On Instability in Data Assimilation

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Outline

1. Motivation and Introduction.

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2. **Variational Data Assimilation**
   - Tikhonov and 3dVar
   - 4dVar
   - Spectral Representation

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   - Setup: Constant System
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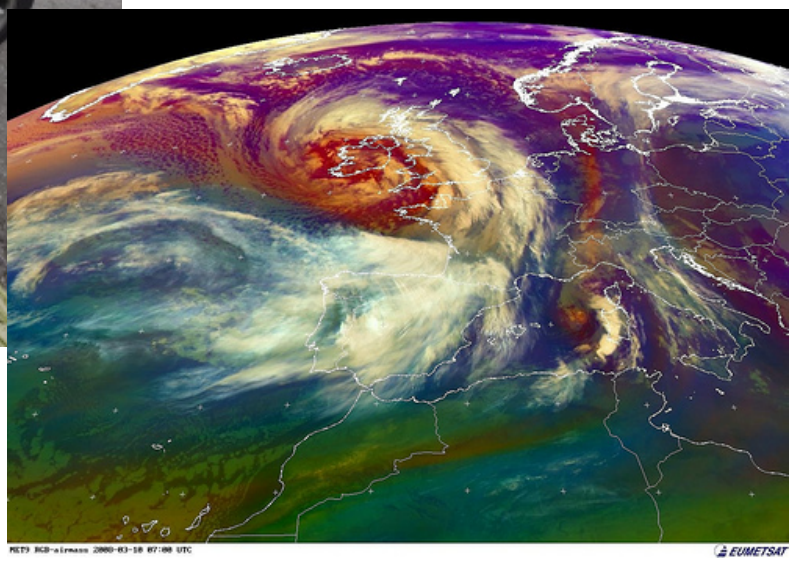
   - Setup: High-Frequency Damping Systems
   - Analysis Error Bounds

Motivation I: Numerical Weather Forecast ...

Warn and Protect

Plan Travel



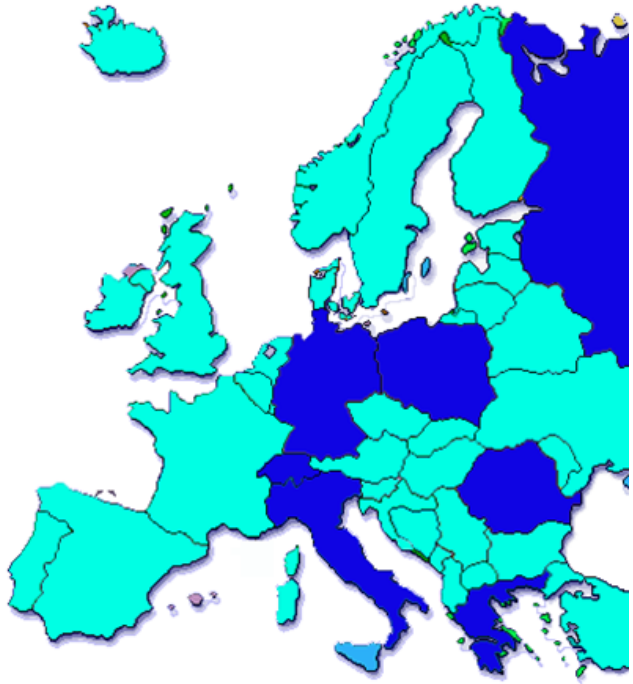
Motivation II: Numerical Weather Forecast ...

Logistics

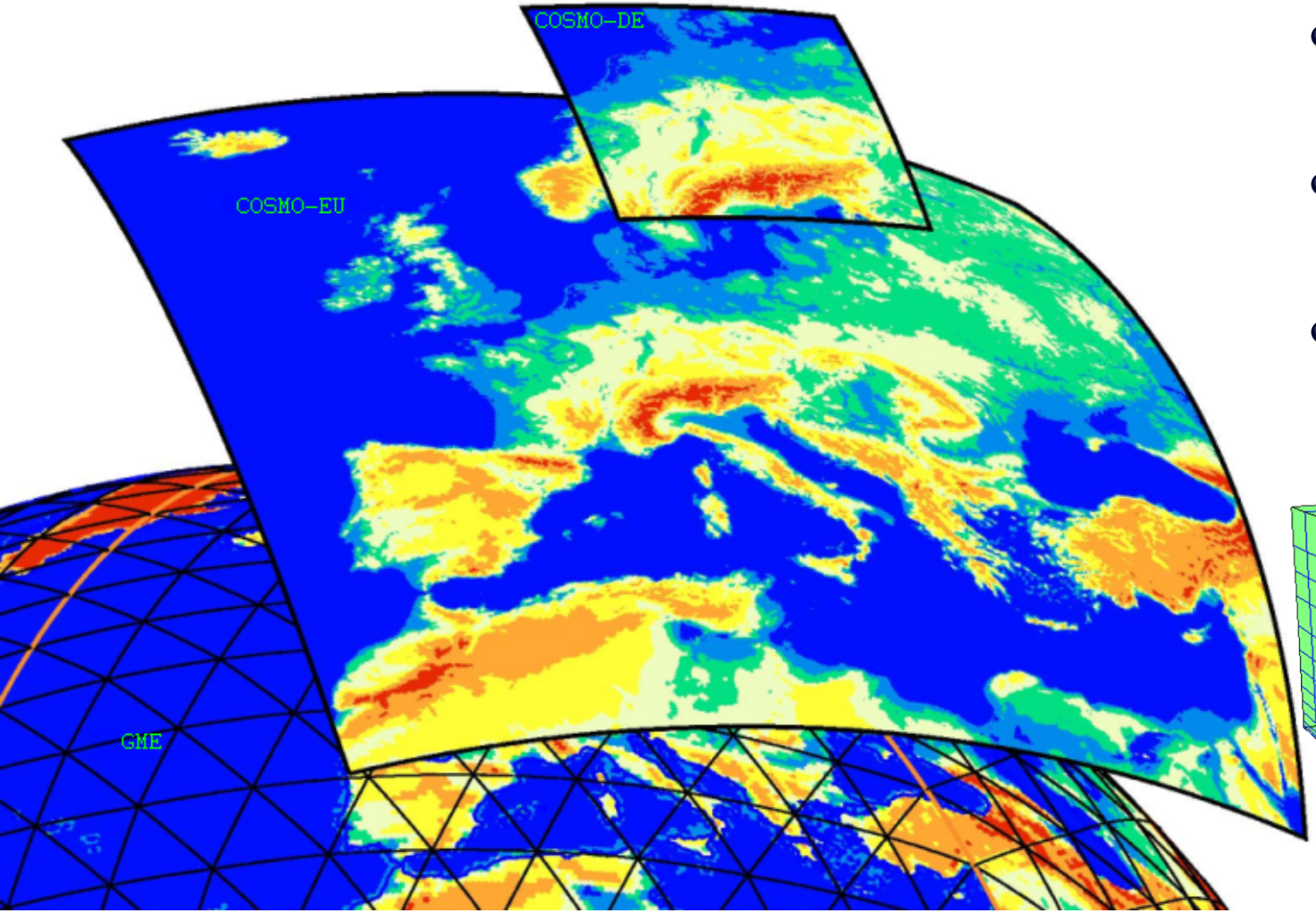
Rivers and Environment

Air Control

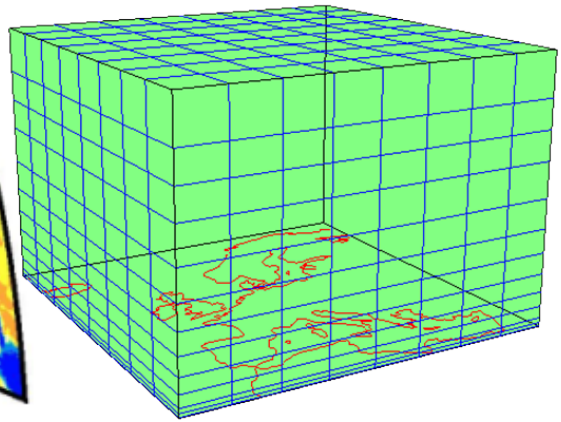
Data Assimilation at the Deutscher Wetterdienst



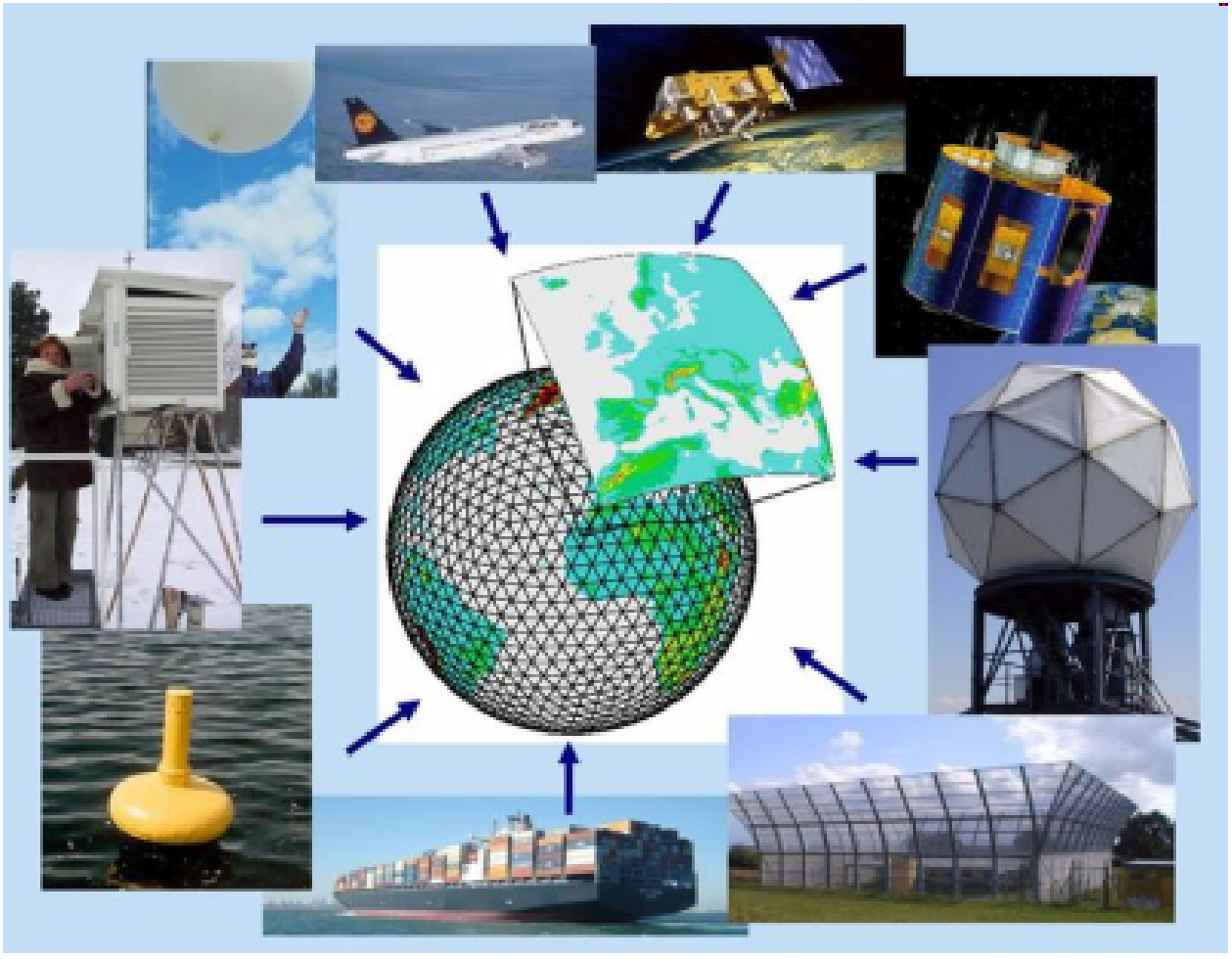
Modelling of the Atmosphere: Geometry



- GME/ICON
  Resolution 30km
- COSMO-EU
  Resolution 7km
- COSMO-DE
  Resolution 2.8km

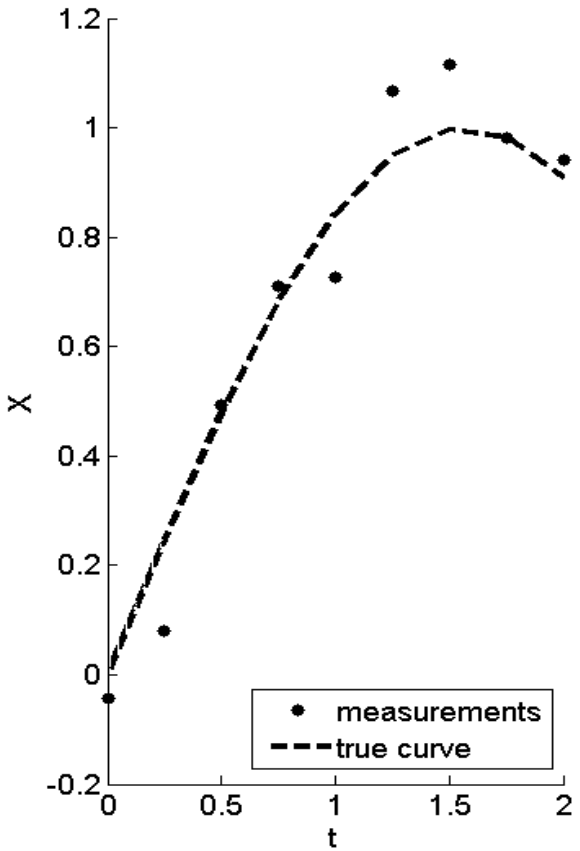


Measurements for State Determination ...



- Synop,
- TEMP,
- Radiosondes,
- Buoys,
- Airplanes (AMDAR),
- Radar,
- Wind Profiler,
- Scatterometer,
- Radiances,
- GPS/GNSS,
- Ceilometer,
- Lidar

Mathematical Setup for Data Assimilation



State Space:

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

φ state of the atmosphere

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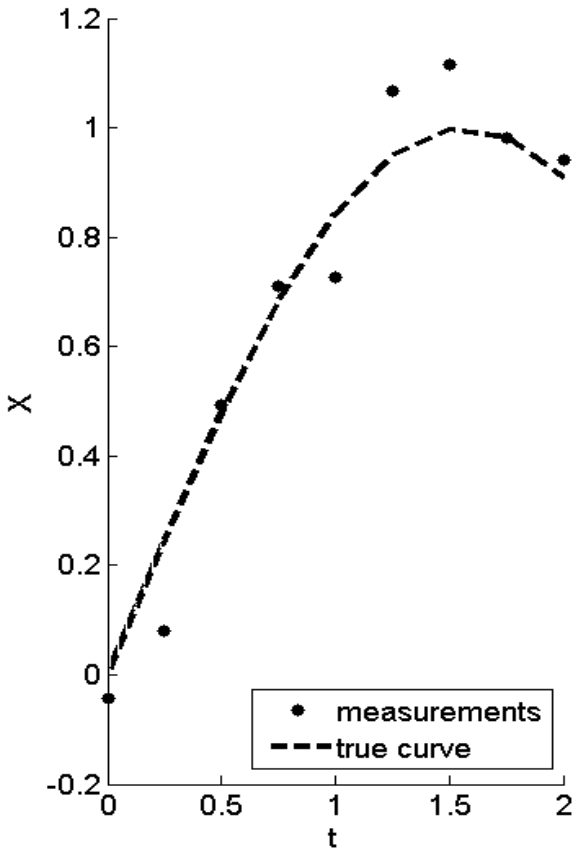

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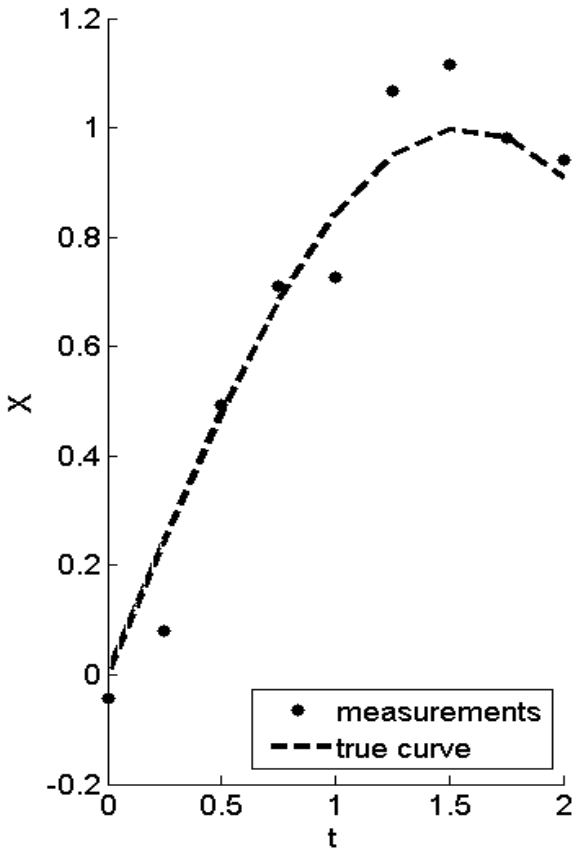

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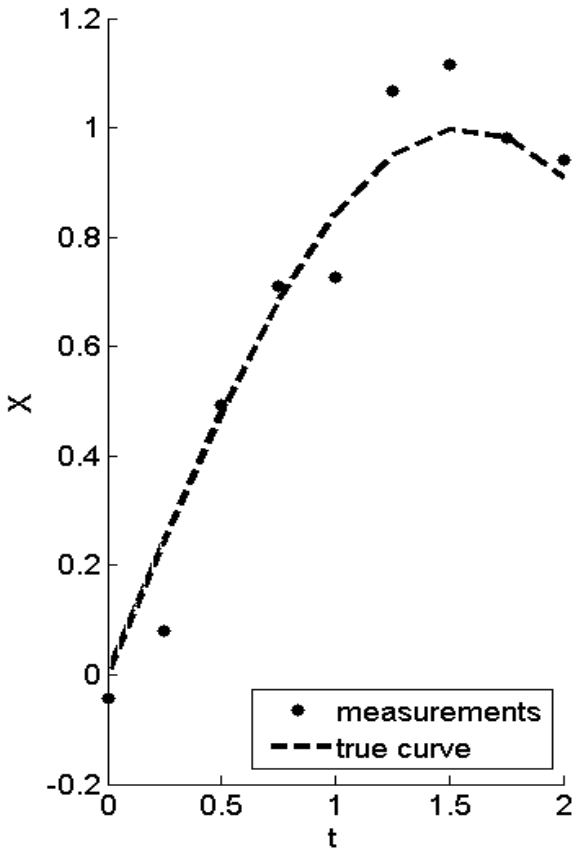

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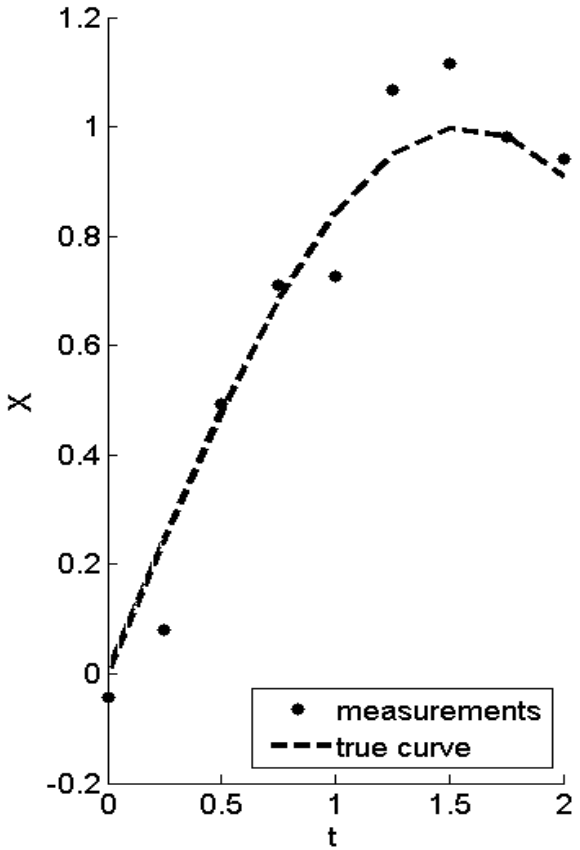
Observation Space

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 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

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

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

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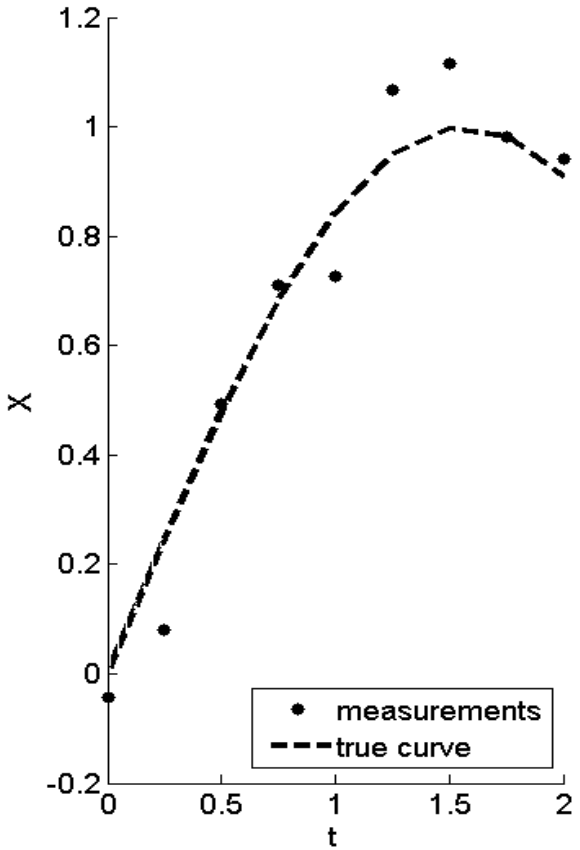

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- Usually the measurement space is dynamic, i.e. changing in every time-step.
- In general H is a non-linear operator, non-injective, ill-posed.
- The value f_k contains significant data error with stochastic components and a dynamic bias.

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Tikhonov Data Assimilation

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

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

where

$$\varphi_{k+1}^{(b)} := M\varphi_k^{(a)}, \quad k = 0, 1, 2, \ldots \tag{3}$$

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

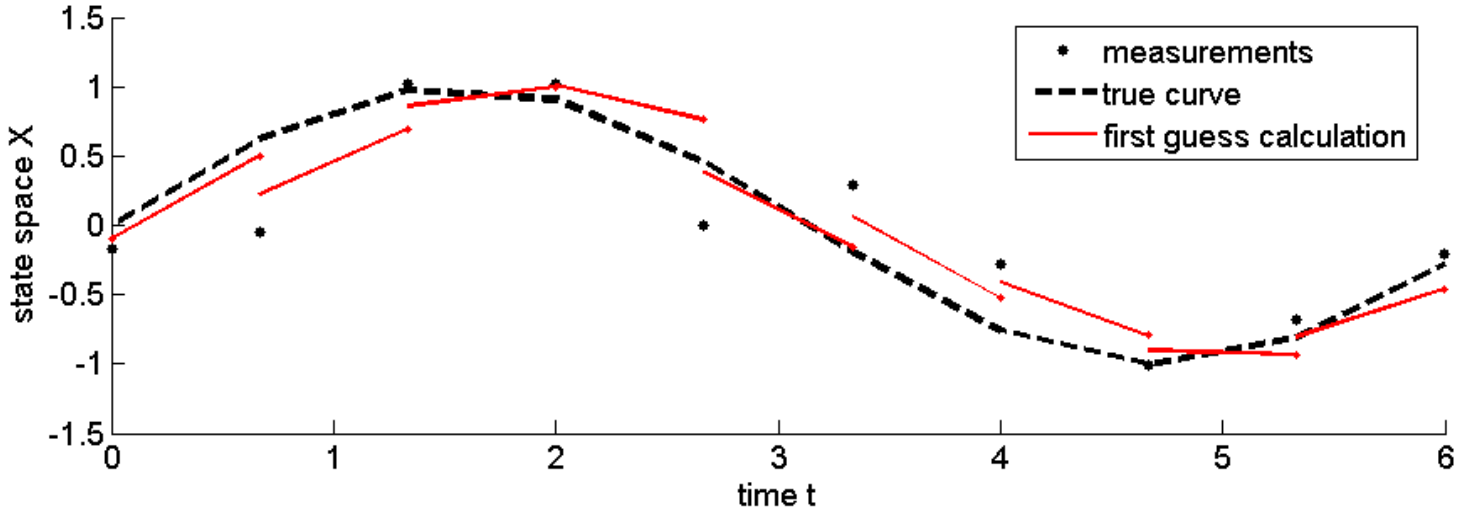
$$\varphi_{k+1}^{(a)} = \varphi_{k+1}^{(b)} + R_\alpha \left(f_{k+1} - H\varphi_{k+1}^{(b)} \right) \tag{4}$$

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

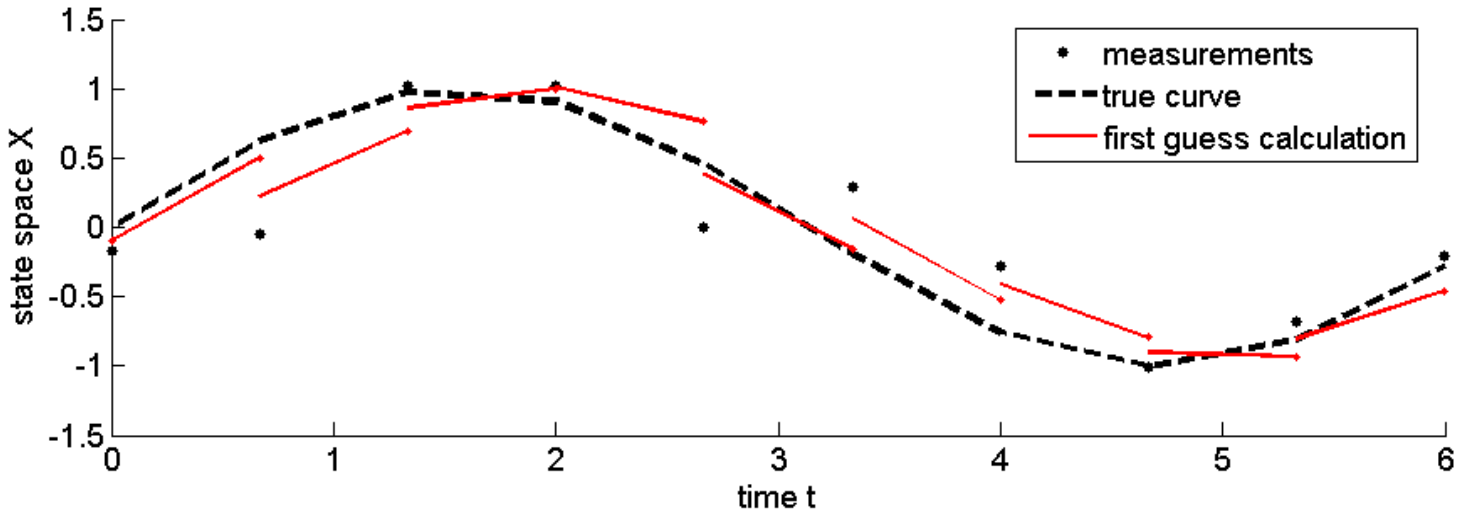
$$\varphi_{k+1}^{(a)} = M\varphi_k^{(a)} + R_\alpha \left(f_{k+1} - HM\varphi_k^{(a)} \right) \tag{5}$$

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

3dVAR - 1


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

3dVAR - 1



1. Start with $\varphi_0^{(a)}$ and for $k = 1, 2, 3, \ldots$ do:

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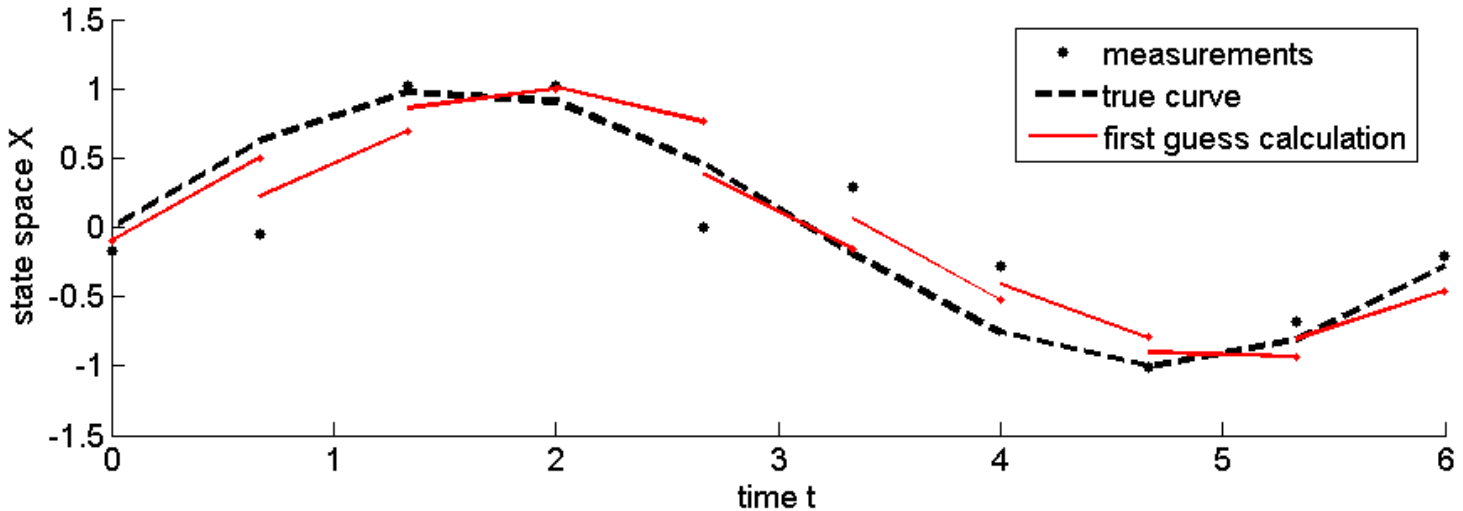

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2. Calculate **first guess**

$$\varphi_k^{(b)} = M_{k-1}\varphi_{k-1}^{(a)} \tag{6}$$

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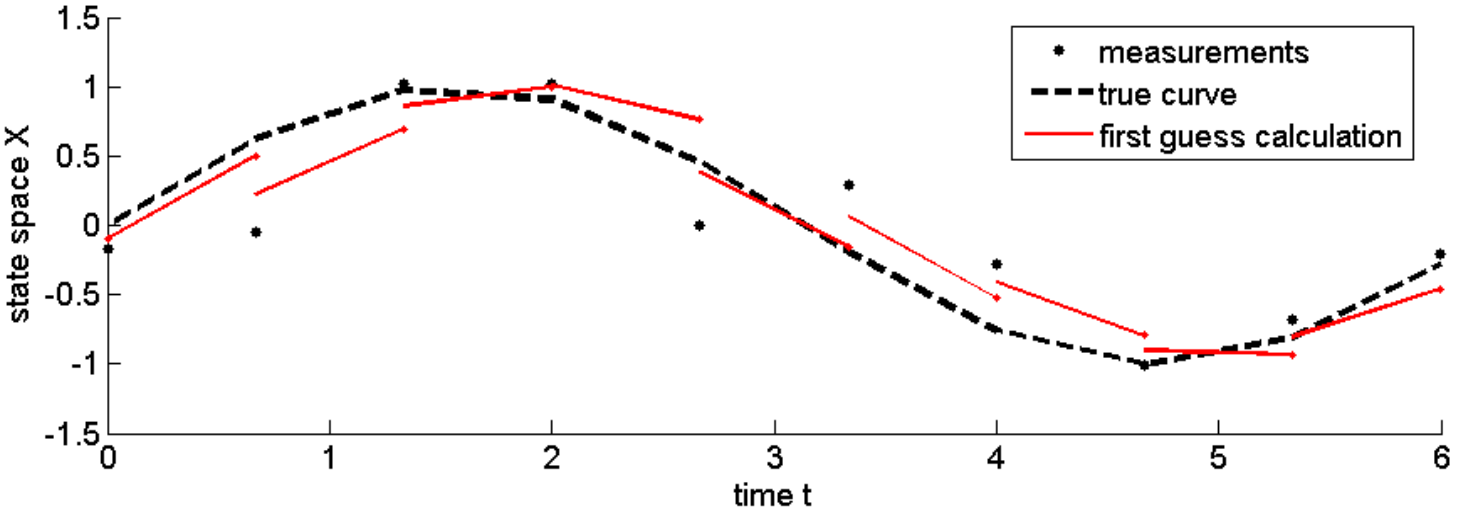

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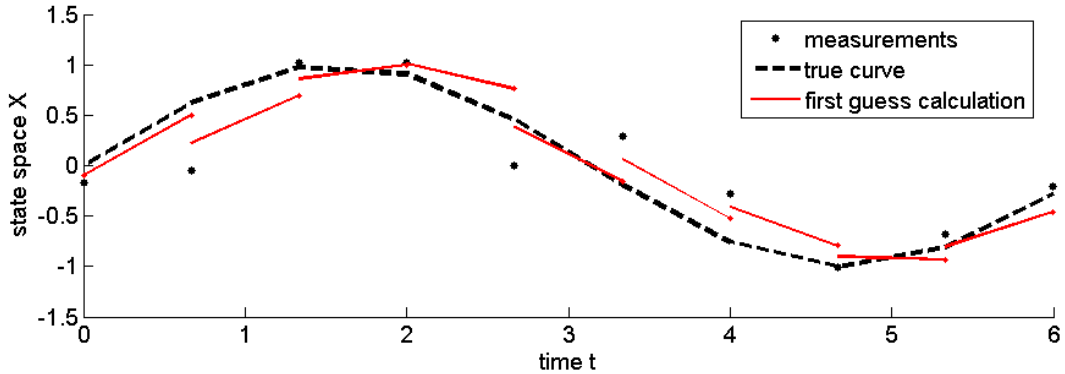
3. **Assimilate data** f_k at time t_k calculating $\varphi_k^{(a)}$.

3dVAR - 2



Functional at **time slice**

$$J(\varphi) = ||\varphi - \varphi^{(b)}||^2_{B^{-1}} + ||f - H\varphi||^2_{R^{-1}} \tag{7}$$

Update Formula

$$\begin{aligned} \varphi_k^{(a)} &= \varphi_k^{(b)} + \left(B^{-1} + H^* R^{-1} H\right)^{-1} H^* R^{-1} \left(f_k - H(\varphi_k^{(b)})\right) \\ &= \varphi_k^{(b)} + \underbrace{BH^*\left(R + HBH^*\right)^{-1}}_{\text{Kalman gain matrix}} \Big(\underbrace{f_k - H(\varphi_k^{(b)})}_{\text{obs - first guess}} \Big). \end{aligned} \tag{8}$$

3dVar = Tikhonov Regularization in a weighted space

We study a **weighted scalar product**

$$\left\langle \varphi, \psi \right\rangle := \left\langle \varphi, B^{-1}\psi \right\rangle_{L^2}, \quad \left\langle f, g \right\rangle := \left\langle f, R^{-1}g \right\rangle_{L^2} \tag{9}$$

with some self-adjoint invertible matrices B and R. The adjoint with respect to the weighted scalar product is denoted by H'.

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This leads to

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$$H' = BH^*R^{-1} \tag{10}$$

and thus

$$\begin{aligned} BH^*\left(R + HBH^*\right)^{-1} &= BH^*R^{-1}\left(I + HBH^*R^{-1}\right)^{-1} \\ &= H'\left(I + HH'\right)^{-1} = \left(I + H'H\right)^{-1}H'. \end{aligned}$$

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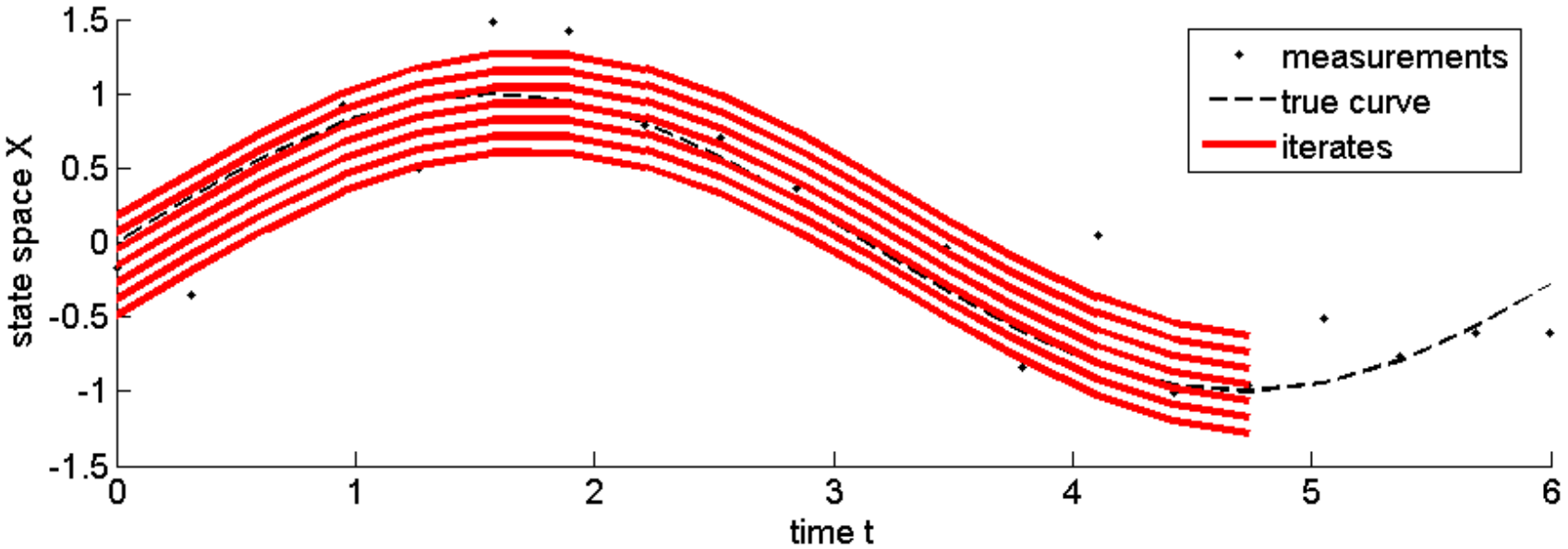
4dVar - 1 (functional)

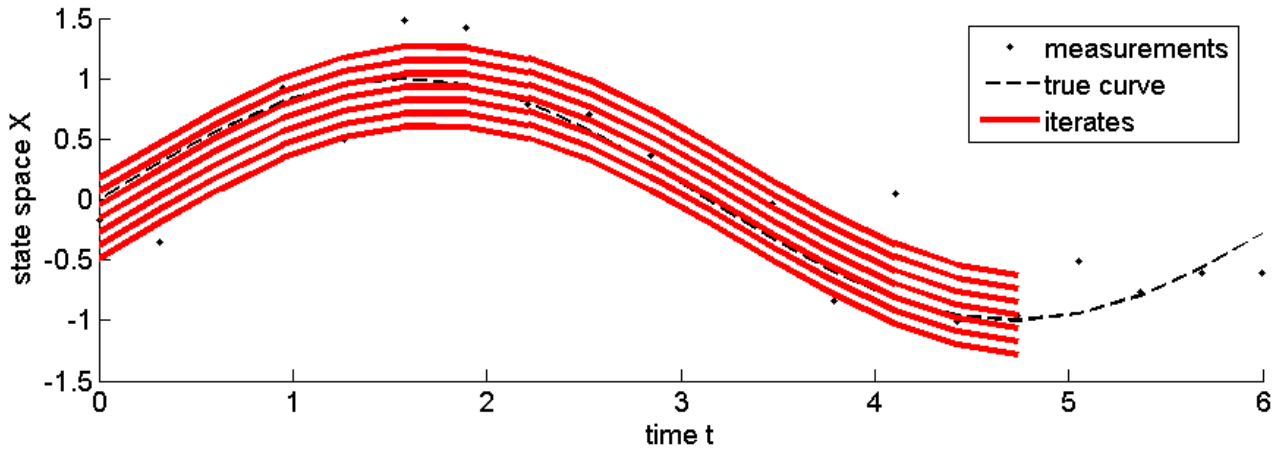


Functional on **time interval**, minimize by a **Gradient Method**

$$J(\varphi) = ||\varphi - \varphi^{(b)}||^2_{B^{-1}} + \sum_{k=1}^{K} ||f_k - H\varphi_k||^2_{R^{-1}}, \qquad \varphi_k = M[t_0, t_k]\varphi$$

where $M[s, t]$ denotes the **model operator** from time s to time t.

4dVar - 2 (cycling)



Functional

$$J(\varphi) = ||\varphi - \varphi_\ell^{(b)}||^2_{B^{-1}} + \sum_{k=1}^{K} ||f_k - H\varphi_{\ell+k}||^2_{R^{-1}}, \quad \varphi_{\ell+k} = M[t_\ell, t_{\ell+k}]\varphi$$

for $\ell = 0, K, 2K, 3K, \ldots$

Minimizer gives the *analysis* $\varphi_\ell^{(a)}$, next **background** is

$$\varphi_{\ell+K}^{(b)} = M[t_\ell, t_{\ell+K}]\varphi_\ell^{(a)} \tag{11}$$

4dVar - 3 (with linear M rewrite as Tikhonov)

Assume that M is linear. Then by

$$\tilde{H}_\ell \varphi := \begin{pmatrix} H\varphi \\ HM[t_\ell, t_{\ell+1}]\varphi \\ HM[t_\ell, t_{\ell+2}]\varphi \\ \vdots \\ HM[t_\ell, t_{\ell+K}]\varphi \end{pmatrix} \quad \tilde{f}_\ell := \begin{pmatrix} f_{\ell+1} \\ f_{\ell+2} \\ \vdots \\ f_{\ell+K} \end{pmatrix} \tag{12}$$

we can rewrite 4*dVar* as a three-dimensional assimilation algorithm solving

$$\tilde{H}\varphi = \tilde{f}_\ell. \tag{13}$$

The regularized solution provides $\varphi_\ell^{(a)}$, from which $\varphi_{\ell+K}^{(b)}$ is calculated by an application of $M[t_\ell, t_{\ell+K}]$.

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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

$$H' H \psi_n = \mu_n^2 \psi_n, \tag{14}$$

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With measurements

$$f = \sum_{n=1}^{\infty} f_n g_n \quad \in Y \tag{16}$$

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**

$$\gamma_n = \frac{\mu_n}{\alpha + \mu_n^2} f_n, \quad n \in \mathbb{N}. \tag{17}$$

Spectral Representation 2

The true Inverse is

$$\gamma_n^{true} = \frac{1}{\mu_n} f_n^{true}. \tag{18}$$

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

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

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

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

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A system with constant dynamics

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

$$\varphi_{k+1}^{(b)} = \varphi_k^{(a)}, \quad k = 1, 2, 3, \ldots \tag{20}$$

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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(This coincides with work of Engl on 'iterated Tikhonov regularization'!)

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$$\varphi_k = \varphi_{k-1} + \left(\alpha I + H'H\right)^{-1} H'\left(f - H\varphi_{k-1}\right), \quad k = 1, 2, 3, \ldots \tag{21}$$

(This coincides with work of Engl on 'iterated Tikhonov regularization'!)

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

$$\gamma_{n,k} = \gamma_{n,k-1} + \frac{\mu_n}{\alpha + \mu_n^2}\left(f_{n,k} - \mu_n \gamma_{n,k-1}\right) \tag{22}$$

Spectral Formula I

We employ

$$f = H\varphi^{(true)} + \delta, \quad f_{n,k} = \mu_n \gamma_n^{(true)} + \delta_n. \tag{23}$$

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**

$$\gamma_{n,k} = (1 - q_n)\gamma_n^{(true)} + q_n \gamma_{n,k-1} + \frac{(1 - q_n)}{\mu_n}\delta_n \tag{24}$$

using

$$q_n = \frac{\alpha}{\alpha + \mu_n^2} = 1 - \frac{\mu_n^2}{\alpha + \mu_n^2}. \tag{25}$$

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*

$$\gamma_{n,k} = (1 - q_n^k)\gamma_n^{(true)} + q_n^k \gamma_{\mathbf{n,0}} + \frac{(1 - q_n^k)}{\mu_n}\delta_n \tag{26}$$

using

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

Proof. Induction over k. □

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Convergence for $f \in R(H)$

Theorem (Convergence for $f \in R(H)$)

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

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

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for $k \to \infty$.

Since $0 < q_n < 1$, we have

$$q_n^k \to 0, \quad k \to \infty, \quad (1 - q_n^k) \to 1, \quad k \to \infty. \tag{29}$$

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* $k \to \infty$.

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 $k \to \infty$.*

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 $k \to \infty$. 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 $k \in \mathbb{N}$

$$\left|\frac{(1 - q_n^k)}{\mu_n}\right| = \left|\frac{(\alpha + \mu_n^2)^k - \alpha^k}{(\alpha + \mu_n^2)^k \mu_n}\right| \tag{31}$$

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

Divergence for $f \notin R(H)$

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

$$S_L := \sum_{n=1}^{L} \left| \frac{\delta_n}{\mu_n} \right|^2 \to \infty, \quad L \to \infty. \tag{32}$$

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

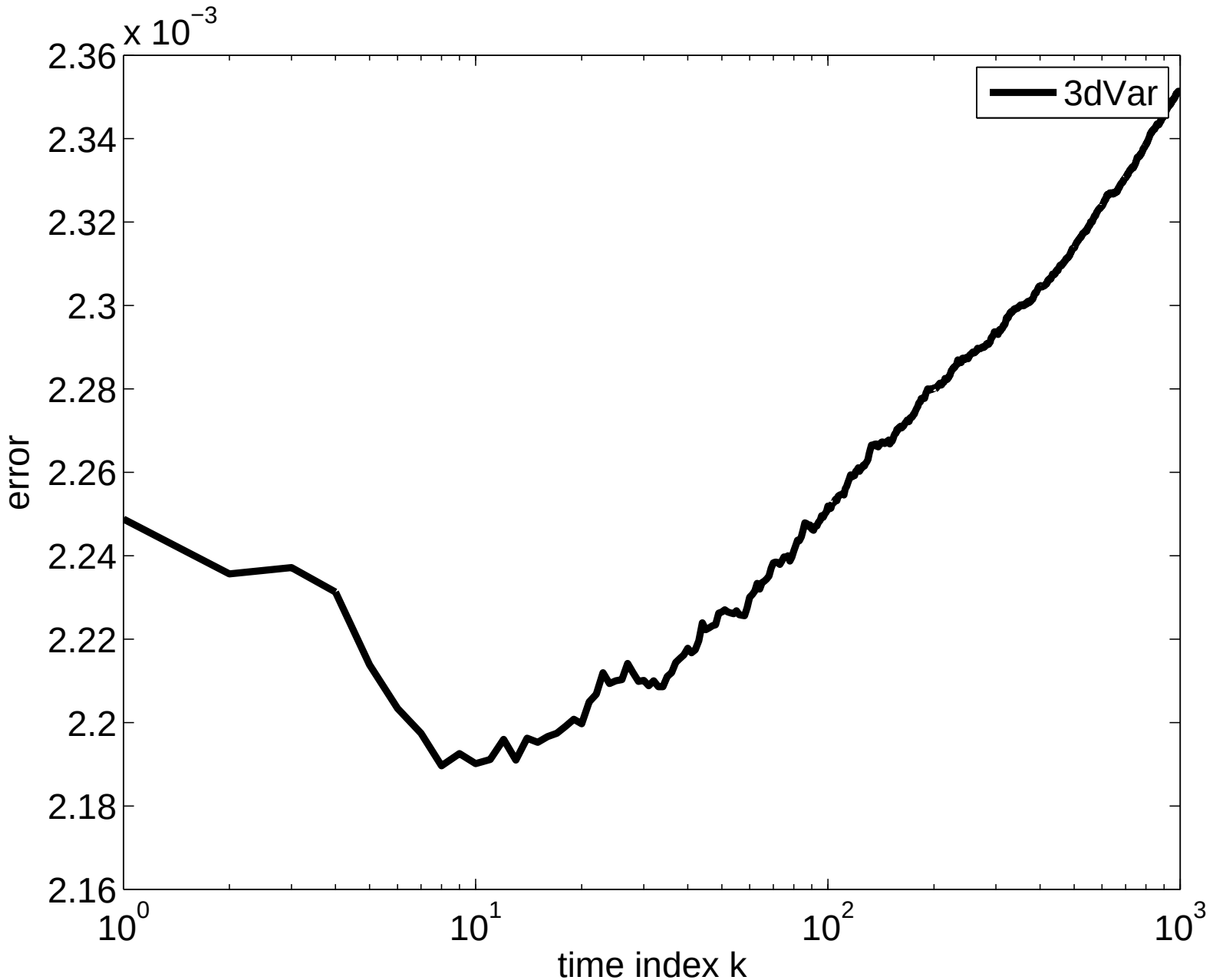
$$||\sigma_k||^2 \geq \sum_{n=1}^{L} \left| \frac{(1 - q_n^k)\delta_n}{\mu_n} \right|^2 > C \tag{33}$$

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

$$||\sigma_k|| \to \infty, \quad k \to \infty \tag{34}$$

and the proof is complete. □

Numerical Example: Dynamic Magnetic Tomography



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$$\begin{aligned}\varphi_{k+1}^{(a)} - \varphi_{k+1}^{(true)} &= M\left(\varphi_k^{(a)} - \varphi_k^{(true)}\right) + R_\alpha HM\left(\varphi_k^{(true)} - \varphi_k^{(a)}\right) + R_\alpha f_{k+1}^{(\delta)} \\ &= \left(I - R_\alpha H\right)M\left(\varphi_k^{(a)} - \varphi_k^{(true)}\right) + R_\alpha f_{k+1}^{(\delta)}. \end{aligned} \tag{35}$$

We abbreviate the analysis error by

$$\mathbf{e_k} := \varphi_k^{(a)} - \varphi_k^{(true)}, \quad k = 1, 2, \ldots \tag{36}$$

and define

$$\Lambda := \left(I - R_\alpha H\right)M \tag{37}$$

to obtain the iteration formula

$$e_{k+1} = \Lambda e_k + R_\alpha f_{k+1}^{(\delta)}, \quad k = 0, 1, 2, \ldots \tag{38}$$

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 (38) evolve according to

$$e_k = \Lambda^k e_0 + \left(\sum_{\ell=0}^{k-1} \Lambda^\ell \right) e^{(\delta)} \tag{39}$$

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

$$e_k = \Lambda^k e_0 + (I - \Lambda)^{-1}(I - \Lambda^k) e^{(\delta)} \tag{40}$$

- 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.

Frobenius Norm

Let $\{\psi_\ell : \ell \in \mathbb{N}\}$ be a complete orthonormal system in X. Then, any vector $\varphi \in X$ can be decomposed into its Fourier sum

$$\varphi = \sum_{\ell=1}^{\infty} \alpha_\ell \psi_\ell \tag{41}$$

with $\alpha_\ell := \langle \varphi, \psi_\ell \rangle$ for $\ell \in \mathbb{N}$. We apply this to $M\varphi$ to derive

$$M\varphi = \sum_{\ell=1}^{\infty} \langle M\varphi, \psi_\ell \rangle \psi_\ell = \sum_{\ell=1}^{\infty} \sum_{j=1}^{\infty} \alpha_j \langle M\varphi_j, \psi_\ell \rangle \psi_\ell = \sum_{\ell=1}^{\infty} \sum_{j=1}^{\infty} \psi_\ell M_{\ell,j} \alpha_j.$$

with the infinite matrix $M_{\ell,j} = \langle M\psi_j, \psi_\ell \rangle$. The **Frobenius norm** of M with respect to the orthonormal system $\{\psi_\ell : \ell \in \mathbb{N}\}$ is defined as

$$||M||_{Fro} := \sum_{\ell=1}^{\infty} \sum_{j=1}^{\infty} |M_{\ell,j}|^2. \tag{42}$$

Frobenius Systems: Damping of High Frequencies

Lemma

If M is self-adjoint with respect to the scalar product $\langle \cdot, \cdot \rangle$, then its Frobenius norm (42) is independent of the orthonormal system $\{\psi_\ell : \ell \in \mathbb{N}\}$.

- The identity operator I does *not* have a bounded Frobenius norm.
- Systems with bounded Frobenius norm are damping on higher modes or frequencies.

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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 $N = (I - R_\alpha H)$ 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**

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

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

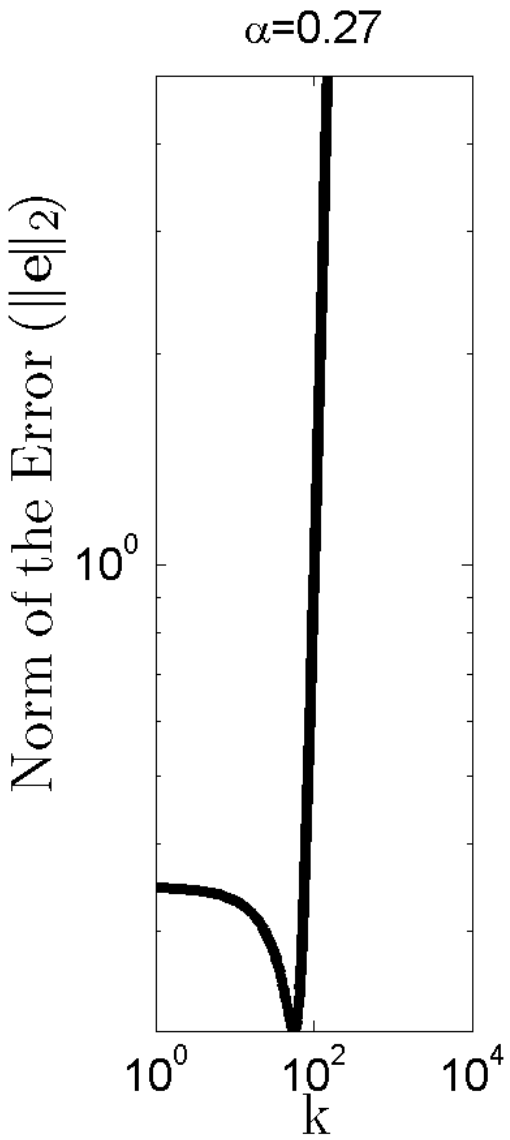
$$e_k = \Lambda^k e_0 + (I - \Lambda)^{-1}(I - \Lambda^k)e^{(\delta)} \tag{55}$$

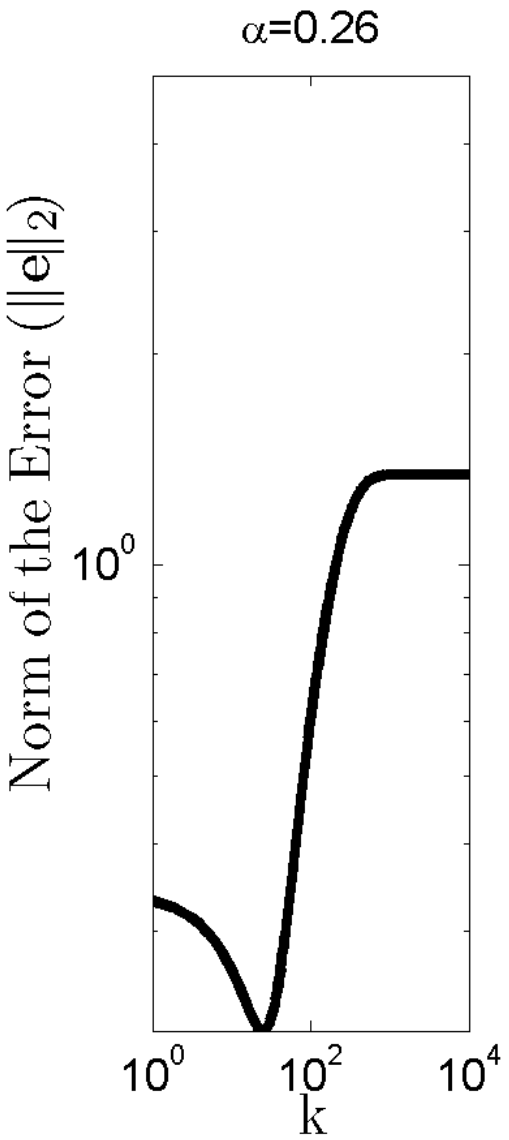
Theorem

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 DA Instability

- 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.

- 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 $||M||_2 > 1$.