

Data assimilation from a viewpoint of regularization theory

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J. Cheng, L. Ding, M. Iglesias, L. Lin, P. Niu, A. Stuart, F. Werner.

Outline

Motivation and Introduction Filter Based Methods Data Models

Discrete dynamic systems

Main assumptions and general filter properties Asymptotic behavior

Continuous dynamic systems

From discrete setting to continuous one Asymptotic behavior

Conclusion

Motivation: history

Bayes' theorem

Proposed by Thomas Bayes and summarized by Richard Price (1763)



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Motivation: history

Tikhonov–Phillips regularization

Independently by Andrey Tikhonov (1963) and David L. Phillips (1962)



 $T\varphi=g$

$$\varphi_{\alpha}^{\delta} \mapsto \min J_{\alpha}(\varphi) := \|T\varphi - g^{\delta}\|^2 + \alpha \|\varphi - \varphi_0\|^2$$

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Motivation: history

Kalman filter

By Rudolph Kalman (1960)



What we know and what we want to know

Deterministic		Statistical		
Regularization \iff		Bayesian Approach		
??	\iff	Filter based methods		
	Deterministic Regularization ??	DeterministicRegularization??		



T. Bayes 18th Century

R. Kalman 1960





A. Tikhonov 1963

What we know and what we want to know

	Deterministic		Statistical		
Steady equations	Regularization	\iff	Bayesian Approach		
Dynamic system	??	\Leftrightarrow	Filter based methods		

Filter based methods:

- Kalman Filter, 3DVAR (Online);
- 4DVAR (Offline);
- Kalman-Bucy Filter (Online, continuous dynamic).
- Ensemble Kalman Filter, Particle Filter (Online);

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Filter based methods:

- Kalman Filter, 3DVAR (Online);
- 4DVAR (Offline);
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- Ensemble Kalman Filter, Particle Filter (Online);

Task: deriving optimal error estimates and asymptotic behavior.

Linear Inverse Problems

We consider the linear inverse problem

$$y=Au^{\dagger}+\eta,$$

- *A* is an injective linear bounded operator acting from a Hilbert space *X* to *Y*.
- The exact solution $u^{\dagger} \in X$.
- Noise $\eta \sim \mathcal{N}(0, \gamma^2 I)$.

Artificial Dynamic

Dynamic System

$$u_n = u_{n-1}$$

$$y_n = Au_n + \eta_n,$$

Artificial Dynamic

Dynamic System

 $u_n = u_{n-1}$ $y_n = Au_n + \eta_n,$

Inverse problems

- Steady setting: reconstruct the unknown solution. Method: regularization schemes.
- Artificial dynamic: identify the stationary state and quantify the uncertainty. Method: filter based methods.

M. A. Iglesias, K. J. Law, and A. M. Stuart, *Ensemble Kalman methods for inverse problems*, Inverse Problems **29** (2013), no. 4, 045001.

Prediction step:

$$\begin{array}{rcl} \mathscr{N}(m_{n-1},C_{n-1}) & \to & \mathscr{N}(\hat{m}_n,\hat{C}_n) \\ \pi(u_{n-1}|y_1,\ldots,y_{n-1}) & & \pi(u_n|y_1,\ldots,y_{n-1}) \end{array}$$

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Analysis step:

$$\begin{aligned} \mathcal{N}(\hat{m}_n, \hat{C}_n) &\to & \mathcal{N}(m_n, C_n) \\ \pi(u_n | y_1, \dots, y_{n-1}) & & \pi(u_n | y_1, \dots, y_{n-1}, \mathbf{y_n}) \end{aligned}$$

🛸 K. J. Law, A.M. Stuart, and K.C. Zygalakis, Data Assimilation: A Mathematical Introduction, Springer, 2015.

Dynamic System

$$u_n = Du_{n-1}$$
$$y_n = Hu_n + \eta_n$$

Dynamic System

$$u_n = Du_{n-1}$$
$$y_n = Hu_n + \eta_n$$

Prediction:

$$\hat{m}_n = Dm_{n-1}$$

 $\hat{C}_n = DC_{n-1}D^*$

Analysis:

$$m_n = \hat{m}_n + K_n(y_n - H\hat{m}_n)$$

$$C_n = (I - K_n H)\hat{C}_n,$$

with Kalman gain

$$K_n = \hat{C}_n H^T \left(H \hat{C}_n H^T + \gamma^2 I \right)^{-1}.$$

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Kalman Filter for Artificial Dynamic

Kalman filter

Let D = I and H = A. Take $\mathcal{N}(m_0, C_0)$ with $C_0 = \frac{\gamma^2}{\alpha} \Sigma_0$ as the initial guess

$$K_n = C_{n-1}A^* (AC_{n-1}A^* + \gamma^2 I)^{-1}$$

$$m_n = m_{n-1} + K_n(y_n - Am_{n-1})$$

$$C_n = (I - K_n A)C_{n-1}.$$

3DVAR for Artificial Dynamic

3DVAR

Let D = I and H = A. Take $\mathcal{N}(m_0, C_0)$ with $C_0 = \frac{\gamma^2}{\alpha} \Sigma_0$ as the initial guess and fix the Kalman gain

$$K_n \equiv \mathscr{K} := C_0 A^* \left(A C_0 A^* + \gamma^2 I \right)^{-1}$$

$$\zeta_n = \zeta_{n-1} + \mathscr{K} (y_n - A \zeta_{n-1})$$

$$\mathscr{C}_n \equiv (I - \mathscr{K} A) C_0.$$

Iterative Regularization Methods

Iterative Tikhonov Regularization

$$u_n = \arg \min \frac{1}{2} ||y - Au||^2 + \frac{\alpha}{2} ||u - u_{n-1}||^2,$$

or equivalently

$$u_n = u_{n-1} + (A^*A + \alpha I)^{-1}A^*(y - Au_{n-1}).$$

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Weighted operator in regularization:

 $(A^*A + \alpha I)^{-1}A^*;$

• Kalman gain in filter based methods:

$$K_{n} = C_{n-1}A^{*} \left(AC_{n-1}A^{*} + \gamma^{2}I\right)^{-1}$$

Tikhonov & Arsenin 1977], [Hofmann 1986], [Louis 1989], Tikhonov, Goncharsky, Stepanov & Yagola 1995],
 [Engl, Hanke & Neubauer 1996], [Nair 2009], [Kabanikhin 2012], [Lu & Pereverzev 2013] ...

Statistical Inverse Problems

Spectral methods of the form

$$u_{\gamma}^{\delta} = q_{\gamma}(A^*A)A^*y^{\delta}$$

Variational ones of the form

$$u_{\gamma}^{\delta} \in \operatorname{arg\,min}_{u \in X} \left[\|Au\|_{Y}^{2} - 2\left\langle Au, y^{\delta} \right\rangle_{Y \times Y^{*}} + \gamma R(u) \right]$$

Table 1. R	ates for o	leterministic	and	stochastic	model
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	Deterministic	Stochastic
Direct	ε^2	$\varepsilon^{\frac{4\alpha}{2\alpha+1}}$
Polynomial	$\varepsilon^{\frac{4\alpha}{2\alpha+2\beta}}$	$\varepsilon^{rac{4lpha}{2lpha+2eta+1}}$
Exponential	$\varepsilon^{\frac{4\alpha}{2\alpha+2\beta}}$	$\varepsilon^{\frac{4\alpha}{2\alpha+2\beta}}$

L. Cavalier, *Ch.1 Inverse Problems in Statistics*, P. Alquier et al. (eds.), Inverse Problems and High-Dimensional Estimation, Lecture Notes in Statistics 203, Springer-Verlag Berlin Heidelberg 2011.

Data model 1: updating observation

$$u_n = u_{n-1}$$
$$y_n = Au_n + \eta_n$$

Here each η_n is i.i.d Gaussian noise drawn from $\mathcal{N}(0, \gamma^2 I)$.

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Here each η_n is i.i.d Gaussian noise drawn from $\mathcal{N}(0, \gamma^2 I)$.

Decreased uncertainty

Auxiliary element (the law of large number)

$$\bar{y} = \frac{1}{n} \sum_{j=1}^{n} y_j = A u^{\dagger} + \frac{1}{n} \sum_{j=1}^{n} \eta_j.$$

with $\bar{\eta} = \frac{1}{n} \sum_{j=1}^{n} \eta_j$ whose distribution is $\mathcal{N}(0, \frac{\gamma^2}{n}I)$.

B. T. Knapik; A. W. Van Der Vaart and J. H. Van Zanten, *Bayesian inverse problems with Gaussian priors*, The Annals of Statistics 39 (2011), 2626–2657.





Nonlinear problems extension:

- Deterministic: Levenberg–Marquardt Methods;
- Statistical: Extended Kalman Filter Method; Ensemble Kalman Filter Method.

M. A. Iglesias, K. J. Law, and A. M. Stuart, *Ensemble Kalman methods for inverse problems*, Inverse Problems **29** (2013), no. 4, 045001.

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General Filter Properties

General formulae:

Updated mean: $m_n = (I - K_n A)m_{n-1} + K_n y_n;$ True solution: $u^{\dagger} = (I - K_n A)u^{\dagger} + K_n A u^{\dagger}.$

General Filter Properties

Bias-Variance Decomposition:

Total error $e_n := m_n - u^{\dagger}$:

$$e_n = \prod_{j=1}^n (I - K_j A) e_0 + \sum_{j=1}^{n-1} \left(\prod_{i=n-j}^{n-1} (I - K_{i+1} A) \right) K_{n-j} \eta_{n-j} + K_n \eta_n$$

:= J₁ + J₂

with an initial guess m_0 and

$$e_{0} = m_{0} - u^{\dagger};$$

$$J_{1} = \prod_{j=1}^{n} (I - K_{j}A)e_{0} \quad \text{(Bias)};$$

$$J_{2} = \sum_{j=1}^{n-1} \left(\prod_{i=n-j}^{n-1} (I - K_{i+1}A)\right) K_{n-j}\eta_{n-j} + K_{n}\eta_{n} \quad \text{(Variance)}.$$

Mean Squared Error

Mean squared error:

$$\mathbb{E}||m_n - u^{\dagger}||^2 = ||J_1||^2 + \mathbb{E}||J_2||^2.$$

Mean Squared Error

Mean squared error:

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Key formula:

Kalman filter:

$$\prod_{j=1}^{n} (I - K_j A) = C_n C_0^{-1} = (C_0^{-1} + nA^* A/\gamma^2)^{-1} C_0^{-1}$$
$$= C_0^{\frac{1}{2}} \gamma^2 (\gamma^2 I + nC_0^{\frac{1}{2}} A^* A C_0^{\frac{1}{2}})^{-1} C_0^{-\frac{1}{2}}.$$

3DVAR:

$$(I - \mathscr{K}A)^n = C_0^{\frac{1}{2}} \gamma^2 (\gamma^2 I + C_0^{\frac{1}{2}} A^* A C_0^{\frac{1}{2}})^{-n} C_0^{-\frac{1}{2}}.$$

Main Assumptions

Assumption 1

- 1. the initial variance $C_0 = \frac{\gamma^2}{\alpha} \Sigma_0$ and $\mathscr{R}(\Sigma_0^{1/2}) \subset \mathscr{D}(A)$, where α is a positive constant and Σ_0 is positive self-adjoint, and Σ_0^{-1} is a densely defined unbounded self-adjoint strictly positive operator;
- 2. the forward operator A satisfies

$$C^{-1} \|\Sigma_0^{\frac{a}{2}} x\| \le \|Ax\| \le C \|\Sigma_0^{\frac{a}{2}} x\|$$

on *X* for some constants a > 0 and $1 \le C < \infty$;

- 3. the initial mean satisfies $m_0 u^{\dagger} \in \mathscr{D}(\Sigma_0^{-\frac{s}{2}})$ (or $\zeta_0 u^{\dagger} \in \mathscr{D}(\Sigma_0^{-\frac{s}{2}})$) with $0 \le s \le a + 2$;
- 4. the operator Σ_0 in item 1. is trace-class on *X*.

H. W. Engl; M. Hanke and A. Neubauer, *Regularization of inverse problems*. Kluwer Academic Publishers Group, Dordrecht, 1996.

Main Assumptions

Assumption 2

1. Let the initial variance $C_0 = \frac{\gamma^2}{\alpha} \Sigma_0$. The operators Σ_0 and A^*A have the same eigenfunctions $\{e_i\}$ with their eigenvalues $\{\lambda_i\}$ and $\{\kappa_i^2\}$ satisfying

$$\lambda_i = i^{-1-2\varepsilon}, \qquad C^{-1}i^{-p} \le \kappa_i \le Ci^{-p}$$

for some $\varepsilon > 0$, p > 0 and $C \ge 1$.

2. By choosing the initial mean $m_0 = 0$, the true solution u^{\dagger} with its coordinates $\{u^{\dagger,i}\}$ in the basis $\{e_i\}$ obeys $\sum_{i=1}^{\infty} (u^{\dagger,i})^2 i^{2\beta} < \infty$.

Assumptions 1 and 2 are identical if $a = \frac{2p}{1+2\epsilon}$ and $s = \frac{2\beta}{1+2\epsilon}$.

B. T. Knapik; A. W. Van Der Vaart and J. H. Van Zanten, *Bayesian inverse problems with Gaussian priors*, The Annals of Statistics 39 (2011), 2626–2657.

Asymptotic Analysis

Setup revisit:

Two data models: Updating or fixed observation; Two assumptions: General operators or SVD systems;

Asymptotic Analysis

Setup revisit:

Two data models: Updating or fixed observation; Two assumptions: General operators or SVD systems;

Initial values revisit: Initial mean: $m_0 = 0$; Initial variance: $C_0 = \frac{\gamma^2}{\alpha} \Sigma_0$ with noise variance $\gamma^2 I$ and an operator Σ_0 . The parameter α is a tuning parameter.

Kalman Filter: Data Model 1

Kalman filter (Assumption 1)

Let Assumption 1 hold. Then the Kalman filter method yields a bias-variance decomposition of the mean squared error

$$\mathbb{E}\|m_n - u^{\dagger}\|^2 \leq C\left(\frac{\alpha}{n}\right)^{\frac{s}{a+1}} + \frac{\gamma^2}{\alpha} \operatorname{tr}(\Sigma_0)$$

for the Data Model 1. Setting $\alpha = N^{\frac{s}{s+a+1}}$ and stopping the iteration when n = N then gives

$$\mathbb{E}\|m_N - u^{\dagger}\|^2 \leq \left(C + \gamma^2 \operatorname{tr}(\Sigma_0)\right) N^{-\frac{s}{s+a+1}}.$$

Asymptotical boundness of Kalman filter (for any fixed α and γ).

3DVAR: Data Model 1

3DVAR (Assumption 1)

Let Assumption 1 hold. Then 3DVAR filter yields a bias-variance decomposition of the mean squared error

$$\mathbb{E}\|\zeta_n - u^{\dagger}\|^2 \le C\left(\frac{\alpha}{n}\right)^{\frac{s}{\alpha+1}} + C\frac{\gamma^2 \ln n}{\alpha} \operatorname{tr}(\Sigma_0)$$

for the Data Model 1. Setting $\alpha = N^{\frac{s}{s+a+1}}$ and stopping the iteration when n = N then gives

$$\mathbb{E}\|\zeta_N - u^{\dagger}\|^2 \leq C \left(1 + \gamma^2 \operatorname{tr}(\Sigma_0)\right) N^{-\frac{s}{s+a+1}} \ln N.$$

Blow up of 3DVAR (for any fixed α and γ).

Kalman Filter: Data Model 1

Kalman filter (Assumption 2)

Let Assumption 2 hold. Then the Kalman filter method yields a bias-variance decomposition of the mean squared error

$$\mathbb{E}\|m_n-u^{\dagger}\|^2 \leq C\left(\frac{\alpha}{n}\right)^{\frac{2\beta}{1+2\varepsilon+2\rho}} + \gamma^2 n^{-\frac{2\varepsilon}{1+2\varepsilon+2\rho}} \alpha^{-\frac{1+2\rho}{1+2\varepsilon+2\rho}}$$

for the Data Model 1. Setting $\alpha = N^{\frac{2(\beta-\varepsilon)}{1+2\beta+2p}}$ and stopping the iteration when n = N then gives following minimax convergence rate:

$$\mathbb{E}||m_N-u^{\dagger}||^2 \leq CN^{-\frac{2\beta}{1+2\beta+2p}}.$$

Unconditional convergence of Kalman filter (for any fixed α and γ).

Kalman Filter: Data Model 2

Kalman Filter: Assumption 1

Let Assumption 1 hold. Then the Kalman filter method yields a bias-variance decomposition of the mean squared error

$$\mathbb{E}\|m_n - u^{\dagger}\|^2 \leq C\left(\frac{\alpha}{n}\right)^{\frac{s}{a+1}} + \frac{n\gamma^2}{\alpha} \operatorname{tr}(\Sigma_0)$$

for Data Model 2. Fix $\alpha = 1$ and assume that the noise variance $\gamma^2 = N^{-\frac{a+s+1}{a+1}}$. If the iteration is stopped at n = N then following convergence rate is valid:

$$\mathbb{E}\|m_N - u^{\dagger}\|^2 \le (C + \operatorname{tr}(\Sigma_0)) N^{-\frac{s}{a+1}}.$$

Blow up of Kalman filter (for any fixed α and γ).

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Linear Inverse Problems

We consider the linear inverse problem

$$y = Au^{\dagger} + \eta,$$

- *A* is an injective linear bounded operator acting from a Hilbert space *X* to *Y*.
- The exact solution $u^{\dagger} \in X$.
- Noise $\eta \sim \mathcal{N}(0, \varepsilon^2 I)$.

Towards a continuous analog

Artificial dynamical system (Data model 1)

$$u_n = u_{n-1}$$
$$y_n = Au_n + \eta_n$$

with $\eta_n \sim \mathcal{N}(0, \tau^{-1}\Sigma)$.

The continuous analog

Denote $z_1, ..., z_n$ be equidistant (approximate) samples of a random process z such that $y_n = \left(\frac{z_n - z_{n-1}}{\tau}\right)$ with a time step $\tau > 0$, let $\tau \to 0$ and

$$du = 0, \quad u(0) = u^{\dagger};$$

$$dz = Audt + \sqrt{\Sigma}dW, \quad z(0) = 0.$$

Consistency check

Original steady problem

$$y^{\delta} = A u^{\dagger} + \delta \eta$$

with a noise level δ and we assume $\delta \rightarrow 0$.

Consistency check

$$y^{\delta} := \frac{1}{T} z(T) = A u^{\dagger} + \frac{1}{T} \sqrt{\Sigma} \left(W(T) - W(0) \right),$$

$$\sqrt{\Sigma} \left(W(T) - W(0) \right) \sim \mathcal{N}_{Y} \left(0, T \Sigma \right).$$

Hence, the ending point of the observable process *z* carries the same information as the data observed in the original inverse problem with $\delta = 1/\sqrt{T}$.

Kalman-Bucy filter: Non-stationary Asymptotical Regularization Method

The Kalman-Bucy filter:

$$dm = CA^* \Sigma^{-1} (dz - Amdt), \quad m(0) = m_0;$$

$$dC = -CA^* \Sigma^{-1} ACdt, \quad C(0) = C_0.$$

Solve the Riccati equation to obtain

$$C(t) = (C_0^{-1} + tA^*\Sigma^{-1}A)^{-1}, \quad t > 0.$$

Thus the Kalman-Bucy filter is

$$dm = (C_0^{-1} + tA^*\Sigma^{-1}A)^{-1}A^*\Sigma^{-1}(dz - Amdt), \quad m(0) = m_0.$$

3DVAR: Stationary Asymptotical Regularization Method

$$d\zeta = \mathscr{C}A^*\Sigma^{-1}(dz - A\zeta dt), \quad \zeta(0) = m_0,$$

$$d\mathscr{C} = 0, \quad \mathscr{C}(0) = C_0.$$

Non-stationary (and stationary) ARMs

Non-stationary ARM (Kalman-Bucy filter)

$$(u-m)(t) = e^{-\int_0^t (C_0^{-1} + sA^*\Sigma^{-1}A)^{-1}A^*\Sigma^{-1}Ads} (u-m)(0)$$

- $\int_0^t e^{-\int_s^t (C_0^{-1} + \tau A^*\Sigma^{-1}A)^{-1}A^*\Sigma^{-1}Ad\tau} (C_0^{-1} + sA^*\Sigma^{-1}A)^{-1}A^*\Sigma^{-1/2}dW(s).$

Stationary ARM (3DVAR)

$$(u-\zeta)(t) = e^{-C_0 A^* \Sigma^{-1} A t} (u-\zeta)(0) - \int_0^t e^{-\int_s^t C_0 A^* \Sigma^{-1} A d\tau} C_0 A^* \Sigma^{-1/2} dW(s)$$

Niu, Lu and Cheng [IPI 2019]

Main ingredients

Effective dimension

$$\mathscr{D}(\gamma) = \mathscr{D}_B(\gamma) := \operatorname{tr}\left((\gamma I + B^* B)^{-1} B^* B\right), \gamma > 0.$$

Stochastic integration (Infinite-dimensional Itô-isometry)

The stochastic integral $\Phi \rightarrow \int_0^t \Phi(s) d\mathcal{W}(s)$ with respect to a *Y*-valued *Q*-Wiener process $\mathcal{W}(s)$ satisfies

$$\mathbb{E}\left\|\int_0^t \Phi(s) \mathrm{d}\mathscr{W}(s)\right\|_X^2 = \mathbb{E}\int_0^t \|\Phi(s)\|_{\mathscr{L}_2(Y_Q,X)}^2 \mathrm{d}s < \infty$$

for $t \in [0,T]$.

L. Gawarecki and V. Mandrekar, Stochastic Differential Equations in Infinite Dimensions with Applications to Stochastic Partial Differential Equations. Springer-Verlag Berlin Heidelberg 2011.

Convergence rate of Non-stationary ARM

Let appropriate Assumptions hold, then the non-stationary ARM yields MSE estimates

• If the function $\lambda \mapsto \phi(\lambda)/\lambda^{p+1}$ is non-increasing, then

$$\mathbb{E}\|m(t)-u^{\dagger}\|^{2} \leq \phi^{2}\left(\left(\frac{\alpha}{t}\right)^{\frac{1}{p+1}}\right) + \alpha^{-\frac{1}{p+1}}t^{-\frac{p}{p+1}}\mathscr{D}\left(\frac{\alpha}{t}\right)$$

for all $0 \le t \le T$.

 If there is a constant c < ∞ with φ(λ) ≤ cλ^{p+1} as λ → 0, then

$$\mathbb{E}\|m(t) - u^{\dagger}\|^{2} \leq c \left(\frac{\alpha}{t}\right)^{2} + \alpha^{-\frac{1}{p+1}} t^{-\frac{p}{p+1}} \mathscr{D}\left(\frac{\alpha}{t}\right)^{2}$$

for all $0 \le t \le T$.

Convergence rate of Stationary ARM

Let appropriate Assumptions hold, then the stationary ARM yields the MSE estimate

$$\mathbb{E}\|\zeta(t) - u^{\dagger}\|^{2} \leq c\phi^{2}\left(\left(\frac{\alpha}{t}\right)^{\frac{1}{p+1}}\right) + \frac{1}{2}\alpha^{-1}\mathrm{tr}\left(\Omega\right)$$

for all $0 \le t \le T$ with a constant $c = \max\{(v_0/(p+1))^{v_0/(p+1)}, 1\}$.

Answers to what we want to know!

	Deterministic		Statistical
Steady equations	Tikhonov	\iff	Bayesian approach
Discrete Dynamic	Tikhonov Iterative Tikhonov Tikhonov	$\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	Kalman filter 3DVAR 4DVAR (offline)
Continuous Dynamic	Tikhonov Showalter	$ \underset{\Longleftrightarrow}{\Leftrightarrow} $	Kalman-Bucy filter 3DVAR



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When inverse problems meet

- Randomness (Statistical inverse problems)
- Dynamic systems (Online inversion algorithms)

Kügler 2008], [Boiger & Kaltenbacher 2016], [Parzer & Scherzer 2022] ...



Thank you for your attention and have a good time in Linz!

Iglesias, Lin, Lu and Stuart [CMS 2017]; Ding, Lu and Cheng [J. Complexity 2018];
Niu, Lu and Cheng [IPI 2019]; Lu, Niu and Werner [JUQ 2021]; Wang, Han and Lu [Q J R Meteorol Soc 2021].