Krylov subspace methods

- Introduction to Krylov subspace techniques
- FOM, GMRES, practical details.
- Symmetric case: Conjugate gradient
- See Chapter 6 of text for details.

Motivation

➤ Common feature of one-dimensional projection techniques:

$$x_{new} = x + \alpha d$$

where d = a certain direction.

➤ α is defined to optimize a certain function.

➤ Equivalently: determine α by an orthogonality constraint

Example

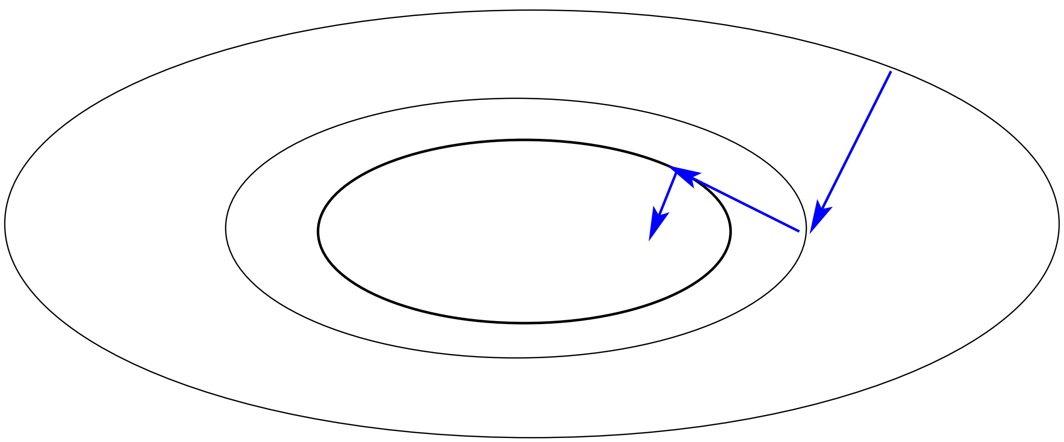
In MR:
$x(\alpha) = x + \alpha d$, with $d = b - Ax$.
$\min_\alpha \|b - Ax(\alpha)\|_2$ reached iff $b - Ax(\alpha) \perp r$

➤ One-dimensional projection methods are greedy methods. They are 'short-sighted'.

Example:

Recall in Steepest Descent: New direction of search $\tilde{r}$ is $\perp$ to old direction of search r.

$$\boxed{\begin{array}{l} r \leftarrow b - Ax, \\ \alpha \leftarrow (r, r)/(Ar, r) \\ x \leftarrow x + \alpha r \end{array}}$$



Question: can we do better by combining successive iterates?

➤ Yes: Krylov subspace methods..

Krylov subspace methods: Introduction

➤ Consider MR (or steepest descent). At each iteration:

$$\begin{aligned} r_{k+1} &= b - A(x^{(k)} + \alpha_k r_k) \\ &= r_k - \alpha_k A r_k \\ &= (I - \alpha_k A) r_k \end{aligned}$$

➤ In the end:

$$r_{k+1} = (I - \alpha_k A)(I - \alpha_{k-1} A) \cdots (I - \alpha_0 A) r_0 = p_{k+1}(A) r_0$$

where $p_{k+1}(t)$ is a polynomial of degree $k + 1$ of the form

$$p_{k+1}(t) = 1 - t q_k(t)$$

✍ Show that: $x^{(k+1)} = x^{(0)} + q_k(A) r_0$, with deg $(q_k) = k$

➤ Krylov subspace methods: iterations of this form that are 'optimal' [from m-dimensional projection methods]

Krylov subspace methods

Principle: Projection methods on Krylov subspaces:

$$K_m(A, v_1) = \text{span}\{v_1, Av_1, \cdots, A^{m-1}v_1\}$$

- The most important class of iterative methods.
- Many variants exist depending on the subspace L.

Simple properties of K_m

➤ Notation: μ = deg. of minimal polynomial of v. Then:

- $K_m = \{p(A)v | p = \text{polynomial of degree} \leq m - 1\}$
- $K_m = K_\mu$ for all $m \geq \mu$. Moreover, K_μ is invariant under A.
- $dim(K_m) = m$ iff $\mu \geq m$.

A little review: Gram-Schmidt process

Goal: given $X = [x_1, \ldots, x_m]$ compute an orthonormal set $Q = [q_1, \ldots, q_m]$ which spans the same susbpace.

ALGORITHM : 1. *Classical Gram-Schmidt*

1. *For* $j = 1, ..., m$ *Do:*
2. *Compute* $r_{ij} = (x_j, q_i)$ *for* $i = 1, \ldots, j-1$
3. *Compute* $\hat{q}_j = x_j - \sum_{i=1}^{j-1} r_{ij} q_i$
4. $r_{jj} = \|\hat{q}_j\|_2$ *If* $r_{jj} == 0$ *exit*
5. $q_j = \hat{q}_j / r_{jj}$
6. *EndDo*

ALGORITHM : 2. *Modified Gram-Schmidt*

1. *For* $j = 1, ..., m$ *Do:*
2. $\quad \hat{q}_j := x_j$
3. $\quad$ *For* $i = 1, \ldots, j-1$ *Do*
4. $\quad\quad r_{ij} = (\hat{q}_j, q_i)$
5. $\quad\quad \hat{q}_j := \hat{q}_j - r_{ij} q_i$
6. $\quad$ *EndDo*
7. $\quad r_{jj} = \|\hat{q}_j\|_2$. *If* $r_{jj} == 0$ *exit*
8. $\quad q_j := \hat{q}_j / r_{jj}$
9. *EndDo*

Let:

$\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m]$ ($\boldsymbol{n} \times \boldsymbol{m}$ matrix)

$\boldsymbol{Q} = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_m]$ ($\boldsymbol{n} \times \boldsymbol{m}$ matrix)

$\boldsymbol{R} = \{\boldsymbol{r}_{ij}\}$ ($\boldsymbol{m} \times \boldsymbol{m}$ upper triangular matrix)

- At each step,

$$\boldsymbol{x}_j = \sum_{i=1}^{j} \boldsymbol{r}_{ij} \boldsymbol{q}_i$$

Result:

$$\boxed{\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{R}}$$

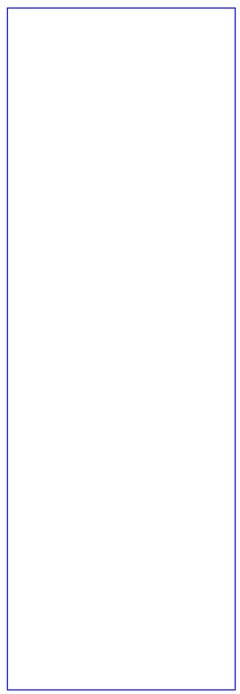
Arnoldi's algorithm

- Goal: to compute an orthogonal basis of K_m.
- Input: Initial vector v_1, with $\|v_1\|_2 = 1$ and m.

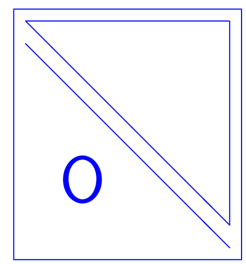
For $j = 1, ..., m$ Do:
  Compute $w := Av_j$
  For $i = 1, \ldots, j$ Do:
    $h_{i,j} := (w, v_i)$
    $w := w - h_{i,j}v_i$
  EndDo
  Compute: $h_{j+1,j} = \|w\|_2$ and $v_{j+1} = w/h_{j+1,j}$
EndDo

Result of orthogonalization process (Arnoldi):

1. $V_m = [v_1, v_2, ..., v_m]$ orthonormal basis of K_m.
2. $AV_m = V_{m+1}\overline{H}_m$
3. $V_m^T AV_m = H_m \equiv \overline{H}_m -$ last row.

$V_m =$ 

$$AV_m = V_{m+1}\overline{H}_m$$

$\overline{H}_m =$ 

$$V_{m+1} = [V_m, v_{m+1}]$$

Arnoldi's Method for linear systems ($L_m = K_m$)

From Petrov-Galerkin condition when $L_m = K_m$, we get

$$x_m = x_0 + V_m H_m^{-1} V_m^T r_0$$

If, in addition we choose $v_1 = r_0/\|r_0\|_2 \equiv r_0/\beta$ in Arnoldi's algorithm, then

$$\boxed{x_m = x_0 + \beta V_m H_m^{-1} e_1}$$

Several algorithms mathematically equivalent to this approach:

* FOM [Y. Saad, 1981] (above formulation), Young and Jea's ORTHORES [1982], Axelsson's projection method [1981],..

* Also Conjugate Gradient method [see later]

Minimal residual methods ($L_m = AK_m$)

When $L_m = AK_m$, we let $W_m \equiv AV_m$ and obtain relation

$$\begin{aligned} x_m &= x_0 + V_m[W_m^T AV_m]^{-1}W_m^T r_0 \\ &= x_0 + V_m[(AV_m)^T AV_m]^{-1}(AV_m)^T r_0. \end{aligned}$$

➤ Use again $v_1 := r_0/(\beta := \|r_0\|_2)$ and the relation

$$\boxed{AV_m = V_{m+1}\bar{H}_m}$$

➤ $x_m = x_0 + V_m[\bar{H}_m^T \bar{H}_m]^{-1}\bar{H}_m^T \beta e_1 = x_0 + V_m y_m$
where y_m minimizes $\|\beta e_1 - \bar{H}_m y\|_2$ over $y \in \mathbb{R}^m$.

➤ Gives the Generalized Minimal Residual method (GMRES) ([Saad-Schultz, 1986]):

$$\begin{aligned} x_m &= x_0 + V_m y_m \quad \text{where} \\ y_m &= \min_y \|\beta e_1 - \bar{H}_m y\|_2 \end{aligned}$$

➤ Several Mathematically equivalent methods:

- Axelsson's CGLS
- Orthomin (1980)
- Orthodir
- GCR

A few implementation details: GMRES

Issue 1 : How to solve the least-squares problem ?

Issue 2: How to compute residual norm (without computing solution at each step)?

- Several solutions to both issues. Simplest: use Givens rotations.
- Recall: We want to solve least-squares problem

$$\min_y \|\beta e_1 - \overline{H}_m y\|_2$$

- Transform the problem into upper triangular one.

➤ Rotation matrices of dimension $m+1$. Define (with $s_i^2 + c_i^2 = 1$):

$$\Omega_i = \begin{array}{cl} \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & s_i & & & \\ & & & -s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix} & \begin{array}{l} \\ \\ \\ \leftarrow \text{row } i \\ \leftarrow \text{row } i+1 \\ \\ \\ \\ \end{array} \end{array}$$

➤ Multiply $\bar{H}_m$ and right-hand side $\bar{g}_0 \equiv \beta e_1$ by a sequence of such matrices from the left. ➤ s_i, c_i selected to eliminate $h_{i+1,i}$

$$\bar{H}_5 = \begin{bmatrix} h_{11} & h_{12} & h_{13} & h_{14} & h_{15} \\ h_{21} & h_{22} & h_{23} & h_{24} & h_{25} \\ & h_{32} & h_{33} & h_{34} & h_{35} \\ & & h_{43} & h_{44} & h_{45} \\ & & & h_{54} & h_{55} \\ & & & & h_{65} \end{bmatrix}, \quad \bar{g}_0 = \begin{bmatrix} \beta \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- 1-st Rotation:

$$\Omega_1 = \begin{bmatrix} c_1 & s_1 & & & \\ -s_1 & c_1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix} \text{ with: } \quad \begin{aligned} s_1 &= \frac{h_{21}}{\sqrt{h_{11}^2 + h_{21}^2}}, \\ c_1 &= \frac{h_{11}}{\sqrt{h_{11}^2 + h_{21}^2}} \end{aligned}$$

$$\bar{H}_m^{(1)} = \begin{bmatrix} h_{11}^{(1)} & h_{12}^{(1)} & h_{13}^{(1)} & h_{14}^{(1)} & h_{15}^{(1)} \\ & h_{22}^{(1)} & h_{23}^{(1)} & h_{24}^{(1)} & h_{25}^{(1)} \\ & h_{32} & h_{33} & h_{34} & h_{35} \\ & & h_{43} & h_{44} & h_{45} \\ & & & h_{54} & h_{55} \\ & & & & h_{65} \end{bmatrix}, \quad \bar{g}_1 = \begin{bmatrix} c_1\beta \\ -s_1\beta \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Repeat with $\Omega_2, \ldots, \Omega_i$. Result:

$$\bar{H}_5^{(5)} = \begin{bmatrix} h_{11}^{(5)} & h_{12}^{(5)} & h_{13}^{(5)} & h_{14}^{(5)} & h_{15}^{(5)} \\ & h_{22}^{(5)} & h_{23}^{(5)} & h_{24}^{(5)} & h_{25}^{(5)} \\ & & h_{33}^{(5)} & h_{34}^{(5)} & h_{35}^{(5)} \\ & & & h_{44}^{(5)} & h_{45}^{(5)} \\ & & & & h_{55}^{(5)} \\ & & & & 0 \end{bmatrix}, \quad \bar{g}_5 = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \cdot \\ \cdot \\ \gamma_6 \end{bmatrix}$$

Define

$$\begin{aligned} Q_m &= \Omega_m \Omega_{m-1} \ldots \Omega_1 \\ \bar{R}_m &= \bar{H}_m^{(m)} = Q_m \bar{H}_m, \\ \bar{g}_m &= Q_m(\beta e_1) = (\gamma_1, \ldots, \gamma_{m+1})^T. \end{aligned}$$

- Since Q_m is unitary,

$$\min \|\beta e_1 - \bar{H}_m y\|_2 = \min \|\bar{g}_m - \bar{R}_m y\|_2.$$

- Delete last row and solve resulting triangular system.

$$R_m y_m = g_m$$

Proposition:

1. The rank of AV_m is equal to the rank of R_m. In particular, if $r_{mm} = 0$ then A must be singular.
2. The vector y_m which minimizes $\|\beta e_1 - \bar{H}_m y\|_2$ is given by

$$y_m = R_m^{-1} g_m.$$

3. The residual vector at step m satisfies

$$\begin{aligned} b - Ax_m &= V_{m+1}\left[\beta e_1 - \bar{H}_m y_m\right] \\ &= V_{m+1} Q_m^T (\gamma_{m+1} e_{m+1}) \end{aligned}$$

4. As a result, $\|b - Ax_m\|_2 = |\gamma_{m+1}|$.