The Conjugate Gradient Algorithm

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References

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Introduction

Problem: efficiently solve

$$A\mathbf{x} = \mathbf{b}$$

where $A \in \mathbb{R}^{n\times n}$ is symmetric and positive-definite.
Typical example: A is a 3D finite element stiffness matrix with n of order 10^7 to 10^8.
Iterative method: starting from an initial guess $\mathbf{x}_0$, generate (cheaply)

$$\mathbf{x}_1, \quad \mathbf{x}_2, \quad \mathbf{x}_3, \quad \ldots$$

such that $\mathbf{x}_k \to \mathbf{x}$ (rapidly) as $k \to \infty$.
Residuals:

$$\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k.$$

Obviously

$$\mathbf{x}_k \to \mathbf{x} \iff \mathbf{r}_k \to 0.$$

Krylov subspaces:

$$V_k = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, A^2\mathbf{r}_0, \ldots, A^{k-1}\mathbf{r}_0\} \quad \text{for } k = 1, 2, 3, \ldots.$$

Euclidean inner product and norm:

$$\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^T \mathbf{w} \quad \text{and} \quad \|\mathbf{v}\| = \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle}.$$

Definition

The kth CG iterate is the unique vector $\mathbf{x}_k \in \mathbb{R}^n$ satisfying the Galerkin equations

$$\mathbf{x}_k - \mathbf{x}_0 \in V_k \quad \text{and} \quad \langle A\mathbf{x}_k, \mathbf{w} \rangle = \langle \mathbf{b}, \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in V_k.$$

Galerkin orthogonality:

$$\langle A(\mathbf{x}_k - \mathbf{x}), \mathbf{w} \rangle = 0 \quad \text{for all } \mathbf{w} \in V_k.$$

Optimality Property

Inner product and norm induced by A:

$$\langle \mathbf{v}, \mathbf{w} \rangle_A = \mathbf{v}^T A \mathbf{w} \quad \text{and} \quad \|\mathbf{v}\|_A = \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle_A}.$$

Equivalent definition of $\mathbf{x}_k - \mathbf{x}_0 \in V_k$ is

$$\langle \mathbf{x}_k - \mathbf{x}_0, \mathbf{w} \rangle_A = \langle \mathbf{r}_0, \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in V_k,$$

so existence and uniqueness of $\mathbf{x}_k$ follows.
Since

$$V_1 \subseteq V_2 \subseteq V_3 \subseteq \cdots$$

the next lemma implies that the error decreases monotonically,

$$\|\mathbf{x}_0 - \mathbf{x}\|_A \geq \|\mathbf{x}_1 - \mathbf{x}\|_A \geq \|\mathbf{x}_2 - \mathbf{x}\|_A \geq \cdots .$$

Theorem

The CG iterates have the best-approximation property

$$\|\mathbf{x}_k - \mathbf{x}\|_A = \min_{\mathbf{y} \in \mathbf{x}_0 + V_k} \|\mathbf{y} - \mathbf{x}\|_A$$

Proof.

Since

$$\mathbf{x}_k - \mathbf{y} = (\mathbf{x}_k - \mathbf{x}_0) - (\mathbf{y} - \mathbf{x}_0) \in V_k,$$

Galerkin orthogonality and the Cauchy–Schwarz inequality give

$$\begin{aligned} \|\mathbf{x}_k - \mathbf{x}\|_A^2 &= \langle A(\mathbf{x}_k - \mathbf{x}), \mathbf{x}_k - \mathbf{x} \rangle \\ &= \underbrace{\langle A(\mathbf{x}_k - \mathbf{x}), \mathbf{x}_k - \mathbf{y} \rangle}_{=0} + \langle A(\mathbf{x}_k - \mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \\ &= \langle \mathbf{x}_k - \mathbf{x}, \mathbf{y} - \mathbf{x} \rangle_A \le \|\mathbf{x}_k - \mathbf{x}\|_A \|\mathbf{y} - \mathbf{x}\|_A. \end{aligned}$$

□

Finite Termination Property

Recall that

$$V_k = \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, A^2\mathbf{r}_0, \ldots, A^{k-1}\mathbf{r}_0\}.$$

Lemma

$\mathbf{r}_k \in V_{k+1}$ *for* $k = 0, 1, 2, \ldots$.

Proof.

Since $\mathbf{x}_k - \mathbf{x}_0 \in V_k$ we have

$$\mathbf{x}_k = \mathbf{x}_0 + \sum_{j=1}^{k} c_j A^{j-1}\mathbf{r}_0$$

for some $c_1, c_2, \ldots, c_k \in \mathbb{R}$, and thus

$$\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k = \underbrace{\mathbf{b} - A\mathbf{x}_0}_{\mathbf{r}_0} - \sum_{j=1}^{k} c_j A^j \mathbf{r}_0 \in V_{k+1}.$$

Lemma

$\langle \mathbf{r}_j, \mathbf{r}_k \rangle = 0$ *if* $j \neq k$.

Proof.

Galerkin orthogonality implies that

$$\langle \mathbf{r}_k, \mathbf{w} \rangle = \langle \mathbf{b} - A\mathbf{x}_k, \mathbf{w} \rangle = \langle A(\mathbf{x} - \mathbf{x}_k), \mathbf{w} \rangle = 0$$

for all $\mathbf{w} \in V_k$, so $\mathbf{r}_k \perp V_k$, and thus $\langle \mathbf{r}_k, \mathbf{r}_j \rangle = 0$ for $j < k$. □

Theorem

$\mathbf{x}_k = \mathbf{x}$ *for some* $k \leq n$.

Proof.

Suppose for a contradiction that $\mathbf{x}_k \neq \mathbf{x}$ for $0 \leq k \leq n$. Thus, $\mathbf{r}_k \neq \mathbf{0}$ for $0 \leq k \leq n$, which is impossible because we cannot have $n + 1$ linearly independent vectors in $\mathbb{R}^n$. □

Thus, we have an index $k^* < n$ such that

$$\mathbf{x}_k \neq \mathbf{x} \quad \text{for } 0 \leq k \leq k^*,$$

and

$$\mathbf{x}_k = \mathbf{x} \quad \text{for } k \geq k^* + 1.$$

Lemma

If $k \leq k^*$ then the residuals $\mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_{k-1}$ form an orthogonal basis for the Krylov subspace V_k.

Proof.

The residuals are linearly independent vectors in V_k, and $\dim V_k \leq k$. □

Lemma

The Krylov subspaces satisfy

$$V_1 \subsetneq V_2 \subsetneq V_3 \subsetneq \cdots \subsetneq V_{k^*} \subsetneq V_{k^*+1} = V_{k^*+2} = \cdots .$$

Proof.

If suffices to show that $A^{k^*+1}\mathbf{r}_0 \in V_{k^*+1}$. We have

$$\mathbf{x} = \mathbf{x}_{k^*+1} = \mathbf{x}_0 + \sum_{k=1}^{k^*+1} c_j A^{j-1}\mathbf{r}_0,$$

and $c_{k^*+1} \neq 0$ because otherwise $\mathbf{x} \in \mathbf{x}_0 + V_{k^*}$, which would imply $\mathbf{x}_{k^*} = \mathbf{x}$. Thus,

$$A^{k^*+1}\mathbf{r}_0 = \frac{1}{c_{k^*+1}}\left(\underbrace{A(\mathbf{x} - \mathbf{x}_0)}_{\mathbf{r}_0} - \sum_{j=1}^{k^*} c_j A^j \mathbf{r}_0\right) \in V_{k^*+1}.$$

□

Iterative Algorithm

Strategy: construct an A-conjugate basis for V_k.

Gramm–Schmidt procedure: define

$$\mathbf{p}_0 = \mathbf{r}_0 \quad \text{and} \quad \mathbf{p}_k = \mathbf{r}_k - \sum_{j=0}^{k-1} \frac{\langle \mathbf{r}_k, \mathbf{p}_j \rangle_A}{\|\mathbf{p}_j\|_A^2} \mathbf{p}_j \quad \text{for } 1 \le k \le k^*,$$

so that

$$\langle \mathbf{p}_j, \mathbf{p}_k \rangle_A = 0 \quad \text{if } j \ne k,$$

and

$$V_k = \operatorname{span}\{\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_{k-1}\} = \operatorname{span}\{\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{k-1}\}.$$

Happily, in the sum over j, all terms with $j \le k-2$ vanish.

Lemma

$$\mathbf{p}_k = \mathbf{r}_k + \beta_k \mathbf{p}_{k-1} \quad \textit{where} \quad \beta_k = -\frac{\langle \mathbf{r}_k, \mathbf{p}_{k-1} \rangle_A}{\|\mathbf{p}_{k-1}\|_A^2}.$$

Proof.

Since $\mathbf{p}_j \in V_{j+1}$ we have $A\mathbf{p}_j \in V_{j+2}$. Thus, if $j \leq k-2$ then $A\mathbf{p}_j \in V_k$ and so $\langle \mathbf{r}_k, \mathbf{p}_j \rangle_A = \langle \mathbf{r}_k, A\mathbf{p}_j \rangle = 0$ because $\mathbf{r}_k \perp V_k$. □

Recall that for $\mathbf{w} \in V_k$,

$$\langle A\mathbf{x}_k, \mathbf{w} \rangle = \langle \mathbf{b}, \mathbf{w} \rangle$$

so

$$\langle A(\mathbf{x}_k - \mathbf{x}_0), \mathbf{w} \rangle = \langle \mathbf{b} - A\mathbf{x}_0, \mathbf{w} \rangle.$$

Since

$$\mathbf{x}_k - \mathbf{x}_0 \in V_k \quad \text{and} \quad \langle \mathbf{x}_k - \mathbf{x}_0, \mathbf{w} \rangle_A = \langle \mathbf{r}_0, \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in V_k,$$

we see by taking $\mathbf{w} = \mathbf{p}_j$ that for $1 \leq k \leq k^*$,

$$\mathbf{x}_k - \mathbf{x}_0 = \sum_{j=0}^{k-1} \alpha_j \mathbf{p}_j \quad \text{where} \quad \alpha_j = \frac{\langle \mathbf{r}_0, \mathbf{p}_j \rangle}{\|\mathbf{p}_j\|_A^2}.$$

In turn,

$$-\mathbf{r}_k = A(\mathbf{x}_k - \mathbf{x}) = A(\mathbf{x}_0 - \mathbf{x}) + \sum_{j=0}^{k-1} \alpha_j A \mathbf{p}_j$$

so

$$\mathbf{r}_k = \mathbf{r}_0 - \sum_{j=0}^{k-1} \alpha_j A \mathbf{p}_j.$$

Lemma

$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A\mathbf{p}_k \quad \textit{and} \quad \alpha_k = \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{p}_k\|_A^2} \quad \textit{for } 0 \le k \le k^*.$$

Proof.

The recursion for $\mathbf{r}_k$ follows from

$$\mathbf{r}_{k+1} - \mathbf{r}_k = \sum_{j=0}^{k} \alpha_j A\mathbf{p}_j - \sum_{j=0}^{k-1} \alpha_j A\mathbf{p}_j = \alpha_k A\mathbf{p}_k,$$

and the formula for α_k follows from

$$0 = \langle \mathbf{r}_k, \mathbf{r}_{k+1} \rangle = \|\mathbf{r}_k\|^2 - \alpha_k \langle \mathbf{r}_k, A\mathbf{p}_k \rangle$$

together with

$$\langle \mathbf{r}_k, A\mathbf{p}_k \rangle = \langle \mathbf{p}_k - \beta_k \mathbf{p}_{k-1}, A\mathbf{p}_k \rangle = \langle \mathbf{p}_k, A\mathbf{p}_k \rangle.$$

Lemma

$$\beta_k = \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{r}_{k-1}\|^2} \quad \textit{for } 1 \le k \le k^*.$$

Proof.

Since $\mathbf{r}_k \perp \mathbf{r}_{k-1}$,

$$\alpha_{k-1}\beta_k = -\frac{\langle \mathbf{r}_k, \alpha_{k-1} A\mathbf{p}_{k-1}\rangle}{\|\mathbf{p}_{k-1}\|_A^2} = \frac{\langle \mathbf{r}_k, \mathbf{r}_{k-1} - \alpha_{k-1} A\mathbf{p}_{k-1}\rangle}{\|\mathbf{p}_{k-1}\|_A^2}$$
$$= \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{p}_{k-1}\|_A^2},$$

so

$$\beta_k = \frac{1}{\alpha_{k-1}} \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{p}_{k-1}\|_A^2} = \frac{\|\mathbf{p}_{k-1}\|_A^2}{\|\mathbf{r}_{k-1}\|^2} \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{p}_{k-1}\|_A^2} = \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{r}_{k-1}\|^2}.$$

□

Summing up, the CG algorithm looks as follows:

$$
\begin{aligned}
&\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0 \\
&\mathbf{p}_0 = \mathbf{r}_0 \\
&\alpha_0 = \|\mathbf{r}_0\|^2/(\mathbf{p}_0^T A\mathbf{p}_0) \\
&\mathbf{x}_1 = \mathbf{x}_0 + \alpha_0\mathbf{p}_0 \\
&\text{do } k = 1,\ n-1 \\
&\qquad \mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k = \mathbf{r}_{k-1} - \alpha_{k-1}A\mathbf{p}_{k-1} \\
&\qquad \text{if (} \|\mathbf{r}_k\| < \text{tol) then} \\
&\qquad\qquad \text{exit} \\
&\qquad \text{end if} \\
&\qquad \beta_k = \|\mathbf{r}_k\|^2/\|\mathbf{r}_{k-1}\|^2 \\
&\qquad \mathbf{p}_k = \mathbf{r}_k + \beta_k\mathbf{p}_{k-1} \\
&\qquad \alpha_k = \|\mathbf{r}_k\|^2/(\mathbf{p}_k^T A\mathbf{p}_k) \\
&\qquad \mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k\mathbf{p}_k \\
&\text{end do}
\end{aligned}
$$