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GMRES in variable accuracy: a case study in low rank tensor linear systems

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GAMM, Prague, 23-09-2022

Concace - Inria joint team with Airbus and Cerfacs

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1

Background on GMRES

To solve $Ax = b$ with initial guess $x_0 = 0$, at the k -th iteration GMRES minimizes the norm of residual

$$\|r_k\| = \min_{x \in \mathcal{K}_k(A, b)} \|Ax - b\|$$

in the space

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

From [Drkosova et al. 1995; Paige, Miroslav, and Strakoš 2006], the recommended stopping criterion is the backward error

$$\eta_{A,b}(x_k) = \min_{\Delta A, \Delta b} \{\tau > 0 : \|\Delta A\| \leq \tau \|A\|, \|\Delta b\| \leq \tau \|b\| \text{ and } (A + \Delta A)x_k = b + \Delta b\}$$

$$\eta_{A,b}(x_k) = \frac{\|Ax_k - b\|}{\|A\|_2 \|x_k\| + \|b\|}$$

Denoting by u the unit roundoff of the working precision for solving the linear system $Ax = b$, then

Householder-GMRES [Drkosova et al. 1995]

Under technical assumptions [Drkosova et al. 1995, Corollary 4.2], it is shown that the normwise backward error at the last iterate x_n of Householder-GMRES is such that $\eta_{A,b}(x_n) = \mathcal{O}(u)$.

MGS-GMRES [Paige, Miroslav, and Strakoš 2006]

If $\sigma_{\min}(A) \gg n^2 \|A\| u$, then normwise backward error at the k -th iterate x_k of MGS-GMRES is such that $\eta_{A,b}(x_k) = \mathcal{O}(u)$, where $k \in \mathbb{N}$ is the first integer such that $\kappa_2(\tilde{V}_{k+1}) > 4/3$.

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δ -componentwise
perturbation

δ -componentwise storage model

Denoting by u the unit roundoff of the working precision,

Standard IEEE model [Higham 2002]

$$fl(x \text{ op } y) = (x \text{ op } y)(1 + \varepsilon)$$

with $|\varepsilon| \leq u$ and $\text{op} \in \{+, -, \times, \div\}$.

δ -componentwise storage

$$\delta\text{-storage}(x) = x(1 + \xi)$$

with $|\xi| \leq \delta$.

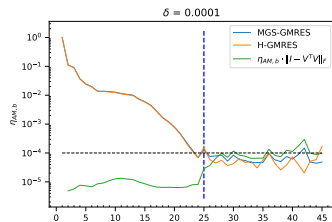
δ -representation

$$fl_{\delta}(x \text{ op } y) = \delta\text{-storage}(fl(x \text{ op } y)) = (x \text{ op } y)(1 + \varepsilon + \xi)$$

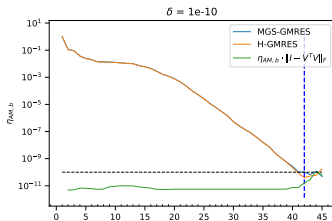
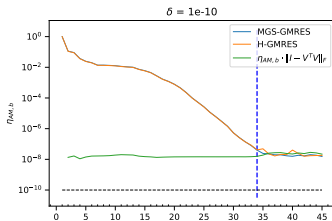
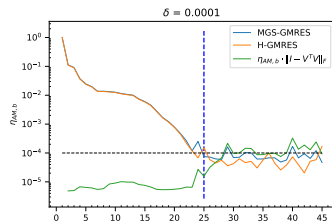
with $|\varepsilon| \leq u$, $|\xi| \leq \delta$ and $\text{op} \in \{+, -, \times, \div\}$.

Numerical experiments δ -componentwise perturbation

fp32



fp64



The variable accuracy approach reveals the dominating error part.

3

δ -normwise perturbation

Length n vectors are stored in compressed format with δ -normwise representation

δ -normwise representation

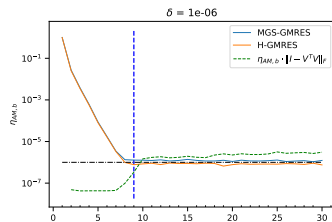
Any vector $z \in \mathbb{R}^n$ is replaced by $\bar{z} \in \mathbb{R}^n$ such that

$$\frac{\|z - \bar{z}\|}{\|z\|} \leq \delta.$$

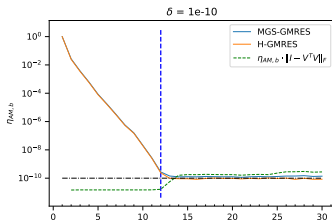
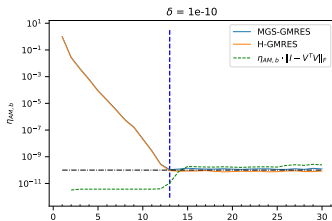
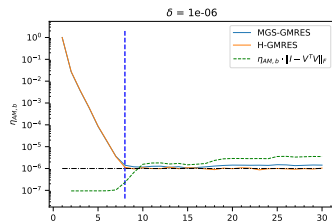
Remark

The technical details of the theoretical backward stability results in [Drkosova et al. 1995; Paige, Miroslav, and Strakoš 2006] do not readily apply.

δ -componentwise



δ -normwise



The δ -componentwise and δ -normwise perturbation lead to similar results.

4

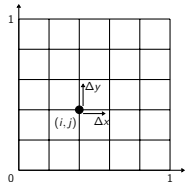
Tensor linear systems

The problem

$$\begin{cases} \mathcal{L}(u) = f & \text{in } \Omega \\ u = f_0 & \text{in } \partial\Omega \end{cases}$$

for $\Omega \subseteq \mathbb{R}^{n_1 \times \dots \times n_d}$.

$\xrightarrow{\text{discretization}}$



$$\mathbf{Ax} = \mathbf{b}$$

where $\mathbf{A} : \mathbb{R}^{n_1 \times \dots \times n_d} \rightarrow \mathbb{R}^{n_1 \times \dots \times n_d}$ is a multilinear operator and $\mathbf{b} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ a tensor.

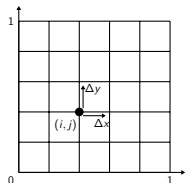
- Curse of dimensionality
- TT-formalism [Oseledets 2011]

The problem

$$\begin{cases} \mathcal{L}(u) = f & \text{in } \Omega \\ u = f_0 & \text{in } \partial\Omega \end{cases}$$

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→
discretization



$$\mathbf{Ax} = \mathbf{b}$$

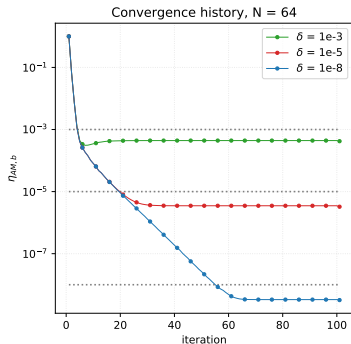
where $\mathbf{A} : \mathbb{R}^{n_1 \times \dots \times n_d} \rightarrow \mathbb{R}^{n_1 \times \dots \times n_d}$ is a multilinear operator and $\mathbf{b} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ a tensor.

- Curse of dimensionality
- Memory cost growing with iterations
- TT-formalism [Oseledets 2011]
- TT-rounding [Oseledets 2011]

TT-representation at accuracy δ

For every TT-vector $\mathbf{z} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ we compress it getting $\bar{\mathbf{z}} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ such that

$$\frac{\|\mathbf{z} - \bar{\mathbf{z}}\|}{\|\mathbf{z}\|} \leq \delta.$$



Convection-Diffusion problem

$$\begin{cases} -\Delta \mathbf{u} + \mathbf{v} \cdot \nabla \mathbf{u} & = 0 \\ \mathbf{u}|_{\{y=1\}} & = 1 \end{cases} \quad \text{in} \quad \Omega = [-1, 1]^3$$

5

Parameter dependent
tensor linear system

Let the parametric convection-diffusion problem be

$$\begin{cases} -\alpha \Delta \mathbf{u} + \mathbf{v} \cdot \nabla \mathbf{u} & = 0 \\ \mathbf{u}|_{\{y=1\}} & = 1 \end{cases} \quad \text{in } \Omega = [-1, 1]^d \text{ and } \alpha \in [1, 10]$$

Solve independently p tensor linear systems of order d

$$\mathbf{A}_{\alpha_i} \mathbf{x}_{\alpha_i} = \mathbf{b}_{\alpha_i}$$

$$\forall \alpha_i \in \{\alpha_1, \dots, \alpha_p\}.$$

Solve once the tensor linear system $\mathbf{A} \mathbf{x} = \mathbf{b}$ of order $(d + 1)$

$$\begin{bmatrix} \mathbf{A}_{\alpha_1} & & \\ & \ddots & \\ & & \mathbf{A}_{\alpha_p} \end{bmatrix} \begin{bmatrix} \mathbf{x}^{[\alpha_1]} \\ \vdots \\ \mathbf{x}^{[\alpha_p]} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{\alpha_1} \\ \vdots \\ \mathbf{b}_{\alpha_i} \end{bmatrix}$$

What is the numerical quality of $\mathbf{x}^{[\alpha_i]}$ slice of \mathbf{x} solution of the $(d + 1)$ tensor linear system and by construction the solution of the problem $\mathbf{A}_{\alpha_i} \mathbf{x}_{\alpha_i} = \mathbf{b}_{\alpha_i}$?

Let the backward error of the $(d + 1)$ system $\mathbf{Ax} = \mathbf{b}$ be

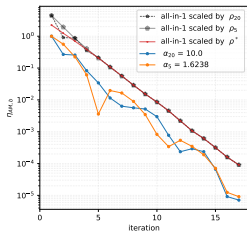
$$\eta_{\mathbf{A},\mathbf{b}}(\mathbf{x}) = \frac{\|\mathbf{b} - \mathbf{Ax}\|}{\|\mathbf{A}\|_2\|\mathbf{x}\| + \|\mathbf{b}\|}.$$

Let $\mathbf{A}_i, \mathbf{b}_i$ be the multilinear operator and the right-hand side of the parametric problem for the parameter value α_i , then define

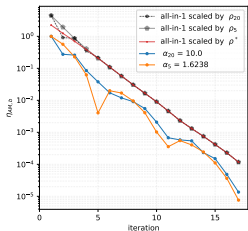
$$\eta_{\mathbf{A}_i,\mathbf{b}_i}(\mathbf{x}^{[i]}) = \frac{\|\mathbf{b}_i - \mathbf{A}_i\mathbf{x}^{[i]}\|}{\|\mathbf{A}_i\|_2\|\mathbf{x}^{[i]}\| + \|\mathbf{b}_i\|}$$

with $\mathbf{x}^{[i]}$ denotes the i -th slice of \mathbf{x} on the parameter mode for $i \in \{1, \dots, p\}$. Then we prove that

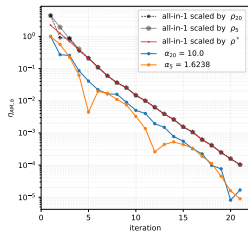
$$\eta_{\mathbf{A},\mathbf{b}}(\mathbf{x}) \rho_i(\mathbf{x}) \geq \eta_{\mathbf{A}_i,\mathbf{b}_i}(\mathbf{x}^{[i]}) \quad \text{where} \quad \rho_i(\mathbf{x}) = \frac{\|\mathbf{A}\|_2\|\mathbf{x}\| + \sqrt{p}}{\|\mathbf{A}_i\mathbf{x}^{[i]}\| + 1}.$$



(I) $n = 63$



(J) $n = 127$



(K) $n = 255$

Figure: 4-d Parametric convection diffusion $\eta_{AM,b}$ bound using $\delta = \varepsilon = 10^{-5}$ and $p = 20$ uniformly logarithmically distributed parameter values $\alpha_i \in [1, 10]$.

- Backward stability of GMRES holds numerically [Inria RR-9483] when data are stored with
 - > componentwise perturbation
 - > normwise perturbationboth have practical implementations, for example SZ lossy compressor [S. Di, F. Cappello at Argonne National Lab]
- GMRES in Tensor Train format with TT-rounding seems to be backward stable [Inria RR-9484]
- Special parameter dependent problems of order d can be solved at once through an order $(d + 1)$ problem, guaranteeing backward stable bounds linking the $(d + 1)$ and d solutions [Inria RR-9484]

Thanks for the attention.

Questions?

If \mathbf{M} is a preconditioner, the previous stopping criterion gets

$$\eta_{AM,b}(\mathbf{t}_k) = \frac{\|\mathbf{AMt}_k - \mathbf{b}\|}{\|\mathbf{AM}\|_2 \|\mathbf{t}_k\| + \|\mathbf{b}\|} \quad \text{and} \quad \mathbf{x}_k = \mathbf{Mt}_k.$$

Another possible one based just on the right-hand side is

$$\begin{aligned} \eta_b(\mathbf{x}_k) &= \min_{\Delta A, \Delta b} \{ \tau > 0 : \|\Delta b\| \leq \tau \|b\| \text{ and } A\mathbf{x}_k = b + \Delta b \} \\ &= \frac{\|\mathbf{Ax}_k - \mathbf{b}\|}{\|\mathbf{b}\|}. \end{aligned}$$