Randomized Orthogonal Projection Methods for Krylov solvers

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Preliminaries

ROPMs

Short recurrence orthonormalization

arCG

Conclusion
Introduction to Krylov solvers

**Krylov solvers** A mathematical setting describing several iterative methods.

Define linear system of equations with first guess $x_0 \in \mathbb{R}^n$

$$Ax = b, \quad A \in \mathbb{R}^{n \times n}, \quad b \in \mathbb{R}^n$$

Seek solution in the **Krylov subspace**, $r_0 = b - Ax_0$

$$\mathcal{K}_k(A, r_0) = x_0 + \text{Span} \langle r_0, Ar_0, \ldots, A^{k-1}r_0 \rangle$$
Designing a Krylov solver

For all $k \leq n$, find $x_k \in \mathcal{K}_k(A, r_0)$ that \textbf{minimizes some measure of the error} $x - x_k$

\textbf{Example} : Choose $x_k = \arg \min_{y \in \mathcal{K}_k(A, r_0)} \| x - y \|_2$

Reformulate with the \textbf{residual} $r_k = b - Ax_k$

\[ x_k = \arg \min_{y \in \mathcal{K}_k(A, r_0)} \| x - y \|_2 \iff r_k \perp A\mathcal{K}_k(A, r_0) \]

(a) Some Krylov design

(b) Equivalent formulation
Mathematical formulation

We’ve designed a Krylov solver. An iterative method producing \((x_k)_k\) s.t:

1. \(\forall k, \ x_k \in \mathcal{K}_k(A, r_0)\) (subspace condition)
2. \(\forall k, \ r_k \perp \mathcal{L}_k\), with \(\mathcal{L}_k\) some \(k\)-dimensional vector subspace (Petrov-Galerkin condition)

Examples [6]:

- **CG**: \(r_k \perp \mathcal{K}_k(A, r_0) \iff x_k = \arg \min_{y \in \mathcal{K}_k(A, r_0)} \|x - y\|_A\)
- **GMRES**: \(r_k \perp A\mathcal{K}_k(A, r_0) \iff x_k = \arg \min_{y \in \mathcal{K}_k(A, r_0)} \|b - Ay\|_2\)
A problem arises

How to enforce the Petrov-Galerkin condition?

\[ P_{L_k}(b - Ax_k) = 0 \iff (P_{L_k}A)x_k = (P_{L_k}b) \quad (x_k \in K_k(A, r_0)) \]

Usually requires access to bases of \( L_k \) and of \( K_k(A, r_0) \). For numerical stability, these bases should be well conditioned. Not the case of \( \{r_0, Ar_0, \ldots, A^{k-1}r_0\} \)!

\[ \implies \quad \text{Proceed with a subsequent orthonormalization process of these bases.} \]

**Dilemma**: often the most expensive part of the solver (typical asymptotic cost is \( O(nk^2) \) flops)
Introduction to randomization

**Randomization?** A dimension reduction technique that approximates geometry of a vector-subspace \( \mathcal{V}_k \subset \mathbb{R}^n, k \ll n \).

We say that a linear mapping \( \Omega : \mathbb{R}^n \rightarrow \mathbb{R}^\ell \) is an \( \epsilon \)-embedding of \( \mathcal{V}_k \) if and only if

\[
\forall x \in \mathcal{V}_k, \quad (1 - \epsilon)\|x\|_2^2 \leq \|\Omega x\|_2^2 \leq (1 + \epsilon)\|x\|_2^2
\]  

(1)

see [8]. Due to parallelogram identity, eq. (1) is equivalent to

\[
\forall x, y \in \mathcal{V}_k, \quad |\langle \Omega x, \Omega y \rangle - \langle x, y \rangle| \leq \epsilon\|x\|_2\|y\|_2
\]

Typical \( \epsilon = \frac{1}{2} \). Designed to preserve orders of magnitude, not to be a fine approximation.
An analogy with projections (1)

(a) Enough to guess geometry...   (b) ...but can be misleading!

Figure: Good and bad projections
An analogy with projections (2)

Figure: A set of high-dimensional vectors projected in $\mathbb{R}^3$ (*diadema urchin*)
Oblivious subspace embeddings

Oblivious subspace embedding with parameters $\epsilon, k, \delta$: a linear mapping $^3 \Omega : \mathbb{R}^n \rightarrow \mathbb{R}^\ell$ such that, for any $k$-dimensional subspace $\mathcal{V}_k$, it is an $\epsilon$-embedding of $\mathcal{V}_k$ with probability at least $1 - \delta$ (see [8]).

Examples:

- Gaussian OSE: Independent $\Omega_{i,j} \sim \mathcal{N}(0, \sqrt{\ell^{-1}}), \ 1 \leq j \leq \ell$.
  Dense matrix.

- SRHT OSE: Independent $\ell$ rows sampling of $HD$ where $H \in \mathbb{R}^{n \times n}$ is Hadamard transform and $D$ is random cheap rotation. Fast transform, but not suited for distributed computing [9]

$\ell$: the sampling size. The more successful and fine we want $\Omega$, the greater the sampling size. Typical $\ell = 5k$.

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$^3$The theory is simplified here
Some new notions

Let $\Omega : \mathbb{R}^n \to \mathbb{R}^\ell$ an $\epsilon$-embedding for vector subspace $\mathcal{V}_k$. Let $\mathcal{V}_p \subset \mathcal{V}_k$ a vector subspace.

- We say that $\nu_1, \cdots, \nu_p \in \mathcal{V}_p$ are a sketch orthonormal basis of $\mathcal{V}_p$ if and only if they are a basis of $\mathcal{V}_p$ and verify

\[
\forall i, j \in \{1, \cdots, p\}, \quad \langle \Omega \nu_i, \Omega \nu_j \rangle = \delta_{i,j} \quad \left(\text{Cond}(\mathcal{V}_p) \leq \sqrt{\frac{1 + \epsilon}{1 - \epsilon}}\right)
\]

- We say that $z \perp^\Omega \mathcal{V}_p$ if and only if

\[
\forall x \in \mathcal{V}_p, \quad \langle \Omega z, \Omega x \rangle = 0
\]

- We define the sketch orthogonal projector from $\mathcal{V}_k$ onto $\mathcal{V}_p$ as

\[
\mathcal{P}_{\mathcal{V}_p}^\Omega : \begin{cases} 
\mathcal{V}_k & \to & \mathcal{V}_p \\
x & \mapsto & \arg\min_{y \in \mathcal{V}_p} \|\Omega(x - y)\|_2^2
\end{cases}
\]
Problem identified

Replace the orthogonalization step of Krylov solvers by sketch-orthogonalization step?

What has been done:

- Randomized Gram-Schmidt [2] and block version [1]: Half the flops of modified Gram-Schmidt (MGS), with similar stability.
- Applied to GMRES [2], same convergence rate, stable.
- Applied to eigenvalue solvers [5]

The case $r_k \perp_{\Omega} A K_k(A, r_0)$ is now well documented. What about $r_k \perp_{\Omega} K_k(A, r_0)$?

Considered in [3, 4], but still no error minimizing characterization.
Randomized Orthogonal Projection Method over the Krylov subspace (ROPM) : an iterative algorithm producing $(x_k)_k$ s.t.:

1. $\forall k, x_k \in \mathcal{K}_k(A, r_0)$ (subspace condition)
2. $\forall k, r_k \perp \Omega \mathcal{K}_k(A, r_0)$ (sketched Petrov-Galerkin condition)
The following algorithm is an ROPM.

**Input:** Matrix $A \in \mathbb{R}^{n \times n}$, vector $b \in \mathbb{R}^n$, $\epsilon$-embedding $\Omega \in \mathbb{R}^{\ell \times n}$ of $\mathcal{K}_{k_{\max}}$, $k_{\max} < \ell \ll n$, first guess $x_0$

**Output:** Approximation $x_k \in \mathcal{K}_k (A, r_0)$ of solution to $Ax = b$.

1. $r_0 \leftarrow b - Ax_0$
2. Compute $\Omega r_0$
3. $v_1 \leftarrow \|\Omega r_0\|^{-1} r_0$
4. Compute/deduce $\Omega v_1$
5. while $k \leq k_{\max}$ and $\|\Omega r_k\| > \eta$ do
6.     $w \leftarrow A v_k$
7.     Compute $\Omega w$
8.     $(h_{i,k})_{1 \leq i \leq k} \leftarrow (\Omega V_k)^t \Omega w$ where $V_k$ is the matrix formed by $v_1, \ldots, v_k$
9.     $w \leftarrow w - V_k (h_{i,k})_{1 \leq i \leq k}$
10.    Compute/deduce $\|\Omega w\|$
11.    $h_{k+1,k} \leftarrow \|\Omega w\|$
12.    $w \leftarrow h_{k+1,k}^{-1} w$
13.    $v_{k+1} \leftarrow w$
14.    Compute/deduce $\Omega v_{k+1}$
15.    $x_k \leftarrow x_0 + H_k^{-1} (\Omega V_k)^t \Omega r_0$, where $H_k = (h_{i,j})_{1 \leq i \leq k}$, $1 \leq j \leq k$
16.    $k \leftarrow k + 1$
17. return $x_k$

**Algorithm 0:** RFOM, a.k.a Randomized Arnoldi
Is the sketched Petrov-Galerkin condition met?

This algorithm builds sketch orthonormal vectors $v_1, v_2 \cdots$ s.t:

$$\forall k, \ h_{k+1,k}v_{k+1} = Av_k - \langle \Omega Av_k, \Omega v_1 \rangle v_1 - \cdots \langle \Omega Av_k, \Omega v_k \rangle$$

We get the randomized Arnoldi relation:

$$\forall k, \ AV_k = V_{k+1}H_{k+1,k}, \ (\Omega V_k)^t\Omega V_k = I_k, \ H_{k+1,k} = (h_{i,j})_{1 \leq i \leq k+1, 1 \leq j \leq k}$$

Using the sketch orthogonality, we get $H_k = (\Omega V_k)^t\Omega AV_k$. Finally,

$$r_k \perp^\Omega K_k(A, r_0) \iff (\Omega V_k)^t\Omega r_k = 0_k \iff x_k = x_0 + H_k^{-1}(\Omega V_k)^t\Omega r_0$$
Figure: Easy problem

This is the desired behavior.
Some testing (2)

(a) Reasonably difficult system, $\text{Cond}(A) \approx 4000$

(b) Harder system, $\text{Cond}(P^{-1}A) \approx 10^5$

(c) Even harder, $\text{Cond}(P^{-1}A) \approx 10^9$

Figure: Convergence of ROPM

Similar convergence rate overall.

Apparition of spikes of the randomized error. Are they random?
Straightforward bound

Using the $\epsilon$-embedding property straightforwardly:

Proposition

Let $\Omega \in \mathbb{R}^{\ell \times n}$ be an $\epsilon$-embedding of $K_{k+1} + \text{Span}\langle x \rangle$, with $\epsilon \leq \text{cond}(A)^{-\frac{1}{2}}$. Assume that $A$ is positive-definite. Then the estimate $x_k \in K_k$ produced by ROPM and $\tilde{x}_k \in K_k$ produced by standard OPM satisfy

$$
\|x - x_k\|_A \leq \frac{1 + \epsilon \text{cond}(A)^{\frac{1}{2}}}{1 - \epsilon \text{cond}(A)^{\frac{1}{2}}} \|x - \tilde{x}_k\|_A.
$$

Pessimistic bound. Not well-defined for ill-conditioned systems. Doesn’t describe the spikes.
Isolating the spikes

(a) Spectrum of randomly generated symmetric matrix

(b) Early convergence

Figure: Spike study

Spikes seem related to the properties of the system after all.
Our main contribution

**Theorem**
Assume that $A$ is positive-definite. We have

$$\|x - x_k\|_A \leq \left(1 + \alpha_k^2 \beta_k^2\right)^{\frac{1}{2}} \|x - \tilde{x}_k\|_A,$$

where $x_k \in \mathcal{K}_k$ and $\tilde{x}_k \in \mathcal{K}_k$ are the sketched and the classical Petrov-Galerkin projections, respectively, and

$$\alpha_k := \frac{\langle x - \tilde{x}_{k-1}, \mathcal{P}_{\mathcal{K}_k}^\Omega A\tilde{v}_k \rangle}{\langle x - \tilde{x}_{k-1}, \mathcal{P}_{\mathcal{K}_k} A\tilde{v}_k \rangle},$$

$$\beta_k := \|A^{-\frac{1}{2}} \mathcal{P}_{\mathcal{K}_k}^\Omega \tilde{v}_{k+1}\| \langle \tilde{v}_{k+1}, A\tilde{v}_k \rangle \frac{\langle \tilde{v}_k, \tilde{x}_k \rangle}{\|x - \tilde{x}_k\|_A},$$

and where $\tilde{v}_k$ is a unit vector spanning the range of $(I - \mathcal{P}_{\mathcal{K}_{k-1}})\mathcal{P}_{\mathcal{K}_k}$. 
Numerical testing

Figure: RFOM convergence for the shifted $Si_{41}Ge_{41}H_{72}$ system.

Fine bound. Truthful to the spikes.
Indirect bound

Proposition

If $x_k \in \mathcal{K}_k$ satisfies the sketched Petrov-Galerkin condition, and if $\tilde{x}_k$ satisfies the Petrov-Galerkin condition,

$$\|r_k\|_2 \leq \|\tilde{r}_k\|_2 + \|r_0\| \left| \tilde{s}_{k,1} \right| + \sqrt{\frac{1 + \epsilon}{1 - \epsilon}} |s_{k,1}| .$$

(4)

where $s_{k,1}$ (resp. $\tilde{s}_{k,1}$) denote the product of $h_{k+1,k}$ and the bottom left corner of $H_{k}^{-1}$ (resp ...)

Figure: Indirect residual bound
Future development

(a) Spectra at spike’s iteration 30

(b) Spectra after spike iteration 32

(c) Discrete second derivative of OPM error ($D^2\text{OPM}$)

Figure: Spike study

Is there a synthetic bound, only featuring spectral properties of Hessenberg matrices?

Deflation of the bad Ritz vectors?
Short recurrences

The randomized Arnoldi relation for symmetric system $A$ is not symmetric anymore.

$$\tilde{H}_k = \tilde{V}_k^t A \tilde{V}_k$$ symmetric, but $(\Omega V_k)^t \Omega AV_k \neq (\Omega AV_k)^t \Omega V_k$

Short recurrence is lost

(a) 4096 sampling size

(b) Overall distribution

(c) $\Gamma_{i_0,j_0}$ distribution

Figure: Distribution of $H_k$ (noise above the superdiagonal)
Noise seems Gaussian

Experimentally, Gaussian distributed noise of great magnitude above the superdiagonal.

Empirical implications: not compressible, stable by isometric transformations.

Randomization extended to CG is not trivial.

What happens if we use it anyway?
**Input:** $A \in \mathbb{R}^{n \times n}$ an SPD matrix, $b \in \mathbb{R}^n$, $\eta \in \mathbb{R}^+$, $k_{\text{max}} \in \mathbb{N}^*$, $x_0 \in \mathbb{R}^n$, $\Omega$ an $\epsilon$-embedding of $\mathcal{K}_{k_{\text{max}}}$

**Output:** $x_k$ an estimate of the solution of $Ax = b$

1. $r_0 \leftarrow b - Ax_0$
2. $p_0 \leftarrow r_0$
3. Compute $\Omega r_0$
4. while $\|\Omega r_k\| \geq \eta \|b\|$ and $k \leq k_{\text{max}}$ do
   5. if $k \geq 1$ then
      6. $\delta_k \leftarrow \frac{\|\Omega r_k\|^2}{\|\Omega r_{k-1}\|^2}$
      7. $p_k \leftarrow r_k + \delta p_{k-1}$
   8. Compute $Ap_k$, $\Omega Ap_k$, $\Omega p_k$
   9. $\gamma_k \leftarrow -\frac{\|\Omega r_k\|^2}{\langle \Omega Ap_k, \Omega p_k \rangle}$
10. $x_{k+1} \leftarrow x_k + \gamma_k p_k$
11. $r_{k+1} \leftarrow r_k - \gamma_k Ap_k$
12. Compute $\Omega r_{k+1}$
13. $k \leftarrow k + 1$
14. Return $x_k$

**Algorithm 0:** arCG
An indirect bound

arCG only imposes local orthogonality between $r_k$ and $\mathcal{K}_k(A, r_0)$.

**Proposition**

Assume an $\tilde{\varepsilon}$-embedding property applies to the coefficients $\gamma_k$ and $\delta_k$ computed by arCG. Let $k, d \in \mathbb{N}$ such that $k + d \leq k_{\text{max}}$. Then

$$\|x - x_k\|_A^2 - \|x - x_{k+d}\|_A^2 \leq \frac{1 + \tilde{\varepsilon} + 2\varepsilon}{1 - \varepsilon} \sum_{j=k}^{k+d-1} |\gamma_j|\|\Omega p_j\|_2^2.$$  (5)

**Indirect bound** of the error if we know the algorithm has converged, same as [7]
Experimental testing of arCG

(a) Typical application

(b) Harder problem

(c) Well-conditioned, smooth spectral decay

(d) Ill-conditioned, smooth spectral decay

(e) Well-conditioned, clustered spectral decay

(f) Ill-conditioned, clustered spectral decay
Conclusion

- ROPMs should be considered for solving very ill-conditioned problems that disqualify CG
- Short recurrence sketched orthonormalization is not trivial
- arCG should be considered for solving high dimensional easy problems
- Check our preprint!
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