Data assimilation as an optimal control problem and applications to UQ

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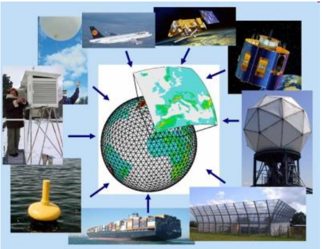
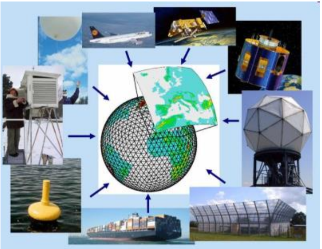
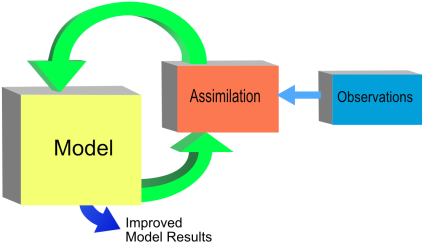
Numerical Weather Prediction



- **Model**: highly nonlinear discretized partial differential equations
- **Data**: heterogeneous mix of ground-, airborne-, satellite-based and radar data
- 24/7 **data assimilation** service for optimal weather prediction





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Problem setting

Model:

$$\mathrm{d}x_t = f(x_t,\lambda)\,\mathrm{d}t + \sigma(x_t)\circ \mathrm{d}W_t, \qquad (x_0,\lambda) \sim \pi_0$$

Data/Observations:

(A) continuous-in-time

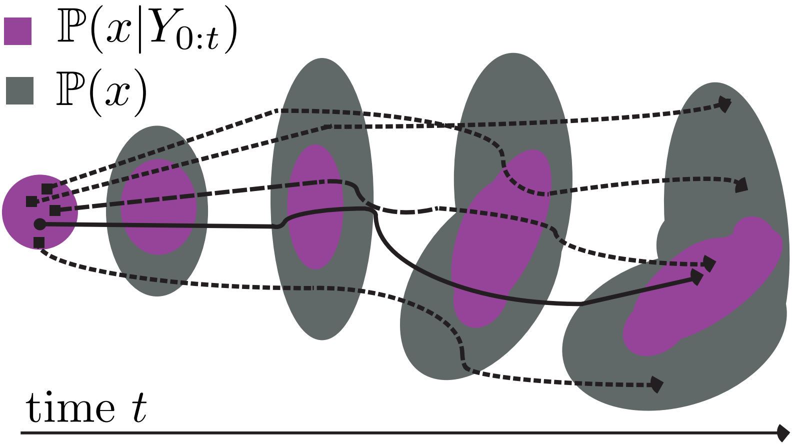
$$\mathrm{d}y_t = h(x_t,\lambda)\,\mathrm{d}t + R^{1/2}\mathrm{d}V_t$$

(B) discrete-in-time

$$y_{t_n} = h(x_{t_n},\lambda) + R^{1/2}\,\Xi_{t_n}\,.$$

Goal: Approximate conditional PDF $\tilde{\pi}_t(x,\lambda) = \pi_t(x,\lambda|Y_t)$ where Y_t contains all the data up to time t and $\tilde{\pi}_0 = \pi_0$ at initial time.

Time evolved marginal distributions:



Applications

- assimilation of observations into computer model (e.g. weather forecasting),
- assimilation of synthetic data from a high resolution model into a model of lower resolution (e.g. parameter estimation),
- rare event simulation (data comes from possible rare event scenarios),
- solution of inverse problems, minimization (model dynamics is trivial, e.g., $\mathrm{d}x_t = 0$).

Problem setting

Particle filters: Approximate conditional PDF $\tilde{\pi}_t$ by a set of particles

$$z_t^i = (x_t^i, \lambda_t^i), \qquad i = 1, \ldots, M,$$

with weights

$$w_t^i \geq 0, \qquad \text{s.t.} \sum_i w_t^i = 1.$$

E.g. sequential Monte Carlo.

Eulerian:

$$z_t^i = z_0^i \qquad \text{(particle locations are fixed)}$$

E.g., grid-based methods.

Lagrangian:

$$w_t^i = 1/M \qquad \text{(weights are fixed)}$$

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A control approach to the continuous-in-time filtering problem:

Kalman gain factor:

$$K_t = P_{xh} R^{-1} ,$$

P_{xh} denotes the covariance matrix between x_t and $h(x_t)$

Innovation:

$$\mathrm{d}I_t = \mathrm{d}y_t - \frac{1}{2}(h(x_t) - \bar{h}_t)\,\mathrm{d}t$$

or

$$\mathrm{d}I_t = \mathrm{d}y_t - h(x_t)\,\mathrm{d}t - R^{1/2}\mathrm{d}U_t$$

Ensemble Kalman-Bucy filter:

$$\mathrm{d}x_t = f(x_t, \lambda)\,\mathrm{d}t + \sigma(x_t) \circ \mathrm{d}W_t + K_t \circ \mathrm{d}I_t$$

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$$\mathrm{d}x_t = f(x_t,\lambda)\,\mathrm{d}t + \sigma(x_t)\circ \mathrm{d}W_t + K_t \circ \mathrm{d}I_t$$

(i) Draw samples x_0^i, $i = 1, \dots, M$ from the initial distribution π_0.

(ii) Solve the **interacting particle system**

$$\mathrm{d}x_t^i = f(x_t^i, \lambda)\mathrm{d}t + \sigma(x_t^i) \circ \mathrm{d}W_t^i + K_t \circ \mathrm{d}I_t^i,$$

with **innovation**

$$\mathrm{d}I_t^i = \mathrm{d}y_t - \mathrm{d}y_t^i, \qquad \mathrm{d}y_t^i := h(x_t^i)\mathrm{d}t + R^{-1/2}\mathrm{d}U_t^i,$$

and **gain factor**

$$K_t = P_{xh}R^{-1},$$

$$P_{xh} := \frac{1}{M-1}\sum_{i=1}^{M}(x_t^i - \bar{x}_t)(h(x_t^i) - \bar{h}_t)^{\mathrm{T}},$$

$i = 1, \dots, M$.

Consider zero-drift & scalar SDE

$$\mathrm{d}x_t = \sigma(x_t) \circ \mathrm{d}W_t$$

with time-evolved expectation values:

$$\pi_t[f] = \pi_0[f] + \int_0^t \pi_s[\mathcal{L}f]\,\mathrm{d}s, \qquad \mathcal{L}f := \frac{1}{2}\sigma\,\partial_x(\sigma\,\partial_x f)$$

Interacting particle representation:

$$\dot{x}_t = \frac{1}{2}\sigma(x_t)I_t(x_t), \qquad I_t := -\pi_t^{-1}\partial_x(\pi_t\,\sigma)$$

It holds that (Liouville plus integration by parts)

$$\hat{\pi}_t[f] := \pi_0[f] + \frac{1}{2}\int_0^t \pi_s[(\partial_x f)(\sigma I_s)]\,\mathrm{d}s$$

$$= \pi_0[f] + \int_0^t \pi_s[\mathcal{L}f]\,\mathrm{d}s = \pi_t[f]\,.$$

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Generalization of the ensemble Kalman-Bucy filter:

$$\mathrm{d}x_t = f(x_t, \lambda)\,\mathrm{d}t + \sigma(x_t) \circ \mathrm{d}W_t + K_t \circ \mathrm{d}I_t$$

Innovation $\mathrm{d}I_t$ as before, i.e.,

$$\mathrm{d}I_t = \mathrm{d}y_t - \frac{1}{2}(h(x_t) - \bar{h}_t)\,\mathrm{d}t$$

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Kalman gain matrix $K_t = \nabla\psi_t$ with

$$-\nabla_x \cdot (\hat{\pi}_t \nabla_x \psi_t) = R^{-1}\hat{\pi}_t(h - \tilde{\pi}_t[h])\,.$$

It can be shown that $\tilde{\pi}_t[f] = \hat{\pi}_t[f]$.

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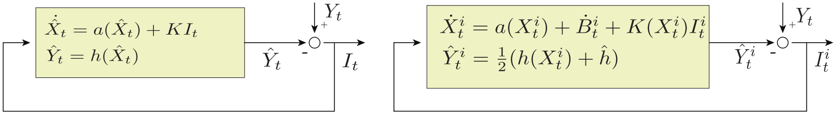
Structural form of filter formulations:



(a): Kalman Filter (b): Feedback Particle Filter

A) **Diffusion maps**: Define elliptic operator

$$\mathcal{L}_\pi \psi := -\pi^{-1} \nabla_x \cdot (\pi \nabla_x \psi)$$

and introduce the approximation

$$\frac{e^{\epsilon \mathcal{L}_\pi} - \mathrm{Id}}{\epsilon} \psi \approx h - \pi[h]$$

The exponential $e^{\epsilon \mathcal{L}_\pi}$ can be approximated using diffusion maps.

B) **Optimal transport**: Find optimal coupling T_ϵ between π and

$$\pi_\epsilon = \pi(1 + \epsilon(h - \pi[h])\,.$$

Then

$$\nabla_x \psi(x) \approx \frac{T_\epsilon(x) - x}{\epsilon}\,.$$

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The time-evolution of an ensemble of M particles x_t^i is given by

$$\mathrm{d}x_t^i = f(x_t^i, \lambda)\,\mathrm{d}t + \sigma(x_t^i) \circ \mathrm{d}W_t^i - \tilde{K}_t^i \circ \mathrm{d}I_t^i$$

Gain:

$$\tilde{K}_t^i := \sum_{j=1}^{M} x_t^j d_{ji} \approx \nabla_x \psi_t(x_t^i)$$

Innovation:

$$\mathrm{d}I_t^i = \mathrm{d}y_t - \frac{1}{2}(h(x_t^i) - \bar{h}_t)\,\mathrm{d}t$$

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References

EnKBF:

- SR (BIT, 2011), Bergemann & SR (Meteorol. Zeitschrift, 2012)
- de Wiljes, Stannat & SR (ArXiv:1612.06065, 2016), Del Moral, Kurtzmann & Tugaut (ArXiv:1606.082566, 2016)

FPF:

- Yang, Mehta & Meyn (IEEE Trans. Autom. Contr., 2013)
- Taghvaei, de Wiljes, Mehta & SR (ArXiv:1702.07241), David, de Wiljes & SR (ArXiv:1709.09199)

Alternative control formulation:

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Bayes:

$$\pi(x|y) \propto \pi(y|x)\,\pi(x)$$

Task: Given a set of samples $x_0^i \sim \pi(x)$, produce an estimator for expectation values with respect to the posterior distribution.

Application: Learn models

$$y_{\text{out}} = \Psi_x(y_{\text{in}}),$$

parametrized by x, which gives rise to the likelihood $\pi(y|x)$.

Standard methodologies:

- importances sampling
- MCMC
- homotopy methods: **learning models by making them interact**

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Homotopy method I

Homotopy: Define family of distributions

$$\pi_\alpha(x) \propto e^{-\alpha L}\, \pi(x)\,,$$

where $L(x) := -\ln \pi(y|x)$ and $\alpha \geq 0$. The posterior is obtained for $\alpha = 1$.

The function L can also stand for a tilting potential in rare event simulations/ importance sampling.

Dynamic formulation:

- **Bayes**

$$\frac{\partial}{\partial \alpha}\pi_\alpha = -\pi_\alpha\,(L - \pi_\alpha[L])\,, \qquad \pi[e^{-L}] = 1 + \int_0^1 \pi_\alpha[L]\mathrm{d}t\,,$$

- **Liouville**

$$\frac{\partial}{\partial \alpha}\pi_\alpha = -\nabla_x \cdot (\pi_\alpha \nabla_x \psi_\alpha)$$

and parameter dynamics given by

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Particle flow filter:

$$\dot{x}^i_\alpha = \nabla_x \psi_\alpha(x^i_\alpha), \qquad x^i_0 \sim \pi(x)\,,$$

$\alpha \in [0,1]$, with potential ψ_α solving

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Numerical implementation:

- diffusion maps
- optimal transportation
- (iterative) ensemble Kalman filter

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Homotopy method III

Extensions:

- **Randomized particle flow:**

$$\begin{aligned} dx_\alpha &= \varepsilon \nabla_x \ln \pi_\alpha(x)\,dt + \sqrt{2\varepsilon}\,dW_\alpha + \nabla_x \psi_\alpha(x)\,dt \\ &= \nabla_x \left\{ \psi_\alpha(x) + \epsilon \ln \pi_0(x) - \epsilon \alpha L(x) \right\} dt + \sqrt{2\varepsilon}\,dW_\alpha\,, \end{aligned}$$

  for $\alpha \geq 0$. Here $\epsilon \geq 0$ is a parameter.

  It still holds that

$$\partial_\alpha \pi_\alpha = -\pi_\alpha (L - \pi_\alpha[L])\,.$$

- **Minimization:** Method for finding

$$x^* = \arg\min V(x)$$

  if $\alpha \to \infty$, $\epsilon \propto \alpha^{-1}$, and

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- Moser (1965),
- Daum et al. (SPIE, 2010), Daum et al. (SPIE, 2017)
- SR (BIT, 2011)
- Heng, Doucet & Pokern (2015, ArXiv:1509.08787)

Extensions:

- iterative Kalman filters (Dean Oliver, Mark Bocquet, Marco Iglesias, SR ...)
- sequential Monte Carlo & rejuvenation (..., Beskos, Crisan & Jasra (Annals of Applied Prob, 2014), ...)
- Kalman filter as minimizer (Schilling & Stuart (2016, ArXiv:1602.02020))
- stochastic minimization techniques/ simulated annealing (...)

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Conclusions

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- stability and accuracy of the resulting interacting particle systems is largely unknown
- many applications outside classic filtering context such as rare event simulations and whenever a change of measure arises
- exploitation of geometric properties? E.g. data assimilation for highly oscillatory Hamiltonian systems (Reinhardt, Hastermann, Klein, SR, ArXiv:1708.03570)
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