Krylov subspace methods for linear systems with tensor product structure

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Outline

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Linear system with tensor product structure

We consider the linear system

$$\mathcal{A}x = b$$

with

$$\mathcal{A} = \sum_{s=1}^{d} I_{n_1} \otimes \cdots \otimes I_{n_{s-1}} \otimes A_s \otimes I_{n_{s+1}} \otimes \cdots \otimes I_{n_d},$$

$$b = b_1 \otimes \cdots \otimes b_d,$$

$A_s \in \mathbb{R}^{n_s \times n_s}$ positive definite, $b_s \in \mathbb{R}^{n_s}$.

Example for 3 dimensions:

$$(A_1 \otimes I \otimes I + I \otimes A_2 \otimes I + I \otimes I \otimes A_3)x = b_1 \otimes b_2 \otimes b_3$$

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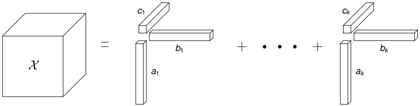
Tensor decompositions

CP decomposition:

$$\mathrm{vec}(\mathcal{X}) = \sum_{r=1}^{k} a_r \otimes b_r \otimes c_r$$

$$a_r \in \mathbb{R}^m, b_r \in \mathbb{R}^n, c_r \in \mathbb{R}^p$$



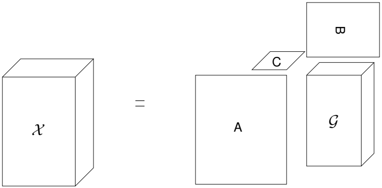
Tucker decomposition:

$$\mathrm{vec}(\mathcal{X}) = \sum_{i=1}^{\tilde{m}} \sum_{s=1}^{\tilde{n}} \sum_{l=1}^{\tilde{p}} \mathcal{G}_{ijl}\, a_i \otimes b_j \otimes c_l$$

$$= (A \otimes B \otimes C)\,\mathrm{vec}(\mathcal{G})$$

$$\mathcal{G} \in \mathbb{R}^{\tilde{m} \times \tilde{n} \times \tilde{p}},$$

$$a_i \in \mathbb{R}^m, b_j \in \mathbb{R}^n, c_l \in \mathbb{R}^p$$



About this system

The eigenvalues of the matrix $\mathcal{A}$ are given by all possible sums

$$\lambda_{i_1}^{(1)} + \lambda_{i_2}^{(2)} + \ldots + \lambda_{i_d}^{(d)}$$

where $\lambda_{i_s}^{(s)}$ denotes an eigenvalue of A_s. For A_s positive definite, the system has a unique solution.

Note that x and b are vector representations of tensors in $\mathbb{R}^{n_1 \times \cdots \times n_d}$, and b represents a rank-one tensor.

A tensor arising from the discretization of a sufficiently smooth function f can be approximated by a short sum of rank-one tensors. By superposition, we can insert such a tensor as right-hand side into our system.

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Tensorized Krylov subspaces

A Krylov subspace is defined as

$$\mathcal{K}_k(A, b) = \text{span}\{b,\ Ab,\ \ldots,\ A^{k-1}b\}.$$

We define a tensorized Krylov subspace as

$$\mathcal{K}^{\otimes}_{\mathfrak{K}}(\mathcal{A}, b) := \operatorname{span}\big(\mathcal{K}_{k_1}(A_1, b_1) \otimes \cdots \otimes \mathcal{K}_{k_d}(A_d, b_d)\big).$$

Note that

$$\mathcal{K}_{k_0}(\mathcal{A}, b) \subset \mathcal{K}^{\otimes}_{\mathfrak{K}}(\mathcal{A}, b)$$

for $\mathfrak{K} = (k_0, \ldots, k_0)$.

$\Rightarrow$ Tensorized Krylov subspaces are richer than standard Krylov subspaces.

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Outline

Reminder: CG method ($Ax = b$)

The best approximation of x in $\mathcal{K}_k(A, b)$ is defined by:

$$\|x_k - x\|_A = \min_{\tilde{x} \in \mathcal{K}_k(A,b)} \|\tilde{x} - x\|_A.$$

Find U_k with (orthonormal) columns that span the Krylov subspace $\mathcal{K}_k(A, b)$. Set $x_k = U_k y$, then y is the solution of the compressed system

$$H_k y = \tilde{b}, \qquad H_k = U_k^\top A U_k, \tilde{b} = U_k^\top b.$$

Convergence bound ($\kappa = \kappa_2(A)$)

$$\|x_k - x\|_A \leq C(A, b, \kappa)\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k.$$

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Tensorized Krylov: $\mathcal{A}\,\mathrm{vec}(\mathcal{X}) = b$

Applying the Arnoldi method to A_s, b_s results in U_s, H_s with

$$U_s^\top A_s U_s = H_s,$$

U_s column-orthogonal, H_s upper Hessenberg matrix.

The columns of U_s span $\mathcal{K}_{k_s}(A_s, b_s)$, and similarly the columns of $\mathcal{U} := U_1 \otimes \cdots \otimes U_d$ span $\mathcal{K}^{\otimes}_{\mathfrak{K}}(\mathcal{A}, b)$.

Solve the compressed system

$$\mathcal{H} y = \tilde{b}$$

with $x_{\mathfrak{K}} = \mathcal{U} y$, $\tilde{b} = \mathcal{U}^\top b$ and $\mathcal{H} = \mathcal{U}^\top \mathcal{A} \mathcal{U}$.

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Compressed system

The structure of $\mathcal{H}y = \tilde{b}$ corresponds to that of $\mathcal{A}x = b$:

$$\mathcal{H} = \sum_{s=1}^{d} I_{k_1} \otimes \cdots \otimes I_{k_{s-1}} \otimes H_s \otimes I_{k_{s+1}} \otimes \cdots \otimes I_{k_d}$$

$$\tilde{b} = \tilde{b}_1 \otimes \cdots \otimes \tilde{b}_d = \|b\|_2 \, (e_1 \otimes \cdots \otimes e_1)$$

For dense core tensor y, $x_{\mathfrak{K}}$ is a tensor in Tucker decomposition:

$$x_{\mathfrak{K}} = (U_1 \otimes \cdots \otimes U_d) y$$

Outline

Convergence, s.p.d. case (1)

Similarly to CG, we have:

$$\|x_{\mathfrak{K}} - x\|_{\mathcal{A}} = \min_{\tilde{x} \in \mathcal{K}_{\mathfrak{K}}^{\otimes}(\mathcal{A}, b)} \|\tilde{x} - x\|_{\mathcal{A}}$$

Every vector in a Krylov subspace $\mathcal{K}_{k_s}(A_s, b_s)$ can be seen as $p(A_s)b_s$, with p a polynomial of order at most $k_s - 1$. A similar thought reduces the bound calculation to the min-max problem

$$E_{\Omega}(\mathfrak{K}) := \min_{p \in \Pi_{\mathfrak{K}}^{\otimes}} \|p(\lambda_1, \ldots, \lambda_d) - \frac{1}{\lambda_1 + \cdots + \lambda_d}\|_{\Omega},$$

where $\Pi_{\mathfrak{K}}^{\otimes}$ is a space of multivariate polynomials, and Ω contains the eigenvalues $(\lambda_1, \ldots, \lambda_d)$, with $\lambda_i \in [\lambda_{\min}(A_i), \lambda_{\max}(A_i)]$.

Convergence, s.p.d. case (2)

Inserting an upper bound for $E_\Omega(\mathfrak{K})$, we find

$$\|x_{\mathfrak{K}} - x\|_{\mathcal{A}} \leq \sum_{s=1}^{d} C(\mathcal{A}, b, \kappa_s)\left(\frac{\sqrt{\kappa_s} - 1}{\sqrt{\kappa_s} + 1}\right)^{k_s},$$

with $\kappa_s = 1 + \frac{\lambda_{\max}(A_s) - \lambda_{\min}(A_s)}{\lambda_{\min}(\mathcal{A})}$.

For the case A_s, k_s constant:

$$\|x_{\mathfrak{K}} - x\|_{\mathcal{A}} \leq C(\mathcal{A}, b, d)\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{k},$$

with $\kappa = \frac{d-1}{d} + \frac{\kappa_2(\mathcal{A})}{d}$.

Note that the convergence rate improves with increasing dimension.

Convergence, non-symmetric positive definite case

General convergence bound:

$$\|x_{\mathfrak{K}} - x\|_2 \leq \sum_{s=1}^{d} \int_0^{\infty} e^{-\hat{\alpha}_s t} \, \|U_s e^{-tH_s} e_1 - e^{-tA_s} b_s\|_2 \, \mathrm{d}t$$

with $\hat{\alpha}_s := \sum_{j \neq s} \alpha_j$ and $\alpha_j = \lambda_{\min}(A_j + A_j^\top)/2$.

The bound on $\|U_s e^{-tH_s} e_1 - e^{-tA_s} b_s\|_2$ will depend on additional knowledge on A_s.

For example, when the field of values of each matrix A_s is contained in a known ellipse, an explicit convergence bound can be found.

Outline

Grasedyck's method, system $\mathcal{H}y = \tilde{b}$

For $\mathcal{H}$ positive definite:

$$\mathcal{H}^{-1} = \int_0^\infty \exp(-t\mathcal{H})dt$$

The exponential of $\mathcal{H}$ has a Kronecker product structure, too:

$$\exp(-t\mathcal{H}) = \exp(-t\sum_{s=0}^{d} \hat{H}_s) = \prod_{s=1}^{d} \exp(-t\hat{H}_s) = \bigotimes_{s=1}^{d} \exp(-tH_s),$$

Approximation y_m:

$$y_m = \sum_{j=1}^{m} \omega_j \bigotimes_{s=1}^{d} \exp\Big(-\alpha_j H_s\Big)\tilde{b}_s,$$

with certain coefficients α_j, ω_j.

Coefficients of the exponential sum (1)

The coefficients α_j, ω_j should minimize

$$\sup_{z \in \Lambda(\mathcal{H})} \left| \frac{1}{z} - \sum_{j=1}^{m} \omega_j e^{-\alpha_j z} \right|$$

Case 1: $\mathcal{H}$ symmetric and condition number known
The eigenvalues of $\mathcal{H}$ are real: $\Lambda(\mathcal{H}) \subset [\lambda_{\min}, \lambda_{\max}]$. There are coefficients α_j, ω_j s.t.

$$\|y - y_m\|_2 \leq C(\mathcal{H}, \tilde{b}) \exp\left(\frac{-m\pi^2}{\log(8\kappa_2(\mathcal{H}))} \right).$$

These coefficients may be found using a variant of the Remez algorithm. Tabellated values have been made available by Hackbusch.

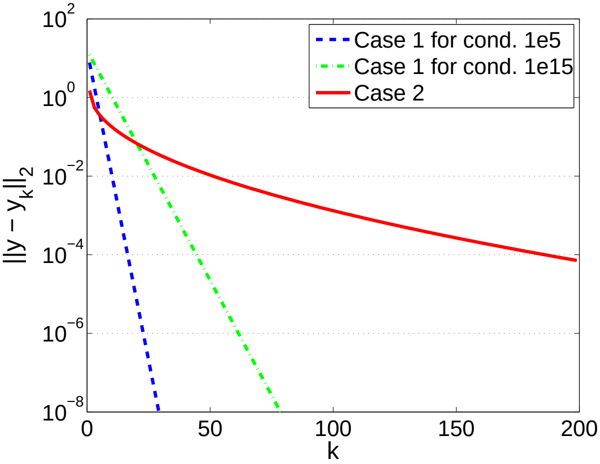
Coefficients of the exponential sum (2)

Case 2: Nonsymmetric $\mathcal{H}$ and/or unknown condition number
There is an explicit formula for α_j, ω_j, where the eigenvalues of $\mathcal{H}$ only need to have positive real part.

$$\|y - y_{2m+1}\|_2 \leq C(\mathcal{H}, \tilde{b}) \exp(\mu/\pi) \exp(-\sqrt{m}),$$
$$\text{where } \mu = \max\{|\Im m(\Lambda(\mathcal{H}))|\}.$$

The convergence is significantly slower than for Case 1.

Theoretical convergence bounds for the coefficients



Outline

Symmetric example: Poisson Equation

Finite difference discretization of the Poisson equation in d dimensions:

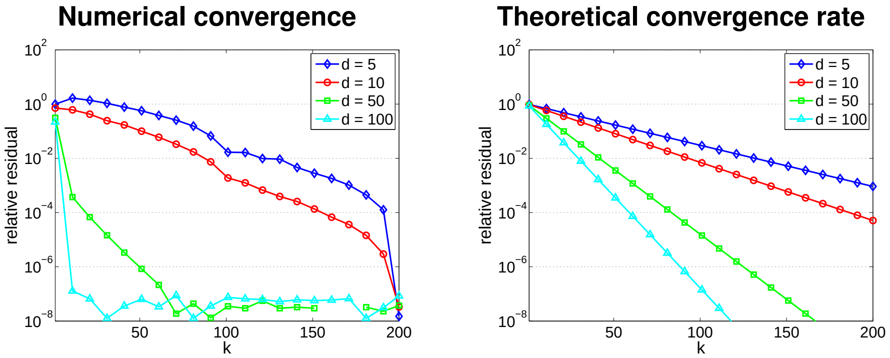
$$\begin{aligned} \Delta u &= f \quad \text{in } \Omega = [0,1]^d \\ u &= 0 \quad \text{on } \Gamma := \partial\Omega, \end{aligned}$$

where the right-hand side f is a separable function.

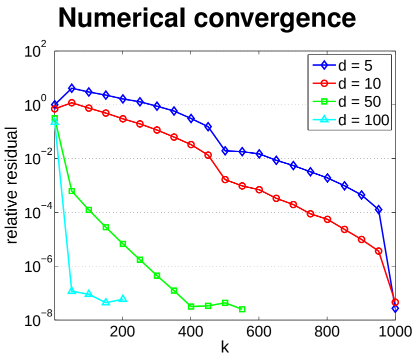
$$A_s = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}, b_s : \text{random numbers.}$$

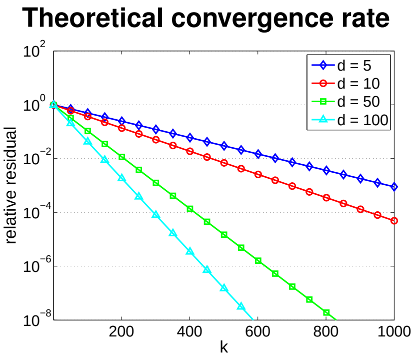
The approximation error is measured by *relative residual*, $\frac{\|\mathcal{A}x_{\mathfrak{K}} - b\|_2}{\|b\|_2}$.

Convergence for system size 200^d



Convergence for system size 1000^d





Extended Krylov subspaces

Using *extended Krylov subspaces*

$$\widetilde{\mathcal{K}}_{k_s}(A_s, b_s) := \mathrm{span}(\mathcal{K}_{k_s}(A_s, b_s) \cup \mathcal{K}_{k_s+1}(A_s^{-1}, b_s)),$$

the algorithm works analogously.
Convergence bound (A_s, k_s constant):

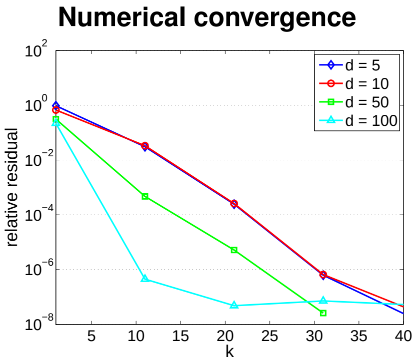
$$\|x_{\mathfrak{K}} - x\|_2 \le C(\mathcal{A}, b, d)\left(\frac{\sqrt{\tilde{\kappa}} - 1}{\sqrt{\tilde{\kappa}} + 1}\right)^k.$$

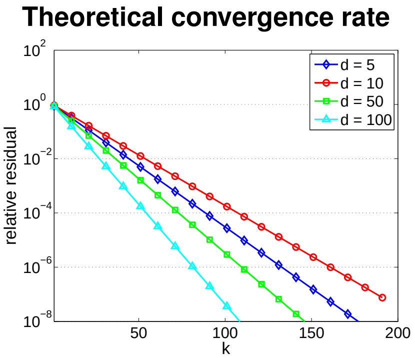
The convergence rate depends on $\tilde{\kappa}$:

$$\tilde{\kappa} \approx \frac{d-1}{d} + \frac{1}{d^2}(d-1)^{\frac{d-1}{d}}\kappa_2(\mathcal{A})^{\frac{d-1}{d}}$$

$$d = 2 : \tilde{\kappa} = \frac{1}{2} + \frac{\sqrt{\kappa_2(\mathcal{A})}}{4}, \qquad d \gg 0 : \tilde{\kappa} \approx \frac{d-1}{d} + \frac{\kappa_2(\mathcal{A})}{d}.$$

Extended Krylov, system size 200^d





Non-symmetric example

Finite difference discretization in d dimensions of the convection-diffusion equation

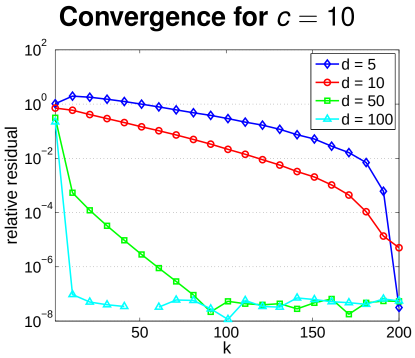
$$\begin{aligned} \Delta u - (c, \dots, c)\nabla u &= f \quad \text{in } \Omega = [0,1]^d \\ u &= 0 \quad \text{on } \Gamma := \partial\Omega, \end{aligned}$$

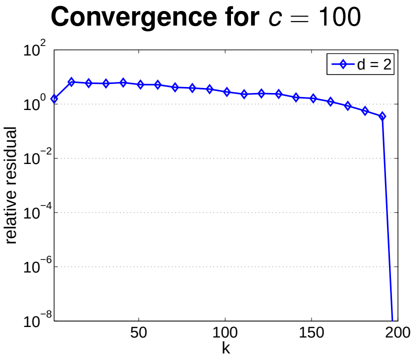
where f is again a separable function.

$$A_s = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} + \frac{c}{4h}\begin{pmatrix} 3 & -5 & 1 & & \\ 1 & 3 & -5 & \ddots & \\ & \ddots & \ddots & \ddots & 1 \\ & & 1 & 3 & -5 \\ & & & 1 & 3 \end{pmatrix}.$$

For $c = 10$, all eigenvalues of $\mathcal{A}$ are real. For $c = 100$, this is not the case, and the convergence is significantly worsened.

Non-symmetric case, system size 200^d





Conclusions

- An efficient algorithm to calculate a low-rank approximation of the solution tensor
- The computational complexity is linear in the number of dimensions
- Only matrix-vector operations with the full system matrices are required
- A theoretical convergence bound was found.

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Thank you for your attention!

Literature

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