathbf{a}} \right)^{-1} \right]^{\mathrm{T}} \rho \circ \mathbf{P}_i^{\mathbf{a}} \mathbf{h}_{i+1}^{\mathrm{T}} \left(\mathbf{h}_{i+1} \rho \circ \mathbf{P}^{\mathbf{a}} \mathbf{h}_{i+1}^{\mathrm{T}} + \mathbf{R} \right)^{-1} \left(y_{i+1}^{o} - \mathbf{h}_{i+1} \mathbf{x}_i^{\mathbf{a}} \right) \right\}$$

$$= \alpha \circ \left\{ \mathbf{J}_{\mathbf{e}}^{\mathrm{T}} \left[\mathbf{X}_i^{\mathbf{a}} \left(\mathbf{X}_i^{\mathbf{a}\,\mathrm{T}} \mathbf{X}_i^{\mathbf{a}} \right)^{-1} \right]^{\mathrm{T}} \delta \mathbf{x}^{\mathbf{a}} \right\}$$

- Covariance localization, or tapering, can be applied
  - at the assimilation step with ρ
  - to the regressions with α
- ρ is typically a function of space alone
- α is function of space and time, here from a Bayesian hierarchical estimate (Anderson 2007)

Experiment Details (1)

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- Nature/truth from Lorenz (2005) one-scale Model II or two-scale Model III
  - Perfect-model experiments
  - Model error simulated by retaining fast scale in nature run/ truth and eliminating it in the assimilating model
- Ensemble-filter data assimilation every 6 h
  - 80 cycles
    - Network of every-other grid point; or
    - Network of one-half of domain totally observed
- Forecast metric (J) is root-mean square error (RMSE)

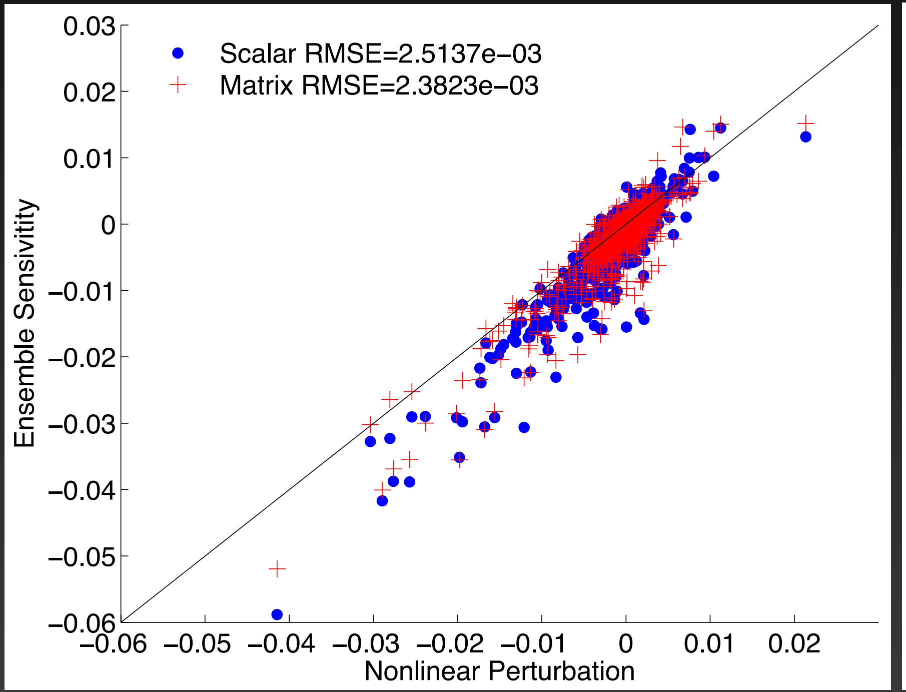
Experiment Details (2)

- Apply individual perturbations by assimilating individual observation at randomly-chosen unobserved gridpoints
- Evaluate 6-h forecast response with nonlinear model
- Compare to 6-h response as predicted by linear method: $$\delta J = \left(\frac{\partial J_e}{\partial \mathbf{x}^{\mathbf{a}}} \right)^{\mathbf{T}} \delta \mathbf{x}^{\mathbf{a}}$$

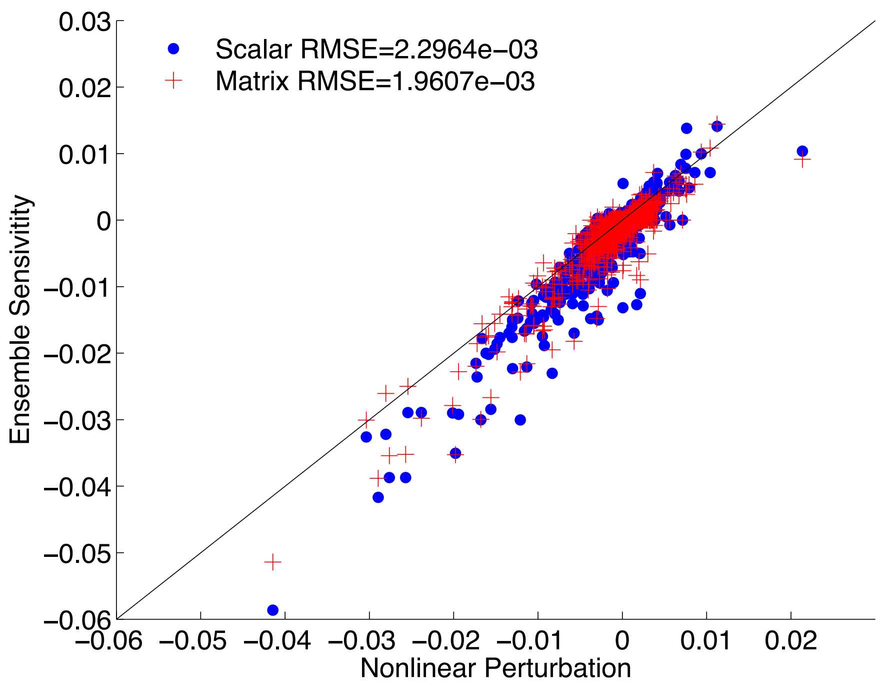
Perfect Model II

When only smooth/slow scales present, little difference between univariate (scalar) and multivariate (matrix) predictions of response to perturbation.

Sensitivity *without* localization



Sensitivity *with* localization

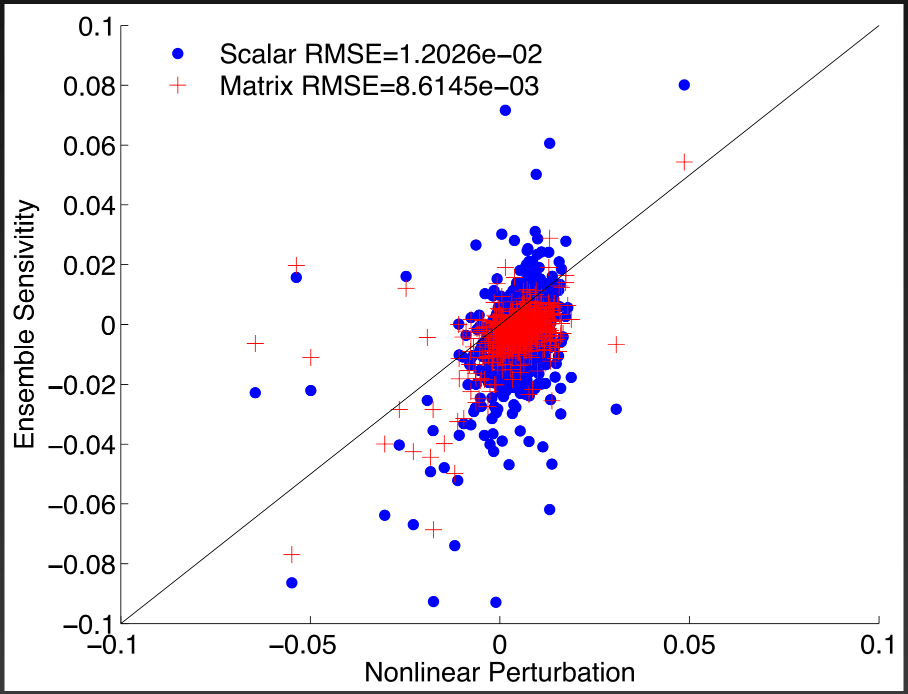


Here observations are randomly chosen from every other gridpoint (which are un-observed for sensitivity calculations).

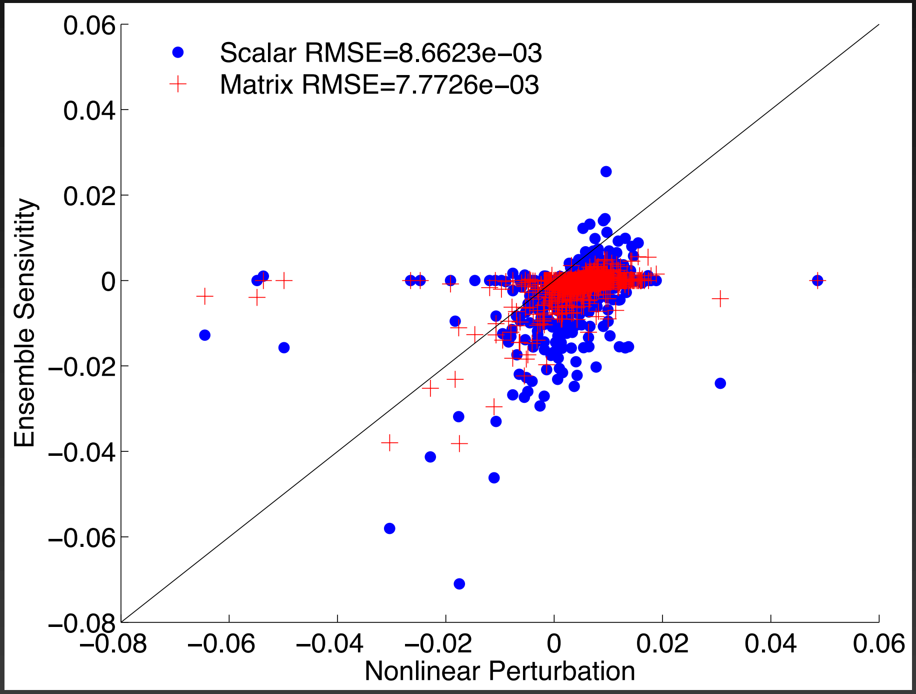
Perfect Model III

When both slow and fast scales are present, diagonal approximation is less accurate. Localization slightly improves predictions of response.

Sensitivity *without* localization



Sensitivity *with* localization



Here observations are randomly chosen from every other gridpoint (which are un-observed for sensitivity calculations).

Imperfect Model

For imperfect model, diagonal approximation results in greater over-prediction of response; multivariate sensitivities account for presence of fast scales in real system, which appears as noise.

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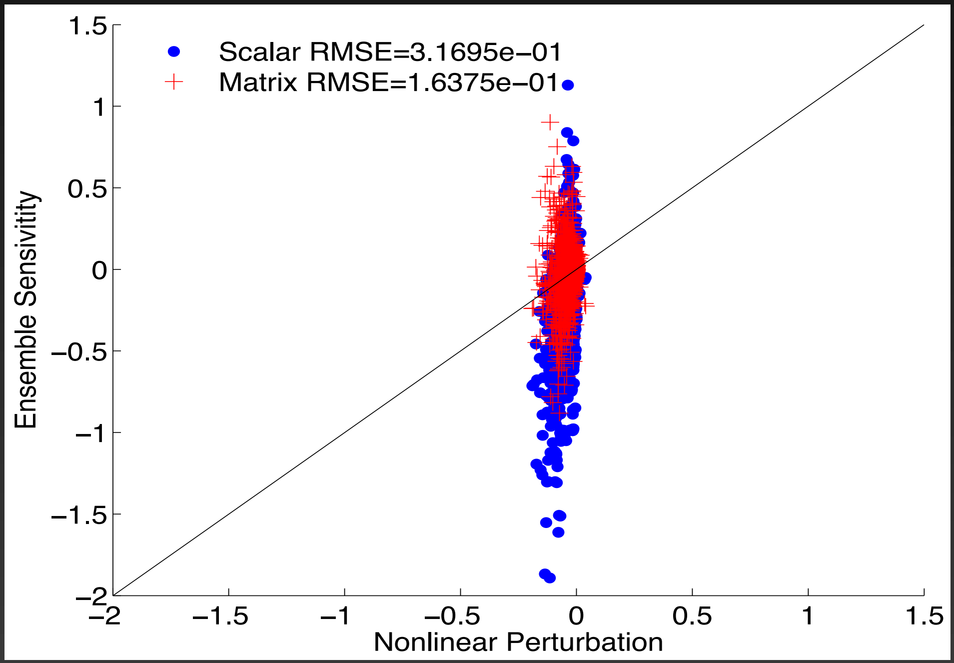
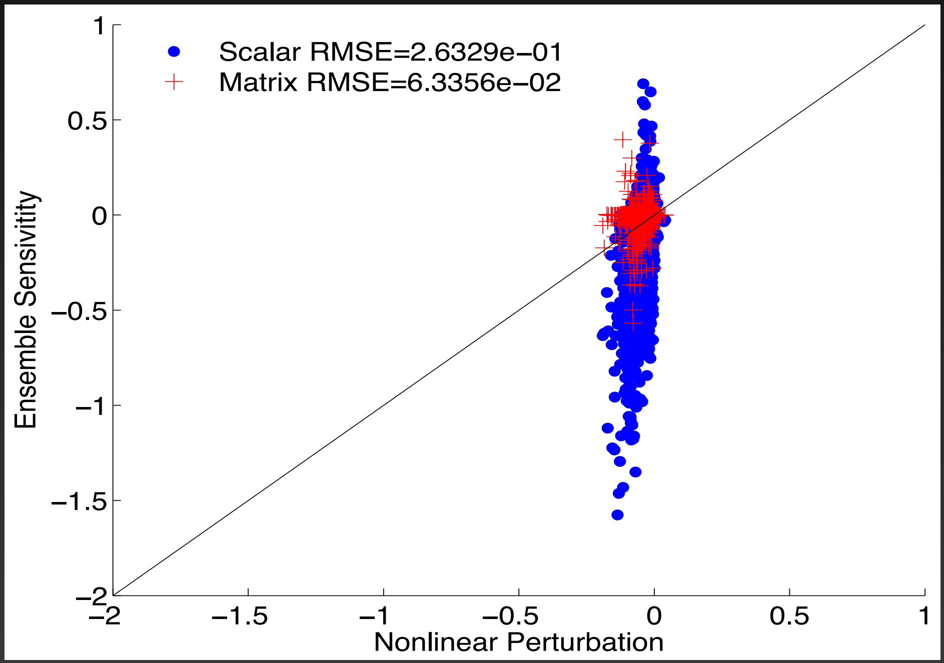
Sensitivity *without* localization

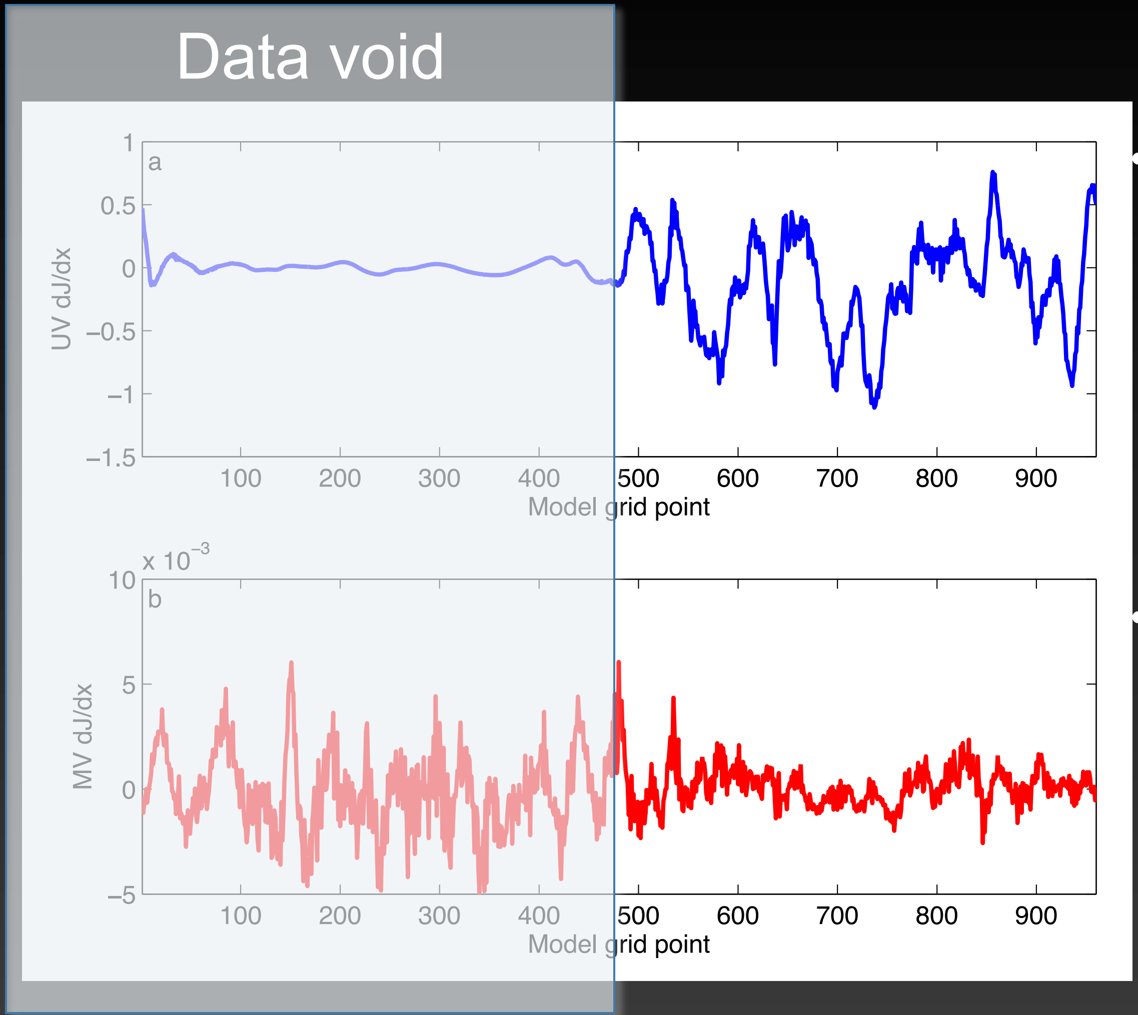


Sensitivity *with* localization



Here observations are assimilated on half of domain that is data void; more impact from observations because greater uncertainty in analysis.

Sensitivities in a data void



- Top: univariate sensitivities are small in the data void because analysis uncertainty is large
- Bottom: multivariate sensitivities larger over data void than over densely observed region, consistent with expectations

Summary (II)

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- Multivariate sensitivities are possible to estimate by finding a minimum-norm solution to the resulting underdetermined matrix problem.
- Whether univariate or multivariate methods are employed, sampling error is a problem.
- Sensitivities used to predict the perturbation response in the nonlinear system are more accurate when localized/tapered to account for sampling error.
- Multivariate sensitivities better predict the nonlinear response when:
  - Fast scales are present
  - Model error is present
  - Part of the state is poorly observed and can benefit from additional observations

Results suggest mesoscale sensitivities for real atmospheric problems will be more useful if using multivariate estimates.

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