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 $x_0 + K_m(A, r_0)$

$$K_m(A r_0) = \{ r_0, Ar_0, \ldots, A^{m-1}r_0 \}$$

That is

$$x^m = x_0 + \theta^m \quad \theta^m \in K_m$$

and such that

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

$$\leq \frac{1}{2} A(x-x_0-\phi), x-x_0-\phi) - \frac{1}{2} (Ax, x)$$

for any $\phi$ in $K_m$

$$x-x^m = e^m \quad x-x_0 = e_0$$

As a result we get

$$(A e^m, e^m) \leq (A(e_0-\phi), e_0-\phi)$$

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

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

Thus

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

But $r^0 = 6 - A x^0 = A (x - x^0) = A e^0$

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

Thus we set

$$
(A e^m, e^m) \leq (A P_m(A) e^0, P_m(A) e^0)
$$

If we use the standard notation of a new inner product

$$(x, y)_A = (A x, y)$$

and norm $(A x)_A = 11 \times 1_A$

we set

$$
(e^m, e^m)_A \leq (P(A) e^0, e^0)_A
$$

$$
\| e^m \|_A^2 \leq \| P_m(A) \|_A^2 \| e^0 \|_A^2
$$

$A$ is an SPD matrix, thus has eigenvalues

$$
0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n
$$
One proves in this case that

$$\| Q_m(A) \|_A = \max_{1 \leq j \leq n} | Q_m(y_j) |$$

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 $(\lambda_2, \lambda_n)$. This problem was already studied in Chebyshev method and we know that

$$\max_j | Q_m(y_j) | \leq 2 \left( \frac{1 - \sqrt{\kappa}}{1 + \sqrt{\kappa}} \right)^m \xi = \frac{1}{A} = \frac{A_1}{\lambda_n}$$

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

\[ 0 < \lambda_1 << \lambda_2 \leq \ldots \leq \lambda_n \]

This phenomenon is called spectrum clustering.

E.g. \( \lambda_n = 0.000001 \), \( 1/\lambda_1 \approx 1/2 \).

This is the case of clustering of the eigenvalues.

The convergence from the general point of view will be still

\[ \| \mathbf{x}^m \| \leq 2 \left( \frac{1 - \sqrt{\varepsilon}}{1 + \sqrt{\varepsilon}} \right)^m 10^{0.4} \]

For example, if we have the above case \( \varepsilon = 10^{-6} \)

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

you will need about 7000 iterations.
You might be surprised that CG will run much less. Why?

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

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

\[
\tilde{Q}_m(A) = (I - \frac{1}{x_n} A)(I - \frac{1}{x_1} A) \ldots (I - \frac{1}{x_{m-1}} A)
\]

where the parameters \( x_1, \ldots, x_{m-1} \) are chosen using Chebyshev technique on \([x_2, x_n]\). From the theory of Chebyshev acceleration we know that

\[
\| (I - x_1 A) \ldots (I - x_{m-1} A) \| \leq 2 \frac{1 - \sqrt{\xi_1}}{1 + \sqrt{\xi_1}}
\]

where \( \xi_1 = \frac{x_2}{x_n} \). Then for the overall norm of \( \tilde{Q}_m(A) \) we shall have

\[
\| \tilde{Q}_m(A) \| \leq \left| 1 - \frac{1}{x_1} \right| \cdot 2 \left( \frac{1 - \sqrt{\xi_1}}{1 + \sqrt{\xi_1}} \right)^{m-1} \approx 2 \frac{1 - \sqrt{\xi_1}}{1 + \sqrt{\xi_1}}^{m-1}
\]

Remember that CG will do better than \( \tilde{Q}_m(A) \).
Why $\tilde{Q}_m(A)$ is good? Let us go back to Fourier mode analysis

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

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

But now the error is spanned by the remaining eigenvectors and it is in the space $\{\psi_2, \ldots, \psi_n\}$.

But on this subspace, $\lambda_2/\lambda_m$ is not that close to 1.

Which factor

$$q_1 = 2 \left(\frac{1 - \sqrt{\varepsilon}}{\sqrt{1 + \sqrt{\varepsilon}}}\right)^m \quad \text{general theory}$$

$$q_2 = \frac{2}{\varepsilon} \left(\frac{1 - \sqrt{\varepsilon_1}}{\sqrt{1 + \sqrt{\varepsilon_1}}}\right)^{m-1} \quad \text{special consideration}$$

is smaller. Often $q_2$ is much smaller.

For example $\lambda_1 = 10^{-6} \quad \varepsilon = 10^{-8} \quad \lambda_2 = \frac{1}{2} \quad \lambda_1 = 1$.

General theory will predict that you need about 100 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.

\[ Ax = b \] in the original system

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

\[ BAx = Bb \Rightarrow \tilde{Ax} = \tilde{b} \]

the system \( \tilde{Ax} = \tilde{b} \) has

1. \( \tilde{A} \) symmetric, may be in a special inner product
2. spectrum of \( \tilde{A} \) are either clustered, or have reduced ratio \( \frac{x_n}{x_1} = \text{cond} (A) \) in \( L^2 \)

\( B \) is called preconditioner of \( A \). The corresponding variant is called

preconditioned conjugate gradient \( \text{PCG} \)
MINRES

There are many other Krylov based methods. Now consider the case when $A$ is nonsingular and symmetric but not positive definite. In this case $A^2$ is SPD matrix and we consider the minimization problem: minimize

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

over the space $K_m + \{x_0\}$ where

$$K_m = \text{span}\{r_0, A r_0, \ldots, A^{m-1} r_0\}$$

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

$$\|e^m\|_{A^2} = \min_{y \in \{x_0\} + K_m} \|x - y\|_{A^2} = \min_{y \in \{x_0\} + K_m} (A(x-y), A(x-y))$$
Minres: A symmetric matrix in $\mathbb{R}^{n \times n}$.
For $x^0$, give set $r^0 = p^0 = b - Ax^0$. Then for $m = 0, 1,\ldots$ define

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

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

$$p^{m+1} = r^{m+1} + \beta_m p^m$$
$$\beta_m = \frac{(A r^{m+1}, A p^m)}{(A p^m, A p^m)}$$

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

Example: FE approximation of the problem

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

may lead to such problem (Symmetric but not PD)