October 15, 2013

This week: Tue / Thur

Next Tues: Eldad Haber

Only one more assignment
- project proposal & more questions

Assign 1 - this week by Friday

GMRES + CG: the gory details:

GMRES:

$$x_k = x_0 + V z_k$$

where $z_k = \underset{z}{\operatorname{argmin}} \|\rho e_1 - H_{k+1,k} z\|_2$

$$\rho = \|r_0\|_2$$

To generate $H_{k+1,k}$: Arnoldi $(AQ_k = Q_{k+1} H_{k+1,k})$

Outline of algorithm:

$r_0 = b - Ax_0$

$\rho = \|r_0\|_2$

$q_1 = \frac{r_0}{\rho}$

For $j = 1, \ldots, k$ do Arnoldi-Modified Gram-Schmidt

  Compute $w_j = Aq_j$

  For $i = 1, \ldots, j$

    $h_{ij} = (w_j, q_i)$

    $w_j = w_j - h_{ij} q_i$

  end do

  $h_{j+1,j} = \|w_j\|_2$

  if $h_{j+1,j} = 0$ set $k = j$ and jump out of loop

  $q_{j+1} = w_j / h_{j+1,j}$

$$H_{k+1,k} = \{h_{ij}\}$$

end do

$$z_k \leftarrow \min \|\rho e_1 - H_{k+1,k} z\|$$

$$x_k \leftarrow x_0 + Q z_k$$

We generate $H_{k+1,k}$ using Arnoldi MGS

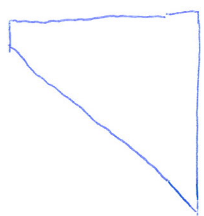
↳ a (probably) better way: Householder Arnoldi

* Note: solution is not explicitly given at every step

When do we stop?

look at the least squares problem...

$$\min \|\rho e_1 - H_{k+1,k} z\|$$

$H_{k+1,k} =$  $=$

$k=5$

$$\begin{matrix} h_{11} & h_{12} & h_{13} & h_{14} & h_{15} \\ h_{21} & \ddots & & & \vdots \\ & \ddots & \ddots & & \\ & & \ddots & & h_{55} \\ & & & \ddots & h_{56} \end{matrix}$$

problem: $\min \|b - Ax\|$ (note: not same A, b, x).

$$\phi(x) = \|b - Ax\|^2$$
$$= (b-Ax)^T(b-Ax)$$

$$\nabla\phi = 0 \Rightarrow A^TAx = A^Tb \leftarrow \text{normal equations}$$ very good if A is well-conditioned, otherwise use QR

$$QR: A = QR \Rightarrow R^T \underbrace{Q^TQ}_{I} Rx = R^TQ^Tb$$
$$x = R^{-1}(Q^Tb) \leftarrow \text{economy size.}$$

How to form QR:

① Gram-Schmidt: triangularly orthogonalize

② Householder: force $A \to R$

$$\|V\|_2 = 1 \qquad (I - 2VV^*)x$$

$$\underbrace{(I - 2VV^*)}_{Q_1} a_1 = \beta e_1$$

$$\begin{pmatrix} | & | & \\ a_1 & a_2 & \cdots \\ | & | & \end{pmatrix} \xrightarrow[\text{transform}]{\text{orthogonal}} \begin{pmatrix} \beta & \cdots & \vdots \\ & \ddots & \vdots \\ 0 & & \vdots \end{pmatrix}$$

$a_1 - \gamma v = \beta e_1$ * to choose sign, try to add rather than subtract (to reduce cancellation errors).

$\gamma v = a_1 - \beta e_1$

$|\beta| = \|a_1\|$

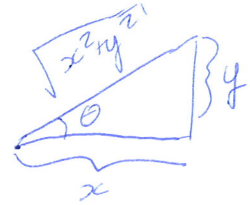
take norms

$|\gamma| = \|a_1 - \beta e_1\|$

$$v = \frac{a_1 - \beta e_1}{\|a_1 - \beta e_1\|}$$

③ Givens rotations:

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix}\begin{pmatrix} x & x \\ x & x \end{pmatrix} = \begin{pmatrix} x & x \\ 0 & x \end{pmatrix}$$



$c \equiv \cos\theta$

$s \equiv \sin\theta$

$c^2 + s^2 = 1$

$$c = \frac{x}{\sqrt{x^2+y^2}} \qquad s = \frac{y}{\sqrt{x^2+y^2}}$$

so

* Rotation is an orthogonal transformation (preserves the norm)

zero out the -1 diagonal

↳ so you get an upper triangular matrix

$$s_1 = \frac{h_{21}}{\sqrt{h_{11}^2 + h_{21}^2}} \qquad c_1 = \frac{h_{11}}{\sqrt{h_{11}^2 + h_{21}^2}}$$

Apply

$$P_1 = \begin{pmatrix} c_1 & s_1 & \\ -s_1 & c_1 & \\ & & I \end{pmatrix} \qquad H \to \begin{pmatrix} x & x & \cdots & x \\ 0 & x & \cdots & x \\ & x & x \cdots & x \\ & & \ddots & \vdots \\ & & & x \end{pmatrix} = P_1 H$$

$$P_2 = \begin{pmatrix} 1 & & & \\ & c_2 & s_2 & \\ & -s_2 & c_2 & \\ & & & I \end{pmatrix} \to P_2 P_1 H = \begin{pmatrix} x & & & & \\ 0 & x & & & \\ & 0 & x & & \\ & & x & x & \\ & & & \ddots & x \\ & & & & x \end{pmatrix}$$

$H_{k+1,k}\, z \approx \beta e_1$

$$\begin{pmatrix} \beta \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{k+1 \text{ elements}} \xrightarrow{\text{apply } P_1} \begin{pmatrix} c_1 \beta \\ -s_1 \beta \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

in the end, we will have

$$\begin{array}{c} k \\ \left(\begin{array}{cc} & R \\ O & \end{array}\right)_{k+1} \end{array} \qquad \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_{k+1} \end{pmatrix}$$

we have taken

$$H_{k+1,k}\, z \approx \beta e_1 \longrightarrow \begin{pmatrix} R \\ 0 \end{pmatrix} z \approx \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_{k+1} \end{pmatrix}$$

residual : γ_{k+1} : $|\gamma_{k+1}|$ = norm of residual.

↳ don't need to work extra to form residual.

so $|\gamma_{k+1}|$ can be used as a stopping criteria

One final comment:

$h_{j+1,j} = 0$

↳ lucky breakdown: means we have constructed the entire basis for Krylov subspace : quit + be happy!

↳ how small is zero

FGMRES: flexible GMRES - use $\{M_j\}$ preconditioners throughout...