Iterative Solution methods

Iterative solution methods

- Steepest descent
- conjugate gradient method (CG)
- Generalized conjugate gradient method (GCG)
- ORTHOMIN
- Minimal residual method (MINRES)
- Generalized minimal residual method (GMRES)
- Lanczos method
- Arnoldi method
- Orthogonal residual method (ORTHORES)
- Full orthogonalization method (FOM)
- Incomplete orthogonalization method (IOM)

Iterative solution methods

- SYMMLQ
- Biconjugate gradient method (BiCG)
- BiCGStab
- Conjugate gradients squared (CGS)
- Minimal residual method (MR)
- Quasiminimal residual method
- . . .

Projection methods

General framework – projection methods

Want to solve $\mathbf{b} - A\mathbf{x} = \mathbf{0}, \mathbf{b}, \mathbf{x} \in R^n, A \in R^{n,n}$

Instead, choose two subspaces $L \subset R^n$ and $K \subset R^n$ and

$$* \text{ find } \widetilde{\mathbf{x}} \in \mathbf{x}^{(0)} + K, \text{ such that } \mathbf{b} - A\widetilde{\mathbf{x}} \perp L$$

K - search space
L - subspace of constraints

$*$ - basic projection step

The framework is known as Petrov-Galerkin conditions.

There are two major classes of projection methods:

- orthogonal - if $K \equiv L$,
- oblique - if $K \neq L$.

Notations:
$\widetilde{\mathbf{x}} = \mathbf{x}^0 + \delta$ - (δ - correction)

$\mathbf{r}^0 = \mathbf{b} - A\mathbf{x}^0$ ($\mathbf{r}^0$ - residual)

$*$ find $\delta \in K$, such that $\mathbf{r}^0 - A\delta \perp L$

Matrix formulation

Choose a basis in K and L: $V = \{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_m\}$ and $W = \{\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_m\}$.
Then, $\widetilde{\mathbf{x}} = \mathbf{x}^0 + \delta = \mathbf{x}^0 + V\mathbf{y}$ for some $\mathbf{y} \in R^m$.

The orthogonality condition can be written as

$$(**) \quad \boxed{W^T(\mathbf{r}^0 - AV\mathbf{y})}$$

which is exactly the Petrov-Galerkin condition.
From $(**)$ we get

$$\begin{aligned} W^T\mathbf{r}^0 &= W^T AV\mathbf{y} \\ \mathbf{y} &= (W^T AV)^{-1} W^T \mathbf{r}^0 \\ \widetilde{\mathbf{x}} &= \mathbf{x}^0 + V(W^T AV)^{-1} W^T \mathbf{r}^0 \end{aligned}$$

In practice, $m < n$, even $m \ll n$, for instance, $m = 1$.

The matrix $W^T AV$ will be small and, hopefully, with a nice structure.

A prototype projection-based iterative method:

Given $\mathbf{x}^{(0)}$; $\mathbf{x} = \mathbf{x}^{(0)}$
Until convergence do:
Choose K and L
Choose basis V in K and W in L
Compute $\mathbf{r} = \mathbf{b} - A\mathbf{x}$

$$\mathbf{y} = (W^T A V)^{-1} W^T \mathbf{r}$$
$$\mathbf{x} = \mathbf{x} + V\mathbf{y}$$

Degrees of freedom: m, K, L, V, W.
Clearly, if $K \equiv L$, then $V = W$.

Plan:
(1) Consider two important cases: $L = K$ and $L = AK$
(2) Make a special choice of K.

Property 1:

Theorem 1 *Let A be square, $L = AK$. Then a vector $\widetilde{\mathbf{x}}$ is an oblique projection on K orthogonally to AK with a starting vector $\mathbf{x}^0$ if and only if $\widetilde{\mathbf{x}}$ minimizes the 2-norm of the residual over $\mathbf{x}^0 + K$, i.e.,*

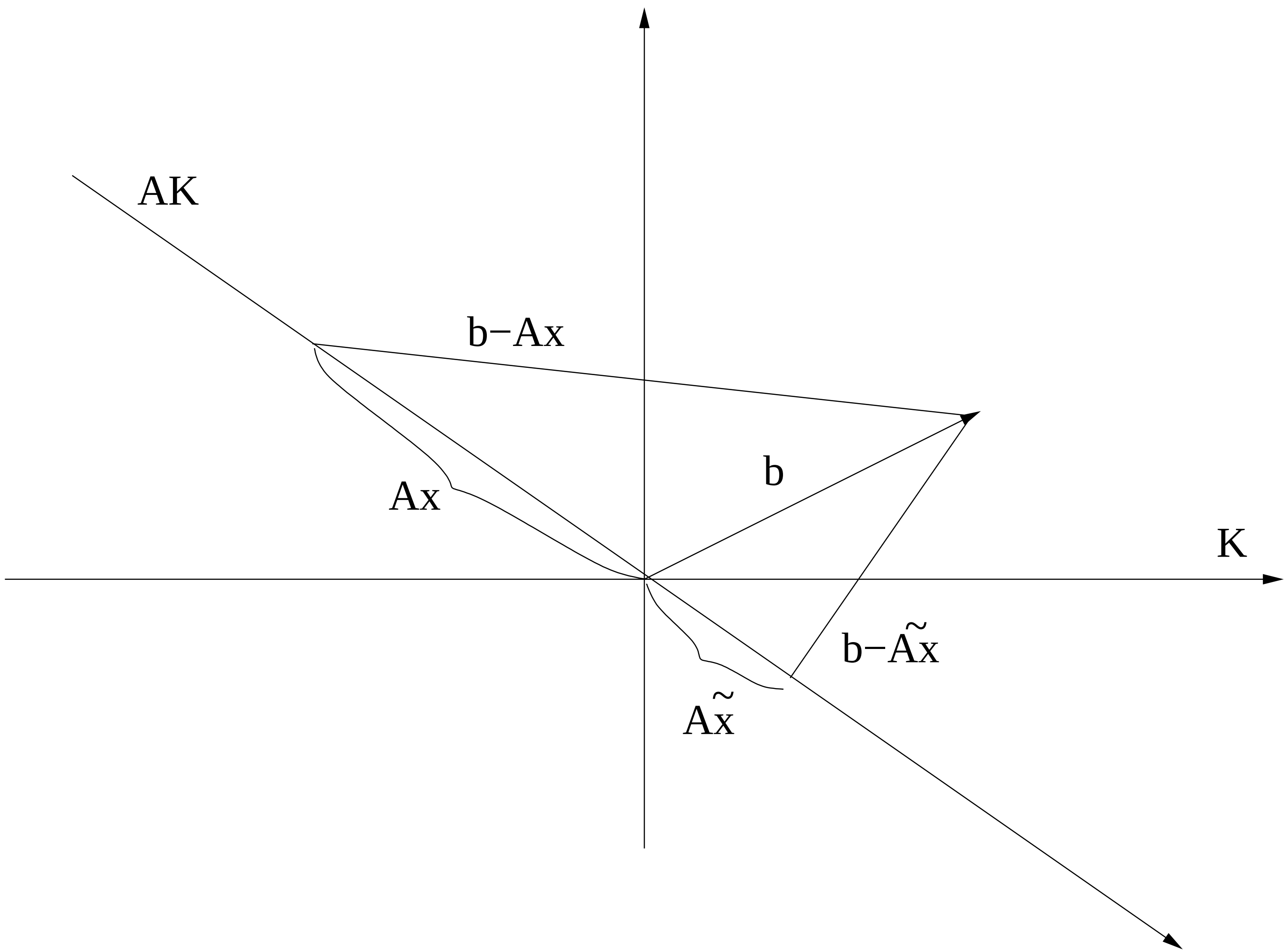
$$\|\mathbf{r} - A\widetilde{\mathbf{x}}\|_2 = \min_{\mathbf{x} \in \mathbf{x}^0 + K} \|\mathbf{r} - A\mathbf{x}\|_2. \tag{1}$$

Thus, the residual decreases monotonically.

Referred to as *minimal residual methods*

CR, GCG, GMRES, ORTHOMIN

Property 1:



Property 2:

Theorem 2 *Let A be symmetric positive definite, i.e., it defines a scalar product $(A\cdot, \cdot)$ and a norm $\|\cdot\|_A$. Let $L = K$, i.e., $\mathbf{r}^0 - A\widetilde{\mathbf{x}} \perp K$. Then a vector $\widetilde{\mathbf{x}}$ is an orthogonal projection onto K with a starting vector $\mathbf{x}^0$ if and only if it minimizes the A-norm of the error $\mathbf{e} = \mathbf{x}^* - \mathbf{x}$ over $\mathbf{x}^0 + K$, i.e.,*

$$\|\mathbf{x}^* - \widetilde{\mathbf{x}}\|_A = \min_{\mathbf{x} \in \mathbf{x}^0 + K} \|\mathbf{x}^* - \mathbf{x}\|_A. \tag{2}$$

The error decreases monotonically in the A-norm.

Error-projection methods.

Example: $m = 1$

Consider two vectors: $\mathbf{d}$ and $\mathbf{e}$. Let $K = span\{\mathbf{d}\}$ and $L = span\{\mathbf{e}\}$.
Then $\widetilde{\mathbf{x}} = \mathbf{x}^0 + \alpha\mathbf{d}$ ($\delta = \alpha\mathbf{d}$) and the orthogonality condition reads as:

$$\mathbf{r}^0 - A\delta \perp \mathbf{e} \Rightarrow (\mathbf{r}^0 - A\delta, \mathbf{e}) = 0 \Rightarrow \alpha(A\mathbf{d}, \mathbf{e}) = (\mathbf{r}^0, \mathbf{e}) \Rightarrow \alpha = \frac{(\mathbf{r}^0, \mathbf{e})}{(A\mathbf{d}, \mathbf{e})}.$$

If $\mathbf{d} = \mathbf{e}$ - Steepest Descent method (minimization on a line.

If we minimize over a plane - ORTHOMIN.

Choice of K:

$$K = \mathcal{K}^m(A, \mathbf{v}) = \{\mathbf{v}, A\mathbf{v}, A^2\mathbf{v}, \cdots, A^{m-1}\mathbf{v}\}$$

Krylov subspace methods

- $L = K = \mathcal{K}^m(A, \mathbf{r}^0)$ and A spd $\Rightarrow$ CG
- $L = AK = A\mathcal{K}^m(A, \mathbf{r}^0)$ $\Rightarrow$ GMRES

How to construct a basis for $\mathcal{K}$?

CG

Arnoldi's method for general matrices

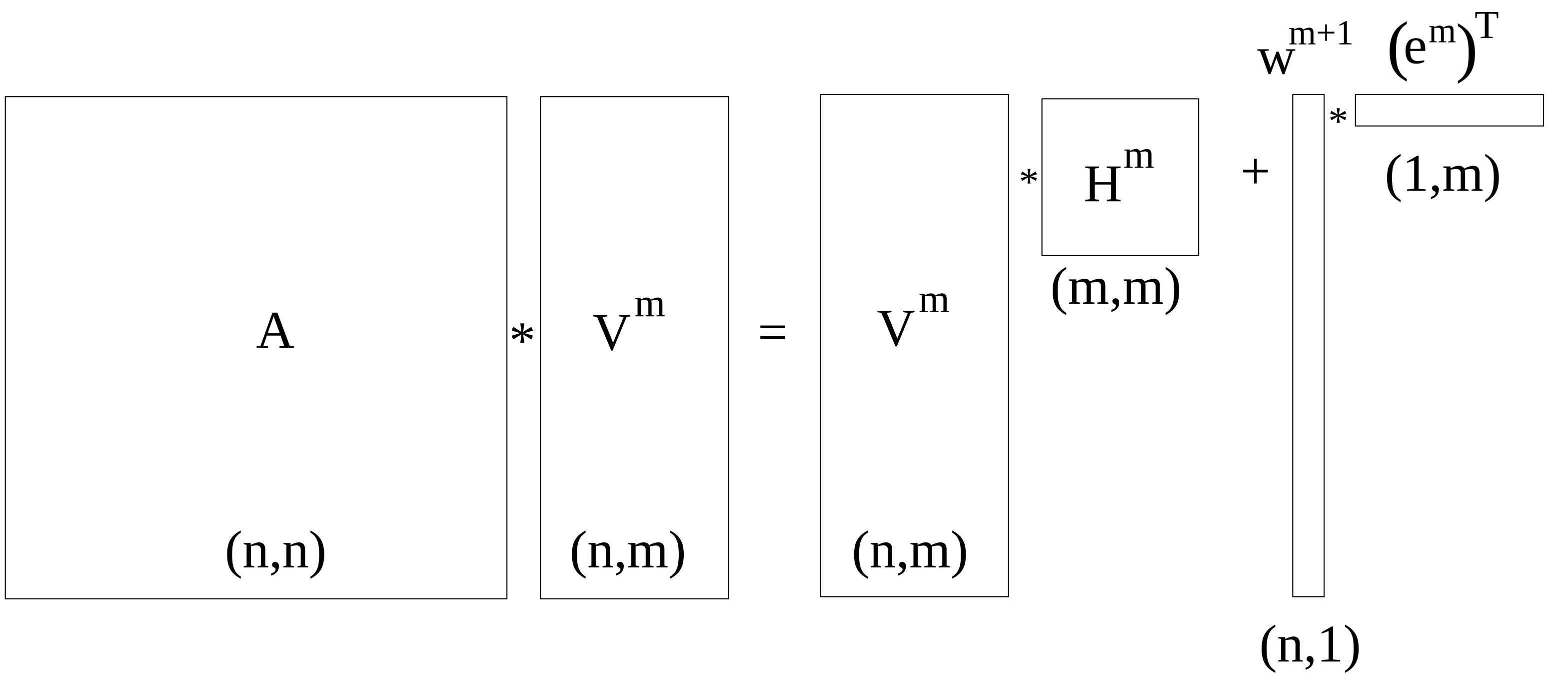
Consider $\mathcal{K}^m(A, \mathbf{v}) = \{\mathbf{v}, A\mathbf{v}, A^2\mathbf{v}, \cdots, A^{m-1}\mathbf{v}\}$, generated by some matrix A and vector $\mathbf{v}$.

1. Choose a vector $\mathbf{v}_1$ such that $\|\mathbf{v}_1\| = 1$
2. For $j = 1, 2, \cdots, m$
3. For $i = 1, 2, \cdots, j$
4. $h_{ij} = (A\mathbf{v}_j, \mathbf{v}_i)$
5. End
6. $\mathbf{w}_j = A\mathbf{v}_j - \sum_{i=1}^{j} h_{ij}\mathbf{v}_i$
7. $h_{j+1,j} = \|\mathbf{w}_j\|$
8. If $h_{j+1,j} = 0$, stop
9. $\mathbf{v}_{j+1} = \mathbf{w}_j / h_{j+1,j}$
10. End

The algorithm breaks down in step j, i.e., $h_{j+1,j} = 0$, if and only if the minimal polynomial of A is of degree j.

The result of Arnoldi's process

- $V^m = \{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_m\}$ is an orthonormal basis in $\mathcal{K}^m(A, \mathbf{v})$
- $AV^m = V^m H^m + \mathbf{w}_{m+1}\mathbf{e}_m^T$



Arnoldi's process - example

$$H^3 = \begin{bmatrix} (A\mathbf{v}_1, \mathbf{v}_1) & (A\mathbf{v}_2, \mathbf{v}_1) & (A\mathbf{v}_3, \mathbf{v}_1) \\ \|\mathbf{w}_1\| & (A\mathbf{v}_2, \mathbf{v}_2) & (A\mathbf{v}_3, \mathbf{v}_2) \\ 0 & \|\mathbf{w}_2\| & (A\mathbf{v}_3, \mathbf{v}_3) \end{bmatrix}$$

Since $V^{m+1} \perp \{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_m\}$ then it follows that $(V^m)^T A V^m = H^m$.

H^m is an upper-Hessenberg matrix.

Arnoldi's method for symmetric matrices

Let now A be real symmetric matrix. Then the Arnoldi method reduces to the Lanczos method.

Recall: $H^m = (V^m)^T A V^m$
If A is symmetric, then H^m must be symmetric too, i.e., H^m is three-diagonal

$$H^m = \begin{bmatrix} \gamma_1 & \beta_2 & & \\ \beta_2 & \gamma_2 & \beta_3 & \\ & & \ddots & \\ & & \beta_m & \gamma_m \end{bmatrix}$$

Thus, the vectors $\mathbf{v}^j$ satisfy a three-term recursion:

$$\beta_{i+1}\mathbf{v}^{i+1} = A\mathbf{v}^i - \gamma_i \mathbf{v}^i - \beta_i \mathbf{v}^{i-1}$$

Lanczos algorithm to solve symmetric linear systems

Given:	$\mathbf{x}^{(0)}$
Compute	$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\beta = \|\mathbf{r}^{(0)}\|$, $\mathbf{v}^1 = \mathbf{r}^{(0)}/\beta$
Set	$\beta_1 = 0$ and $\mathbf{v}^0 = \mathbf{0}$
For	$j = 1 : m$
	$\mathbf{w}^j = A\mathbf{v}^j - \beta_j \mathbf{v}^{j-1}$
	$\gamma_j = (\mathbf{w}^j, \mathbf{v}^j)$
	$\mathbf{w}^j = \mathbf{w}^j - \gamma_j \mathbf{v}^j$
	$\beta_{j+1} = \|\mathbf{w}^j\|_2$, if $\beta_{j+1} = 0$, go out of the loop
	$\mathbf{v}^{j+1} = \mathbf{w}^j / \beta_{j+1}$
End	
Set	$T_m = tridiag\{\beta_i, \gamma_i, \beta_{i+1}\}$
Compute	$\mathbf{y}^m = T_m^{-1}(\beta \mathbf{e}_1)$
	$\mathbf{x}^m = \mathbf{x}^0 + V^m \mathbf{y}^m$

Leads to three-term CG.

To solve, factor first $T_m = LL^T$ and then $\mathbf{x}^m = \mathbf{x}^{(0)} + V^m L^{-T} L^{-1} \beta \mathbf{e}_1$

The CG method:

The CG algorithm using the above relations:

Initialize:	$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b}$, $\mathbf{g}^{(0)} = \mathbf{r}^{(0)}$
For	$k = 0, 1, \cdots$, until convergence
	$\tau_k = \frac{(\mathbf{r}^{(k)},\mathbf{r}^{(k)})}{(A\mathbf{g}^k,\mathbf{g}^{(k)})}$
	$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \tau_k \mathbf{g}^k$
	$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} + \tau_k A\mathbf{g}^k$
	$\beta_k = \frac{(\mathbf{r}^{(k+1)},\mathbf{r}^{(k+1)})}{(\mathbf{r}^{(k)},\mathbf{r}^{(k)})}$
	$\mathbf{g}^{k+1} = \mathbf{r}^{(k+1)} + \beta_k \mathbf{g}^k$
end	

$\mathbf{r}^{(k)}$ – iteratively computed residuals
$\mathbf{g}^k$ – search directions

Note: the coefficients β_k are different from those in the Lanczos method.

CG: computer implementation

```
x = x0
r = A*x-b
delta0 = (r,r)
g = -r
Repeat: h   = A*g
        tau = delta0/(g,h)
        x   = x + tau*g
        r   = r + tau*h
        delta1 = (r,r)
        if delta1 <= eps, stop
        beta = delta1/delta0
        g    = -r + beta*g
```

Optimality properties of the CG method

Opt1: Mutually orthogonal search directions: $(\mathbf{g}^{k+1}, A\mathbf{g}^j) = 0, j = 0, \cdots, k$

Opt2: There holds $\mathbf{r}^{(k+1)} \perp K_m(A, \mathbf{r}^{(0)}$, i.e.,
$(\mathbf{r}^{(k+1)}, A\mathbf{r}^{(k)}) = 0, j = 0, \cdots, k$

Opt3: Optimization property: $\|\mathbf{r}^{(k)}\|$ smallest possible at any step, since CG minimizes the functional $f(\mathbf{x}) = 1/2(\mathbf{x}, A\mathbf{x}) - (\mathbf{x}, \mathbf{b})$

Opt4: $(\mathbf{e}^{(k+1), A\mathbf{g}^j}) = (\mathbf{g}^{k+1}, A\mathbf{g}^j) = (\mathbf{r}^{(k+1)}, \mathbf{r}^{(k)}) = 0, j = 0, \cdots, k$

Opt5: Finite termination property: there are n breakdowns of the CG algorithm.
Reasoning: if $\mathbf{g}^j = \mathbf{0}$ then τ_k is not defined. the vectors $\mathbf{g}^j$ are computed from the formula $\mathbf{g}^k = \mathbf{r}^{(k)} + \beta_k \mathbf{g}^{k-1}$. Then
$0 = (\mathbf{r}^{(k)}, \mathbf{g}^j) = -(\mathbf{r}^{(k)}, \mathbf{r}^{(k)}) + \beta_k \underbrace{(\mathbf{r}^{(k)}, \mathbf{g}^{k-1})}_{0}, \Rightarrow \; \mathbf{r}^{(k)}\mathbf{0}$, i.e., the solution is already found.
As soon as $\mathbf{x}^{(k)} \neq \mathbf{x}_{exact}$, then $\mathbf{r}^{(k)} \neq \mathbf{0}$ and then $\mathbf{g}^{k+1}) \neq \mathbf{0}$.
However, we can generate at most n mutually orthogonal vectors in R^n, thus, CG has a finite termination property.

Convergence analysis

Convergence of the CG method

Theorem: In exact arithmetic, CG has the property that $\mathbf{x}_{exact} = \mathbf{x}^{(m)}$ for some $m \le n$, where n is the order of A.

Rate of convergence of the CG method

Theorem: Let A is symmetric and positive definite.
Suppose that for some set S, containing all eigenvalues of A, for some polynomial $\widetilde{P}(\lambda) \in \Pi_k^1$ and some constant M there holds $\max\limits_{\lambda \in S} \left|\widetilde{P}(\lambda)\right| \le M$.

Then,

$$\|\mathbf{x}_{exact} - \mathbf{x}^{(k)}\|_A \le M \|\mathbf{x}_{exact} - \mathbf{x}^{(0)}\|_A.$$

$$\|\mathbf{e^k}\|_A \le 2 \left[\frac{\varkappa(A) + 1}{\varkappa(A) - 1}\right]^k \|\mathbf{e^0}\|_A$$

Rate of convergence (cont)

Repeat:

$$\|\mathbf{e^k}\|_A \leq 2 \left[\frac{\varkappa(A)+1}{\varkappa(A)-1} \right]^k \|\mathbf{e^0}\|_A$$

Seek now the smallest k, such that

$$\|\mathbf{e}^k\|_A \leq \varepsilon \|\mathbf{e}^0\|_A$$

$$\text{we want } \left(\tfrac{\varkappa+1}{\varkappa-1}\right)^k > \tfrac{2}{\varepsilon}$$

$$\Rightarrow \ k \ ln\left(\tfrac{\varkappa+1}{\varkappa-1}\right) > ln(\tfrac{2}{\varepsilon})$$

$$\Rightarrow \ k > ln(\tfrac{2}{\varepsilon})/ln\left(\tfrac{\varkappa+1}{\varkappa-1}\right)$$

$$\Rightarrow \ k > \tfrac{1}{2}\sqrt{\varkappa}\, ln(\tfrac{2}{\varepsilon})$$

The GMRES method

Basic GMRES

Choose $\mathbf{v}_1$ to be the normalized $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$.
Any vector $\mathbf{x} \in \mathbf{x}_0 + K$ is of the form $\mathbf{x} = \mathbf{x}_0 + V_m\mathbf{y}$. Then

$$\begin{aligned}
\mathbf{b} - A\mathbf{x} &= \mathbf{b} - A(\mathbf{x}_0 + V_m\mathbf{y}) \\
&= \mathbf{r}_0 - AV_m\mathbf{y} \\
&= \beta\mathbf{v}_1 - V_{m+1}\widetilde{H}_m\mathbf{y} \\
&= V_{m+1}(\beta\mathbf{e}_1 - \widetilde{H}_m\mathbf{y}).
\end{aligned}$$

Since the columns of V_{m+1} are orthonormal, then

$$\|\mathbf{b} - A\mathbf{x}\|_2 = \|\beta\mathbf{e}_1 - \widetilde{H}_m\mathbf{y}\|_2.$$

Basic GMRES

1. Compute $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$, $\beta = \|\mathbf{r}_0\|_2$ and $\mathbf{v}_1 = \mathbf{r}_0/\beta$
2. For $j = 1, 2, \cdots, m$
3.   Compute $\mathbf{w}_j = A\mathbf{v}_j$
4.   For $i = 1, 2, \cdots, j$
5. $h_{ij} = (\mathbf{w}_j, \mathbf{v}_i)$
6. $\mathbf{w}_j = \mathbf{w}_j - h_{ij}\mathbf{v}_i$
7.   End
8. $h_{j+1,j} = \|\mathbf{w}_j\|_2$; if $h_{j+1,j} = 0$, set $m = j$, goto 11
9. $\mathbf{v}_{j+1} = \mathbf{w}_j / h_{j+1,j}$
10. End
11. Define the $(m+1) \times m$ Hessenberg matrix $\widetilde{H}_m = \{h_{ij}\}, 1 \leq i \leq m+1, 1 \leq j \leq m$
12. Compute $\mathbf{y}_m$ as the minimizer of $\|\beta \mathbf{e}_1 - \widetilde{H}_m \mathbf{y}\|_2$ and $\mathbf{x}_m = \mathbf{0} + V_m \mathbf{y}_m$

GMRES:

- No breakdown of GMRES
- As m increases, storage and work per iteration increase fast. Remedies:
  - Restart (keep m constant)
  - Truncate the orthogonalization process
- The norm of the residual in the GMRES method is monotonically decreasing. However, the convergence may stagnate. The rate of convergence of GMRES canot be determined so easy as that of CG.

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