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Convergence of CG method

CG iterate x^m was defined as a minimizer of the quadratic functional

$$J(y) = \frac{1}{2}(A(x-y), x-y) - \frac{1}{2}(Ax, x)$$

over all y in the space $\{x^0\} + K_m(A, r^0)$

$$K_m(A, r^0) = \{r^0, Ar^0, \dots, A^{m-1}r^0\}$$

That is

$$x^m = x^0 + \theta^m \qquad \theta^m \in K_m$$

is a minimizer of $J(y)$

and such that

$$\frac{1}{2}(A(x-x^m), x-x^m) - \cancel{\frac{1}{2}(Ax, x)} \le$$

$$\le \frac{1}{2}A(x-x^0-\phi), x-x^0-\phi) - \cancel{\frac{1}{2}(Ax, x)}$$

for any ϕ in K_m

$x - x^m = e^m \qquad x - x^0 = e^0$

$$\boxed{\text{As a result we get } (Ae^m, e^m) \le (A(e^0-\phi), e^0-\phi) \text{ for any } \phi \in K_m}$$

How $\phi \in K_m$ looks like? Well

$$\phi = a_0 r^0 + a_1 A r^0 + \dots + a_{m-1} A^{m-1} r^0 = P_{m-1}(A) r^0$$

Thus

$$(Ae^m, e^m) \le (A(e^0 - P_{m-1}(A) r^0), e^0 - P_{m-1}(A) r^0)$$

but $r^0 = b - Ax^0 = A(x - x^0) = Ae^0$

$$e^0 - \phi = e^0 - P_{m-1}(A) r^0 = e^0 - P_{m-1}(A) A e^0$$

$$= \underbrace{(I - P_{m-1}(A) A)}_{Q_m(A)} e^0$$

Thus we get

$$(Ae^m, e^m) \le (A Q_m(A) e^0, Q_m(A) e^0)$$

If we use the standard notation of a new inner product

$$(x, y)_A = (Ax, y) \quad \& \text{ norm } (Ax, x)^{1/2} = \|x\|_A$$

we get

$$(e^m, e^m)_A \le (Q(A) e^0, e^0)_A$$

$$\|e^m\|_A^2 \le \|Q_m(A)\|_A^2 \, \|e^0\|_A^2$$

A is an SPD matrix, thus has eigenvalues

$$0 < \lambda_1 \le \lambda_2 \le \dots \le \lambda_n$$

One proves in this case that

$$\|Q_m(A)\|_A = \max_{1\le j\le n} |Q_m(\lambda_j)|$$

Thus CG methods choses the iterates in such a way that the A-norm of the error of the m-th iterate has minimal A-norm of $Q_m(A)$ on the interval (λ_1, λ_n). This problem was already studied in Chebyshev method and we know that

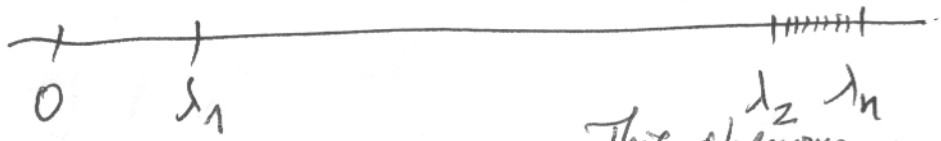
$$\max_j |Q_m(\lambda_j)| \le 2\left(\frac{1-\sqrt{\xi}}{1+\sqrt{\xi}}\right)^m \qquad \xi = \frac{\lambda}{\Lambda} = \frac{\lambda_1}{\lambda_n}$$

The bottom line is that CG performs in the same way as Chebyshev method.

Important: it does more work, but it work without knowledge of the spectrum and requires optimal # of iterations

There is a number of very attractive properties of CG method that are not available for Chebyshev acceleration. Consider the following case

$$0 < \lambda_1 << \lambda_2 \leq \dots \leq \lambda_n$$



This phenomenon is called spectrum clustering

E.g. $\lambda_1 = 0.000001$ $\quad \lambda_2/\lambda_n \approx 1/2$

This is the case of clustering of the eigenvalues

The convergence from the general point of view will be still

$$\|e^m\|_A \leq 2\left(\frac{1-\sqrt{\xi}}{1+\sqrt{\xi}}\right)^m \|e^0\|_A$$

For example if we have the above case $\xi = 10^{-6}$

So if you want $2\left(\frac{1-\sqrt{\xi}}{1+\sqrt{\xi}}\right)^m \leq 10^{-6} \equiv$

you will need about 7000 iterations.

You might be surprized that CG will run much less! Why?

Remember CG minimizes the norm $\max_j |Q_m(\lambda_j)|$, i.e. it is the best polynomial in terms of minimal norm.

Now let us construct (say by hand) the following polynomial

$$\tilde{Q}_m(A) \equiv \left(I - \frac{1}{\lambda_1} A\right)(I - \tau_1 A) \cdots (I - \tau_{m-1} A)$$

where the parameters $\tau_1, \ldots, \tau_{m-1}$ are chosen using Chebyshev technique on $[\lambda_2, \lambda_n]$. From the theory of Chebyshev acceleration we know that

$$\| (I - \tau_1 A) \cdots (I - \tau_{m-1} A) \|_A \leq 2 \frac{1 - \sqrt{\xi_1}}{1 + \sqrt{\xi_1}}$$

where $\xi_1 = \frac{\lambda_2}{\lambda_n}$. Then for the overall norm of $\tilde{Q}_m(A)$ we shall have

$$\|\tilde{Q}_m(A)\| \leq \left|1 - \frac{\lambda_n}{\lambda_1}\right| \cdot 2 \left(\frac{1 - \sqrt{\xi_1}}{1 + \sqrt{\xi_1}}\right)^{m-1} \approx \frac{2}{\xi} \left(\frac{1 - \sqrt{\xi_1}}{1 + \sqrt{\xi_1}}\right)^{m-1}$$

Remember that CG will do better that $\tilde{Q}_m(A)$!

Why $\tilde{Q}_m(A)$ is good? Let us go back to Fourier mode analysis

$$e^0 = \sum c_j \psi_j \quad A\psi_j = \lambda_j \psi_j \quad (\psi_j, \psi_i) = \delta_{ij}$$

$$e^1 = \left(I - \frac{1}{\lambda_n} A\right) e^0 = \sum_{j=1}^{n} c_j \left(1 - \frac{\lambda_j}{\lambda_n}\right) \psi_j \approx \sum_{j=1}^{n-1} c_j \left(1 - \frac{\lambda_j}{\lambda_n}\right) \psi_j$$

$$= \sum_{j=1}^{n-1} \tilde{c}_j \psi_j$$

But now the error is spanned by the remaining eigenvectors and it is in the space $\{\psi_2, \dots, \psi_n\}$. But on this subspace λ_2/λ_n is not that close to 1.

Which factor $q_1 = 2\left(\frac{1-\sqrt{\xi}}{1+\sqrt{\xi}}\right)^m$ general theory

$q_2 = \frac{2}{\xi}\left(\frac{1-\sqrt{\xi_1}}{1+\sqrt{\xi_1}}\right)^{m-1}$ special consideration

is smaller. Often q_2 is much smaller.

For example $\lambda_1 = 10^{-6}$ $\varepsilon = 10^{-\varepsilon}$ $\lambda_2 = \frac{1}{2}$ $\lambda_n = 1$

general theory will predict that you need about 1000 iterations to make $q_1 < \varepsilon$. But in fact based on above consideration we can see that you need only 20 iterations to get $q_2 < \varepsilon$

The above observation has tremendous consequences in the practical use of CG. This is what is done in practice.

$Ax=b$ is the original system

Try to an equivalent system by multiplying the equation by another matrix B - called preconditioner so that

$$BAx = Bb \Rightarrow \tilde{A}\tilde{x} = \tilde{b}$$

the system $\tilde{A}\tilde{x}=\tilde{b}$ has

(1) $\tilde{A}$ symmetric maybe in a special inner product

(2) eigenvalues $\tilde{\lambda}_i$ of $\tilde{A}$ are either clustered, or spectrum of $\tilde{A}$ have reduced ratio $\frac{\tilde{\lambda}_n}{\tilde{\lambda}_1} = \text{cond}(A)$ in L^2

B is called preconditioner of A. The corresponding variant is called

preconditioned conjugate gradient PCG

MINRES

There are many other Krylov based methods

Now consider the case when A is nonsingular and symmetric but <u>not</u> positive definite. In this case A^2 is SPD matrix and we consider the minimization problem: minimize

$$\bar{J}(y) = \frac{1}{2}(A^2 y, y) - (Ab, y)$$

over the space $K_m + \{x^0\}$ where

$$K_m = \text{span}\{r^0, Ar^0, \ldots, A^{m-1} r^0\}$$

In fact this minimizes the A^2-norm of the error, i.e.

$$\|e^m\|_{A^2} = \min_{y \in \{x^0\} + K_m} \|x - y\|_{A^2} = \min_{y \in \{x^0\} + K_m} (A(x-y), A(x-y))$$

<u>Minres:</u> A symmetric matrix in $\mathbb{R}^{n\times n}$.
For x^0 - given set $r^0 = p^0 = b - Ax^0$. Then for $m = 0, 1, \ldots$ define

$$x^{m+1} = x^m + \alpha_m p_m \qquad \alpha_m = \frac{(r^m, Ap^m)}{(Ap^m, Ap^m)}$$

$$r^{m+1} = r^m - \alpha_m A p_m$$

$$p^{m+1} = r^{m+1} + \beta_m p^m \qquad \beta_m = \frac{-(Ar^{m+1}, Ap^m)}{(Ap^m, Ap^m)}$$

On each step we need two evaluations of $A\xi$ per step, namely Ap^m & Ar^{m+1}. But there is a variant that leads to only one such evaluation

<u>Example</u> FE approximation of the problem

$$-\Delta u - k^2 u = f \quad \Omega$$
$$u = 0 \quad \partial\Omega$$

may lead to such problem (Symmetric but <u>not</u> PD)