Lecture 25

Intro slides and overview of other iterative methods.

An optimized GMRES method for non-symmetric systems with Arnoldi.
* Updating only what is needed.
* QR of upper-Hessenberg matrices
* updating the right hand side

Then we go back to CG using as a very round-about way with orthogonal polynomials.

Goal: to understand the relationship between orthogonal polynomials and matrix computations

Orthogonal polynomials
- Three-term recurrences
- Three-term recurrences and tridiagonal matrices
- Evaluating orthogonal polys in Julia

(We'll probably only get here...)

Polys and residuals with matrix arguments.
Picking a set of orthogonal polynomials.

GMRES Overview

Given $\boldsymbol{A}, \mathbf{b}$ where we can only multiply by $\boldsymbol{A}$.

for $k = 1$ to maxiter

Update the Arnoldi factorization $\boldsymbol{Q}_k, \boldsymbol{H}_{k+1}$. → $O(k)$ mdots, + one mvproduct

Solve for $\mathbf{z}_k$ by minimizing $\|\boldsymbol{H}_{k+1}\mathbf{z}_k - \|\mathbf{b}\|\mathbf{e}_1\|$.

i.e. $\mathbf{z}_k = \operatorname{argmin} \|\boldsymbol{H}_{k+1}\mathbf{z}_k - \|\mathbf{b}\|\mathbf{e}_1\|$

Let $\mathbf{x}_k = \boldsymbol{Q}_k \mathbf{z}_k$.

Check $\|\boldsymbol{A}\mathbf{x}_k - \mathbf{b}\|$ = $\|b - A\mathbf{x}_k\|$ when $\mathbf{x}_k \approx \mathbf{x}_*$ & $\|\mathbf{r}_k\| \approx 0$

$O(k)$ mdots

Mdots: Project a vector onto the orthogonal basis. $O(k^2 n)$ flops. $O(k^2)$ for the upper-triangular solve.

Given $\boldsymbol{A}, \mathbf{b}$ where we can only multiply by $\boldsymbol{A}$.
for $k=1$ to maxiter
Update the Arnoldi factorization $\boldsymbol{Q}_k, \boldsymbol{H}_{k+1}$.
Compute $\|\mathbf{r}_k\|$ where
$\mathbf{r}_k = \boldsymbol{A}\mathbf{x}_k - \mathbf{b}$
$\mathbf{x}_k = \boldsymbol{Q}_k \mathbf{z}_k$
$\mathbf{z}_k = \operatorname{argmin} \|\boldsymbol{H}_{k+1}\mathbf{z}_k - \|\mathbf{b}\|\mathbf{e}_1\|$
and stop once $\|\mathbf{r}_k\|$ is sufficiently small, i.e.
Explicitly compute $\mathbf{z}_k = \operatorname{argmin} \|\boldsymbol{H}_{k+1}\mathbf{z}_k - \|\mathbf{b}\|\mathbf{e}_1\|$ and
and return $\mathbf{x}_k = \boldsymbol{Q}_k \mathbf{z}_k$ only at the end of the iteration

We want $\|r_k\|_2$ when
$\|r_k\|_2 = \|Ax_k - b\|_2 = \|Ax - AQ_k y_k\|_2$
$= \|H_{k+1} z_k - \|b\| e_1\|_2$

Future figure 0.1 how to get that to the right place.

H_k is:

$$\begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix} y_k = \|b\| \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

H_k

For LS, we know QR. Let $H_k = Q_k R_k$.

$\|r_k\| = \|Q_{k+1} R_k y_k - \|b\| e_1\|_2$

$= \|R_k y_k - Q_{k+1}^T \|b\| e_1\|_2$

$= \left\| \begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & 0 \end{pmatrix} y_k - \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ g_5 \end{pmatrix} \right\|_2$

$\Rightarrow$

$\|r_k\| = \|g_5\|$

We need to find y_k to get the result back.

How to do QR on H_k.

Step

$$\begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix} \xrightarrow{U_1} \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix} \xrightarrow{U_2} \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix} \xrightarrow{U_3} \begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{pmatrix}$$

(explicit)

$$\xrightarrow{2nd} \begin{bmatrix} \times \\ \times \\ \times \\ \times \\ \times \end{bmatrix} \xrightarrow{U_2^T} \begin{bmatrix} \times \\ \times \\ 0 \\ \times \\ \times \end{bmatrix} \xrightarrow{\text{Add pivot}} \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix}$$

Apply U_3^T to it

$$\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix} \xrightarrow{U_3^T} \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix}$$

$$U_4^T U_3^T U_2^T U_1^T H_k = \begin{pmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Its Weight:

$U_4 = J_1 U_3^T U_2^T \cdots U_1^T$

$U_4 R_k = H_k$

$$H_k = \begin{bmatrix} H_k & b \\ 0 & h_{k,k} \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} U_k^T & 0 \\ 0 & 1 \end{bmatrix} H_k = \begin{bmatrix} U_k^T H_k & U_k^T b \\ 0 & h_{k,k} \end{bmatrix}$$

Given $U_k^T b$, Compt

J_k st. we can at basis.

$\Rightarrow U_k^T = J_k U_k - J_1$

Let $g_k = U_k^T e_1$

$U_k^T = J_k - J_1 e_1$

$g_{k+1} = J_{k+1} \begin{bmatrix} g_k \\ 0 \end{bmatrix}$

Just apply J_{k+1} to last 2

Start with g^1

Clearly g_k is the leading vector used in the polynomial.

Q. Degree O poly?

Orthogonal Polys

$$p(x) = \sum_{j=0}^{k} c_j x^j$$

is a convenient poly!

Ex. $p(x) = \frac{1}{2}x^2 - \frac{1}{2}$

$q(x) = \frac{1}{2}x^2 - \frac{3}{2}x + \frac{2}{3}$

Degree 2 $\Rightarrow$ Degree 2

$\Rightarrow p(x), q(x)$ are orthogonal!

Vectors:

$u^T v = 0$ if u, v are orthog

$u^T u = \sum_{i=1}^{n} u_i u_i$

2 polys f, g are orthogonal if $\int_{a}^{b} f(x) g(x)\, dx = 0$.

① on weights interval $\int_{a}^{b} f(x) g(x) w(x)\, dx = 0$. Weight function

If $w(x) = 1$ such times $\int f(x) g(x)\, dx$. $\int_{-1}^{1} f(x) g(x)\, dx = 0$.

② More generally poly C_k orthog. w.r.t. $\int_{a}^{b} f(x) g(x) w(x)\, dx = 0$.

③ on arbitrary interval $\int_{a}^{b} f(x) g(x) w(x)\, dx = 0$.

④ $w(x) = \begin{cases} 1 & x \in [x_1, x_2] \\ 0 & \text{otherwise} \end{cases}$ $\Rightarrow \int_{x_1}^{x_2} f(x) g(x)\, dx$

Orth poly sequence:

Let $P_k(x)$ be a deg k poly that then

$P_0(x) = 1$

$P_1(x) = x$

$P_2(x) = \frac{1}{2}(3x^2 - 1)$

$P_3(x) = \frac{1}{2}(5x^3 - x)$

$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$

are orthog. w.r.t. $\int_{-1}^{1} f(x) g(x)\, dx = 0$.

Called Legendre polys

Other tools:

Lagrange poly: if $\int_{0}^{\infty} f(x) e^{-x}\, dx$

Hermite: $\int_{-\infty}^{\infty} f(x) e^{-x^2}\, dx$.

Chebyshev: $\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\, dx$

Tools:

Gaussian —

All orthogonal polys satisfy a 3-term recurrence

Ex. Legendre

$$P_{k+1}(x) = \frac{(2k+1)}{k+1} x P_k(x) - \frac{k}{k+1} P_{k-1}(x)$$

$$P_2(x) = \frac{(2+1)}{(1+1)} (x^2) - \frac{1}{(1+1)} [1]$$

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In general

$$P_{n+1}(t) = p_n(P_n(t) - q_n t P_n(t)) + q_n P_{n-1}(t)$$

Claim by p_n, q_n, q_n..

And any seq. gives you a orthog. poly!

3-term Recurrence gives you matrix:

$$\begin{bmatrix} -t & 1 & & \\ 1 & -3t & 2 & \\ 0 & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} P_0(t) \\ P_1(t) \\ P_2(t) \\ \vdots \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$(-2k+1)\,P_{k-1}$

(a) $P_0(t) = 1$

(b) $-tP_0(t) + P_1(t) = 0 \Rightarrow P_1(t) = t$

(c) $P_0(t) - 3tP_1(t) + 2P_2(t) = 0 \Rightarrow$

$P_2(t) = \frac{3}{2}t^2 - \frac{1}{2}P_0(t)$

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