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Krylov Subspace Methods

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Research School on Iterative Methods for PDEs 2023
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Outline

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References

- Y. Saad. Iterative Methods for Sparse Linear Systems
- J. Liesen and Z. Strakoš. Krylov Subspace Methods
- G. Ciarmella and M. Gander. Iterative Methods and Preconditioners for Systems of Linear Equations

Notation

- $n \gg 1$, integer
- $A \in \mathbb{R}^{n \times n}$, nonsingular matrix
- $b \in \mathbb{R}^n$, vector
- $\| \cdot \|_2$, the Euclidean norm
- $A^\top$ is the transpoe of A
- A is symmetric if $A^\top = A$
- A is symmetric positive definite (SPD) if $A^\top = A$ and $\|x\|_A = x^\top Ax > 0, \; \forall x \neq 0$
- When available and real $\lambda_1(A) \geq \ldots \geq \lambda_n(A)$ the eigenvalues of A
- $nnz(A)$ is the number of nonzero values in A

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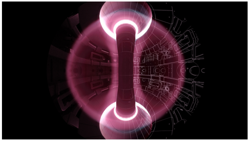
Linear Systems of Equations

$$Ax = b$$

arises in a most scientific applications

- Control
- Optimizatioin
- Simulations
- etc

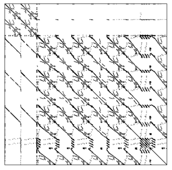
Example

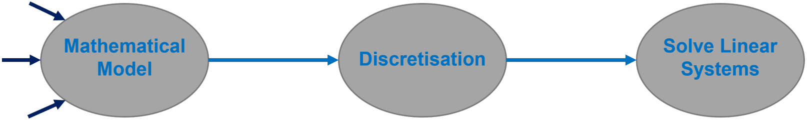


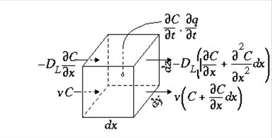
$$\frac{du_1}{dx} = \frac{-3u_1 + 4u_2 - u_3}{2h}$$

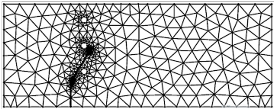
$$\frac{du_i}{dx} = \frac{-u_{i+1} + u_{i+1}}{2h}, \ i = 2(1)N-2$$

$$\frac{du_{N-1}}{dx} = \frac{u_{N-3} - 4u_{N-2} + 3u_{N-1}}{2h}.$$









```
procedure pcg(A, Θ^k, b̄)
    Compute Δy_0 as a guess of Δy^k;
    r_0 := b̄ − AΘ^k A^⊤ Δy_0;
    solve M z_0 = r_0;
    p_0 := z_0;
    i := 0;
    do stopping criterion not satisfied →
        q_i := AΘ^k A^⊤ p_i;
        α_i := z_i^⊤ r_i / p_i^⊤ q_i;
        Δy_{i+1} := Δy_i + α_i p_i;
        r_{i+1} := r_i − α_i q_i;
        solve M z_{i+1} = r_{i+1};
        β_i := z_{i+1}^⊤ r_{i+1} / z_i^⊤ r_i;
        p_{i+1} := z_{i+1} + β_i p_i;
        i := i + 1
    od;
    Δy^k := Δy_i
end pcg;
```

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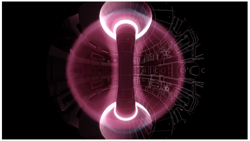
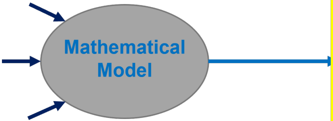
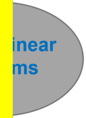
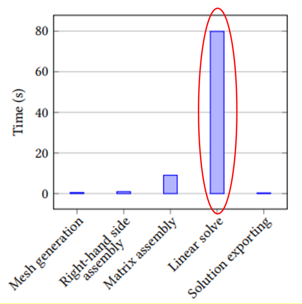
Example

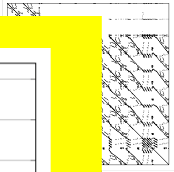


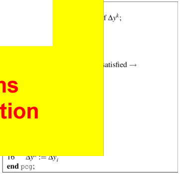


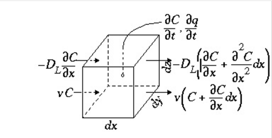


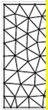


Solving linear systems dominates time to solution









Runtime figure from Pierre Jolivet's PhD thesis

Sparse Matrices

$nnz(A)/n \ll n$

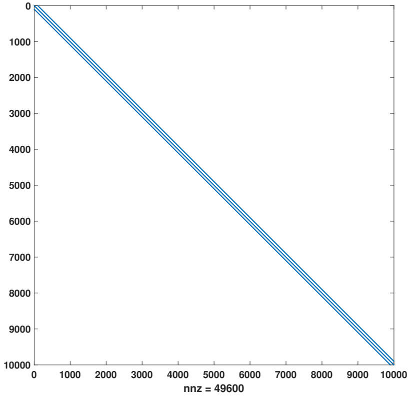


Figure: Sparsirty pattern of a discretized 2D Laplacian

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Direct Sparse Solvers

- A SPD, $A = PLL^\top P^\top$
- A Symmetric, $A = PLDL^\top P^\top$
- A nonsingular, $A = LUP^\top$
- $A = QRP^\top$

Software available: **HSL**, MUMPS, PARDISO, SuperLU, UMFPACK, CholMOD

Direct Sparse Solvers: Properties

- Robust
- Black box
- Requires access to its elements values
- Memory demanding
- Too much unnecessary accuracy most of the times
- Not easy to parallelize

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Direct Sparse Solvers: Fill-in

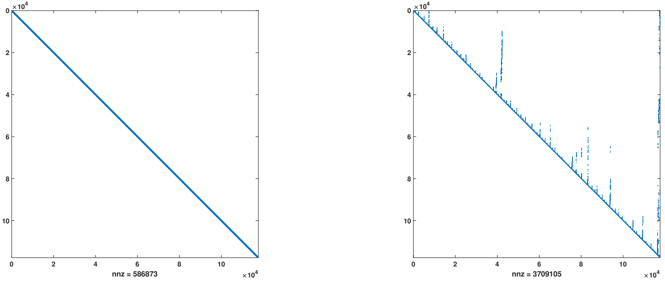

Figure: Sparsirty pattern of a A and L^T for discretized 2D Laplacian

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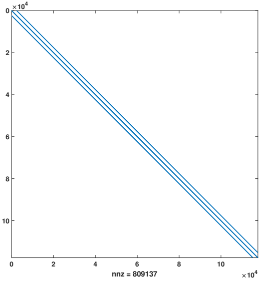
Direct Sparse Solvers: Fill-in



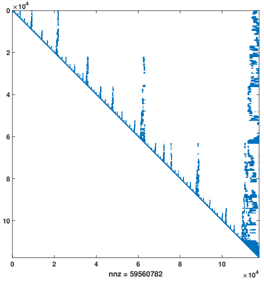


Figure: Sparsirty pattern of a A and L^T for discretized 3D Laplacian

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Introduction

Krylov Subspace Methods

Projection Methods

Minimization Properties

Algorithms

Arnoldi and GMRES

Lanczos and CG

Convergence and Preconditioning

Recent Advances

Cayley–Hamilton Theorem

- $\chi_A(\lambda) = det(\lambda I - A) = \sum_{k=0}^{n} a_k \lambda^k$
- $\chi_A(A) = 0$
- $A^{-1}b = \sum_{k=1}^{n} -a_k/a_0 A^k b$ for any $b \in \mathbb{R}^n$

$Ax = b$ yields $x \in$ span$\{b, Ab, A^2b, \ldots, A^{n-1}b\}$

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Krylov Subspace: Definition

The kth Krylov subspace associated with A and b is

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

- Requires only matrix-vector product
- $\mathcal{K}_1(A, b) \subset \cdots \subset \mathcal{K}_k(A, b) \subset \cdots \subset \mathcal{K}_\nu(A, b) = \mathcal{K}_{\nu+1}(A, b)$
- $k \leq \nu, \;\; \dim(\mathcal{K}_k) = k$
- $z \in \mathcal{K}_k(A, b)$, $\exists q$ of order $< k$, $z = q(A)b$

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Search and Constraint Subspaces

- $\mathcal{K}_k, \mathcal{L}_k \subset \mathbb{R}^n$ of dim k
- Look for $x_k \in \mathcal{K}_k$ for $r_k = b - Ax_k \perp \mathcal{L}_k$.
- There are k DOFs: $x_k = V_{\mathcal{K}_k} u_k$.
- There are k constraints $V_{\mathcal{L}_k}^\top A V_{\mathcal{K}_k} u_k = V_{\mathcal{L}_k} b$.

Hence, if $V_{\mathcal{L}_k}^\top A V_{\mathcal{K}_k}$ is nonsingular, x_k is unique!
Let's build $\mathcal{K}_1 \subset \mathcal{K}_2 \cdots$, $\mathcal{L}_1 \subset \mathcal{L}_2 \cdots$ and solve iteratively $Ax = b$

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Krylov Subspace as Projection Methods

The kth Krylov subspace associated with A and b is

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

- A is nonsingular and $\mathcal{K}_k = \mathcal{K}_k(A, b)$ spanned by V_k, $\mathcal{L} = A\mathcal{K}_k$
- $V_k^\top A^\top A V_k$ is nonsingular
- $x_k = V_k(V_k^\top A^\top A V_k)^{-1} V_k^\top A^\top b$

- A is SPD and $\mathcal{K}_k = \mathcal{L}_k = \mathcal{K}_k(A, b)$ spanned by V_k
- $V_k^\top A V_k$ is nonsingular
- $x_k = V_k(V_k^\top A V_k)^{-1} V_k^\top b$

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Minimizing Residual

A is nonsingular $\mathcal{K}_k = \mathcal{K}_k(A, b)$ spanned by V_k, $\mathcal{L}_k = A\mathcal{K}_k(A, b)$

- $x_k = V_k(V_k^\top A^\top A V_k)^{-1} V_k^\top A^\top b$

$$\|b - Ax_k\|_2 = \min_{z \in \mathcal{K}_k} \|b - Az\|_2$$

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Minimizing Error

A is SPD $\mathcal{K}_k = \mathcal{L}_k = \mathcal{K}_k(A, b)$ spanned by V_k

- $x_k = V_k(V_k^\top A V_k)^{-1} V_k^\top b$

$$\|x - x_k\|_A = \min_{z \in \mathcal{K}_k} \|x - z\|_A$$

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Krylov subspace basis

Is $\{b, Ab, \ldots, A^{k-1}b\}$ practical basis? Remember the power method?

If $V_k = \begin{pmatrix} b & Ab & \cdots & A^{k-1}b \end{pmatrix}$, it will most likely be very badly conditioned even for small k and hence poor approximate solution.

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Arnoldi Procedure I

Algorithm Arnoldi Procedure, Classical Gram–Schmidt Orthogonalization

Require: $A,\ b \neq 0,\ k > 0$

Ensure: orthonormal vectors $V_k = [v_1, \ldots, v_k]$ spanning $\mathcal{K}_k(A, b)$.

1: $v_1 = b/\|b\|_2$
2: **for** $j = 1 : k-1$ **do**
3: $\quad \hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$, where $h_{i,j} = v_i^\top A v_j$,
4: $\quad h_{j+1,j} = \|\hat{v}_{j+1}\|_2$, if $h_{j+1,j} = 0$ then stop
5: $\quad v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$

$$\forall j \leq k,\ AV_j = V_{j+1} H_j$$

where $H_j \in \mathbb{R}^{(j+1)\times j}$ is Hessenberg matrix

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Arnoldi Procedure II

Algorithm Arnoldi Procedure, Modified Gram–Schmidt Orthogonalization

Require: $A,\ b \neq 0,\ k > 0$

Ensure: orthonormal vectors $V_k = [v_1, \dots, v_k]$ spanning $\mathcal{K}_k(A, b)$.

1: $v_1 = b / \|b\|_2$
2: **for** $j = 1 : k-1$ **do**
3:     $\hat{v}_{j+1} = Av_j$
4:     **for** $i = 1 : j$ **do**
5:         $h_{i,j} = v_i^\top \hat{v}_{j+1}$
6:         $\hat{v}_{j+1} = \hat{v}_{j+1} - v_i h_{i,j}$
7:     $h_{j+1,j} = \|\hat{v}_{j+1}\|_2$, if $h_{j+1,j} = 0$ then stop
8:     $v_{j+1} = \hat{v}_{j+1} / h_{j+1,j}$

$$\forall j \leq k,\ AV_j = V_{j+1} H_j$$

where $H_j \in \mathbb{R}^{(j+1) \times j}$ is Hessenberg matrix

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GMRES

Saad and Schultz 1986

Algorithm GMRES, Classical Gram–Schmidt Orthogonalization

Require: $A,\; b \neq 0, k > 0$

Ensure: x_k approximate solution to $Ax = b$

1: $\beta = \|b\|_2,\; v_1 = b/\beta$

2: **for** $j = 1 : k$ **do**

3: $\quad \hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$, where $h_{i,j} = v_i^\top A v_j$,

4: $\quad h_{j+1,j} = \|\hat{v}_{j+1}\|_2$, if $h_{j+1,j} = 0$ set $k := j$ and go to 6

5: $\quad v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$

6: $x_k = \beta V_k y_k$ where y_k minimizes $\|H_k y - \beta e_1\|_2$

GMRES

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

$$\begin{aligned}
\|b - AV_k y\|_2 &= \|\beta V_{k+1}e_1 - AV_k y\|_2 \\
&= \|\beta V_{k+1}e_1 - V_{k+1}H_k y\|_2 \\
&= \|\beta e_1 - H_k y\|_2 \\
&\geq \|\beta e_1 - H_k y_k\|_2 \\
&= \|b - Ax_k\|_2
\end{aligned}$$

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The Hessenberg Matrix in GMRES

$$\forall j \leq k, \; AV_j = V_{j+1} H_j$$

$$H_{j+1} = \begin{pmatrix} H_j & h_{1:j+1,j+1} \\ 0_{1,j} & h_{j+2,j+1} \end{pmatrix}$$

Its QR decomposition can be updated cheaply.

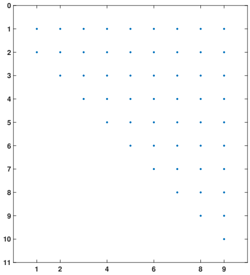

Figure: 10×9 Hessenberg matrix

Arnoldi Procedure with SPD A

Algorithm Arnoldi Procedure, Classical Gram–Schmidt Orthogonalization

Require: A SPD, $b \neq 0$, $k > 0$

Ensure: orthonormal vectors $V_k = [v_1, \ldots, v_k]$ spanning $\mathcal{K}_k(A, b)$.

1: $v_1 = b/\|b\|_2$

2: **for** $j = 1 : k-1$ **do**

3: $\quad \hat{v}_{j+1} = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$, where $h_{i,j} = v_i^\top A v_j$,

4: $\quad h_{j+1,j} = \|\hat{v}_{j+1}\|_2$, if $h_{j+1,j} = 0$ then stop

5: $\quad v_{j+1} = \hat{v}_{j+1}/h_{j+1,j}$

$$\forall j \leq k,\ AV_j = V_{j+1} H_j = V_j \bar{H}_j + v_{j+1} h_{j+1,j} e_j^\top$$

where $\bar{H}_j \in \mathbb{R}^{j \times j}$ is tridiagonal matrix

Lanczos Procedure

Lanczos 1950

Algorithm Lanczos Procedure

Require: A SPD, $b \neq 0$, $k > 0$

Ensure: orthonormal vectors $V_k = [v_1, \ldots, v_k]$ spanning $\mathcal{K}_k(A, b)$.

$v_0 = 0$, $\beta_1 = 0$, $v_1 = b / \|b\|_2$
for $j = 1 : k-1$ **do**
  $\hat{v}_{j+1} = A v_j - \beta_j v_{j-1}$
  $\alpha_j = \hat{v}_{j+1}^\top v_j$
  $\hat{v}_{j+1} = \hat{v}_{j+1} - \alpha_j v_j$
  $\beta_j = \|\hat{v}_{j+1}\|_2$, if $\beta_j = 0$ then stop
  $v_{j+1} = \hat{v}_{j+1} / \beta_j$

$$\forall j \leq k,\ AV_j = V_{j+1} T_j = V_j \bar{T}_j + v_{j+1} \beta_{j+1} e_j^\top$$

where $T_j \in \mathbb{R}^{(j+1)\times j}$ is tridiagonal matrix $((\alpha_j), (\beta_j))$

CG I

A is SPD. Consider the quadratic function

$$\phi(x) = \frac{1}{2}x^\top Ax - x^\top b$$

Its gradient

$$\nabla\phi(x) = Ax - b$$

Then, minimizing ϕ is equivalent to solving $Ax = b$ (unique stationary point).
Given x_j and some p_j, line search to find a minimizing α_j

$$x_{j+1} = x_j + \alpha_j p_j.$$

$$\|x - x_{j+1}\|_A^2 = \|x - x_j\|_A^2 + \alpha_j^2 p_j^\top Ap_j - 2\alpha_j p_j^\top r_j.$$

Minimum attained at $\alpha_j = \dfrac{p_j^\top r_j}{p_j^\top Ap_j}$ resulting also in $p_j^\top r_{j+1} = 0$

CG, II

Remains to define the search directions. $p_0 = b$ and

$p_{j+1} = r_{j+1} + \frac{r_{j+1}^\top r_{j+1}}{r_j^\top r_j} p_j$ ensures $p_i^\top A p_j = 0$, $r_i^\top r_j = 0$ if $i \neq j$.

($\nabla \phi(x_j) = -r_j$, hence the name)

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CG, II

Remains to define the search directions. $p_0 = b$ and

$p_{j+1} = r_{j+1} + \frac{r_{j+1}^\top r_{j+1}}{r_j^\top r_j} p_j$ ensures $p_i^\top A p_j = 0$, $r_i^\top r_j = 0$ if $i \neq j$.

($\nabla \phi(x_j) = -r_j$, hence the name)

Note $x - x_{j+1} = (x - x_j) - \alpha_j p_j$ where $\alpha_j = \frac{p_j^\top r_j}{p_j^\top A p_j} = \frac{p_j^\top A(x - x_j)}{p_j^\top A p_j}$

yields

$$\|x - x_j\|_A^2 = \|x - x_{j+1}\|_A^2 + \alpha_j^2 \|p_j\|_A^2$$

$$\|x - x_0\|_A^2 = \|x\|_A^2 = \|x - x_{j+1}\|_A^2 + \sum_{k=1}^{j} \alpha_k^2 \|p_k\|_A^2$$

$$\|x - x_{j+1}\|_A = \min_{z \in \text{ span}\{p_0, \ldots, p_j\}} \|x - z\|_A$$

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CG, III

Actually, $\operatorname{span}\{p_0, p_1, \ldots, p_j\} = \operatorname{span}\{b, Ab, \ldots, A^j b\}$.
Indeed, $p_0 = b$, $p_k \in \operatorname{span}\{r_k, p_{k-1}\}$ and $p_k^\top A p_{k-1} = 0$

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CG

Hestenes and Stiefel 1952

Algorithm CG

Require: A SPD, $b \neq 0, k > 0$

Ensure: x_k approximate solution to $Ax = b$

$x_0 = 0,\ r_0 = b,\ p_0 = r_0$

for $j = 1, 2, \cdots$ **do**

$$\alpha_j = \frac{r_j^\top r_j}{p_j^\top A p_j}$$

$$x_{j+1} = x_j + \alpha_j p_j$$

$$r_{j+1} = r_j - \alpha_j A p_j$$

$$\beta_j = \frac{r_{j+1}^\top r_{j+1}}{r_j^\top r_j}$$

$$p_{j+1} = r_{j+1} + \beta_j p_j$$

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Convergence

Suppose $A = V\Lambda V^{-1}$ GMRES:

$$\begin{aligned}
\|b - Ax_k\|_2 &= \min_{y \in \mathcal{K}_k(A,b)} \|b - Ay\|_2 \\
&= \min_{p \in \mathcal{P}_{k-1}} \|b - Ap(A)b\|_2 \\
&= \min_{q \in \mathcal{P}_k, q(0)=1} \|q(A)b\|_2 \\
&= \min_{q \in \mathcal{P}_k, q(0)=1} \|Vq(\Lambda)V^{-1}b\|_2 \\
&\leq \|V\|_2 \|V^{-1}\|_2 \|b\|_2 \min_{q \in \mathcal{P}_k, q(0)=1} \|q(\Lambda)\|_2
\end{aligned}$$

Convergence

CG:

$$\begin{aligned}
\|x - x_k\|_A &= \min_{y \in \mathcal{K}_k(A,b)} \|x - y\|_A \\
&= \min_{q \in \mathcal{P}_k, q(0)=1} \|q(A)x\|_A \\
&\leq \min_{q \in \mathcal{P}_k, q(0)=1} \max_{\lambda \in [\lambda_n, \lambda_1]} |q(\lambda)| \|x\|_A \\
&\leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x\|_A
\end{aligned}$$

where $\kappa = \dfrac{\lambda_1}{\lambda_n}$ is the condition number

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Preconditioning I

Transform

$$Ax = b$$

into

$$M^{-1}Ax = M^{-1}b$$

s.t. $M^{-1}A$ has nicer properties.
General requirements

- Easy to set up
- Cheap to multiply by a vector
- Approximate A^{-1} in a certain way

For CG, the convergence depends heavily on $\kappa_2(A)$.
For GMRES, yet to be discovered! Nonetheless, even though eigenvalues do not cover the whole picture, they are widely considered in practice.