Overview: Data Assimilation and Model Reduction

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Outline

Introduction to data assimilation

Sequential and variational techniques

- Ensemble Filters
- Incremental 4DVar

Numerical experiments

Conclusions

The Data Assimilation Problem

Data Assimilation

Aim:

Find the best estimate (analysis) of the expected states of a system, consistent with both observations and the system dynamics given:

- Numerical prediction model
- Observations of the system (over time)
- Background state (prior estimate)
- Estimates of error statistics

Significant Properties:

- Very large number of unknowns (10^8 – 10^9)
- Few observations (10^5 – 10^6)
- System nonlinear unstable/chaotic
- Multi-scale dynamics

System Equations

$$\mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i) \equiv \mathcal{S}(t_{i+1}, t_i, \mathbf{x}_i)$$ States

$$\mathbf{y}_i = H_i[\mathbf{x}_i^{(k)}] + \boldsymbol{\eta}_i$$ Observations

$$\boldsymbol{\eta}_i \sim N(0, \mathbf{R}_i)$$ Noise

Best Unbiased Estimate

$$\min \; J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}_0^{-1}(\mathbf{x}_0 - \mathbf{x}^b)$$

$$+ \sum_{i=0}^{n} (H_i[\mathbf{x}_i] - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (H_i[\mathbf{x}_i] - \mathbf{y}_i)$$

subject to $\quad \mathbf{x}_i = S(t_i, t_0, \mathbf{x}_0)$

$\mathbf{x}^b$ - Background state (prior estimate)

$\mathbf{y}_i$ - Observations

H_i - Observation operator

$\mathbf{B}_0$ - Background error covariance matrix

$\mathbf{R}_i$ - Observation error covariance matrix

Sequential and Variational Assimilation Techniques

Sequential and Variational Assimilation Techniques

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Sequential Assimilation

Sequential Filter

Predict: $$\mathbf{x}_i^b = \mathcal{S}(t_i, t_{i-1}, \mathbf{x}_{i-1}^a)$$

Correct: $$\mathbf{x}_i^a = \mathbf{x}_i^b + \mathbf{K}_i(H_i[\mathbf{x}_i^b] - \mathbf{y}_i)$$

where $$\mathbf{K}_i = \mathbf{B}_i\mathbf{H}_i^T(\mathbf{H}_i\mathbf{B}_i\mathbf{H}_i^T + \mathbf{R}_i)^{-1}$$

$\mathbf{H}_i$ = the linearized observation operator

and $$\mathbf{B}_i = \mathcal{E}\{(\mathbf{x}_i - \mathbf{x}_i^b)(\mathbf{x}_i - \mathbf{x}_i^b)^T\} .$$

Difficulties:

- Need to propagate covariance matrices at each step
- Need to solve large inverse problem at each step.

Solutions:

- Approximate covariances – use ensemble methods
- Use iterative methods and truncate

Ensemble Square Root Filter (EnRF)

At time t_i we have an ensemble of forecast states generated by the model, initiated from perturbed analysis states at time t_{i-1}. The ensemble is given by

$$\left(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \right) \in \mathcal{R}^{n \times N}$$

We define the ensemble mean and covariance using

$$\overline{\mathbf{x}} = \frac{1}{N} \sum_{j=1}^{N} \mathbf{x}_j \quad , \quad \mathbf{X}' = (\mathbf{x}_1 - \overline{\mathbf{x}}, \ldots, \mathbf{x}_N - \overline{\mathbf{x}})$$

$$\mathbf{P}_e = \frac{1}{N-1} \mathbf{X}' \mathbf{X}'^T$$

EnSRF

Then the analysis at time t_i is given by

$$\overline{\mathbf{x}}^a = \overline{\mathbf{x}}^f + \tilde{\mathbf{K}}(\mathbf{y} - \overline{H(\mathbf{x}^f)})$$

where

$$\tilde{\mathbf{K}} = \frac{1}{N-1}\mathbf{X}'^f\mathbf{X}'^{f^T}\mathbf{H}^T\left(\frac{1}{N-1}\mathbf{H}\mathbf{X}'^f\mathbf{X}'^{f^T}\mathbf{H}^T + \mathbf{R}\right)^{-1}$$

Obtain the analysis ensemble for the next forecast from

$$\mathbf{X}^a = \mathbf{X}'^a + \bar{\mathbf{X}}^a \qquad \mathbf{X}'^a = \mathbf{X}'^f\boldsymbol{\Upsilon}$$

where $\boldsymbol{\Upsilon}$ is a square root found from $\mathbf{X}'$

EnSRF

Problems: arise because the covariance is not full rank, which leads to

- spurious long range correlations
- filter collapse
- filter divergence

Treatments:

- inflation of variances
- localization methods
- regularization methods

Variational Assimilation

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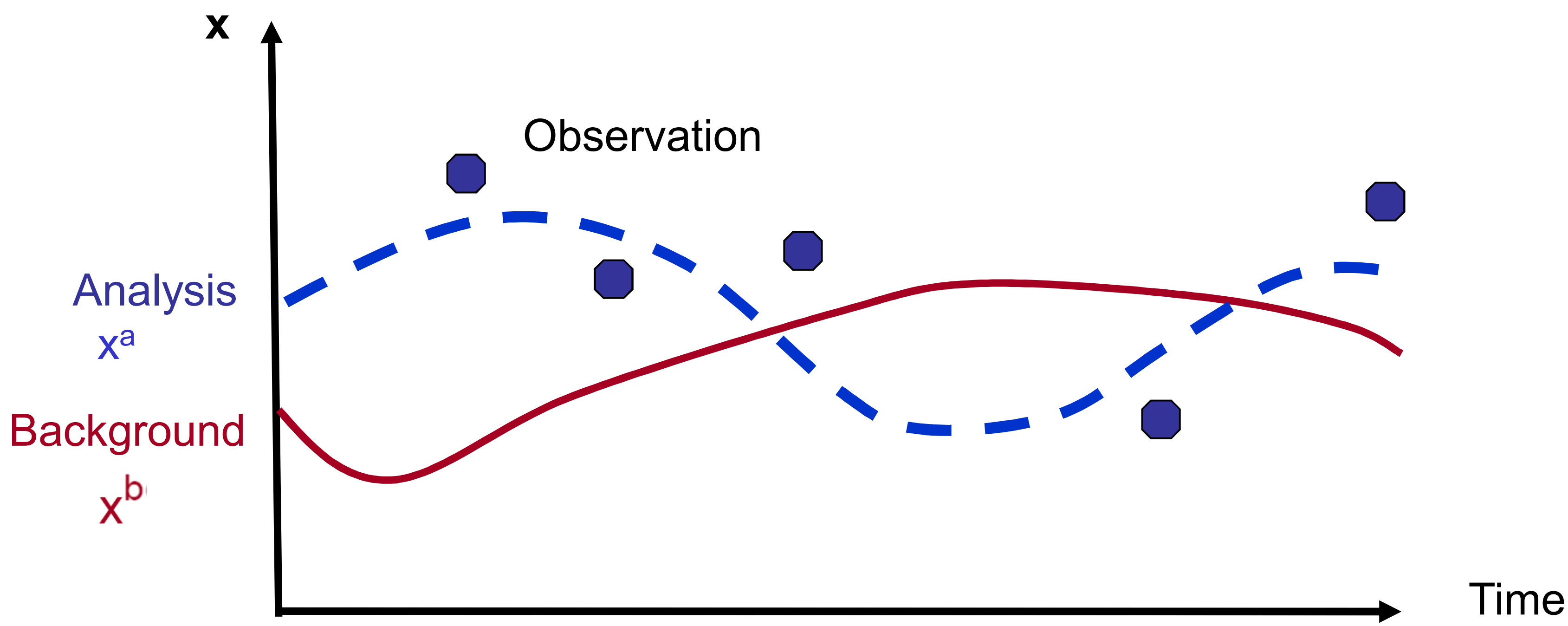
Variational Assimilation

Aim: Find the initial state x_0^a (analysis) such that the distance between the state trajectory and the observations is minimized, subject to x_0^a remaining close to the prior estimate x^b



4DVar Assimilation

$$\min \ J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}_0^{-1}(\mathbf{x}_0 - \mathbf{x}^b)$$

$$+\sum_{i=0}^{n}(H_i[\mathbf{x}_i] - \mathbf{y}_i)^T \mathbf{R}_i^{-1}(H_i[\mathbf{x}_i] - \mathbf{y}_i)$$

subject to $\quad \mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i) \equiv \mathcal{S}(t_{i+1}, t_i, \mathbf{x}_i)$

Solve iteratively by gradient optimization methods.

Use adjoint methods to find the gradients.

3DVar if n = 0 $\qquad$ 4DVar if n $\geq$ 1

Difficulties:

- Time constraints – solve in real time
- Need to build adjoints
- Conditioning of the problem

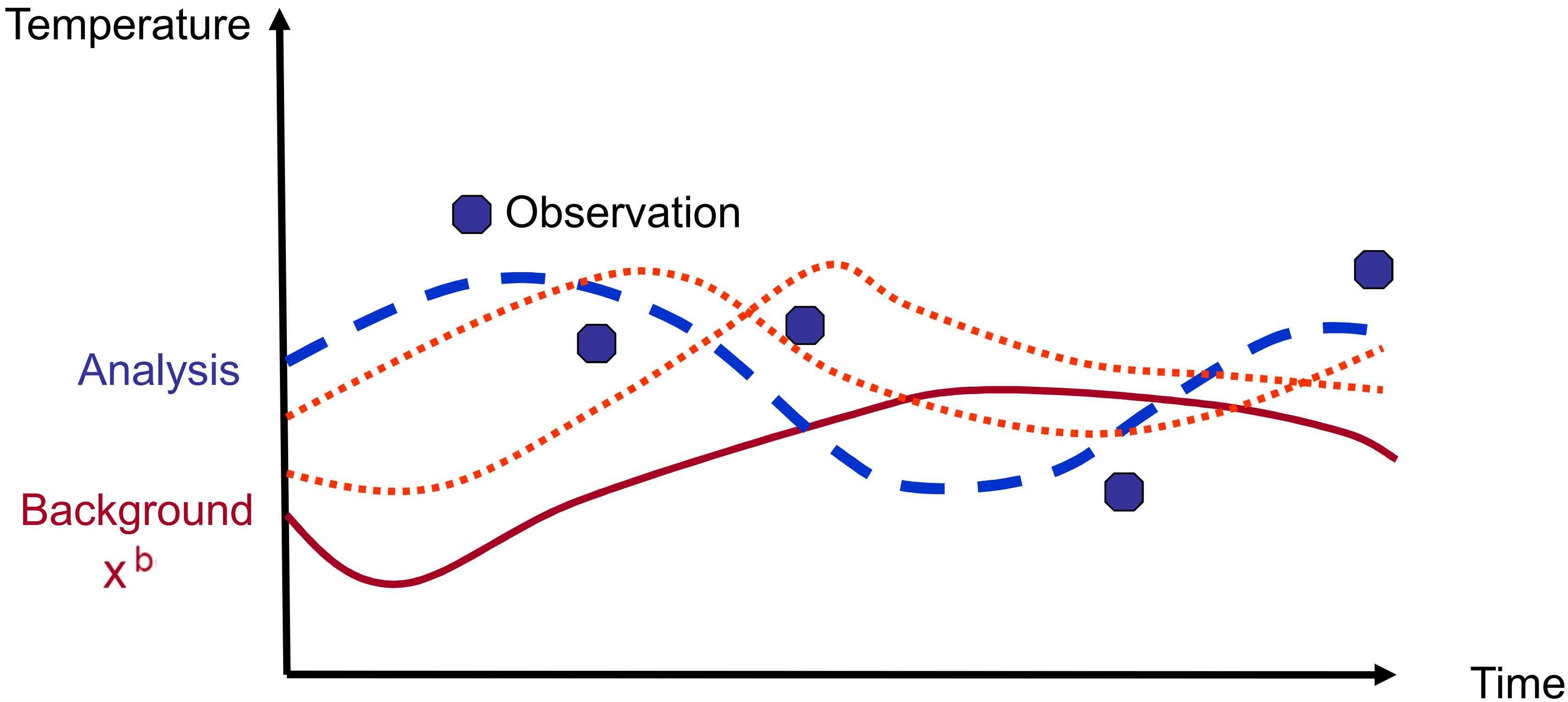
Treatment:

- Precondition using control variable transforms
- Use incremental method = Gauss Newton
- Use approximate linearization

(See *Gratton, Lawless and Nichols, SIOPT, 2007*)

- Solve on short windows and cycle sequentially
- Solve in restricted space (lower resolution)

Incremental 4D-Var



Solve by iteration a sequence of linear least squares problems that approximate the nonlinear problem.

Incremental 4D-Var

Set $\mathbf{x}_0^{(0)}$ (usually equal to background)

For k = 0, …, K find: $\mathbf{x}_i^{(k)} = S(t_i, t_0, \mathbf{x}_0^{(k)})$

Solve inner loop linear minimization problem:

$$\boxed{\begin{aligned}\tilde{\mathcal{J}}^{(k)}[\delta\mathbf{x}_0^{(k)}] &= \frac{1}{2}(\delta\mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])^{\mathrm{T}}\mathbf{B}_0^{-1}(\delta\mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}]) \\ &+ \frac{1}{2}\sum_{i=0}^{N}(\mathbf{H}_i\delta\mathbf{x}_i^{(k)} - \mathbf{d}_i^{(k)})^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\delta\mathbf{x}_i^{(k)} - \mathbf{d}_i^{(k)})\end{aligned}}$$

subject to $\boxed{\delta\mathbf{x}_{i+1}^{(k)} = \mathbf{M}_i\delta\mathbf{x}_i^{(k)}}$, $\quad \mathbf{d}_i = \mathbf{y}_i - H_i[\mathbf{x}_i^{(k)}]$

Update: $\mathbf{x}_0^{(k+1)} = \mathbf{x}_0^{(k)} + \delta\mathbf{x}_0^{(k)}$

Low Order Models in Incremental 4DVar

Find: restriction operators $\mathbf{U}_i \in \mathbb{R}^{r \times n}$ and prolongation operators $\mathbf{V}_i \in \mathbb{R}^{r \times n}$ with $\mathbf{U}_i^T \mathbf{V}_i = \mathbf{I}_r$, $r << N$, and $\mathbf{V}_i \mathbf{U}_i^T$ a projection.

Define: a reduced order system in $\mathbb{R}^r$

$$\delta \hat{\mathbf{x}}_{i+1}^{(k)} = \hat{\mathbf{M}}_i \delta \hat{\mathbf{x}}_i^{(k)}, \qquad \hat{\mathbf{d}}_i = \hat{\mathbf{H}}_i \delta \hat{\mathbf{x}}_i^{(k)}$$

where $\mathbf{V}_i \hat{\mathbf{M}}_i \mathbf{U}_i^T$, $\hat{\mathbf{H}}_i \mathbf{U}_i^T$ approximate $\mathbf{M}_i$, $\mathbf{H}_i$

Reduced Order Assimilation Problem

The reduced order inner loop problem is to minimize

$$\hat{\mathcal{J}}^{(k)}[\delta\hat{\mathbf{x}}_0^{(k)}] =$$

$$\frac{1}{2}(\delta\hat{\mathbf{x}}_0^{(k)} - \mathbf{U}_0^T[\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])^{\mathrm{T}}(\mathbf{U}_0^T\mathbf{B}_0\mathbf{U}_0)^{-1}(\delta\hat{\mathbf{x}}_0^{(k)} - \mathbf{U}_0^T[\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])$$

$$+ \quad \frac{1}{2}\sum_{i=0}^{N}(\mathbf{H}_i\mathbf{V}_i\delta\hat{\mathbf{x}}_i^{(k)} - \mathbf{d}_i^{(k)})^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\mathbf{V}_i\delta\hat{\mathbf{x}}_i^{(k)} - \mathbf{d}_i^{(k)})$$

subject to the reduced order system

and set $\delta\mathbf{x}_0^{(k)} = \mathbf{V}_0\delta\hat{\mathbf{x}}_0^{(k)}$

(See *Lawless et al, Monthly Weather Review, 2008*)

Projection Operators

A variety of ways are used for choosing the projection operators:

- Low resolution model of full nonlinear system
- Use ensemble filter method to provide a low order basis.
- POD methods to determine a low order basis (EOFs).
- Use balanced truncation / rational interpolation to find projections (feasible for linear TI systems).

Recent Developments

Derive some of the coefficients from an ensemble (Berre and Desroziers, 2010): *hybrid-Var*
(Use some ensembles for low order covariance basis)

Direct use of localised ensemble perturbations to define covarianc:. *ensemble-Var (EnVar)*

Combine ensemble and climatological covariances: *hybrid-EnVar*

Use ensemble trajectories to define time-evolution of covariances: *4D-Ensemble-Var (4DEnVar)*

Ensembles of 4DEnVar: (*En4DVar)*

Lorenz, 2013

Application and Numerical Results

Model Reduction

Aims:

- Find approximate linear system models using optimal reduced order modeling techniques to improve the efficiency of the incremental 4DVar method.
- Test feasibility of approach in comparison with low resolution models using balanced truncation with a nonlinear model of shallow water flow.

Balanced Truncation

Find: Ψ such that $\Psi^{-1}\mathbf{P}\mathbf{Q}\Psi = \Sigma^2$

where Σ is diagonal and

$$\begin{aligned}\mathbf{P} &= \mathbf{M}\mathbf{P}\mathbf{M}^T + \mathbf{B}_0 \\ \mathbf{Q} &= \mathbf{M}^T\mathbf{Q}\mathbf{M} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}\end{aligned}$$

Then: near optimal projections are given by

$$\mathbf{U}^T = [\mathbf{I}_r, 0]\,\Psi^{-1}, \qquad \mathbf{V} = \Psi \begin{bmatrix} \mathbf{I}_r \\ 0 \end{bmatrix}$$

1D Shallow Water Model

Nonlinear continuous equations

$$\frac{\mathrm{D}u}{\mathrm{D}t} + \frac{\partial \varphi}{\partial x} = -g\,\frac{\partial \overline{h}}{\partial x}$$

$$\frac{\mathrm{D}(\ln \varphi)}{\mathrm{D}t} + \frac{\partial u}{\partial x} = 0$$

with

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + u\,\frac{\partial}{\partial x}$$

We discretize using a semi-implicit semi-Lagrangian scheme and linearize to get linear model (TLM).

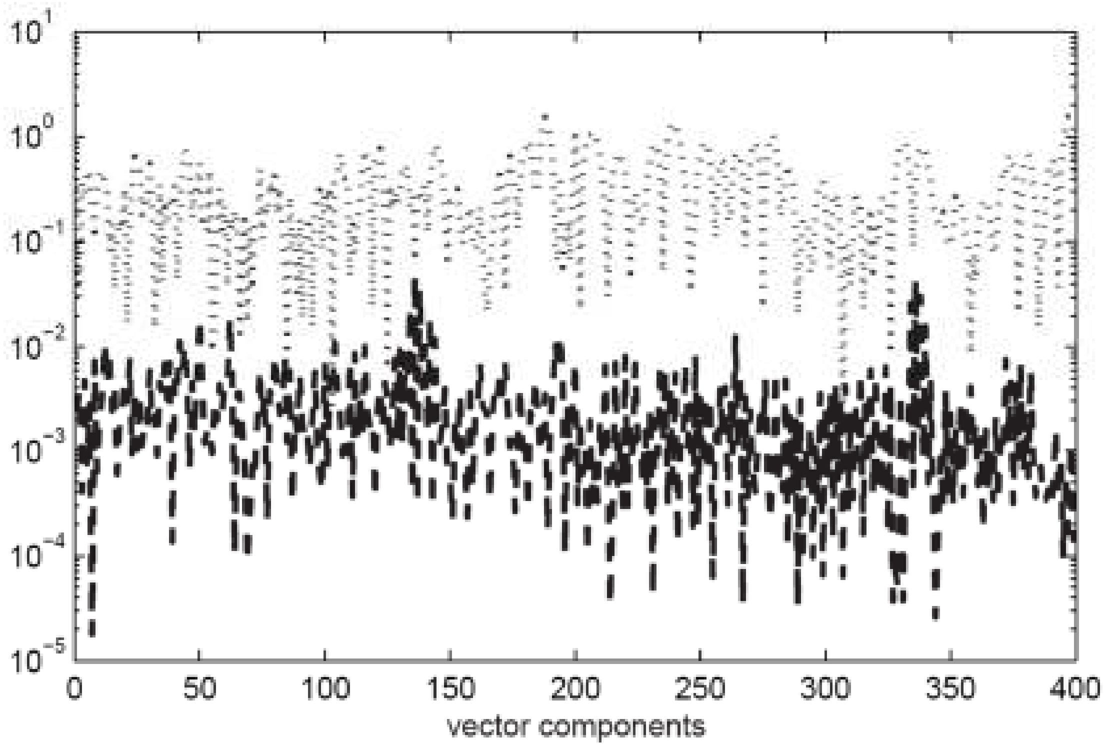
Numerical Experiments
Error Norms

Test matrices:

$\mathbf{M} \in \mathbb{R}^{400\times 400}$	from linear model
$\mathbf{H} \in \mathbb{R}^{200\times 400}$	observations at every other point
$\mathbf{B}_0^{\frac{1}{2}} \in \mathbb{R}^{400\times 400}$	quite realistic test matrix

Error norm $nrm = \dfrac{\| \delta x_0 - \delta x_0^{(lift)} \|_2}{\| \delta x_0 \|_2}$, $\quad \delta x_0^{(lift)} := \mathbf{V}\, \delta \hat{x}_0.$

Errors between exact and approximate analysis for 1-D SWE model

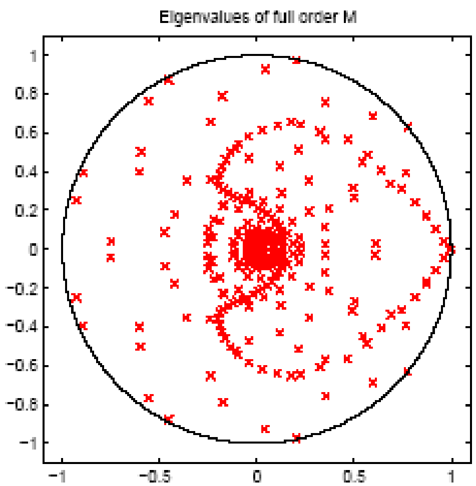


Low resolution model – dotted line
Reduced order model – dashed line

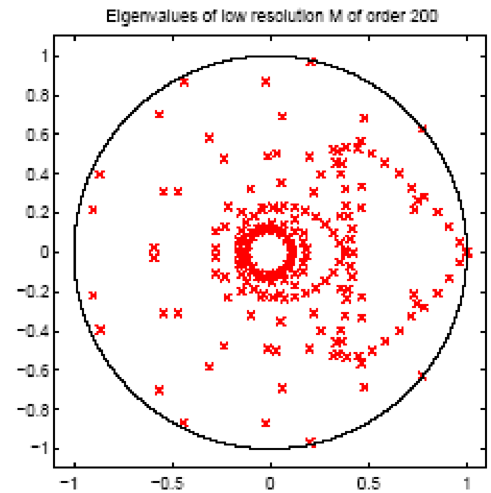
Comparison of Error Norms
Low resolution vs Reduced order models

	reduced order	low resolution
l=200	0.0027	0.2110
l=150	0.0134	—
l=100	0.0623	—
l=90	0.1015	—
l=80	0.1726	—
l=70	0.2327	—

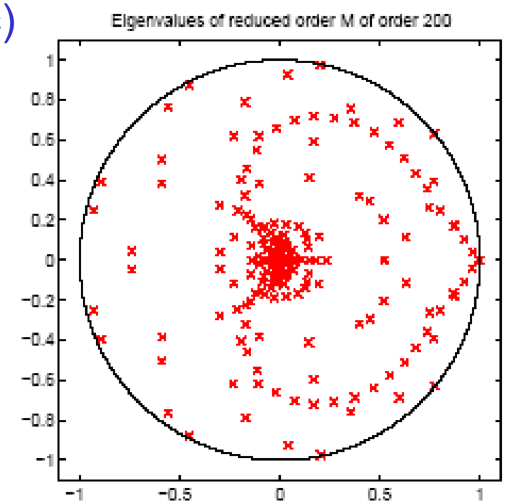
(a)



(b)



(c)



Eigenvalues of (a) full, (b) low resolution (c) reduced order system matrices

Summary of experiments

- Reduced rank linear models obtained by optimal reduction techniques give more accurate analyses than low resolution linear models that are currently used in practice.
- Incorporating the background and observation error covariance information is necessary to achieve good results
- Reduced order systems capture the optimal growth behaviour of the model more accurately than low resolution models
- Can be extended to unstable systems

(See *Boess et al, CAF, 2011*)

Conclusions

Conclusions

The use of model reduction in data assimilation is generally based on low rank approximations to the prior error covariances, which leads to a low rank set of basis vectors.

+ This reduces the degrees of freedom in the optimization problem.

- Does not necessarily reduce the work needed to integrate the dynamical model

Ideally want both, and that the low rank system minimizes the expected error between the outputs from the full system and those from the reduced model.

Future

Many more challenges left!

References:

Nichols, N. K. (2010) Mathematical concepts of data assimilation. In: Lahoz, W., Khattatov, B. and Menard, R. (eds.) Data assimilation: making sense of observations. Springer, pp. 13-40. ISBN 9783540747024