MA5233 Computational Mathematics

Lecture 10: Krylov Subspace Methods: Algorithms

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Krylov Subspace Methods: Algorithms

Krylov subspace methods

A new class of algorithms for solving linear systems.

Review: LU factorisation for solving $Ax = b$

Good: black-box algorithm.

- Pass A and b, get x with errors close to machine precision without any extra input from user.

Bad: expensive!

- Typically does not scale linearly in the matrix size, even for sparse matrices.

Krylov subspace methods outperform LU factorisation for some important linear systems (when used correctly).

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Problem statement

Given invertible $A \in \mathbb{R}^{N \times N}$ and $b \in \mathbb{R}^N$, find $x \in \mathbb{R}^N$ such that $Ax = b$.

Note that the problem dimension is denoted by N rather than n.

Subspace methods

Given $V \in \mathbb{R}^{N \times n}$, approximate x by

$$\tilde{x} := Vy \qquad \text{where} \qquad y = \arg\min \|AVy - b\|.$$

Terminology: $r := b - A\tilde{x}$ is called the *residual* of $\tilde{x}$.

Krylov subspace methods

Choose $V := \begin{pmatrix} b & Ab & \dots & A^{n-1}b \end{pmatrix} \iff \tilde{x} = \sum_{k=0}^{n-1} y_k \, A^k b$.

The approximate solution $\tilde{x}$ is thus given by

$$\tilde{x} := p_{n-1}(A)\, b \qquad \text{where} \qquad p_{n-1} := \operatorname*{arg\,min}_{p_{n-1} \in \mathcal{P}_{n-1}} \left\| \big(A p_{n-1}(A) - I\big)\, b \right\|$$

and $\mathcal{P}_n := \left\{ p(x) \mid p(x) = \sum_{k=0}^{n} c_k x^k \right\}$.

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Remarks on Krylov subspace methods

- Terminology: Krylov subspace $= \operatorname{span}\{b, Ab, \dots, A^{n-1}b\}$.
- We will discuss pros and cons of Krylov subspaces later.
  For now, let us focus on the *how* rather than the *why*.
- There are several distinct but related Krylov subspace methods.
  For now, we will focus on the Generalised Minimal Residual (GMRES) method, which solves

  $$\tilde{x} := p_{n-1}(A)\, b \qquad \text{where} \qquad p_{n-1} := \operatorname*{arg\,min}_{p_{n-1} \in \mathcal{P}_{n-1}} \big\| \big(A p_{n-1}(A) - I\big)\, b \big\|_2,$$

  i.e. GMRES minimises the two-norm of the residual.

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Implementing GMRES, the bad way

1. Assemble $V := \begin{pmatrix} b & Ab & \dots & A^{n-1}b \end{pmatrix}$.
2. Solve least squares problem $y = \arg\min \|AVy - b\|_2$.
3. Set $\tilde{x} = Vy$.

See `10_krylov_subspace_methods.jl`.

Observation

Algorithm breaks down for $n \gtrsim 8$!
Educated guess: since algorithm works for small n, break-down is likely due to rounding errors.
The following slides will look into this more closely.

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Recap: conditioning of least squares problem

Least-squares problem $\arg\min_x \|Ax - b\|_2$ is well-conditioned if

- columns of A are linearly independent, and
- the angle between $\operatorname{span}(A)$ and b is not too large.

Application to GMRES

Least squares problem to solve is $\arg\min_y \|AVy - b\|_2$.

Observations regarding angle:

- $\operatorname{span}(AV) = \{Ab, \dots, A^n b\}$ and b are prescribed, so there is nothing we can do about the angle between them.
- If angle is large, then least squares problem is ill-conditioned. However, in this case $\tilde{x}$ will be a bad approximation to x anyway; hence we don't care.
- In previous example, angle must be zero since $\dim(V) = N$.
- Conclusion: angle is not responsible for failure.

The following slide studies linear independence of the columns of V.

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Why the naive implementation of GMRES breaks down

Let λ_ℓ, u_ℓ be the eigenvalues and -vectors of A, sorted such that

$$|\lambda_1| \leq |\lambda_2| \leq \ldots \leq |\lambda_N|.$$

Let $b = \sum_{\ell=1}^{N} c_\ell u_\ell$. Then,

$$A^k b = \sum_{\ell=1}^{N} c_\ell \, A^k u_\ell = \sum_{\ell=1}^{N} c_\ell \, \lambda_\ell^k u_\ell.$$

Observation: If $|\lambda_1| < |\lambda_2|$, then $\frac{|\lambda_1|^k}{|\lambda_2|^k}$ vanishes exponentially.

Conclusion:

- $\frac{A^k b}{\|A^k b\|_2}$ approaches u_N for large k.
- Columns of V become almost linearly dependent.
- $\arg\min_y \|AVy - b\|_2$ becomes ill-conditioned.

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Key to stabilising GMRES

Find orthogonal basis for span$\{b, Ab, \ldots, A^{n-1}b\}$.

Such a basis can be found using the following algorithm.

Algorithm 1 Arnoldi iteration

$q_0 = b/\|b\|_2$.
for $k = 0, \ldots, n-1$ **do**
  $\tilde{q}_{k+1} = Aq_k$.
  for $\ell = 0, \ldots, k$ **do**
    $H_{\ell k} = q_\ell^T \tilde{q}_{k+1}$
    $\tilde{q}_{k+1} = \tilde{q}_{k+1} - H_{\ell k} q_\ell$
  end for
  $H_{k+1,k} = \|\tilde{q}_{k+1}\|_2$
  $q_{k+1} = \tilde{q}_{k+1}/H_{k+1,k}$
end for

Following slides list the key properties of this algorithm.

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Lemma (Arnoldi relations)

$$AQ_n = Q_{n+1} H_n$$

where

- $Q_k = \begin{pmatrix} q_0 & \dots & q_{k-1} \end{pmatrix} \in \mathbb{R}^{N \times k}$, and
- $H_n \in \mathbb{R}^{(n+1)\times n}$ is the matrix whose entries are given in the algorithm.

Proof. Rewrite lines 3, 6, 9 in the form

$$H_{k+1,k} q_{k+1} = Aq_k - \sum_{\ell=0}^{k} H_{\ell k} q_\ell,$$

which can be rearranged to

$$Aq_k = H_{k+1,k} q_{k+1} + \sum_{\ell=0}^{k} H_{\ell,k} q_\ell.$$

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Lemma

$$\text{span}\{q_0, \ldots, q_{n-1}\} = \text{span}\{b, Ab, \ldots, A^{n-1}b\}$$

Proof. Show by induction that $q_k = \sum_{\ell=0}^{k} c_\ell A^\ell b$ with $c_k \neq 0$:
Base: $q_0 = b/\|b\|_2 = c_0 A^0 b$.
Induction: We have

$$H_{k+1,k}\, q_{k+1} = Aq_k - \sum_{\ell=0}^{k} H_{\ell,k}\, q_\ell$$

By induction hypothesis, the highest power of A in Aq_k is A^{k+1} while all other terms only go up to A^k.

Lemma

$$q_k^T q_\ell = \delta_{k\ell}$$

Proof. Arnoldi iteration is effectively the Gram-Schmidt orthogonalisation procedure applied to $b, Ab, \ldots, A^{n-1}b$.

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Corollary

$q_0, \ldots, q_{n-1}$ is an orthogonal basis for $\operatorname{span}\{b, Ab, \ldots, A^{n-1}b\}$;
hence $\arg\min_y \|AQy - b\|_2$ is well-conditioned.

Implementing GMRES, the stable way

1. Run Arnoldi iteration to obtain Q_{n+1}, H_n.
2. Solve least squares problem $y = \arg\min \|AQ_n y - b\|_2$
3. Set $\tilde{x} = Q_n\, y$.

Assembling AQ_n is unnecessarily costly.
See next slide for how we can do better.

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The GMRES least squares problem

Least squares problem can be rewritten as

$$\begin{aligned} y &= \arg\min \|AQ_n y - b\|_2 \\ &= \arg\min \|Q_{n+1} H_n y - b\|_2 \\ &= \arg\min \left\| H_n y - Q_{n+1}^T b \right\|_2 \qquad (Q_{n+1} \text{ is orthogonal}) \\ &= \arg\min \left\| H_n\, y - \|b\|_2\, e_1 \right\|_2 \qquad (q_0 = b/\|b\|_2,\ (e_1)_k = \delta_{k1}). \end{aligned}$$

Advantages:

- No more matrix products to assemble least squares matrix.
- $H \in \mathbb{R}^{(n+1)\times n}$ is much smaller than $AQ_n \in \mathbb{R}^{N\times n}$.
- H has special structure: $H_{ij} = 0$ if $i > j+1 \iff H = \begin{pmatrix} x & x & x & x \\ x & x & x & x \\ & x & x & x \\ & & x & x \\ & & & x \end{pmatrix}$.

  Such matrices are called *Hessenberg*.
  QR factorisation of Hessenberg matrix can be computed in $\mathcal{O}(n^2)$ rather than $\mathcal{O}(n^3)$ FLOP.

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Cost of Arnoldi iteration

- Line 3: n matrix-vector products.
- Lines 5, 6: $\mathcal{O}\left(Nn^2\right)$ FLOP.
  - $\mathcal{O}(N)$ FLOP per execution of either line.
  - Number of executions: $\sum_{k=0}^{n-1} \sum_{\ell=0}^{k} 1 = \sum_{k=0}^{n-1}(k+1) = \frac{n\,(n+1)}{2}$.
- Lines 8, 9: $\mathcal{O}(Nn)$ FLOP.

Summary: n matrix-vector products, $\mathcal{O}\left(Nn^2\right)$ other FLOP.

Cost of Arnoldi-based GMRES

- Arnoldi: n matrix-vector products, $\mathcal{O}\left(Nn^2\right)$ other FLOP.
- Least squares: $\mathcal{O}(n^2)$ FLOP.
- $\tilde{x} = Q_n y$: $\mathcal{O}\left(Nn\right)$ FLOP.

Summary: n matrix-vector products, $\mathcal{O}\left(Nn^2\right)$ other FLOP.

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Summary GMRES

Given A, b and n, find $\tilde{x} := p_{n-1}(A)\, b$ where

$$p_{n-1} := \operatorname*{arg\,min}_{p_{n-1} \in \mathcal{P}_{n-1}} \left\| \left(A p_{n-1}(A) - I\right) b \right\|_2.$$

Cost: n matrix-vector products and $\mathcal{O}\left(Nn^2\right)$ other FLOP.

Discussion

- Linear scaling in N if matrix-vector product is $\mathcal{O}(N)$ (unlike LU factorisation).
- Expensive for large n due to $\mathcal{O}(Nn^2)$ FLOP for orthogonalisation.
- Good news: orthogonalisation simplifies for symmetric matrices!

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GMRES applied to symmetric matrices

Key observation: A symmetric $\implies$ H is tridiagonal.

Proof 1. Multiplying $AQ_n = Q_{n+1}H_n$ with Q_n^T from left yields

$$Q_n^T A Q_n = \begin{pmatrix} Q_n^T Q_n & Q_n^T q_n \end{pmatrix} H_n = \begin{pmatrix} I & 0 \end{pmatrix} H_n =: \tilde{H}_n$$

($\tilde{H}_n \in \mathbb{R}^{n\times n}$ is obtained from H_n by removing last row).
$\tilde{H}_n$ is Hessenberg and symmetric $\implies$ H_n is tridiagonal.

Proof 2. By construction, $q_k = \sum_{m=0}^{k} c_m A^m b$ and

$$q_k^T \left(\sum_{m'=0}^{k'} c'_{m'} A^{m'} b\right) = 0 \qquad \text{if } k' < k.$$

Thus, for $\ell < k-1$ we obtain

$$H_{\ell k} = (Aq_k)^T q_\ell = q_k^T A q_\ell = q_k^T \left(\sum_{m=0}^{\ell} c_m A^{m+1} b\right) = 0.$$

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GMRES applied to symmetric matrices

Consequence of observation from last slide:
we only have to orthogonalise $\tilde{q}_{k+1} = Aq_k$ against q_k and q_{k-1}.
All other inner products $q_\ell^T \tilde{q}_{k+1}$ are automatically 0.

The resulting modification of Arnoldi is known as Lanczos iteration.

Algorithm 2 Lanczos iteration

$q_0 = b/\|b\|_2$
for $k = 0, \ldots, n-1$ **do**
  $\tilde{q}_{k+1} = Aq_k$
  $H_{kk} = q_k^T \tilde{q}_{k+1}$
  if $k = 0$ **then**
    $\tilde{q}_{k+1} = \tilde{q}_{k+1} - H_{kk} q_k$
  else
    $\tilde{q}_{k+1} = \tilde{q}_{k+1} - H_{kk} q_k - H_{k-1,k} q_{k-1}$
  end if
  $H_{k+1,k} = H_{k,k+1} = \|\tilde{q}_{k+1}\|$
  $q_{k+1} = \tilde{q}_{k+1}/H_{k+1,k}$
end for

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Terminology

GMRES applied to symmetric matrices and using Lanczos instead of Arnoldi is known as MinRes (Minimal Residual).

Discussion of MinRes

- Cost of MinRes reduces to n matrix-vector products and $\mathcal{O}(Nn)$ other FLOP.
- It is possible to interleave the Lanczos iteration and the QR factorisation of H such that only five vectors (rather than all the q_k as in GMRES) need to be stored. This is important for very large-scale computations where memory constraints are a concern.
- In practice, the q_k computed by Lanczos may fail to be orthogonal due to rounding errors. This limits the accuracy reachable with this algorithm. Some implementations include additional steps to improve orthogonality.

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Conjugate Gradients (CG)

Let A be symmetric positive definite (SPD, $v^T A v > 0$ for all nonzero v).
Conjugate gradient approximation $\tilde{x}$ to the solution to $Ax = b$ is given by

$$\tilde{x} := p_{n-1}(A)\, b \qquad \text{where} \qquad p_{n-1} := \operatorname*{arg\,min}_{p_{n-1} \in \mathcal{P}_{n-1}} \left\| \left(A p_{n-1}(A) - I \right) b \right\|_{A^{-1}}$$

and $\|v\|_{A^{-1}} := \sqrt{v^T A^{-1} v}$ (note that this is a norm since A is SPD).

Discussion

- Conjugate gradients is most well-known Krylov subspace method.
- It can be implemented using only four vectors and somewhat fewer FLOP than MinRes (but cost is still n matrix-vector products and $\mathcal{O}(Nn)$ other FLOP).
- Let $r = A\tilde{x} - b = A(\tilde{x} - x) = Ae$. Then,

  $$\|r\|_{A^{-1}}^2 = r^T A^{-1} r = e^T A A^{-1} A e = e^T A e = \|e\|_A^2.$$

  Hence, CG minimises error norm $\|e\|_A$.
  Small $\|e\|_A$ is sometimes more relevant than small $\|r\|_2$.

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Summary of Krylov subspace methods

- GMRES:

$$\tilde{x} := p_{n-1}(A)\, b \qquad \text{where} \qquad p_{n-1} := \operatorname*{arg\,min}_{p_{n-1} \in \mathcal{P}_{n-1}} \left\| \left(A p_{n-1}(A) - I\right) b \right\|_2$$

  Cost: n matrix-vector products, $\mathcal{O}(Nn^2)$ other FLOP.

- MinRes: GMRES applied to symmetric matrix.
  Cost: n matrix-vector products, $\mathcal{O}(Nn)$ other FLOP.

- Conjugate gradients:

$$\tilde{x} := p_{n-1}(A)\, b \qquad \text{where} \qquad p_{n-1} := \operatorname*{arg\,min}_{p_{n-1} \in \mathcal{P}_{n-1}} \left\| \left(A p_{n-1}(A) - I\right) b \right\|_{A^{-1}}$$

  Slightly cheaper than MinRes, but same cost in $\mathcal{O}$-sense.
  Only works for symmetric positive definite (SPD) matrices.

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Discussion

- Krylov subspace methods are perhaps the most confusing topic of this module. I recommend to stick with high-level definitions as much as possible and fill in details only when needed.
- Conjugate gradient is algorithm of choice for SPD matrices. MinRes is algorithm of choice for symmetric indefinite matrices.
- $\mathcal{O}(Nn^2)$ scaling of GMRES is often a problem in practice. Many alternative algorithms exist which avoid the n^2 factor at the price of other disadvantages
  - Conjugate gradients applied to $A^T A x = A^T b$
  - Restarted GMRES
  - BiCGSTAB

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References and further reading

Recommended since closest to presentation above:

- L. N. Trefethen and D. Bau. *Numerical Linear Algebra.* Society for Industrial and Applied Mathematics (1997),

Other references:

- G. H. Golub and C. F. Van Loan. *Matrix Computations.* Johns Hopkins University Press (1996),
- J. W. Demmel. *Applied Numerical Linear Algebra.* Society for Industrial and Applied Mathematics (1997), `doi:10.1137/1.9781611971446`
- N. J. Higham. *Accuracy and Stability of Numerical Algorithms.* Society for Industrial and Applied Mathematics (2002), `doi:10.1137/1.9780898718027`