Iterative Methods for Large Linear Systems

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Projection Methods

$$Ax = b$$

- A is $n \times n$ real matrix
- Idea: approximate solution $\hat{x} \in x_0 + \mathcal{K}$ such that $b - A\hat{x} \perp \mathcal{L}$

$$r_0 = b - Ax_0$$
$$\hat{x} = x_0 + \delta \qquad \delta \in \mathcal{K}$$
$$< r_0 - A\delta, w >= 0 \qquad \forall w \in \mathcal{L}$$

Projection Methods

- Two classes of projections:
  - Oblique
  - Orthogonal $\mathcal{L} = \mathcal{K}$
- Matrix Representation
  - $V = [v_1 \cdots v_m]$ basis for $\mathcal{K}$
  - $W = [w_1 \cdots W_m]$ basis for $\mathcal{L}$

$$
\begin{aligned}
x &= x_0 + Vy \\
W^T AVy &= W^T r_0 \\
\hat{x} = x_0 + V(W^T AV)^{-1} W^T r_0
\end{aligned}
$$

- $W^T AV$ non-singular
- never compute Mat-Mat products

Projection Methods

Theorem

$W^T A V$ *is non-singular in case :*

- A *is positive definite and* $\mathcal{L} = \mathcal{K}$
- A *is non-singular and* $\mathcal{L} = A\mathcal{K} \iff W = AVG$

Theorem

$\hat{x}$ *is the optimal solution in the above cases : min* $||Ax - b||$

Krylov Subspace

$$\mathcal{K}_m(A, r_0) = span\{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\}$$
$$r_0 = b - Ax - 0$$

- Krylov subspace methods $\mathcal{K} = \mathcal{K}_m$
- Different methods have different choices of $\mathcal{L}_m$
- Idea: $A^{-1} b \approx p(A) b$

Arnoldi Iteration

- Based on Gram-Schmidt orthogonalization

```
Choose v_1 where ||v_1||=1
for j=1:m do
    w_j = A v_j
    for i=1:j do
        h_ij = < w_j, v_i >
        w_j = w_j - h_ij v_j
    end
    h_{j+1,j} = ||w_j||_2
    if h_{j+1,j}=0 then
        Stop
    end
    v_{j+1} = w_j / h_{j+1,j}
end
```

Arnoldi Iteration

$$h_{j+1,j}v_{j+1} = Av_j - \sum_{i=1}^{j} h_{ij}v_j$$

$$Av_j = \sum_{i=1}^{j+1} h_{ij}v_j \quad j = 1, 2, \ldots m$$

- $AV_m = V_m H_m + w_m e_m^T = V_{m+1}\bar{H}_m$
- $V_m^T AV_m = H_m$
- $\bar{H}_m$ is $(m+1) \times m$ Hessenberg matrix
- V_m and V_{m+1} Orthonormal matrices

Arnoldi Iteration

- (FOM) Arnoldi method for linear systems
  - $\mathcal{K} = \mathcal{L} = \mathcal{K}_m(A, r_0)$
  - $V_m^T A V_m = H_m$
  - $V_m^T r_0 = V_m^T(||r_0|| v_1) = \beta e_1$

$$x_m = x_0 + V_m y_m$$
$$y_m = H_m^{-1}(\beta e_1)$$

- Flavors:
  - CGS
  - MGS
  - Householder : QR factorization of $[v_1, Av_1, \ldots, Av_m]$

Arnoldi Iteration

Full orthogonalization method:

- Computational and storage cost to orthogonalize against previous v_j
- Truncation
- Restart with $x_0^{new} = x_m$

GMRES

- $\mathcal{K} = \mathcal{K}_m$ and $\mathcal{L} = A\mathcal{K}_m$
- Idea : $\min ||b - Ax||_2$ for $x = x_0 + V_m y$

$$
\begin{aligned}
b - Ax &= b - A(x_0 + V_m y) \\
&= r_0 - AV_m y \\
&= \beta v_1 - V_{m+1}\bar{H}_m y \\
&= V_{m+1}(\beta e_1 - \bar{H}_m y) \\
&\rightarrow ||b - Ax|| = ||\beta e_1 - \bar{H}_m y||
\end{aligned}
$$

GMRES

$$x_m = x_0 + V_m y_m$$
$$y_m = argmin_y ||\beta e_1 - \bar{H}_m y||_2$$

- $W_m = AV_m$
- $(m+1) \times m$ LSQ problem
- $\bar{H}_m$ can be transformed to upper triangular via a series of rotations
- Flavors: Householder variant is more stable
- if A is symmetric : Lanczos method

Lanczos

- What if A is symmetric ?
- $H_m = V_m^T A V_m$ is symmetric
- H_m is tridiagonal (think of storage and computation effort)
- Arnoldi iteration is simplified: $\alpha_j = h_{ij}$ and $\beta_j = h_{j-1,j}$

Set $\beta_1 = 0, v_0 = 0, ||v_1|| = 1$ **for** *j=1:m* **do**

$w_j = Av_j - \beta_j v_{j-1}$

$\alpha_j =< w_j, v_j >$

$w_j = w_j - \alpha_j v_j$

$\beta_{j+1} = ||w_j||$ **if** $\beta_{j+1,j}$*=0* **then**

Stop

end

$v_{j+1} = w_j / \beta_{j+1}$

end

What remains ...

- CG (Symmetric positive definite A)
- BiCG (non-Symmetric A)
- Convergence of CG, GMRES
- Block Krylov methods