Lecture 7
Conjugate Gradient Method (CG)

Jinn-Liang Liu

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The CG method is used for solving *symmetric* and *positive definite* (SPD) systems

$$A\vec{x} = \vec{b} \tag{7.1}$$

with

$$\begin{aligned} A &= A^T, & (7.2)\\ \vec{x}^T A \vec{x} &> 0 \ \text{ for all non-zero vectors } \vec{x} \in R^N. & (7.3) \end{aligned}$$

Algorithm CG: Conjugate Gradient Method

$$\begin{array}{ll}
 & \vec{x}^{(0)} = \vec{0} \qquad \text{(Arbitrary)} \\
 & \vec{r}^{(0)} = \vec{b} - A\vec{x}^{(0)} \quad \text{(Residual vector)} \\
 & \vec{p}^{(1)} = \vec{r}^{(0)} \\
 & \text{for } k = 1, \cdots, N \qquad \text{(Why } N \text{ not } k\,\text{max ?)} \\
\text{(S1)} & \quad \alpha_k := \dfrac{\left\langle \vec{p}^{(k)}, \vec{r}^{(k-1)} \right\rangle}{\left\langle \vec{p}^{(k)}, A\vec{p}^{(k)} \right\rangle} = \dfrac{\left\langle \vec{r}^{(k-1)}, \vec{r}^{(k-1)} \right\rangle}{\left\langle \vec{p}^{(k)}, A\vec{p}^{(k)} \right\rangle} \qquad \text{(Why ??)} \\
\text{(S2)} & \quad \vec{x}^{(k)} = \vec{x}^{(k-1)} + \alpha_k \vec{p}^{(k)} \\
\text{(S3)} & \quad \vec{r}^{(k)} = \vec{b} - A\vec{x}^{(k)} = \vec{r}^{(k-1)} - \alpha_k A \vec{p}^{(k)} \quad \text{(Why ?)} \\
 & \quad \text{check convergence; continue if necessary} \\
\text{(S4)} & \quad \beta_k := -\dfrac{\left\langle \vec{r}^{(k)}, A\vec{p}^{(k)} \right\rangle}{\left\langle \vec{p}^{(k)}, A\vec{p}^{(k)} \right\rangle} = \dfrac{\left\langle \vec{r}^{(k)}, \vec{r}^{(k)} \right\rangle}{\left\langle \vec{r}^{(k-1)}, \vec{r}^{(k-1)} \right\rangle} \quad \text{(Why ??)} \\
\text{(S5)} & \quad \vec{p}^{(k+1)} = \vec{r}^{(k)} + \beta_k \vec{p}^{(k)} \\
 & \text{end for}
\end{array}$$

In this algorithm, α_k is called a *stepping length* and $\vec{p}^{(k)}$ is called a search direction (or *predictor*, or prediction vector). We can geometrically interpret (S2) as that we are currently at $\vec{x}^{(k-1)}$ and then take a next step with the length α_k in the direction of $\vec{p}^{(k)}$ to go to the point $\vec{x}^{(k)}$. Therefore, it is critical to determine the next α_k and $\vec{p}^{(k)}$.

Example 7.1. Given $A = \begin{bmatrix} 1 & 0 \\ 0 & 9 \end{bmatrix}$ and $\overrightarrow{b} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$, find the solution of $A\overrightarrow{x} = \overrightarrow{b}$ by using the conjugate method with the initial guess $\overrightarrow{x}^{(0)} = \begin{bmatrix} 1 \\ 1/9 \end{bmatrix}$.

Project 7.1. First, write a program for the CG algorithm and test it by Example 7.1. Second, run your CG program for the 1D Poisson Problem (1.1) (with $f(x) = 2$, $g_D = 0$, and $g_N = 0$) discretized by FDM.

Input: N, A, $\overrightarrow{b}$, TOL (write the input in the program).

Output:

N	k	$E^{\overrightarrow{x}}$	E^u	α
5				
9				
17				
33				
65				
129				

The CG is a *nonstationary* iterative method, i.e., in matrix form

$$\overrightarrow{x}^{(k)} = B\overrightarrow{x}^{(k-1)} + \overrightarrow{c} \tag{7.4}$$

where B and $\overrightarrow{c}$ depend on the iteration (i.e., B and $\overrightarrow{c}$ change from iteration to iteration).

Table 7.1. Time Complexity of Various Methods

Method	2D	3D
GE	$O(N^3)$	$O(N^3)$
JM	$O(N^2)$	$O(N^{\frac{5}{3}})$
GS	$O(N^2)$	$O(N^{\frac{5}{3}})$
SOR	$O(N^{\frac{3}{2}})$	$O(N^{\frac{4}{3}})$
CG	$O(N^{\frac{3}{2}})$	$O(N^{\frac{4}{3}})$
PCG	$O(N^{1.2})$	$O(N^{1.17})$
Multigrid	$O(N \log N)$	$O(N \log N)$

Remark 7.1.

(1) CG can also be used to solve unconstrained optimization problems.

(2) The biconjugate gradient method (BiCG) is a generalization of CG for non-symmetric systems.

(3) CG with preconditioning requires about $\sqrt{N}$ steps to determine an approximate solution.

We say that two non-zero vectors $\overrightarrow{u}$ and $\overrightarrow{v}$ are *conjugate* with respect to A if

$$\langle \overrightarrow{u}, \overrightarrow{v} \rangle_A := \overrightarrow{u}^T A \overrightarrow{v} = 0 \tag{7.5}$$

The left hand side defines an inner product since A is SPD, i.e.,

$$\begin{aligned} \langle \overrightarrow{u}, \overrightarrow{v} \rangle_A &= \overrightarrow{u}^T A \overrightarrow{v} = \langle \overrightarrow{u}, A\overrightarrow{v} \rangle \\ &= \left\langle A^T \overrightarrow{u}, \overrightarrow{v} \right\rangle = \langle A\overrightarrow{u}, \overrightarrow{v} \rangle \\ &= \langle \overrightarrow{v}, \overrightarrow{u} \rangle_A, \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the standard inner product defined in R^N. This conjugate is not related to the notion of complex conjugate.

Example 7.2. Show that $A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ is SPD. Let $\overrightarrow{u} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and $\overrightarrow{v} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$. Show that $\langle \overrightarrow{u}, \overrightarrow{v} \rangle = 0$, i.e., $\overrightarrow{u} \perp \overrightarrow{v}$ in the sense of $\langle \cdot, \cdot \rangle$. Does $\langle \overrightarrow{u}, \overrightarrow{v} \rangle_A = 0$? Find any two vectors $\overrightarrow{x}$ and $\overrightarrow{y}$ such that $\langle \overrightarrow{x}, \overrightarrow{y} \rangle_A = 0$, i.e., $\overrightarrow{x} \perp \overrightarrow{y}$ in the sense of $\langle \cdot, \cdot \rangle_A$.

Minimization Problem: With A being SPD, solve (7.1) for $\overrightarrow{x}$ via minimizing the **quadratic function**

$$\phi(\overrightarrow{x}) = \frac{1}{2}\overrightarrow{x}^T A \overrightarrow{x} - \overrightarrow{x}^T \overrightarrow{b} = \frac{1}{2}\langle A\overrightarrow{x}, \overrightarrow{x} \rangle - \left\langle \overrightarrow{b}, \overrightarrow{x} \right\rangle \quad \forall \overrightarrow{x} \in R^N \tag{7.6}$$

Example 7.3. A simplest example for (7.1) and (7.6) is given by $N = 1$, $A = 2$, $b = 1$. The solution of the *linear* problem $2x = 1$ is $x^* = 1/2$. Find the minimizer x^* for the following quadratic function (a *nonlinear* problem)

$$\begin{aligned} \phi(\overrightarrow{x}) &= \frac{1}{2}x^T A x - x^T b \\ &= \frac{1}{2} \cdot 2 \cdot x^2 - x = x^2 - x \end{aligned} \tag{7.7}$$

Example 7.4. Solve the linear problem $\begin{bmatrix} 1 & 0 \\ 0 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and then solve it via minimizing the quadratic function

$$\begin{aligned} \phi(\overrightarrow{x}) &= \frac{1}{2} x^T A x - x^T b \\ &= \frac{1}{2} \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad (7.8) \end{aligned}$$

1 Minimization of the Quadratic Function

As noted above, $\phi(\overrightarrow{x})$ is *nonlinear* and $A\overrightarrow{x} = \overrightarrow{b}$ is *linear*. Given any vectors $\overrightarrow{x}$ and $\overrightarrow{p}$, let h be a function of α defined by

$$\begin{aligned} h(\alpha) &= \phi(\overrightarrow{x} + \alpha \overrightarrow{p}) \qquad (7.9) \\ &= \frac{1}{2} \langle A(\overrightarrow{x} + \alpha \overrightarrow{p}), \overrightarrow{x} + \alpha \overrightarrow{p} \rangle - \left\langle \overrightarrow{b}, \overrightarrow{x} + \alpha \overrightarrow{p} \right\rangle \\ &= \frac{\alpha^2}{2} \langle A\overrightarrow{p}, \overrightarrow{p} \rangle + \alpha \langle A\overrightarrow{p}, \overrightarrow{x} \rangle + \frac{1}{2} \langle A\overrightarrow{x}, \overrightarrow{x} \rangle - \left\langle \overrightarrow{b}, \overrightarrow{x} + \alpha \overrightarrow{p} \right\rangle \\ &= \frac{1}{2} \langle A\overrightarrow{p}, \overrightarrow{p} \rangle \alpha^2 + \left\langle A\overrightarrow{x} - \overrightarrow{b}, \overrightarrow{p} \right\rangle \alpha + \phi(\overrightarrow{x}) \qquad (7.10) \end{aligned}$$

Theorem 7.1.

$$\overrightarrow{x}^* \text{ minimizes } \phi(\overrightarrow{x}) \iff A\overrightarrow{x}^* = \overrightarrow{b} \qquad (7.11)$$

Proof: ($\Longrightarrow$) For any vector $\overrightarrow{p}$, define

$$h(\alpha) = \phi(\overrightarrow{x}^* + \alpha \overrightarrow{p})$$

Since $\phi(\overrightarrow{x}^*)$ is minimum, the function $h(\alpha)$ attains its minimum at $\alpha = 0$

with the minimum value of $h(0) = \phi(\overrightarrow{x}^*)$. This implies that

$$
\begin{aligned}
0 &= \frac{dh(0)}{d\alpha} = \lim_{\alpha \to 0} \frac{h(\alpha) - h(0)}{\alpha} \\
&= \lim_{\alpha \to 0} \frac{\phi(\overrightarrow{x}^* + \alpha \overrightarrow{p}) - \phi(\overrightarrow{x}^*)}{\alpha} \\
&= \lim_{\alpha \to 0} \frac{\frac{1}{2} \langle A\overrightarrow{p}, \overrightarrow{p} \rangle \alpha^2 + \left\langle A\overrightarrow{x}^* - \overrightarrow{b}, \overrightarrow{p} \right\rangle \alpha + \phi(\overrightarrow{x}^*) - \phi(\overrightarrow{x}^*)}{\alpha} \\
&= \lim_{\alpha \to 0} \left(\frac{1}{2} \langle A\overrightarrow{p}, \overrightarrow{p} \rangle \alpha + \left\langle A\overrightarrow{x}^* - \overrightarrow{b}, \overrightarrow{p} \right\rangle \right) \\
&= \left\langle A\overrightarrow{x}^* - \overrightarrow{b}, \overrightarrow{p} \right\rangle, \ \forall \overrightarrow{p} \neq \overrightarrow{0}. \\
&\Longrightarrow A\overrightarrow{x}^* = \overrightarrow{b}.
\end{aligned}
$$

$$(\Longleftarrow) \quad A\overrightarrow{x}^* = \overrightarrow{b} \ \Longrightarrow$$

$$
\begin{aligned}
\phi(\overrightarrow{x}^* + \overrightarrow{p}) &= \phi(\overrightarrow{x}^*) + \left\langle A\overrightarrow{x}^* - \overrightarrow{b}, \overrightarrow{p} \right\rangle + \frac{1}{2} \langle A\overrightarrow{p}, \overrightarrow{p} \rangle \geq \phi(\overrightarrow{x}^*), \quad \forall \overrightarrow{p} \\
&\Longrightarrow \phi(\overrightarrow{x}^*) \text{ is minimum.}
\end{aligned}
$$

As a by-product from the proof, we see that, for any given vectors $\overrightarrow{x}$ and $\overrightarrow{p} \neq 0$,

$$
\begin{aligned}
0 &= \frac{d}{d\alpha} \phi(\overrightarrow{x} + \alpha \overrightarrow{p}) = h'(\alpha) = \langle A\overrightarrow{p}, \overrightarrow{p} \rangle \alpha + \left\langle A\overrightarrow{x} - \overrightarrow{b}, \overrightarrow{p} \right\rangle \\
&\Longrightarrow \alpha = \frac{\left\langle A\overrightarrow{x} - \overrightarrow{b}, \overrightarrow{p} \right\rangle}{\langle A\overrightarrow{p}, \overrightarrow{p} \rangle} \qquad (7.12)
\end{aligned}
$$

which gives an optimal stepping length as defined in (S1).

Remark 7.2. This theorem says that solving the linear system (7.1) is equivalent to minimizing the nonlinear function. In general, a linear problem is much easier to solve than a nonlinear one.

Question 7.1. Why do we make a detour from an easy road to a rough road?

2 Directional Derivative (Gradient Operator)

$$
\begin{aligned}
D_{\vec{p}}\phi(\vec{x}) &= D_{\vec{p}}\phi(x_1,x_2) \ = \lim_{t\to 0}\frac{\phi(\vec{x}+t\vec{p})-\phi(\vec{x})}{t} && (7.13\\
(\vec{x} &= (x_1,x_2) \text{ any fixed point, } \vec{p} = (p_1,p_2) \text{ any unit direction.)}\\
&= \lim_{t\to 0}\frac{\phi(x_1+tp_1,x_2+tp_2)-\phi(x_1,x_2)}{t}\\
&= \lim_{t\to 0}\frac{\phi(x_1+tp_1,x_2+tp_2)-\phi(x_1,x_2+tp_2)+\phi(x_1,x_2+tp_2)-\phi(x_1,x_2)}{t}\\
&= \lim_{t\to 0}\frac{[\phi(x_1+tp_1,x_2+tp_2)-\phi(x_1,x_2+tp_2)]p_1}{tp_1}+\frac{[\phi(x_1,x_2+tp_2)-\phi(x_1,x_2)]p_2}{tp_2}\\
&= \lim_{t\to 0}\frac{[\phi(x_1+\Delta x_1,x_2+tp_2)-\phi(x_1,x_2+tp_2)]p_1}{\Delta x}+\frac{[\phi(x_1,x_2+\Delta x_2)-\phi(x_1,x_2)]p_2}{\Delta x_2}\\
&= \frac{\partial\phi(x_1,x_2)}{\partial x_1}p_1+\frac{\partial\phi(x_1,x_2)}{\partial x_2}p_2\\
(\nabla &= \left\langle\frac{\partial}{\partial x_1},\frac{\partial}{\partial x_2}\right\rangle = \text{grad} = \text{del, the vector differential operator gradient)}\\
&= \nabla\phi(x_1,x_2)\cdot\vec{p} && (7.14\\
&= |\nabla\phi|\,|\vec{p}|\cos\theta && (7.15\\
&\Rightarrow \text{ Max value of } D_{\vec{p}}\phi \text{ is } |\nabla\phi| \text{ with } \theta=0 \text{ and } |\vec{p}|=1\\
&\Rightarrow \text{ Min value of } D_{\vec{p}}\phi \text{ is} - |\nabla\phi| \text{ in } \vec{p} = -\nabla\phi/|\nabla\phi| \text{ direction } \theta=180^\circ
\end{aligned}
$$

Conclusion 7.1. At any point $\vec{x}$, the functional ϕ decreases most rapidly (steepest) in the direction of the negative gradient $-\nabla\phi(\overrightarrow{x})$.

$$
\begin{aligned}
\phi(\overrightarrow{x}) &= \phi(x_1, x_2, \cdots\cdots, x_N) \\
&= \frac{1}{2}\langle A\overrightarrow{x}, \overrightarrow{x}\rangle - \left\langle \overrightarrow{b}, \overrightarrow{x} \right\rangle \\
&= \frac{1}{2}\begin{bmatrix} x_1 & \cdots & \cdots & x_N \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & \cdots & a_{1N} \\ a_{21} & \cdots & \cdots & a_{2N} \\ \vdots & & & \vdots \\ a_{N1} & \cdots & \cdots & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_N \end{bmatrix} \\
&\quad - \begin{bmatrix} b_1 & \cdots & \cdots & b_N \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_N \end{bmatrix} \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} a_{ij}x_j x_i - \sum_{i=1}^{N} x_i b_i \\
&= \frac{1}{2}\sum_{i=1}^{N}(a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{ii}x_i + \cdots + a_{ik}x_k + \cdots)x_i - \sum_{i=1}^{N} x_i b_i \\
&= \frac{1}{2}(a_{11}x_1 + a_{12}x_2 + \cdots + a_{1i}x_i + \cdots + a_{1k}x_k + \cdots)x_1 \\
&\quad + \frac{1}{2}(a_{21}x_1 + a_{22}x_2 + \cdots + a_{2i}x_i + \cdots + a_{2k}x_k + \cdots)x_2 \\
&\quad + \cdots \\
&\quad + \frac{1}{2}(a_{k1}x_1 + a_{k2}x_2 + \cdots + a_{ki}x_i + \cdots + a_{kk}x_k + \cdots)x_k \qquad (7.16) \\
&\quad + \cdots \\
&\quad + \frac{1}{2}(a_{N1}x_1 + a_{N2}x_2 + \cdots + a_{Ni}x_i + \cdots + a_{Nk}x_k + \cdots)x_N - \sum_{i}^{N} x_i b_i
\end{aligned}
$$

$$
\begin{aligned}
\phi_{x_k}(\overrightarrow{x}) &= \frac{\partial\phi(\overrightarrow{x})}{\partial x_k} = \sum_{i=1}^{N} a_{ik}x_i - b_k, \quad (\because a_{ik} = a_{ki}) \qquad (7.17) \\
-\nabla\phi(\overrightarrow{x}) &= -\left(\phi_{x_1}, \phi_{x_2}, \cdots, \phi_{x_N}\right) = \overrightarrow{b} - A\overrightarrow{x} \qquad (7.18)
\end{aligned}
$$

The slope (grade) of a line $\phi(x) = ax + b$ (a scalar function) is defined as the rise over the run, $m = \frac{\Delta\phi}{\Delta x} = \phi'(x) = \frac{d\phi}{dx}$. The gradient (or gradient vector field) of a scalar function $\phi(\overrightarrow{x})$ with respect to a vector variable $\overrightarrow{x}$ is denoted by $\nabla\phi = \text{grad}\phi$ where ∇ (the nabla symbol) denotes the vector differential operator del (grad). By definition, the gradient is a vector field whose components are the partial derivatives of ϕ as (7.18).

HW 7.1. Consider a unit circle. Define the unit circle by using a quadratic functional $\phi(\overrightarrow{x})$. Find $\nabla\phi$ at the point (1,0) on the circle. What can you say (geometrically) about the gradient at that point and then at any point? Tangent vector? Normal vector? So what is your conclusion? If we change the unit circle to a set of level curves, does your conclusion still hold? Prove and draw a picture to explain the conclusion.

3 Method of Steepest Descent

Therefore, we should choose the direction $\overrightarrow{p}$ as $\overrightarrow{b} - A\overrightarrow{x}$ if we want to minimize $\phi(x, y)$ in the steepest way, i.e.,

$$\begin{aligned} D_{\overrightarrow{p}}\phi(x,y) &= \nabla\phi(\overrightarrow{x}) \cdot \overrightarrow{p} && (7.19)\\ \overrightarrow{p} &= -\nabla\phi(\overrightarrow{x}) && (7.20)\\ \overrightarrow{p} &= \overrightarrow{b} - A\overrightarrow{x} && (7.21)\\ \overrightarrow{r} &= \overrightarrow{b} - A\overrightarrow{x} && (7.22) \end{aligned}$$

Iteration:

$$\begin{aligned} \overrightarrow{x}^{(k)} &= \overrightarrow{x}^{(k-1)} + \alpha_k \overrightarrow{p}^{(k)} && (7.23)\\ \overrightarrow{p}^{(k)} &= -\bigtriangledown \phi(\overrightarrow{x}^{(k-1)}) = \overrightarrow{r}^{(k-1)} && (7.24) \end{aligned}$$

Algorithm MSD: Method of Steepest Descent

$\overrightarrow{x}^{(0)} = \overrightarrow{0}$ (initial guess or any other vector)
for $k = 1, 2, \cdots, k\max$
$\overrightarrow{r}^{(k-1)} = \overrightarrow{b} - A\overrightarrow{x}^{(k-1)}$ (search direction $\overrightarrow{p} = -\bigtriangledown \phi$)
if $\overrightarrow{r}^{(k-1)} = \overrightarrow{0}$ then quit (solution found)
else $\overrightarrow{p}^{(k)} = \overrightarrow{r}^{(k-1)}$

$$\alpha_k = \frac{\left\langle \overrightarrow{p}^{(k)}, \overrightarrow{r}^{(k-1)} \right\rangle}{\left\langle \overrightarrow{p}^{(k)}, A\overrightarrow{p}^{(k)} \right\rangle} = \frac{\left\langle \overrightarrow{r}^{(k-1)}, \overrightarrow{r}^{(k-1)} \right\rangle}{\left\langle \overrightarrow{r}^{(k-1)}, A\overrightarrow{r}^{(k-1)} \right\rangle} \quad \text{(by (7.12))}$$

$$\overrightarrow{x}^{(k)} = \overrightarrow{x}^{(k-1)} + \alpha_k \overrightarrow{p}^{(k)}$$

Remark 7.3. The convergence results for MSD are (see J. R. Shewchuk 1994)

$$\begin{aligned}
\left\| \overrightarrow{e}^{(k)} \right\|_A &\leq \left(\frac{\kappa - 1}{\kappa + 1} \right)^k \left\| \overrightarrow{e}^{(0)} \right\|_A && (7.25) \\
\overrightarrow{e}^{(0)} &= \overrightarrow{x}^{*} - \overrightarrow{x}^{(0)} \\
\overrightarrow{e}^{(k)} &= \overrightarrow{x}^{*} - \overrightarrow{x}^{(k)} \\
\left\| \overrightarrow{e}^{(k)} \right\|_A &= \left\langle \overrightarrow{e}^{(k)}, A\overrightarrow{e}^{(k)} \right\rangle \\
\kappa &= \frac{\lambda_{\max}}{\lambda_{\min}}, \ \{\lambda_i\} \text{ are eigenvalue of } A && (7.26) \\
A \ \text{SPD} &\Rightarrow 0 < \lambda_1 \leqslant \lambda_2 \leqslant \lambda_3 \leqslant \cdots\cdots \leqslant \lambda_N \\
\kappa &= \frac{\lambda_N}{\lambda_1}
\end{aligned}$$

(iii) The convergence is slow if A is ill-conditioned, i.e., $\kappa >> 1$.

HW 7.2. Prove (7.25).

Example 7.5.

$$A = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix}$$

Solution:

$$\begin{aligned}
\det(A - \lambda I) &= \det \begin{vmatrix} 3-\lambda & 2 \\ 2 & 6-\lambda \end{vmatrix} = 0 \\
&\Rightarrow (3-\lambda)(6-\lambda) - 4 = 0 \\
0 &= \lambda^2 - 9\lambda + 14 \\
\lambda &= \frac{9 \pm \sqrt{81 - 56}}{2} \\
\lambda_{\max} &= 7 \\
\lambda_{\min} &= 2 \\
\kappa &= \frac{7}{2}
\end{aligned}$$

Example 7.6.

$$A = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \qquad \overrightarrow{b} = \begin{bmatrix} 2 \\ -8 \end{bmatrix}$$

Solution:

$$\begin{aligned}
\phi(\overrightarrow{x}) &= \frac{1}{2}\langle A\overrightarrow{x}, \overrightarrow{x}\rangle - \left\langle \overrightarrow{b}, \overrightarrow{x}\right\rangle \\
&= \frac{1}{2}\left\langle \begin{bmatrix} 3x_1+2x_2 \\ 2x_1+6x_2 \end{bmatrix}, \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right\rangle - \left\langle \begin{bmatrix} 2 \\ -8 \end{bmatrix}, \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right\rangle \\
&= \frac{1}{2}\left(3x_1^2+4x_1x_2+6x_2^2\right) - (2x_1-8x_2) \\
&= C \text{ (Different contours with different constants } C\text{)}
\end{aligned}$$

$$\begin{aligned}
x_1 &= x_1'\cos\theta + x_2'\sin\theta \\
x_2 &= -x_1'\sin\theta + x_2'\cos\theta \\
&\Rightarrow \frac{(x_1'-p_1)^2}{a^2} + \frac{(x_2'-p_2)^2}{b^2} = 1
\end{aligned}$$

Example 7.7.

$$N=2, A = \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix}, \overrightarrow{b} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \overrightarrow{x} = \begin{bmatrix} x \\ y \end{bmatrix}, \; d_2 \geq d_1 > 0$$

Solution:

$$\begin{aligned}
\phi(\overrightarrow{x}) &= \frac{1}{2}\langle A\overrightarrow{x}, \overrightarrow{x}\rangle = \frac{1}{2}\begin{bmatrix} x, & y \end{bmatrix}\begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} \\
&= \frac{1}{2}(d_1x^2+d_2y^2) \\
&= C_1(\text{constant}) > 0 \Rightarrow \text{a level curve} \\
&\Rightarrow \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \\
&\Rightarrow \frac{a}{b} \approx \sqrt{\frac{d_2}{d_1}} \approx \sqrt{\kappa}
\end{aligned}$$

HW 7.3. Let $d_1 = 1$ and $d_2 = 1/9$. Draw level curves (contours) of the function $\phi(\overrightarrow{x})$ and the gradient $\nabla\phi(\overrightarrow{x})$ at some point $\overrightarrow{x} = (1, 1/9)$. Find the tangent line at $\overrightarrow{x} = (1, 1/9)$ to the level curve passing through $(1, 1/9)$. What is the relation between $\nabla\phi(1, 1/9)$ and this line? Find the minimum value and minimizer of $\phi(\overrightarrow{x})$ by MSD starting from the point $(1, 1/9)$.

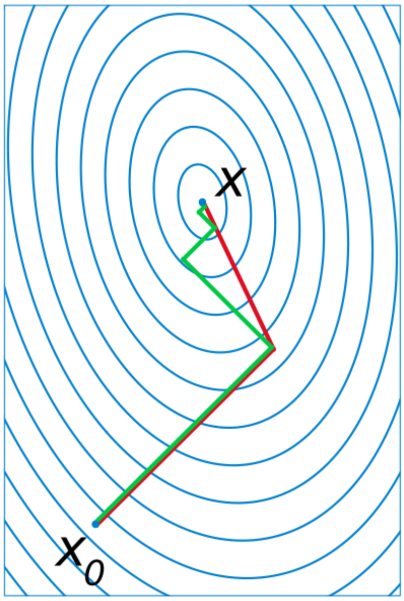

Figure 1: Steepest Descent vs. Conjugate Gradient

Conclusion 7.2. Case (1) If the contour is a circle, i.e. $\kappa = 1$, the solution is found in *one* step by MSD. Case (2) A is ill-conditioned $\Rightarrow \kappa \gg 1 \Rightarrow$ level curves very elongated $\Rightarrow$ requires a lot of iterations to find an approximation solution $\Rightarrow$ MSD converges very slowly.

HW 7.4. Prove Case (1).

Example 7.8. A comparison (Fig. 1) of the convergence of *gradient (steepest) descent* with optimal step size (in green) and conjugate gradient (in red) for minimizing the quadratic form associated with a given linear system. *Conjugate gradient* converges in at most N steps where N is the size of the matrix of the system (here $N = 2$).

4 Conjugate Gradient Method

To avoid Case (2), another approach was proposed by choosing

$$\{\overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots\} \neq \{\overrightarrow{r}^{(0)}, \overrightarrow{r}^{(1)}, \overrightarrow{r}^{(2)}, \cdots\} \tag{7.27}$$

that satisfy

$$\left\langle \overrightarrow{p}^{(i)}, A\overrightarrow{p}^{(j)} \right\rangle = 0 \qquad \forall \;\; i \neq j \tag{7.28}$$

This is called an A-**orthogonal** (A-**conjugate**) condition and the set $\left\{ \overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots \right\}$ is said to be A-**orthogonal**. The vectors $\overrightarrow{p}^{(i)}$ are called **conjugate directions**. Since A is SPD, the set $\left\{ \overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots, \overrightarrow{p}^{(N)} \right\}$ is linearly independent, i.e.,

$$\begin{aligned}
R^N &= \text{span } \left\{ \overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots, \overrightarrow{p}^{(N)} \right\} ? && (7.29)\\
(7.12) \quad h'(\alpha) &= 0 \Rightarrow && \\
\alpha_k &= \frac{\left\langle \overrightarrow{b} - A\overrightarrow{x}^{(k-1)}, \overrightarrow{p}^{(k)} \right\rangle}{\left\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)} \right\rangle} = \frac{\left\langle \overrightarrow{r}^{(k-1)}, \overrightarrow{p}^{(k)} \right\rangle}{\left\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)} \right\rangle} && (7.30)\\
\overrightarrow{x}^{(k)} &= \overrightarrow{x}^{(k-1)} + \alpha_k \overrightarrow{p}^{(k)} \quad \text{(Next Iterate)} && (7.31)
\end{aligned}$$

Theorem 7.2. Let $\left\{ \overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots, \overrightarrow{p}^{(N)} \right\}$ be an A-orthogonal set of nonzero vectors associated with the SPD matrix A and let $\overrightarrow{x}^{(0)}$ be arbitrary. Define the iterates (7.31) for $k = 1, 2, 3, \cdots$, with (7.30). Then, assuming exact arithmetic, we have

$$A\overrightarrow{x}^{(N)} = \overrightarrow{b} \qquad (N \text{ steps to get solution}) \tag{7.32}$$

Proof:

$$
\begin{aligned}
A\overrightarrow{x}^* &= b, \quad A: N\times N,\ \overrightarrow{x}^* \in R^N \\
\phi(\overrightarrow{x}) &= \frac{1}{2}\langle A\overrightarrow{x}, \overrightarrow{x}\rangle - \left\langle \overrightarrow{b}, \overrightarrow{x}\right\rangle, \quad \forall \overrightarrow{x} \in R^N \\
h(\alpha) &= \phi(\overrightarrow{x} + \alpha\overrightarrow{p}) = \phi(\overrightarrow{x}) + \alpha\left\langle A\overrightarrow{x} - \overrightarrow{b}, \overrightarrow{p}\right\rangle + \frac{\alpha^2}{2}\langle A\overrightarrow{p}, \overrightarrow{p}\rangle \\
-\bigtriangledown\phi(\overrightarrow{x}) &= \overrightarrow{r} = \overrightarrow{b} - A\overrightarrow{x} \\
\overrightarrow{x}^{(k)} &= \overrightarrow{x}^{(k-1)} + \alpha_k\overrightarrow{p}^{(k)} \\
A\overrightarrow{x}^{(N)} &= A\overrightarrow{x}^{(N-1)} + \alpha_N A\overrightarrow{p}^{(N)} \\
&= A\overrightarrow{x}^{(N-2)} + \alpha_{N-1}A\overrightarrow{p}^{(N-1)} + \alpha_N A\overrightarrow{p}^{(N)} \\
&= A\overrightarrow{x}^{(0)} + \alpha_1 A\overrightarrow{p}^{(1)} + \alpha_2 A\overrightarrow{p}^{(2)} + \cdots + \alpha_{N-1}A\overrightarrow{p}^{(N-1)} + \alpha_N A\overrightarrow{p}^{(N)} \\
A\overrightarrow{x}^{(N)} - \overrightarrow{b} &= A\overrightarrow{x}^{(0)} - \overrightarrow{b} + \sum_{i=1}^{N}\alpha_i A\overrightarrow{p}^{(i)} \\
\left\langle A\overrightarrow{x}^{(N)} - \overrightarrow{b}, \overrightarrow{p}^{(k)}\right\rangle &= \left\langle A\overrightarrow{x}^{(0)} - \overrightarrow{b}, \overrightarrow{p}^{(k)}\right\rangle + \sum_{i=1}^{N}\alpha_i\left\langle A\overrightarrow{p}^{(i)}, \overrightarrow{p}^{(k)}\right\rangle \\
&= \left\langle A\overrightarrow{x}^{(0)} - \overrightarrow{b}, \overrightarrow{p}^{(k)}\right\rangle + \alpha_k\left\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)}\right\rangle \\
&\quad \left(\because \left\{\overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots, \overrightarrow{p}^{(N)}\right\} \text{ is } A\text{-orthogonal}\right) \\
&= \left\langle A\overrightarrow{x}^{(0)} - \overrightarrow{b}, \overrightarrow{p}^{(k)}\right\rangle + \frac{\left\langle \overrightarrow{b} - A\overrightarrow{x}^{(k-1)}, \overrightarrow{p}^{(k)}\right\rangle}{\left\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)}\right\rangle}\left\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)}\right\rangle \\
&= \left\langle A\overrightarrow{x}^{(0)} - A\overrightarrow{x}^{(k-1)}, \overrightarrow{p}^{(k)}\right\rangle \\
(A\overrightarrow{x}^{(k-1)} &= A\overrightarrow{x}^{(k-2)} + \alpha_{k-1}A\overrightarrow{p}^{(k-1)} = A\overrightarrow{x}^{(0)} + \alpha_1 A\overrightarrow{p}^{(1)} + \cdots + \alpha_{k-1}A\overrightarrow{p}^{(k-1)}) \\
&= -\sum_{i=1}^{k-1}\alpha_i\left\langle A\overrightarrow{p}^{(i)}, \overrightarrow{p}^{(k)}\right\rangle = 0 \qquad \forall k = 1, \cdots, N \\
&\Longrightarrow A\overrightarrow{x}^{(N)} = \overrightarrow{b}
\end{aligned}
$$

How to determine the A-orthogonal set $\left\{\overrightarrow{p}^{(1)}, \overrightarrow{p}^{(2)}, \overrightarrow{p}^{(3)}, \cdots, \overrightarrow{p}^{(N)}\right\}$ (set of search directions, conjugate directions)?

Lemma 7.1. Show that

$$\begin{aligned}
\left\langle \overrightarrow{r}^{(k)}, \overrightarrow{p}^{(k)} \right\rangle &= 0 \ \text{ for } k = 1, \cdots, N, && (7.33)\\
\left\langle \overrightarrow{p}^{(k+1)}, A\overrightarrow{p}^{(k)} \right\rangle &= 0 \ \text{ for } k = 1, \cdots, N-1, && (7.34)\\
\left\langle \overrightarrow{p}^{(k)}, A\overrightarrow{p}^{(k)} \right\rangle &= \left\langle \overrightarrow{r}^{(k-1)}, A\overrightarrow{p}^{(k)} \right\rangle \ \text{ for } k = 1, \cdots, N, && (7.35)\\
\left\langle \overrightarrow{r}^{(k)}, \overrightarrow{r}^{(k-1)} \right\rangle &= 0 \ \text{ for } k = 1, \cdots, N, && (7.36)
\end{aligned}$$

Proof:

$$\begin{aligned}
\overrightarrow{r}^{(k)} &= \overrightarrow{b} - A\overrightarrow{x}^{(x)}\\
(\ \overrightarrow{x}^{(k)} &= \overrightarrow{x}^{(k-1)} + \alpha_k \overrightarrow{p}^{(k)} \ )\\
&= \overrightarrow{b} - A\overrightarrow{x}^{(k-1)} - \frac{\left\langle \overrightarrow{b} - A\overrightarrow{x}^{(k-1)}, \overrightarrow{p}^{(k)} \right\rangle}{\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)} \rangle} A\overrightarrow{p}^{(k)}\\
\left\langle \overrightarrow{r}^{(k)}, \overrightarrow{p}^{(k)} \right\rangle &= \left\langle \overrightarrow{b} - A\overrightarrow{x}^{(k-1)}, \overrightarrow{p}^{(k)} \right\rangle - \left\langle \overrightarrow{b} - A\overrightarrow{x}^{(k-1)}, \overrightarrow{p}^{(k)} \right\rangle\\
&= 0 \Rightarrow (7.33)
\end{aligned}$$

$$\begin{aligned}
(S5) &\Rightarrow A\overrightarrow{p}^{(k+1)} = A\overrightarrow{r}^{(k)} + \beta_k A\overrightarrow{p}^{(k)}\\
\left\langle A\overrightarrow{p}^{(k+1)}, \overrightarrow{p}^{(k)} \right\rangle &= \left\langle A\overrightarrow{r}^{(k)}, \overrightarrow{p}^{(k)} \right\rangle + \beta_k \left\langle A\overrightarrow{p}^{(k)}, \overrightarrow{p}^{(k)} \right\rangle = 0\\
&\Rightarrow (7.34) \text{ by (S4) and this is the answer to the first ? in (S4).}
\end{aligned}$$

For $k = 1$,

$$\left\langle \overrightarrow{p}^{(1)}, A\overrightarrow{p}^{(1)} \right\rangle = \left\langle \overrightarrow{r}^{(0)}, A\overrightarrow{p}^{(1)} \right\rangle \quad \text{by the definition of } \overrightarrow{p}^{(1)}.$$

For $2 \le k \le N$,

$$\begin{aligned}
\left\langle \overrightarrow{p}^{(k)}, A\overrightarrow{p}^{(k)} \right\rangle &= \left\langle \overrightarrow{r}^{(k-1)} + \beta_{k-1} \overrightarrow{p}^{(k-1)}, A\overrightarrow{p}^{(k)} \right\rangle \quad \text{by (S5)}\\
&= \left\langle \overrightarrow{r}^{(k-1)}, A\overrightarrow{p}^{(k)} \right\rangle + \beta_{k-1} \left\langle \overrightarrow{p}^{(k-1)}, A\overrightarrow{p}^{(k)} \right\rangle\\
&= \left\langle \overrightarrow{r}^{(k-1)}, A\overrightarrow{p}^{(k)} \right\rangle \quad \text{by (7.34)} \Rightarrow (7.35)
\end{aligned}$$

HW 7.5. Show the second equality in (S1) first and then (7.36).
Theorem 7.3.

$$\left\langle \overrightarrow{p}^{(j)}, A\overrightarrow{p}^{(m)} \right\rangle = 0, \quad \left\langle \overrightarrow{r}^{(j-1)}, \overrightarrow{r}^{(m-1)} \right\rangle = 0 \qquad \forall j \neq m. \tag{7.37}$$

Proof: This result is proved by induction on m. From (7.34) and (7.36), we first note that $\left\langle \overrightarrow{p}^{(2)}, A\overrightarrow{p}^{(1)} \right\rangle = \left\langle \overrightarrow{r}^{(1)}, \overrightarrow{r}^{(0)} \right\rangle = 0$. Assume now that

$$\left\langle \overrightarrow{p}^{(l)}, A\overrightarrow{p}^{(k)} \right\rangle = \left\langle \overrightarrow{r}^{(l-1)}, \overrightarrow{r}^{(k-1)} \right\rangle = 0 \quad \text{for} \quad 1 \leq k < l \leq m. \tag{7.38}$$

We want to show that the same relation holds true for $0 \leq k < l \leq m+1$. It has been shown in Lemma 7.1 for $k = m$ and $l = m+1$. Taking $1 \leq k < m$ and $l = m+1$, it follows

$$\begin{aligned}
\left\langle \overrightarrow{r}^{(m)}, \overrightarrow{r}^{(k-1)} \right\rangle &= \left\langle \overrightarrow{r}^{(m-1)}, \overrightarrow{r}^{(k-1)} \right\rangle - \alpha_m \left\langle A\overrightarrow{p}^{(m)}, \overrightarrow{r}^{(k-1)} \right\rangle \\
&= -\alpha_m \left\langle A\overrightarrow{p}^{(m)}, \overrightarrow{r}^{(k-1)} \right\rangle \quad \text{by (7.38)} \\
&= -\alpha_m \left\langle A\overrightarrow{p}^{(m)}, \overrightarrow{p}^{(k)} - \beta_{k-1}\overrightarrow{p}^{(k-1)} \right\rangle \quad \text{by (S5)} \\
&= 0 \quad \text{by (7.38)}
\end{aligned} \tag{7.39}$$

$$\begin{aligned}
\left\langle \overrightarrow{p}^{(m+1)}, A\overrightarrow{p}^{(k)} \right\rangle &= \left\langle \overrightarrow{r}^{(m)} + \beta_m \overrightarrow{p}^{(m)}, A\overrightarrow{p}^{(k)} \right\rangle \\
&= \left\langle \overrightarrow{r}^{(m)}, A\overrightarrow{p}^{(k)} \right\rangle + \beta_m \left\langle \overrightarrow{p}^{(m)}, A\overrightarrow{p}^{(k)} \right\rangle \\
&= \left\langle \overrightarrow{r}^{(m)}, A\overrightarrow{p}^{(k)} \right\rangle \quad \text{by (7.38)} \\
&= \left\langle \overrightarrow{r}^{(m)}, \overrightarrow{r}^{(k-1)} - \overrightarrow{r}^{(k)} \right\rangle \alpha_k^{-1} \quad \text{by (S3)} \\
&= 0 \quad \text{by (7.39)}
\end{aligned}$$