Optimization Theory and Methods

Prof. Xiaoe Ruan

Email: wruanxe@xjtu.edu.cn
Tel:13279321898

2019, Fall

Chap.2 Numerical Techniques for Optimization

1. Solution to Linear Equations

2. Decomposition of Matrix

3. Line Search

4. Trust-Region Method

1. Solution to Linear Equations

Th.1. Let $f(x)=\frac{1}{2}x^{\mathrm{T}}Ax-b^{\mathrm{T}}x,$

where A is real symmetric positive definite (RSPD). Then

x^* is a solution to Eq. $Ax=b$

$\Leftrightarrow$ x^* is an extreme minimizer of $f(x)$.

Proof: $\Rightarrow$ Let $Ax^*=b.$ For $\forall x\in R^n$ we have

$$f(x)-f(x^*)=\frac{1}{2}x^{\mathrm{T}}Ax-b^{\mathrm{T}}x-\frac{1}{2}x^{*\mathrm{T}}Ax^*+b^{\mathrm{T}}x^*$$

$$=\frac{1}{2}\left(x^{\mathrm{T}}Ax-2b^{\mathrm{T}}x+x^{*\mathrm{T}}Ax^*\right)-x^{*\mathrm{T}}Ax^*+b^{\mathrm{T}}x^*$$

$$=\frac{1}{2}\left(x^{\mathrm{T}}Ax-2\left(Ax^*\right)^{\mathrm{T}}x+x^{*\mathrm{T}}Ax^*\right)$$

$$=\frac{1}{2}\left(x-x^*\right)^{\mathrm{T}}A\left(x-x^*\right)\geq 0$$

$\Leftarrow$ Obvious from necessity cond.

Then

$$\min_{x\in R^n} f(x)=\frac{1}{2}x^{\mathrm{T}}Ax-b^{\mathrm{T}}x,$$

$$\Longrightarrow \quad \nabla f(x)=Ax-b=0 \quad \Longleftrightarrow \quad Ax=b$$

Theoretically $x^*=A^{-1}b$

But inversion computing is sensitive to computing error which may lead the algorithm unstable.

Possible way:

Solve linear Eqs by matrix decomposition,

LU decomposition, QR decomposition, etc

Conjugate Gradient Method

Def.1 (Conjugate directions) Let $d^{(0)}, d^{(1)}, \cdots, d^{(m-1)}$ be m nonzero directions. If there exists a RSPD matrix A s.t.

$$\left\langle d^{(i)}, Ad^{(j)} \right\rangle = d^{(i)\mathrm{T}} Ad^{(j)} = 0 \left(i, j = 0,1,\cdots,m-1, i \neq j\right)$$

Then $d^{(0)}, d^{(1)}, \cdots, d^{(m-1)}$ are called conjugate directions w.r.t A or $d^{(i)} \left(i = 0,1,\cdots,m-1\right)$ are conjugate w.r.t A.

Th.1. Conjugate directions $d^{(0)}, \cdots, d^{(m-1)}$ w.r.t A are independent.

Proof: Let $k_0 d^{(0)} + k_1 d^{(1)} + \cdots + k_{m-1} d^{(m-1)} = \sum_{j=0}^{m-1} k_j d^{(j)} = 0$

Then $$\left\langle \sum_{j=0}^{m-1} k_j d^{(j)}, Ad^{(i)} \right\rangle = \sum_{j=0}^{m-1} \left\langle k_j d^{(j)}, Ad^{(i)} \right\rangle = k_i \left\langle d^{(i)}, Ad^{(i)} \right\rangle = 0$$

Thus $$k_i = 0 \left(i = 0,1,\cdots,m-1\right)$$

Th.2. Let vectors $p^{(0)}, p^{(1)}, \cdots, p^{(m-1)}$ be independent.

Then conjugate directions $d^{(0)}, d^{(1)}, \cdots, d^{(m-1)}$ w.r.t A constructive.

Proof: Let $d^{(0)} = p^{(0)}$. $\beta_{1,0} = \dfrac{\langle p^{(1)}, Ad^{(0)} \rangle}{\langle d^{(0)}, Ad^{(0)} \rangle}$,

Construct $d^{(1)} = p^{(1)} - \beta_{1,0} d^{(0)}$. Then

$$\langle d^{(1)}, Ad^{(0)} \rangle = \langle p^{(1)}, Ad^{(0)} \rangle - \frac{\langle p^{(1)}, Ad^{(0)} \rangle}{\langle d^{(0)}, Ad^{(0)} \rangle} \langle d^{(0)}, Ad^{(0)} \rangle = 0.$$

Let $\beta_{2,0} = \dfrac{\langle p^{(2)}, Ad^{(0)} \rangle}{\langle d^{(0)}, Ad^{(0)} \rangle}$, $\beta_{2,1} = \dfrac{\langle p^{(2)}, Ad^{(1)} \rangle}{\langle d^{(1)}, Ad^{(1)} \rangle}$,

Construct $d^{(2)} = p^{(2)} - \beta_{2,0} d^{(0)} - \beta_{2,1} d^{(1)}$.

Testify results $\langle d^{(2)}, Ad^{(0)} \rangle = 0$ and $\langle d^{(2)}, Ad^{(1)} \rangle = 0$.

Analogously, let

$$\beta_{k,0}=\frac{\left\langle p^{(k)},Ad^{(0)}\right\rangle}{\left\langle d^{(0)},Ad^{(0)}\right\rangle},\quad \beta_{k,1}=\frac{\left\langle p^{(k)},Ad^{(1)}\right\rangle}{\left\langle d^{(1)},Ad^{(1)}\right\rangle},\quad \cdots,\beta_{k,k-1}=\frac{\left\langle p^{(k)},Ad^{(k-1)}\right\rangle}{\left\langle d^{(k-1)},Ad^{(k-1)}\right\rangle},$$

Construct $d^{(k)}=p^{(k)}-\beta_{k,0}d^{(0)}-\beta_{k,1}d^{(1)}-\cdots-\beta_{k,k-1}d^{(k-1)}$

$$(k=1,2,\cdots,m-1)$$

Then $\left\langle d^{(k)},Ad^{(j)}\right\rangle=0\left(j=0,1,\cdots,k-1\right)$

Th.3. Let A be a RSPD matrix and $d^{(0)}, d^{(1)}, \cdots, d^{(n-1)}$ are conjugate directions w.r.t A. Solve the quadratic optimization

$$\min f(x) = \frac{1}{2} x^{\mathrm{T}} A x - b^{\mathrm{T}} x.$$

Start from $x^{(0)}$ and search along directions $d^{(0)}, d^{(1)}, \cdots, d^{(n-1)}$ by exact line search. Then at most n iterations gets the minimizer.

Proof: Let $x^{(k+1)} = x^{(k)} + \alpha_k d^{(k)}$ be iterative sequence.

where $f\left(x^{(k)} + \alpha_k d^{(k)}\right) = \min\limits_{\alpha \geq 0} f\left(x^{(k)} + \alpha d^{(k)}\right).$ -Exact line search

Then

$$0 = \left.\frac{\mathrm{d} f\left(x^{(k)} + \alpha d^{(k)}\right)}{\mathrm{d}\alpha}\right|_{\alpha=\alpha_k} = \nabla f\left(x^{(k)} + \alpha_k d^{(k)}\right)^{\mathrm{T}} d^{(k)} = \nabla f\left(x^{(k+1)}\right)^{\mathrm{T}} d^{(k)}$$

In particular $\nabla f\left(x^{(n)}\right)^{\mathrm{T}} d^{(n-1)} = \left\langle \nabla f\left(x^{(n)}\right), d^{(n-1)} \right\rangle = 0$

From $\nabla f(x) = Ax - b$ results that for $k = 0,1,\cdots,n-1.$

$$\nabla f\left(x^{(k+1)}\right) = Ax^{(k+1)} - b = A\left(x^{(k)} + \alpha_k d^{(k)}\right) - b = \nabla f\left(x^{(k)}\right) + \alpha_k A d^{(k)}$$

Particularly $\nabla f\left(x^{(n)}\right) = \nabla f\left(x^{(n-1)}\right) + \alpha_{n-1} A d^{(n-1)}$

$$= \nabla f\left(x^{(n-2)}\right) + \alpha_{n-2} A d^{(n-2)} + \alpha_{n-1} A d^{(n-1)}$$

$$= \nabla f\left(x^{(k+1)}\right) + \alpha_{k+1} A d^{(k+1)} + \alpha_{k+2} A d^{(k+2)} + \cdots + \alpha_{n-1} A d^{(n-1)}$$

Thus $\left\langle \nabla f\left(x^{(n)}\right), d^{(k)} \right\rangle = \left\langle \nabla f\left(x^{(k+1)}\right), d^{(k)} \right\rangle = 0 \ (k = 0,1,\cdots,n-2)$

That is $\left\langle \nabla f\left(x^{(n)}\right), d^{(k)} \right\rangle = 0 \quad (k = 0,1,\cdots,n-1)$

Due to $d^{(0)}, d^{(1)}, \cdots, d^{(n-1)}$ independence, we have $\nabla f\left(x^{(n)}\right) = 0.$

Then $x^{(n)}$ is a stationary point or minimizer of $f(x)$.

Conjugate Gradient Method(CGM): $\min f(x)=\frac{1}{2}x^{\mathrm{T}}Ax-b^{\mathrm{T}}x$

(1) Computing α_k **Let** $f\left(x^{(k)}+\alpha_k d^{(k)}\right)=\min_{\alpha\geq 0} f\left(x^{(k)}+\alpha d^{(k)}\right).$

Then $$0=\left.\frac{df\left(x^{(k)}+\alpha d^{(k)}\right)}{d\alpha}\right|_{\alpha=\alpha_k}=\nabla f\left(x^{(k)}+\alpha_k d^{(k)}\right)^{\mathrm{T}}d^{(k)}$$

$$=\left[A\left(x^{(k)}+\alpha_k d^{(k)}\right)-b\right]^{\mathrm{T}}d^{(k)}=-\left(b-Ax^{(k)}\right)^{\mathrm{T}}d^{(k)}+\alpha_k d^{(k)\mathrm{T}}Ad^{(k)}$$

Define $r^{(k)}=b-Ax^{(k)}$ **as residual error vector**

-negative gradient vector

Then $$\alpha_k=\frac{\left(b-Ax^{(k)}\right)^{\mathrm{T}}d^{(k)}}{d^{(k)\mathrm{T}}Ad^{(k)}}=\frac{r^{(k)\mathrm{T}}d^{(k)}}{d^{(k)\mathrm{T}}Ad^{(k)}}$$

Conjugate Gradient Method(CGM):

$$\forall x^{(0)},$$
$$r^{(0)} = b - Ax^{(0)} = -\nabla f\left(x^{(0)}\right)$$

$$d^{(0)} = r^{(0)}, \alpha_0 = \frac{r^{(0)\mathrm{T}} d^{(0)}}{d^{(0)\mathrm{T}} A d^{(0)}}$$

$$x^{(1)} = x^{(0)} + \alpha_0 d^{(0)}$$
$$r^{(1)} = b - Ax^{(1)}$$

$$d^{(1)} = r^{(1)} - \frac{r^{(1)\mathrm{T}} A d^{(0)}}{d^{(0)\mathrm{T}} A d^{(0)}} d^{(0)},$$
$$\alpha_1 = \frac{r^{(1)\mathrm{T}} d^{(1)}}{d^{(1)\mathrm{T}} A d^{(1)}}$$

$$x^{(2)} = x^{(1)} + \alpha_1 d^{(1)}$$
$$r^{(2)} = b - Ax^{(2)}$$

$$d^{(k)} = r^{(k)} - \frac{r^{(k)\mathrm{T}} A d^{(0)}}{d^{(0)\mathrm{T}} A d^{(0)}} d^{(0)} - \cdots - \frac{r^{(k)\mathrm{T}} A d^{(k-1)}}{d^{(k-1)\mathrm{T}} A d^{(k-1)}} d^{(k-1)}$$
$$\alpha_k = \frac{r^{(k)\mathrm{T}} d^{(k)}}{d^{(k)\mathrm{T}} A d^{(k)}}$$

$$x^{*} = x^{(n)} = x^{(n-1)} + \alpha_{n-1} d^{(n-1)}$$

（2） Formula simplification of CGM:

Th.4. Let A be a RSPD matrix and $d^{(0)}, d^{(1)}, \cdots, d^{(k)} \ (k \le n)$ conjugate directions w.r.t A. $r^{(0)}, r^{(1)}, \cdots, r^{(k)} \ (k \le n-1)$ are nonzero residual directions of CGM.

Then

(1) $\left\langle r^{(k+1)}, d^{(j)} \right\rangle = 0, \ j = 0, 1, \cdots, k.$

(2) $\left\langle r^{(k)}, d^{(k)} \right\rangle = \left\langle r^{(k)}, r^{(k)} \right\rangle.$

(3) $r^{(0)}, r^{(1)}, \cdots, r^{(k)} \ (k \le n-1)$ are orthogonal.

Proof:(1) $r^{(k+1)}=r^{(k)}-\alpha_k Ad^{(k)}=r^{(k-1)}-\alpha_{k-1}Ad^{(k-1)}-\alpha_k Ad^{(k)}$

$$=\cdots=r^{(j)}-\alpha_j Ad^{(j)}-\alpha_{j+1}Ad^{(j+1)}-\cdots-\alpha_k Ad^{(k)}$$ **Then**

$$\left\langle r^{(k+1)},d^{(j)}\right\rangle=\left\langle r^{(j)},d^{(j)}\right\rangle-\frac{\left\langle r^{(j)},d^{(j)}\right\rangle}{\left\langle Ad^{(j)},d^{(j)}\right\rangle}\left\langle Ad^{(j)},d^{(j)}\right\rangle-\sum_{i=j+1}^{k}\alpha_i\left\langle Ad^{(i)},d^{(j)}\right\rangle=0.$$

$j=0,1,\cdots,k.$

(2) $d^{(k)}=r^{(k)}-\frac{\left\langle r^{(k)},Ad^{(0)}\right\rangle}{\left\langle d^{(0)},Ad^{(0)}\right\rangle}d^{(0)}-\cdots-\frac{\left\langle r^{(k)},Ad^{(k-1)}\right\rangle}{\left\langle d^{(k-1)},Ad^{(k-1)}\right\rangle}d^{(k-1)}$ **Then**

$$\left\langle r^{(k)},d^{(k)}\right\rangle=\left\langle r^{(k)},r^{(k)}\right\rangle-\sum_{j=0}^{k-1}\frac{\left\langle r^{(k)},Ad^{(j)}\right\rangle}{\left\langle d^{(j)},Ad^{(j)}\right\rangle}\left\langle r^{(k)},d^{(j)}\right\rangle=\left\langle r^{(k)},r^{(k)}\right\rangle.$$

(3) By Induction **Step1.** $k=1,\quad \left\langle r^{(1)},r^{(0)}\right\rangle=\left\langle r^{(1)},d^{(0)}\right\rangle=0.$

Step2. Suppose that $\left\{r^{(0)},r^{(1)},\cdots,r^{(k)}\right\}$ **are orthogonal,**

that is $\left\langle r^{(i)},r^{(j)}\right\rangle=0, i,j=0,1,\cdots,k, i\neq j.$

$$\begin{cases} r^{(k+1)} = b - Ax^{(k+1)} \\ r^{(k)} = b - Ax^{(k)} \end{cases} \Longrightarrow \quad r^{(k+1)} - r^{(k)} = -A\left(x^{(k+1)} - x^{(k)}\right)$$

Then $r^{(k+1)} = r^{(k)} - \alpha_k A d^{(k)}$ **Thus, for** $j = 0, 1, \cdots, k-1$

$$\left\langle r^{(k+1)}, r^{(j)} \right\rangle = \left\langle r^{(k)}, r^{(j)} \right\rangle - \alpha_k \left\langle Ad^{(k)}, r^{(j)} \right\rangle$$

$$= -\alpha_k \left\langle Ad^{(k)}, d^{(j)} + \frac{\left\langle r^{(j)}, Ad^{(0)} \right\rangle}{\left\langle d^{(0)}, Ad^{(0)} \right\rangle} d^{(0)} + \cdots + \frac{\left\langle r^{(j)}, Ad^{(j-1)} \right\rangle}{\left\langle d^{(j-1)}, Ad^{(j-1)} \right\rangle} d^{(j-1)} \right\rangle = 0$$

$$\left\langle r^{(k+1)}, r^{(k)} \right\rangle = \left\langle r^{(k)} - \alpha_k Ad^{(k)}, r^{(k)} \right\rangle = \left\langle r^{(k)}, r^{(k)} \right\rangle$$

$$-\alpha_k \left\langle Ad^{(k)}, d^{(k)} + \frac{\left\langle r^{(k)}, Ad^{(0)} \right\rangle}{\left\langle d^{(0)}, Ad^{(0)} \right\rangle} d^{(0)} + \cdots + \frac{\left\langle r^{(k)}, Ad^{(k-1)} \right\rangle}{\left\langle d^{(k-1)}, Ad^{(k-1)} \right\rangle} d^{(k-1)} \right\rangle$$

$$= \left\langle r^{(k)}, r^{(k)} \right\rangle - \frac{\left\langle r^{(k)}, d^{(k)} \right\rangle}{\left\langle d^{(k)}, Ad^{(k)} \right\rangle} \left\langle Ad^{(k)}, d^{(k)} \right\rangle = \left\langle r^{(k)}, r^{(k)} \right\rangle - \left\langle r^{(k)}, d^{(k)} \right\rangle = 0$$

Th.5. Conjugate Gradient Method(CGM):

(1) $$\alpha_k = \frac{r^{(k)\mathrm{T}} d^{(k)}}{d^{(k)\mathrm{T}} A d^{(k)}} = \frac{\left\| r^{(k)} \right\|_2^2}{d^{(k)\mathrm{T}} A d^{(k)}}$$

(2) $$\beta_{k+1,j} = \frac{\left\langle r^{(k+1)}, Ad^{(j)} \right\rangle}{\left\langle d^{(j)}, Ad^{(j)} \right\rangle} = \left\langle r^{(k+1)}, \frac{1}{\alpha_j}\left(r^{(j)} - r^{(j+1)}\right) \right\rangle = 0$$

$$(j = 0, 1, \cdots, k-1)$$

(3) $$\beta_{k+1,k} = \frac{\left\langle r^{(k+1)}, Ad^{(k)} \right\rangle}{\left\langle d^{(k)}, Ad^{(k)} \right\rangle} = \frac{\left\langle r^{(k+1)}, \frac{1}{\alpha_k}\left(r^{(k)} - r^{(k+1)}\right) \right\rangle}{\left\langle d^{(k)}, Ad^{(k)} \right\rangle} = -\frac{\left\| r^{(k+1)} \right\|_2^2}{\left\| r^{(k)} \right\|_2^2}$$

$$\forall x^{(0)},$$

$$r^{(0)} = b - Ax^{(0)} = -\nabla f\left(x^{(0)}\right)$$

$$d^{(0)} = r^{(0)}, \alpha_0 = \frac{\left\|r^{(0)}\right\|_2^2}{d^{(0)\mathrm{T}} A d^{(0)}}$$

$$x^{(1)} = x^{(0)} + \alpha_0 d^{(0)}$$

$$r^{(1)} = b - Ax^{(1)}$$

$$d^{(1)} = r^{(1)} + \frac{\left\|r^{(1)}\right\|_2^2}{\left\|r^{(0)}\right\|_2^2} d^{(0)},$$

$$\alpha_1 = \frac{\left\|r^{(1)}\right\|_2^2}{d^{(1)\mathrm{T}} A d^{(1)}}$$

$$x^{(2)} = x^{(1)} + \alpha_1 d^{(1)}$$

$$r^{(2)} = b - Ax^{(2)}$$

$$d^{(k)} = r^{(k)} + \frac{\left\|r^{(k)}\right\|_2^2}{\left\|r^{(k-1)}\right\|_2^2} d^{(k-1)}$$

$$\alpha_k = \frac{\left\|r^{(k)}\right\|_2^2}{d^{(k)\mathrm{T}} A d^{(k)}}$$

$$x^* = x^{(n)} = x^{(n-1)} + \alpha_{n-1} d^{(n-1)}$$

Homework#1:

Find the minimizer of a higher-dimensional quadratic objective function by Conjugate Gradient Method Programming.

Requirements:

（1）Cover page: Homework#1
Name & student ID number

（2）Problem description

（3）Solution & Programming

（4）Results

（5）Conclusion and acquirement

2. Matrix Decomposition

(1) LU Decomposition

Th.6.

If ordinal principal sub-determinants

$$A_{ii}=\begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1i} \\ a_{21} & a_{22} & \cdots & a_{2i} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i1} & a_{i2} & \cdots & a_{ii} \end{vmatrix} \neq 0\left(i=1,\cdots,n\right).$$

Then

There exists a unique identical lower-triangular matrix L **and an invertible matrix** U **as**

$$L=\begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & 1 \end{bmatrix}, \qquad U=\begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{bmatrix}.$$

s.t. $A=LU$ **Then** $Ax=b \Longrightarrow Ly=b, Ux=y$

$$u_{11} = a_{11} \neq 0,$$

$$u_{1j} = a_{1j} \; (j = 2, \cdots, n)$$

$$l_{21} u_{11} = a_{21}$$

$$\Rightarrow \quad l_{21} = \frac{a_{21}}{u_{11}}$$

$$l_{21} u_{1j} + u_{2j} = a_{2j} \; (j \geq i = 2)$$

$$\Rightarrow$$

$$u_{2j} = a_{2j} - l_{21} u_{1j} \; (j \geq i = 2)$$

$$\sum_{k=1}^{j-1} l_{ik} u_{kj} + l_{ij} u_{jj} = a_{ij} \; (i > j)$$

$$\Rightarrow \quad l_{ij} = \frac{\left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right)}{u_{jj}}$$

$$\sum_{k=1}^{j-1} l_{ik} u_{kj} + u_{ij} = a_{ij} \; (i \leq j)$$

$$\Rightarrow \quad u_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \; (i \leq j)$$

(2) LDL^{T} decomposition of symmetric positive definite matrix

$$A = LU = \begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{bmatrix}.$$

$$= \begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & & & \\ & u_{22} & & \\ & & \ddots & \\ & & & u_{nn} \end{bmatrix} \begin{bmatrix} 1 & m_{12} & \cdots & m_{1n} \\ & 1 & \cdots & m_{2n} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix} = LDM^{\mathrm{T}}$$

If $A^{\mathrm{T}} = A$ **Then** $M = L$ **that is** $A = LDL^{\mathrm{T}}$

Thus $Ax = LDL^{\mathrm{T}}x = b \Longrightarrow \{ Ly = b, Dz = y, L^T x = z$

From $u_{ij} = d_i l_{ji}\,(i > j)$ **yields**

$$d_1 = a_{11} \neq 0$$

$$l_{21}u_{11} = a_{21} \Rightarrow l_{21} = \frac{a_{21}}{d_1}$$

$$l_{21}u_{1j} + u_{2j} = a_{2j}\,(j \geq i = 2)$$

$$\Rightarrow d_2 = a_{22} - l_{21}^2 d_1$$

$$\sum_{k=1}^{j-1} l_{ik}u_{kj} + l_{ij}u_{jj} = a_{ij}\,(i > j)$$

$$\Rightarrow l_{ij} = \frac{\left(a_{ij} - \sum_{k=1}^{j-1} l_{ik}d_k l_{jk}\right)}{d_j}$$

$$\sum_{k=1}^{j-1} l_{ik}u_{kj} + u_{ij} = a_{ij}\,(i \leq j)$$

$$\Rightarrow d_j = a_{jj} - \sum_{k=1}^{j-1} l_{jk} d_k$$

$$A = LDL^{\mathrm{T}} = LD^{\frac{1}{2}}D^{\frac{1}{2}}L^{\mathrm{T}}$$

$$= GG^{\mathrm{T}}$$

(3) QR **decomposition**

Householder Transform (H-transform)

Given $u=[u_1,\cdots,u_n]^{\mathrm{T}}\in R^n$, $\|u\|_2=\left(\sum_{i=1}^{n}u_i^2\right)^{\frac{1}{2}}=1.$

Let $H=I-2uu^{\mathrm{T}}$ **Then** $y=Hx$ **is called a H-transform.**

Testify $H^{\mathrm{T}}H=\left(I-2uu^{\mathrm{T}}\right)\left(I-2uu^{\mathrm{T}}\right)=I$

or $\|y\|^2=\langle Hx,Hx\rangle=x^{\mathrm{T}}H^{\mathrm{T}}Hx=\|x\|^2$

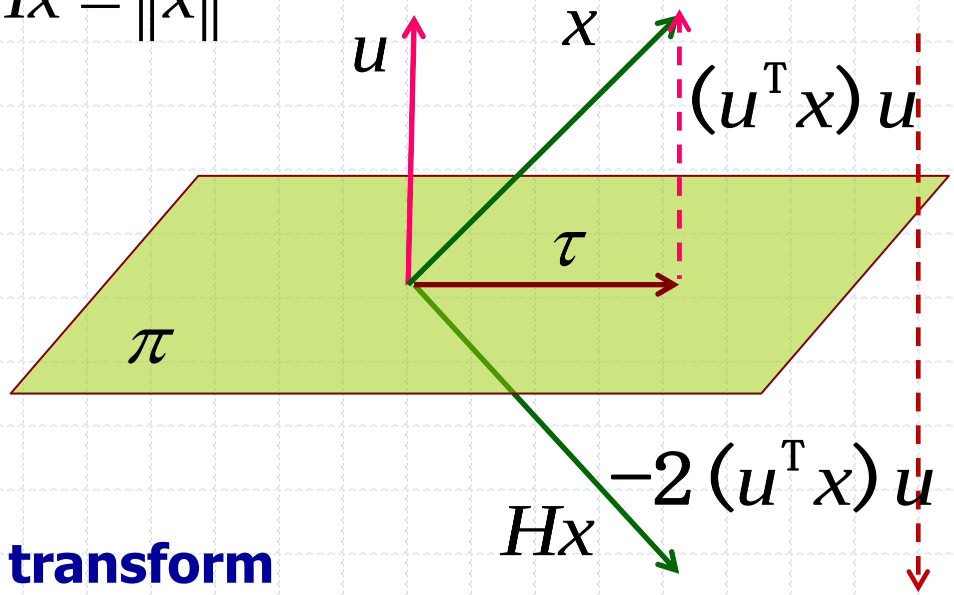
Namely $H=I-2uu^{\mathrm{T}}$

is an orthogonal matrix.

-Elementary reflecting matrix

or Householder matrix

or $y=Hx$ **is an orthogonal transform**



Th.7. **For any given vector** $0 \neq x \in R^n$, **Given** $v,\ \|v\|_2 = 1.$

Then there exists H-matrix $H = I - 2uu^{\mathrm{T}}$ **s.t.** $Hx = \sigma v.$

Proof: **Let** $\sigma^2 = x^{\mathrm{T}}x,\quad u = \dfrac{x - \sigma v}{\|x - \sigma v\|},\quad H = I - 2uu^{\mathrm{T}}.$

Then

$$uu^{\mathrm{T}} = \frac{(x - \sigma v)(x - \sigma v)^{\mathrm{T}}}{\|x - \sigma v\|^2} = \frac{xx^{\mathrm{T}} - \sigma xv^{\mathrm{T}} - \sigma vx^{\mathrm{T}} + \sigma^2 vv^{\mathrm{T}}}{(2\sigma^2 - 2\sigma x^{\mathrm{T}}v)}$$

Thus

$$Hx = x - 2uu^{\mathrm{T}}x = x - \frac{xx^{\mathrm{T}}x - \sigma xv^{\mathrm{T}}x - \sigma vx^{\mathrm{T}}x + \sigma^2 vv^{\mathrm{T}}x}{(\sigma^2 - \sigma x^{\mathrm{T}}v)}$$

$$= x - \frac{(\sigma^2 - \sigma x^{\mathrm{T}}v)x - (\sigma^3 - \sigma^2 x^{\mathrm{T}}v)v}{(\sigma^2 - \sigma x^{\mathrm{T}}v)} = \sigma v$$

Th.8. $A = QR$ **with** Q **Orthogonal & R upper triangular**

Proof: **Step1.** **Denote** $A_{m\times n} = A^{(1)} = \left[A_1^{(1)}, A_2^{(1)}, \cdots, A_n^{(1)}\right]$

If $A_1^{(1)} = 0$, **choose** $\sigma_1 = 0$, $H_1 = I_n$

Otherwise

Let $x^{(1)} = A_1^{(1)}$, $\sigma_1 = \left\|x^{(1)}\right\|$, $v^{(1)} = e^{(1)} = [1, 0, \cdots, 0]^{\mathrm{T}} \in R^n$

$$u^{(1)} = \frac{x^{(1)} - \sigma_1 v^{(1)}}{\left\|x^{(1)} - \sigma_1 v^{(1)}\right\|}, \qquad H_1 = I_n - 2u^{(1)}u^{(1)\mathrm{T}},$$

Then $\tilde{A}^{(2)} = H_1 A^{(1)} = \begin{bmatrix} \sigma_1 & \tilde{A}_{12}^{(2)} \\ 0 & \tilde{A}_{22}^{(2)} \end{bmatrix}$. **Denote** $A^{(2)} = \tilde{A}_{22}^{(2)}$.

Step2. **Let** $A^{(2)}=\left[A_1^{(2)},\cdots,A_{n-1}^{(2)}\right]$

If $A_1^{(2)}=0$, **choose** $\sigma_2=0,\quad \tilde{H}_2=I_{n-1}$. **Otherwise**

Let $x^{(2)}=A_1^{(2)},\quad \sigma_2=\left\|x^{(2)}\right\|,\quad v^{(2)}=e^{(2)}=[1,0,\cdots,0]^{\mathrm{T}}\in R^{n-1}$

$$u^{(2)}=\frac{x^{(2)}-\sigma_2 v^{(2)}}{\left\|x^{(2)}-\sigma_2 v^{(2)}\right\|},\quad \tilde{H}_2=I_{n-1}-2u^{(2)}u^{(2)\mathrm{T}}.$$

Then $\tilde{H}_2 x^{(2)}=\sigma_2 v^{(2)}$ **and** $\tilde{H}_2 A^{(2)}=\begin{bmatrix}\sigma_2 & \tilde{A}_{23}^{(3)}\\ 0 & \tilde{A}_{33}^{(3)}\end{bmatrix}.$

Let $H_2=\begin{bmatrix}1 & 0\\ 0 & \tilde{H}_2\end{bmatrix}$. **Then** $H_2H_1A=\begin{bmatrix}\sigma_1 & \tilde{a}_{12}^{(2)} & \tilde{A}_{13}^{(2)}\\ 0 & \sigma_2 & \tilde{A}_{23}^{(3)}\\ 0 & \mathbf{0} & \tilde{A}_{33}^{(3)}\end{bmatrix}.$

Stepk. Let $A^{(k)} = \tilde{A}^{(k)}_{kk}$. Repeating above operation

makes $\tilde{H}_k = I_{n-k+1} - 2u^{(k)}u^{(k)\mathrm{T}}$.

Let $H_k = \begin{bmatrix} I_{k-1} & 0 \\ 0 & \tilde{H}_k \end{bmatrix}$, $k = 1,\cdots,s$, $s = min\{m,n\}$

Then

If $m \le n$

$$Q^{-1}A = H_m \cdots H_2 H_1 A = \begin{bmatrix} \sigma_1 & \tilde{a}^{(2)}_{12} & \cdots & \tilde{a}^{(2)}_{1m} & \tilde{A}^{(2)}_{1,m+1} \\ 0 & \sigma_2 & \cdots & \tilde{a}^{(3)}_{2m} & \tilde{A}^{(3)}_{2,m+1} \\ 0 & \mathbf{0} & \ddots & \vdots & \\ 0 & 0 & \cdots & \sigma_m & \tilde{A}^{(m+1)}_{m,m+1} \end{bmatrix} = R$$

Therefore $A = QR$

Analogously,

If $m > n$ **then** $A = \tilde{Q}\begin{bmatrix} \tilde{R} \\ 0 \end{bmatrix} = QR$

where Q **Orthogonal &** R **upper triangular**

3. Line search strategies

$$\varphi(\alpha) = f\left(x^{(k)} + \alpha d^{(k)}\right)$$

(1) Exactly line search

From $$f\left(x^{(k)} + \alpha_k d^{(k)}\right) = \min_{\alpha \geq 0} f\left(x^{(k)} + \alpha d^{(k)}\right)$$

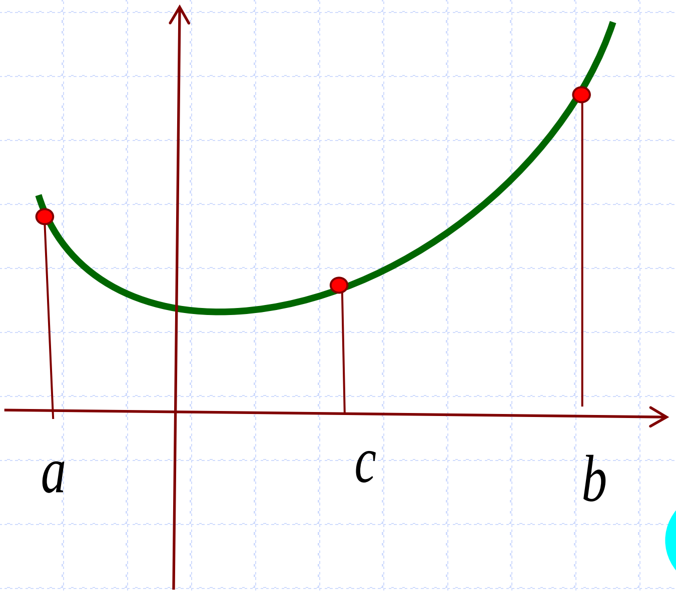
Solving following Eq to get α_k

$$0 = \varphi'(\alpha)\big|_{\alpha=\alpha_k} = \left.\frac{\mathrm{d}f\left(x^{(k)} + \alpha d^{(k)}\right)}{\mathrm{d}\alpha}\right|_{\alpha=\alpha_k} = \left\langle \nabla f\left(x^{(k)} + \alpha_k d^{(k)}\right), d^{(k)} \right\rangle$$

(2) Determination of search interval

Determine $a < c < b$

s.t. $\varphi(a) > \varphi(c) < \varphi(b)$

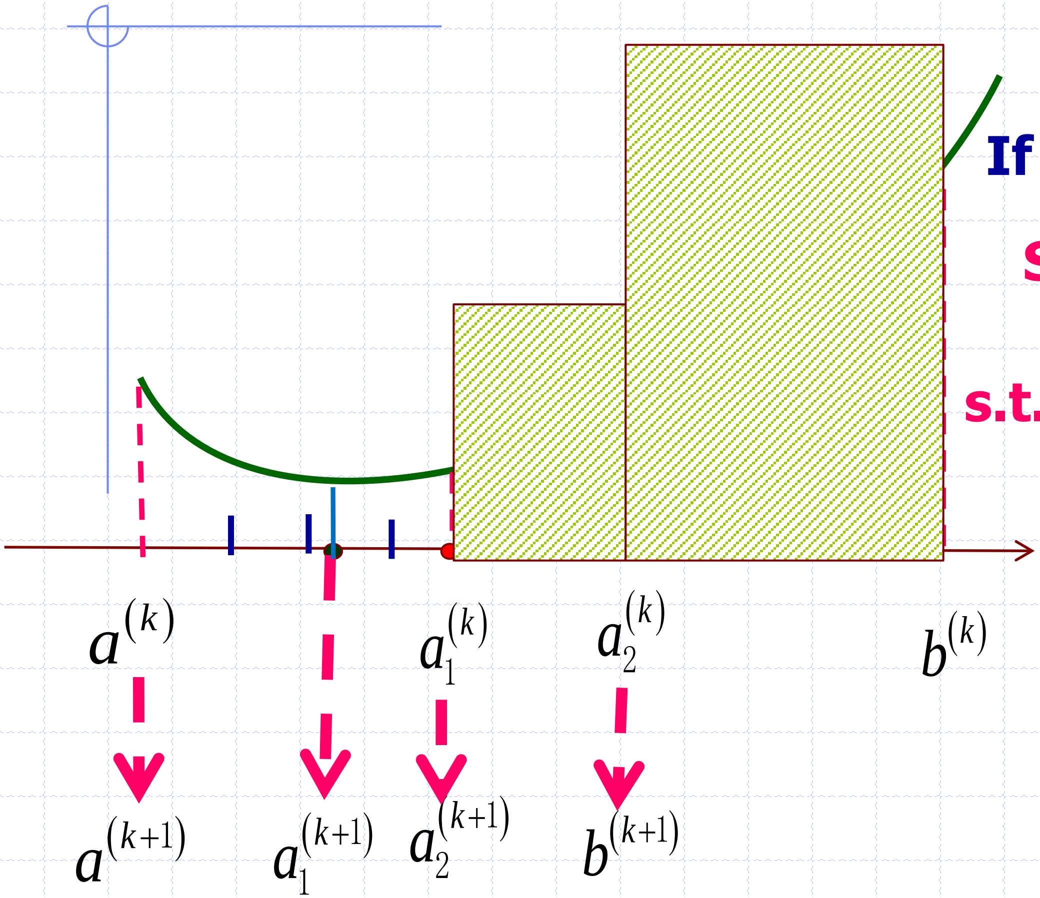


(3)0.618 Method（Golden Section Method）

Step k: Interpolate $a_1^{(k)}, \quad a_2^{(k)}$ **s.t.**

$$a_2^{(k)} - a^{(k)} = \lambda\left(b^{(k)} - a^{(k)}\right)$$

$$b^{(k)} - a_1^{(k)} - = \lambda\left(b^{(k)} - a^{(k)}\right)$$



If $\varphi\left(a_1^{(k)}\right) < \varphi\left(a_2^{(k)}\right)$ **delete** $\left[a_2^{(k)}, b^{(k)}\right]$

Step k+1: Update. Add $a_1^{(k+1)}$

s.t.

$$a_2^{(k+1)} - a^{(k+1)} = \lambda\left(b^{(k+1)} - a^{(k+1)}\right)$$

$$b^{(k+1)} - a_1^{(k+1)} = \lambda\left(b^{(k+1)} - a^{(k+1)}\right)$$

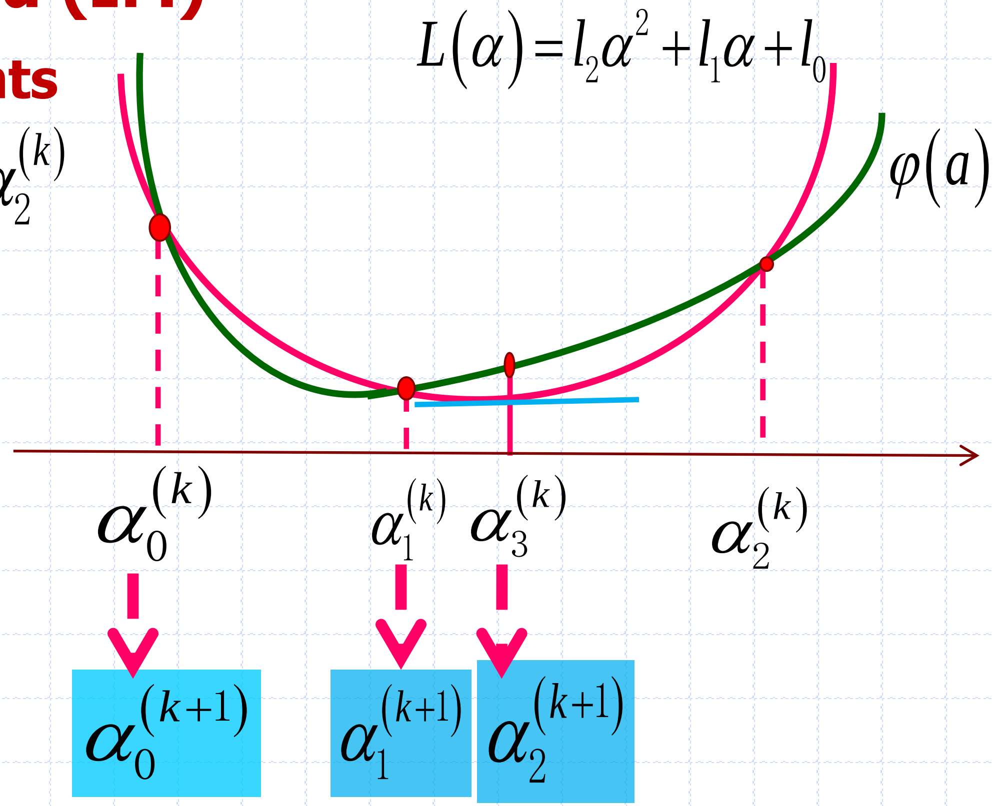
$$\lambda = \frac{a_2^{(k+1)} - a^{(k+1)}}{b^{(k+1)} - a^{(k+1)}} = \frac{a_1^{(k)} - a^{(k)}}{a_2^{(k)} - a^{(k)}} = \frac{1-\lambda}{\lambda}$$

Then $\lambda = \frac{\sqrt{5}-1}{2} \approx 0.618$

Otherwise, delete $\left[a^{(k)}, a_1^{(k)}\right]$ **Step k+1: Update**

(4) Interpolation Method (IM)

(4.1) Quadratic IM with 3 pnts



Step k: **Select** $\alpha_0^{(k)} < \alpha_1^{(k)} < \alpha_2^{(k)}$

s.t. $\varphi\left(\alpha_0^{(k)}\right) > \varphi\left(\alpha_1^{(k)}\right) < \varphi\left(\alpha_2^{(k)}\right)$

Construct quadratic Lagrangian interpolation fcn $L(\alpha)$ **passing through** $\left(\alpha_0^{(k)},\varphi\left(\alpha_0^{(k)}\right)\right)$, $\left(\alpha_1^{(k)},\varphi\left(\alpha_1^{(k)}\right)\right)$

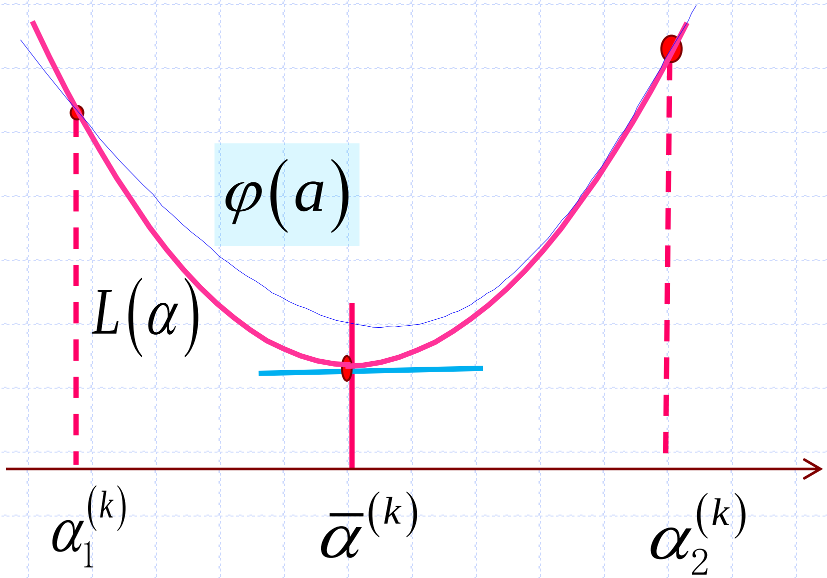
and $\left(\alpha_2^{(k)},\varphi\left(\alpha_2^{(k)}\right)\right)$ **Then solve the minimizer** $\alpha_3^{(k)}$

(1) If $\alpha_1^{(k)} < \alpha_3^{(k)}, \varphi\left(\alpha_1^{(k)}\right) < \varphi\left(\alpha_3^{(k)}\right)$ **update1** $\alpha_2^{(k+1)} = \alpha_3^{(k)}$

(2) If $\alpha_1^{(k)} < \alpha_3^{(k)}, \varphi\left(\alpha_1^{(k)}\right) > \varphi\left(\alpha_3^{(k)}\right)$, **update2** $\alpha_1^{(k+1)} = \alpha_3^{(k)}$

(3) If $\alpha_1^{(k)} > \alpha_3^{(k)}$, **(Exercise)**

(4.2) Quadratic IM with 2 pnts



Step k: **Given** $\alpha_1^{(k)} < \alpha_2^{(k)}$

and $\varphi\left(\alpha_1^{(k)}\right),\ \varphi\left(\alpha_2^{(k)}\right),\ \varphi'\left(\alpha_2^{(k)}\right)$

Construct quadratic interpolation fcn $L(\alpha)$

s.t. $L\left(\alpha_1^{(k)}\right)=\varphi\left(\alpha_1^{(k)}\right),\ L\left(\alpha_2^{(k)}\right)=\varphi\left(\alpha_2^{(k)}\right)$ **and** $L'\left(\alpha_2^{(k)}\right)=\varphi'\left(\alpha_2^{(k)}\right)$

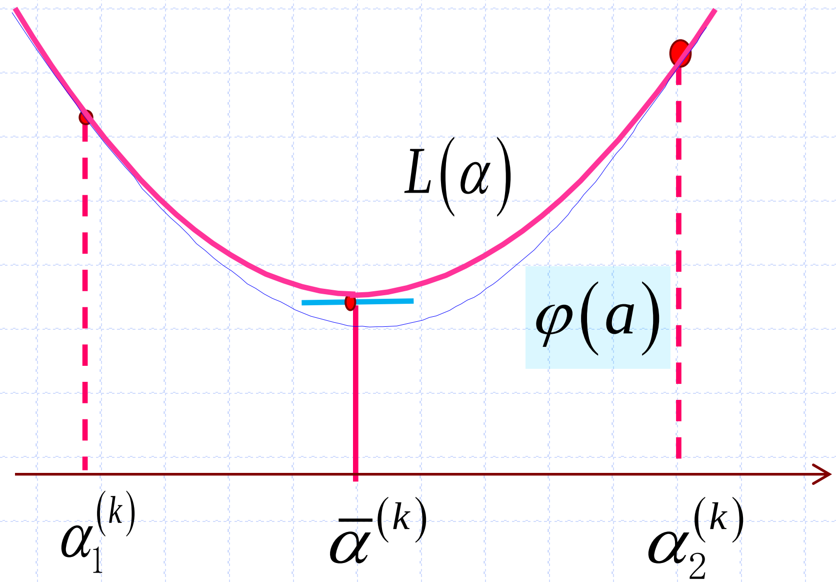
Solve the minimizer of $L(\alpha)$ **as** $\bar{\alpha}^{(k)}$

(1) If $\varphi'\left(\bar{\alpha}^{(k)}\right)\cdot\varphi'\left(\alpha_2^{(k)}\right)>0$ **update1** $\alpha_1^{(k+1)}=\alpha_1^{(k)}$ $\alpha_2^{(k+1)}=\bar{\alpha}^{(k)}$

(2) If $\varphi'\left(\bar{\alpha}^{(k)}\right)\cdot\varphi'\left(\alpha_2^{(k)}\right)<0$ **update2** $\alpha_1^{(k+1)}=\bar{\alpha}^{(k)}$ $\alpha_2^{(k+1)}=\alpha_2^{(k)}$

(3) If $\varphi'\left(\bar{\alpha}^{(k)}\right)=0$ **then** $\alpha^*=\bar{\alpha}^{(k)}$

(4.3) Quadratic IM with 2 pnts



Step k: **Given** $\alpha_1^{(k)} < \alpha_2^{(k)}$

and $\varphi\left(\alpha_1^{(k)}\right),\ \varphi'\left(\alpha_1^{(k)}\right),\ \varphi'\left(\alpha_2^{(k)}\right)$

Construct quadratic interpolation fcn $L(\alpha)$ **s.t.**

$$L\left(\alpha_1^{(k)}\right)=\varphi\left(\alpha_1^{(k)}\right),\ L'\left(\alpha_1^{(k)}\right)=\varphi'\left(\alpha_1^{(k)}\right) \text{ and } L'\left(\alpha_2^{(k)}\right)=\varphi'\left(\alpha_2^{(k)}\right)$$

Solve the minimizer of $L(\alpha)$ **as** $\bar{\alpha}^{(k)}$

(1) If $\varphi'\left(\bar{\alpha}^{(k)}\right)\cdot\varphi'\left(\alpha_2^{(k)}\right)>0$ **update1** $\alpha_1^{(k+1)}=\alpha_1^{(k)}$ $\alpha_2^{(k+1)}=\bar{\alpha}^{(k)}$

(2) If $\varphi'\left(\bar{\alpha}^{(k)}\right)\cdot\varphi'\left(\alpha_2^{(k)}\right)<0$ **update2** $\alpha_1^{(k+1)}=\bar{\alpha}^{(k)}$ $\alpha_2^{(k+1)}=\alpha_2^{(k)}$

(3) If $\varphi'\left(\bar{\alpha}^{(k)}\right)=0$ **then** $\alpha^*=\bar{\alpha}^{(k)}$

(5) Goldstein criterion of inexactly line search:

Given $\rho, \sigma, 0 < \rho < \sigma < 1$ **e.g.** $\rho \in \left(0, \frac{1}{2}\right), \sigma \in \left(\frac{1}{2}, 1\right).$

Choose $\alpha_k > 0,$ **satisfying**

$$f(x_k + \alpha_k d_k) \le f(x_k) + \rho \alpha_k \nabla f(x_k)^{\mathrm{T}} d_k,$$ **sufficient descending**

$$f(x_k + \alpha_k d_k) \ge f(x_k) + \sigma \alpha_k \nabla f(x_k)^{\mathrm{T}} d_k,$$ α_k **not very small**

(6) Wolfe criterion of inexactly line search:

Given $\rho, \sigma, 0 < \rho < \sigma < 1$

e.g. $\rho \in \left(0, \frac{1}{2}\right), \sigma \in \left(\frac{1}{2}, 1\right).$ **choose** $\alpha_k > 0,$

s.t. $$f(x_k + \alpha_k d_k) \le f(x_k) + \alpha_k \rho \nabla f(x_k)^{\mathrm{T}} d_k,$$

$$\nabla f(x_k + \alpha_k d_k)^{\mathrm{T}} d_k \ge \sigma \nabla f(x_k)^{\mathrm{T}} d_k, \sigma \in (\rho, 1)$$

4.Trust-Region Method $\quad min\ f\left(x\right), \quad x^{(k+1)} = x^{(k)} + \delta^{(k)}$

where $\quad \delta^{(k)} = \min_{\delta} q_k\left(\delta\right) = f\left(x^{(k)}\right) + \nabla f\left(x^{(k)}\right)^{\mathrm{T}} \delta + \frac{1}{2}\delta^{\mathrm{T}} B_k \delta$

satisfying $\quad \|\delta\| \le \rho^{(k)}.$ $\quad B_k \approx \nabla^2 f\left(x^{(k)}\right)$

Denote $\quad Q_k = \dfrac{f\left(x^{(k)}\right) - f\left(x^{(k)} + \delta^{(k)}\right)}{f\left(x^{(k)}\right) - q_k\left(\delta^{(k)}\right)}.$

If $\quad Q_k \approx 1,$ **then** $\quad q_k\left(\delta^{(k)}\right) \approx f\left(x^{(k)} + \delta^{(k)}\right).$ **Enlarge or no change of** $\rho^{(k)}$

If $\quad Q_k \approx 0$ **or** $Q_k < 0,$ **then lessen** $\quad \rho^{(k)}$

Advantage:

Convergence no requirements: convexity of objective fcn, initial pnt nearing minimizer, positive definite of approximate Hesse matrix.

THANK YOU FOR ATTENDING