Stability and Instability of Cycled Inverse Scattering Problems

Roland Potthast[1,2], Boris Marx[3], Alexander Moodey[2], Amos Lawless[2], Peter Jan van Leeuwen[2], Melina Freitag[4]

[1]German Meteorological Service (DWD),
[2]University of Reading, United Kingdom
[3]University of Göttingen, Germany
[4]University of Bath, United Kingdom

Outline

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1. **Motivation and Introduction.**
2. **Cycled Inverse Scattering Problems**
   - Cycled Tikhonov and 3dVar
   - Spectral Representation

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   - Setup: Constant System
   - Convergence for Data $f \in R(H)$ / Divergence for $f \notin R(H)$

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4. **Convergence Analysis 2: Regularization of Cycled Inversion**
   - Setup: High-Frequency Damping Systems
   - Analysis Error Bounds

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5. **Reading $\leftrightarrow$ Rennes**

Literature

- Marx and P.: **On Instabilities for Data Assimilation Algorithms**, GEM - International Journal on Geomathematics November 2012, Volume 3, Issue 2, pp 253-278

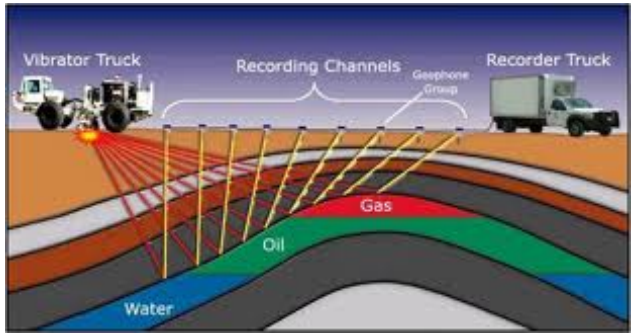
- Moodey, Lawless, P. and van Leeuwen: **Nonlinear error dynamics for cycled data assimilation methods** 2013 Inverse Problems 29 025002

- Freitag and P.: **Synergy of Inverse Problems and Data Assimilation Techniques,** 2013, in Press. in ”Large Scale Inverse Problems - Computational Methods and Applications in the Earth Sciences” Hrsg. v. Cullen, Mike / Freitag, Melina A / Kindermann, Stefan / Scheichl, Robert http://www.degruyter.com/view/product/182025

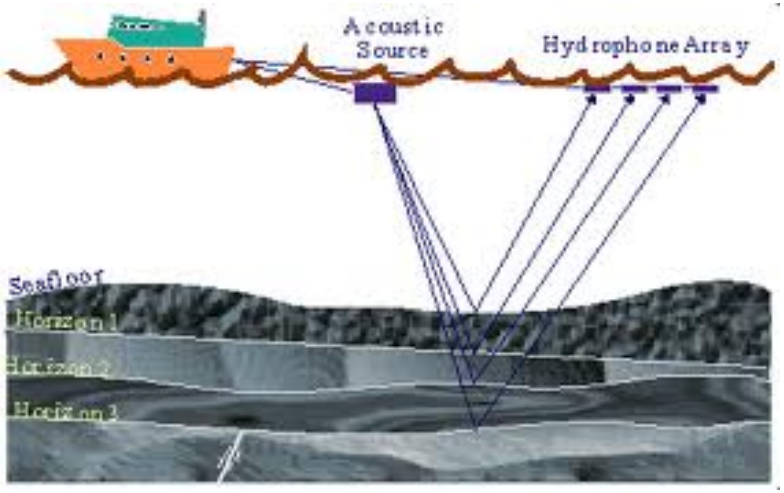
- Marx and P.: Data Assimilation Algorithms for Dynamic Magnetic Tomography and Parameter Reconstruction, Preprint.

Motivation I: Inverse Scattering in Applications ...

Medical Imaging via Scattering and Inverse Source Problems



Seismic Exploration



Motivation II: Inversion and Dynamics ...

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Inverse scattering +

further knowledge

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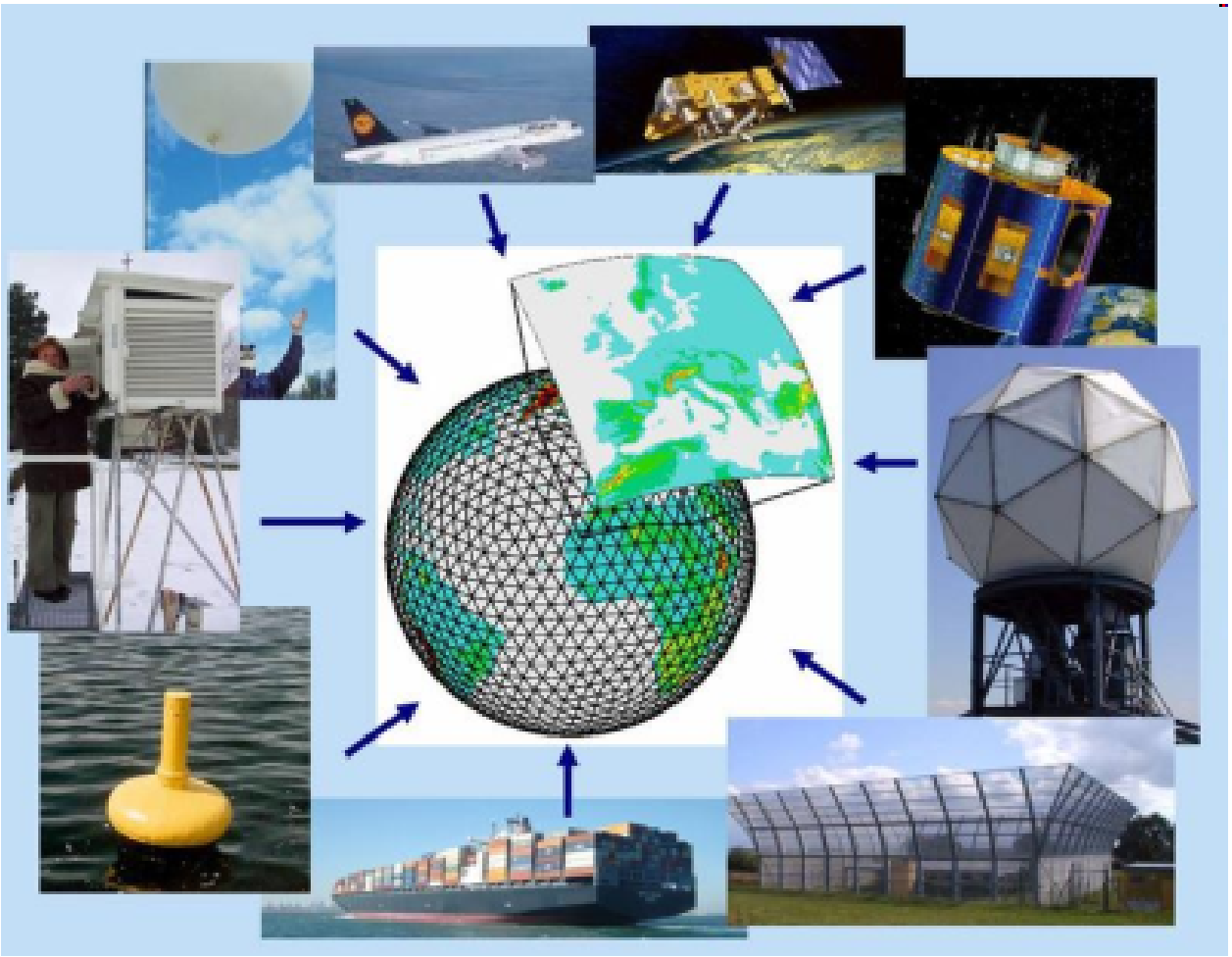
  - the **first guess** $\varphi_{k+1}^{(b)}$.

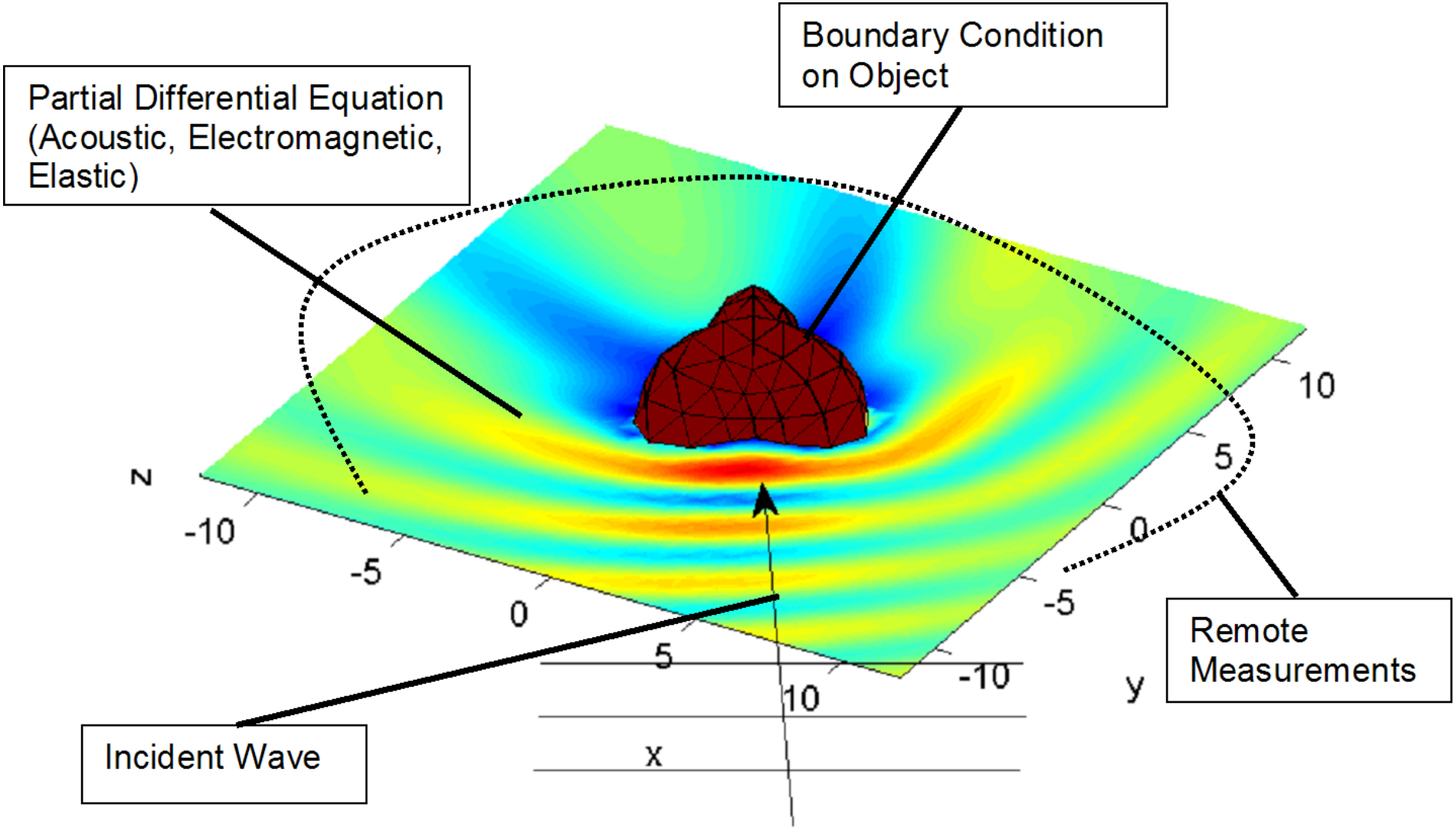
NWP: Measurements for State Determination ...



- Synop,
- TEMP,
- Radiosondes,
- Buoys,
- Airplanes (AMDAR),

- **Radar**,
- Wind Profiler,
- **Scatterometer**,
- Radiances,
- GPS/GNSS,
- Ceilometer,
- **Lidar**

Setting for reconstruction problem



Electromagnetic scattering problem

- Bounded scatterer in three dimensions with boundary of class C^2, incident field E^i
- Scattered field E^s solves Maxwell equations

$$\mathrm{curl}\mathrm{E}^{\mathrm{s}} - \mathrm{i}\kappa\mathrm{H}^{\mathrm{s}} = 0 \qquad \mathrm{curl}\mathrm{H}^{\mathrm{s}} + \mathrm{i}\kappa\mathrm{E}^{\mathrm{s}} = 0 \tag{1}$$

in $\mathbb{R}^3 \setminus \overline{D}$ and satisfies the Silver-Müller radiation condition

$$E^s \times x + rH^s \to 0, \quad r = |x| \to \infty. \tag{2}$$

- On the boundary $\Gamma := \partial D$ the tangential component of the total field $E = E^i + E^s$ vanishes, i.e. we have the perfect conductor boundary condition

$$\nu \times E|_\Gamma = 0 \tag{3}$$

Measured data

Measured data are either the scattered field E^s on some surface Λ or the far field pattern E^∞ defined by

$$E^s(x) = \frac{e^{i\kappa|x|}}{|x|}\left\{E^\infty(\hat{x}) + O\left(\frac{1}{x}\right)\right\}, \quad \hat{x} := x/|x| \tag{4}$$

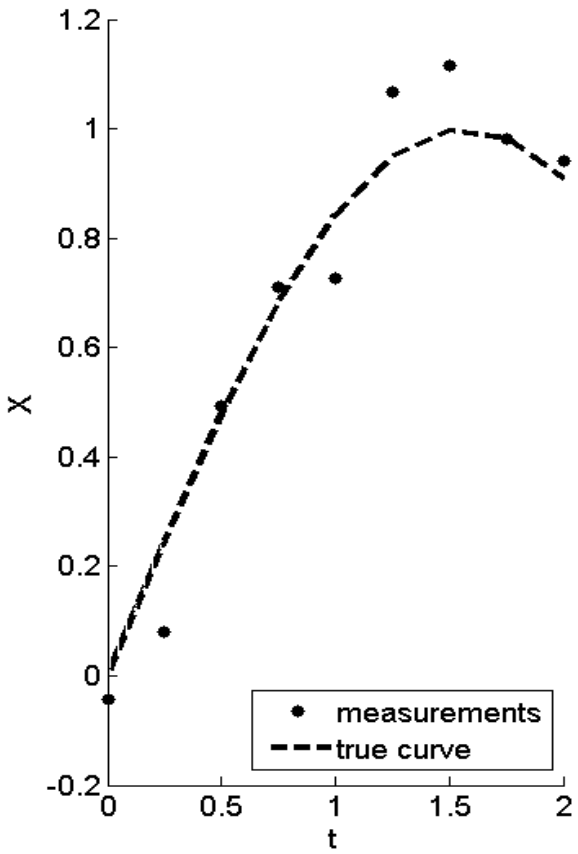
uniformly on $\mathbb{S}$ for $|x| \to \infty$.

For the above scattering problem the far field pattern can be calculated via integral equations of the second kind.

$$E^s(\partial D) = \mathcal{H}(\partial D) \qquad \text{or} \qquad f(\varphi) = \mathcal{H}(\varphi) \tag{5}$$

when $\varphi := \partial D(t)$.

Mathematical Setup for Cycled Inversion



State Space:

X	**state space**, containing all state variables in one vector φ
φ	state of the system

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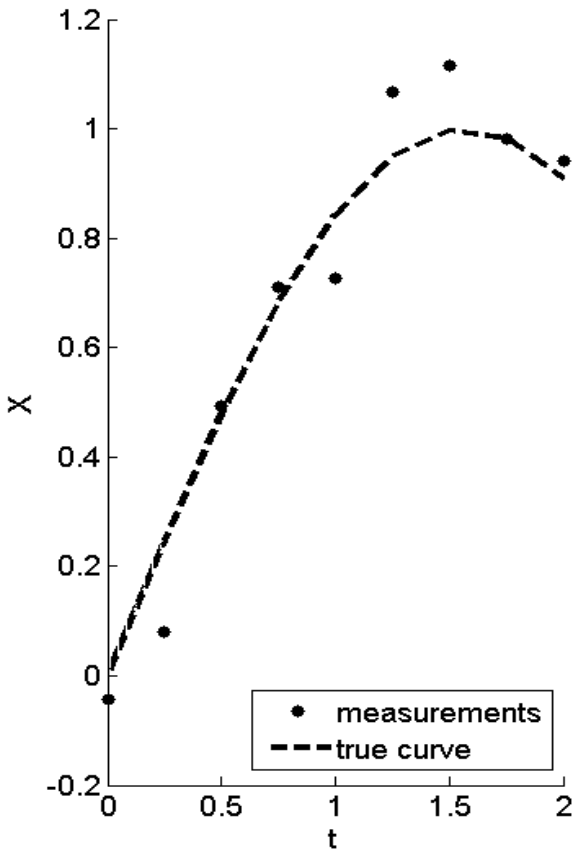

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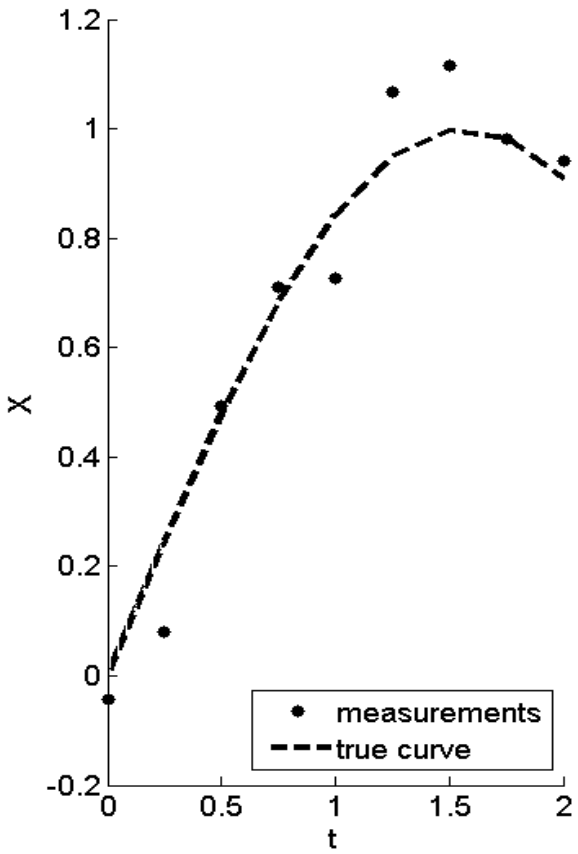

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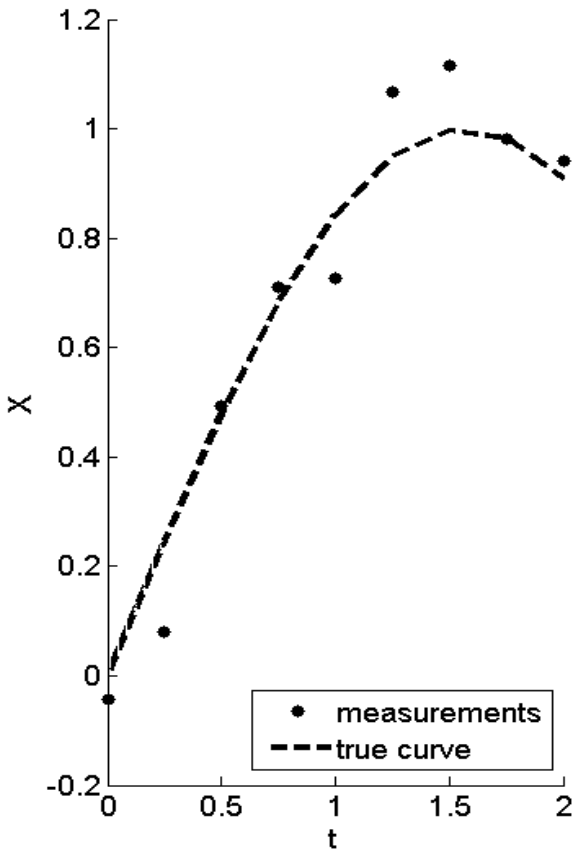

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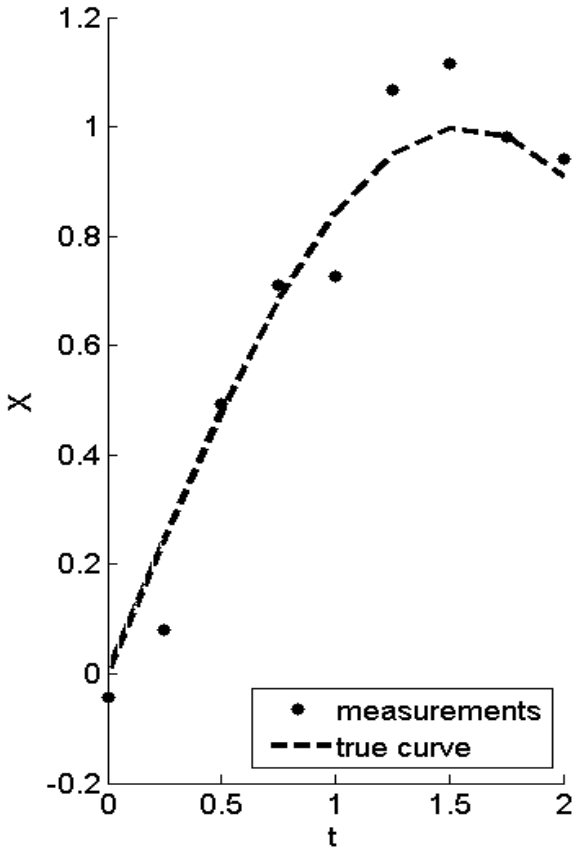
Observation Space

Y_k	**observation space** at time t_k
f_k	observation vector at time t_k
$H_k : X \to Y_k$	**observation operator**
x, y	points in physical space

Data Assimilation or Cycled Inversion Task



Definition (Data Assimilation Task)

Given measurements f_k at t_k for $k = 1, 2, 3, \ldots$ determine the states φ_k from the equations

$$H\varphi_k = f_k, \quad k = 1, 2, 3, \ldots \tag{6}$$

taking care of the *model dynamics* given by M_k.

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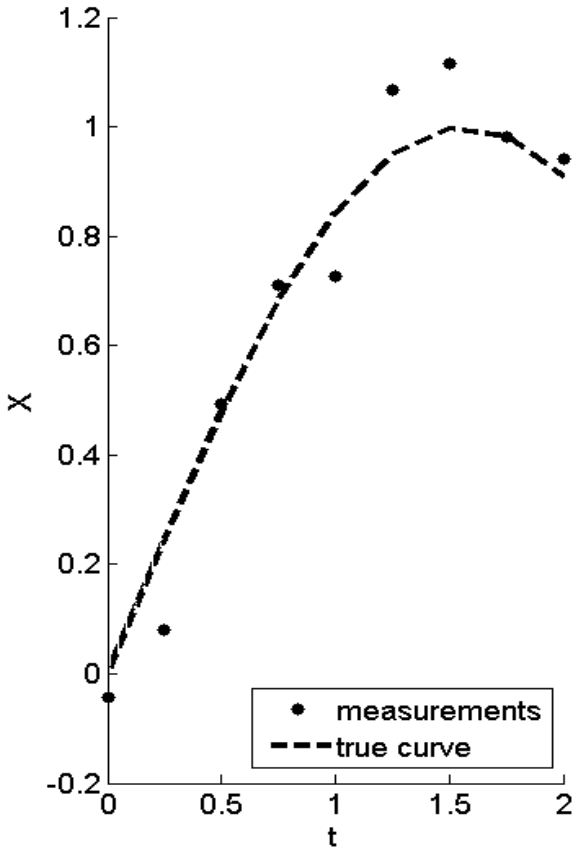

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- Usually the measurement space is dynamic, i.e. changing in every time-step.
- In general H is a non-linear operator, non-injective, ill-posed.
- The value f_k contains significant data error with stochastic components and a dynamic bias.

Outline

Tikhonov Data Assimilation

In every assimilation step $k \in \mathbb{N}$ we solve the variational minimization problem to find the minimum of

$$J(\varphi) := \alpha ||\varphi - \varphi_{k+1}^{(b)}||^2 + ||f_{k+1} - H\varphi_{k+1}^{(b)}||^2, \quad \varphi \in X, \tag{7}$$

where

$$\varphi_{k+1}^{(b)} := M\varphi_k^{(a)}, \quad k = 0, 1, 2, \ldots \tag{8}$$

For linear operators the minimum is given by the *normal equations*, which can be reformulated into the update formula

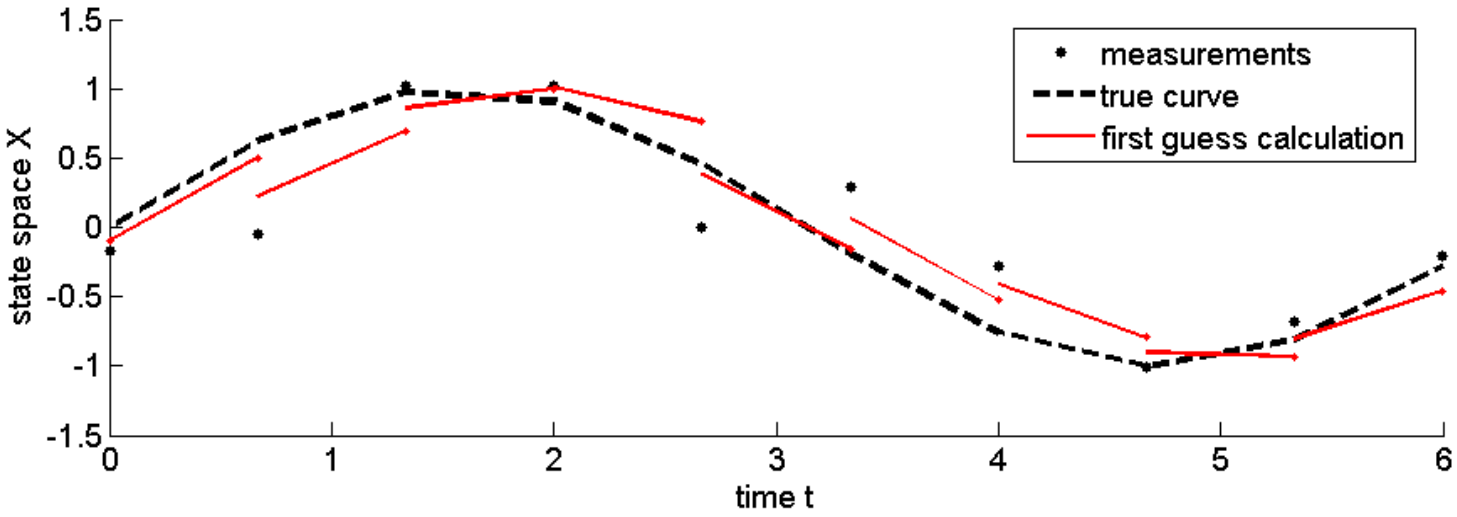
$$\varphi_{k+1}^{(a)} = \varphi_{k+1}^{(b)} + R_\alpha \left(f_{k+1} - H\varphi_{k+1}^{(b)} \right) \tag{9}$$

with $R_\alpha = (\alpha I + H^* H)^{-1} H^*$, or in terms of the analysis fields $\varphi_k^{(a)}$

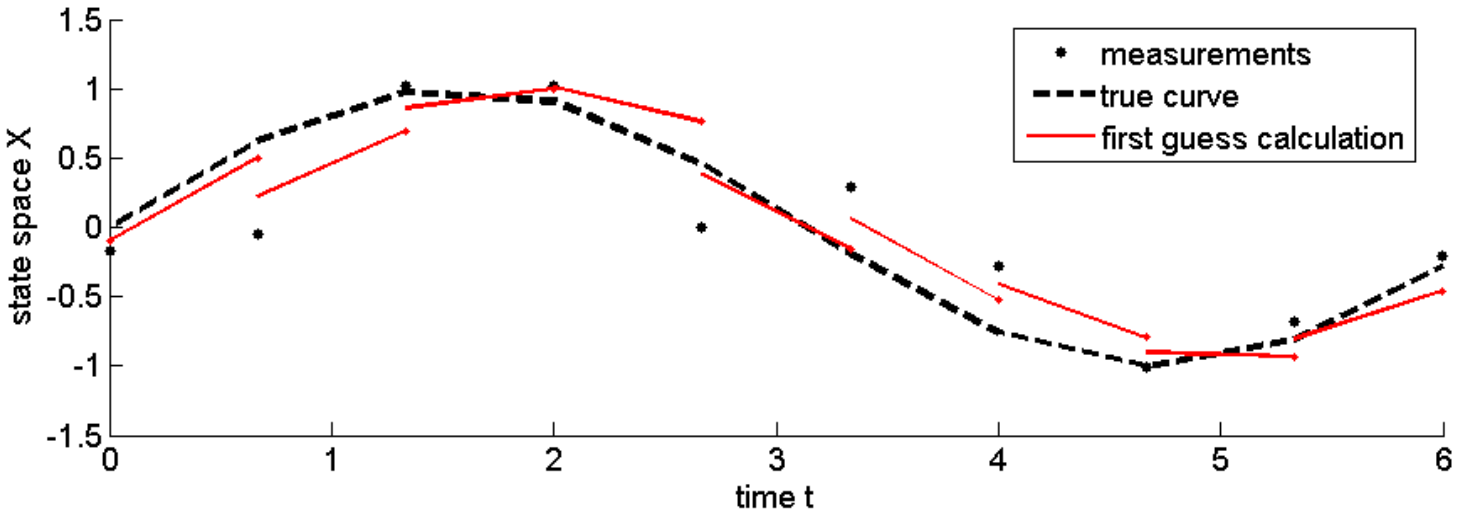
$$\varphi_{k+1}^{(a)} = M\varphi_k^{(a)} + R_\alpha \left(f_{k+1} - HM\varphi_k^{(a)} \right) \tag{10}$$

for $k = 0, 1, 2, \ldots$.

3dVAR - 1


1.5
1
0.5
0
-0.5
-1
-1.5
state space X
0
1
2
3
4
5
6
time t
measurements
true curve
first guess calculation

3dVAR - 1



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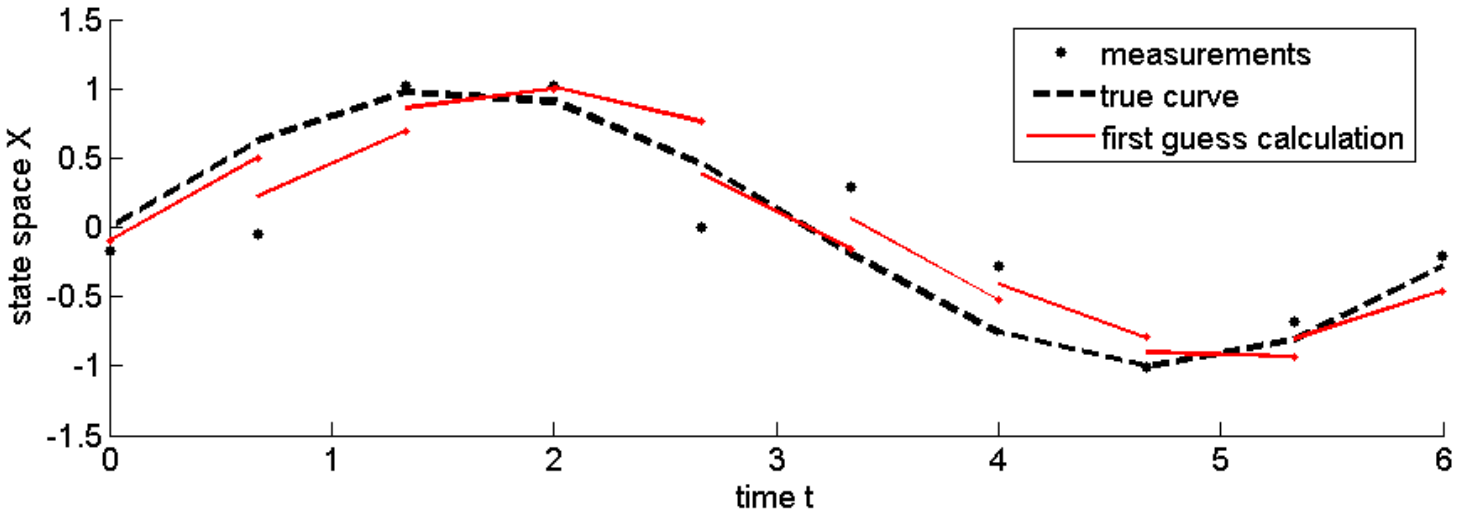

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2. Calculate **first guess**

$$\varphi_k^{(b)} = M_{k-1}\varphi_{k-1}^{(a)} \tag{11}$$

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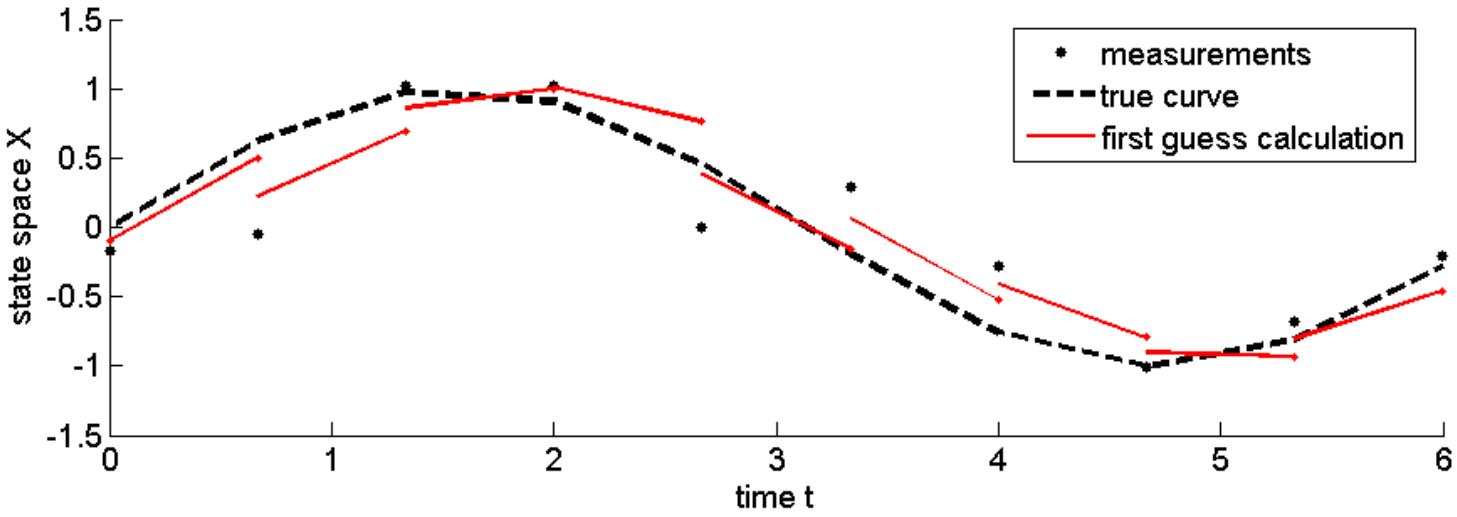

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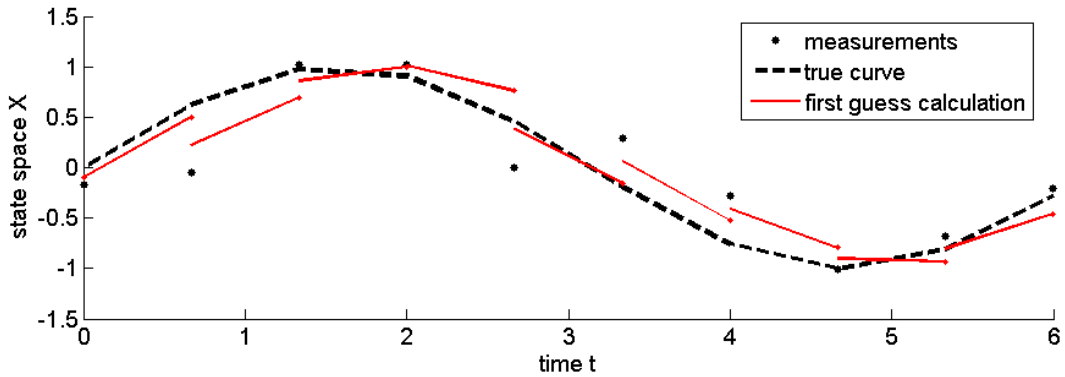
3. **Assimilate data** f_k at time t_k calculating $\varphi_k^{(a)}$.

3dVAR - 2



Functional at **time slice**

$$J(\varphi) = ||\varphi - \varphi^{(b)}||^2_{B^{-1}} + ||f - H\varphi||^2_{R^{-1}} \tag{12}$$

Update Formula

$$\begin{aligned} \varphi_k^{(a)} &= \varphi_k^{(b)} + (B^{-1} + H^* R^{-1} H)^{-1} H^* R^{-1} (f_k - H(\varphi_k^{(b)})) \\ &= \varphi_k^{(b)} + \underbrace{BH^*(R + HBH^*)^{-1}}_{\text{Kalman gain matrix}} (\underbrace{f_k - H(\varphi_k^{(b)})}_{\text{obs - first guess}}). \end{aligned} \tag{13}$$

Nonlinear Observation Operators

In the case of nonlinear observation operators $\mathcal{H}$ we employ linearization

$$\mathcal{H}(\varphi^{(b)} + \delta\varphi) = \mathcal{H}(\varphi^{(b)}) + H\delta\varphi + O(||\delta\varphi||^2).$$

with **H being the linearization of $\mathcal{H}$ at $\varphi^{(b)}$**. Then, we need to minimize

$$J(\delta\varphi) = ||\delta\varphi||^2 + ||(f - \mathcal{H}(\varphi^{(b)})) - H\delta\varphi||^2.$$

Nonlinear three-dimensional Variational Data Assimilation (3dVar)

The **variational update formula** of 3dVar is

$$\begin{aligned} \varphi_k^{(a)} &= \varphi_k^{(b)} + (B^{-1} + H'R^{-1}H)^{-1}H'R^{-1}(f_k - \mathcal{H}(\varphi_k^{(B)})) \\ &= \varphi_0 + BH'(R + HBH')^{-1}(f_k - \mathcal{H}\varphi_k^{(b)}). \qquad (14) \\ \varphi_{k+1}^{(b)} &= M_k\varphi_k^{(a)}, \quad k = 1, 2, 3, \ldots \qquad (15) \end{aligned}$$

Outline

Spectral Representation 1

Assume that $H : X \to Y$ is linear and compact. Then, there is a **singular system** $\{(\psi_n, g_n, \mu_n),\ n \in \mathbb{N}\}$ such that $H\psi_n = \mu_n g_n$, $H' g_n = \mu_n \psi_n$ and

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With measurements

$$f = \sum_{n=1}^{\infty} f_n g_n \quad \in Y \tag{18}$$

and denote the spectral coefficients of the Tikhonov solution φ by γ_n. 3dVar or Tikhonov regularization, respectively, $(\alpha I + H' H)\varphi = H' f$ is equivalent to the **spectral damping scheme**

$$\gamma_n = \frac{\mu_n}{\alpha + \mu_n^2} f_n, \quad n \in \mathbb{N}. \tag{19}$$

Spectral Representation 2

The true Inverse is

$$\gamma_n^{true} = \frac{1}{\mu_n} f_n^{true}. \tag{20}$$

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This inversion is **unstable**, if $\mu_n \to 0$, $n \to \infty$!

Tikhonov regularization is **stable** for $\alpha > 0$

$$\gamma_n = \frac{\mu_n}{\alpha + \mu_n^2} f_n, \quad n \in \mathbb{N}. \tag{21}$$

Tikhonov **shifts the eigenvalues** of $H'H$ by α.

Outline

A system with constant dynamics

As a simple model system for study we use **constant dynamics** $M = \mathit{Identity}$, i.e

$$\varphi_{k+1}^{(b)} = \varphi_k^{(a)}, \quad k = 1, 2, 3, \ldots \tag{22}$$

for 3dVar. Also, we employ **identical measurements** $f_k \equiv f$, $k \in \mathbb{N}$.

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Then, **3dVar** is given by the iteration

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For the **spectral coefficients** $\gamma_{n,k}$ of φ_k this leads to the iteration

$$\gamma_{n,k} = \gamma_{n,k-1} + \frac{\mu_n}{\alpha + \mu_n^2}\left(f_{n,k} - \mu_n \gamma_{n,k-1}\right) \tag{24}$$

Spectral Formula I

We employ

$$f = H\varphi^{(true)} + \delta, \quad f_{n,k} = \mu_n \gamma_n^{(true)} + \delta_n. \tag{25}$$

and obtain

$$\gamma_{n,k} = \gamma_{n,k-1} + \frac{\mu_n^2}{\alpha + \mu_n^2}(\gamma_n^{(true)} - \gamma_{n,k-1}) + \frac{\mu_n^2}{\alpha + \mu_n^2}\frac{\delta_n}{\mu_n}$$

Theorem (Spectral Formula I)

The **3dVar cycling for a constant dynamics** *with identical measurements* $f = H\varphi^{(true)} + \delta$ *lead to the* **spectral update formula**

$$\gamma_{n,k} = (1 - q_n)\gamma_n^{(true)} + q_n \gamma_{n,k-1} + \frac{(1 - q_n)}{\mu_n}\delta_n \tag{26}$$

using

$$q_n = \frac{\alpha}{\alpha + \mu_n^2} = 1 - \frac{\mu_n^2}{\alpha + \mu_n^2}. \tag{27}$$

Spectral Formula II

Theorem (Spectral Formula II)

The **3dVar cycling for a constant dynamics** *with identical measurements* $f = H\varphi^{(true)} + \delta$ *can be carried out explicitly. The development of its spectral coefficients is given by*

$$\gamma_{n,k} = (1 - q_n^k)\gamma_n^{(true)} + q_n^k \gamma_{\mathbf{n,0}} + \frac{(1 - q_n^k)}{\mu_n}\delta_n \tag{28}$$

using

$$q_n = \frac{\alpha}{\alpha + \mu_n^2} = 1 - \frac{\mu_n^2}{\alpha + \mu_n^2}. \tag{29}$$

Proof. Induction over k. □

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Convergence for $f \in R(H)$

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Cycled 3dVar for a constant dynamics and identical measurements $f^{(true)} + \delta \in R(H)$ tends to the true solution $\varphi^{(true)} + \sigma$ with $H\sigma = \delta$ for $k \to \infty$.

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Proof. We study

$$\gamma_{n,k} = (1 - q_n^k)\gamma_n^{(true)} + q_n^k \gamma_{n,0} + \frac{(1 - q_n^k)}{\mu_n}\delta_n \tag{30}$$

for $k \to \infty$.

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Cycled 3dVar for a constant dynamics and identical measurements $f^{(true)} + \delta \in R(H)$ tends to the true solution $\varphi^{(true)} + \sigma$ with $H\sigma = \delta$ for $k \to \infty$.

Proof. We study

$$\gamma_{n,k} = (1 - q_n^k)\gamma_n^{(true)} + q_n^k \gamma_{n,0} + \frac{(1 - q_n^k)}{\mu_n}\delta_n \tag{30}$$

for $k \to \infty$.

Since $0 < q_n < 1$, we have

$$q_n^k \to 0, \quad k \to \infty, \quad (1 - q_n^k) \to 1, \quad k \to \infty. \tag{31}$$

Since $\delta = H\sigma$ the element σ with spectral coefficients δ_n/μ_n is in X and cycled 3dVar converges towards $\varphi^{(true)} + \sigma$. □

Divergence for $f \notin R(H)$

Theorem (Divergence for $f \notin R(H)$)

For a constant dynamics and identical measurements $f^{(true)} + \delta \notin R(H)$ **cycled 3dVar diverges** *for $k \to \infty$.*

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$$\gamma_{n,k} = (1 - q_n^k)\gamma_n^{(true)} + q_n^k \gamma_{n,0} + \frac{(1 - q_n^k)}{\mu_n}\delta_n \tag{32}$$

for $k \to \infty$. Let $\sigma_k \in X$ denote the element with spectral coefficients

$$\sigma_{n,k} = \frac{(1 - q_n^k)}{\mu_n}\delta_n, \quad k, n \in \mathbb{N}.$$

which is well defined since for every fixed $k \in \mathbb{N}$

$$\left|\frac{(1 - q_n^k)}{\mu_n}\right| = \left|\frac{(\alpha + \mu_n^2)^k - \alpha^k}{(\alpha + \mu_n^2)^k \mu_n}\right| \tag{33}$$

is bounded uniformly for $n \in \mathbb{N}$.

Divergence for $f \notin R(H)$

Since $\delta \notin R(H)$ we know that

$$S_L := \sum_{n=1}^{L} \left| \frac{\delta_n}{\mu_n} \right|^2 \to \infty, \quad L \to \infty. \tag{34}$$

Given $C > 0$ we can choose L such that $S_L > 2C$. Then

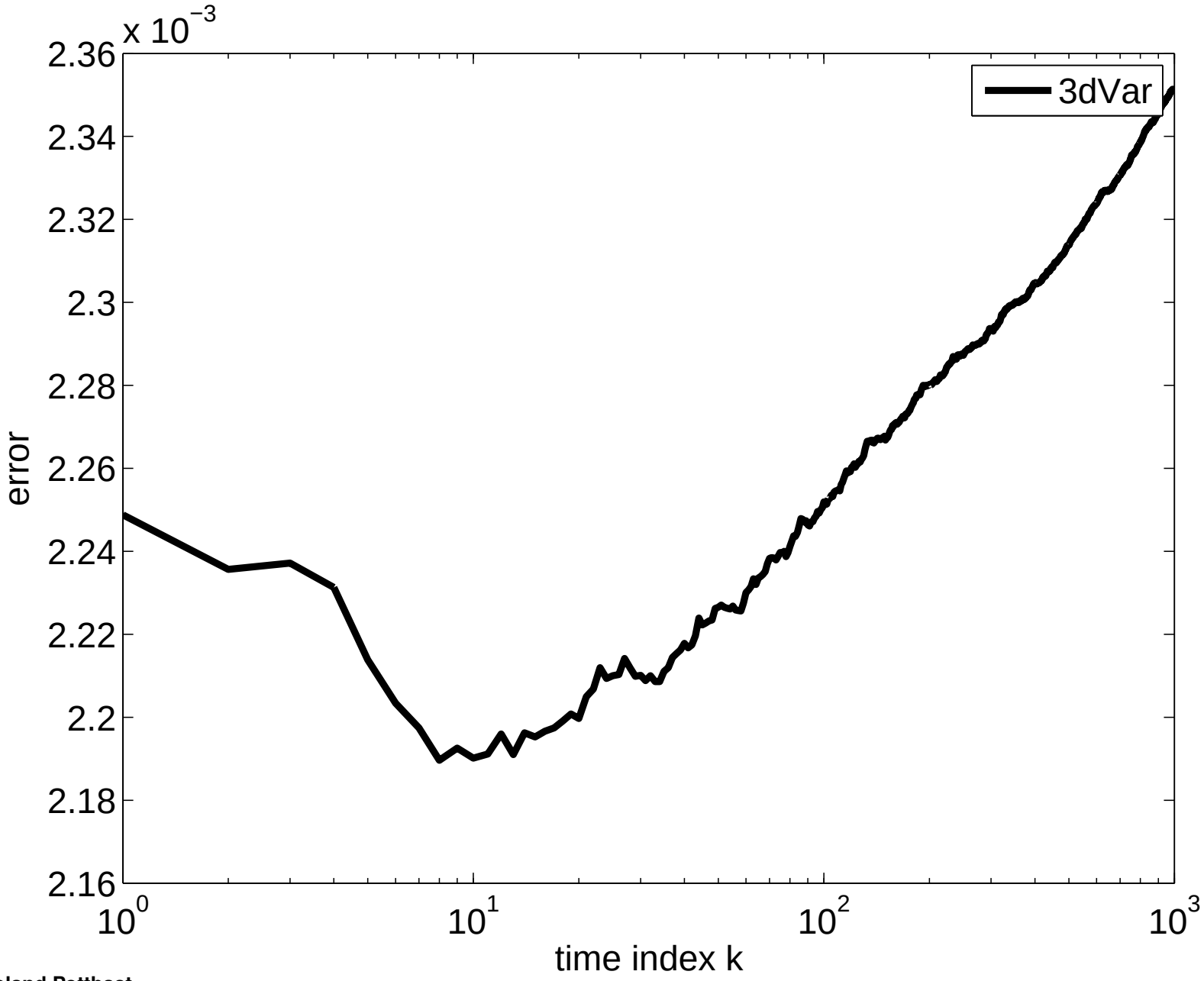
$$||\sigma_k||^2 \geq \sum_{n=1}^{L} \left| \frac{(1 - q_n^k)\delta_n}{\mu_n} \right|^2 > C \tag{35}$$

for $k \in \mathbb{N}$ sufficiently large, which proves

$$||\sigma_k|| \to \infty, \quad k \to \infty \tag{36}$$

and the proof is complete. $\square$

Numerical Example: Dynamic Magnetic Tomography



Outline

$$\begin{aligned}\varphi_{k+1}^{(a)} - \varphi_{k+1}^{(true)} &= M\big(\varphi_k^{(a)} - \varphi_k^{(true)}\big) + R_\alpha HM\Big(\varphi_k^{(true)} - \varphi_k^{(a)}\Big) + R_\alpha f_{k+1}^{(\delta)} \\ &= \big(I - R_\alpha H\big)M\Big(\varphi_k^{(a)} - \varphi_k^{(true)}\Big) + R_\alpha f_{k+1}^{(\delta)}. \end{aligned} \tag{37}$$

We abbreviate the analysis error by

$$\mathbf{e_k} := \varphi_k^{(a)} - \varphi_k^{(true)}, \quad k = 1, 2, \ldots \tag{38}$$

and define

$$\Lambda := \big(I - R_\alpha H\big)M \tag{39}$$

to obtain the iteration formula

$$e_{k+1} = \Lambda e_k + R_\alpha f_{k+1}^{(\delta)}, \quad k = 0, 1, 2, \ldots \tag{40}$$

System Evolution

Theorem

Assume that the error $f_k^{(\delta)}$ does not depend on k, i.e. that we feed some constant error into the data assimilation scheme. Then, the error terms e_k with initial error e_0 described by the update formula (40) evolve according to

$$e_k = \Lambda^k e_0 + \Big(\sum_{\ell=0}^{k-1} \Lambda^\ell \Big) e^{(\delta)} \tag{41}$$

with $e^{(\delta)} := R_\alpha f^{(\delta)}$. If $(I - \Lambda)^{-1}$ exists, it can be written as

$$e_k = \Lambda^k e_0 + (I - \Lambda)^{-1} (I - \Lambda^k) e^{(\delta)} \tag{42}$$

- The update formula has been already known in the 1970s.
- It was derived for a finite dimensional system with some well-posed observation operator in a stochastic framework for the Kalman filter.

Outline

Space Decomposition

Let the orthonormal system $\{\psi_\ell : \ell \in \mathbb{N}\}$ in X be given by the **singular system** of the **observation operator** $H : X \to Y$. In this case we define an **orthogonal decomposition** of the space X by

$$X_1^{(n)} := \underbrace{\mathrm{span}\{\psi_1, ..., \psi_n\}}_{lowermodes}, \quad X_2^{(n)} := \overbrace{\mathrm{span}\{\psi_{n+1}, \psi_{n+2}, ...\}}^{highermodes}. \tag{43}$$

Using the orthogonal projection operators P_1 of X onto X_1 and P_2 of X onto X_2, we decompose M into

$$M_1 := P_1 M, \quad M_2 := P_2 M. \tag{44}$$

Using $N = \left(I - R_\alpha H\right)$ and $\Lambda = NM$ we obtain

$$\Lambda = \underbrace{N|_{X_1} M_1}_{lower\ modes} + \overbrace{N|_{X_2} M_2}^{higher\ modes}. \tag{45}$$

Norm estimates for N

The operator N maps X_j, $j = 1, 2$, into itself. This leads to the **norm estimate**

$$\begin{aligned} ||\Lambda\varphi||^2 &= ||(N|_{X_1} M_1 + N|_{X_2} M_2)\varphi||^2 \\ &= ||N|_{X_1} M_1 \varphi||^2 + ||N|_{X_2} M_2 \varphi||^2, \end{aligned} \tag{46}$$

leading to

$$||\Lambda||^2 \leq ||N|_{X_1}||^2 ||M_1||^2 + ||N|_{X_2}||^2 ||M_2||^2. \tag{47}$$

- We derive estimates for all the above terms.

Norm Estimates 1

$$||\Lambda||^2 \leq ||N|_{X_1}||^2 ||M_1||^2 + ||N|_{X_2}||^2 ||M_2||^2. \tag{48}$$

Lemma

The norm of the operator $N|_{X_2}$ is given by

$$||N|_{X_2}|| = 1 \tag{49}$$

for all $n \in \mathbb{N}$ and $\alpha > 0$.

Lemma

Assume that M is self-adjoint with bounded Frobenius norm. Then, given $\rho > 0$ there is $n \in \mathbb{N}$ such that for $M_2 = M_2^{(n)}$ we have

$$||M_2|| < \rho. \tag{50}$$

Norm Estimates 2

$$||\Lambda||^2 \leq ||N|_{X_1}||^2 ||M_1||^2 + ||N|_{X_2}||^2 ||M_2||^2. \tag{51}$$

We need the freedom

$$||M_1|| = c. \tag{52}$$

Lemma

On X_1 for $N = I - R_\alpha H$ we have the norm estimate

$$||N|_{X_1}|| = \sup_{\ell=1,..,n} |\frac{\alpha}{\alpha + \mu_n^2}| \tag{53}$$

where μ_n are the singular values of the operator H ordered according to their size and multiplicity. In particular, given $\epsilon > 0$ and $n \in \mathbb{N}$ we can choose $\alpha > 0$ sufficiently small such that

$$||N|_{X_1}|| < \epsilon. \tag{54}$$

Stabilization of data assimilation

Recall

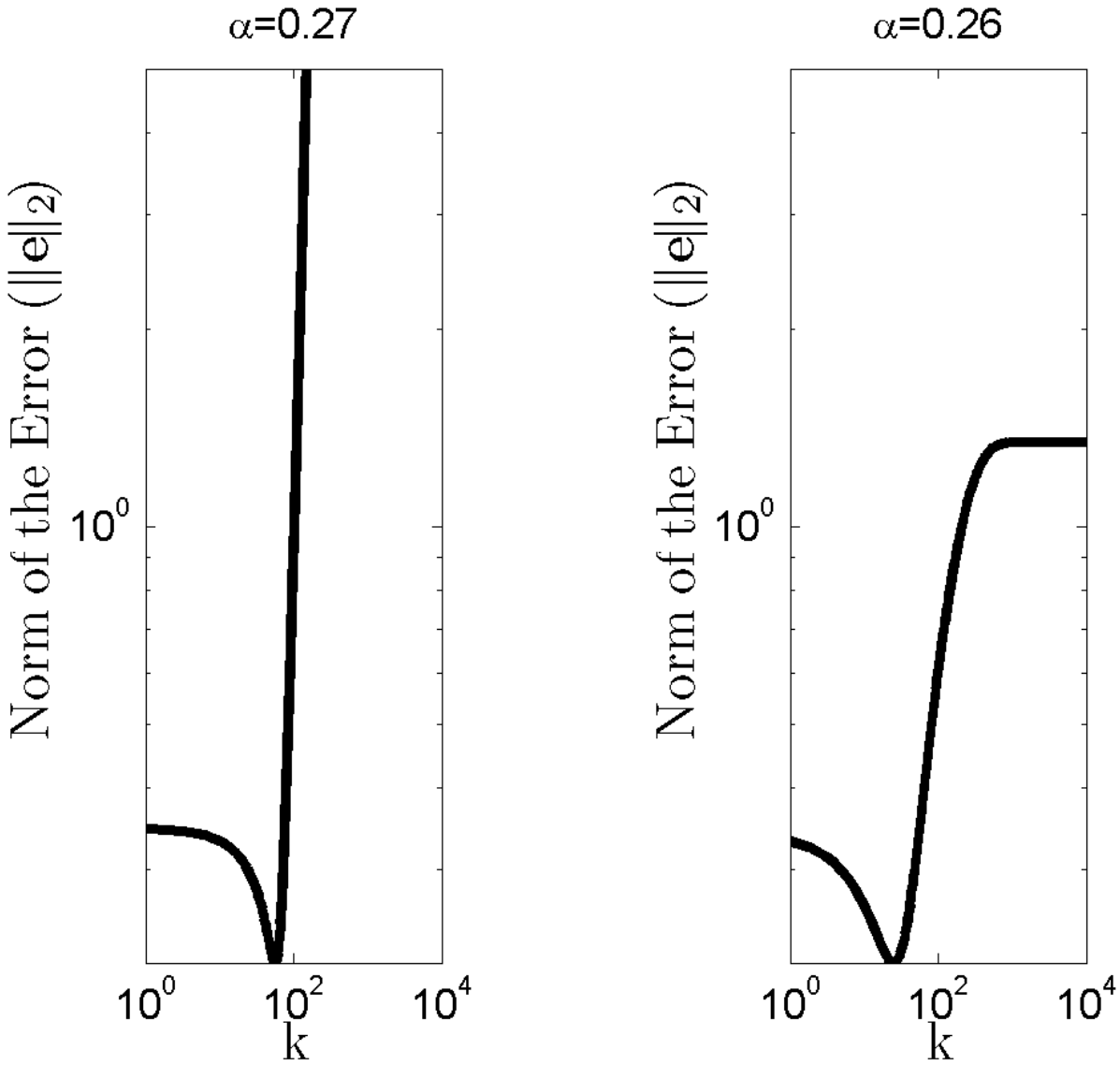
$$e_k = \Lambda^k e_0 + (I - \Lambda)^{-1}(I - \Lambda^k)e^{(\delta)} \tag{55}$$

Theorem

Assume that the system M is self-adjoint and its Frobenius norm is bounded and let α denote the regularization parameter for a cycled data assimilation scheme. Then, for $\alpha > 0$ sufficiently small, we have $||\Lambda|| < 1$. Assume that the observation error $f^{(\delta)}$ is bounded in norm by $\delta > 0$. In this case, the analysis error is bounded over time with

$$\limsup_{k\to\infty} ||e_k|| \leq \frac{||R_\alpha||\delta}{1 - ||\Lambda||}. \tag{56}$$

Numerical Example



Summary

Summary on Cycled Inversion Instability I

- 3dVar (and 4dVar for linear systems) can be analysed as a **cycled Tikhonov regularization**.
- We have shown that even for very stable dynamics where $M = const$ cycled Tikhonov with ill-posed observation operators **diverges** if we have data $f \notin R(H)$.
- The divergence carries over to 3dVar and 4dVar for simple systems.

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- The divergence carries over to 3dVar and 4dVar for simple systems.

Summary on Cycled Inversion Instability II

- For systems damping high frequencies we have shown that stability depends on the choice of the regularization parameter α
- For self-adjoint systems M with bounded Frobenius norm we can always achieve a stable assimilation by choosing α appropriately, even if $||M_2|| > 1$.

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