Simulation and High-Performance Computing

Part 8: Krylov Methods

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Positive definite matrices

Task: We want to solve a linear system $Ax = b$.

Assumption: The matrix $A \in \mathbb{R}^{n \times n}$ is symmetric and positive definite, i.e.,

$$\begin{aligned} \langle x, Ay \rangle &= \langle y, Ax \rangle && \text{for all } x, y \in \mathbb{R}^n, \\ \langle x, Ax \rangle &> 0 && \text{for all } x \in \mathbb{R}^n,\ x \neq 0. \end{aligned}$$

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Approach: Characterize the solution x via a minimization problem.

Example: For $a > 0$, the function $f(x) = \frac{1}{2}ax^2 - bx$ takes its minimum at $ax = b$, since $f'(x) = ax - b$.

Minimization problem

Goal: Prove that the function

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takes its minimum if $Ax = b$.

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Approach: Given a direction $p \in \mathbb{R}^n$, we prove that

$$f(x) \leq f(x + \theta p) \qquad \text{holds for all } \theta \in \mathbb{R}$$

if and only if p and $Ax - b$ are orthogonal, i.e.,

$$\langle p, Ax - b\rangle = 0.$$

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Result: If $Ax = b$, the minimality condition holds for all $p \in \mathbb{R}^n$, and f takes its global minimum in x.
If f takes its global minimum in x, we can choose $p = Ax - b$ and obtain $\|Ax - b\|^2 = \langle Ax - b, Ax - b\rangle = 0$, i.e., $Ax = b$.

Orthogonality implies minimality

Binomial equation: Given $p \in \mathbb{R}^n$, $\theta \in \mathbb{R}$, we have

$$\begin{aligned}
f(x+\theta p) &= \tfrac{1}{2}\langle x+\theta p, A(x+\theta p)\rangle - \langle b, x+\theta p\rangle \\
&= f(x) + \tfrac{1}{2}\theta\langle x, Ap\rangle + \tfrac{1}{2}\theta\langle p, Ax\rangle + \tfrac{1}{2}\theta^2\langle p, Ap\rangle - \theta\langle b, p\rangle \\
&= f(x) + \tfrac{1}{2}\theta\langle x, Ap\rangle + \tfrac{1}{2}\theta\langle x, Ap\rangle + \tfrac{1}{2}\theta^2\langle p, Ap\rangle - \theta\langle b, p\rangle \\
&= f(x) + \theta\langle p, Ax-b\rangle + \tfrac{1}{2}\theta^2\langle p, Ap\rangle.
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Minimality: If p and $Ax - b$ are orthogonal, i.e., if $\langle p, Ax - b\rangle = 0$ holds, we have

$$f(x+\theta p) = f(x) + \frac{1}{2}\theta^2\langle p, Ap\rangle \geq f(x),$$

since A is positive definite, i.e., x cannot be reduced any further along the direction p.

Minimality implies orthogonality

We choose $p \in \mathbb{R}^n$ with $p \neq 0$ and assume that we cannot improve our solution in direction p, i.e.,

$$f(x) \leq f(x + \theta p) \qquad \text{for all } \theta \in \mathbb{R}.$$

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$$f(x) \leq f(x + \theta p) \qquad \text{for all } \theta \in \mathbb{R}.$$

We can choose $\theta = -\frac{\langle p, Ax - b\rangle}{\langle p, Ap\rangle}$ and obtain

$$\begin{aligned} f(x) \leq f(x + \theta p) &= f(x) + \theta \langle p, Ax - b\rangle + \tfrac{1}{2}\theta^2 \langle p, Ap\rangle \\ &= f(x) - \frac{\langle p, Ax - b\rangle^2}{\langle p, Ap\rangle} + \frac{\langle p, Ax - b\rangle^2}{2\langle p, Ap\rangle} \\ &= f(x) - \frac{\langle p, Ax - b\rangle^2}{2\langle p, Ap\rangle} \leq f(x), \end{aligned}$$

since $\langle p, Ap\rangle > 0$. This implies $\langle p, Ax - b\rangle = 0$.

Iterative minimization

Idea: Given $x_m \in \mathbb{R}^n$, pick a direction $p_m \in \mathbb{R}^n$ and a stepsize $\theta_m \in \mathbb{R}$ with

$$f(x_m + \theta_m p_m) \leq f(x_m).$$

The next approximation is $x_{m+1} = x_m + \theta_m p_m$.

Locally optimal direction: If θ is small, we have

$$f(x + \theta p) \approx f(x) + \theta \langle p, Ax - b \rangle,$$

and the best direction is $p = b - Ax$.

Optimal stepsize: For $p \in \mathbb{R}^n$ with $p \neq 0$, the best stepsize satisfies

$$0 = \langle p, A(x + \theta p) - b \rangle = \langle p, Ax - b \rangle + \theta \langle p, Ap \rangle,$$

i.e., we have $\theta = -\frac{\langle p, Ax - b \rangle}{\langle p, Ap \rangle} = \frac{\langle p, b - Ax \rangle}{\langle p, Ap \rangle}$.

Gradient iteration

Simple version:

$\texttt{for } m = 0, 1, \ldots \texttt{ do}$

$\quad p_m \leftarrow b - Ax_m$

$\quad \theta_m \leftarrow \frac{\|p_m\|^2}{\langle p_m, Ap_m \rangle}$

$\quad x_{m+1} \leftarrow x_m + \theta_m \, p_m$

$\texttt{end}$

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Improved version avoiding unnecessary matrix-vector multiplications:

$$
\begin{array}{l}
p_0 \leftarrow b - Ax_0 \\
\texttt{for } m = 0, 1, \ldots \texttt{ do} \\
\quad a_m \leftarrow Ap_m \\
\quad \theta_m \leftarrow \frac{\|p_m\|^2}{\langle p_m, a_m \rangle} \\
\quad x_{m+1} \leftarrow x_m + \theta_m \, p_m \\
\quad p_{m+1} \leftarrow p_m - \theta_m \, a_m \\
\texttt{end}
\end{array}
$$

Gradient iteration: Implementation

```
copy(n, b, 1, p, 1);
addeval_laplace(-1.0, x, 1, p, 1);
error = nrm2(n, p, 1);

while(error > eps) {
  clear(n, a, 1);
  addeval_laplace(1.0, p, 1, a, 1);

  omega = dot(n, p, 1, a, 1);
  theta = dot(n, p, 1, p, 1) / omega;
  axpy(n, theta, p, 1, x, 1);
  axpy(n, -theta, a, 1, p, 1);
  error = nrm2(n, p, 1);
}
```

Experiment: Gradient iteration

Task: Solve the linear system $-\Delta_h u_h = f$.

m	$\|b - Ax_m\|$	$f(x_m)$
0	2.33_{+3}	0.00_{+0}
1	1.21_{+3}	-1.27_{+3}
2	8.92_{+2}	-1.61_{+3}
3	7.31_{+2}	-1.80_{+3}
4	6.34_{+2}	-1.92_{+3}
10	4.20_{+2}	-2.25_{+3}
100	1.89_{+2}	-3.02_{+3}
1000	3.04_{+0}	-3.45_{+3}
2000	3.14_{-2}	-3.45_{+3}

Observation: Very slow convergence, rate $\sim 1 - ch^2$.

Preserving optimality

Optimality: Our choice of θ_m guarantees

$$\langle p_m, Ax_{m+1} - b \rangle = 0,$$

i.e., x_{m+1} cannot be improved in the direction p_m.

Problem: Optimality is lost in later steps, usually already in the next.

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Idea: Modify the directions in order to preserve optimality. If x_m is already optimal with respect to $p_0, \ldots, p_{m-1}$, we need

$$\begin{aligned} 0 &\overset{!}{=} \langle p_\ell, Ax_{m+1} - b \rangle = \langle p_\ell, A(x_m + \theta_m\, p_m) - b \rangle \\ &= \langle p_\ell, Ax_m - b \rangle + \theta_m \langle p_\ell, Ap_m \rangle = \theta_m \langle p_\ell, Ap_m \rangle. \end{aligned}$$

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Conjugate direction: We have to ensure

$$\langle p_\ell, Ap_m \rangle = 0 \qquad\qquad \text{for all } \ell \in [0 : m-1].$$

Conjugate gradients

Idea: Start with the residual

$$r_m := b - Ax_m$$

and apply the Gram-Schmidt procedure:

$$p_m := r_m - \sum_{k=0}^{m-1} \frac{\langle p_k, Ar_m \rangle}{\langle p_k, Ap_k \rangle} p_k.$$

Result: Due to $\langle p_\ell, Ap_k \rangle = 0$ for $\ell \neq k$, we obtain

$$\langle p_\ell, Ap_m \rangle = \langle p_\ell, Ar_m \rangle - \sum_{k=0}^{m-1} \frac{\langle p_k, Ar_m \rangle}{\langle p_k, Ap_k \rangle} \langle p_\ell, Ap_k \rangle = 0.$$

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Problem: This procedure is not particularly efficient.

Krylov spaces

Krylov space: We have

$$\operatorname{span}\{p_0, \ldots, p_m\} = \operatorname{span}\{r_0, \ldots, r_m\} = \operatorname{span}\{r_0, Ar_0, \ldots, A^m r_0\}$$

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First inclusion: We start with $p_0 = r_0$ and use induction with

$$p_{m+1} = r_{m+1} - \sum_{k=0}^{m} \alpha_k \, p_k = r_{m+1} - \sum_{k=0}^{m} \beta_k \, r_k.$$

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Second inclusion: We again use induction with

$$r_{m+1} = r_m - \theta_m \, Ap_m = r_m - \theta_m \sum_{k=0}^{m} \alpha_k A r_k.$$

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Equality: The conjugate directions $p_0, \ldots, p_m$ are linear independent, therefore all spaces have full dimension $m + 1$.

Efficient orthogonalization

Krylov space: We have

$$\mathcal{K}_m := \operatorname{span}\{r_0, Ar_0, \ldots, A^m r_0\} = \operatorname{span}\{p_0, \ldots, p_m\}.$$

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Optimality: By construction, we have

$$\langle q, r_{m+1} \rangle = \langle q, b - Ax_{m+1} \rangle = 0 \qquad \text{for all } q \in \mathcal{K}_m.$$

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Symmetry: Since A is symmetric and $Ap_k \in \mathcal{K}_{k+1}$, we have

$$\langle p_k, Ar_{m+1} \rangle = \langle Ap_k, r_{m+1} \rangle = 0 \qquad \text{for all } k \in [0 : m-1]$$

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Result: New direction can be computed efficiently via

$$p_{m+1} := r_{m+1} - \frac{\langle p_m, Ar_{m+1} \rangle}{\langle p_m, Ap_m \rangle} p_m = r_{m+1} - \frac{\langle Ap_m, r_{m+1} \rangle}{\langle p_m, Ap_m \rangle} p_m.$$

Conjugate gradient method

$r_0 \leftarrow b - Ax_0$
$p_0 \leftarrow r_0$
$\texttt{for } m = 0, 1, \ldots \texttt{ do}$
  $a_m \leftarrow Ap_m$
  $\omega_m \leftarrow \langle p_m, a_m \rangle$
  $\theta_m \leftarrow \frac{\langle p_m, r_m \rangle}{\omega_m}$
  $x_{m+1} \leftarrow x_m + \theta_m \, p_m$
  $r_{m+1} \leftarrow r_m - \theta_m \, a_m$
  $\mu_m \leftarrow \frac{\langle a_m, r_{m+1} \rangle}{\omega_m}$
  $p_{m+1} \leftarrow r_{m+1} - \mu_m p_m$
$\texttt{end}$

Experiment: Conjugate gradient method

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50	4.95_{-4}	-3.45_{+3}
100	6.11_{-15}	-3.45_{+3}

Observation: Significantly faster than the gradient method, rate $\sim 1 - ch$.

Summary

Minimization problem: $\langle p, Ax - b \rangle = 0$ is equivalent with

$$f(x) \leq f(x + \theta p) \qquad \text{for all } \theta \in \mathbb{R}.$$

The global minimum of f corresponds with the solution of $Ax = b$.

Gradient method approximates the minimum.

$$p_m = b - Ax_m \qquad x_{m+1} = x_m + \frac{\|p_m\|^2}{\langle p_m, Ap_m \rangle} p_m.$$

Conjugate gradient method ensures that x_m is optimal with respect to $p_0, \ldots, p_{m-1}$ and converges significantly faster than the gradient method.

Krylov spaces allow us to implement the cg method efficiently.