Low-rank cross approximation approach for reducing stochastic collocation models

Sergey Dolgov

joint work with Robert Scheichl

UNIVERSITY OF BATH

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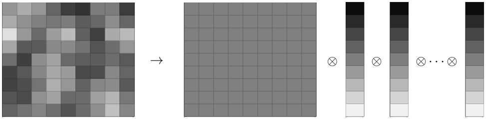
Stochastic partial differential equation

- Uncertainty quantification (UQ)
  - Subsurface flow
  - Calibration
  - Fluid dynamics



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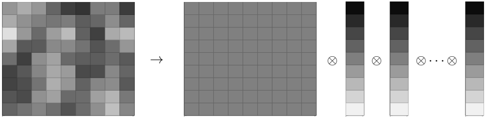

- Example: $-\nabla_{\mathbf{x}} \kappa(\mathbf{x}, \theta_1, \dots, \theta_d) \nabla_{\mathbf{x}} u = f$

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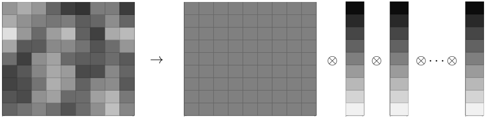


- Example: $-\nabla_{\mathbf{x}}\kappa(\mathbf{x}, \theta_1, \ldots, \theta_d)\nabla_{\mathbf{x}} u = f$

- Many uncertain quantities $\rightarrow$ many dimensions
- Discretize: n DOFs for each θ_k $\rightarrow$ n^d elements in total.

High-dimensional problem $\rightarrow$ low-dimensional output

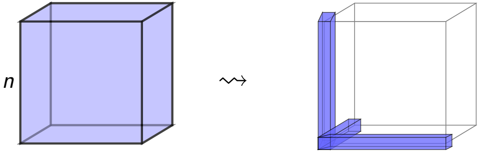
However, the output of interest is **low**-dimensional.

- Eliminate space $Q(\boldsymbol{\theta}) = \mathcal{Q}\left[u(x, \boldsymbol{\theta})\right]$.
- Eliminate parameters by computing
  - moments $\mathbb{E}Q^p$,
  - distribution function/event probabilities $P(Q < \xi)$,
  - quantiles $\xi : P(Q < \xi) > 0.95$

Approximate the solution by a **low-dimensional representation**.

Mathematical insights for data compression

Low-rank tensor decomposition $\Leftrightarrow$ separation of variables:



- Approximate: $\underbrace{u(i_1,\ldots,i_d)}_{\text{tensor}} \approx \underbrace{\sum_{\alpha} u_{\alpha}^{(1)}(i_1)u_{\alpha}^{(2)}(i_2)\cdots u_{\alpha}^{(d)}(i_d)}_{\text{tensor product decomposition}}.$

Goals:

- Store and integrate u $\qquad \mathcal{O}(dn)$ cost **instead of $\mathcal{O}(n^d)$.**
- Solve equations $Au = f$ $\qquad \mathcal{O}(dn^2)$ cost **instead of $\mathcal{O}(n^{2d})$**.

Stochastic PDEs: solution methods

	Cost vs. accuracy	Use of structure
Monte Carlo/Quasi MC	$-$	$+$
Sparse grids (collocation)	$\pm$	$+$
Low-rank decompositions	$+$	$-$

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Sparse grids (collocation)	$\pm$	$+$
Low-rank decompositions	$+$	?

?

- Stochastic PDE $\rightarrow$ **block-diagonal** linear system.
- Generic low-rank algorithms discard the sparsity.
- Can we fix that?

Tensor decompositions: the two workhorses

Goals:

- Store and integrate u

  How to construct u directly?

- Solve equations $Au = f$

  In general?

  How to leverage sparsity?

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Alternating Least Squares

Cross interpolation

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my talk

Tensor decompositions: the two workhorses

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my talk

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The story starts in two dimensions...

2D: low-rank matrices

- Discrete **Separation of variables**:

$$\begin{bmatrix} u_{1,1} & \cdots & u_{1,n} \\ \vdots & & \vdots \\ u_{n,1} & \cdots & u_{n,n} \end{bmatrix} = \sum_{\alpha=1}^{r} \begin{bmatrix} v_{1,\alpha} \\ \vdots \\ v_{n,\alpha} \end{bmatrix} \begin{bmatrix} w_{\alpha,1} & \cdots & w_{\alpha,n} \end{bmatrix} + \mathcal{O}(\varepsilon).$$

- **Rank** $r \ll n$.
- $\mathtt{mem}(v) + \mathtt{mem}(w) = 2nr \ll n^2 = \mathtt{mem}(u)$.
- **Singular Value Decomposition** $\rightarrow$ optimal approximation:

$$\|U - VW^*\|_F^2 \rightarrow \min_{V,W}$$

Cross approximation methods

Singular Value Decomposition is not always good:

- impossible to start from full arrays
- analytical low-rank forms may not exist

Cross algorithms: reconstruct a low-rank form from **a few entries**.

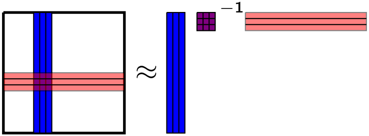
Cross interpolation

- Recall SVD: minimization of the error $\|U - VW^*\|_F^2$.
- **Interpolate** instead:

$$U(\mathcal{I},:) = V(\mathcal{I},:)W^*, \qquad U(:,\mathcal{J}) = VW^*(:,\mathcal{J})$$

for some **index sets** $\mathcal{I},\mathcal{J} \subset \{1,\ldots,n\}$.

- Equivalent to **cross** decomposition:



How to **find** index sets?

Cross approximation: alternating iteration

Practically realizable strategy: assume **initial guess** $U \approx VW^\top$.

1. $\mathcal{J} = \texttt{pivots}(W) \quad \rightarrow \quad V = U(:, \mathcal{J})$.
2. $\mathcal{I} = \texttt{pivots}(V) \quad \rightarrow \quad W = U(\mathcal{I}, :)$.
3. repeat...

V, W are $n \times r$ matrices $\Rightarrow$ `pivots` are feasible (LU, **Maxvol**[1])

Cost: $2nr$ samples $+ \mathcal{O}(nr^2)$ other flops per iteration.

[1] Goreinov, Tyrtyshnikov '01

Cross approximation algorithm

Improvements:

- $V = \mathrm{qr}(V)$ numerical stability.
- $V = \begin{bmatrix} V & Z \end{bmatrix}$ rank update.

Use cross approximation to construct **low-rank PDE coefficients**.

Similar algorithms exist: ACA[2], (D)EIM[3].

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[2] [Bebendorf]

[3] [Maday, Chaturantabut/Sorensen] This week: ask Chris?

Stochastic PDE $\to$ block-diagonal matrix

- We are solving $-\nabla\kappa(x,\theta)\nabla u = f$
- n Finite Elements for x, m collocation points for θ.

$$\int \kappa(x,\theta_j)\nabla\psi_i(x)\cdot\nabla u(x,\theta_j)\;dx = \int \psi_i(x) f(x,\theta_j) dx$$

Independent equations over x for different θ.

$$\begin{bmatrix} A_1 & & & \\ & A_2 & & \\ & & \ddots & \\ & & & A_m \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix}$$

But: every block A_j is **not** diagonal.

Cross approximation and Alternating Least Squares (ALS)

Cross approximation algorithm:

+ Good for functions defined pointwise.
− Not applicable for linear systems.

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Cross interpolation for linear systems

- Rewrite interpolation as projection:

$$E_{\mathcal{J}}^{\top}\mathrm{vec}(VW^*) = E_{\mathcal{J}}^{\top}\mathrm{vec}(U),$$

where $E_{\mathcal{J}}$ is a **submatrix of identity** at $\mathcal{J}$.

Cross interpolation for linear systems

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- Replace I by the stiffness matrix:

$$E_{\mathcal{J}}^{\top} \cdot \mathbf{A} \cdot \mathrm{vec}(VW^*) = E_{\mathcal{J}}^{\top} \mathrm{vec}(F)$$

... and $\mathbf{A} \cdot \mathrm{vec}(U)$ by the right hand side.

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- Replace I by the stiffness matrix:

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- Still: any benefit for UQ?

How we represent the matrix?

- **Coefficient** is low-rank:

$$\kappa(x, \theta) \approx \sum_{\beta=1}^{R} g_\beta(x) h_\beta(\theta).$$

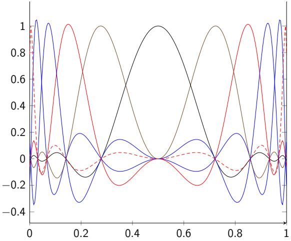
- Hence $\mathbf{A}$ is low-**Kronecker**-rank:

$$\mathbf{A} = \sum_{\beta=1}^{R} A_\beta \otimes D_\beta$$

- A_β is FEM-related, but
- $D_\beta = \mathrm{diag}(d_\beta)$ is **diagonal**.

Interpolatory representation

- VW^* is not unique $\to$ ensure $W(\mathcal{J}) = I$.



...as a by-product $V = U(:, \mathcal{J})$.

- **Distribute** the products

$$E_{\mathcal{J}}^{\top} \cdot \mathbf{A} \cdot \mathrm{vec}(VW^*) = \sum_{\beta=1}^{R} A_\beta \otimes [D_\beta(\mathcal{J}, :)W] \cdot v = \sum_{\beta=1}^{R} A_\beta \otimes \mathrm{diag}(d_\beta(\mathcal{J})) \cdot v$$

Block diagonal system, stage 1: space

The first step:

$$\{j_1, \dots, j_r\} = \texttt{pivots}(W)$$

$$\begin{bmatrix} A_{j_1} & & \\ & A_{j_2} & \\ & & A_{j_r} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_r \end{bmatrix} = \begin{bmatrix} f_{j_1} \\ f_{j_2} \\ f_{j_r} \end{bmatrix}$$

- Solve r independent deterministic problems.
  - Similar to Monte Carlo and stochastic collocation.
  - Can use specialized tools (preconditioners/software).

Block diagonal system, stage 2: parameters

A_j is not diagonal $\rightarrow$ ALS-projection:

1. Make V orthogonal $\rightarrow$ projection matrix $\mathcal{V} = V \otimes I$.
2. Solve $\left(\mathcal{V}^\top \mathbf{A} \mathcal{V}\right) w = \mathcal{V}^\top \mathbf{f}$.

- Solve m systems of size $r \times r$.
- Similar to Reduced Basis MOR (**in 2 dimensions**).
- Extensible to **many dimensions**.

Back to many variables

- What about $-\nabla\kappa(x, \theta_1, \dots, \theta_d)\nabla u = f$?

Tensor Train (TT) decomposition

- Many dimensions: Matrix Product States/Tensor Train[4]:

$$u(i_1 \dots i_d) = \sum_{\alpha_k=1}^{r_k} u^{(1)}_{\alpha_1}(i_1) \cdot u^{(2)}_{\alpha_1,\alpha_2}(i_2) \cdot u^{(3)}_{\alpha_2,\alpha_3}(i_3) \cdots u^{(d)}_{\alpha_{d-1}}(i_d)$$

- TT blocks $u^{(k)}$ are **three-dimensional**.
- Storage: $\mathcal{O}(dnr^2)$.

[4] Wilson '75, White '93, Verstraete '04, Oseledets '09

Tensor Train for stochastic PDEs

TT format of the coefficient $\rightarrow$ TT format of the matrix:

- Space $\rightarrow$ first TT block $\rightarrow$ FEM stiffness pattern
- Parameters $\rightarrow$ other TT blocks $\rightarrow$ diagonal

$$\mathbf{A} = \sum_{\beta_k=1}^{R_k} A^{(1)}_{\beta_1} \otimes \mathrm{diag}(d^{(2)}_{\beta_1,\beta_2}) \otimes \cdots \otimes \mathrm{diag}(d^{(d)}_{\beta_{d-1}})$$

Tensor Train for stochastic PDEs

The algorithm in a nutshell:

1. $\mathcal{J}_k = \texttt{pivots}\left(U_{>k}\right)$.
2. Generate and solve $\left[\mathcal{U}_{<k}{}^{\top} \mathbf{A}_{\mathcal{J}_k} \mathcal{U}_{<k}\right] u^{(k)} = \mathcal{U}_{<k}^{\top} \mathbf{f}_{\mathcal{J}_k}$.
3. $\mathcal{U}_{<k+1} = \mathcal{U}_{<k} \cdot u^{(k)}$.
4. Set $k = k+1$ or $k = k-1$ and repeat...

$$\xrightarrow{\qquad\qquad}$$

$$u^{(1)} \cdot u^{(2)} \ldots u^{(k)} \ldots u^{(d-1)} \cdot u^{(d)}$$

$$\xleftarrow{\qquad\qquad}$$

1. Problem setting
2. Low-rank UQ algorithms
   - Singular value decomposition
   - Cross approximation for matrices
   - Cross approximation for sPDEs
3. Numerical experiments

Log-normal diffusion coefficient

$$
\begin{aligned}
&-\nabla\kappa(x,\theta)\nabla u = 0 \quad \text{in} \quad (0,1)^2 \\
&u|_{x_1=0} = 1, \qquad u|_{x_1=1} = 0, \\
&\frac{\partial u}{\partial n}|_{x_2=0} = \frac{\partial u}{\partial n}|_{x_2=1} = 0.
\end{aligned}
$$

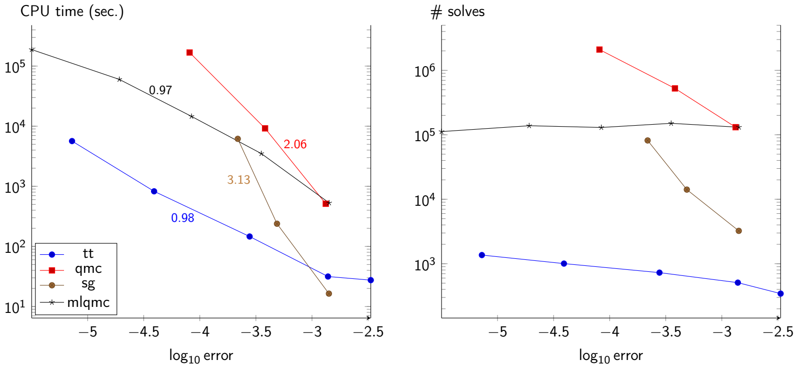
- $\kappa(x,\theta) = \exp\left(\sum_{k=1}^{d} \phi_k(x)\theta_k\right)$
- ϕ_k: Karhunen-Loeve expansion of the Matern covariance with parameters $\sigma^2 = 1$ and (different) ν.

Methods

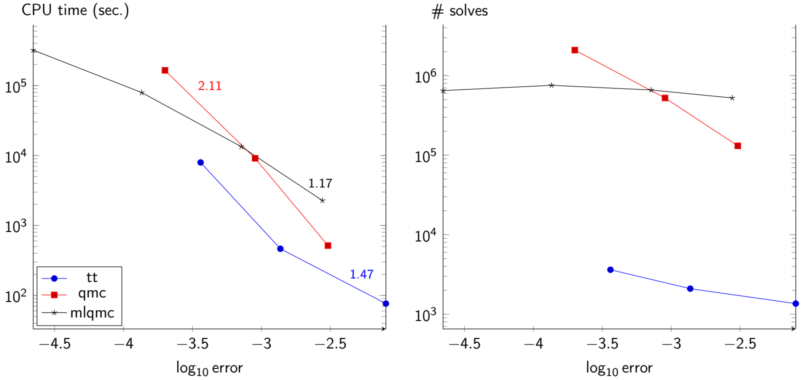
- Quasi Monte Carlo with a special lattice vector[5].
- Multilevel QMC.
- Adaptive Sparse Grids toolbox[6].
- TT Cross algorithm.

[5] `lattice-39102-1024-1048576.3600.txt` from F. Kuo
[6] Andreas Klimke '08 `http://www.ians.uni-stuttgart.de/spinterp/`

Smooth ($\nu = 4$) uniform field



Rougher ($\nu = 2.5$) normal field



Conclusion

Cross interpolation can be used as a low-rank solver...

- ...which preserves sparsity in sPDEs.
- Faster than QMC/SG if the problem has low-rank structure.
- Less efficient if the problem is "more" random.
- Reference and code: [arXiv:1707.04562]
- Future plans: inverse problems.

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Thank you for your attention!