Iterative Methods

Part 4: Lanczos Iterations & Conjugate Gradient

Recap

$$K_n(A,b) = \text{span}\{b, Ax, \dots, A^{n-1}x\}$$

$$\begin{bmatrix} | & | & & | \\ b & Ab & \cdots & A^{n-1}b \\ | & | & & | \end{bmatrix} = Q_n R_n, \qquad AQ_n = H_n Q_n + h q_{n+1} e_n^T$$

QR factor of Krylov Mat — Arnoldi Decomposition

$\Rightarrow$ Approximate solutions to $Ax = \lambda x$ and $Ax = b$ constructed from Q_n and H_n

Lanczos Iterations

When A is real-symmetric (or Hermitian), the matrix H_n is actually tridiagonal.

$$H_n = Q_n^T A Q_n \iff H_n^T = (Q_n^T A Q_n)^T$$
$$= Q_n^T A^T Q_n$$
$$= Q_n^T A Q_n$$
$$= H_n$$

$\Rightarrow$ H_n is upper Hessenberg & symmetric, therefore it is tridiagonal, $H_n = T_n$.

$$A \begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ & & \beta_{n-1} & \alpha_n \end{bmatrix}$$

$$\qquad Q_n \qquad\qquad\qquad Q_n \qquad\qquad T_n$$

$$A q_k = \beta_{k-1} q_{k-1} + \alpha_k q_k + \beta_k q_{k+1} \qquad (\beta_0 = 0)$$

$$\beta_k q_{k+1} = (A - \alpha_k I) q_k - \beta_{k-1} q_{k-1}$$

Three term recurrence means that we don't <u>explicitly</u> orthogonalize against $q_1, \ldots, q_{k-2}$!

$\Rightarrow$ T_n and its eigenvalues are intimately connected with the theory of orthogonal polynomials and their roots.

$\Rightarrow$ In floating point arithmetic, Q_n suffers loss of orthogonalization related to convergence of Ritz values: one needs to explicitly reorthogonalize.

<u>The method of Conjugate Gradients (CG)</u>

$\Rightarrow$ Like GMRES, CG approximates $x_* = A^{-1}b$ by solving an optimization problem over the Krylov subspace $K_n(A,b)$.

Let A be (real) symmetric positive definite (SPD) so that $x^T A x > 0$ for every nonzero $x \in \mathbb{R}^m$.

Then $\langle x,y\rangle_A = x^T A y$ defines an inner product and $\|x\|_A = \sqrt{\langle x,x\rangle_A} = \sqrt{x^T A x}$ defines a norm.

$\Rightarrow$ CG minimizes $e_n = x_* - x_n$ over $x_n \in K_n(A,b)$ in the norm $\|\cdot\|_A$ with n mat-vecs.

<u>CG Iteration</u>

$x_0 = 0$, $r_0 = b$, $p_0 = r_0$

for $n = 1,2,3,\ldots$

	$\alpha_n = (r_{n-1}^T r_{n-1})/(p_{n-1}^T A p_{n-1})$	step size
	$x_n = x_{n-1} + \alpha_n p_{n-1}$	approx. soln.
	$r_n = r_{n-1} - \alpha_n A p_{n-1}$	residual
	$\beta_n = (r_n^T r_n)/(r_{n-1}^T r_{n-1})$	improvement
	$p_n = r_n + \beta_n p_{n-1}$	search direction

Note: only one mat-vec required. Everything else is vector operations.

The optimality of CG is due to orthogonality relations of the residuals and search directions.

<u>Thm 1</u> If A is SPD and $r_{n-1} \neq 0$ (not yet converged), then

$$K_n = \text{span}\{x_1, x_2, \ldots, x_n\} = \text{span}\{p_1, p_2, \ldots, p_{n-1}\}$$

$$= \text{span}\{r_0, r_1, \ldots, r_{n-1}\} = \text{span}\{b, Ab, \ldots, A^{n-1}b\}$$

Also, $r_n^T r_j = 0$ for $j<n$ and $p_n^T A p_j = 0$ for $j<n$.

<u>Pf</u> (Sketch) $x_0 = 0$ and $x_n = x_{n-1} + \alpha p_{n-1}$ means $S = \text{span}\{x_1, x_2, \ldots, x_n\} = \text{span}\{p_0, \ldots, p_{n-1}\}$. Similarly, $p_n = r_n + \beta_n p_{n-1} \Rightarrow r_n = p_n - \beta_n p_{n-1}$ means $S = \text{span}\{r_0, r_1, \ldots, r_{n-1}\}$. And since $r_n = r_{n-1} - \alpha_n A p_{n-1}$ with $r_0 = p_0 = b$, we have $S = \text{span}\{b, Ab, \ldots, A^{n-1}b\}$.

Now,
$$r_n^T r_j = (r_{n-1} - \alpha_n A p_{n-1})^T r_j$$
$$= r_{n-1}^T r_j - \alpha_n p_{n-1}^T A r_j \quad (A^T = A)$$

for $j < n-1$, induction hyp. $\Rightarrow r_{n-1}^T r_j = 0$ and

$$p_{n-1}^T A r_j = p_{n-1}^T A(p_j - \beta_n p_{j-1}) = p_{n-1}^T A p_j - p_{n-1}^T A p_{j-1} = 0.$$

for $j = n-1$, $r_n^T r_{n-1} = r_{n-1}^T r_{n-1} - \alpha_n p_{n-1}^T A r_{n-1}$

$$= r_{n-1}^T r_{n-1} - \alpha_n p_{n-1}^T A(p_{n-1} - \beta_n p_{n-2})$$

$$= r_{n-1}^T r_{n-1} - \alpha_n p_{n-1}^T A p_{n-1}$$

$$= r_{n-1}^T r_{n-1} - \frac{r_{n-1}^T r_{n-1}}{p_{n-1}^T A p_{n-1}} p_{n-1}^T A p_{n-1}$$

$$= r_{n-1}^T r_{n-1} - r_{n-1}^T r_{n-1} = 0 \checkmark$$

Similar calculation shows $p_n^T A p_j = 0$ for $j < n$.

Now, we can explain how CG minimizes $\|e_n\|_A$ over $K_n(A,b)$

<u>Thm 2</u> Under hypotheses of Thm 1, x_n is the unique minimizer of $\|e_n\|_A$ in $K_n(A,b)$. Moreover, $\|e_n\|_A \le \|e_{n-1}\|_A$ and $e_n = 0$ is achieved for some $n \le m$.

<u>Pf</u> (Sketch)

Take $x = x_n - \Delta x \in K_n$ with

$e = x_* - x = e_n + \Delta x$. Then,

$$\|e\|_A^2 = (e_n + \Delta x)^T A (e_n + \Delta x)$$
$$= e_n^T A e_n + (\Delta x)^T A (\Delta x) + 2 e_n^T A (\Delta x)$$

Now, $e_n^T A = (x_n - x)^T A = (A(x_n - x))^T = (A x_n - b)^T = r_n^T$

$$\Rightarrow \quad 2 e_n^T A (\Delta x) = 2 r_n^T (\Delta x)$$

Since $\Delta x = x_n - x \in K_n(A, b) = \text{span}\{r_0, \ldots, r_{n-1}\}$

and $r_n^T r_j = 0,\ j < n \Rightarrow r_n^T (\Delta x) = 0$

Therefore $\|e\|_A^2 = e_n^T A e_n + \underbrace{(\Delta x)^T A (\Delta x)}_{> 0 \text{ by } A \text{ SPD}}$

$$\Rightarrow \quad \|e\|_A > \|e_n\|_A$$

$\Rightarrow$ e_n is unique minimizer.