Numerical Model Error in 4D-Variational Data Assimilation

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Centre for Nonlinear Mechanics

What is Data Assimilation?

Data assimilation is used to solve a particular kind of inverse problem:

Given a set of observations and a numerical model for a dynamical system, find the best estimate as to the true state of the system.

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There are many different methods for data assimilation such as,

- the Kalman filter,
- 3D-Variational (3D-Var) data assimilation,
- 4D-Variational (4D-Var) data assimilation.

What is Variational Data Assimilation?

Variational data assimilation solves a specific formulation of the data assimilation problem:

Given a set of observations and a numerical model for a dynamical system, find an initial condition for the numerical model that provides the best approximation to the true state of the system, when a priori information for the initial condition is available.

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- There are two different methods generally used for answering this question,
  - 3D-Variational (3D-Var) data assimilation,
  - 4D-Variational (4D-Var) data assimilation.
- Both methods are used in current operational weather forecast centres to make short and long range weather predictions.

4D-Var Cost Function

4D-Var is formulated as a minimisation problem, where the 4D-Var cost function is minimised with respect to the initial condition for the system.

$$\min_{\mathbf{x}_0} J(\mathbf{x}_0)$$

where,

$$\begin{aligned} J(\mathbf{x}_0) &= (\mathbf{x}_0 - \mathbf{x}_b)^T B^{-1} (\mathbf{x}_0 - \mathbf{x}_b) \\ &\quad + \sum_{l=0}^{L} [\mathbf{y}_l - \mathcal{H}_l(\mathbf{x}_l)]^T \mathcal{R}_l^{-1} [\mathbf{y}_l - \mathcal{H}_l(\mathbf{x}_l)] \\ \mathbf{x}_{l+1} &= \mathcal{M}_{l+1,l}(\mathbf{x}_l) \end{aligned}$$

- The cost function finds the weighted least squares solution between the sets of observations and the results of the numerical model using $\mathbf{x}_b$ as the initial condition.

Errors in Variational Data Assimilation

The errors in variational data assimilation can be divided into four sources,

- background errors,
- observational errors: miscalibration of instrumentation,
- representative errors: discretisation errors,
- model error $\begin{cases} \text{inaccurate model equations,} \\ \text{inaccurate numerical model.} \end{cases}$

Assumptions

Remove all forms of error other than numerical model error and observations errors,

- Neglect the background term of the cost function,
- Take observations at every temporal and spatial grid point $\Rightarrow \mathcal{H}_l = I_N \ \ \forall l$,
- Observations: $\mathbf{y}_l = \tilde{\mathbf{y}}_l + \boldsymbol{\epsilon}_l$ such that $\boldsymbol{\epsilon}_l$ iid $\mathcal{N}(\mathbf{0}, \sigma_o^2 I_N)$, $\sigma_o \in \mathbb{R}$, $\Rightarrow \mathcal{R}_l = \sigma_o^2 I_N \ \ \forall l$.

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\end{aligned}
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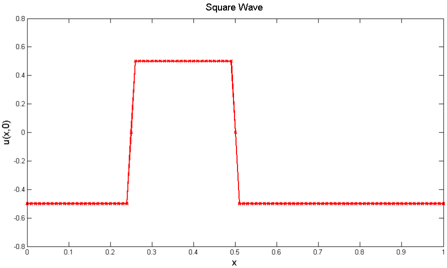
Linear Advection Equation

- Consider the linear advection equation,
  $u : \mathbb{R} \times \mathbb{R} \to \mathbb{R}, \quad (d, t) \mapsto u(d, t),$

$$\begin{aligned} u_t + \eta u_d &= 0, & d \in [0,1), t > 0 \\ u(d,t) &= u(d+1,t), & d \in \mathbb{R}, t \geq 0 \\ u(d,0) &= u_0(d), & d \in [0,1). \end{aligned}$$

  Here the *wave speed* is $\eta \in \mathbb{R}$.
- The true solution is $u(d, t) = u_0(d - \eta t)$ for some function $f : \mathbb{R} \to \mathbb{R}$.

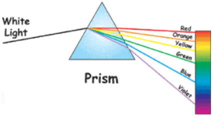


Numerical Dissipation and Dispersion

The initial condition $u_0(d)$ can be considered in the form of a Fourier series,

$$u_0(d) \approx \sum_{p=-\infty}^{\infty} c_p e^{2\pi i p d}, \text{ where } c_p = \int_0^1 u(d,0) e^{-2\pi i p d} dd.$$

http://harishmaas.blogspot.com



www.earthlyissues.com

Definition

- Dissipation - The amplitude of the component waves decrease over time.
- Dispersion - The component waves move out of phase over time.

Numerical Schemes: $u_t(d,t) + \eta u_d(d,t) = 0$

Consider a uniform grid with $N+1$ spatial mesh points with a spatial step size Δd and timestep Δt. Let $U_j^n \approx u(x_j, t^n)$ at each grid point, $t^n = n\Delta t$, $x_j = j\Delta x$. Also, let $h = \eta\frac{\Delta t}{\Delta x}$. The following finite difference schemes are considered,

- the Upwind (explicit) scheme,

$$U_j^{n+1} = hU_{j-1}^n + (1-h)U_j^n,$$

- the Preissman Box (implicit) scheme,

$$(1-h)U_j^{n+1} + (1+h)U_{j+1}^{n+1} = (1+h)U_j^n + (1-h)U_{j+1}^n.$$

- the Lax-Wendroff (explicit) scheme,

$$U_j^{n+1} = \frac{h}{2}(h+1)U_{j-1}^n + (1-h^2)U_j^n + \frac{h}{2}(h-1)U_{j+1}^n,$$

Eigenvalue and Eigenvector Analysis

- Each of the methods discussed can be expressed in the form:

$$\mathbf{U}^{n+1} = M\mathbf{U}^{n},$$

where the jth element of $\mathbf{U}^n$ is U_{j-1}^n, $M \in \mathbb{R}^{N \times N}$.

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- For the Upwind scheme,

$$M = \begin{bmatrix} 1-h & 0 & & & h \\ h & 1-h & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & h & 1-h & 0 \\ 0 & & & h & 1-h \end{bmatrix}.$$

Eigenvectors of M

$$M = V \Lambda V^*$$

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$$[\mathbf{v}_p]_q = \frac{1}{\sqrt{N}} e^{\frac{2\pi i(p-1)(q-1)}{N}} = \frac{1}{\sqrt{N}} e^{2\pi i(p-1)d_q}.$$

- The pth eigenvector is the $(p-1)$th wavenumber component of the Fourier series for $u_0(d)$, sampled at the N mesh points.

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$$\mathbf{U}^0 = \sum_{p=1}^{N} (\mathbf{v}_p^* \mathbf{U}^0)\mathbf{v}_p$$

Eigenvalues of M

The eigenvalues determine the propagation of the wavenumber components of $u_0(d)$,

$$\mathbf{U}^n = V\Lambda^n V^* \mathbf{U}^0$$

The eigenvalues of M control the magnitude and phase shift of each eigenvector,

$$\lambda_p = |\lambda_p| e^{i\theta_p}, \quad \theta_p \in (-2\pi, 0].$$

- $|\lambda_p|$ affects the amplitude of $\mathbf{v}_p$,
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The ideal model would possess $|\lambda_p| = 1$.

Sample Error

- The system is constructed from the N distinguishable wavenumber components on the spatial mesh, represented by the eigenvectors, $\{\mathbf{v}_p\}_{p=1}^N$.
- The unresolvable wavenumber components are aliased to these.
- The coefficient of $\mathbf{v}_p$ in $\mathbf{U}^0$ is given by the Poisson equation,

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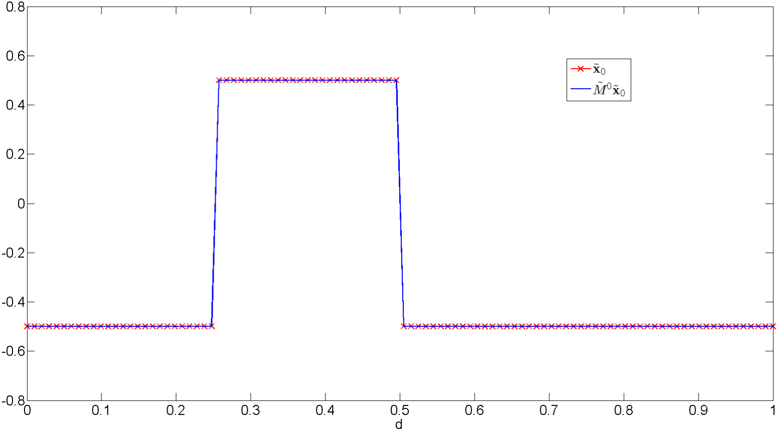
- If λ_p applies no numerical dissipation or dispersion to $\mathbf{v}_p$, it may still apply numerical dispersion to the aliased wavenumber components.

Sample Error: MNIMC scheme, $h = 0.5$

- $t = 0$:



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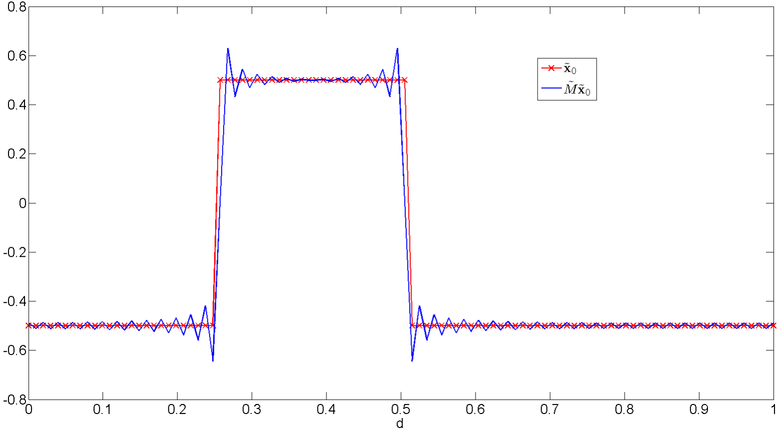
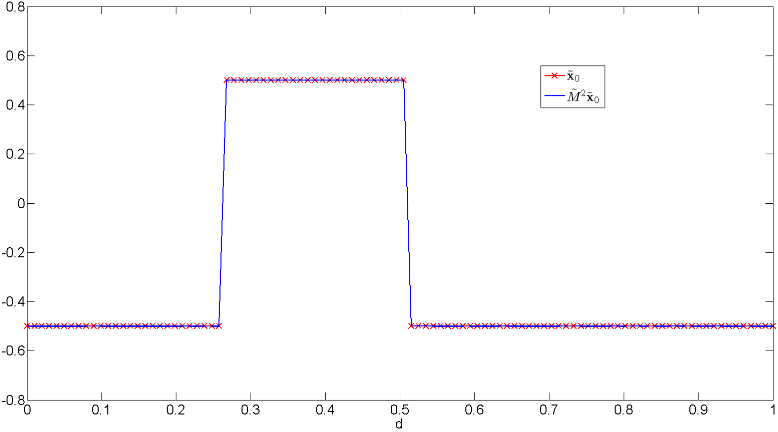
- $t = \Delta t$



Sample Error: MNIMC scheme, $h = 0.5$

- $t = 2\Delta t = \Delta x$ (as $\eta = 1$)



Perfect Observations: NIMC

- Could construct perfect observations using the Numerical Implementation of the Method of Characteristics

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- Only numerically stable and non-dissipative when $h = 1$.

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implemented by the matrix M_{NIMC}.

- Always numerically non-dispersive and does not introduce sample error.
- Only numerically stable and non-dissipative when $h = 1$.
- As a result, produces perfect observations every $\Delta t = \frac{\Delta d}{\eta}$.
- Imperfect scheme produces observations every $\Delta t = \frac{h\Delta d}{\eta}$.

Perfect Observations: MNIMC

- Perfect observations are generated by the Modified NIMC (MNIMC) finite difference scheme implemented by the matrix $\tilde{M} = V\tilde{\Lambda}V^*$, where $\tilde{\lambda}_p = e^{i\tilde{\theta}_p}$ and N is odd such that

$$\tilde{\theta}_p = \begin{cases} \frac{-2\pi i(p-1)h}{N}, & \text{for } p \leq \frac{N+1}{2} \\ 2\pi\left[(h-1) - \frac{(p-1)h}{N}\right], & \text{for } p > \frac{N+1}{2} \end{cases}$$

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- Eigenvectors do not introduce numerical dissipation or dispersion into the resolvable wavenumber components.
- Introduces sample error, so need to add a correction term $\mathbf{r}_l$

$$\tilde{\mathbf{y}}_l = \tilde{M}^l \mathbf{U}^0 + \mathbf{r}_l$$

Dissipation and Dispersion

Choosing $h = 0.5$ results in,

- Upwind: Dissipative,
- Box: Dispersive,
- Lax-Wendroff: Dissipative and Dispersive.

with respect to the resolvable wavenumber components represented by the eigenvectors.

4D-Var Cost Function

Using the finite difference scheme implemented by the matrix M as the forward model, $\mathcal{M}_{l+1,l} := M$ and $\mathbf{x}_l := \mathbf{U}^l \;\; \forall l$. Hence,

$$J(\mathbf{x}_0) = \frac{1}{\sigma_o^2} \sum_{l=0}^{L} [\mathbf{y}_l - M^l \mathbf{x}_0]^T [\mathbf{y}_l - M^l \mathbf{x}_0]$$

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Consider,

- Initially consider perfect observations ie: $\mathbf{y}_l = \tilde{\mathbf{y}}_l \;\; \forall l$. Arbitrarily choose $\sigma_o^2 = 1$.
- Then re-introduce observation errors.

Analysing Fourier Components

Let $h = \frac{q}{a}$, $q, a, \in \mathbb{Z}$ such that $\gcd(q,a) = 1$. Then the analysis vector for perfect observations can be written as,

$$\mathbf{x}_a = A_L \tilde{\mathbf{x}}_0 + \boldsymbol{\rho}_L$$

where the *model resolution matrix* $A_L \in \mathbb{R}^{N \times N}$ and $\boldsymbol{\rho}_L \in \mathbb{R}^N$ are,

$$A_L = V \left[\sum_{r=0}^{L} (\Lambda^* \Lambda)^r \right]^{-1} \left[\sum_{l=0}^{L} (\Lambda^* \tilde{\Lambda})^l \right] V^*,$$

$$\begin{aligned} \boldsymbol{\rho}_L &= V \left[\sum_{r=0}^{L} (\Lambda^* \Lambda)^r \right]^{-1} \left[\left\{ \sum_{l=0}^{\frac{L-[L]_a}{a}-1} (\Lambda^* \tilde{\Lambda})^{la} \right\} \left\{ \sum_{y=1}^{a-1} (\Lambda^*)^y V^* \mathbf{r}_y \right\} \right. \\ &\quad \left. + \left(\Lambda^* \tilde{\Lambda} \right)^{L-[L]_a} \left\{ \sum_{y=1}^{[L]_a} (\Lambda^*)^y V^* \mathbf{r}_y \right\} \right], \end{aligned}$$

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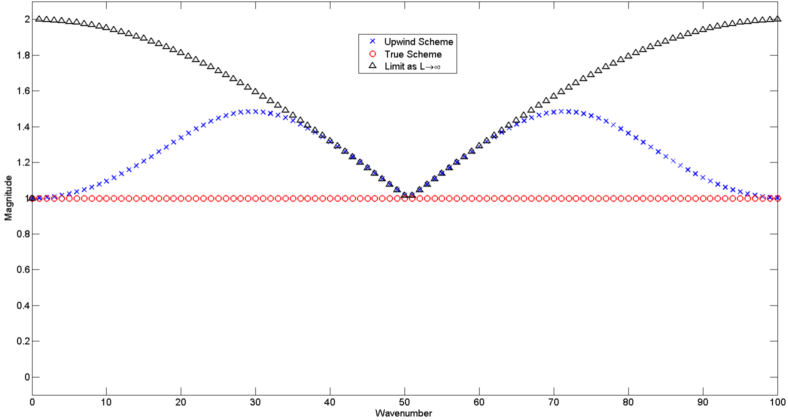
Non-Dispersive Eigenvalues: Upwind Scheme

$N = 101$, $L = 4$: $A_L = V \text{diag}(\nu_p) V^*$



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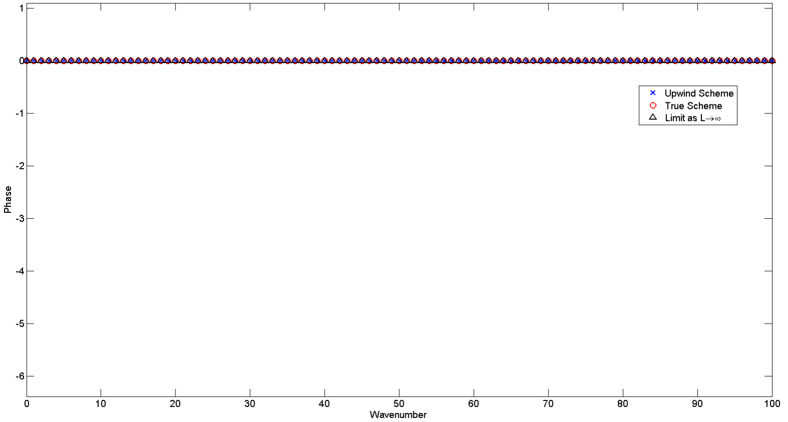
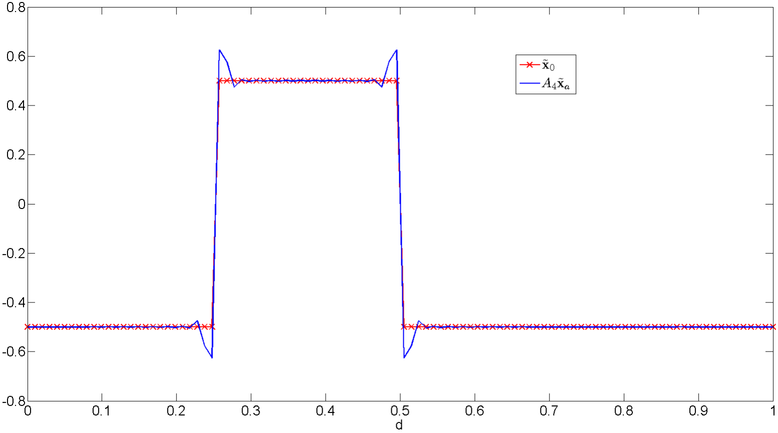


Non-Dispersive Eigenvalues: Upwind Scheme

$N = 101,\ L = 4$: $A_L \tilde{\mathbf{x}}_0$



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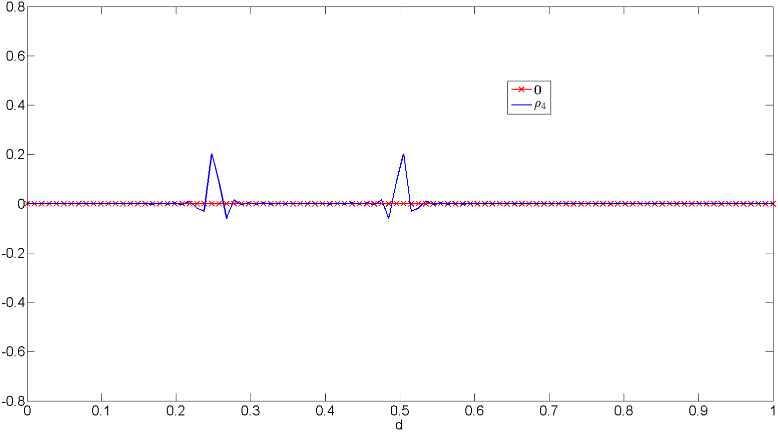

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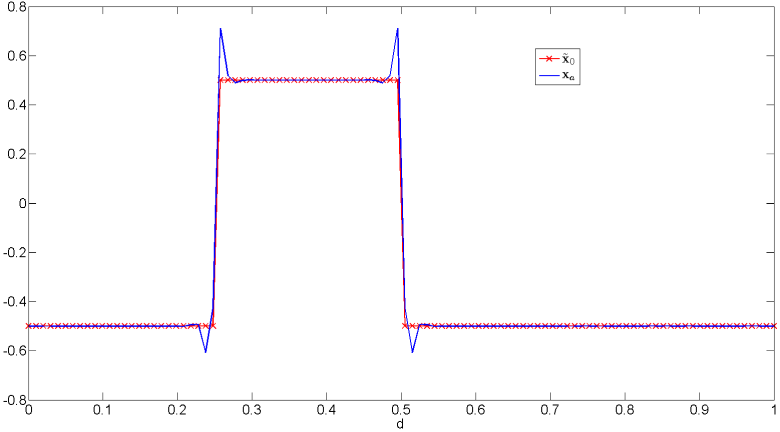

Non-Dissipative Eigenvalues: Preissman Box Scheme

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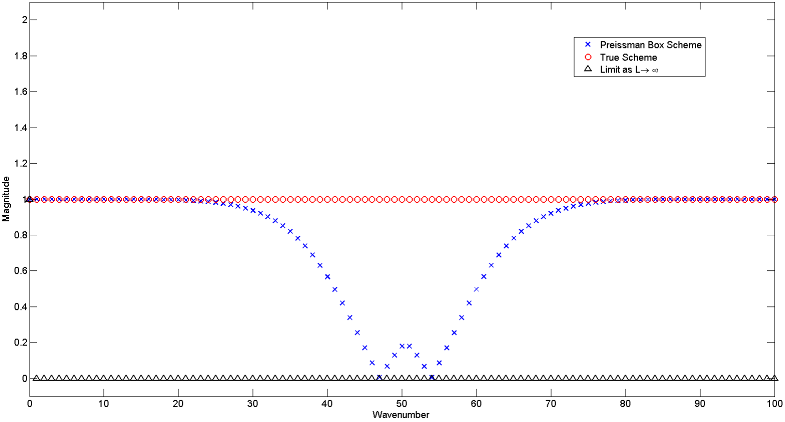

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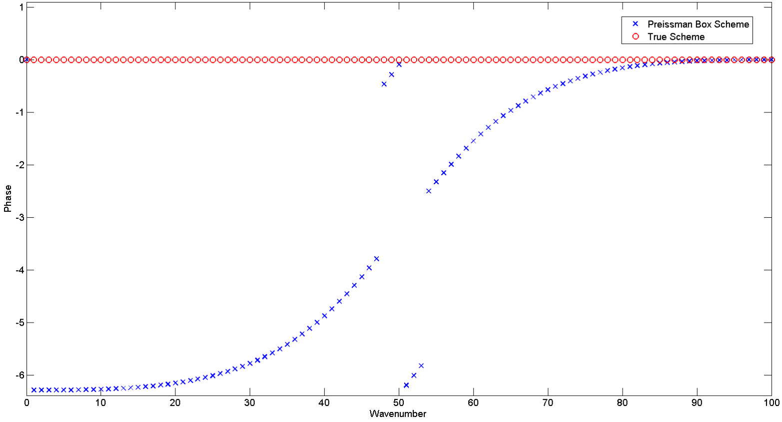

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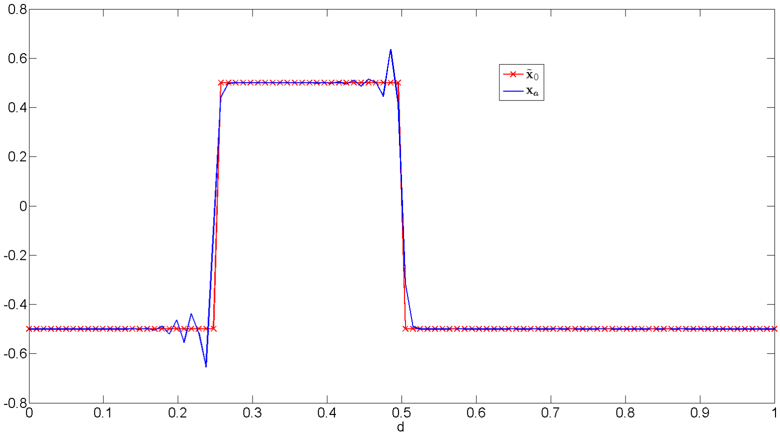

Dissipative and Dispersive Eigenvalues: Lax-Wendroff Scheme

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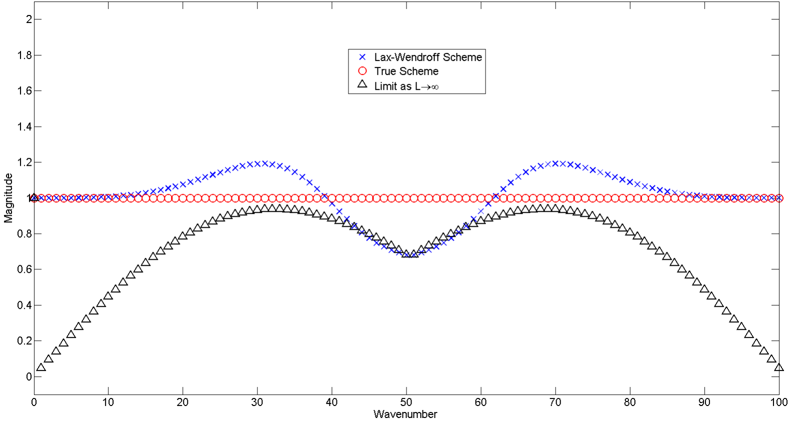

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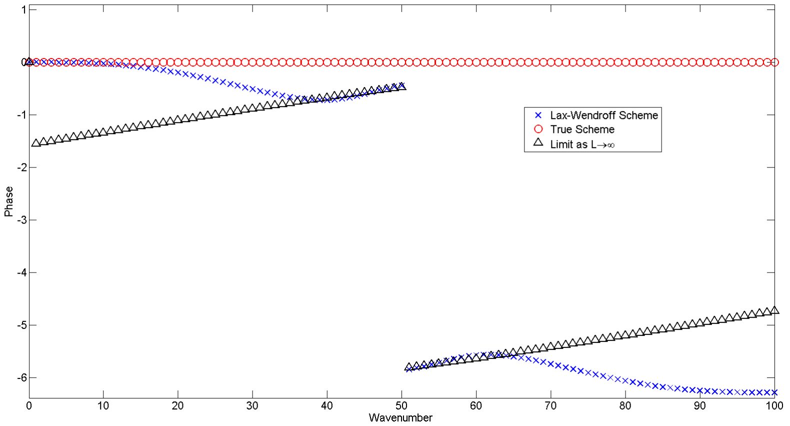
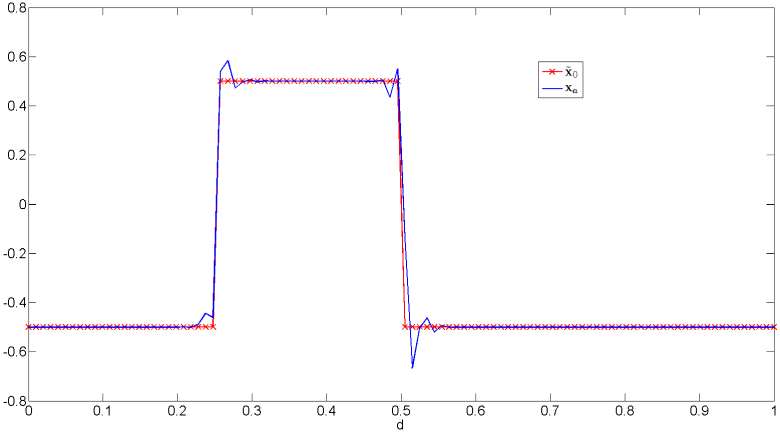


Dissipative and Dispersive Eigenvalues: Lax-Wendroff Scheme

$N = 101$, $L = 4$: $\mathbf{x}_a = A_L \tilde{\mathbf{x}}_0 + \boldsymbol{\rho}_L$



Upper Bound

$$\|\tilde{\mathbf{x}}_0 - \mathbf{x}_a\|_2^2 \leq N\left\{|1-\nu_1|D_1 + (|1-\nu_1| - 2\xi_1)\frac{D_3}{N^{\mathbf{r}+1}}\right\}^2$$
$$+N\sum_{p=2}^{\frac{N+1}{2}}\left\{|1-\nu_p|\frac{D_2}{(p-1)^{\mathbf{r}+1}} + (|1-\nu_p| - 2\xi_p)\frac{D_3}{N^{\mathbf{r}+1}}\right\}^2$$
$$+N\sum_{p=\frac{N+3}{2}}^{N}(|1-\nu_p| - 2\xi_p)^2\left(\frac{D_2}{(p-1)^{\mathbf{r}+1}} + \frac{D_3}{N^{\mathbf{r}+1}}\right)^2,$$

where D_1, D_2 and D_3 are constants independent of p and N, $\mathbf{r} \in \mathbb{N}_0$ denotes the regularity of the initial condition $u(d,0)$ and

$$\xi_p = \frac{\left|\sum_{l=0}^{\frac{L-[L]_a}{a}-1}\left[|\lambda_p|^a e^{ia\phi_p}\right]^l\right|\left\{\sum_{y=1}^{a-1}|\lambda_p|^y\right\} + |\lambda_p|^{L-[L]_a}\sum_{y=1}^{[L]_a}|\lambda_p|^y}{\sum_{s=0}^{L}|\lambda_p|^{2s}}.$$

Upper Bound

$$\begin{aligned}\|\tilde{\mathbf{x}}_0 - \mathbf{x}_a\|_2^2 \quad \leq \quad & N\left\{|1-\nu_1|D_1 + (|1-\nu_1| - 2\xi_1)\frac{D_3}{N^{\mathbf{r}+1}}\right\}^2 \\ & + N\sum_{p=2}^{\frac{N+1}{2}}\left\{|1-\nu_p|\frac{D_2}{(p-1)^{\mathbf{r}+1}} + (|1-\nu_p| - 2\xi_p)\frac{D_3}{N^{\mathbf{r}+1}}\right\}^2 \\ & + N\sum_{p=\frac{N+3}{2}}^{N}(|1-\nu_p| - 2\xi_p)^2\left(\frac{D_2}{(p-1)^{\mathbf{r}+1}} + \frac{D_3}{N^{\mathbf{r}+1}}\right)^2,\end{aligned}$$

where D_1, D_2 and D_3 are constants independent of p and N, $\mathbf{r} \in \mathbb{N}_0$ denotes the regularity of the initial condition $u(d, 0)$ and

$$\xi_p = \frac{\left|\sum_{l=0}^{\frac{L-[L]_a}{a}-1}\left[|\lambda_p|^a e^{ia\phi_p}\right]^l\right|\left\{\sum_{y=1}^{a-1}|\lambda_p|^y\right\} + |\lambda_p|^{L-[L]_a}\sum_{y=1}^{[L]_a}|\lambda_p|^y}{\sum_{s=0}^{L}|\lambda_p|^{2s}}.$$

Upper Bound

$$
\begin{aligned}
\|\tilde{\mathbf{x}}_0 - \mathbf{x}_a\|_2^2 \leq \; & N \left\{ |1-\nu_1| D_1 + (|1-\nu_1| - 2\xi_1) \frac{D_3}{N^{\mathbf{r}+1}} \right\}^2 \\
& + N \sum_{p=2}^{\frac{N+1}{2}} \left\{ |1-\nu_p| \frac{D_2}{(p-1)^{\mathbf{r}+1}} + (|1-\nu_p| - 2\xi_p) \frac{D_3}{N^{\mathbf{r}+1}} \right\}^2 \\
& + N \sum_{p=\frac{N+3}{2}}^{N} (|1-\nu_p| - 2\xi_p)^2 \left(\frac{D_2}{(p-1)^{\mathbf{r}+1}} + \frac{D_3}{N^{\mathbf{r}+1}} \right)^2,
\end{aligned}
$$

where D_1, D_2 and D_3 are constants independent of p and N, $\mathbf{r} \in \mathbb{N}_0$ denotes the regularity of the initial condition $u(d,0)$ and

$$
\xi_p = \frac{\left| \sum_{l=0}^{\frac{L-[L]_{\mathbf{a}}}{\mathbf{a}}-1} \left[|\lambda_p|^{\mathbf{a}} e^{i\mathbf{a}\phi_p} \right]^l \right| \left\{ \sum_{y=1}^{\mathbf{a}-1} |\lambda_p|^y \right\} + |\lambda_p|^{L-[L]_{\mathbf{a}}} \sum_{y=1}^{[L]_{\mathbf{a}}} |\lambda_p|^y}{\sum_{s=0}^{L} |\lambda_p|^{2s}}.
$$

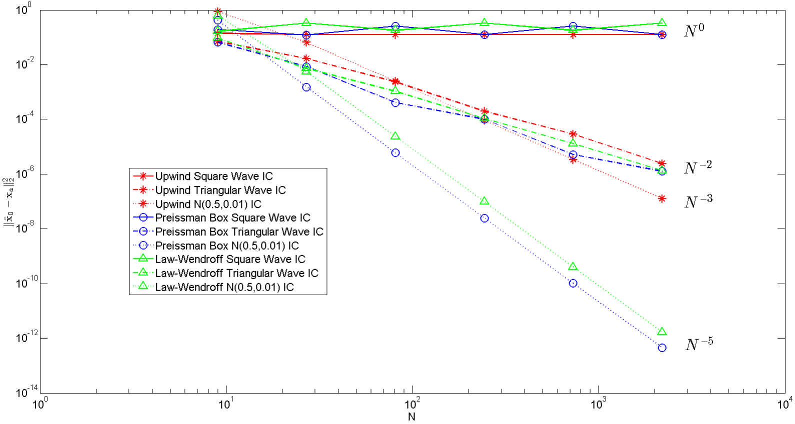
Numerical Results

Order of convergence to zero wrt N^α or L^β.

r	α		β	
	Upper Bound	Data Assimilation	Upper Bound	Data Assimilation
0	-6.7708×10^{-15}	1.4148×10^{-15}	5.7945×10^{-1}	5.6939×10^{-1}
1	-2.0000	-2.2612	1.5053	1.5096
∞	-3.0000	-3.0000	2.0000	2.0000

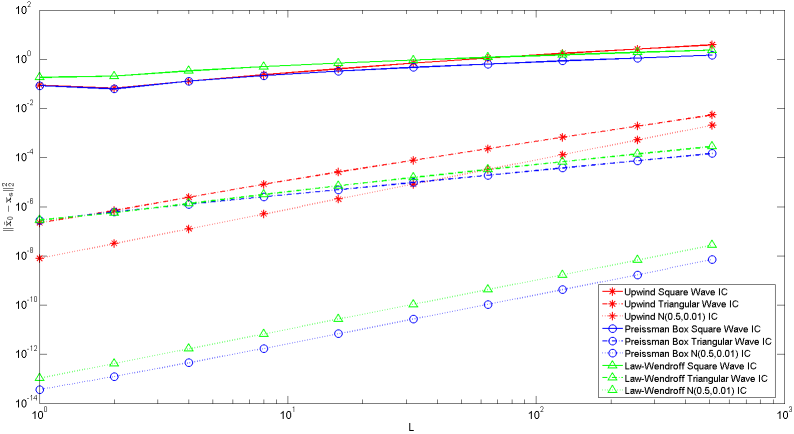
Numerical Model Error

The order of convergence of $\|\mathbf{x}_a - \tilde{\mathbf{x}}_0\|_2^2$ to zero, with respect to N. $L = 4$ and $\alpha = 2:7$ such that $N = 3^\alpha$.



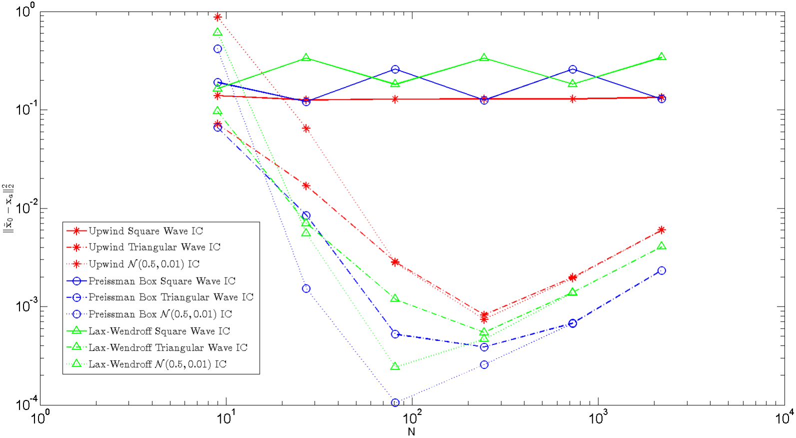
Numerical Model Error

The order of convergence of $\|\mathbf{x}_a - \tilde{\mathbf{x}}_0\|_2^2$ to zero, with respect to L.
$N = 3^7$ and $\alpha = 0 : 9$ such that $L = 2^\beta$.



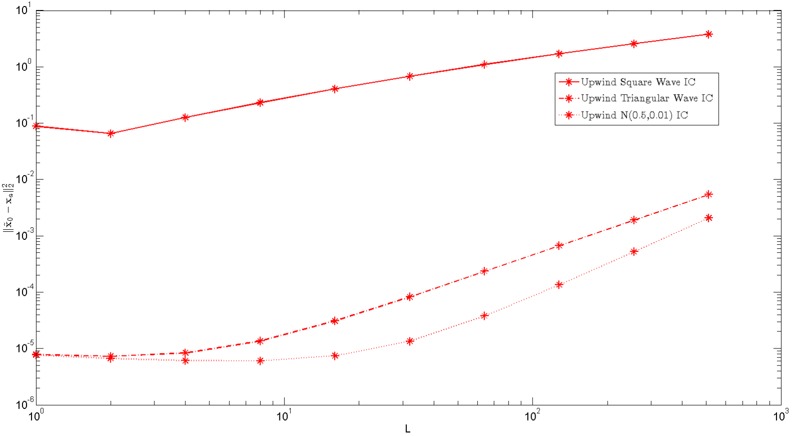
Observation and Numerical Model Errors

The order of convergence of $\|\mathbf{x}_a - \tilde{\mathbf{x}}_0\|_2^2$ to zero, with respect to N.
$L = 4$, $\sigma_o^2 = 5 \times 10^{-6}$ and $\alpha = 2 : 7$ such that $N = 3^\alpha$.



Observation and Numerical Model Errors

The order of convergence of $\|\mathbf{x}_a - \tilde{\mathbf{x}}_0\|_2^2$ to zero, with respect to L.
$N = 3^7$, $\sigma_o^2 = 5 \times 10^{-9}$ and $\alpha = 0:9$ such that $L = 2^\beta$.



Summary

Conclusion

- Dispersive schemes result in destructive interference. This leads to a loss of information in the analysis vector and its subsequent forecast.
- The order of convergence of $\|\tilde{\mathbf{x}}_o - \mathbf{x}_a\|_2^2$ to zero, with respect to N, is dependent on the regularity of $u_0(d)$.
- There is a critical value of N where the effects of both numerical model error and observation error are minimised.

Future Work

In the future we aim to,

- Quantify and reduce the effects of numerical dispersion and dissipation on the forecast,
- Consider the linearised shallow water equations,
- Investigate realistic meteorological methods and models.