Ensemble Kalman Inversion As A Dynamical System

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Overview

Some Notation

Please Internalize

$$\text{Notation:} \quad |\cdot| \ \textbf{Euclidean},$$
$$\text{Assumption:} \quad A^T = A, \ \ A > 0,$$
$$\text{Notation:} \quad \langle \cdot, \cdot \rangle_A := \langle \cdot, A^{-1} \cdot \rangle,$$
$$\text{Notation:} \quad |\cdot|_A := |A^{-\frac{1}{2}} \cdot |.$$

Nonlinear Filtering

- 3DVAR: Lorenc (1986) [22]
- EnKF: Evensen (1994) [12]
- OT: Reich (2011) [25]
- Text: Reich & Cotter (2015) [26]
- Text: Law, S & Zygalakis (2015) [21]
- 3DVAR accuracy: Hayden, Olson & Titi [15]
- 3DVAR accuracy: Brett et al (2013) [8]

Nonlinear Filtering

State Space Model

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

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

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

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

Sequential Optimization Approach 3DVAR

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

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

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

Ensemble Nonlinear Filtering

State Space Model

$$\text{Dynamics Model:} \quad v_{n+1} = \Psi(v_n) + \xi_n, \quad n \in \mathbb{Z}^+$$
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$$\text{Probabilistic Structure:} \quad v_0 \perp \{\xi_n\} \perp \{\eta_n\} \text{ independent}$$

Sequential Optimization Perspective

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

Ensemble Nonlinear Filtering

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

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

Non-Autonomous Dynamical System: EnKF

Formulation 1: $v_{n+1}^{(j)} = \Psi(v_n^{(j)}) + K_n\big(y_{n+1} - H\Psi(v_n^{(j)})\big) \quad n \in \mathbb{Z}^+$

Formulation 2: $v_{n+1}^{(j)} = \big(I - K_nH\big)\Psi(v_n^{(j)}) + K_n y_{n+1} \quad n \in \mathbb{Z}^+$

Kalman Gain: $K_n = K_n\big(\{v_n^{(k)}\}_{k=1}^J\big)$

Ensemble Nonlinear Filtering

State Space Model

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

Non-Autonomous Dynamical System: EnKF Synchonization: see [15], [8]

$$
\begin{aligned}
\text{Formulation 1:} \quad & v_{n+1}^{(j)} = \Psi(v_n^{(j)}) + K_n\big(y_{n+1} - H\Psi(v_n^{(j)})\big) \quad n \in \mathbb{Z}^+ \\
\text{Formulation 2:} \quad & v_{n+1}^{(j)} = (I - K_nH)\Psi(v_n^{(j)}) + K_n y_{n+1} \quad n \in \mathbb{Z}^+ \\
\text{Kalman Gain:} \quad & K_n = K_n\big(\{v_n^k\}_{k=1}^J\big)
\end{aligned}
$$

Inverse Problems

- Oil Reservoir: Chen & Oliver (2012) [9]
- Oil Reservoir: Emerick & Reynolds (2013) [11]
- General: Iglesias, Law & S (2015) [16]
- With Constraints: Albers, Blancquart, Levine, Esmaeilzadeh Seylabi & S (2019) [1]

Inverse Problem

Problem Statement

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

$$y = \mathrm{G}(u) + \eta.$$

Optimization $\Phi(u) = \frac{1}{2}|y - G(u)|_{\Gamma}^{2} + \frac{1}{2}|u|_{\Sigma}^{2};$ Probability $e^{-\Phi(u)}.$

Dynamical Formulation Iterative inversion: see [9], [11], [16]

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

EKI Algorithm

Dynamical Formulation

$$\text{Dynamics Model:} \quad u_{n+1} = u_n, \quad n \in \mathbb{Z}^+$$

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

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

State Space Estimation Formulation

$$\text{Reformulate:} \quad v = (u, w), \quad \Psi(v) = (u, \mathsf{G}(u)), \quad H = (0, I)$$

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

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

Employ EnKF with $y_{n+1} \equiv y$.

Discrete Time EKI Algorithm

Covariances

$$C_n^{ww} = \frac{1}{J}\sum_{j=1}^{J}\big(\mathsf{G}(u_n^{(j)}) - \overline{w}_n\big) \otimes \big(\mathsf{G}(u_n^{(j)}) - \overline{w}_n\big), \quad \overline{w}_n = \frac{1}{J}\sum_{j=1}^{J}\mathsf{G}(u_n^{(j)}),$$

$$C_n^{uw} = \frac{1}{J}\sum_{j=1}^{J}\big(u_n^{(j)} - \overline{u}_n\big) \otimes \big(\mathsf{G}(u_n^{(j)}) - \overline{w}_n\big), \quad \overline{u}_n = \frac{1}{J}\sum_{j=1}^{J}u_n^{(j)}.$$

Iteration $n \mapsto n+1$

$$u_{n+1}^{(j)} = u_n^{(j)} + C_n^{uw}\big(C_n^{ww} + \Gamma\big)^{-1}\big(y - \mathsf{G}(u_n^{(j)})\big)$$

Gradient Flow In Parameter Space

- Ensemble Filtering Continuous Time: Bergemann & Reich (2010a, 2010b, 2012) [4, 5, 6]
- Ensemble Filtering Continuous Time: Reich (2011) [25]
- 3DVAR Filtering Continuous Time: Blömker, Law, S & Zygalakis (2013) [7]
- Ensemble Filtering Continuous Time: Kelly, Law & S (2015) [18]
- Ensemble Inversion Continuous Time: Schillings & S (2017) [28]
- Text: Reich & Cotter (2015) [26]
- Text: Law, S & Zygalakis (2015) [21]
- Ensemble Filtering Continuous Time: Lange & Stannat [20]
- Ensemble Square Root Filtering Continuous Time: Lange & Stannat [19]

Discrete Time EKI Algorithm

Compensating For Repeated Use Of Data

Iterative inversion: see [9], [11], [25], [28]

$$Nh = 1,$$
$$\Gamma \to h^{-1}\Gamma$$

Iteration $n = 0, \ldots, N-1$

$$u_{n+1}^{(j)} = u_n^{(j)} + C_n^{uw}\left(C_n^{ww} + h^{-1}\Gamma\right)^{-1}\left(y - \mathsf{G}(u_n^{(j)})\right)$$

Ensemble Kalman Inversion (EKI)

Continuous Time Formulation

$$\dot{u}^{(j)} = -\frac{1}{J}\sum_{k=1}^{J}\left\langle \mathsf{G}(u^{(k)}) - \bar{\mathsf{G}}, \mathsf{G}(u^{(j)}) - y\right\rangle_{\Gamma}\left(u^{(k)} - \bar{u}\right)$$

$$\bar{u} = \frac{1}{J}\sum_{k=1}^{J} u^{(k)}, \quad \bar{\mathsf{G}} = \frac{1}{J}\sum_{k=1}^{J} G(u^{(k)}),$$

$$C(u) = \frac{1}{J}\sum_{k=1}^{J}\left(u^{(k)} - \bar{u}\right) \otimes \left(u^{(k)} - \bar{u}\right).$$

Ensemble Kalman Inversion – Linear Approximation

Linear Approximation

$$(\mathrm{G}(u^{(k)}) - \bar{\mathrm{G}}) \approx D\mathrm{G}(u^{(j)})(u^{(k)} - \bar{u}).$$

Converts EKI To Self-Preconditioned Gradient Descent See [25], [28]

$$\dot{u}^{(j)} \approx -C(u)\nabla\Phi_0(u^{(j)}),$$

$$\Phi_0(u) = \frac{1}{2\gamma^2}\left|y - G(u)\right|_\Gamma^2.$$

Gradient Flow In Space Of Probability Measures

- Jordan, Kinderlehrer & Otto 1998 [17]
- Otto 2001 [23]
- Benamou & Brenier 2000 [3]
- Ambrosio, Gigli & Savare 2008 [2]
- Villani 2008 [29]
- Reich & Cotter 2013 [27]
- Garbuno-Inigo, Hoffmann, Li & Stuart 2020 [13]
- Garbuno-Inigo, Nüsken & Reich [14]

Ensemble Kalman Sampling (EKS)

Continuous Time Formulation: Put EKI in a heat bath

$$\dot{u}^{(j)} = -\frac{1}{J}\sum_{k=1}^{J}\Big\langle \mathsf{G}(u^{(k)}) - \bar{\mathsf{G}}, \mathsf{G}(u^{(j)}) - y\Big\rangle_{\Gamma}\left(u^{(k)} - \bar{u}\right) - C(u)\Sigma^{-1}u^{(j)} + \sqrt{2C(u)}\,\dot{W}^{(j)},$$

$$C(u) = \frac{1}{J}\sum_{k=1}^{J}\left(u^{(k)} - \bar{u}\right)\otimes\left(u^{(k)} - \bar{u}\right).$$

Ensemble Kalman Sampling – Linear Approximation

Linear Approximation

$$(\mathrm{G}(u^{(k)}) - \bar{\mathrm{G}}) \approx D\mathrm{G}(u^{(j)})(u^{(k)} - \bar{u}).$$

Converts EKS To Self-Preconditioned Langevin Equation

$$\dot{u}^{(j)} \approx -C(u)\nabla\Phi(u^{(j)}) + \sqrt{2C(u)}\,\dot{W}^{(j)},$$

$$\Phi(u) = \frac{1}{2\gamma^2}\left|y - G(u)\right|_\Gamma^2 + \frac{1}{2}\left|u\right|_\Sigma^2.$$

Ensemble Kalman Sampling – Mean Field Approximation

Mean Field Limit $J \to \infty$ (Preconditioned Langevin-McKean Equation)

$$\dot{u} = -\mathcal{C}(\rho)\nabla\Phi(u) + \sqrt{2C(\rho)}\dot{W},$$

$$\mathcal{C}(\rho) = \int (u - \bar{u}) \otimes (u - \bar{u})\rho(u,t)du, \quad \bar{u} = \int u\rho(u,t)du.$$

Nonlinear Nonlocal Fokker-Planck Equation For $\rho(u,t)$

$$\partial_t \rho = \nabla \cdot \big(\rho\,\mathcal{C}(\rho)\,\nabla\Phi\big) + \mathcal{C}(\rho) : D^2\rho, \quad \rho(0) = \rho_0.$$

$$\Phi(u) = \frac{1}{2\gamma^2}|y - G(u)|_\Gamma^2 + \frac{1}{2}|u|_\Sigma^2.$$

Linear Fokker-Planck Equation

SDE & Fokker-Planck [17]

$$\dot{u} = -\nabla\Phi(u) + \sqrt{2}\dot{W}$$

$$\star$$

$$u \sim \mu, \quad \text{with pdf } \rho(u,t).$$

$$\star$$

$$\partial_t\rho = \nabla\cdot\left(\rho\,\nabla\Phi\right) + \triangle\rho\,,$$
$$\partial_t\rho = \nabla\cdot\left(\rho\,\nabla\left(\Phi + \ln\rho\right)\right).$$

Linear Fokker-Planck Equation (Energy)

Theorem [17]

The linear Fokker-Planck equation may be written as

$$\partial_t \rho = \nabla \cdot \left(\rho \nabla \frac{\delta \mathcal{E}}{\delta \rho} \right) \ , \mathcal{E}(\rho) = \int (\Phi + \ln \rho) \rho \, \mathrm{d} u .$$

This gives a Lyapunov function:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}(\rho) = - \int \rho \left| \nabla (\Phi + \ln \rho) \right|^2 \mathrm{d} u .$$

Linear Fokker-Planck Equation (Energy & Metric)

Proof Of Theorem [17, 23]

Formally taking L^2 inner-products in the linear Fokker-Planck equation

$$\left\langle \frac{\delta \mathcal{E}}{\delta \rho}, \partial_t \rho \right\rangle_{L^2} = \left\langle \frac{\delta \mathcal{E}}{\delta \rho}, \nabla \cdot \left(\rho \nabla \frac{\delta \mathcal{E}}{\delta \rho} \right) \right\rangle_{L^2}.$$

Gradient flow in $\mathcal{P}_+$ (probability measures) w.r.t. metric g_ρ (on the tangent space):

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\rho) &= -\int \rho \left| \nabla(\Phi + \ln \rho) \right|^2 \mathrm{d}u \\ &= -g_\rho(\partial_t \rho, \partial_t \rho). \end{aligned}$$

Linear Fokker-Planck Equation (Metric)

Wasserstein Metric Tensor

Define $g_\rho : T_\rho\mathcal{P}_+ \times T_\rho\mathcal{P}_+ \to \mathbb{R}$ by

$$g_\rho(\sigma_1, \sigma_2) := \int_\Omega \langle \nabla\psi_1 \,, \nabla\psi_2 \rangle \, \rho \, \mathrm{d}x,$$

where $\sigma_i = -\nabla \cdot (\rho \nabla \psi_i) \in T_\rho\mathcal{P}_+$ for $i = 1, 2$.

Wasserstein Metric $\mathcal{W}$: $\mathcal{P}_+ \times \mathcal{P}_+ \to \mathbb{R}$ (Transport Form[3])

For $\rho^0, \rho^1 \in \mathcal{P}_+$,

$$\mathcal{W}(\rho^0, \rho^1)^2 := \inf_{(\rho_t, \psi_t)} \int_0^1 \int_\Omega \langle \nabla\psi_t \,, \nabla\psi_t \rangle \, \rho_t \, \mathrm{d}x$$

$$\text{subject to} \quad \partial_t \rho_t + \nabla \cdot (\rho_t \nabla \psi_t) = 0, \;\; \rho_0 = \rho^0, \;\; \rho_1 = \rho^1,$$

Nonlinear Nonlocal Fokker-Planck Equation

Mean Field SDE & Nonlinear Nonlocal Fokker-Planck [13]

$$\dot{u} = -\mathcal{C}(\rho)\nabla\Phi(u) + \sqrt{2C(\rho)}\dot{W}$$

$$\mathcal{C}(\rho) = \int (u - \bar{u}) \otimes (u - \bar{u})\rho(u,t)du \quad \& \quad \bar{u} = \int u\rho(u,t)du.$$

$\star$

$$u \sim \mu, \quad \text{with pdf } \rho(u,t).$$

$\star$

$$\partial_t \rho = \nabla \cdot \big(\rho\,\mathcal{C}(\rho)\,\nabla\Phi\big) + \mathcal{C}(\rho) : D^2\rho$$

$$\partial_t \rho = \nabla \cdot \Big(\rho\,\mathcal{C}(\rho)\,\nabla\left(\Phi + \ln\rho\right)\Big).$$

Nonlinear Nonlocal Fokker-Planck Equation (Change The Metric)

Theorem

The nonlinear Fokker-Planck equation may be written as

$$\partial_t \rho = \nabla \cdot \left(\rho \mathcal{C}(\rho) \nabla \frac{\delta \mathcal{E}}{\delta \rho} \right) \,, \mathcal{E}(\rho) = \int (\Phi + \ln \rho) \, \rho \, \mathrm{d}u.$$

Gradient flow in $\mathcal{P}_+$ (probability measures) w.r.t. metric $g_{\rho,\mathcal{C}}$ (on the tangent space):

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}(\rho) &= - \int \rho \left| \mathcal{C}(\rho)^{\frac{1}{2}} \nabla (\Phi + \ln \rho) \right|^2 \mathrm{d}u \\ &= -g_{\rho,\mathcal{C}}(\partial_t \rho, \partial_t \rho). \end{aligned}$$

Nonlinear Nonlocal Fokker-Planck Equation (Metric)

Kalman-Wasserstein Metric Tensor [27],[13]

Define $g_{\rho,\mathcal{C}} : T_\rho\mathcal{P}_+ \times T_\rho\mathcal{P}_+ \to \mathbb{R}$ by

$$g_{\rho,\mathcal{C}}(\sigma_1, \sigma_2) := \int_\Omega \langle \nabla\psi_1 \,,\, \mathcal{C}(\rho)\nabla\psi_2 \rangle \; \rho \, \mathrm{d}x,$$

where $\sigma_i = -\nabla \cdot (\rho\mathcal{C}(\rho)\nabla\psi_i) \in T_\rho\mathcal{P}_+$ for $i = 1, 2$.

Kalman-Wasserstein Metric $\mathcal{W}_\mathcal{C} : \mathcal{P}_+ \times \mathcal{P}_+ \to \mathbb{R}$ (Transport Form)

For ρ^0, $\rho^1 \in \mathcal{P}_+$,

$$\mathcal{W}_\mathcal{C}(\rho^0, \rho^1)^2 := \inf_{(\rho_t,\psi_t)} \int_0^1 \int_\Omega \langle \nabla\psi_t \,,\, \mathcal{C}(\rho_t)\nabla\psi_t \rangle \; \rho_t \, \mathrm{d}x$$

$$\text{subject to} \quad \partial_t\rho_t + \nabla \cdot (\rho_t\mathcal{C}(\rho_t)\nabla\psi_t) = 0, \;\; \rho_0 = \rho^0, \;\; \rho_1 = \rho^1,$$

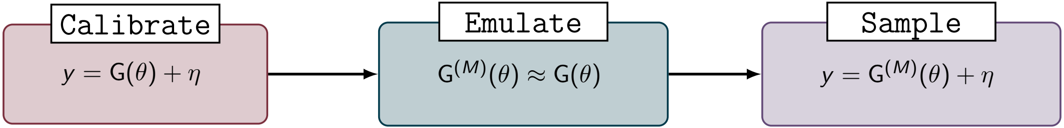
Closing

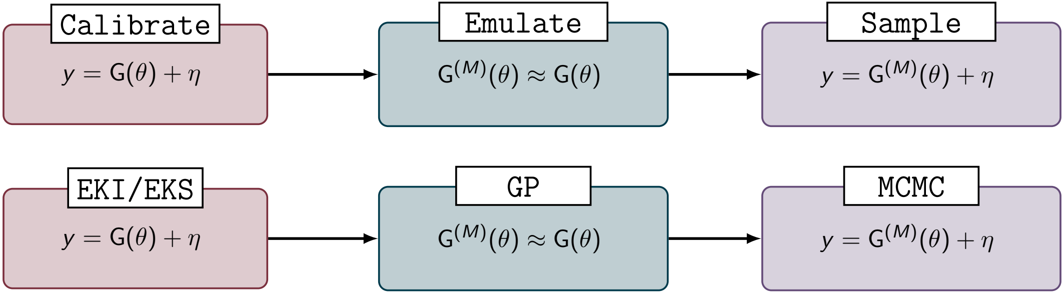
Conclusions: Ensemble Kalman Inversion

- Flexible inversion methodology: black box.
- Optimization and probabilistic approaches both possible.
- Approximate (noisy) gradient flow structure: parameter space.
- Approximate (noisy) gradient flow structure: probability space.
- Connections to Wasserstein gradient flows, optimal transport.
- Applications in calibration and UQ for complex models.
- Many open (nonautonomous/stochastic) dynamical systems questions.

Application To Climate Model

- O'Gorman and Schneider 2008 [24]
- Cleary, Garbuno-Inigo, Lan, Schneider & S 2020, [10]


Calibrate
$y = G(\theta) + \eta$
Emulate
$G^{(M)}(\theta) \approx G(\theta)$
Sample
$y = G^{(M)}(\theta) + \eta$


Calibrate
$y = G(\theta) + \eta$
Emulate
$G^{(M)}(\theta) \approx G(\theta)$
Sample
$y = G^{(M)}(\theta) + \eta$
EKI/EKS
$y = G(\theta) + \eta$
GP
$G^{(M)}(\theta) \approx G(\theta)$
MCMC
$y = G^{(M)}(\theta) + \eta$

Example: Idealized Climate Model

Forward Model

$$\text{Moisture Conservation:} \quad \frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q = -\frac{q - q_{ref}(T; u)}{\tau_q(q, T; u)}$$

$$\text{Energy Conservation:} \quad \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \frac{T - T_{ref}(q, T; u)}{\tau_T(q, T; u)} + \text{RAD} + \ldots$$

- Coupled with mass and momentum conservation equations.
- $\mathcal{O}(10^5)$ unknowns
- Employs 2 unknown parameters:
  - u_{RH}: reference relative humidity
  - u_τ: default relaxation timescale

Data From Dynamics

Time-Averaged Data

$$\frac{du}{dt} = F(u; u), \quad u(0) = u_0,$$
$$y = G_T(u; u_0) = \frac{1}{T}\int_0^T \varphi\big(u(t)\big)\,dt.$$

Central Limit Theorem

$$G_T(u; u_0) = G(u) + \frac{1}{\sqrt{T}}N(0, \Sigma),$$
$$y = G(u) + \frac{1}{\sqrt{T}}N(0, \Sigma).$$

Example: Idealized Climate Model

Objective Function

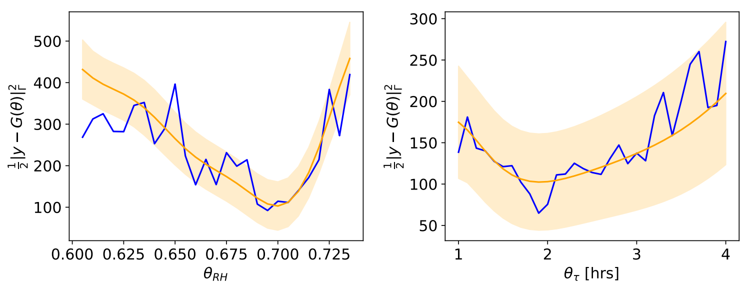


Figure: GP trained from EKI data

Dark orange: GP mean; shaded orange: GP 2 std.

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