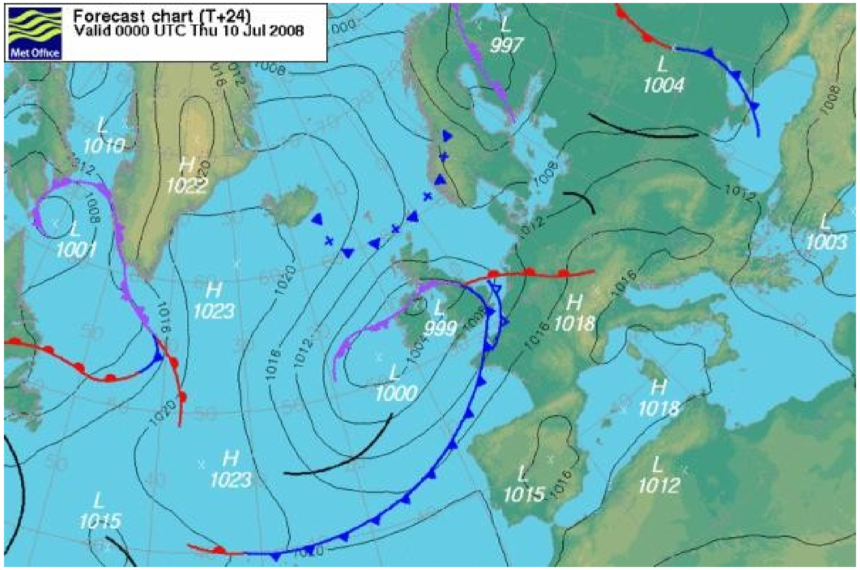
Optimal State Estimation Using Reduced Order Models



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Outline

- State estimation / Data assimilation
- Incremental 4D variational assimilation
- Model reduction using balanced truncation
- Balanced truncation in incremental 4DVar
- Numerical experiments
- Conclusions

State estimation / Data Assimilation

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

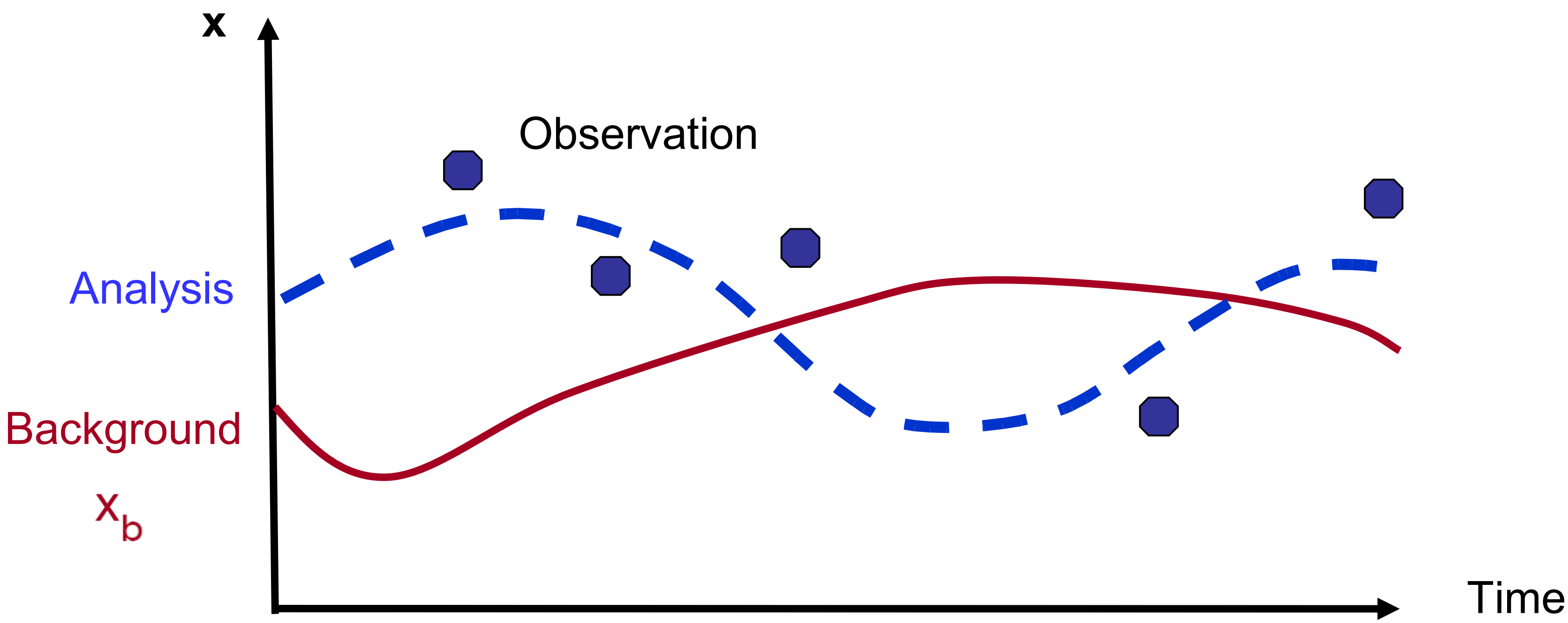
- Numerical prediction model
- Observations of the system (over time)
- Background state (prior estimate)
- Estimates of the errors

Significant Properties:

- Very large number of unknowns (10^7 – 10^8)
- Few observations (10^5 – 10^6)
- System nonlinear unstable/chaotic
- Multi-scale dynamics

4DVar Assimilation

Aim: Find the initial state x_0 such that the distance between the state trajectory and the observations is minimized, subject to x_0 remaining close to the prior estimate x_b.



4D-Var Nonlinear Problem

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

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

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

$\mathbf{x}_b$ - Background state (prior)

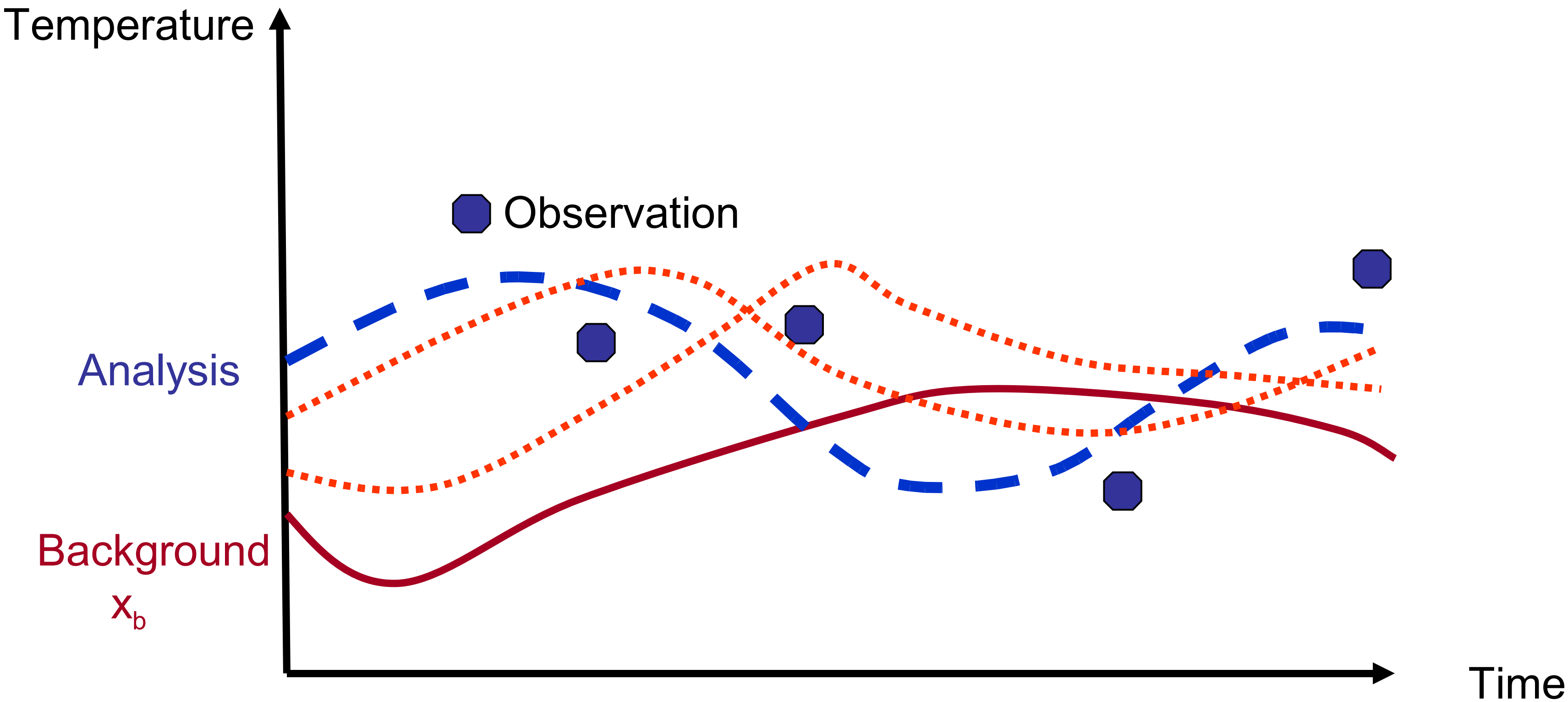
$\mathbf{y}_i^o$ - Observations

H_i - Observation operator

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

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

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

Solve inner loop linear minimization problem:

$$\min J^{(k)}[\delta\mathbf{x}_0^{(k)}] = \left(\delta\mathbf{x}_0^{(k)} - \delta\mathbf{x}_b^{(k)}\right)^T \mathbf{B}_0^{-1}(\delta\mathbf{x}_0^{(k)} - \delta\mathbf{x}_b^{(k)})$$

$$+ \sum_{i=0}^{n} (\mathbf{H}_i\delta\mathbf{x}_i^{(k)} - \mathbf{d}_i^{o})^T \mathbf{R}_i^{-1}(\mathbf{H}_i\delta\mathbf{x}_i^{(k)} - \mathbf{d}_i^{o})$$

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

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

On each outer iteration the linear least squares problem is solved subject to the linearized dynamical system

$$\delta \mathbf{x}_{i+1} = \mathbf{M}_i \delta \mathbf{x}_i \qquad \delta \mathbf{x}_i \in \mathbb{R}^N$$

$$\mathbf{d}_i = \mathbf{H}_i \delta \mathbf{x}_i \qquad \mathbf{M}_i \in \mathbb{R}^{N \times N}$$

$$\mathbf{H}_i \in \mathbb{R}^{p \times N}$$

In practice this problem is too computationally expensive to solve. Approximations to the inner minimization problem are therefore used.

Previous Results

- Incremental 4D-Var without approximations is equivalent to a Gauss-Newton iteration for nonlinear least squares problems.
- In operational implementation the solution procedure is approximated:
  - Truncate inner loop iterations
  - Use approximate linear system model
- Theoretical convergence results obtained by reference to Gauss-Newton method (*SIOPT, 07*).

New Research

Aims:

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

Model Reduction via Oblique Projections

Given:
$$\delta\mathbf{x}_{i+1} = \mathbf{M}\delta\mathbf{x}_i + \mathbf{u}_i, \qquad \mathbf{u}_i \sim \mathcal{N}(0, \mathbf{B}_0)$$
$$\mathbf{d}_i = \mathbf{H}\delta\mathbf{x}_i$$

Find: projections $\mathbf{U}, \mathbf{V}$ with $\mathbf{U}^T\mathbf{V} = \mathbf{I}_r$, $\mathbf{r} << \mathrm{N}$,
such that the output of the reduced order system

$$\begin{aligned} \delta\hat{\mathbf{x}}_{i+1} &= \mathbf{U}^T\mathbf{M}\mathbf{V}\delta\hat{\mathbf{x}}_i + \mathbf{u}_i, \\ \hat{\mathbf{d}}_i &= \mathbf{H}\mathbf{V}\delta\hat{\mathbf{x}}_i \end{aligned}$$

minimizes:
$$\boxed{\lim_{i\to\infty} \mathcal{E}\left\{\left[\hat{\mathbf{d}}_i - \mathbf{d}_i\right]^T \mathbf{R}^{-1}\left[\hat{\mathbf{d}}_i - \mathbf{d}_i\right]\right\}}$$

(over all inputs with expected norm equal to a constant)

Balanced Truncation

Balanced truncation removes states that are least affected by inputs and that have least effect on outputs (in a statistical sense).

There are 2 steps:

1. Balancing – Transform system to one in which these states are the same.
2. Truncation – Truncate states related to the smallest singular values of the transformed covariance matrices (Hankel singular values).

Projected system exactly matches the largest Hankel singular values of the full system.

Balanced Truncation

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

where $\boldsymbol{\Sigma}$ 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

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

Reduced Order Assimilation Problem

The reduced order inner loop problem is to minimize

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

subject to

$$\begin{aligned}\delta\hat{\mathbf{x}}_{i+1}^{(k)} &= \mathbf{U}^T\mathbf{M}\mathbf{V}\delta\hat{\mathbf{x}}_i{}^{(k)}, \\ \hat{\mathbf{d}}_i &= \mathbf{H}\mathbf{V}\delta\hat{\mathbf{x}}_i{}^{(k)}\end{aligned}$$

and set

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

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).

Methodology

- Define an initial random perturbation $\delta\mathbf{x}_0$ from a distribution B_0.
- Calculate 'true' solution by solving full linear least squares problem.
- Calculate 'observations' $\mathbf{d}_i = \mathrm{H}\delta\mathbf{x}_i$ for 5 steps (t=0 to t=5)
- Compare solutions using
  - Low resolution linear model.
  - Reduced order model.
- Size of full dimension is 400.

Numerical Experiments -
Error Norms and Condition Numbers

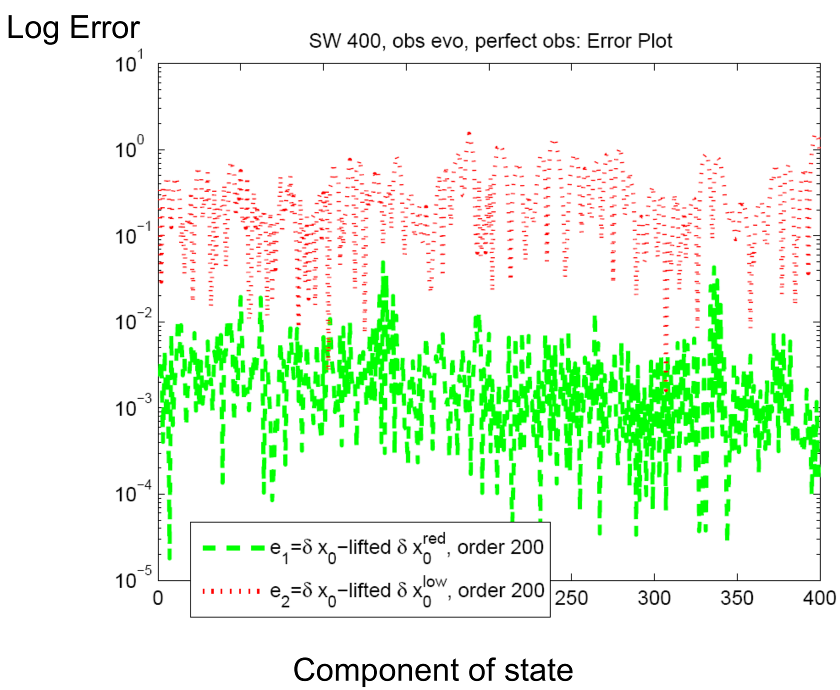
Test matrices:

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

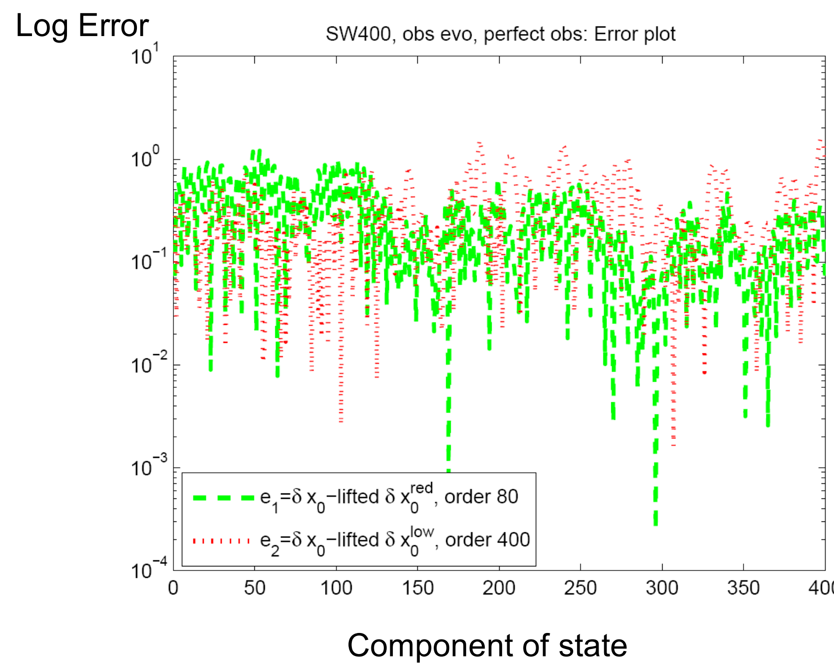
Error norm $nrm = \frac{\|\delta x_0 - \delta x_0^{(lift)}\|_2}{\|\delta x_0\|_2}$, $\qquad \delta x_0^{(lift)} := V\delta\hat{x}_0$.

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

Low Res Model of order = **200**
vs Reduced Model of order = **200**



Low Res Model of order = **200**
vs Reduced Model of order = **80**



Red (dotted) = Low Res Model **Green** (dashed) = Reduced Rank Model

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	—

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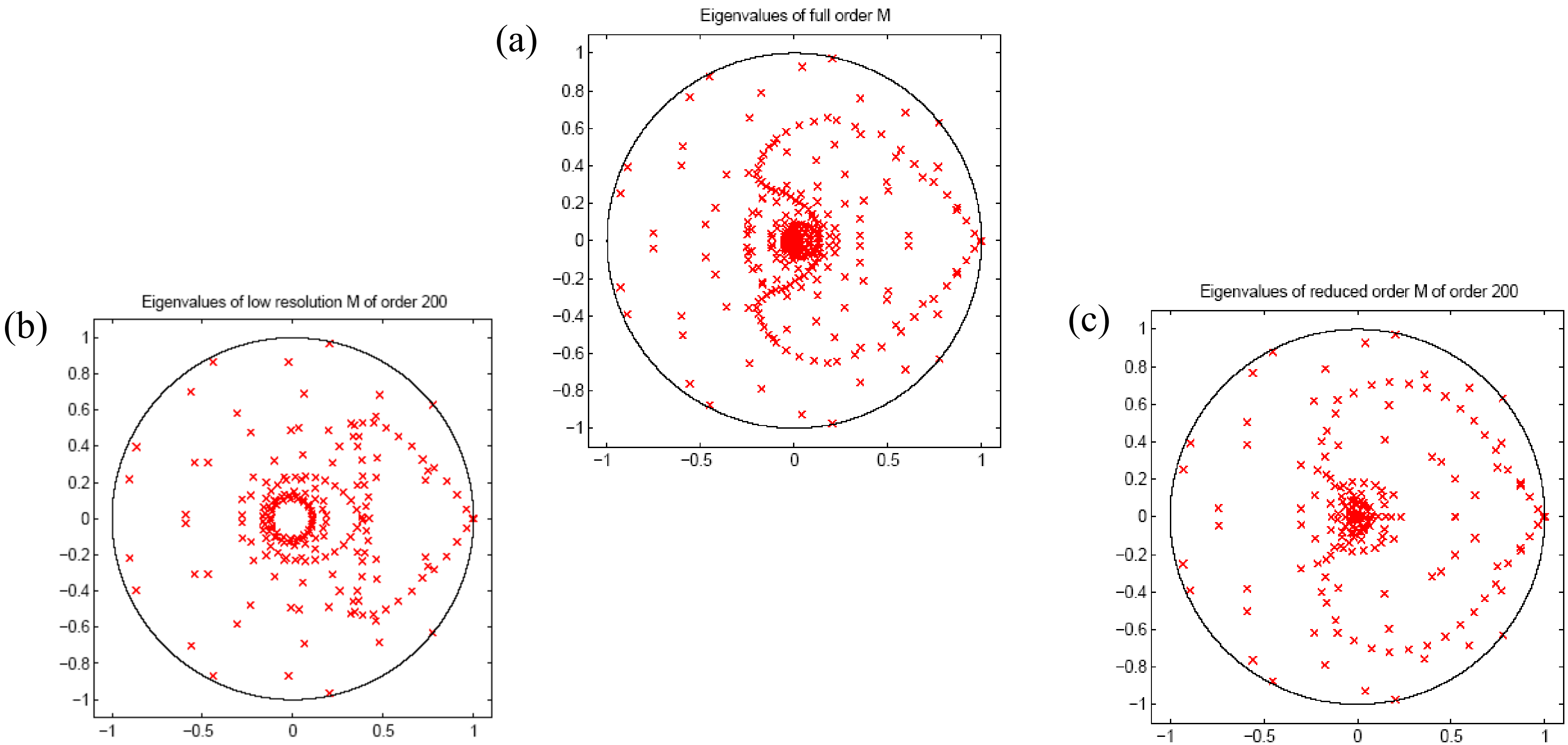
Comparison of Model Eigenvalues



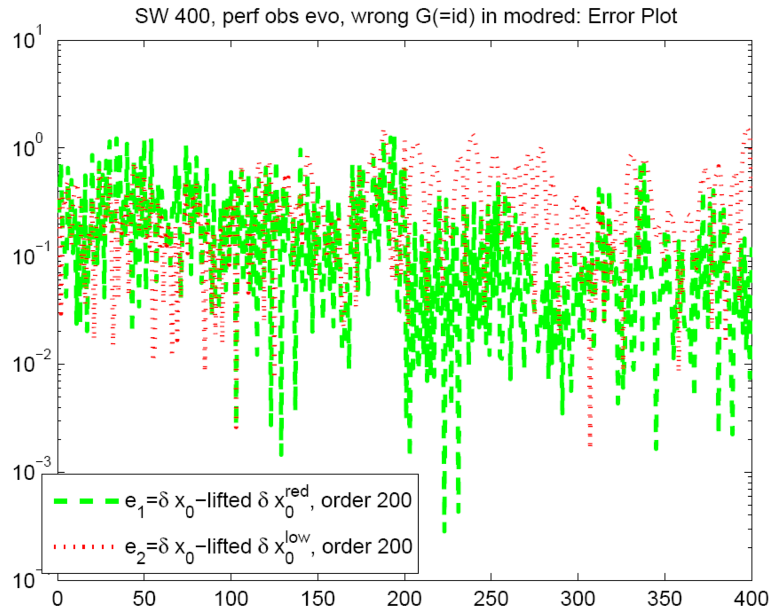
Eigenvalues plotted on the complex plane for (a) full resolution model; (b) low resolution model of order 200; (c) reduced rank model of order 200.

Importance of B Matrix

Errors where covariance B_0 is not used in model reduction

Low Res Model of order = 200 vs Reduced Model of order = 200

Log Error



Component of state

Red (dotted) = Low Res Model **Green** (dashed) = Reduced Rank Model

Conclusions

- 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

Monthly Weather Rev, 2008

Work in progress:

- to obtain efficient model reduction techniques for use in data assimilation
- to demonstrate convergence of the Incremental 4DVar method using low order models.