

# Parametric Problems, Stochastics, and Identification

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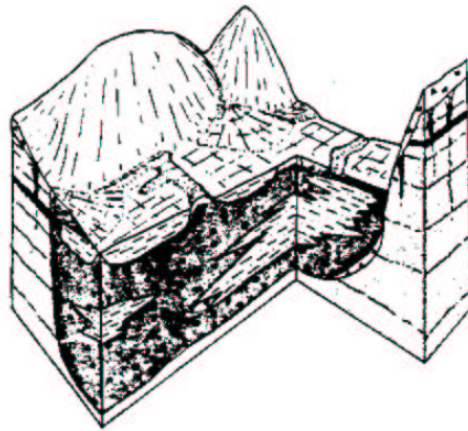


# Overview

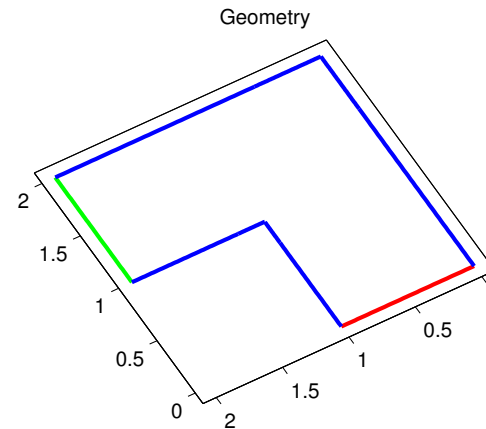
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1. Parameter identification
2. Parametric forward problem
3. Bayesian updating, inverse problems
4. Tensor approximation
5. Bayesian computation
6. Examples

# To fix ideas: example problem



Aquifer



2D Model

Simple stationary model of groundwater flow with stochastic data

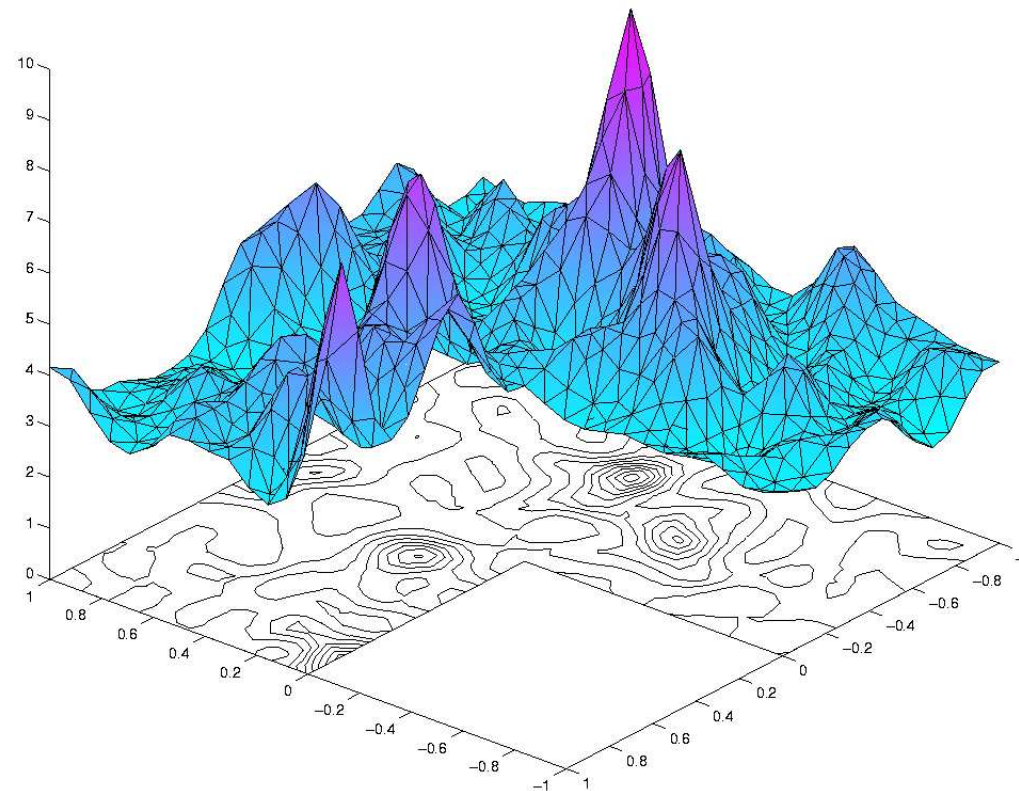
$$-\nabla_x \cdot (\kappa(x, \omega) \nabla_x u(x, \omega)) = f(x, \omega) \quad \& \text{ b.c.}, \quad x \in \mathcal{G} \subset \mathbb{R}^d$$

$$-\kappa(x, \omega) \nabla_x u(x, \omega) = g(x, \omega), \quad x \in \Gamma \subset \partial \mathcal{G}, \quad \omega \in \Omega.$$

Parameter  $q(x, \omega) = \log \kappa(x, \omega)$  is **uncertain**,  
the **stochastic** conductivity  $\kappa$ , as well as  $f$  and  $g$  — sinks and sources.

# Realisation of $\kappa(x, \omega)$

A sample realization



# Mathematical setup

Consider operator equation, physical **system** modelled by  $A$ :

$$A(u) = f \quad u \in \mathcal{U}, f \in \mathcal{F},$$

$$\Leftrightarrow \forall v \in \mathcal{U} : \quad \langle A(u), v \rangle = \langle f, v \rangle,$$

$\mathcal{U}$  — space of **states**,  $\mathcal{F} = \mathcal{U}^*$  — dual space of **actions** / **forcings**.

Solution operator:  $u = U(f)$ , inverse of  $A$ .

Operator depends on **parameters**  $q \in \mathcal{Q}$ ,  
hence state  $u$  is also function of  $q$ :

$$A(u; q) = f(q) \quad \Rightarrow \quad u = U(f; q).$$

**Measurement** operator  $Y$  with values in  $\mathcal{Y}$ :

$$y = Y(q; u) = Y(q, U(f; q)).$$

# Forward parametric problem

**Parametric** elements: operator  $A(\cdot; q)$ , rhs  $f(q)$ , state  $u(q)$ ,  $\rightarrow r(q)$ .

Goal are representations of  $r(q) \in \mathcal{W}$ , i.e.  $r : \mathcal{Q} \rightarrow \mathcal{W}$ .

Help from **inner product**  $\langle \cdot | \cdot \rangle_{\mathcal{R}}$  on subspace  $\mathcal{R} \subset \mathbb{R}^{\mathcal{Q}}$ .

In case  $\mathcal{Q}$  is a measure / probability space,  $\mathcal{R} = L_2$ .

To each parametric element corresponds **linear map**

$$R : \mathcal{W} \ni \hat{r} \mapsto \langle \hat{r} | r(\cdot) \rangle_{\mathcal{R}} \in \mathcal{R}.$$

**Key** is self-adjoint positive map  $C = R^* R : \mathcal{W} \rightarrow \mathcal{W}$ .

Spectral factorisation of  $C$  leads to **Karhunen-Loève** representation,  
a **tensor product** rep., corresponds to **SVD** of  $R$  (a.k.a. POD).

Each **factorisation**  $C = B^* B$  leads to a tensor representation,  
(ex.: smoothed white noise)

a 1–1 correspondence between factorisations and representations.

# Setting for the identification process

General idea:

We observe / measure a system, whose structure we know in principle.

The system behaviour depends on some quantities (parameters),  
which we do not know  $\Rightarrow$  uncertainty.

We model (uncertainty in) our knowledge in a Bayesian setting:  
as a probability distribution on the parameters.

We start with what we know a priori, then perform a measurement.  
This gives new information, to update our knowledge (identification).

Update in probabilistic setting works with conditional probabilities  
 $\Rightarrow$  Bayes's theorem.

Repeated measurements lead to better identification.

# Inverse problem

For given  $f$ , measurement  $y$  is just a function of  $q$ .  
This function is usually **not invertible**  $\Rightarrow$  **ill-posed** problem,  
measurement  $y$  does **not** contain **enough information**.

In **Bayesian** framework state of knowledge **modelled** in a probabilistic way,  
parameters  $q$  are **uncertain**, and **assumed** as **random**.

**Bayesian** setting allows **updating** / **sharpening** of **information**  
about  $q$  when measurement is performed.

The problem of updating **distribution**—state of knowledge of  $q$   
becomes **well-posed**.

Can be applied **successively**, each new measurement  $y$  and  
forcing  $f$  —may also be uncertain—will provide **new information**.



# Model with uncertainties

For simplicity assume that  $\mathcal{Q}$  is a Hilbert space,  
and  $q(\omega)$  has **finite** variance —  $\|q\|_{\mathcal{Q}} \in \mathcal{S} := L_2(\Omega)$ , so that

$$q \in L_2(\Omega, \mathcal{Q}) \cong \mathcal{Q} \otimes L_2(\Omega) = \mathcal{Q} \otimes \mathcal{S} =: \mathcal{Q}.$$

System model is now

$$A(u(\omega); q(\omega)) = f(\omega) \quad \text{a.s. in } \omega \in \Omega,$$

**state**  $u = u(\omega)$  becomes  $\mathcal{U}$ -valued **random variable** (RV),  
element of a **tensor** space  $\mathcal{U} = \mathcal{U} \otimes \mathcal{S}$ .

As **variational** statement:

$$\forall v \in \mathcal{U} : \quad \mathbb{E} (\langle A(u(\cdot); q(\cdot)), v \rangle) = \mathbb{E} (\langle f(\cdot), v \rangle) =: \langle\langle f, v \rangle\rangle.$$

Leads to **well-posed** stochastic PDE (SPDE).

# Representation of randomness

Parameters  $q$  modelled as  $\mathcal{Q}$ -valued (a vector space) **RVs** on some probability space  $(\Omega, \mathbb{P}, \mathfrak{A})$ , with expectation operator  $\mathbb{E}(q) = \bar{q}$ .

RVs  $q : \Omega \rightarrow \mathcal{Q}$  (and  $u(q)$ ) may be represented in the following ways:

**Samples:** the best known representation, i.e.  $q(\omega_1), \dots, q(\omega_N), \dots$

**Distribution** of  $q$ . This is the push-forward measure  $q_*\mathbb{P}$  on  $\mathcal{Q}$ .

**Moments** of  $q$ , like  $\mathbb{E}(q \otimes \dots \otimes q)$  (mean, covariance, ...).

**Functional/Spectral:** Functions of other (**known**) RVs, like Wiener's polynomial chaos, i.e.  $q(\omega) = q(\theta_1(\omega), \dots, \theta_M(\omega), \dots) =: q(\boldsymbol{\theta})$ .

Sampling and functional representation work with **vectors**,  
allows **linear algebra** in computation.

# Computational approaches

Representation determines algorithms:

- **Distributions** → Kolmogorov / Fokker-Planck equations.  
Needs **new** software, deterministic solver  $u = S(f, q)$  **not** used.
- **Moments** → New (sometimes difficult) equations.  
Needs **new** software, deterministic solver **mostly not** used.
- **Sampling** → Domain of **direct integration** methods;  
(quasi) Monte Carlo, sparse (Smolyak) grids, etc.  
**Obviously non-intrusive**; software **interface** → **solve**.
- **Functional / Spectral** →
  - (1) **Interpolation / collocation**. Based on samples of solution,  
**non-intrusive**, **solve** interface.
  - (2) **Galerkin** at first sight **intrusive**, but with **quadrature** is also  
**non-intrusive**, **precond. residual** interface. Allows **greedy** rank-1

# Conditional probability and expectation

With state  $u \in \mathcal{U} = \mathcal{U} \otimes \mathcal{S}$  a RV, the quantity to be measured

$$y(\omega) = Y(q(\omega), u(\omega)) \in \mathcal{Y} := \mathcal{Y} \otimes \mathcal{S}$$

is also **uncertain**, a **random variable**.

A **new** measurement  $z$  is performed, composed from the “true” value  $y \in \mathcal{Y}$  and a **random** error  $\epsilon$ :  $z(\omega) = y + \epsilon(\omega) \in \mathcal{Y}$ .

Classically, **Bayes's theorem** gives **conditional probability**

$$\mathbb{P}(I_q | M_z) = \frac{\mathbb{P}(M_z | I_q)}{\mathbb{P}(M_z)} \mathbb{P}(I_q);$$

expectation with this posterior measure is **conditional expectation**.

**Kolmogorov** starts from **conditional expectation**  $\mathbb{E}(\cdot | M_z)$ ,  
from this **conditional probability** via  $\mathbb{P}(I_q | M_z) = \mathbb{E}(\chi_{I_q} | M_z)$ .

# Update

The conditional expectation is defined as orthogonal projection onto the closed subspace  $L_2(\Omega, \mathbb{P}, \sigma(z))$ :

$$\mathbb{E}(q|\sigma(z)) := P_{\mathcal{Q}_\infty} q = \operatorname{argmin}_{\tilde{q} \in L_2(\Omega, \mathbb{P}, \sigma(z))} \|q - \tilde{q}\|_{L_2}^2$$

The subspace  $\mathcal{Q}_\infty := L_2(\Omega, \mathbb{P}, \sigma(z))$  represents the available information, estimate minimises  $\Phi(\cdot) := \|q - (\cdot)\|^2$  over  $\mathcal{Q}_\infty$ .  
More general loss functions than mean square error are possible.

The update, also called the assimilated value  $q_a(\omega) := P_{\mathcal{Q}_\infty} q = \mathbb{E}(q|\sigma(z))$ , is a  $\mathcal{Q}$ -valued RV and represents new state of knowledge after the measurement.

Reduction of variance—Pythagoras:  $\|q\|_{L_2}^2 = \|q - q_a\|_{L_2}^2 + \|q_a\|_{L_2}^2$

Doob-Dynkin:  $\mathcal{Q}_\infty = \{ \varphi \in \mathcal{Q} : \varphi = \phi \circ Y, \phi \text{ measurable} \}$

# Important points I

The probability measure  $\mathbb{P}$  is not the **object of desire**.  
It is the **distribution** of  $q$ , a measure on  $\mathcal{Q}$ —**push forward** of  $\mathbb{P}$ :

$$q_*\mathbb{P}(\mathcal{E}) := \mathbb{P}(q^{-1}(\mathcal{E})) \quad \text{for measurable } \mathcal{E} \subseteq \mathcal{Q}.$$

Bayes's original formula **changes**  $\mathbb{P}$ , **leaves**  $q$  as is.  
Kolmogorov's conditional expectation **changes**  $q$ , **leaves**  $\mathbb{P}$  as is.  
In both cases the update is a new  $q_*\mathbb{P}$ .

$\mathbb{P}$  (a probability measure) is on positive part of **unit sphere**,  
whereas  $q$  is **free** in a **vector space**.

This will allow the use of (multi-)linear algebra  
and **tensor approximations**.

## Important points II

Identification process:

- Use **forward problem**  $A(u(\omega); q(\omega)) = f(\omega)$  to **forecast** new state  $u_f(\omega)$  and measurement  $y_f(\omega) = Y(q(\omega), u_f(\omega))$ .
- Perform minimisation of **loss function** to obtain **update map / filter**.
- Use innovation in **inverse problem** to update forecast  $q_f$  to obtain **assimilated** (updated)  $q_a$  with update map.
- All operations in vector space, use **tensor approximations** throughout.

# Approximation

Minimisation equivalent to **orthogonality**: find  $\phi \in L_0(\mathcal{Y}, \mathcal{Q})$

$$\forall p \in \mathcal{Q}_\infty : \quad \langle\langle D_{q_a} \Phi(q_a(\phi)), p \rangle\rangle_{L_2} = \langle\langle q - q_a, p \rangle\rangle_{L_2} = 0,$$

**Approximation** of  $\mathcal{Q}_\infty$ : take  $\mathcal{Q}_n \subset \mathcal{Q}_\infty$

$$\mathcal{Q}_n := \{\varphi \in \mathcal{Q} : \varphi = \psi_n \circ Y, \psi_n \text{ a } n^{\text{th}} \text{ degree polynomial}\}$$

$$\text{i.e. } \varphi = {}^0H + {}^1HY + \dots + {}^kHY^{\otimes k} + \dots + {}^nHY^{\otimes n},$$

where  ${}^kH \in \mathcal{L}_s^k(\mathcal{Y}, \mathcal{Q})$  is **symmetric** and  **$k$ -linear**.

With  $q_a(\phi) = q_a({}^0H, \dots, {}^kH, \dots, {}^nH) = \sum_{k=0}^n {}^kH z^{\otimes k} = P_{\mathcal{Q}_n} q$ ,  
orthogonality implies

$$\forall \ell = 0, \dots, n : \quad D_{({}^\ell H)} \Phi(q_a({}^0H, \dots, {}^kH, \dots, {}^nH)) = 0$$





# Bayesian update in components

For **short**  $\forall \ell = 0, \dots, n$  :

$$\sum_{k=0}^n {}^k H \langle z^{\otimes (\ell+k)} \rangle = \langle q \otimes z^{\otimes \ell} \rangle,$$

For finite dimensional spaces, or after discretisation,  
in **components** (or à la Penrose in '**symbolic index**' notation):

let  $q = (q^m)$ ,  $z = (z^j)$ , and  ${}^k H = ({}^k H^m_{j_1 \dots j_k})$ , then:

$\forall \ell = 0, \dots, n$ ;

$$\begin{aligned} &\langle z^{j_1} \dots z^{j_\ell} \rangle ({}^0 H^m) + \dots + \langle z^{j_1} \dots z^{j_{\ell+1}} \dots z^{j_{\ell+k}} \rangle ({}^k H^m_{j_{\ell+1} \dots j_{\ell+k}}) + \\ &\dots + \langle z^{j_1} \dots z^{j_{\ell+1}} \dots z^{j_{\ell+n}} \rangle ({}^n H^m_{j_{\ell+1} \dots j_{\ell+n}}) = \langle q^m z^{j_1} \dots z^{j_\ell} \rangle. \end{aligned}$$

(Einstein summation convention used)

matrix does **not** depend on  $m$ —it is identically **block diagonal**.

## Special cases

For  $n = 0$  (**constant** functions)  $\Rightarrow q_a = {}^0H = \langle q \rangle \quad (= \mathbb{E}(q))$ .

For  $n = 1$  the approximation is with **affine** functions

$${}^0H + {}^1H \langle z \rangle = \langle q \rangle$$

$${}^0H \langle z \rangle + {}^1H \langle z \otimes z \rangle = \langle q \otimes z \rangle$$

$\Rightarrow$  (remember that  $[\text{cov}_{qz}] = \langle q \otimes z \rangle - \langle q \rangle \otimes \langle z \rangle$ )

$${}^0H = \langle q \rangle - {}^1H \langle z \rangle$$

$${}^1H (\langle z \otimes z \rangle - \langle z \rangle \otimes \langle z \rangle) = \langle q \otimes z \rangle - \langle q \rangle \otimes \langle z \rangle$$

$$\Rightarrow {}^1H = [\text{cov}_{qz}][\text{cov}_{zz}]^{-1} \text{ (Kalman's solution),}$$

$${}^0H = \langle q \rangle - [\text{cov}_{qz}][\text{cov}_{zz}]^{-1} \langle z \rangle,$$

and **finally**

$$q_a = {}^0H + {}^1H z = \langle q \rangle + [\text{cov}_{qz}][\text{cov}_{zz}]^{-1}(z - \langle z \rangle).$$

## Case with prior information

Here we have **prior information**  $\mathcal{Q}_f$  and **prior estimate**  $q_f(\omega)$  (forecast) and measurements  $z$  **generating** via  $Y$  a subspace  $\mathcal{Q}_y \subset \mathcal{Q}$ .

We now need **projection** onto  $\mathcal{Q}_a = \mathcal{Q}_f + \mathcal{Q}_y$ , with reformulation as an **orthogonal direct** sum:

$$\mathcal{Q}_a = \mathcal{Q}_f + \mathcal{Q}_y = \mathcal{Q}_f \oplus (\mathcal{Q}_y \cap \mathcal{Q}_f^\perp) = \mathcal{Q}_f \oplus \mathcal{Q}_\infty.$$

The **update** / **conditional expectation** / **assimilated** value is the orthogonal projection

$$q_a = q_f + P_{\mathcal{Q}_\infty} q = q_f + q_\infty,$$

where  $q_\infty$  is the **innovation**.

Compute  $q_a$  by approximating:  $\mathcal{Q}_n \subset \mathcal{Q}_\infty$ . We now take  $n = 1$ .

# Simplification

The case  $n = 1$ —linear functions, projecting onto  $\mathcal{Q}_1$ —is well known:

this is the **linear minimum variance** estimate  $\hat{q}_a$ .

**Theorem:** (Generalisation of **Gauss-Markov**)

$$\hat{q}_a(\omega) = q_f(\omega) + {}^1H(z(\omega) - y_f(\omega)),$$

where the linear **Kalman** gain operator  ${}^1H : \mathcal{Y} \rightarrow \mathcal{Q}$  is

$${}^1H := [\text{cov}_{qz}][\text{cov}_{zz}]^{-1} = [\text{cov}_{qy}][\text{cov}_{yy} + \text{cov}_{\epsilon\epsilon}]^{-1}.$$

(The **normal Kalman** filter is a **special case**.)

Or in tensor space  $q \in \mathcal{Q} = \mathcal{Q} \otimes \mathcal{S}$ :

$$\hat{q}_a = q_f + ({}^1H \otimes I)(z - y_f).$$

# Deterministic model, discretisation, solution

Remember operator equation:  $A(u) = f \quad u \in \mathcal{U}, f \in \mathcal{F}$ .

Solution is usually by first **discretisation**

$$A(u) = f \quad u \in \mathcal{U}_N \subset \mathcal{U}, f \in \mathcal{F}_N = \mathcal{U}_N^* \subset \mathcal{F},$$

and then **(iterative)** numerical **solution** process

$$u_{k+1} = S(u_k), \quad \lim_{k \rightarrow \infty} u_k = u.$$

$S$  evaluates (pre-conditioned) **residual**  $f - A(u_k)$ .

Similarly for model with **uncertainty**:

$$A(u(\omega); q(\omega)) = f(\omega),$$

assume  $\{v_j\}_{j=1}^N$  a basis in  $\mathcal{U}_N$ , then the approx. solution in  $\mathcal{U}_N \otimes \mathcal{S}$

$$u(\omega) = \sum_{j=1}^N u_j(\omega) v_j.$$

# Discretisation by functional approximation

Choose subspace  $\mathcal{S}_B \subset \mathcal{S}$  with basis  $\{X_\beta\}_{\beta=1}^B$ ,  
make **ansatz** for each  $u_j(\omega) \approx \sum_\beta u_j^\beta X_\beta(\omega)$ , giving

$$\mathbf{u}(\omega) = \sum_{j,\beta} u_j^\beta X_\beta(\omega) \mathbf{v}_j = \sum_{j,\beta} u_j^\beta X_\beta(\omega) \otimes \mathbf{v}_j.$$

Solution is in **tensor product**  $\mathcal{U}_{N,B} := \mathcal{U}_N \otimes \mathcal{S}_B \subset \mathcal{U} \otimes \mathcal{S} = \mathcal{U}$ .

State  $\mathbf{u}(\omega)$  represented by **tensor**  $\mathbf{u} := \mathbf{u}_N^B := \{u_j^\beta\}_{j=1,\dots,N}^{\beta=1,\dots,B}$ ,  
( $\beta$  is usually multi-index)

similarly for all other quantities, **fully discrete** forward model  
is obtained by **weighting** residual with  $\Xi_\alpha$  with ansatz inserted:

$$\forall \alpha : \left\langle \Xi_\alpha(\omega), \mathbf{f}(\omega) - \mathbf{A} \left( \sum_{j,\beta} u_j^\beta X_\beta(\omega) \mathbf{v}_j; \mathbf{q}(\omega) \right) \right\rangle_{\mathcal{S}} = 0.$$

# Stochastic forward problem

$\Rightarrow$  generally **coupled** system of equations for  $\mathbf{u} = \{u_j^\beta\}$ :

$$\mathbf{A}(\mathbf{u}; \mathbf{q}) = \mathbf{f}, \quad \mathbf{y} = \mathbf{Y}(\mathbf{q}; \mathbf{u}).$$

- If  $\Xi_\alpha(\cdot) = \delta(\cdot - \omega_\alpha)$ , system **decouples**  $\longrightarrow$  **collocation / interpolation**; may use for each  $\omega_\alpha$  **original** solver  $S$  (obviously **non-intrusive**).
- If  $\Xi_\alpha(\cdot) = X_\alpha(\cdot) \longrightarrow$  **Bubnov-Galerkin** conditions; with **numerical integration** uses also **original** solver  $S$  and is also **non-intrusive**.
- In **greedy** rank-one **update** tensor solver one uses Bubnov-Galerkin conditions (proper gener. decomp. (**PGD**)/ succ. rank-1 upd. (**SR1U**)/ alt. least squ. (**ALS**)), also possible by **non-intrusive** use of **original**  $S$ .

For update:  ${}^1\mathbf{H} = {}^1\mathbf{H} \otimes \mathbf{I}$  computed **analytically** ( $X_\beta = \text{Hermite basis}$ )  
 $[\text{cov}_{qy}] = \sum_{\alpha > 0} \alpha! \mathbf{q}^\alpha (\mathbf{y}^\alpha)^T; \quad [\text{cov}_{yy}] = \sum_{\alpha > 0} \alpha! \mathbf{y}^\alpha (\mathbf{y}^\alpha)^T.$



## Important points III

Update formulation in **vector spaces**.

This makes tensor representation possible .

Parametric problems lead to **tensor** (or separated) representations.

Sparse approximation by **low-rank** representation.

Possible for **forward** problem (progressive or iterative).

Possible for **inverse** problem.

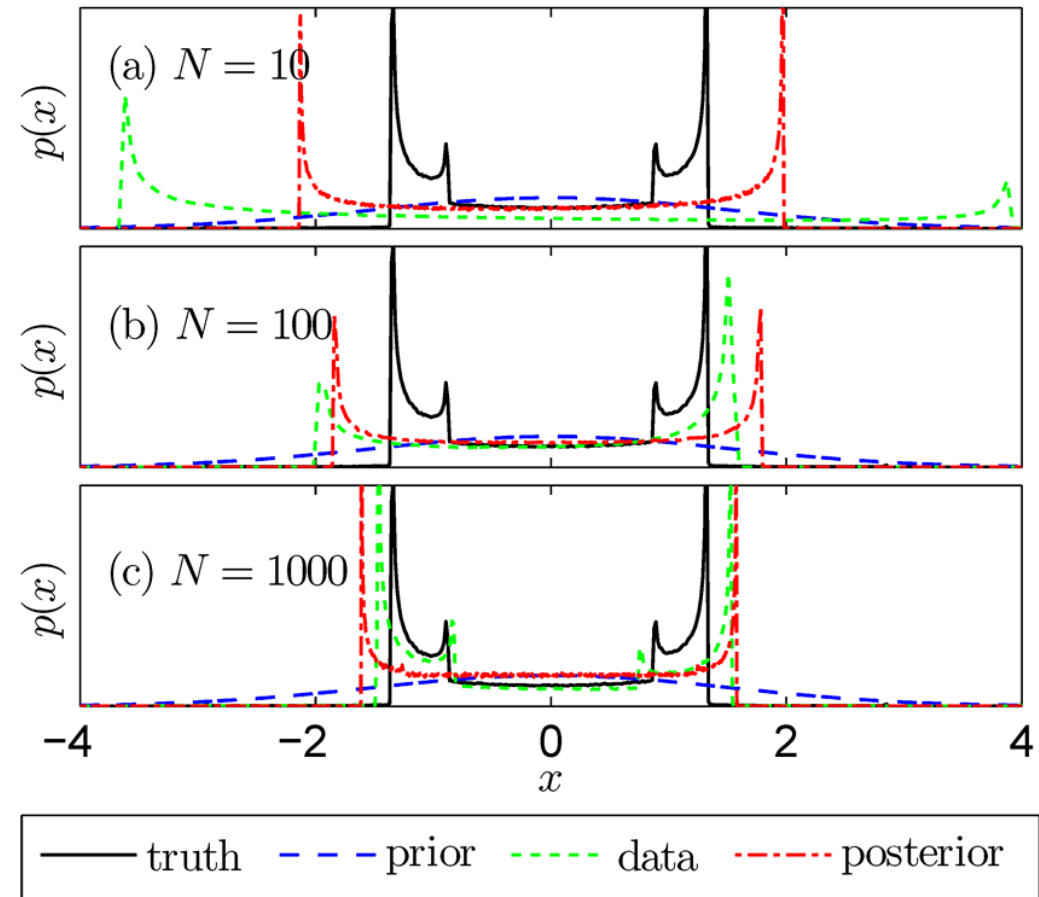
Low-rank approximation can be kept **throughout** update.

# Example 1: Identification of multi-modal dist

**Setup:** Scalar RV  $x$  with **non-Gaussian** multi-modal “truth”  $p(x)$ ; Gaussian prior; Gaussian measurement errors.

**Aim:** Identification of  $p(x)$ .

10 updates of  $N = 10, 100, 1000$  measurements.



## Example 2: Lorenz-84 chaotic model

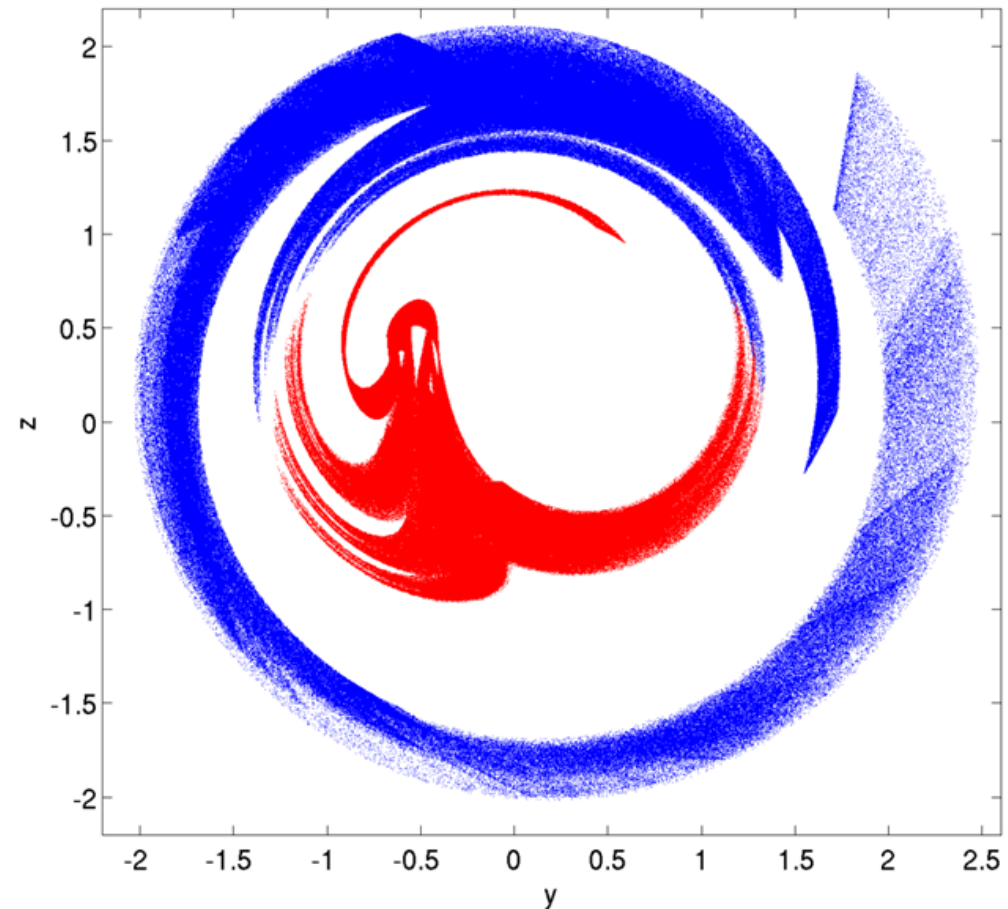
**Setup:** Non-linear, **chaotic** system

$$\dot{u} = f(u), \quad u = [x, y, z]$$

Small uncertainties in initial conditions  $u_0$  have large impact.

**Aim:** Sequentially identify state  $u_t$ .

**Methods:** PCE representation and  
PCE updating and  
sampling representation and  
(Ensemble Kalman Filter)  
EnKF updating.

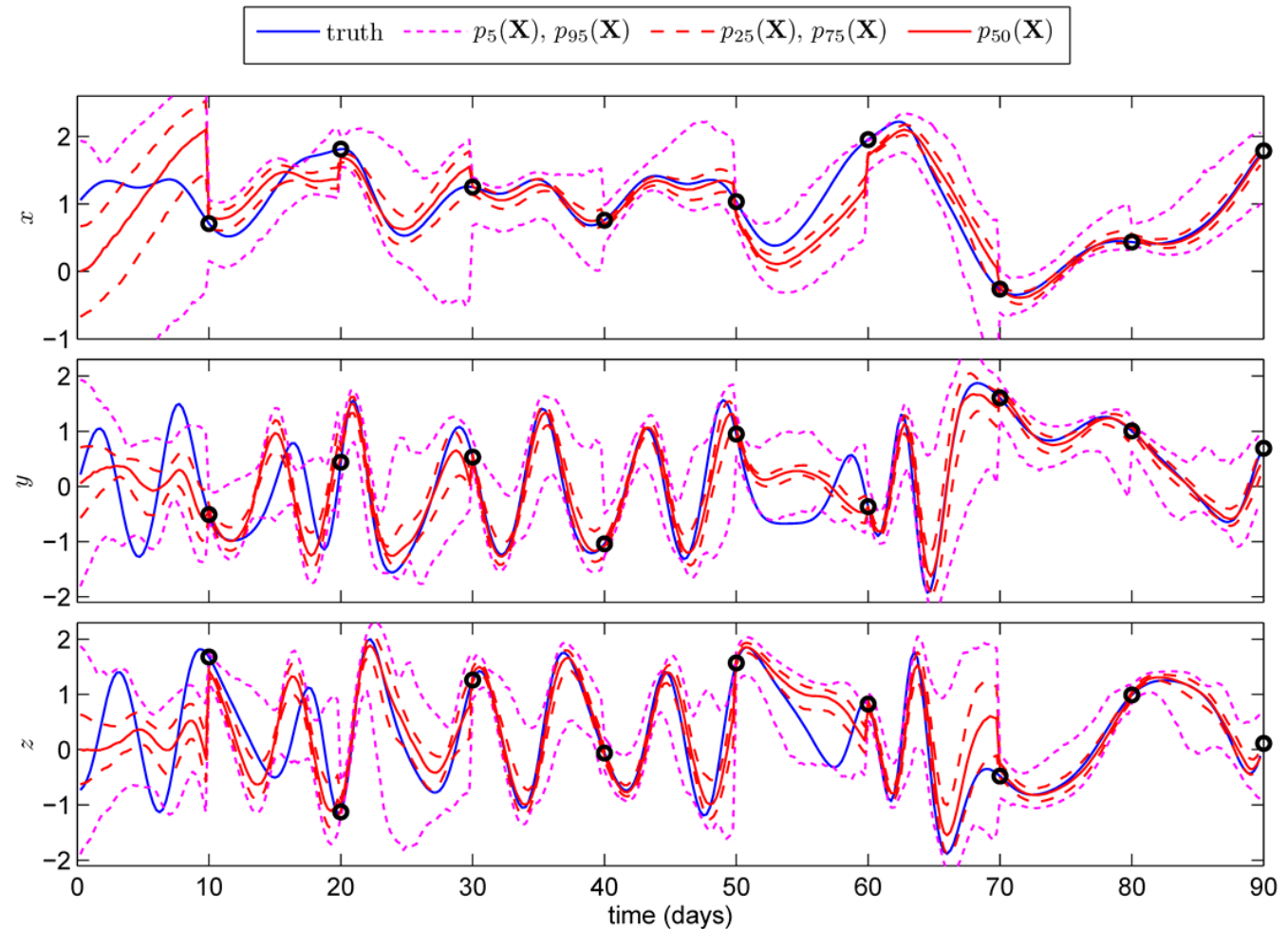


Poincaré cut for  $x = 1$ .

# Example 2: Lorenz-84 PCE representation

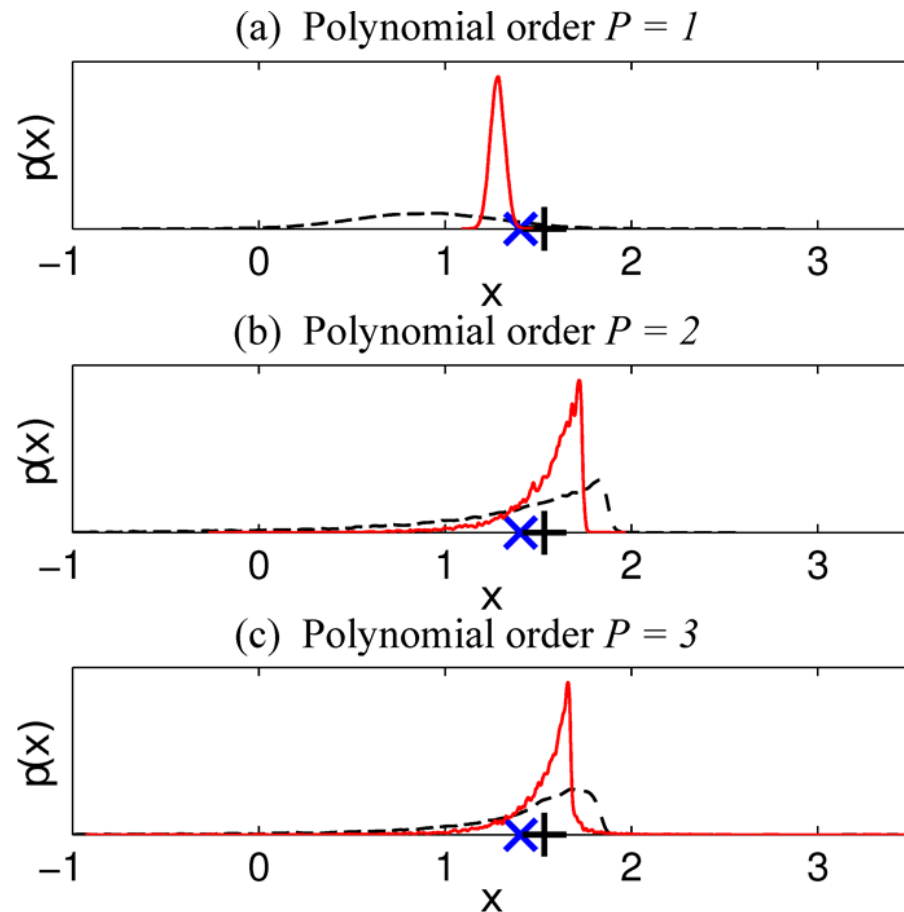
**PCE:** Variance reduction and shift of mean at update points.

Skewed structure clearly visible, preserved by updates.



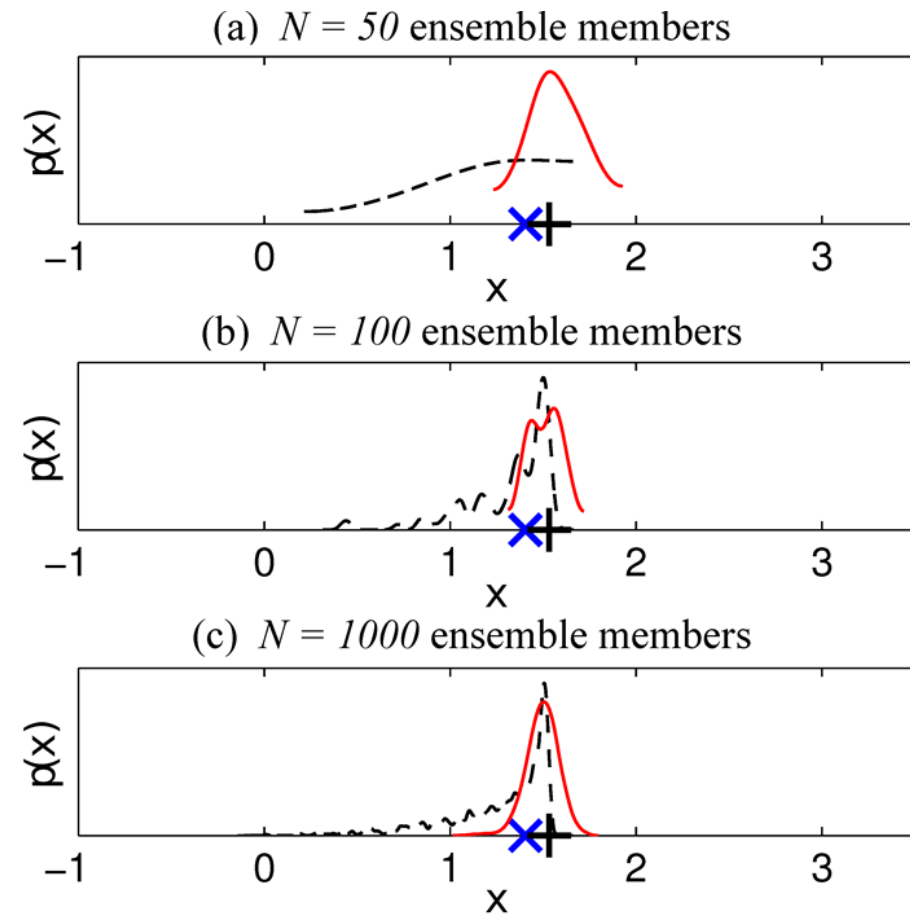
# Example 2: Lorenz-84 non-Gaussian identification

## PCE



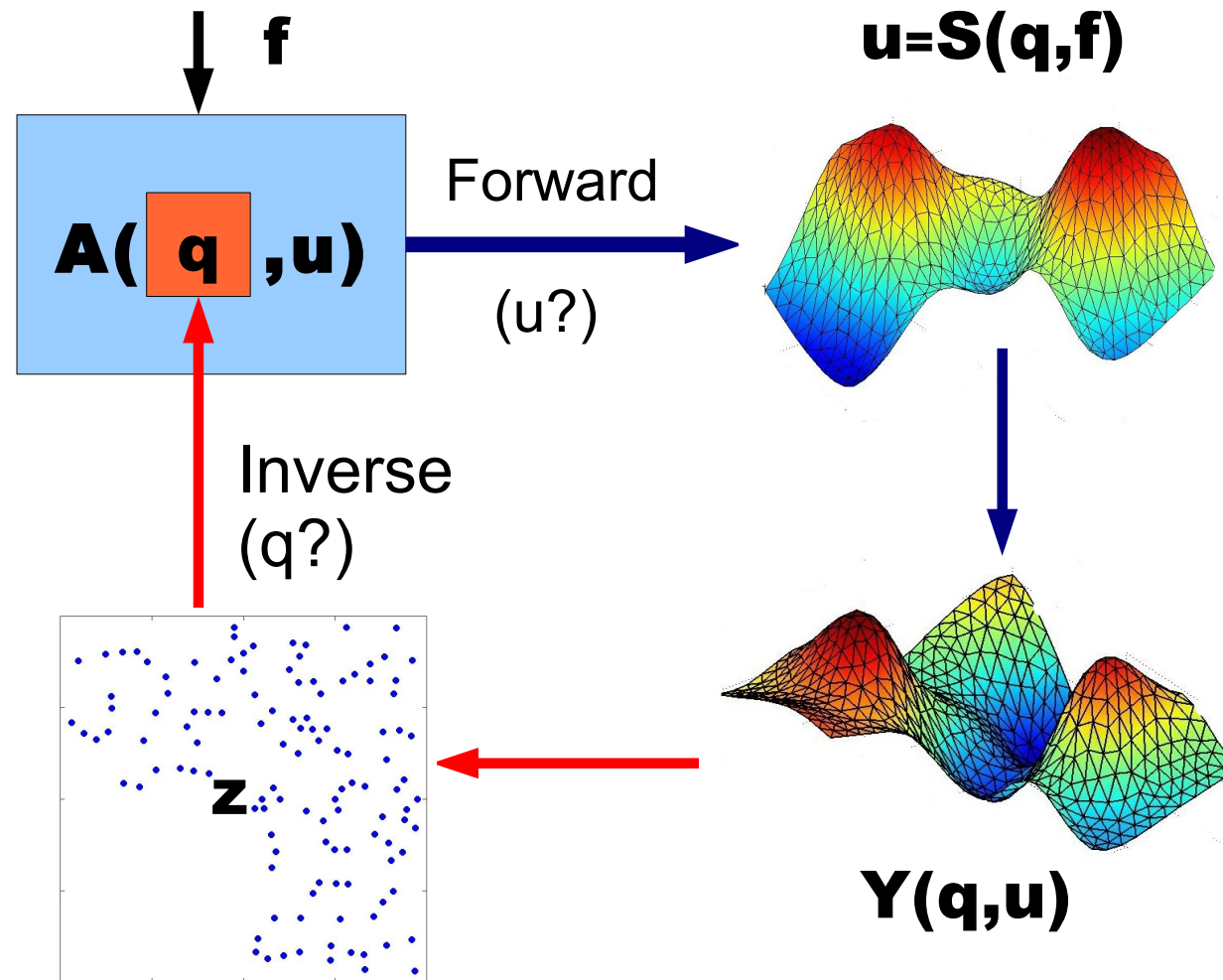
truth  $\times$  measurement  $+$

## EnKF

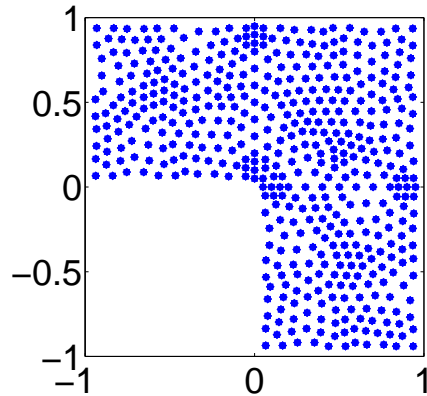


posterior  $p$  prior

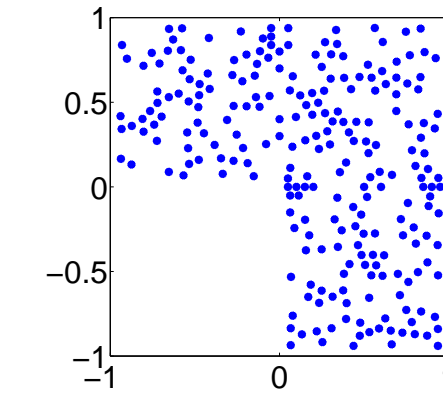
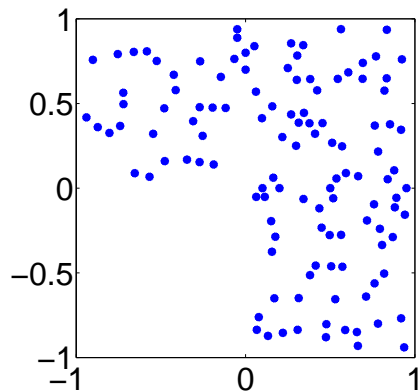
# Example 3: diffusion—schematic representation



# Measurement patches

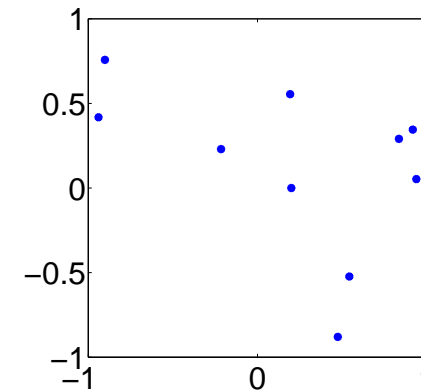


447 measurement patches



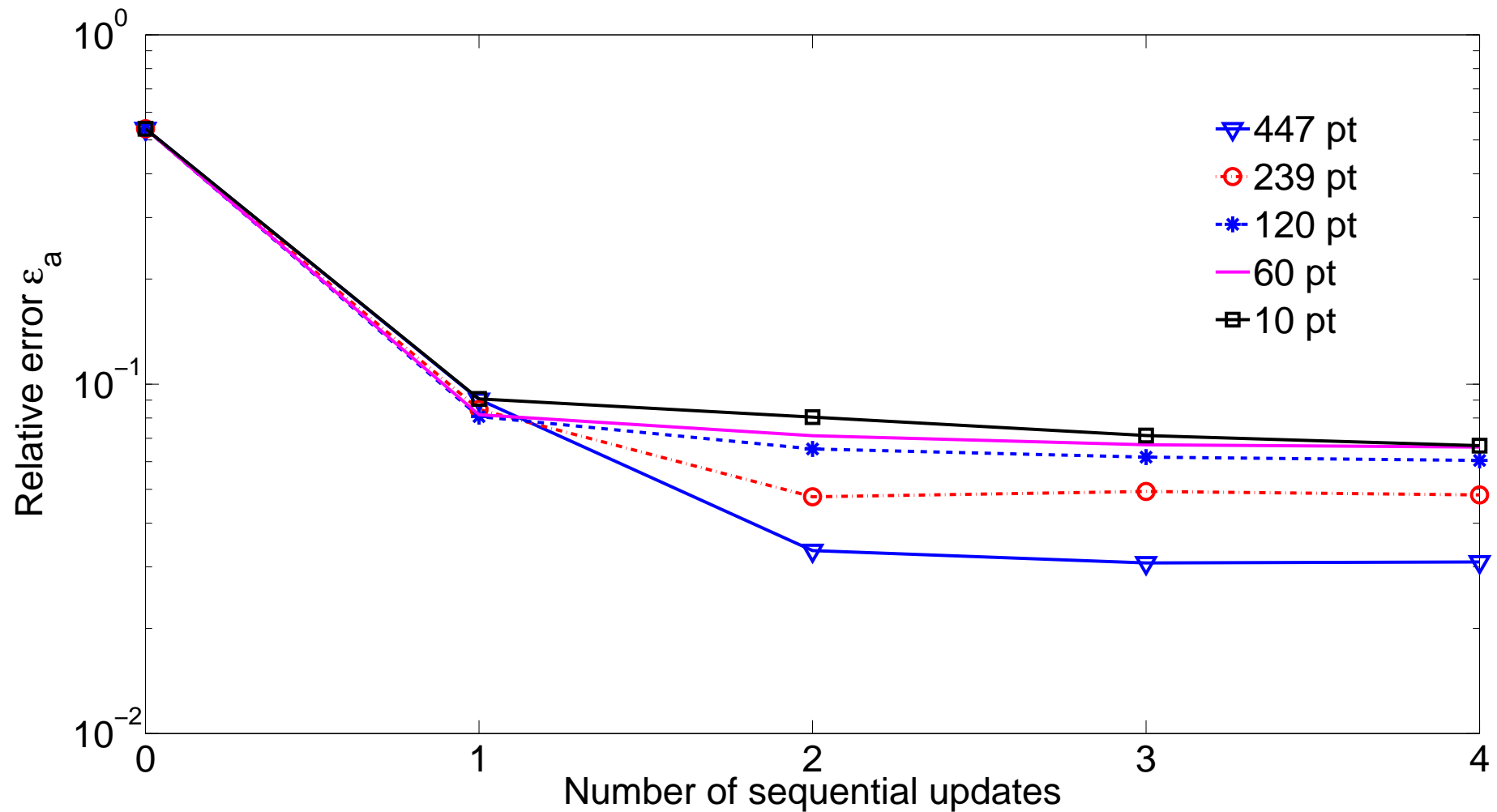
239 measurement patches

120 measurement patches



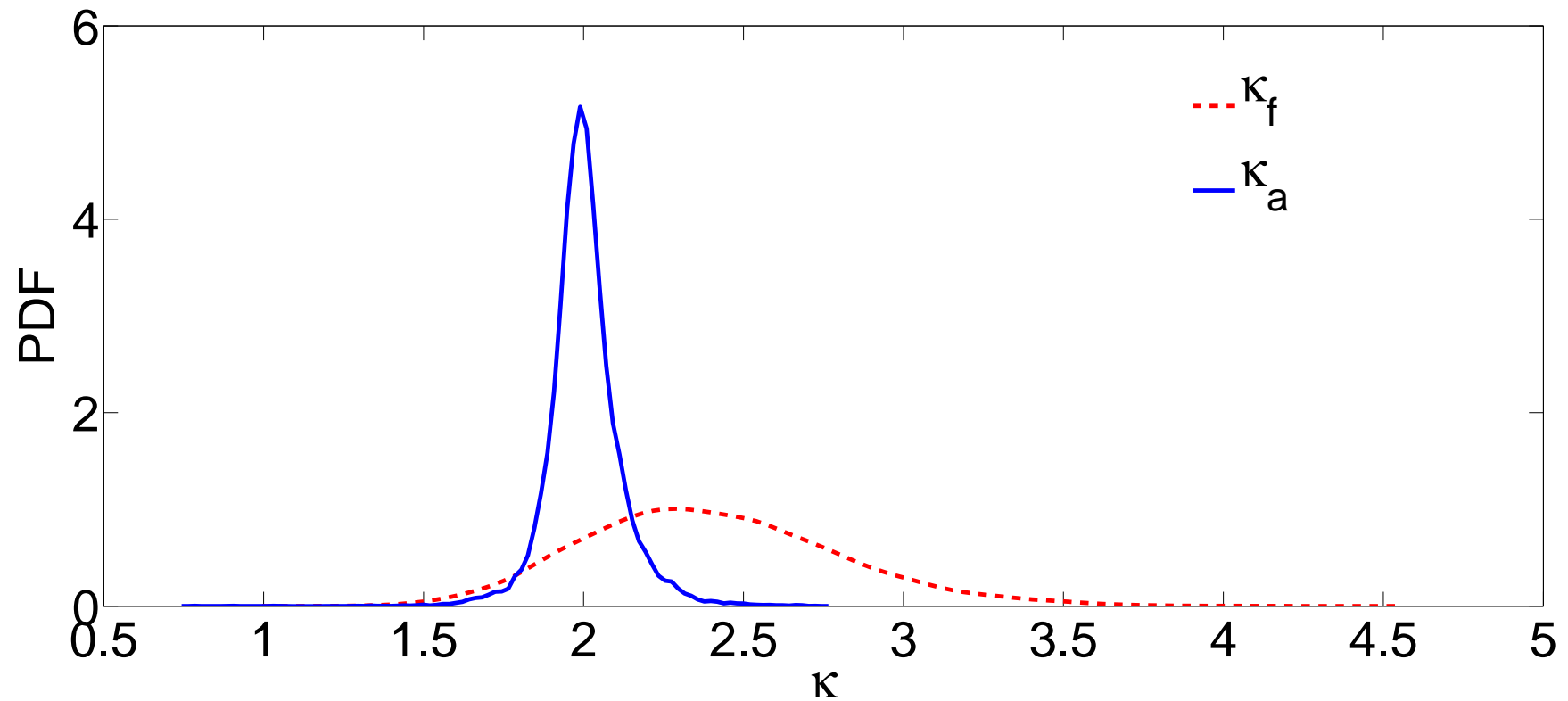
10 measurement patches

# Convergence plot of updates



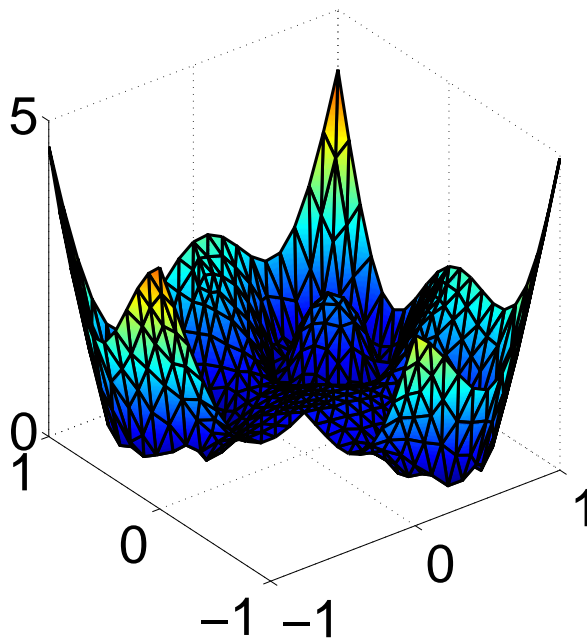


# Forecast and Assimilated pdfs

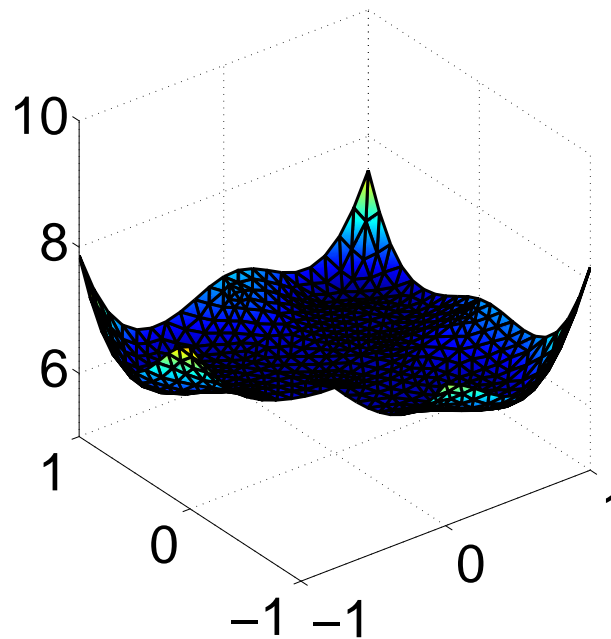


# Spatial Error Distribution

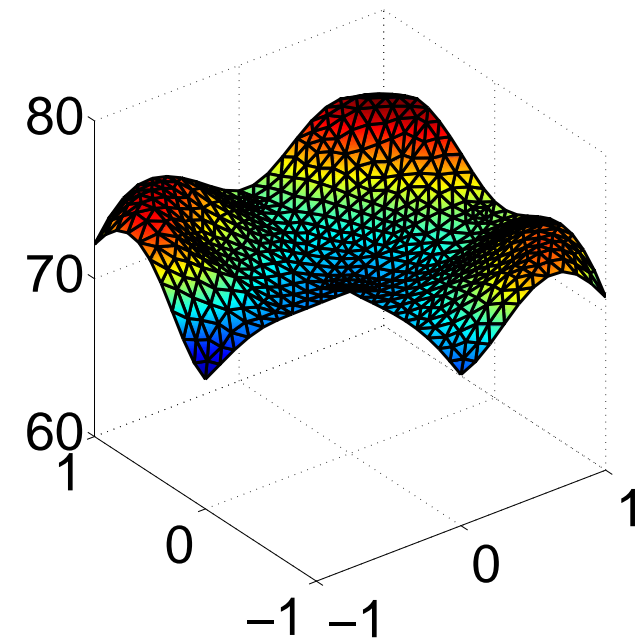
a)  $\bar{\varepsilon}_a$  [%]



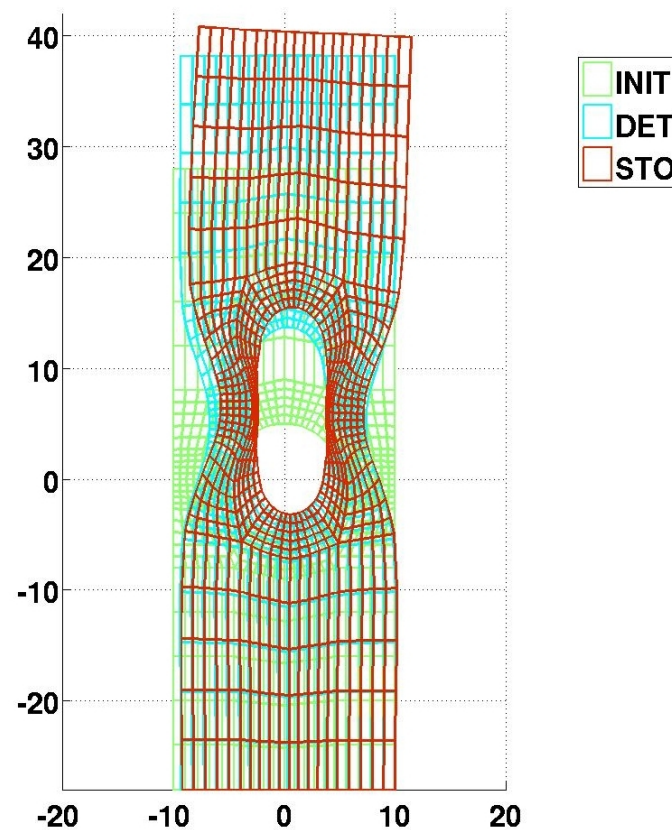
b)  $\varepsilon_a$  [%]



c)  $I$  [%]

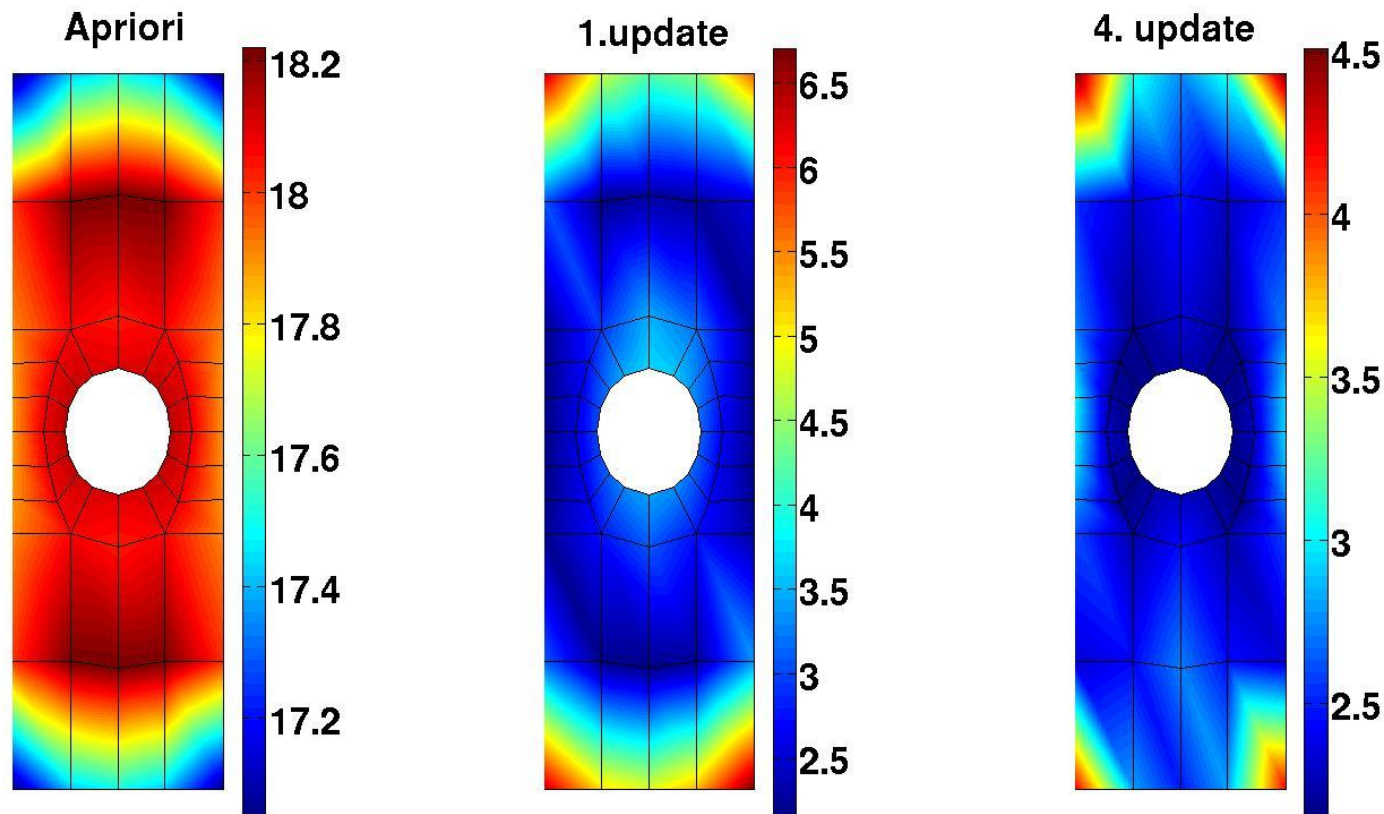


## Example 4: plate with hole



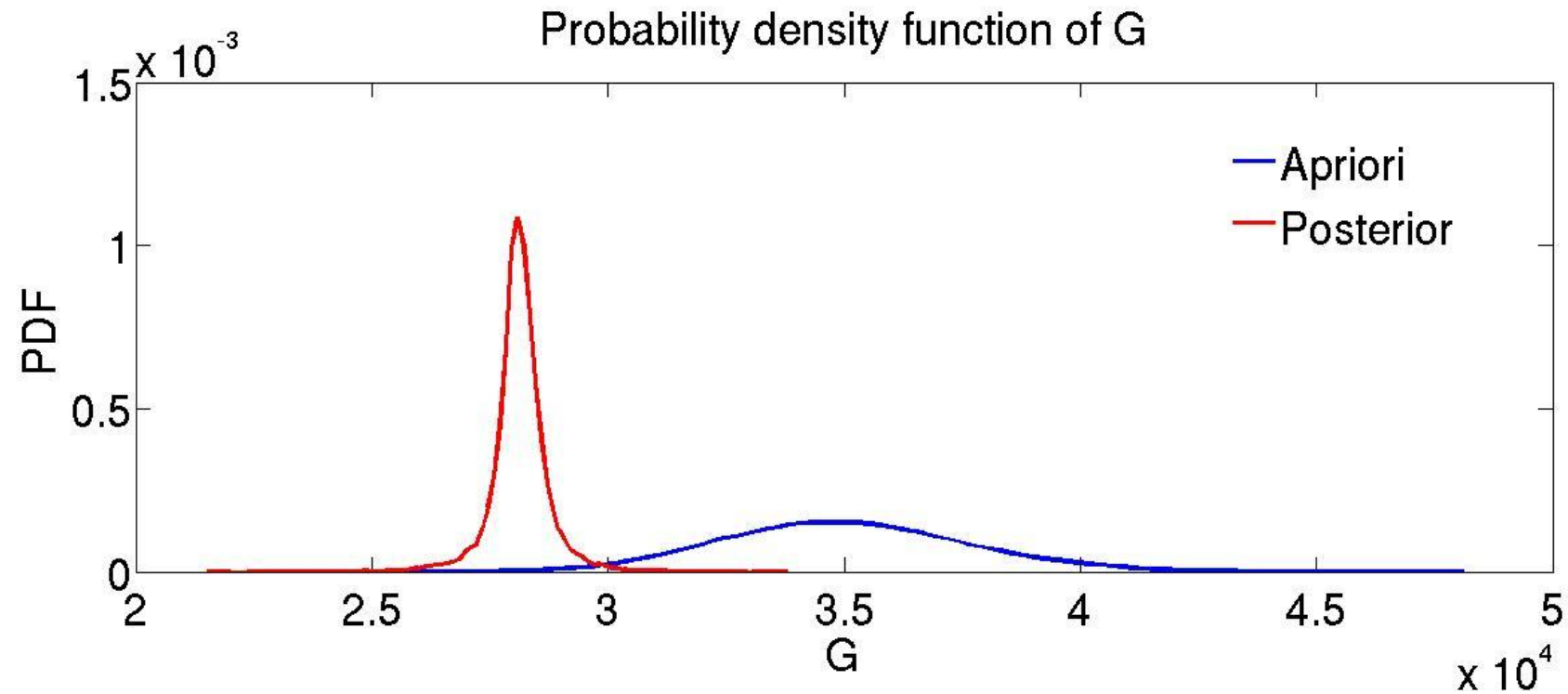
Forward problem: the comparison of the mean values of the total displacement for deterministic, initial and stochastic configuration

# Relative variance of shear modulus estimate



Relative RMSE of variance [%] after 4th update in 10% equally distributed measurement points

# Probability density shear modulus



Comparison of prior and posterior distribution

# Conclusion

- Parametric problems lead to tensor representation.
- **Inverse** problems via Bayes's theorem.
- Bayesian update is a **projection**.
- For efficiency try and use **sparse** representation throughout; ansatz in **low-rank** tensor products, **saves** storage as well as computation.
- Bayesian update **compatible** with **low-rank** representation.