Importance Weighting in Hybrid Iterative Ensemble Smoothers for Data Assimilation[a]

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[a]Hybrid refers to a combination of two methods of estimation gradients.

Parameter estimation and UQ in porous media flow

Two-phase incompressible flow in a porous medium.

$$\phi \frac{\partial}{\partial t} S_\alpha - \nabla \cdot [\lambda_\alpha(S_w) K \nabla p] = q_\alpha \qquad \text{for } \alpha = o,\ w$$

and

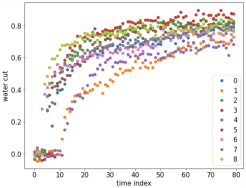
$$S_o + S_w = 1.$$

where permeability $K = e^m$ and porosity ϕ are uncertain.

Observe historical water production rates at a few locations.

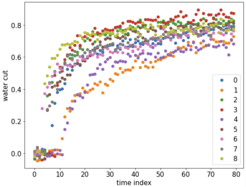
- Typically high-dimensional, relatively few data
- minimization, but no derivatives available
- ensemble-Kalman methods sometimes fail

History matching

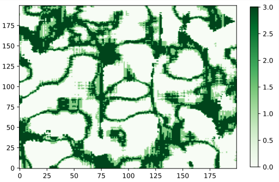


production data

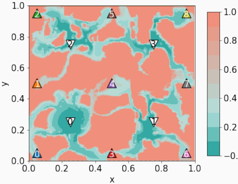
History matching



production data

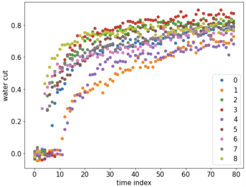


data-generating model



S_w at $t = 10$

History matching



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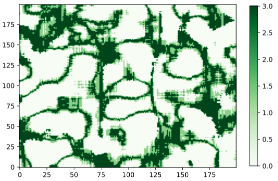

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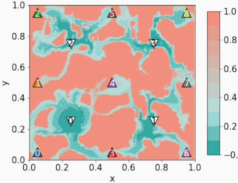

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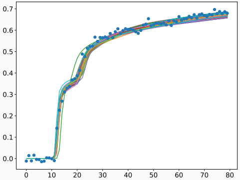
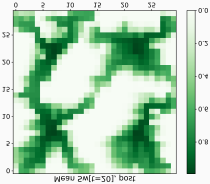


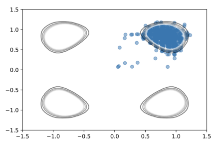
history-matched data



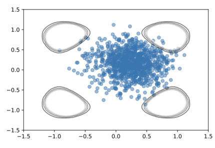
calibrated model

Good data match, but calibrated model not similar to the “truth”.

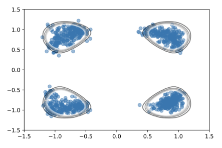
For problems with several similar minima, standard ensemble-based sampling methods will fail[1]



MCMC



ensemble smoother



random minimizer

Random minimizer potentially samples all modes. Example is overly simplistic.

[1] Dunbar et al. (2022) "Ensemble Inference Methods for Models With Noisy and Expensive Likelihoods"

Data assimilation – Minimization for sampling

1. Sample gaussian random variables $x^* \sim N(x^{\mathrm{pr}}, C_x)$
2. Sample the observation error $\epsilon^* \sim N(0, C_d)$
3. Compute $\operatorname{argmin}_x \|d^o - (g(x) + \epsilon^*)\|^2_{C_d^{-1}} + \|x - x^*\|^2_{C_x^{-1}}$

Gauss-Newton minimization

$$\delta x_\ell = x^* - x_\ell - C_x G_\ell^T \left[C_d + G_\ell C_x G_\ell^T \right]^{-1} \times \left[(g(x_\ell) + \epsilon^* - d^o) - G_\ell (x_\ell - x^*) \right].$$

where $G^{\mathrm{T}} = \nabla_x g^{\mathrm{T}}$. (For subsurface flow problems, $\nabla_x g^{\mathrm{T}}$ is often unavailable.)

Hybrid iterative ensemble smoother

Consider composite mappings $\boldsymbol{d} = \boldsymbol{g}(\boldsymbol{m}(\boldsymbol{x}))$

For the hybrid IES, the derivatives of $\boldsymbol{m}$ with respective to $\boldsymbol{x}$ and of data $\boldsymbol{g}$ with respective to $\boldsymbol{m}$ are required.

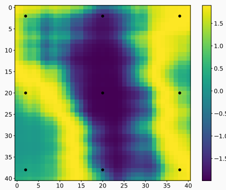
$$\boldsymbol{G} = \nabla_x(g^T) = \boldsymbol{G}_m.(\nabla_x(\boldsymbol{m}^T))^T = \boldsymbol{G}_m\boldsymbol{M}_x$$

A hybrid approximation of the Gauss-Newton update:

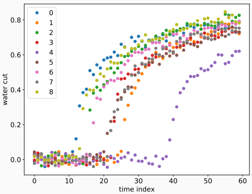
$$\begin{aligned}\delta\boldsymbol{x}_{\ell+1} = -(\boldsymbol{x}_\ell - \boldsymbol{x}^*) - \boldsymbol{C}_x\boldsymbol{M}_x^T\boldsymbol{G}_m^T\Big(\boldsymbol{C}_d + \boldsymbol{G}_m\boldsymbol{M}_x\boldsymbol{C}_x\boldsymbol{M}_x^T\boldsymbol{G}_m^T\Big)^{-1} \\ \times\left(g(\boldsymbol{m}_\ell) + \boldsymbol{\epsilon}^* - \boldsymbol{d}^o - \boldsymbol{G}_m\boldsymbol{M}_x(\boldsymbol{x}_\ell - \boldsymbol{x}^*)\right),\end{aligned}$$

where $\boldsymbol{G}_m = (\Delta\boldsymbol{d}_\ell)(\Delta\boldsymbol{m}_\ell)^{-1}$.

Example: flow in porous medium with multiple rock types[2]



log-permeability, $m(x)$



water rate, $g(m(x))$

$$m = 2\tanh(4x+2) + \tanh(2-4x) - 1$$

Generates channel-like features of high permeability.

[2] Ba and Oliver (2024)

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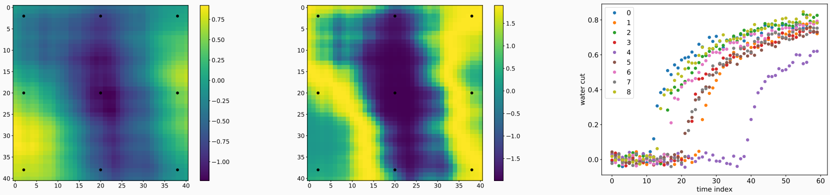

Gaussian variable, x log-permeability, $m(x)$ water rate, $g(m(x))$

$$m = 2\tanh(4x + 2) + \tanh(2 - 4x) - 1$$

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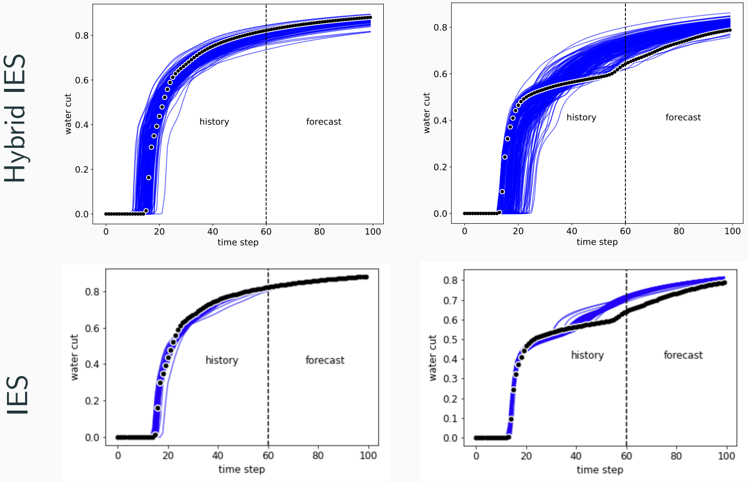
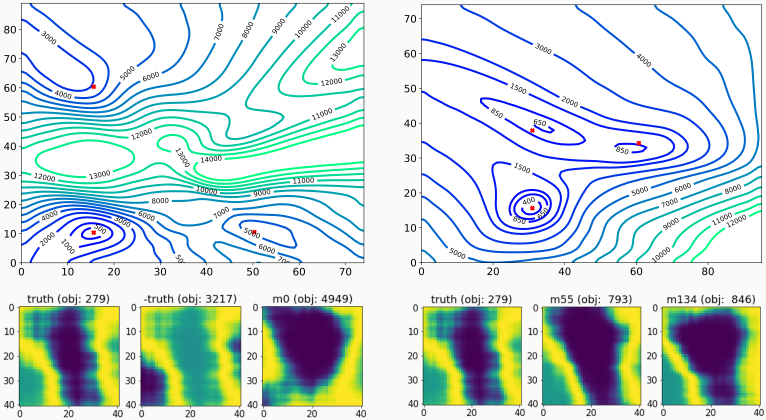
Difficulties with this problem



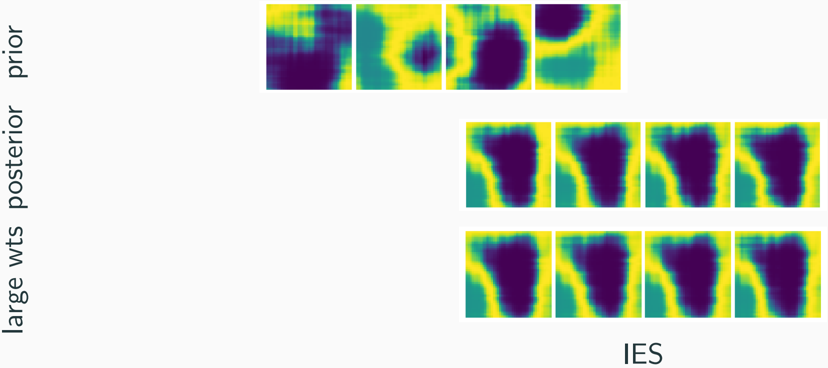
Observations shown by circles. Better match to data with IES.

Fitness landscape



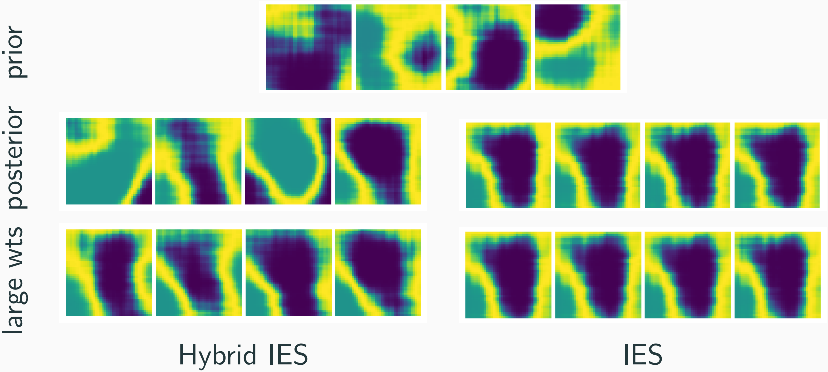
Data misfit function in 2D subspace that includes truth (Oliver, 2022). Many history-matched models end up in “unimportant” local minima.

Posterior sampling



Model realizations for non-monotonic transform of log-permeability using hybrid IES and IES, respectivly. Lack of diversity in IES samples.

Posterior sampling



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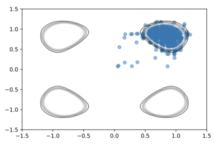

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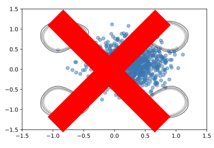
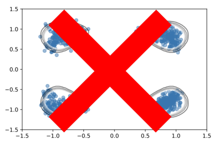


IES



random minimizer

- Modes are probably not equally deep.
- IES likely to migrate to one mode.
- Random minimizer still likely to sample all – but not all of equal importance.

Importance weights (Ba et al., 2022)

The importance weight for a sample obtained using a "minimization" approach is

$$\omega = \frac{\text{Target probability}}{\text{Proposal probability}} \propto \frac{\pi_X(\boldsymbol{x})\pi_\Delta(\boldsymbol{\delta}|\boldsymbol{x})}{p_{X\Delta}(\boldsymbol{x},\boldsymbol{\delta})},$$

Proposal density for samples from the prior pdf:

$$q_{X'\Delta'}(\boldsymbol{x}',\boldsymbol{\delta}') = q_{X'}(\boldsymbol{x}')\, q_{\Delta'}(\boldsymbol{\delta}')$$

An approximate posterior sample is then generated by computing the critical points of the cost functional

$$Q(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}')^T \boldsymbol{C}_x^{-1}(\boldsymbol{x}-\boldsymbol{x}') + \frac{1}{2}(\boldsymbol{g}(\boldsymbol{m})-\delta')^T \boldsymbol{C}_d^{-1}(\boldsymbol{g}(\boldsymbol{m})-\delta').$$

Importance weights

Solving $\nabla_x Q(\boldsymbol{x}) = 0$ leads to a map from $(\boldsymbol{x}, \boldsymbol{\delta})$ to $(\boldsymbol{x}', \boldsymbol{\delta}')$,

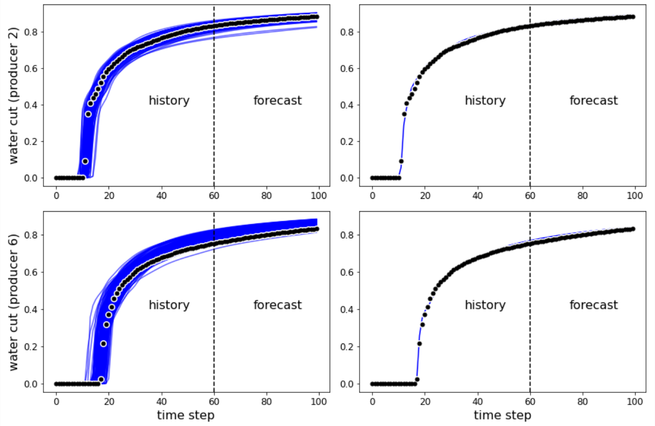
$$\begin{cases} \boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{C}_x \boldsymbol{G}^T \boldsymbol{C}_d^{-1} \big(\boldsymbol{g}(\boldsymbol{m}) - \boldsymbol{\delta} \big) \\ \boldsymbol{\delta}' = \boldsymbol{\delta}. \end{cases}$$

so the proposal pdf is given by[3]

$$p_{X\Delta}(\boldsymbol{x}, \boldsymbol{\delta}) = n(\boldsymbol{x}')^{-1} q_{X'} \Big(\boldsymbol{x} + \boldsymbol{C}_x \boldsymbol{G}^T \boldsymbol{C}_d^{-1} \big(g(\boldsymbol{m}) - \boldsymbol{\delta} \big) \Big) q_{\Delta'}(\boldsymbol{\delta}) J(\boldsymbol{x}, \boldsymbol{\delta}),$$

[3] If $\nabla_x Q(\boldsymbol{x}) = 0$ has multiple solutions, we should either obtain all critical points, or randomly sample.

Effect of weighting (highly non-linear)



Unweighted samples Weighted samples

The posterior predictions for wells 2 and 6 using hybrid IES for the non-monotonic transform. Black points show observations. Effective sampling efficiency is about 1.7%.

Summary

- Possibly many local minima in posterior pdf for parameter estimation in porous media.
- If iterate long enough, IES generally converges to a single minima (but often a “good one”).
- Hybrid IES has much greater diversity, but includes minima with low probability mass.
- Importance weighting of particles from hybrid-IES improves forecasts.

References

Yuming Ba and Dean S. Oliver. Importance weighting in hybrid iterative ensemble smoothers for data assimilation. *Mathematical Geosciences*, 2024. doi: 10.1007/s11004-023-10127-0.

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Oliver R. A. Dunbar, Andrew B. Duncan, Andrew M. Stuart, and Marie-Therese Wolfram. Ensemble inference methods for models with noisy and expensive likelihoods. *SIAM Journal on Applied Dynamical Systems*, 21(2):1539–1572, 2022.

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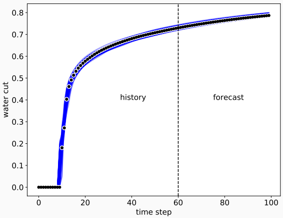
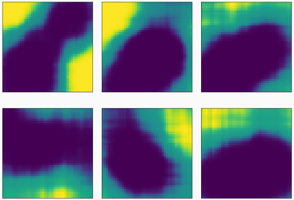
Ensemble collapse?

posterior





Very small spread of data predictions does not imply “collapse” of the ensemble of model realizations.