Nonlinear error dynamics for cycled data assimilation methods

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Dynamical system

- Dynamical system: nonlinear dynamical flow and a linear measurement equation.
- Let M^(t)_k : X → X and M_k : X → X be a true nonlinear model operator and a modelled nonlinear model operator respectively.
- All operators are mapping a state x^(t)_{k-1} ∈ X discretely onto its state x^(t)_k for k ∈ N₀ for the Hilbert space (X, || · ||x).
- The operator $\mathcal{M}_k: \mathbf{X} \to \mathbf{X}$ is modelled, such that

$$\mathcal{M}_{k}\left(\mathbf{x}_{k}^{(t)}\right) = \mathcal{M}_{k}^{(t)}\left(\mathbf{x}_{k}^{(t)}\right) + \boldsymbol{\zeta}_{k+1}, \qquad (1)$$

where ζ_{k+1} is some additive noise which we call *model error* and is bounded by some constant v > 0 for all time t_k for $k \in \mathbb{N}_0$.

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- Let H be an injective linear time-invariant compact observation operator, such that H : X → Y, for Hilbert spaces (X, || · ||_X) and (Y, || · ||_Y).
- Let $\mathbf{y}_k^{(t)} \in \mathbf{Y}$ be the true observations (measurements) located at discrete times t_k linearly, such that

$$\mathbf{y}_{k}^{(t)} = H^{(t)}\mathbf{x}_{k}^{(t)} = H\mathbf{x}_{k}^{(t)} = \mathbf{y}_{k} - \boldsymbol{\eta}_{k}, \qquad (2)$$

where η_k is some additive noise that we call the *observation* error and is bounded by some constant $\delta > 0$ for all time t_k for $k \in \mathbb{N}_0$.

• It is possible to carry through the same analysis using a noise term on *H* modelled,

$$\left(H-H^{(t)}\right)\mathbf{x}_{k}^{(t)}=\boldsymbol{\omega}_{k}.$$
(3)

Definition (p.10 in Kress 1999)

An inner product space, which is complete with respect to the norm

$$\|\mathbf{x}\| := \langle \mathbf{x}, \mathbf{x} \rangle^{1/2}, \qquad (4)$$

for all $\mathbf{x} \in \mathbf{X}$, is called a Hilbert space.

Definition (Definition 7.1 in Rynne and Youngson 2007)

Let **X** and **Y** be normed space. An operator $H \in L(\mathbf{X}, \mathbf{Y})$ is compact if, for any bounded sequence (\mathbf{x}_n) in **X**, the sequence $(H\mathbf{x}_n)$ in **Y** contains a convergent subsequence.

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- Develop theory demonstrating the asymptotic stability of a cycled data assimilation scheme with an ill-posed observation operator in a nonlinear infinite dimensional setting.
- Work within the framework of data assimilation scheme that employ static covariances, such as three dimensional variational data assimilation (3DVar).
- Here we extend previous linear results from *R W E Potthast*, *A J F Moodey*, *A S Lawless and P J van Leeuwen 2012*.

• We define the *analysis error* as the difference between the analysis and the true state of the system, such that

$$\mathbf{e}_k := \mathbf{x}_k^{(a)} - \mathbf{x}_k^{(t)}, \tag{5}$$

where $\mathbf{x}_{k}^{(t)}$ represents the true state of the system at time t_{k} for $k \in \mathbb{N}_{0}$.

• We will call a data assimilation scheme *stable* if given some constant *C* > 0

$$\|\mathbf{e}_k\|_{\mathbf{X}} \le C \tag{6}$$

as $k \to \infty$ with some appropriate norm $\| \cdot \|_{\mathbf{X}}$.

 The analysis error in other fields is known as state reconstruction error, observer error, estimation error, etc.





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 Mathematically, we interpret the data assimilation task as seeking x^(a) at every assimilation step t_k, k ∈ N₀ to solve an operator equation of the first kind

$$H\mathbf{x}_{k}^{(a)} = \mathbf{y}_{k}.$$
 (7)

• This operator equation represents a Fredholm integral equation of the first kind and is ill-posed when the dimension of the state space **X** is infinite.

- Hadamard defined that a well-posed problem must satisfy:
 - **1** There exists a solution to the problem (existence).
 - 2 There is at most one solution to the problem (uniqueness).
 - The solution depends continuously on the data (stability).

If a problem does not satisfy all three of these condition, it is *ill-posed* in the sense of *Hadamard*.

Nashed defined that an operator equation is called well-posed if

• the set of observations is a closed set, that is if H(X) is closed. If a problem does not satisfy this property, then it is *ill-posed*

in the sense of Nashed (Nashed 1981, Nashed 1987).

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Theorem (Theorem 15.4 in *Kress 1999*)

Let **X** and **Y** be normed spaces and $H \in L(\mathbf{X}, \mathbf{Y})$ be a compact operator. If **X** has infinite dimension then H cannot have a bounded inverse and the operator equation of the first kind is ill-posed.

- Regularization methods exist to provide a stable approximate solution to the ill-posed problem.
- Tikhonov-Phillips regularization shifts the the eigenvalues of the operator H*H by a regularization parameter α, where H* is the adjoint to the operator H.

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Definition

Given measurements $\mathbf{y}_k \in \mathbf{Y}$ for $k \in \mathbb{N}_0$ and an initial guess $\mathbf{x}_k^{(b)}$, the objective of cycled Tikhonov-Phillips regularization is to seek an estimate, $\mathbf{x}_k^{(a)}$ that minimises the functional,

$$\mathcal{J}^{(CTP)}(\mathbf{x}_k) := \alpha \left\| \mathbf{x}_k - \mathbf{x}_k^{(b)} \right\|_{\ell^2}^2 + \left\| \mathbf{y}_k - H \mathbf{x}_k \right\|_{\ell^2}^2, \qquad (8)$$

with respect to \mathbf{x}_k for the ℓ^2 norm, where $\mathbf{x}_k^{(b)} = \mathcal{M}_{k-1}(\mathbf{x}_{k-1}^{(a)})$ and $\alpha > 0$.

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Theorem

If H is linear, the minimiser $\mathbf{x}_{k}^{(a)}$ to (8) is given by

$$\mathbf{x}_{k}^{(a)} = \mathcal{M}_{k-1}\mathbf{x}_{k-1}^{(a)} + \mathscr{R}_{\alpha}\left(\mathbf{y}_{k} - \mathcal{H}\mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(a)}\right)\right), \qquad (9)$$

given $\mathbf{x}_{k}^{(b)} = \mathcal{M}_{k-1}(\mathbf{x}_{k-1}^{(a)})$, where

$$\mathscr{R}_{\alpha} = (\alpha I + H^* H)^{-1} H^* \tag{10}$$

is known as the Tikhonov-Phillips inverse, with an adjoint H^* and a regularization parameter α . Here (9) is what we characterise as cycled Tikhonov-Phillips regularization.

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Theorem

If H is linear then the minimiser $\mathbf{x}_{k}^{(a)}$ to

$$\mathcal{J}^{(3D)}(\mathbf{x}_{k}) = \left\langle B^{-1}\left(\mathbf{x}_{k} - \mathbf{x}_{k}^{(b)}\right), \mathbf{x}_{k} - \mathbf{x}_{k}^{(b)} \right\rangle_{\ell^{2}} \\ + \left\langle R^{-1}\left(\mathbf{y}_{k} - H\mathbf{x}_{k}\right), \mathbf{y}_{k} - H\mathbf{x}_{k} \right\rangle_{\ell^{2}}, \qquad (11)$$

is given by

$$\mathbf{x}_{k}^{(a)} = \mathbf{x}_{k}^{(b)} + \mathscr{K}\left(\mathbf{y}_{k} - H\mathbf{x}_{k}^{(b)}\right), \qquad (12)$$

where

$$\mathscr{K} := BH'(HBH' + R)^{-1}$$
(13)

is the Kalman gain and H' is the adjoint with respect to the Euclidean inner product.

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Theorem (Theorem 2.1 in *Marx and Potthast 2012*)

For the Euclidean inner product and the weighted norms

$$\langle \cdot, \cdot \rangle_{B^{-1}} := \left\langle \cdot, B^{-1} \cdot \right\rangle$$
 on X and $\left\langle \cdot, \cdot \right\rangle_{R^{-1}} := \left\langle \cdot, R^{-1} \cdot \right\rangle$ on Y (14)

for self-adjoint, positive definite operators B and R, the Kalman gain \mathcal{K} for 3DVar corresponds to the Tikhonov-Phillips inverse \mathcal{R}_{α} where its adjoint is given by

$$H^* = \alpha B H' R^{-1} \tag{15}$$

for $\alpha = 1$.

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From

$$\mathbf{x}_{k}^{(a)} = \mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(a)}\right) + \mathscr{R}_{\alpha}\left(\mathbf{y}_{k} - \mathcal{H}\mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(a)}\right)\right), \quad (16)$$

we can derive

$$\mathbf{e}_{k} = N\left(\mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(a)}\right) - \mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(t)}\right)\right) + N\boldsymbol{\zeta}_{k} + \mathscr{R}_{\alpha}\boldsymbol{\eta}_{k}, \quad (17)$$

where $\mathbf{e}_k := \mathbf{x}_k^{(a)} - \mathbf{x}_k^{(t)}$, $N := I - \mathscr{R}_{\alpha}H$ and ζ_k and η_k are the noise terms.

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Full deterministic analysis update

As a first attempt,
$$\|\mathbf{e}_{k}\| \leq \|N\| \cdot \left\| \mathcal{M}_{k-1} \left(\mathbf{x}_{k-1}^{(a)} \right) - \mathcal{M}_{k-1} \left(\mathbf{x}_{k-1}^{(t)} \right) \right\| + \|N\| v + \|\mathscr{R}_{\alpha}\| \delta.$$
(18)

Assumption

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The nonlinear mapping $\mathcal{M}_k : \mathbf{X} \to \mathbf{X}$ is Lipschitz continuous with a global Lipschitz constant such that given any $\mathbf{a}, \mathbf{b} \in \mathbf{X}$,

$$\|\mathcal{M}_k(\mathbf{a}) - \mathcal{M}_k(\mathbf{b})\| \le K_k \cdot \|\mathbf{a} - \mathbf{b}\|$$
(19)

where $K_k \leq K$, the global Lipschitz constant for all time t_k , for $k \in \mathbb{N}_0$.

Therefore we obtain

$$e_{k} \leq \nu \cdot e_{k-1} + \|N\| \upsilon + \|\mathscr{R}_{\alpha}\| \delta,$$
(20)

where $\nu := \mathcal{K} \| \mathbf{N} \|$ given the global Lipschitz constant \mathcal{K} ,

Theorem (*Moodey et al. 2013*)

For the Hilbert space $(\mathbf{X}, \|\cdot\|_{B^{-1}})$, let the model error ζ_k , $k \in \mathbb{N}_0$ be bounded by $\upsilon > 0$. Let the observation error η_k , $k \in \mathbb{N}_0$ be bounded by $\delta > 0$. If the nonlinear model operator $\mathcal{M}_k : \mathbf{X} \to \mathbf{X}$ is Lipschitz continuous and satisfies then the analysis error evolution $e_k := \|\mathbf{e}_k\|$ is estimated by

$$e_{k} \leq \nu^{k} e_{0} + \sum_{l=0}^{k-1} \nu^{l} \left(\|\boldsymbol{N}\| \upsilon + \|\mathscr{R}_{\alpha}\| \delta \right),$$

$$(21)$$

for $k \in \mathbb{N}_0$. If $\nu < 1$ then

$$\limsup_{k \to \infty} e_k \le \frac{\|N\| \upsilon + \|\mathscr{R}_{\alpha}\| \delta}{1 - \nu}.$$
 (22)

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Lemma (Potthast et al. 2012)

Let **X** and **Y** be Hilbert spaces and let $H \in L(\mathbf{X}, \mathbf{Y})$ be an injective compact linear operator, then the operator norm of the regularized reconstruction error operator is given by

$$\|N\| = \|I - \mathscr{R}_{\alpha}H\| = 1.$$
(23)

This means to obtain $\nu := K ||N|| < 1$, the model operator \mathcal{M}_k must be strictly damping, that is the global Lipschitz constant K < 1.

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Question: Can we do better than this?

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State space decomposition

- We use the singular system of the observation operator to split the state space. Let (μ_i, φ_i, g_i) be the singular system of H.
- Let $P^{(1)}$ and $P^{(2)}$ be orthogonal projection operators, such that

$$P^{(1)}: \mathbf{X} \to \operatorname{span}\{\varphi_i, i \le n\} \text{ and } P^{(2)}: \mathbf{X} \to \operatorname{span}\{\varphi_i, i > n\},$$
(24)
for $i, n \in \mathbb{N}$.

• We define the following orthogonal subspaces

$$\mathbf{X}^{(1)} := \operatorname{span}\{\varphi_1, \dots, \varphi_n\} \text{ and } \mathbf{X}^{(2)} := \operatorname{span}\{\varphi_{n+1}, \dots, \varphi_\infty\}.$$
(25)

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Then we can expand our error evolution as follows,

$$\mathbf{e}_{k} = N\left(P^{(1)} + P^{(2)}\right)\left(\mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(a)}\right) - \mathcal{M}_{k-1}\left(\mathbf{x}_{k-1}^{(t)}\right)\right) + N\zeta_{k} + \mathscr{R}_{\alpha}\boldsymbol{\eta}_{k}$$
(26)
$$= N|_{\mathbf{X}^{(1)}}\left(\mathcal{M}_{k-1}^{(1)}\left(\mathbf{x}_{k-1}^{(a)}\right) - \mathcal{M}_{k-1}^{(1)}\left(\mathbf{x}_{k-1}^{(t)}\right)\right) + N\zeta_{k} + N|_{\mathbf{X}^{(2)}}\left(\mathcal{M}_{k-1}^{(2)}\left(\mathbf{x}_{k-1}^{(a)}\right) - \mathcal{M}_{k-1}^{(2)}\left(\mathbf{x}_{k-1}^{(t)}\right)\right) + \mathscr{R}_{\alpha}\boldsymbol{\eta}_{k},$$
(27)

where

$$\mathcal{M}_k^{(1)}(\cdot) := P^{(1)} \circ \mathcal{M}_k(\cdot) \text{ and } \mathcal{M}_k^{(2)}(\cdot) := P^{(2)} \circ \mathcal{M}_k(\cdot).$$
 (28)

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Taking norms and rearranging we have,

$$\begin{aligned} \|\mathbf{e}_{k}\| &= \left\| N|_{\mathbf{X}^{(1)}} \left(\mathcal{M}_{k-1}^{(1)} \left(\mathbf{x}_{k-1}^{(a)} \right) - \mathcal{M}_{k-1}^{(1)} \left(\mathbf{x}_{k-1}^{(t)} \right) \right) + N\zeta_{k} \\ &+ N|_{\mathbf{X}^{(2)}} \left(\mathcal{M}_{k-1}^{(2)} \left(\mathbf{x}_{k-1}^{(a)} \right) - \mathcal{M}_{k-1}^{(2)} \left(\mathbf{x}_{k-1}^{(t)} \right) \right) + \mathscr{R}_{\alpha} \eta_{k} \right\| \end{aligned}$$

$$(29)$$

$$\leq \left(K_{k-1}^{(1)} \cdot \|N|_{\mathbf{X}^{(1)}}\| + K_{k-1}^{(2)} \cdot \|N|_{\mathbf{X}^{(2)}}\| \right) \cdot \left\| \mathbf{x}_{k-1}^{(a)} - \mathbf{x}_{k-1}^{(t)} \right\| \\ &+ \|N\zeta_{k}\| + \|\mathscr{R}_{\alpha} \eta_{k}\| \tag{30}$$

where we assume Lipschitz continuity,

$$\left\|\mathcal{M}_{k-1}^{(j)}(\mathbf{x}_{k-1}^{(a)}) - \mathcal{M}_{k-1}^{(j)}(\mathbf{x}_{k-1}^{(t)})\right\| \le \mathcal{K}_{k-1}^{(j)} \left\|\mathbf{x}_{k-1}^{(a)} - \mathbf{x}_{k-1}^{(t)}\right\|$$
(31)

for j = 1, 2, with restrictions according to the singular system of H.

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Lemma (Potthast et al. 2012)

Let $(\mathbf{X}, \|\cdot\|_{B^{-1}})$ be a Hilbert space with weighted norm and let H be an injective linear compact observation operator. Then, by choosing the regularization parameter $\alpha > 0$ sufficiently small we can find a parameter $0 < \rho < 1$, such that $\|N\|_{\mathbf{X}^{(1)}}\| \le \rho < 1$.

Lemma (Potthast et al. 2012)

Let $(\mathbf{X}, \|\cdot\|_{B^{-1}})$ be a Hilbert space with weighted norm and let H be an injective linear compact observation operator, then the operator norm of the regularized reconstruction error operator is given by

$$\|N|_{\mathbf{X}^{(2)}}\| = 1. \tag{32}$$

• We require that $\nu < 1.$ Applying our norm estimates we have that

$$\nu := \mathcal{K}^{(1)} \cdot \|\mathcal{N}|_{\mathbf{X}^{(1)}}\| + \mathcal{K}^{(2)} \cdot \|\mathcal{N}|_{\mathbf{X}^{(2)}}\| \le \mathcal{K}^{(1)} \cdot \rho + \mathcal{K}^{(2)}.$$
 (33)

• The nonlinear system \mathcal{M}_k has to be damping in $\mathbf{X}^{(2)}$ for all time.

Definition

A nonlinear system \mathcal{M}_k , $k \in \mathbb{N}_0$, is *dissipative with respect to H* if it is Lipschitz continuous and damping with respect to higher spectral modes of H, in the sense that $\mathcal{M}_k^{(2)}$ satisfies

$$\left\|\mathcal{M}_{k}^{(2)}(\mathbf{a}) - \mathcal{M}_{k}^{(2)}(\mathbf{b})\right\| \leq \mathcal{K}_{k}^{(2)} \cdot \|\mathbf{a} - \mathbf{b}\|$$
(34)

 $orall \, \mathbf{a}, \mathbf{b} \in \mathbf{X}$, where $\mathcal{K}_k^{(2)} \leq \mathcal{K}^{(2)} < 1$ uniformly for $k \in \mathbb{N}_0.$

Final result

Under this assumption that \mathcal{M}_k is dissipative with respect to H, we can choose the regularization parameter $\alpha > 0$ small enough, such that

$$\rho < \frac{1 - K^{(2)}}{K^{(1)}},\tag{35}$$

to achieve a stable cycled scheme. We are now able to summarise this result in the following theorem.

Theorem (*Moodey et al. 2013*)

Let $(\mathbf{X}, \|\cdot\|_{B^{-1}})$ be a Hilbert space with weighted norm. Let the nonlinear system $\mathcal{M}_k : \mathbf{X} \to \mathbf{X}$ be Lipschitz continuous and dissipative with respect to higher spectral modes of H. Then, for regularization parameter $\alpha > 0$ sufficiently small, we have $\nu := K^{(1)} \|N|_{\mathbf{X}^{(1)}}\| + K^{(2)} \|N|_{\mathbf{X}^{(2)}}\| < 1$. Then,

$$\limsup_{k \to \infty} \|\mathbf{e}_k\| \le \frac{\|N\| \upsilon + \|\mathscr{R}_{\alpha}\| \delta}{1 - \nu}.$$
 (36)

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• The Lorenz '63 equations are as follows,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\sigma(x - y),\tag{37}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \rho x - y - xz, \qquad (38)$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = xy - \beta z, \tag{39}$$

where typically σ , ρ and β are known as the Prandtl number, the Rayleigh number and a non-dimensional wave number respectively.

• We choose the classical parameters, $\sigma = 10$, $\rho = 28$ and $\beta = 8/3$ and discretise the system using a fourth order Runge-Kutta approximation.

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We set up a twin experiment and begin with an initial condition,

$$\left(x_0^{(t)}, y_0^{(t)}, z_0^{(t)}\right) = (-5.8696, -6.7824, 22.3356),$$
 (40)

- We produce a run of the system until time t = 100 with a step-size h = 0.01, which we call a truth run.
- Now we create observations at every tenth time-step from the truth run by adding random normally distributed noise with zero mean and standard deviation $\sigma_{(o)} = \sqrt{2}/40$.
- The background state is calculated in the same way at initial time t_0 with zero mean and standard deviation $\sigma_{(b)} = 1/400$ such that,

$$\left(x_0^{(b)}, y_0^{(b)}, z_0^{(b)}\right) = (-5.8674, -6.7860, 22.3338).$$
 (41)

Now we calculate

$$\mathbf{e}_{k} = (I - \mathscr{R}_{\alpha}H) \left(\mathcal{M}_{k-1} \left(\mathbf{x}_{k-1}^{(a)} \right) - \mathcal{M}_{k-1} \left(\mathbf{x}_{k-1}^{(t)} \right) \right) + \mathscr{R}_{\alpha} \boldsymbol{\eta}_{k}.$$

 We calculate a sampled background error covariance between the background state and true state over the whole trajectory such that

$$B = \begin{pmatrix} 117.6325 & 117.6374 & -2.3513\\ 117.6374 & 152.6906 & -2.0838\\ -2.3513 & -2.0838 & 110.8491 \end{pmatrix}.$$
 (43)

• We simulate the consequence of an ill-posed observation operator H with a random 3×3 matrix with its last singular value $\mu_3 = 10^{-8}$ such that

$$H = \begin{pmatrix} 0.4267 & 0.5220 & 0.5059 \\ 0.8384 & -0.7453 & 1.6690 \\ 0.4105 & 1.6187 & 0.0610 \end{pmatrix}.$$
 (44)

Therefore, H is severely ill-conditioned with a condition number, $\kappa = 2.1051 \times 10^8$.



Figure: (a) ℓ^2 norm of the analysis error $\|\mathbf{e}_k\|_{\ell^2}$ integrated for all assimilation time t_k for k = 1, ..., 1000, varying the regularization parameter, α . (b) Weighted norm of the analysis error $\|\mathbf{e}_k\|_{B^{-1}}$ integrated for all assimilation time t_k for k = 1, ..., 1000, varying the regularization parameter, α .

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Figure: (a) ℓ^2 norm of the analysis error $\|\mathbf{e}_k\|_{\ell^2}$ as the scheme is cycled for index k, with regularization parameter $\alpha = 200$, which corresponds to 3DVar. (b) Trajectories in state space for $t_{200:220}$.



Figure: (a) and (b) Trajectories in state space for $t_{774:805}$ and $t_{858:895}$ respectively.



Figure: (a) ℓ^2 norm of the analysis error $\|\mathbf{e}_k\|_{\ell^2}$ as the scheme is cycled for the index k, with regularization parameter $\alpha = 2$, an inflation in the background variance of 100%. (b) Trajectories in state space for $t_{200:220}$.



Figure: (a) ℓ^2 norm of the analysis error $\|\mathbf{e}_k\|_{\ell^2}$ as the scheme is cycled for the index k, with regularization parameter $\alpha = 10^{-10}$, an inflation in the background variance of 2×10^{12} %. (b) Trajectories in state space for $t_{200:220}$.



Figure: (a) ℓ^2 norm of the analysis error, $\|\mathbf{e}_k\|_{\ell^2}$ as the scheme is cycled for the index k with regularization parameter, $\alpha = 10^{-6}$. (b) Weighted norm of the analysis error, $\|\mathbf{e}_k\|_{B^{-1}}$ as the scheme is cycled for the index k with regularization parameter, $\alpha = 10^{-6}$. Solid line: Nonlinear analysis error. Dashed line: Linear bound. Dotted line: Asymptotic limit.

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Conclusion

- We have developed new stability results for cycled data assimilation schemes with an ill-posed observation operator.
- Under weighted norms, the choice of the α was crucial to keep in the stable range.
- Dissipation in the nonlinear model dynamics is necessary for our stability result to hold.

Future work

• Investigate the analysis error in data assimilation scheme that employ an update in the background error covariance.

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