The Legacy of Rudolph Kalman

Blending Data and Mathematical Models

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Overview

Kalman State Estimation

Kalman Filter

State Space Model

Dynamics Model: $v_{n+1} = Mv_n + \xi_n, \quad n \in \mathbb{Z}^+$

Data Model: $y_{n+1} = Hv_{n+1} + \eta_{n+1}, \quad n \in \mathbb{Z}^+$

Probabilistic Structure: $v_0 \sim N(m_0, C_0), \quad \xi_n \sim N(0, \Sigma), \quad \eta_n \sim N(0, \Gamma)$

Probabilistic Structure: $v_0 \perp \{\xi_n\} \perp \{\eta_n\}$ independent

- Born: Budapest, May 19, 1930.
- Died: Florida, July 2, 2016.
- BS and MS from MIT, 1953, 1954.
- Positions at Stanford, ETH, U of Florida.
- US National Academy of Engineering 1991.
- US National Academy of Sciences 2004.
- US National Medal of Science 2008.
- Draper Prize, Kyoto Prize, Steele Prize . . .

Kalman Filter

State Space Model

$$
\begin{aligned}
\text{Dynamics Model:} \quad & v_{n+1} = Mv_n + \xi_n, \quad n \in \mathbb{Z}^+ \\
\text{Data Model:} \quad & y_{n+1} = Hv_{n+1} + \eta_{n+1}, \quad n \in \mathbb{Z}^+ \\
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\text{Probabilistic Structure:} \quad & v_0 \perp \{\xi_n\} \perp \{\eta_n\} \text{ independent}
\end{aligned}
$$

- J. Basic Engineering **82**(1960); see [1].
- 28,112 Google Scholar citations.
- Navigational and guidance systems.
- Apollo 11.
- $Y_n = \{y_\ell\}_{\ell=1}^{n}$.
- $v_n | Y_n \sim N(m_n, C_n)$.
- $(m_n, C_n) \mapsto (m_{n+1}, C_{n+1})$.

Kalman Filter

Sequential Optimization Perspective

$$\text{Predict:} \quad \widehat{m}_{n+1} = Mm_n, \quad n \in \mathbb{Z}^+$$

$$\text{Model/Data Compromise:} \quad J_n(m) = \frac{1}{2}|m - \widehat{m}_{n+1}|^2_{\widehat{C}_{n+1}} + \frac{1}{2}|y_{n+1} - Hm|^2_{\Gamma}$$

$$\text{Optimize:} \quad m_{n+1} = \operatorname{argmin}_m J_n(m).$$

- $|\cdot|_A = |A^{-\frac{1}{2}} \cdot|$ for $A > 0$.
- Updating $\widehat{C}_{n+1}$ is expensive: $\mathcal{O}(d^2)$ storage.
- d the state space dimension.

3DVAR Filter

State Space Model

$$
\begin{aligned}
\text{Dynamics Model:} \quad & v_{n+1} = \Psi(v_n) + \xi_n, \quad n \in \mathbb{Z}^+ \\
\text{Data Model:} \quad & y_{n+1} = Hv_{n+1} + \eta_{n+1}, \quad n \in \mathbb{Z}^+ \\
\text{Probabilistic Structure:} \quad & v_0 \sim N(m_0, C_0), \quad \xi_n \sim N(0, \Sigma), \quad \eta_j \sim N(0, \Gamma) \\
\text{Probabilistic Structure:} \quad & v_0 \perp \{\xi_n\} \perp \{\eta_n\} \text{ independent}
\end{aligned}
$$

- Introduced in UK Met Office.
- Primary proponent: Andrew Lorenc.
- Quart J. Roy. Met. Soc. **112**(1986).
- J. Met. Soc. Japan **99**(1997).
- $\{v_n\} \mapsto \{v_{n+1}\}$.

3DVAR

Sequential Optimization Perspective

$$\text{Predict:} \quad \widehat{v}_{n+1} = \Psi(v_n), \quad n \in \mathbb{Z}^+$$

$$\text{Model/Data Compromise:} \quad J_n(v) = \frac{1}{2}|v - \widehat{v}_{n+1}|^2_{\widehat{C}} + \frac{1}{2}|y_{n+1} - Hv|^2_{\Gamma}$$

$$\text{Optimize:} \quad v_{n+1} = \operatorname{argmin}_v J_n(v).$$

- $\widehat{C}$ is a fixed model covariance (not updated sequentially).
- $\widehat{C}$ chosen to have simple, computable, structure (Fourier).

Ensemble Kalman Filter

State Space Model

Dynamics Model: $v_{n+1} = \Psi(v_n) + \xi_n, \quad n \in \mathbb{Z}^+$

Data Model: $y_{n+1} = Hv_{n+1} + \eta_{n+1}, \quad n \in \mathbb{Z}^+$

Probabilistic Structure: $v_0 \sim N(m_0, C_0), \quad \xi_n \sim N(0, \Sigma), \quad \eta_j \sim N(0, \Gamma)$

Probabilistic Structure: $v_0 \perp \{\xi_n\} \perp \{\eta_n\}$ independent

- Introduced by Geir Evensen.
- J. Geophysical Research **99**(1994).
- Motivated by extended Kalman filter; see [2].
- Jazwinski (1970) [3], Ghil et al (1981) [4].
- Original paper in ocean dynamics.
- Used in weather forecasting centres worldwide.
- $\{v_n^{(k)}\}_{k=1}^K \mapsto \{v_{n+1}^{(k)}\}_{k=1}^K$.

Ensemble Kalman Filter

Sequential Optimization Perspective

$$
\begin{aligned}
\text{Predict:} \quad & \widehat{v}_{n+1}^{(k)} = \Psi(v_n^{(k)}) + \xi_n^{(k)}, \quad n \in \mathbb{Z}^+ \\
\text{Model/Data Compromise:} \quad & J_n^{(k)}(v) = \frac{1}{2}|v - \widehat{v}_{n+1}^{(k)}|^2_{\widehat{C}_{n+1}} + \frac{1}{2}|y_{n+1}^{(k)} - Hv|^2_\Gamma \\
\text{Optimize:} \quad & v_{n+1}^{(k)} = \mathrm{argmin}_v J_n^{(k)}(v).
\end{aligned}
$$

- $\widehat{C}_{n+1}$ is empirical covariance of the $\{\widehat{v}_{n+1}^{(k)}\}$.
- Updating $\widehat{C}_n$ requires only $\mathcal{O}(Kd)$ storage.

Weather Forecasting

Weather Forecasting: Data

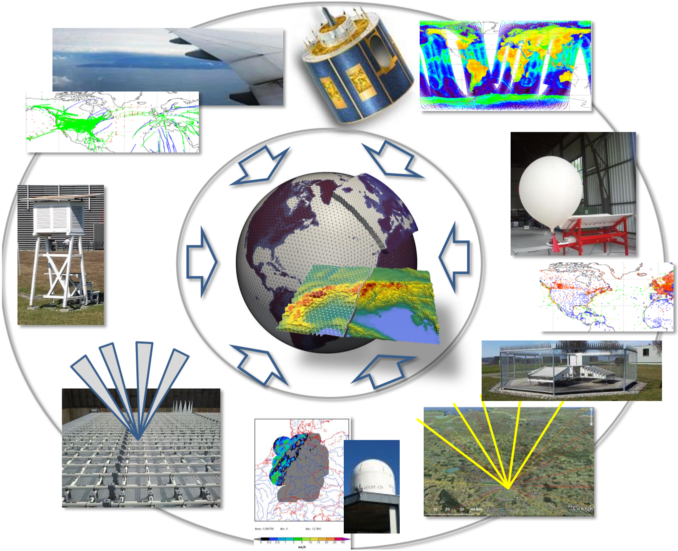


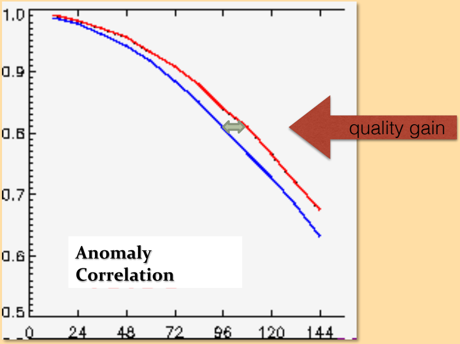
Figure: Big Data $\mathcal{O}(10^6)$/hour; Bigger Models $\mathcal{O}(10^9)$ states.

DWD Weather Forecasting: Impact of Mathematics

Ensemble Kalman Filter (red) versus 3DVAR (blue)

higher skill

lower skill



forecast lead time in hours

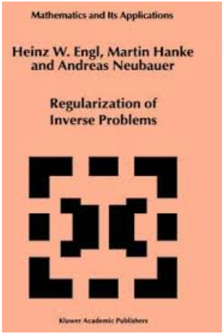
Ensemble Kalman Inversion

Inverse Problem

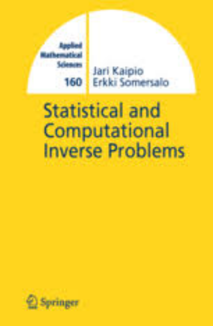
Problem Statement

Find u from y where $G : \mathcal{U} \mapsto \mathcal{Y}$, where $\mathcal{U}, \mathcal{Y}$ are Hilbert spaces, η is noise and

$$y = G(u) + \eta, \quad \eta \sim N(0, \Gamma).$$



A.N. Tikhonov (1963)



J. Franklin (1970) & [6]

Inverse Problem

Dynamical Formulation

$$\text{Dynamics Model:} \quad u_{n+1} = u_n, \quad n \in \mathbb{Z}^+$$
$$\text{Dynamics Model:} \quad w_{n+1} = \mathsf{G}(u_n), \quad n \in \mathbb{Z}^+$$
$$\text{Data Model:} \quad y_{n+1} = w_{n+1} + \eta_{n+1}, \quad n \in \mathbb{Z}^+$$

- $y_{n+1} = y, \quad \eta_{n+1} \sim N(0, h^{-1}\Gamma).$
- Use $\mathcal{O}(1/h)$ steps.
- Evensen moved to Statoil.
- Methodology widely used in oil industry.
- Also in groundwater flow.
- Gier Nævdal 2001, 2002.
- Oliver, Reynolds, Liu (2008) [5].

EKI: Ensemble Kalman Inversion

Reformulate In General State Space Notation

$$
\begin{aligned}
v &= (u, w), \\
\Psi(u, w) &= \big(u, \mathsf{G}(u)\big), \\
Hv &= w.
\end{aligned}
$$

Returns Us To A State Space Model

$$
\begin{aligned}
\text{Dynamics Model:} \quad & v_{n+1} = \Psi(v_n), \quad n \in \mathbb{Z}^+ \\
\text{Data Model:} \quad & y_{n+1} = Hv_{n+1} + \eta_{n+1}, \quad n \in \mathbb{Z}^+.
\end{aligned}
$$

Ensemble Kalman Inversion

Apply EnKF to State Space Model

Properties of EKI

- Linear Case $G(\cdot) = A \cdot$.
- Least Squares Functional:

$$\Phi(u) = \frac{1}{2}\|y - Au\|_\Gamma^2.$$

Theorem (Projected Gradient Structure) Schillings et al [10]

In the linear setting, EKI algorithm minimizes $\Phi(\cdot; y)$ over a finite dimensional subspace defined by the linear span of the initial ensemble.

- Empirically nonlinear problem behaves similarly.
- New variant for which nonlinear theory may be developed. [11]

Inversion Applications

Groundwater Flow 1
Iglesias et al [8,9]

Forward Problem

Given $\kappa \in X := L^\infty(D;\mathbb{R}^+)$ find $p \in H^1_0(D;\mathbb{R})$ such that:

$$\begin{aligned} -\nabla \cdot (\kappa \nabla p) &= f, \quad x \in D, \\ p &= 0, \quad x \in \partial D. \end{aligned}$$

Inverse Problem

Set $\kappa = \exp(u)$. Given K linear functionals of the pressure $\mathsf{G}_k(u) = \mathfrak{o}_k(p)$, $\mathfrak{o}_k \in H^{-1}(D;\mathbb{R})$, find u from noisy measurements y where:

$$y = \mathsf{G}(u) + \eta, \quad \eta \sim \mathsf{N}(0, \Gamma).$$

Grdounwater Flow 2

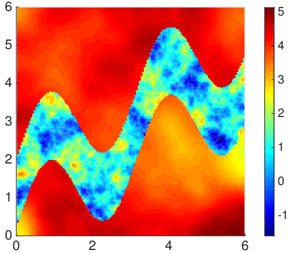


Figure: True log-permeability.

Parameterization

- Five scalars describe channel geometry.
- One random field describes interior of channel.
- One random field describes exterior of channel.
- Lengthscale and smoothness parameters of both random fields.

Groundwater Flow 3

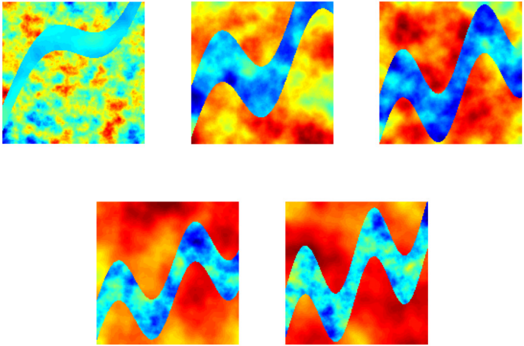


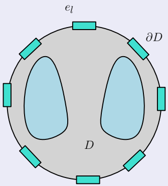
Figure: Five succesive iterations; ensemble mean

Electrical Impedance Tomography (EIT) 1 Iglesias et al [7,9]

Forward Problem

Given $(\kappa, I) \in L^\infty(D; \mathbb{R}^+) \times \mathbb{R}^m$ find $(\nu, V) \in H^1(D) \times \mathbb{R}^m$:

$$\begin{aligned} -\nabla \cdot (\kappa \nabla \nu) = 0 &\quad \in \quad D, \\ \nu + z_\ell \kappa \nabla \nu \cdot n = V_\ell &\quad \in \quad e_\ell, \quad \ell = 1, \ldots, m, \\ \nabla \nu \cdot n = 0 &\quad \in \quad \partial D \setminus \cup_{\ell=1}^m e_\ell, \\ \int \kappa \nabla \nu \cdot n \, ds = I_\ell &\quad \in \quad e_\ell, \quad \ell = 1, \ldots, m. \end{aligned}$$



Ohm's Law: $V = R(\kappa) \times I$.

Inverse Problem

Set $\kappa = \exp(u)$. Given a set of K noisy measurements of voltage $V(k)$ from currents $I(k)$, and $\mathrm{G}_k(u) = R\big(\exp(u)\big) \times I(k)$, find u from y where:

$$y(k) = \mathrm{G}_k(u) + \eta, \quad \eta \sim \mathrm{N}(0, \gamma^2), \quad k = 1, \ldots, K.$$

EIT 2

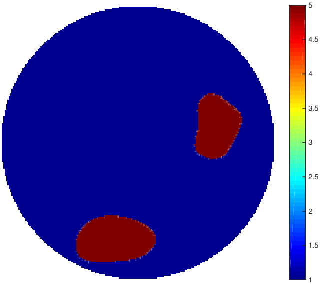


Figure: True Conductivity.

Parameterization

- Continuous level set function.
- Lengthscale of level set function.
- Smoothness of level set function.

EIT 3

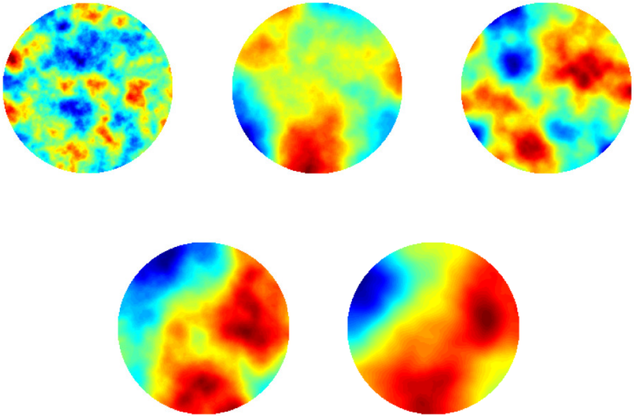


Figure: Five succesive iterations: level set function.

EIT 4

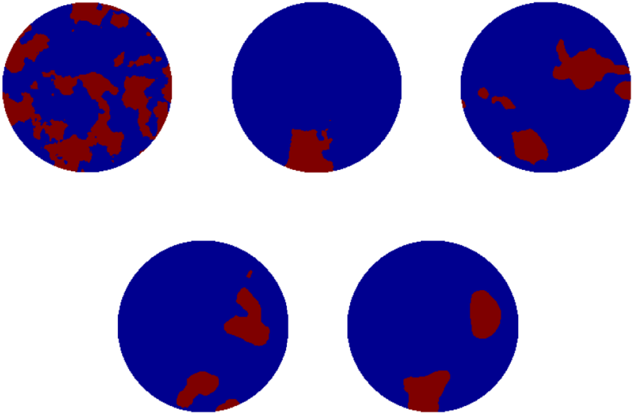


Figure: Five succesive iterations: thresholded level set function.

Supervised Learning – MNIST Kovachki et al [12]

LeCun and Cortes 1999.

Inverse Problem

- 70,000 images (28×28 pixellated.)
- 60,000 are labelled $\in \{0, \ldots, 9\}$.
- Find map **images** $:\mapsto$ **labels**.
- Test on remainder.

MNIST Supervised

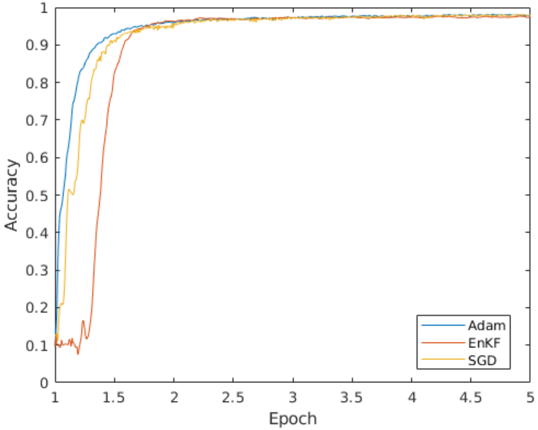


Figure: Test Accuracy of **Net 1** on MNIST (batched).

J	Loss	Momentum	Randomize y	Randomize u
5000	Cross Entropy	✓	✓	χ

Conclusions and References

Conclusions

- Kalman's 1960 paper revoltionized applied mathematics.
- Evensen's 1994 paper introduced a step change in applicability.
- Both state estimation and inverse problems maybe solved.
- Aerospace guidance $\cdots$
- Oceanography, weather forecasting, climate ...
- Geophysical and medical imaging.
- Machine Learning ?

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In preparation

Whittle-Matérn Initial Ensembles

- Create initial ensemble of functions via Gaussian random fields.
- Common choice: Whittle-Matérn family

$$c_{\nu,\tau}(x,x') := \frac{2^{1-\nu}}{\Gamma(\nu)}\left(\tau|x-x'|\right)^{\nu} K_{\nu}\left(\tau|x-x'|\right).$$

  - Smoothness parameter: $\nu \in \mathbb{R}^+$.
  - Inverse length-scale parameter: $\tau \in \mathbb{R}^+$.

- Corresponding covariance operator

$$\mathcal{C}_{\nu,\tau} \propto \tau^{2\nu}(\tau^2 I - \triangle)^{-\nu-\frac{d}{2}}.$$

- Hierarchical: invert for as ν, τ as well as field itself.
- F. Lindgren, H. Rue and J. Lindström, (JRSS-B **73**(2011))

Centred vs Non-centred

- Define $\theta = (\alpha, \tau)$.
- Generate samples u by solving the SPDE

$$(\tau^2 I - \triangle)^{\frac{\nu + \frac{1}{2}d}{2}} u = \tau^{\nu} \xi,$$

  where $\xi \sim \mathrm{N}(0, I)$ is white noise. $u = T(\xi, \theta)$.
  See F. Lindgren, H. Rue and J. Lindström, (JRSS-B **73**(2011))
- Hierarchical: invert for parameters θ as well as field u.
- Centred approach:
  - view (u, θ) as unknowns;
  - initial ensemble samples $\mathbb{P}(u|\theta)\mathbb{P}(\theta)$;
  - $y = \mathcal{G}(u) + \eta$.
- Non-centred approach:
  - view (ξ, θ) as unknowns;
  - initial ensemble samples $\mathbb{P}(\xi)\mathbb{P}(\theta)$;
  - $y = \mathcal{G}\big(T(\xi, \theta)\big) + \eta$.

  See O. Papaspiliopoulos, G. O. Roberts, and M. Sköld, (Statistical Science)**22**(2007))

Supervised Learning

$$\Phi(u) = \frac{1}{2}\|\mathrm{y} - \mathrm{G}(u|\mathrm{x})\|^2_{\mathcal{Y}^N} \quad \text{or} \quad -\sum_{j=1}^{N}\langle y_j, \log \mathcal{G}(u|, x_j)\rangle_{\mathcal{Y}}$$

Algorithms

$$\textbf{SGD}: \dot{u} = -\nabla_u \Phi(u); \quad u(0) = u_0, \quad u_* = u(T)$$

$$\textbf{EnKF}: \dot{u}^{(k)} = -\sum_{\ell=1}^{K} d_{k,\ell}(u)u^{(\ell)}; \quad u^{(k)}(0) = u_0^{(k)}, \qquad u_* = \frac{1}{K}\sum_{\ell=1}^{K} u^{(\ell)}(T)$$

Tricks

- Mini-batching.
- Momentum: $\ddot{u}^{(k)} + \frac{3}{t}\dot{u}^{(k)} = -\sum_{\ell=1}^{K} d_{k,\ell}(u)u^{(\ell)}$.
- Randomize y and u.

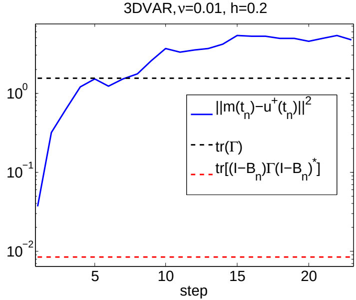
Convolutional Models

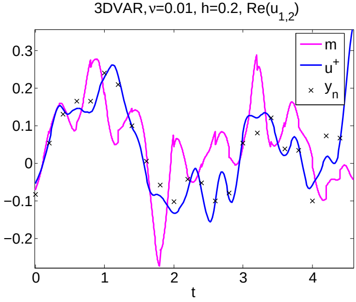
Net 1 $\sim$ 14k	**Net 2** $\sim$ 30k
Conv12x3x3 MaxPool2x2	Conv12x3x3 Conv12x3x3 MaxPool2x2
Conv24x3x3 MaxPool2x2	Conv24x3x3 Conv24x3x3 MaxPool2x2
Conv32x3x3 MaxPool2x2	Conv32x3x3 Conv32x3x3
FC-100	FC-100
FC-10	FC-10

- ReLU: after each block: $\max(0, x)$;
- Layer normalization: Ba, Kiros and Hinton 2016. (NIPS)

Data Fails to Overcome Butterfly Effect

KJH Law and AM Stuart, Monthly Weather Review, 2014.





Theory Backed use of Data Overcomes Butterfly Effect

KJH Law and AM Stuart, Monthly Weather Review, 2014.