# Conjugate gradient method

$A\vec{x} = \vec{b}$ $\quad$ $A$ sym. posdef. $\quad$ $q(\vec{x}) = \langle A\vec{x}, \vec{x}\rangle - 2\langle \vec{b}, \vec{x}\rangle$

$$\vec{x}^{(k+1)} = \vec{x}^{(k)} + t_k \vec{v}^{(k)} \quad \text{where} \quad t_k = \frac{\langle \vec{v}^{(k)}, \vec{r}^{(k)}\rangle}{\langle \vec{v}^{(k)}, A\vec{v}^{(k)}\rangle}$$

search direction

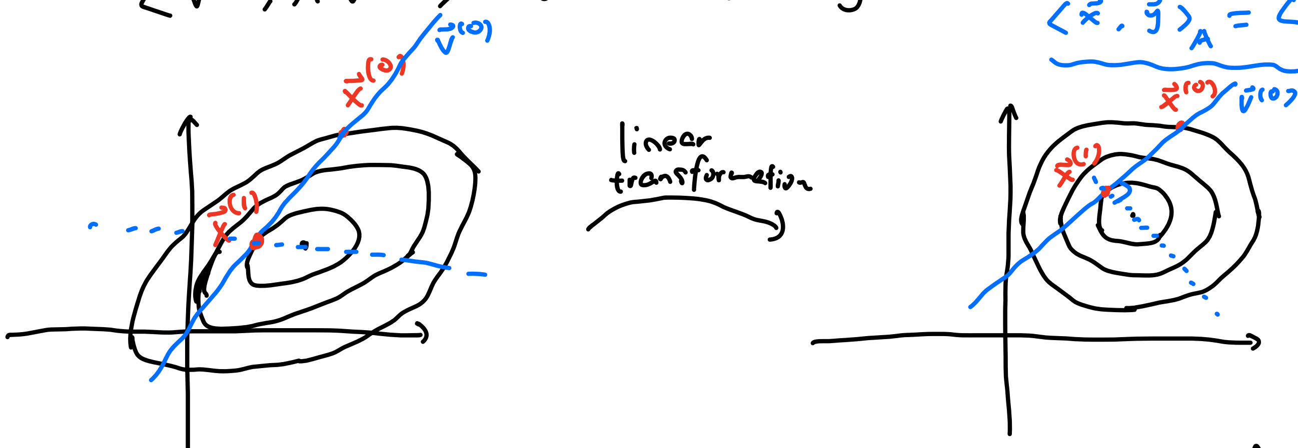
$$\vec{r}^{(k)} = \vec{b} - A\vec{x}^{(k)}$$

In Steepest descent, $\vec{v}^{(k)} = \vec{r}^{(k)}$

- It is desired for the search directions to have <u>$A$-orthogonality</u>, i.e.,

$$\langle \vec{v}^{(i)}, A\vec{v}^{(j)}\rangle = 0 \qquad \forall\, i \neq j$$

$$\langle \vec{x}, \vec{y}\rangle_A = \langle \vec{x}, A\vec{y}\rangle$$




Such a method is called a <u>conjugate direction method</u>

**Thm** A conjugate direction method gets the exact sol'n to $A\vec{x} = \vec{b}$ within $n$ iterations, i.e., for any $\vec{x}^{(0)}$, we have $A\vec{x}^{(n)} = \vec{b}$

**Proof** By normalization, we may assume $\langle \vec{v}^{(i)}, A\vec{v}^{(i)}\rangle = 1$.

Then $\quad \vec{x}^{(k+1)} = \vec{x}^{(k)} + t_k\vec{v}^{(k)} \quad$ where $\quad t_k = \langle \vec{v}^{(k)}, \vec{r}^{(k)}\rangle$

$$\vec{x}^{(n)} = \vec{x}^{(0)} + t_0\vec{v}^{(0)} + t_1\vec{v}^{(1)} + \cdots + t_{n-1}\vec{v}^{(n-1)}$$

$$A\vec{x}^{(n)} - \vec{b} = A\left(\vec{x}^{(0)} + t_0\vec{v}^{(0)} + t_1\vec{v}^{(1)} + \cdots + t_{n-1}\vec{v}^{(n-1)}\right) - \vec{b}$$

For any $k = 0, \cdots, n-1$,

$$\langle A\vec{x}^{(n)} - \vec{b}, \vec{v}^{(k)}\rangle = \langle A\vec{x}^{(0)} - \vec{b}, \vec{v}^{(k)}\rangle + t_0 \langle A\vec{v}^{(0)}, \vec{v}^{(k)}\rangle + \cdots + t_{n-1}\langle A\vec{v}^{(n-1)}, \vec{v}^{(k)}\rangle$$

$$= \langle A\vec{x}^{(0)} - \vec{b}, \vec{v}^{(k)}\rangle + t_k$$

$$t_k = \langle \vec{b} - A\vec{x}^{(k)}, \vec{v}^{(k)}\rangle$$

$$= \langle \vec{b} - A(\vec{x}^{(0)} + \cancel{t_0\vec{v}^{(0)}} + \cdots + \cancel{t_{k-1}\vec{v}^{(k-1)}}), \vec{v}^{(k)}\rangle$$

$$= \langle \vec{b} - A\vec{x}^{(0)}, \vec{v}^{(k)}\rangle$$

$$\Rightarrow \langle A\vec{x}^{(n)} - \vec{b}, \vec{v}^{(k)}\rangle = 0 \qquad k = 0, \cdots, n-1$$

$$\Rightarrow A\vec{x}^{(n)} - \vec{b} = \vec{0}$$

Question : how to make search directions $A$-orthogonal ?

$$\vec{w}^{(0)}, \vec{w}^{(1)}, \cdots, \vec{w}^{(n-1)}$$

$\big\downarrow$ Gram - Schmidt

$$\vec{v}^{(0)} = \vec{w}^{(0)}$$

$$\vec{v}^{(1)} = \vec{w}^{(1)} - \frac{\langle \vec{w}^{(1)}, \vec{v}^{(0)}\rangle_A}{\langle \vec{v}^{(0)}, \vec{v}^{(0)}\rangle_A}\vec{v}^{(0)}$$

$$\vec{v}^{(2)} = \vec{w}^{(2)} - \frac{\cdots}{\cdots}\vec{v}^{(0)} - \frac{\cdots}{\cdots}\vec{v}^{(1)}$$

$\cdots$

too expensive !

- Key observation: if every time we take $\vec{r}^{(k)}$ and do Gram-Schmidt to make it $A$-orthogonal to $\vec{v}^{(0)}, \cdots, \vec{v}^{(k-1)}$ and get $\vec{v}^{(k)}$, then $\vec{r}^{(k)}$ is already $A$-orthogonal to $\vec{v}^{(0)}, \cdots, \vec{v}^{(k-2)}$ so G-S is simplified.

Proof ① $\text{Span}\{\vec{v}^{(0)}, \cdots, \vec{v}^{(k-1)}\} = \text{Span}\{\vec{r}^{(0)}, \cdots, \vec{r}^{(k-1)}\} = D^{(k)}$

② $\langle \vec{r}^{(k)}, \vec{v}^{(i)}\rangle = 0 \quad i = 0, \cdots, k-1$ $\quad \Rightarrow \langle \vec{r}^{(k)}, \vec{r}^{(i)}\rangle = 0 \quad \forall\, i \neq k$

$$\langle \vec{r}^{(k)}, \vec{v}^{(i)} \rangle = \langle \vec{b} - A\vec{x}^{(k)}, \vec{v}^{(i)} \rangle$$

$$= \langle \vec{b} - A(\underbrace{\vec{x}^{(0)} + t_0\vec{v}^{(0)} + \cdots + t_{i-1}\vec{v}^{(i-1)}}_{\vec{x}^{(i)}} + t_i\vec{v}^{(i)} + \cdots$$

$$+ t_{k-1}\vec{v}^{(k-1)}), \vec{v}^{(i)} \rangle$$

$$= \langle \vec{b} - A\vec{x}^{(i)}, \vec{v}^{(i)} \rangle - t_i \langle A\vec{v}^{(i)}, \vec{v}^{(i)} \rangle$$

$$= \langle \vec{r}^{(i)}, \vec{v}^{(i)} \rangle - t_i \langle A\vec{v}^{(i)}, \vec{v}^{(i)} \rangle = 0$$

Since $t_i = \dfrac{\langle \vec{r}^{(i)}, \vec{v}^{(i)} \rangle}{\langle A\vec{v}^{(i)}, \vec{v}^{(i)} \rangle}$

③ $$\vec{r}^{(k-1)} - \vec{r}^{(k-2)} = (\vec{b} - A\vec{x}^{(k-1)}) - (\vec{b} - A\vec{x}^{(k-2)})$$

$$= -A(\vec{x}^{(k-1)} - \vec{x}^{(k-2)}) = -t_{k-2}A\vec{v}^{(k-2)}$$

$$\vec{r}^{(k-2)} - \vec{r}^{(k-3)} = -t_{k-3}A\vec{v}^{(k-3)}$$

any $t_i \neq 0$

$$\vdots$$

$$\vec{r}^{(1)} - \vec{r}^{(0)} = -t_0 A\vec{v}^{(0)}$$

$\Rightarrow A D^{(k-1)} \subset D^{(k)}$ "Krylov subspaces"

Finally, ② gives that $\vec{r}^{(k)}$ is orthogonal to $D^{(k)}$, i.e.,

$$\langle \vec{r}^{(k)}, \vec{x} \rangle = 0 \quad \forall \vec{x} \in D^{(k)}$$

Then, $\forall \vec{y} \in D^{(k-1)}$, ③ gives $A\vec{y} \in D^{(k)}$

$$\Rightarrow \langle \vec{r}^{(k)}, A\vec{y} \rangle = 0$$

Since $D^{(k-1)} = \mathrm{Span}\{\vec{v}^{(0)}, \dots, \vec{v}^{(k-2)}\}$, we get

$\vec{r}^{(k)}$ is $A$-orthogonal to $\vec{v}^{(0)}, \dots, \vec{v}^{(k-2)}$.

This gives the Conjugate gradient method:

$$\vec{v}^{(k)} = \vec{r}^{(k)} - \frac{\langle \vec{r}^{(k)}, A\vec{v}^{(k-1)} \rangle}{\langle \vec{v}^{(k-1)}, A\vec{v}^{(k-1)} \rangle} \vec{v}^{(k-1)} \qquad k = 1, 2, \cdots$$

$$\vec{v}^{(0)} = \vec{r}^{(0)}$$

Simplify: ① $\vec{r}^{(k)} - \vec{r}^{(k-1)} = -t_{k-1} A \vec{v}^{(k-1)}$

$$\langle \vec{r}^{(k)}, \vec{r}^{(k)} \rangle - \cancel{\langle \vec{r}^{(k-1)}, \vec{r}^{(k)} \rangle} = -t_{k-1} \langle A\vec{v}^{(k-1)}, \vec{r}^{(k)} \rangle$$

$$\Rightarrow \langle A\vec{v}^{(k-1)}, \vec{r}^{(k)} \rangle = -\frac{1}{t_{k-1}} \langle \vec{r}^{(k)}, \vec{r}^{(k)} \rangle$$

② $\cancel{\langle \vec{r}^{(k)}, \vec{v}^{(k-1)} \rangle} - \langle \vec{r}^{(k-1)}, \vec{v}^{(k-1)} \rangle = -t_{k-1} \langle A\vec{v}^{(k-1)}, \vec{v}^{(k-1)} \rangle$

$$\Rightarrow \langle A\vec{v}^{(k-1)}, \vec{v}^{(k-1)} \rangle = \frac{1}{t_{k-1}} \langle \vec{r}^{(k-1)}, \vec{v}^{(k-1)} \rangle$$

$$= \frac{1}{t_{k-1}} \langle \vec{r}^{(k-1)}, \vec{r}^{(k-1)} \rangle$$

$\vec{v}^{(k-1)} = \vec{r}^{(k-1)} + \cdots \vec{v}^{(k-2)}$

$\Rightarrow$ Simplified version: $\boxed{\vec{v}^{(k)} = \vec{r}^{(k)} + \frac{\langle \vec{r}^{(k)}, \vec{r}^{(k)} \rangle}{\langle \vec{r}^{(k-1)}, \vec{r}^{(k-1)} \rangle} \vec{v}^{(k-1)}}$

- The $n$-step termination property is not achieved in reality due to round-off errors. However, Conjugate gradient method is a good iterative method (one stops before step $n$ to get an approximate sol'n).

- Error estimate $\|\vec{e}^{(k)}\|_A \leq 2 \left( \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k \|\vec{e}^{(0)}\|_A \qquad \|\vec{x}\|_A := \sqrt{\langle \vec{x}, A\vec{x} \rangle}$.

- For a general system $A\vec{x} = \vec{b}$, one can solve the normal equation

$$\underbrace{A^T A}_{\text{sym. posdef.}} \vec{x} = A\vec{b}$$

and Conjugate gradient applies.

However, this makes condition number worse :

$$\kappa(A^TA) = \kappa(A)^2$$