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Reducing the memory footprint in Krylov methods through lossy compression

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Overview

▶ Introduction

- Krylov methods & inexactness
- Mixed precision & compression

▶ Preliminary results

- Some theory
- Some experiments

▶ Outlook

Introduction

- ▶ Krylov methods & inexactness
- ▶ Mixed precision & compression

Krylov methods

We want to solve

$$Ax = b$$

with $A \in \mathbb{R}^{n \times n}$ and $x, b \in \mathbb{R}^n$.

Krylov methods:

- ▶ Very efficient when A is large and sparse.
- ▶ Typically require 1 matrix-vector multiplication with A and/or A^T per iteration.
- ▶ Construct a Krylov subspace

$$\mathcal{K}_k(A, r_0) = \{r_0, Ar_0, A^2r_0, \dots, A^{k-1}r_0\},$$




with $r_0 = b - Ax_0$ and $x_k \in x_0 + \mathcal{K}_k(A, r_0)$.

Inexact matvec

What happens if the matrix-vector product is not calculated accurately?

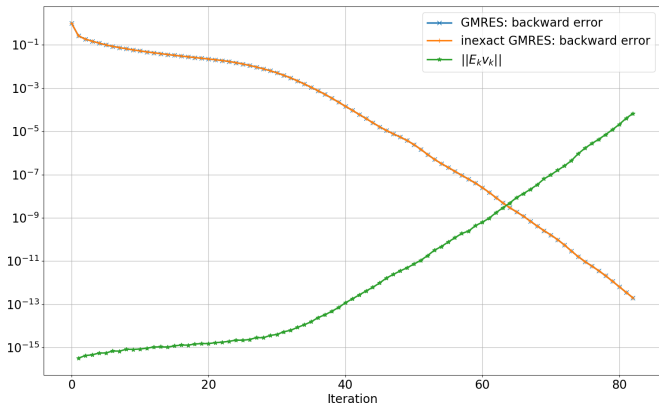
$$z_k = Av_k \quad \longleftrightarrow \quad \begin{cases} z_k = Av_k + p_k \\ z_k = (A + E_k)v_k \end{cases}$$

Recent results:

-  **A. Bouras and V. Frayssé**, *Inexact matrix-vector products in Krylov methods for solving linear systems: a relaxation strategy*, SIAM journal on matrix analysis and applications (2005).
-  **V. Simoncini and D. B. Szyld**, *Theory of inexact Krylov subspace methods and applications to scientific computing*, SIAM journal on scientific computing (2003).
-  **L. Giraud, S. Gratton and J. Langou**, *Convergence in backward error of relaxed GMRES*, SIAM journal on scientific computing (2007).

An example ...

- ▶ $A \in \mathbb{R}^{225 \times 225}$ is PDE225 matrix, $x = (1, \dots, 1)^T \in \mathbb{R}^{225}$.
- ▶ Stopping criterion: $\eta_{A,b}(x_k) = \frac{\|b - Ax_k\|}{\|A\| \|x_k\| + \|b\|} \leq \varepsilon = 1e-12$.






Mixed precision – method I

Method: perform part of the computation in 32 bit or 16 bit, while still achieving full accuracy for the reconstruction.

- ▶ Exploit faster 32 bit & 16 bit calculations on modern hardware.
- ▶ Often it is the preconditioner that is calculated in lower precision.

Recent results:

-  **A. Buttari et al**, *Mixed precision iterative refinement techniques for the solution of dense linear systems*, International journal of high performance computing applications (2007).
-  **M. Arioli and I. S. Duff**, *Using FGMRES to obtain backward stability in mixed precision*, Electronic transactions on numerical analysis (2009).
-  **E. Carson and N. J. Higham**, *Accelerating the solution of linear systems by iterative refinement in three precisions*, MIMS EPrint (2017).

Mixed precision – method II

method: store part of the data in lower precision, while still achieving full accuracy for the reconstruction.

- ▶ Calculations are done in **full precision**.
- ▶ Less communication and lower memory requirements.
- ▶ Read/write operations consume more energy than computations.

Recent results:

- 📄 H. Antz et al., *Adaptive precision in block-Jacobi preconditioning for iterative sparse linear system solvers*, MIMS EPrint (2017).

Why limit ourselves to 64 bit, 32 bit, 16 bit, etc?



Use data compression techniques

The SZ compressor

developed @ Argonne et al.

Lossy compression technique:

- ▶ Higher compression factors than lossless techniques.
- ▶ Designed to deal with irregular data and spiky changes.
- ▶ Compression error can be controlled:
absolute error, relative error or point-wise relative error.

📄 **D. Tao et al.**, *Significantly improving lossy compression for scientific data sets based on multidimensional prediction and error-controlled quantization*, IEEE IPDPS (2017).

📄 <https://github.com/disheng222/SZ>

Project goal:

Incorporate the SZ compressor into a Krylov method in order to reduce the memory and communication costs.

Preliminary results

- ▶ Some theory
- ▶ Some experiments

GMRES

inexact vs. compression

The GMRES algorithm revolves around the Arnoldi-relation

$$AV_k = V_{k+1}H_k.$$

Here $V_k \in \mathbb{R}^{n \times k}$, $V_k^T V_k = I_k$, $\text{span } V_k = \mathcal{K}_k(A, r_0)$, $H_k \in \mathbb{R}^{(k+1) \times k}$ is upper Hessenberg and

$$x_k = x_0 + V_k y_k \quad \text{with} \quad y_k = \arg \min_{y \in \mathbb{R}^k} \left\| \|r_0\| - H_k y \right\|.$$

► **inexact GMRES:**

$$\rightarrow z = (A + E_k)v_k$$

$$\rightarrow A\tilde{V}_k = \tilde{V}_{k+1}\tilde{H}_k$$

→ **still GMRES**

► **compressed GMRES:**

→ compress v_k at some point

→ $z \perp$ the compressed v_k ???

→ **no Arnoldi relation ...**

GMRES: Arnoldi part

1: $v_1 = r_0 / \|r_0\|$

2: **for** $k = 1, 2, \dots$ **do**

3: $z = Av_k$

4: $z \leftarrow \text{Arnoldi}(V_k)$.

5: $v_{k+1} = z / \|z\|$

6: **end for**

FGMRES = GMRES with varying right preconditioner M_k^{-1}

Different Arnoldi-relation:

$$AZ_k = V_{k+1}H_k.$$

Here $V_k \in \mathbb{R}^{n \times k}$, $V_k^T V_k = I_k$, $Z_k \in \mathbb{R}^{n \times k}$, $H_k \in \mathbb{R}^{(k+1) \times k}$ is upper Hessenberg and


$$x_k = x_0 + Z_k y_k \quad \text{with} \quad y_k = \arg \min_{y \in \mathbb{R}^k} \left\| \|r_0\| - H_k y \right\|.$$

- ▶ $\text{span } V_k \neq \mathcal{K}_k(A, r_0)$.
- ▶ Not a Krylov method.
- ▶ z_k can in theory be random.

FGMRES: Arnoldi part

- 1: $v_1 = r_0 / \|r_0\|$
 - 2: **for** $k = 1, 2, \dots$ **do**
 - 3: $z_k = M_k^{-1} v_k$
 - 4: $w = AZ_k$
 - 5: $w \leftarrow \text{Arnoldi}(V_k)$.
 - 6: $v_{k+1} = z / \|z\|$
 - 7: **end for**
-

FGMRES

-  Y. Saad, *A flexible inner-outer preconditioned GMRES algorithm*, SIAM journal on scientific computing (1993).
- ▶ Allows iterative methods to be used as preconditioners.
 - ▶ **Is not guaranteed to converge.**
 - ▶ **Double the memory:** Z_k and V_{k+1}

z_k are not orthogonal \Rightarrow compress z_k instead of v_k .

If compressed FGMRES converges within the same number of iterations, then we gain in memory.

Assumptions & compression model

- ▶ Assume that FGMRES converges with the preconditioners

$$\left\{ M_k^{-1} \right\}_{k=1}^n$$

- ▶ Let ε_k be the maximum relative point-wise error.

We introduce an error after applying the preconditioner M_k^{-1} :

$$z_k = M_k^{-1} v_k \quad \longleftrightarrow \quad \tilde{z}_k = (I + \text{diag}(\delta_k)) z_k = (I + \text{diag}(\delta_k)) M_k^{-1} v_k$$

with $|(\delta_k)_i| \leq \varepsilon_k$, for $i = 1, \dots, n$

- ▶ Still FGMRES, but with the preconditioners

$$\left\{ (I + \text{diag}(\delta_k)) M_k^{-1} \right\}_{k=1}^n$$

Compressed FGMRES

Compressed Arnoldi-relation:

$$A\tilde{Z}_k = \tilde{V}_{k+1}\tilde{H}_k$$

→ optimization in a different subspace of \mathbb{R}^n !!!

If

$$\tilde{y}_k = \arg \min_{\tilde{y} \in \mathbb{R}^k} \|r_0 - A\tilde{Z}_k\tilde{y}\| \quad \text{and} \quad y_k = \arg \min_{y \in \mathbb{R}^k} \|r_0 - AZ_k y\|$$

then

$$\underbrace{\|r_0 - A\tilde{Z}_k\tilde{y}_k\|}_{\text{compressed residual}} \leq \underbrace{\|r_0 - AZ_k y_k\|}_{\text{exact residual}} + \underbrace{\|A[\text{diag}(\delta_1)z_1, \dots, \text{diag}(\delta_k)z_k] y_k\|}_{\text{residual gap}}$$

How large can ε_k become such that $\eta_{A,b}(\tilde{x}_k) \leq \varepsilon$?

Bounding ε_k

For some targeted tolerance ε and $c \in]0, 1[$ we know that there exists a k such that

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

Result:

If, for all $i = 1, \dots, k$,

$$\varepsilon_i \leq (1 - c) \frac{\sigma_{\min}(H_k)}{k^2 \|A\|} \frac{\|b\|}{\|r_{i-1}\|} \varepsilon \quad (1)$$

then

$$\eta_{A,b}(\tilde{x}_k) = \frac{\|b - A\tilde{x}_k\|}{\|A\| \|\tilde{x}_k\| + \|b\|} \leq \varepsilon$$

Some practical bounds

- ▶ (1) contains values that are not available.
- ▶ (1) is a very conservative bound.
- ▶ Consider the relaxed bounds:

$$\varepsilon_i \leq (1 - c) \frac{\sigma_{\min}(A)}{k^2 \|A\|} \frac{\|b\|}{\|\tilde{r}_{i-1}\|} \varepsilon \quad (\text{b1})$$

$$\varepsilon_i \leq (1 - c) \frac{1}{\|A\|} \frac{\|b\|}{\|\tilde{r}_{i-1}\|} \varepsilon \quad (\text{b2})$$

$$\varepsilon_i \leq (1 - c) \frac{\|b\|}{\|\tilde{r}_{i-1}\|} \varepsilon \quad (\text{b3})$$

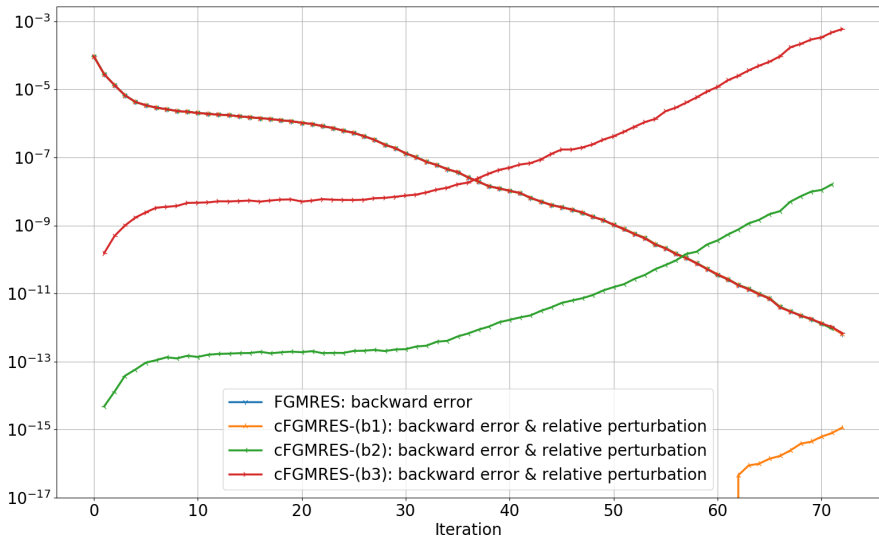
Numerical experiments

- ▶ FMGRES-GMRES(25)
- ▶ Outer stopping criterium: $\eta_{A,b}(x_k) \leq 1e-12$ and $\text{maxit} \leq 256$.
- ▶ Inner stopping criterium: $\eta_{A,v_k}(z_k) \leq 1e-4$ and $\text{maxit} \leq 50$.

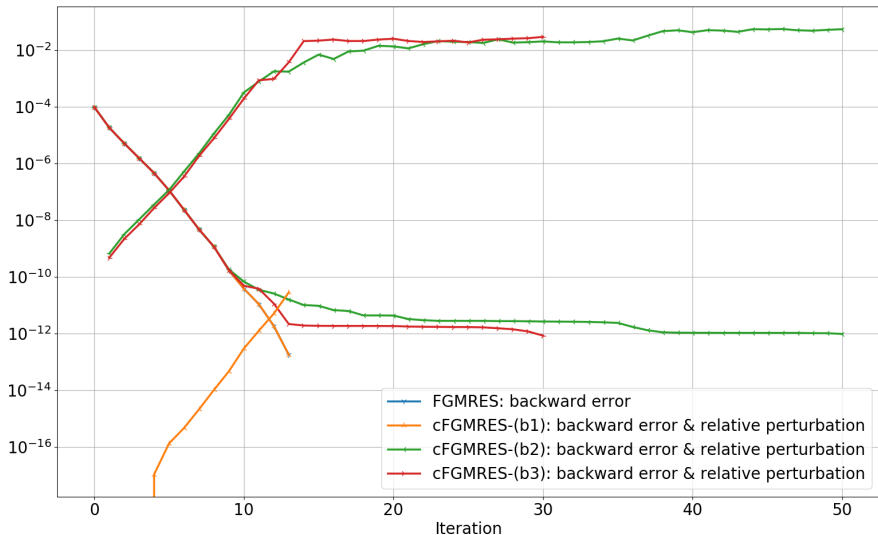
Matrix	n	FGMRES	cFGMRES-(b1)			cFGMRES-(b2)		cFGMRES-(b3)	
pde225	225 × 225	3	3	5.5e-11	3	1.4e-5	3	1.6e-4	
e05r0000	236 × 236	11	11	2.1e-11	11	3.2e-3	11	3.6e-2	
orsirr_1	1030 × 1030	33	33	2.3e-15	33	2.4e-11	33	1.2e-5	
1138_bus	1138 × 1138	72	72	1.1e-15	71	1.6e-8	72	5.9e-4	
cavity05	1182 × 1182	22	22	3.8e-13	22	1.6e-3	24	3.0e-2	
fidap003	1821 × 1821	136	136	0.0	136	4.0e-10	194	9.8e-3	
watt_1	1856 × 1856	138	138	2.9e-16	138	8.8e-2	138	8.7e-2	
bwm2000	2000 × 2000	31	31	6.6e-14	31	8.1e-9	32	2.5e-3	
olm2000	2000 × 2000	113	113	6.8e-15	115	4.1e-9	190	3.0e-3	
add20	2395 × 2395	13	13	2.9e-11	50	5.5e-2	19	2.9e-2	

Matrices taken from matrix market and $x = (1, \dots, 1)^T \in \mathbb{R}^n$.

Results for 1138_bus



Results for add2o



Outlook

Outlook

Done:

- ▶ Theoretical framework for the size of the compression.
- ▶ Initial numerical experiments.
- ▶ A compressor.

To be done:

- ▶ Combine the theoretical results with the compressor.
- ▶ Study the gain in memory & speedup.
- ▶ Empirical generalizations:
 - Compression of blocks.
 - Restarting strategies.
 - ...

Is this the end ...

Thank you for your attention.

Any questions?