M05M11084 最优化理论、算法与应用

5 无约束优化方法 II

无约束优化方法 II

参考：

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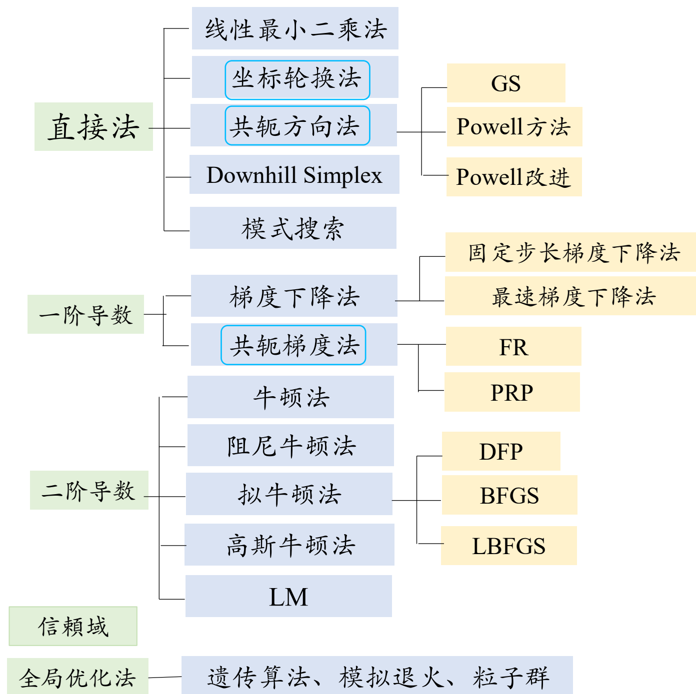
2. 最优化导论，第10章， Edwin K.P. Chong, Stanislaw H. Żak 著, 孙志强等译
3. Practical Optimization Algorithms and Engineering Applications, Chapter 6, A. Antoniou, W. LU



1.基本思想

2.共轭向量的定义与性质

3.共轭方向法

4.共轭梯度法

5.Powell方法

坐标轮换法　如果二次型的Hesse阵是对角的正定阵，那么，迭代n次收敛

$$\min f(x) \qquad f(x)=\frac{1}{2}x^T\Lambda x, \Lambda=\mathrm{diag}(\lambda_i)\succ 0,\quad x\in\mathcal{R}^n$$

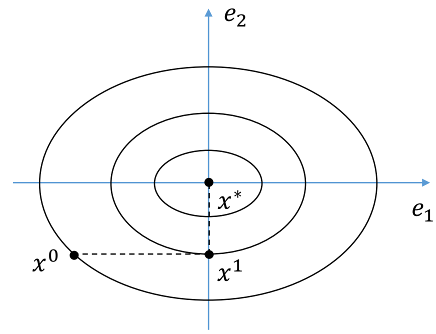
$n=2$　$f(x)=\dfrac{\lambda_1}{2}x_1^2+\dfrac{\lambda_2}{2}x_2^2$

$$x^0 \xrightarrow{e_1} x^1 \xrightarrow{e_2} x^2=x^*$$

$$x^1=x^0+\alpha_1 e_1$$

$$x^2=x^1+\alpha_2 e_2$$

$$x^2=x^*=x^0+\sum_{i=1}^{2}\alpha_i e_i$$



$\forall n>2$　$x^k=x^0+\sum_{i=1}^{k}\alpha_i e_i \quad k=1,\dots,n$　　$x^n=x^*=x^0+\sum_{i=1}^{n}\alpha_i e_i$

二次型的Hesse阵是非对角的正定阵

$f(x)=\dfrac{1}{2}x^TQx \qquad Q=\begin{bmatrix}6 & 2\\ 2 & 8\end{bmatrix}$　非对角阵 $Q\succ 0$　$e_1\to e_2\to$非极小点

正定矩阵Q的分析

$\lambda_1=4.7639$，$\lambda_2=9.2361$

$d_1=\begin{bmatrix}-0.8507\\ 0.5257\end{bmatrix} \quad d_2=\begin{bmatrix}0.5257\\ 0.8507\end{bmatrix}$　特征向量

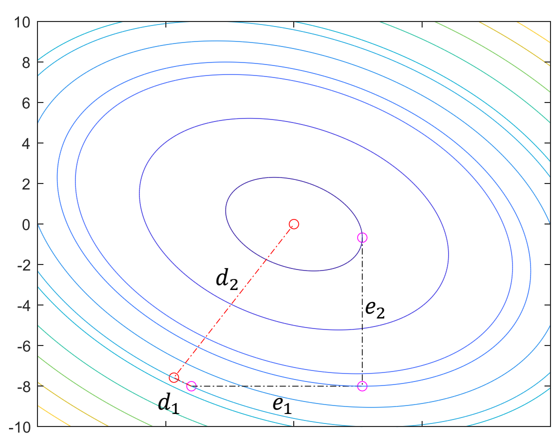
$Q=D\Lambda D^T$，$D^TD=I \qquad \Lambda=\mathrm{diag}(\lambda_i)$

$D=[d_1 \quad d_2]$

$$f(x)=\frac{1}{2}x^T(D\Lambda D^T)x$$

$$=\frac{1}{2}(D^Tx)^T\Lambda(Dx) \qquad \hat{x}=D^Tx, \qquad x=D\hat{x}$$

$$f(\hat{x})=\frac{1}{2}\hat{x}^T\Lambda\hat{x}$$



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$\hat{x}=D^Tx$，　$x=D\hat{x}$　$D=[d_1\ \ d_2]$

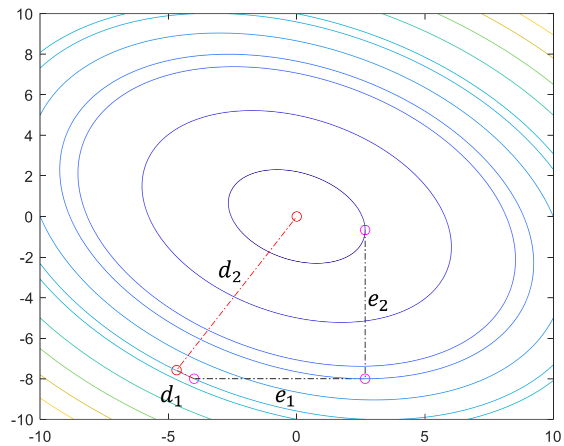
$$f(\hat{x})=\frac{1}{2}\hat{x}^T\Lambda\hat{x}$$

坐标轮换法，得 $\hat{x}^*=(0,0)$

$x^*=D\hat{x}^*$

$x^*=(8.8818\mathrm{e}{-16},2.6645\mathrm{e}{-15})$

$d_1\to d_2\to$极小点



一般地，坐标轮换法如何用？

1. 矩阵正交分解
2. 坐标变换

} 找出特征向量

3. 应用坐标轮换法n次
4. 坐标逆变换→解

} 沿着特征向量迭代n次→解

$$\min f(x) \qquad f(x)=\frac{1}{2}x^TQx, \qquad Q\succ 0, \qquad x\in\mathcal{R}^n$$ 非对角正定阵

$Q=D\Lambda D^T$，$D^TD=I$　$\Lambda=\mathrm{diag}(\lambda_i)$　$D=[d_1\ \cdots\ d_n]$

$\hat{x}=D^Tx$，　$x=D\hat{x}$

$$f(\hat{x})=\frac{1}{2}\hat{x}^T\Lambda\hat{x}$$

$$\hat{x}^k=\hat{x}^0+\sum_{i=1}^{k}\alpha_i\hat{e}_i$$

$$k=1,\dots,n$$

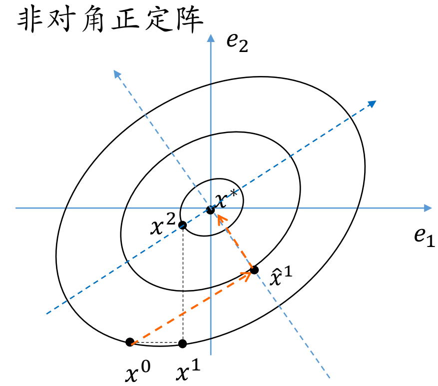
$$\hat{x}^n=\hat{x}^*$$

$$x=D\hat{x}$$

$$D\hat{x}^k=D\hat{x}^0+\sum_{i=1}^{k}\alpha_iD\hat{e}_i$$

$$x^k=x^0+\sum_{i=1}^{k}\alpha_id_i \qquad D\hat{e}_i=d_i$$

$$x^n=x^*$$



分析： $Q = D\Lambda D^T$， $D^T D = I$ $\quad \Lambda = \mathrm{diag}(\lambda_i)$

$D^T Q D = \Lambda$ $\quad$ 记$D = [d_1 \quad \cdots \quad d_n]$

$d_1, \dots, d_n$的性质

$$\begin{bmatrix} d_1^T \\ \vdots \\ d_n^T \end{bmatrix} Q [d_1 \quad \cdots \quad d_n] = \begin{bmatrix} d_1^T Q d_1 & d_1^T Q d_2 & \cdots & d_1^T Q d_n \\ d_2^T Q d_1 & d_2^T Q d_2 & \cdots & d_2^T Q d_n \\ \vdots & \vdots & \ddots & \vdots \\ d_n^T Q d_1 & d_n^T Q d_2 & \cdots & d_n^T Q d_n \end{bmatrix} = \Lambda$$

$$d_i^T Q d_j = \begin{cases} \lambda_i > 0 & i = j \\ 0 & i \neq j \end{cases}$$

称 $d_1, \dots, d_n$为关于Q的一组共轭方向

归纳：

非对角阵 $Q \succ 0$

1. 矩阵正交分解
2. 坐标变换
3. 应用坐标轮换法n次
4. 坐标逆变换→解

$\left.\begin{array}{l}1.\ 2.\end{array}\right\}$ 1.找出矩阵的一组共轭方向

$\left.\begin{array}{l}3.\ 4.\end{array}\right\}$ 2.沿共轭方向搜索迭代n次 → 最优解

1.基本思想

2.共轭向量的定义与性质

n阶正定矩阵的共轭向量组无穷多

共轭向量线性无关

n阶正定矩阵（每组）至多有n个共轭向量

3.共轭方向法

4.共轭梯度法

5.Powell方法

定义

设矩阵$Q \in \mathcal{R}^{n\times n}$为正定矩阵，若存在一组非零向量$d_0, d_1, \dots, d_{n-1} \in \mathcal{R}^n$满足

$$d_i^T Q d_j = 0, \qquad i,j = 0,1,\dots,n-1;\ \ i \neq j$$

则称向量组$d_0, d_1, \dots, d_{n-1}$关于矩阵Q共轭，或称$d_0, d_1, \dots, d_{n-1}$是矩阵Q的一组共轭方向

当$Q = I$时，$d_i^T d_j = 0,\ \ i,j = 0,1,\dots,n-1;\ \ i \neq j$，向量组$d_0, d_1, \dots, d_{n-1}$正交

① n阶正定矩阵Q的共轭向量组有无穷多个 特征向量组只是其中的一组

不妨以$n = 3$为例说明

$n = 3$，一个共轭向量组有3个共轭方向d^0, d^1, d^2 $\quad d^i = [d_1^i \quad d_2^i \quad d_3^i]^T, i = 0,1,2$

共9个未知量

$$d_i^T Q d_j = 0, \qquad i,j = 0,1,2;\ \ i \neq j \quad \Longrightarrow \begin{cases} d_0^T Q d_1 = 0 \\ d_0^T Q d_2 = 0 \\ d_1^T Q d_2 = 0 \end{cases} \quad 共3个方程$$

注意：$d_i^T Q d_j = d_j^T Q d_i$

因而，有无穷多解

一般地，

$$\begin{bmatrix} d_1^T Q d_1 & d_1^T Q d_2 & \cdots & d_1^T Q d_n \\ d_2^T Q d_1 & d_2^T Q d_2 & \cdots & d_2^T Q d_n \\ \vdots & \vdots & \ddots & \vdots \\ d_n^T Q d_1 & d_n^T Q d_2 & \cdots & d_n^T Q d_n \end{bmatrix} = \Lambda$$

定义n个方向有n^2个未知量

$(n-1) + (n-2) + \cdots + 1 = \frac{n(n-1)}{2}$个方程

有无穷多解

例 求矩阵 Q —共轭方向 $Q=\begin{bmatrix}3&0&1\\0&4&2\\1&2&3\end{bmatrix}$, $Q=Q^T$

Q 的特征值: $\lambda_1=1.0968>0, \lambda_2=3.1939>0, \lambda_3=5.7093>0$ $Q\succ 0$

$n=3$，有3个共轭方向

构建矩阵 Q-共轭方向 d^0, d^1, d^2

取 $d^0=[1,0,0]^T$ 设$d^1=(d_1^1, d_2^1, d_3^1)$， $d^2=(d_1^2, d_2^2, d_3^2)$

根据共轭方向的定义， $d^{0T}Qd^1=0$

$$d^{0T}Qd^1=[1\quad 0\quad 0]\begin{bmatrix}3&0&1\\0&4&2\\1&2&3\end{bmatrix}\begin{bmatrix}d_1^1\\d_2^1\\d_3^1\end{bmatrix}=3d_1^1+d_3^1=0$$

$d_1^1=1$， $d_2^1=0$， $d_3^1=-3$ $\Longrightarrow$ $d^1=[1,0,-3]^T$

d^2 与d^0 和 d^1 Q-共轭

$d^{0T}Qd^2=0$ and $d^{1T}Qd^2=0$

$$d^{0T}Qd^2=[1\quad 0\quad 0]\begin{bmatrix}3&0&1\\0&4&2\\1&2&3\end{bmatrix}\begin{bmatrix}d_1^2\\d_2^2\\d_3^2\end{bmatrix}=3d_1^2+d_3^2=0$$

$$d^{1T}Qd^2=[1\quad 0\quad -3]\begin{bmatrix}3&0&1\\0&4&2\\1&2&3\end{bmatrix}\begin{bmatrix}d_1^2\\d_2^2\\d_3^2\end{bmatrix}=-6d_2^2-8d_3^2=0$$

$$\Longrightarrow \begin{cases}3d_1^2+d_3^2=0\\ -6d_2^2-8d_3^2=0\end{cases}$$

令 $d_1^2=1$，解得 $d_2^2=4, d_3^2=-3$ $\Longrightarrow$ $d^2=[1,4,-3]^T$

d^0, d^1和 d^2 关于Q-共轭

$$D=[d_1\quad d_2\quad d_3]\quad D^TQD=\begin{bmatrix}3&0&0\\0&24&0\\0&0&40\end{bmatrix}$$

说明：特征向量只是共轭向量组中的一组

例 同一初始点，不同的共轭方向组

$$f(x)=\frac{1}{2}x^TQx \qquad Q=\begin{bmatrix}1&1\\1&2\end{bmatrix} \qquad x^0=\begin{bmatrix}1.4\\1.4\end{bmatrix}$$

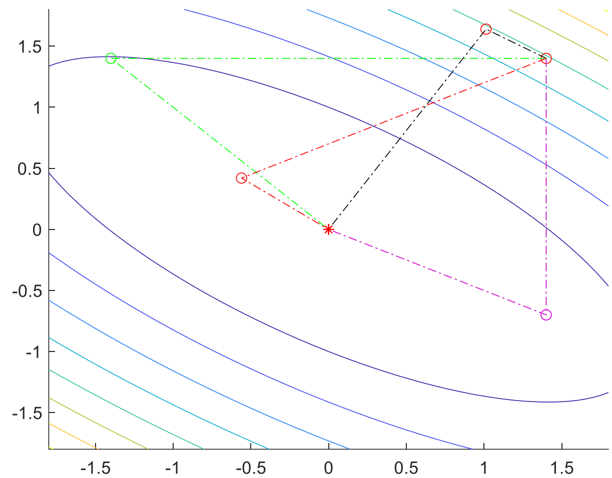
✓ 以特征向量为共轭方向

$$d_1^v=\begin{bmatrix}-0.8507\\0.5257\end{bmatrix}, d_2^v=\begin{bmatrix}0.5257\\0.8507\end{bmatrix}$$

✓ 共轭方向组A $d_1^1=\begin{bmatrix}1\\0\end{bmatrix}, d_2^1=\begin{bmatrix}1\\-1\end{bmatrix}$

✓ 共轭方向组B $d_1^2=\begin{bmatrix}0\\1\end{bmatrix}, d_2^2=\begin{bmatrix}2\\-1\end{bmatrix}$

✓ 共轭方向组C $d_1^3=\begin{bmatrix}1\\0.5\end{bmatrix}, d_2^3=\begin{bmatrix}4\\-3\end{bmatrix}$



例 更换初始点，但，共轭方向组不变

$$x^0=\begin{bmatrix}-0.5\\-1.5\end{bmatrix}$$

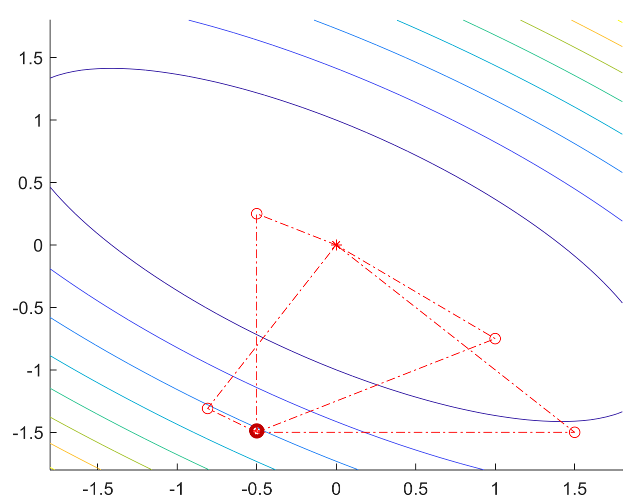
✓ 以特征向量为共轭方向

$$d_1^v=\begin{bmatrix}-0.8507\\0.5257\end{bmatrix}, d_2^v=\begin{bmatrix}0.5257\\0.8507\end{bmatrix}$$

✓ 共轭方向组A $d_1^1=\begin{bmatrix}1\\0\end{bmatrix}, d_2^1=\begin{bmatrix}1\\-1\end{bmatrix}$

✓ 共轭方向组B $d_1^2=\begin{bmatrix}0\\1\end{bmatrix}, d_2^2=\begin{bmatrix}2\\-1\end{bmatrix}$

✓ 共轭方向组C $d_1^3=\begin{bmatrix}1\\0.5\end{bmatrix}, d_2^3=\begin{bmatrix}4\\-3\end{bmatrix}$



不同的初始点，不同的共轭方向组 不影响收敛性

$x^0 = \begin{bmatrix} 1.4 \\ 1.4 \end{bmatrix}$ $x^0 = \begin{bmatrix} -0.5 \\ -1.5 \end{bmatrix}$

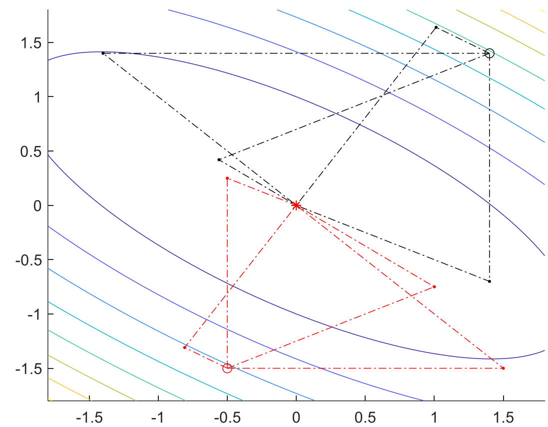
- ✓ 以特征向量为共轭方向

  $d_1^v = \begin{bmatrix} -0.8507 \\ 0.5257 \end{bmatrix}, d_2^v = \begin{bmatrix} 0.5257 \\ 0.8507 \end{bmatrix}$

- ✓ 共轭方向组A $d_1^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, d_2^1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

- ✓ 共轭方向组B $d_1^2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, d_2^2 = \begin{bmatrix} 2 \\ -1 \end{bmatrix}$

- ✓ 共轭方向组C $d_1^3 = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix}, d_2^3 = \begin{bmatrix} 4 \\ -3 \end{bmatrix}$



② 共轭向量线性无关定理

设$Q \in \mathcal{R}^{n\times n}$为正定矩阵，一向量组$d_0, d_1, \ldots, d_{n-1}$关于$Q$共轭，则该向量组线性无关

证：设 $\alpha_0 d_0 + \alpha_1 d_1 + \cdots + \alpha_{n-1} d_{n-1} = \sum_{i=0}^{n-1} \alpha_i d_i = 0$

两边左乘$d_k^T Q$，$k = 0,1, \ldots, n-1$ $d_k^T Q \sum_{i=0}^{n-1} \alpha_i d_i = \alpha_k d_k^T Q d_k = 0$

$\because Q \succ 0$，$d_k \neq 0 \implies d_k^T Q d_k > 0$

$\implies \alpha_k = 0$，$k = 0,1, \ldots, n-1$

$\implies$ 向量组$d_0, d_1, \ldots, d_{n-1}$线性无关

② 共轭向量线性无关定理

设$Q \in \mathcal{R}^{n\times n}$为正定矩阵，一向量组$d_0, d_1, \dots, d_{n-1}$关于$Q$共轭，则该向量组线性无关

推论 向量组$d_0, d_1, \dots, d_{n-1}$可以构成$\mathcal{R}^n$空间的一组基
$\mathcal{R}^n$空间中任意一点可以由它们的线性组合表示

沿着共轭方向搜索，相当于在以这组方向为基的“坐标系”中，进行“坐标”轮换搜索

③ n阶正定矩阵至多有n个共轭向量 定理

设$Q \in \mathcal{R}^{n\times n}$为正定矩阵，一组关于矩阵$Q$共轭的向量至多有$n$个

证：假设有 $n+1$个向量$d_0, d_1, \dots, d_{n-1}, d_n \in \mathcal{R}^n$关于矩阵$Q$共轭
则 $d_0, d_1, \dots, d_{n-1}$也关于矩阵Q共轭

根据共轭方向线性无关定理，$d_0, d_1, \dots, d_{n-1}$线性无关，构成$\mathcal{R}^n$的一组基
即，$\mathcal{R}^n$中的任一非零向量可由这组基线性表示

∃不全为0的系数α_k，$k = 0,1,\dots,n-1$
使

$$d_n = \sum_{k=0}^{n-1} \alpha_k d_k \qquad 0 \neq d_n^T Q d_n = \sum_{k=0}^{n-1} \alpha_k d_n^T Q d_k = 0 \qquad \text{矛盾}$$

所以，一组关于Q共轭的向量不会超过n个

①基本共轭方向法 采用一组共轭方向作为连续搜索方向

$$\min f(x) \qquad f(x)=\frac{1}{2}x^TQx+x^Tb+c, \qquad Q\succ 0, x\in\mathcal{R}^n$$

设$d_0, d_1, \dots, d_{n-1}$关于Q共轭

给定初始点 $x^0\in\mathcal{R}^n$

$k=0$

While $k<n$

$g^k=Qx^k+b$

$\alpha_k=-\dfrac{d_k^Tg^k}{d_k^TQd_k}$?

$x^{k+1}=x^k+\alpha_kd_k$

$k=k+1$

end

$x^*=x^n$?

由基本共轭方向法，第k次迭代可写成

$$\begin{aligned}x^k&=x^{k-1}+\alpha_{k-1}d_{k-1}\\&=x^{k-2}+\alpha_{k-2}d_{k-2}+\alpha_{k-1}d_{k-1}\\&=\cdots\\&=x^0+\sum_{i=0}^{k-1}\alpha_id_i\end{aligned}$$

$$x^n=x^0+\sum_{i=0}^{n-1}\alpha_id_i$$

二次型的精确步长

$$f(x)=\frac{1}{2}x^TQx+x^Tb+c,\qquad Q\succ 0,x\in\mathcal{R}^n$$

$$x^{k+1}=x^k+\alpha d_k \qquad\qquad g^k=\nabla f(x^k)=Qx^k+b$$

$$\phi(\alpha)=f(x^k+\alpha d_k) \qquad\qquad \alpha_k=-\frac{d_k^Tg^k}{d_k^TQd_k}$$

$$\begin{aligned}0=\phi'(\alpha)&=D_xf(x^k+\alpha d_k)D_\alpha(x^k+\alpha d_k)\\&=[\nabla f(x^k+\alpha d_k)]^Td_k\\&=[Q(x^k+\alpha d_k)+b]^Td_k\\&=(Qx^k+b)^Td_k+\alpha d_k^TQd_k\\&=d_k^T(Qx^k+b)+\alpha d_k^TQd_k\\&=d_k^Tg^k+\alpha d_k^TQd_k\end{aligned}$$

②二次收敛性

$$\min f(x)\qquad\qquad f(x)=\frac{1}{2}x^TQx+x^Tb+c,\qquad Q\succ 0,x\in\mathcal{R}^n$$

对于任意给定 $x^0\in\mathcal{R}^n$，基本共轭方向法都能在n次迭代之内收敛到唯一全局极小点x^*，即， $x^n=x^*$

分析:

对给定 $x^0\in\mathcal{R}^n$， $x^0\neq x^*\implies x^*-x^0\in\mathcal{R}^n$

设向量组$d_0,d_1,\dots,d_{n-1}$关于矩阵Q共轭，构成$\mathcal{R}^n$空间的一组基

$$\implies x^*-x^0=\sum_{i=0}^{n-1}\beta_id_i$$

$$\implies x^*=x^0+\sum_{i=0}^{n-1}\beta_id_i$$

基本算法公式 $x^n=x^0+\sum_{i=0}^{n-1}\alpha_id_i$

只要证明$\beta_i=\alpha_i$ $\quad x^*=x^n$

先证明 $\boxed{d_k^T Q(x^* - x^0) = -d_k^T g^k}$

$$Q(x^* - x^0) = Q\left(x^* - x^k\right) + Q\left(x^k - x^0\right)$$
$$= (Qx^* + b) - (Qx^k + b) + Q\left(x^k - x^0\right)$$
$$= 0 - g^k + Q\left(x^k - x^0\right)$$

$$g^k = Qx^k + b$$
$$g^* = Qx^* + b = 0$$

$$d_k^T Q(x^* - x^0) = -d_k^T g^k + d_k^T Q\left(x^k - x^0\right) = -d_k^T g^k$$

由基本共轭方向法，第k次迭代

$$x^k = x^0 + \sum_{i=0}^{k-1} \alpha_i d_i \longrightarrow x^k - x^0 = \sum_{i=0}^{k-1} \alpha_i d_i$$

左乘$d_k^T Q$ $$d_k^T Q\left(x^k - x^0\right) = \sum_{i=0}^{k-1} \alpha_i d_k^T Q d_i = 0$$

$$x^* - x^0 = \sum_{i=0}^{n-1} \beta_i d_i \qquad \boxed{d_k^T Q(x^* - x^0) = -d_k^T g^k}$$

左乘$d_k^T Q$ $$d_k^T Q(x^* - x^0) = \sum_{i=0}^{n-1} \beta_i d_k^T Q d_i = \beta_k d_k^T Q d_k$$

?

$$Q \succ 0 \Longrightarrow d_k^T Q d_k > 0 \longrightarrow \beta_k = \frac{d_k^T Q(x^* - x^0)}{d_k^T Q d_k} = -\frac{d_k^T g^k}{d_k^T Q d_k} = \alpha_k$$

与基本共轭方向法对比，第k次迭代

$$x^k = x^0 + \sum_{i=0}^{k-1} \alpha_i d_i \qquad \boxed{\alpha_k = -\frac{d_k^T g^k}{d_k^T Q d_k}}$$ 二次型精确步长公式

③搜索方向与梯度的正交关系

在二次型共轭方向法中，对于所有k， $0 \le k \le n-1$， $0 \le i \le k$ ，都有

$$d_i^T g_{k+1} = 0 \qquad g_k = \nabla f(x^k)$$

证明　归纳法

首先，证明$k=0$时，定理成立 即 $d_0^T g_1 = 0$

对于精确步长，有

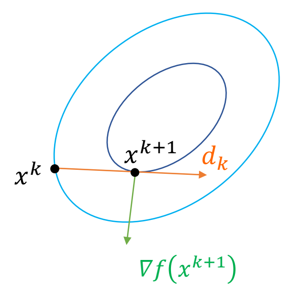
$$\Uparrow \ k = 0$$

$$\left.\begin{aligned} x^{k+1} &= x^k + \alpha_k d_k \\ \alpha_k &= \arg\min_{\alpha \ge 0} f(x^k + \alpha d_k) \end{aligned}\right. \Longrightarrow d_k^T g_{k+1} = 0$$

设 $\phi(\alpha) = f(x^k + \alpha d_k)$

$$\phi'(\alpha) = d_k^T \nabla f(x^k + \alpha d_k)$$

$$0 = \phi'(\alpha_k) = d_k^T \nabla f(x^k + \alpha_k d_k) = d_k^T g_{k+1}$$



在二次型共轭方向法中，对于所有k， $0 \le k \le n-1$， $0 \le i \le k$ ，都有

$$d_i^T g_{k+1} = 0$$

证明　设定理在$k-1$（$k < n-1$）时成立， $d_i^T g_k = 0$，$0 \le i \le k-1$

要证明，在k时也成立；　　　即， $d_i^T g_{k+1} = 0$， $0 \le i \le k$

$$x^{k+1} = x^k + \alpha_k d_k \qquad g_k = Qx^k + b$$

$$Q\alpha_k d_k = Q(x^{k+1} - x^k) = Qx^{k+1} + b - (Qx^k + b) = g_{k+1} - g_k$$

$$\Longrightarrow \ g_{k+1} = g_k + \alpha_k Q d_k$$

固定$k > 0$，考虑$0 \le i < k$　　$d_i^T g_{k+1} = \underbrace{d_i^T g_k}_{\substack{=0 \\ \because 归纳法假设}} + \alpha_k \underbrace{d_i^T Q d_k}_{\substack{=0 \\ \because 共轭向量}} = 0$

$0 \le i \le k-1$

只剩证明$d_k^T g_{k+1} = 0$

在二次型共轭方向法中，对于所有k， $0 \le k \le n-1$， $0 \le i \le k$ ，都有

$$d_i^T g_{k+1} = 0$$

证明 只剩证明$d_k^T g_{k+1} = 0$

$$\begin{aligned} d_k^T g_{k+1} &= d_k^T\left(Qx^{k+1} + b\right) \\ &= d_k^T\left(Qx^k + \alpha_k Q d_k\right) + d_k^T b \\ &= d_k^T\left(Qx^k + b\right) + \alpha_k d_k^T Q d_k \\ &= d_k^T g_k + \left(-d_k^T g_k\right) \\ &= 0 \end{aligned}$$

$$g_k = Qx^k + b$$

$$x^{k+1} = x^k + \alpha_k d_k$$

$$\alpha_k = -\frac{d_k^T g^k}{d_k^T Q d_k}$$ 二次型精确步长公式

证毕

例

$$f(x) = \frac{1}{2} x^T \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix} x - x^T \begin{bmatrix} -1 \\ 1 \end{bmatrix}, \qquad x \in \mathcal{R}^2$$

$x^0 = [0,0]^T$, Q-共轭方向$d_0 = [1,0]^T$ and $d_1 = \left[-\frac{3}{8}, \frac{3}{4}\right]^T$

$$Q = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}, \qquad b = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$\lambda(Q) = 0.7639, 5.2361 > 0 \longrightarrow Q = Q^T \succ 0$

$n = 2 \qquad x^* = x^2$

$k = 0$

$$g^0 = Qx^0 - b = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\alpha_0 = -\frac{d_0^T g^0}{d_0^T Q d_0} = -\frac{\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix}}{\begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix}} = -\frac{1}{4}$$

$$x^1 = x^0 + \alpha_0 d_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \frac{1}{4}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -\frac{1}{4} \\ 0 \end{bmatrix}$$

$k = 1$

$$g^1 = Qx^1 - b = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} -\frac{1}{4} \\ 0 \end{bmatrix} - \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ -\frac{3}{2} \end{bmatrix}$$

$$\alpha_1 = -\frac{d_1^T g^1}{d_1^T Q d_1} = -\frac{\begin{bmatrix} 0 & -\frac{3}{2} \end{bmatrix}\begin{bmatrix} -\frac{3}{8} \\ \frac{3}{4} \end{bmatrix}}{\begin{bmatrix} -\frac{3}{8} & \frac{3}{4} \end{bmatrix}\begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} -\frac{3}{8} \\ \frac{3}{4} \end{bmatrix}} = 2$$

$$x^2 = x^1 + \alpha_1 d_1 = \begin{bmatrix} -\frac{1}{4} \\ 0 \end{bmatrix} + 2\begin{bmatrix} -\frac{3}{8} \\ \frac{3}{4} \end{bmatrix} = \begin{bmatrix} -1 \\ \frac{3}{2} \end{bmatrix}$$

$$x^* = x^2$$

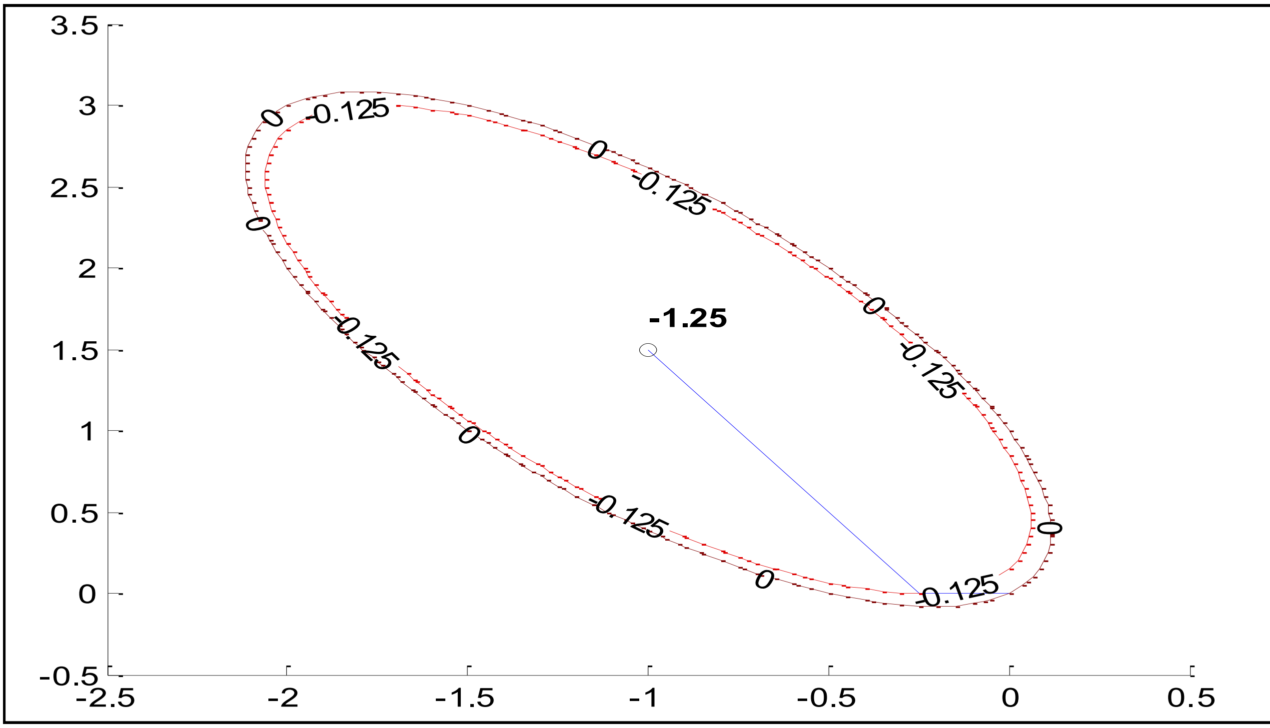
CH10-Example-10.2.xlsx

```
close all
clear
clc
Q = [4,2;2,2];
b = [-1;1];
x0 = [0;0];
d0 = [1;0]; d1 = [-0.375;0.75];
N = 2;

func = @(x)(0.5*x'*Q*x - b'*x);
getx = @(x,d,g)(x - (d'*g)/((d'*Q*d))*d);
getg = @(x)(Q*x - b);

%figure(1);


g0 = getg(x0);

x01 = x0(1);
x02 = x0(2);
v (1)= func(x0);
```

```
hold on;
for i = 1:2
    x1 = getx(x0,d0,g0);
    g1 = getg(x1);

    x01 = [x01 x1(1)];
    x02 = [x02 x1(2)];

    d0 = d1;
    x0 = x1;
    g0 = g1;
    v(i+1) = func(x0);
end
```

```
plot(x01,x02,'b');
f = func(x0);
x = -2.2:0.05:0.2; y = -0.1:0.05:3.2;
[X,Y] = meshgrid(x,y);
Z = 2*X.^2+Y.^2+2*X.*Y+X-Y;
contour (X,Y,Z,v,'ShowText','on');
%contour (X,Y,Z,'ShowText','on')

xx=x0(1)
yy=x0(2)
scatter(xx,yy,‘k’)%标注极小点"o"

text(xx,yy+0.2,{[ num2str(f) ]},‘FontSize’,10,‘FontWeight’,‘bold’);%标出极小值
```

OPT_Example_10_2.m
figure(1);
OPT_Example_10_3.m

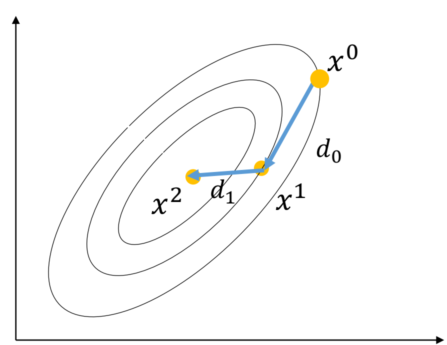


共轭方向法的难点

已知关于矩阵Q的共轭向量组$d_0, d_1, \dots, d_{n-1}$，初始点x^0

$$x^k = x^{k-1} + \alpha_{k-1} d_{k-1} \qquad k = 1,2,\dots,n$$

$$\alpha_k = -\frac{d_k^T g^k}{d_k^T Q d_k} \qquad k = 0,1,2,\dots,n-1$$



迭代前，确定n个共轭方向

但，每次迭代只用1个共轭方向

共轭方向可否随着迭代生成，
即，每次迭代时生成一个?

共轭梯度法

M05M11084 最优化理论、算法与应用

5 无约束优化方法 II

1.基本思想

2.共轭向量的定义与性质

3.共轭方向法

4.共轭梯度法

二次凸目标函数

一般目标函数

5.Powell方法

• 共轭梯度法的基本思想

✓ Hestenes和Stiefel提出解线性方程组

✓ Fletcher和Reeves引入解无约束优化

每一次迭代，产生1个共轭方向

1.第一个方向：$d_0 = -g^0$

2.其余共轭方向：

用当前点x^{k+1}的梯度g^{k+1}和前一点x^k处的搜索方向d^k， 步长α_k?

构造当前搜索方向

$$d_{k+1} = -g^{k+1} + \beta_k d^k, \qquad k = 0,1,\dots,n-2$$

并保证d_{k+1}与之前的搜索方向$d_k, d_{k-1}, \dots, d_0$共轭

3. β_k ?

• 二次凸目标函数的共轭梯度法

$$f(x) = \frac{1}{2}x^TQx + x^Tb, \qquad Q^T = Q \succ 0, \qquad x, b \in \mathcal{R}^n$$

✓ 第一次搜索：在初始点x^0处采用最速下降法

$$d_0 = -g^0, \qquad x^1 = x^0 + \alpha_0 d_0, \qquad \alpha_0 = \operatorname*{argmin}_{\alpha \ge 0} f(x^0 + \alpha d_0)$$

$$\alpha_0 = -\frac{d_0^T g^0}{d_0^T Q d_0}$$

✓ 第k次搜索：x^k出发，沿着d_k方向，确定步长

$$\phi_k(\alpha) = f\left(x^k + \alpha d_k\right)$$

$$\phi_k'(\alpha) = 0$$

$$\boxed{\alpha_k = -\frac{d_k^T g^k}{d_k^T Q d_k}}$$

$$x^{k+1} = x^k + \alpha_k d_k$$

β_k ?

二次凸目标函数的共轭梯度法

$$f(x) = \frac{1}{2}x^TQx + x^Tb, \qquad Q^T = Q \succ 0, \qquad x, b \in \mathcal{R}^n$$

✓ 第一次搜索：在初始点 x^0 处采用最速下降法

$$d_0 = -g^0, \qquad x^1 = x^0 + \alpha_0 d_0, \qquad \alpha_0 = -\frac{d_0^T g^0}{d_0^T Q d_0}$$

✓ 第二次搜索：选择d_0 和g^1的线性组合为d_1，即，$d_1 = -g^1 + \beta_0 d_0$

$$0 = d_1^T Q d_0 = (-g^1 + \beta_0 d_0)^T Q d_0 = -d_0^T Q g^1 + \beta_0 d_0^T Q d_0 \qquad \beta_0 = \frac{d_0^T Q g^1}{d_0^T Q d_0}$$

✓ 第k次搜索：取 $d_{k+1} = -g^{k+1} + \beta_k d_k$

$$0 = d_{k+1}^T Q d_k = \left(-g^{k+1} + \beta_k d_k\right)^T Q d_k = -d_k^T Q g^{k+1} + \beta_k d_k^T Q d_k \qquad \boxed{\beta_k = \frac{d_k^T Q g^{k+1}}{d_k^T Q d_k}}$$

Algorithm FR-CG-Basic

$$f(x) = \frac{1}{2}x^TQx + x^Tb, \qquad Q^T = Q \succ 0, \qquad x, b \in \mathcal{R}^n$$

Given x^0, $k = 0$

Evaluate $f(x^k)$, $g^k = \nabla f(x^k)$

Set $d_k = -g(x^k)$

While $g^k \neq 0$ & $k < n$

  Compute $\alpha_k = -\frac{d_k^T g^k}{d_k^T Q d_k}$ and set $x^{k+1} = x^k + \alpha_k d_k$

  Evaluate $g^{k+1} = \nabla f(x^{k+1})$

    $\beta_k = \frac{d_k^T Q g^{k+1}}{d_k^T Q d_k}$

    $d^{k+1} = -g^{k+1} + \beta_k d_k$

    $k \leftarrow k + 1$

end(while)

例

$$f(x)=\frac{3}{2}{x_1}^2+2{x_2}^2+\frac{3}{2}{x_3}^2+x_1x_3+2x_2x_3-3x_1-x_3$$

给定初始点$x^0=0$，用共轭梯度法求极小值点.

$n=3$ $\quad f(x)=\frac{1}{2}x^TQx-x^Tb,\quad Q=\begin{bmatrix}3&0&1\\0&4&2\\1&2&3\end{bmatrix},\quad b=\begin{bmatrix}3\\0\\1\end{bmatrix}$

$k=0$ $\quad g(x)=\nabla f(x)=Qx-b \quad \longrightarrow g^0=(-3,0,-1) \quad \longrightarrow d_0=-g^0$

$$\alpha_0=-\frac{d_0^Tg^0}{d_0^TQd_0}=\frac{10}{36} \quad \longrightarrow x^1=x^0+\alpha_0d_0=(0.8333,0,0.2778)$$

$k=1$ $\quad g^1=\nabla f(x^1)=[-0.2222 \quad 0.5556 \quad 0.6667]^T$

$$\beta_0=\frac{d_0^TQg^1}{d_0^TQd_0}=0.08025 \quad \longrightarrow d_1=-g^1+\beta_0d_0=[0.4630 \quad -0.5556 \quad -0.5864]^T$$

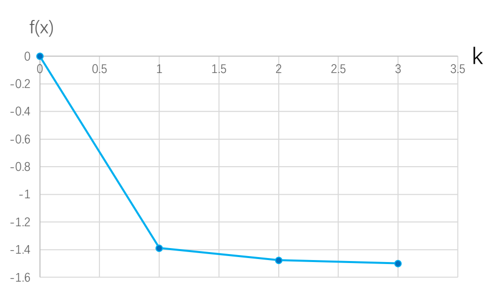
$$\alpha_1=-\frac{d_1^Tg^1}{d_1^TQd_1}=0.2187 \quad \longrightarrow x^2=x^1+\alpha_1d_1=[0.9346 \quad -0.1215 \quad 0.1495]^T$$

$k=2$ $\quad g^2=\nabla f(x^2)=[-0.04673 \quad -0.1869 \quad 0.1402]^T$

$$\beta_1=\frac{d_1^TQg^2}{d_1^TQd_1}=0.07075 \quad \longrightarrow d_2=-g^2+\beta_1d_1=[0.07948 \quad 0.1476 \quad -0.1817]^T$$

$$\alpha_2=-\frac{d_2^Tg^2}{d_2^TQd_2}=0.8231 \quad \longrightarrow x^3=x^2+\alpha_2d_2=[1.000 \quad 0.000 \quad 0.000]^T$$

$$g^3=\nabla f(x^3)=0 \quad \longrightarrow x^*=x^3=[1.000 \quad 0.000 \quad 0.000]^T$$



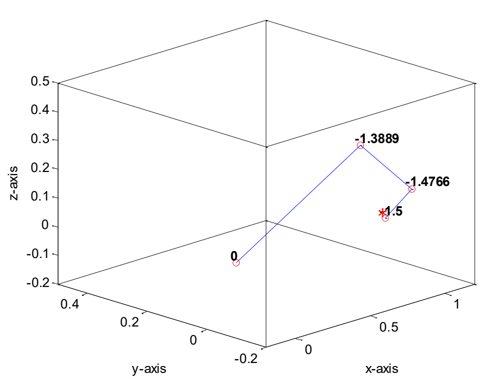
Example 10.3

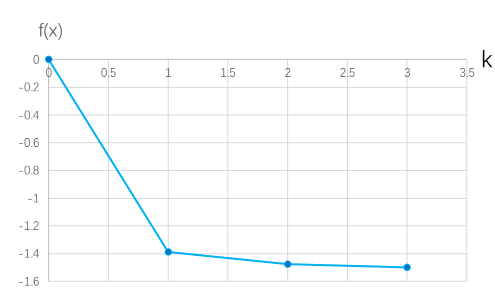
OPT_Example_10_3.m

```
close all
clear
clc
Q = [3,0,1;0,4,2;1,2,3];
b = [3;0;1];
x0 = [0;0;0];

N = 3;

func = @(x)(0.5*x'*Q*x - b'*x);
getd = @(g,d)(-g+(g'*Q*d)/(d'*Q*d)*d);
getx = @(x,d,g)(x - (d'*g)/((d'*Q*d))*d);
getg = @(x)(Q*x - b);

%figure(1);

g0 = getg(x0);
d0 = -g0;
x01 = x0(1);
x02 = x0(2);
x03 = x0(3);
v(1) = func(x0);
```

```
hold on;
for i = 1:N
    x1 = getx(x0,d0,g0);
    g1 = getg(x1);
    d1 = getd(g1,d0);

    x01 = [x01 x1(1)];
    x02 = [x02 x1(2)];
    x03 = [x03 x1(3)];

    d0 = d1;
    x0 = x1;
    g0 = g1;
    v(i+1) = func(x0);
end

plot3(x01,x02,x03,'b');
xlabel('x-axis');ylabel('y-axis');zlabel('z-axis');

axis([-0.2,1.2,-0.2,0.5,-0.2,0.5])
```

```
box on
for i=1:N+1
    scatter3(x01(i),x02(i),x03(i),‘r’)%迭代点"o"
text(x01(i),x02(i)+0.02,x03(i)+0.02,{[ num2str(v(i)) ] },‘FontSize’,10,‘FontWeight’,‘bold’);%迭代点的值
end
```





OPT_Example_10_3.m

• 一般目标函数的共轭梯度法

每一次迭代，产生1个共轭方向

1.第一个方向：$d_0 = -g^0$

2.其余共轭方向：
用当前点x^k的梯度g^k和前一点x^{k-1}处的搜索方向d_{k-1}，非精确一维搜索得步长α_k
构造当前搜索方向

$$d_k = -g^k + \beta_{k-1} d_{k-1}, \qquad k = 1,2,\dots,n-1$$

并保证d_k与之前的搜索方向$d_{k-1}, d_{k-2}, \dots, d_0$共轭

3. β_{k-1}的不同形成若干共轭梯度法

见下表

• 典型的共轭梯度法及其收敛性

名称	β_k的计算公式	提出者	收敛的步长条件
FR	$\dfrac{g^{k\,T} g^k}{g^{k-1\,T}\, g^{k-1}}$	Fletcher-Reeves	强Wolfe条件↓★
PRP	$\dfrac{g^{k\,T}(g^k - g^{k-1})}{g^{k\,T}\, g^{k-1}}$	Polak-Ribiere-Polyak	强Wolfe条件↘
PRP+	$\max\left\{\dfrac{g^{k\,T}(g^k - g^{k-1})}{g^{k\,T}\, g^{k-1}}, 0\right\}$	Powell	强Wolfe条件↓★
DY	$\dfrac{g^{k\,T} g^k}{d_k^T(g^k - g^{k-1})}$	Dai-Yuan	Wolfe条件↓★
HZ	$\left[\gamma^{k-1} - 2d_{k-1}\dfrac{\gamma^{k-1\,T}\gamma^{k-1}}{d_{k-1}^T\gamma^{k-1}}\right]^T \dfrac{g^k}{d_{k-1}^T\gamma^{k-1}}$ $\gamma^k = g^{k+1} - g^k$	Hager-Zhang	Wolfe条件↓★

↓ 共轭方向是下降方向　↘ 共轭方向不一定是下降方向　★ 全局收敛

• 共轭梯度法的特点

1.收敛性

一般形式的目标函数，采用非精确步长法，算法收敛性一般无法保证

典型算法的收敛条件如上表

2.优缺点

优点：

- ✓ 共轭梯度法的收敛速度比最速下降法快
- ✓ 不计算Hesse矩阵及其逆矩阵

缺点：

- ✓ 迭代次数增加
- ✓ 新构造的共轭方向逐渐不精确甚至于不下降，导致收敛速度变慢

改进方法：每迭代n次，令$\beta_k = 0$

Algorithm FR-CG

Given x^0, $k = 0$
Evaluate $f(x^k)$, $g^k = \nabla f(x^k)$;
Set $d_k = -g^k$
While $g^k \neq 0$
  Compute α_k and set $x^{k+1} = x^k + \alpha_k d_k$ 非精线搜，Wolfe准则
  Evaluate $g^{k+1} = \nabla f(x^{k+1})$
    $\beta_{k+1} \leftarrow DY$
      $d_{k+1} = -g^{k+1} + \beta_{k+1} d_k$
    $k \leftarrow k + 1$
    if $k =$ Integer $* n$ $d_{k+1} = -g^{k+1}$
end(while)

$\|x^{k+1} - x^k\| < tol$ 或 $\|g^{k+1}\| < tol$

Conjugate_gradient_DY.m
Wolfe__Search.m

例

例6.1 用Dai-Yuan共轭梯度法求解多维无约束最优化问题

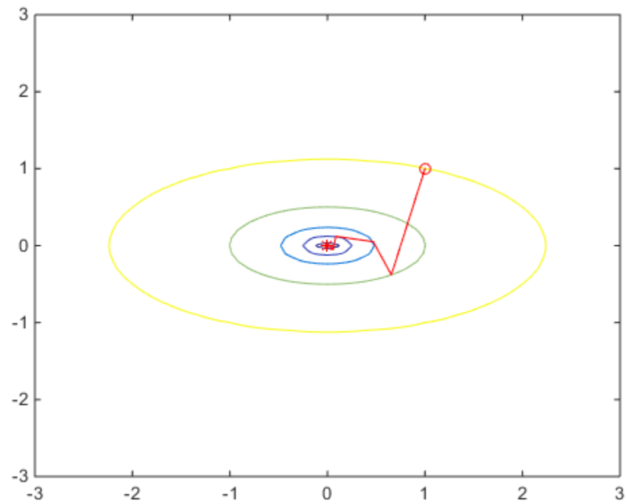
（取初始点$\boldsymbol{x}^0 = (1,1), tol = 1 \times 10^{-6}$）

$$\min f(\boldsymbol{x}) = -0.8e^{-x_1^2-4x_2^2}$$

example_6_1_CH06.m
Conjugate_gradient_DY.m
Wolfe__Search.m

testdata.txt

x_optimal = 1.0e-11 *[-0.7015   0.1358]
f_optimal =-0.8000
k = 10



例6.2 用Dai-Yuan共轭梯度法求解多维无约束最优化问题

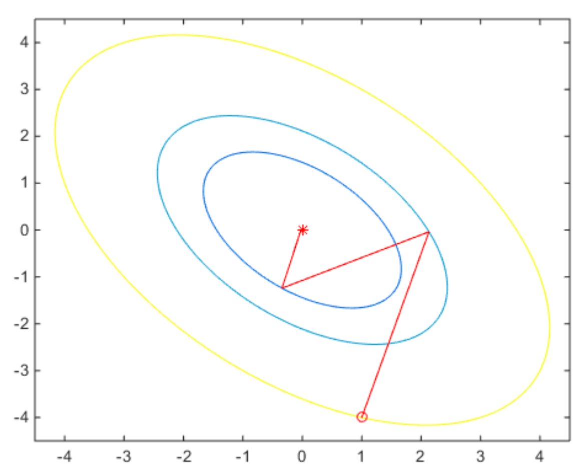
（取初始点$\boldsymbol{x}^0 = (1,-4), tol = 1 \times 10^{-6}$）

$$\min f(\boldsymbol{x}) = x_1^2 + x_2^2 + x_1x_2 + 2$$

example_6_2_CH06.m
Conjugate_gradient_DY.m
Wolfe__Search.m

testdata.txt

x_optimal = 1.0e-17 *[0.2168   -0.520
f_optimal = 2
k = 6



例6.3 用Dai-Yuan共轭梯度法求解多维无约束最优化问题

（取初始点$\boldsymbol{x}^0 = (-4,0,-4,-1,1,1), tol = 1 \times 10^{-6}$）

$$\min f(\boldsymbol{x}) \qquad f(\boldsymbol{x}) = 1 + x_1 + x_2 + x_3 + x_4$$
$$+x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4$$
$$+x_1^2 + x_2^2 + +x_3^2 + x_4^2 - 0.4e^{-x_5^2 - 6x_6^2}$$

```
example_6_3_CH06.m
Conjugate_gradient_DY.m
Wolfe__Search.m
```

x_optimal =[-0.2000 -0.2000
-0.2000 -0.2000
0.0000 0.0000]

f_optimal = 0.2000

k =40

1.基本思想

2.共轭向量的定义与性质

3.共轭方向法

4.共轭梯度法

5.Powell方法

Practical Optimization Algorithms and Engineering Applications,
Chapter 6, A. Antoniou, W. LU

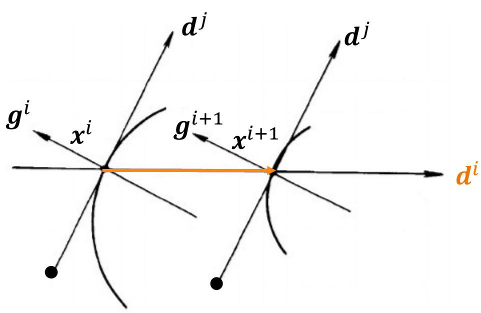
采用一维搜索产生共轭方向

共轭梯度每次迭代计算 $\nabla f(\boldsymbol{x})$

计算量： $n+1$ 函数值 $\Leftrightarrow$ $\nabla f(\boldsymbol{x})$ (n 个分量) + $f(\boldsymbol{x})$ (1个)

Powell每次迭代做一维搜索来产生共轭方向

- 对二次函数，从两个不同的点出发，沿着同一个方向$\boldsymbol{d}^j$，得到两点$\boldsymbol{x}^i$和$\boldsymbol{x}^{i+1}$
- 向量$\boldsymbol{x}^{i+1}-\boldsymbol{x}^i$ 与方向$\boldsymbol{d}^j$是共轭的



无需计算一阶导 $\nabla f(\boldsymbol{x})$

共轭方向生成原理

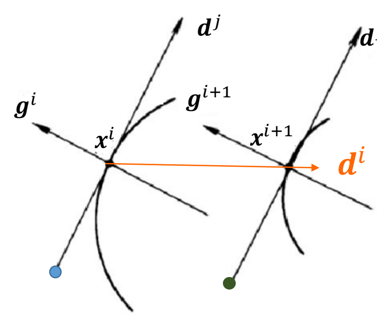
对二次函数，从两个不同的点出发，沿着同一个方向$\boldsymbol{d}^j$，得到两点$\boldsymbol{x}^i$和$\boldsymbol{x}^{i+1}$

$\boldsymbol{d}^i=\boldsymbol{x}^{i+1}-\boldsymbol{x}^i$与$\boldsymbol{d}^j$共轭

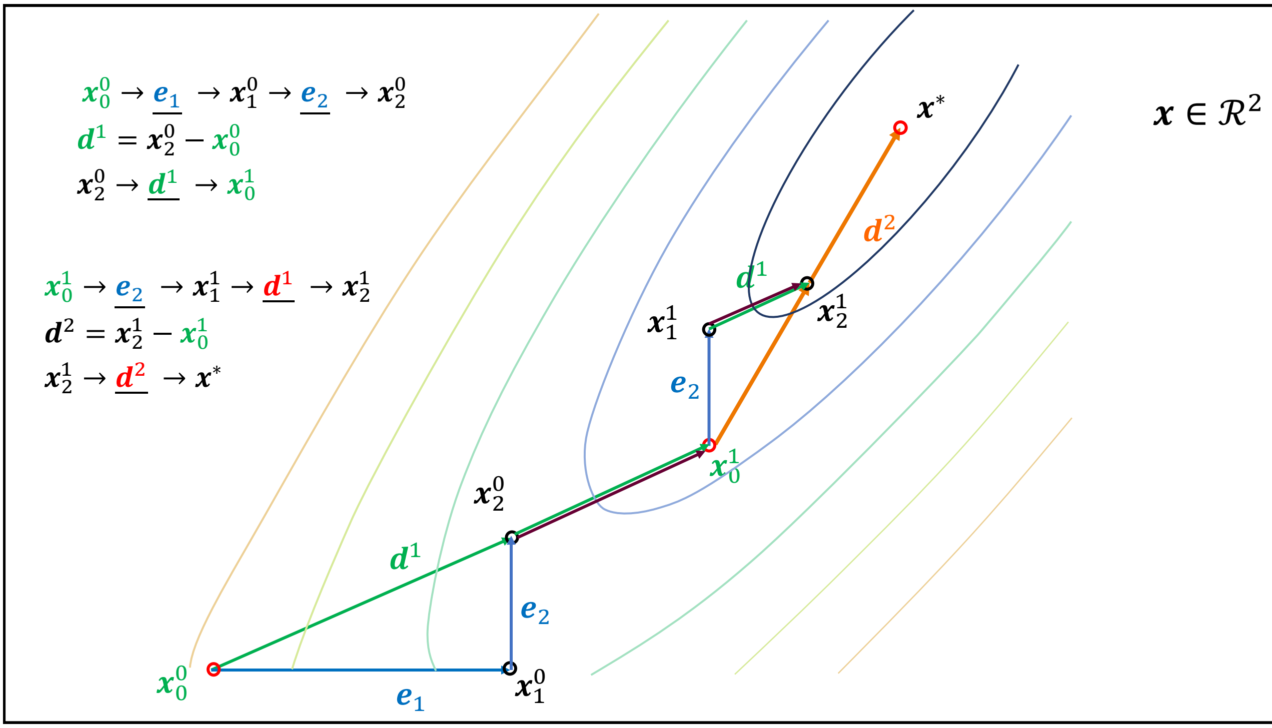
$$\boldsymbol{d}^{j\,T}\boldsymbol{g}^i=0$$
$$\boldsymbol{d}^{j\,T}\boldsymbol{g}^{i+1}=0$$

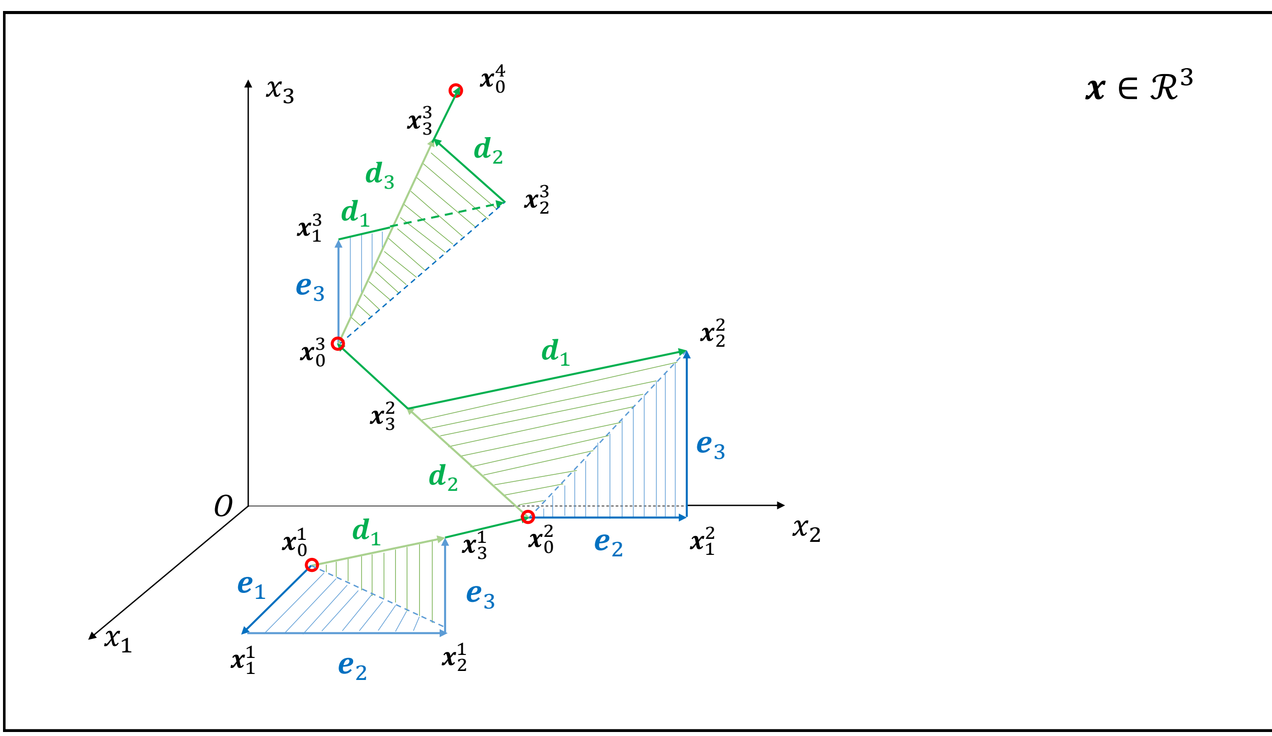
$$\boldsymbol{g}^i=Q\boldsymbol{x}^i-\boldsymbol{b}$$
$$\boldsymbol{g}^{i+1}=Q\boldsymbol{x}^{i+1}-\boldsymbol{b}$$

$$\boldsymbol{g}^{i+1}-\boldsymbol{g}^i=Q\left(\boldsymbol{x}^{i+1}-\boldsymbol{x}^i\right)$$
$$0=\boldsymbol{d}^{j\,T}\left(\boldsymbol{g}^{i+1}-\boldsymbol{g}^i\right)=\boldsymbol{d}^{j\,T}Q\left(\boldsymbol{x}^{i+1}-\boldsymbol{x}^i\right)$$



$$\boldsymbol{d}^i=\boldsymbol{x}^{i+1}-\boldsymbol{x}^i \quad\Rightarrow\quad \boldsymbol{d}^{j\,T}Q\boldsymbol{d}^i=0$$


$x_0^0 \to e_1 \to x_1^0 \to e_2 \to x_2^0$
$d^1 = x_2^0 - x_0^0$
$x_2^0 \to d^1 \to x_0^1$
$x_0^1 \to e_2 \to x_1^1 \to d^1 \to x_2^1$
$d^2 = x_2^1 - x_0^1$
$x_2^1 \to d^2 \to x^*$
$x \in \mathcal{R}^2$
x^*
d^2
d^1
x_1^1
x_2^1
e_2
x_0^1
x_2^0
d^1
e_2
x_0^0
e_1
x_1^0


$x \in \mathcal{R}^3$
x_3
x_0^4
x_3^3
d_2
d_3
x_2^3
x_1^3
d_1
e_3
x_0^3
d_1
x_2^2
x_3^2
e_3
d_2
O
x_2
x_0^1
d_1
x_3^1
x_0^2
e_2
x_1^2
e_1
e_3
x_1
x_1^1
e_2
x_2^1

- Powell算法 $\min_{x} f(\boldsymbol{x}), \boldsymbol{x} = [x_1 \quad x_2 \quad \cdots \quad x_n]^T$

$\{\boldsymbol{d}^i, i = 1, \cdots, n\}$ a given set of linearly independent vectors, $\boldsymbol{x}^0$ an initial approximation to $\boldsymbol{x}^*$

$\boldsymbol{d}^i = \boldsymbol{e}_i$

Step 1
1st Search Basic Search

$$\alpha_i = \arg\min_{\alpha} f(\boldsymbol{x}^{i-1} + \alpha \boldsymbol{d}^i)$$
$$\boldsymbol{x}^i = \boldsymbol{x}^{i-1} + \alpha_i \boldsymbol{d}^i$$

$i = 1, \cdots, n$ $\quad \boldsymbol{d}^1, \boldsymbol{d}^2, \cdots, \boldsymbol{d}^n$

Step 2
Change Direction

$$\boldsymbol{d}^i := \boldsymbol{d}^{i+1}, i = 1, \cdots, n-1$$
$$\boldsymbol{d}^n := \boldsymbol{x}^n - \boldsymbol{x}^0$$

$\boldsymbol{d}^2, \boldsymbol{d}^3, \cdots, \boldsymbol{d}^n, \boldsymbol{x}^n - \boldsymbol{x}^0$

Step 3
2nd Search Accelerated Search

$$\alpha_n = \arg\min_{\alpha} f(\boldsymbol{x}^n + \alpha \boldsymbol{d}^n)$$
$$\boldsymbol{x}^{0\text{ new}} = \boldsymbol{x}^n + \alpha_n \boldsymbol{d}^n = \boldsymbol{x}^n + \alpha_n(\boldsymbol{x}^n - \boldsymbol{x}^0)$$

Go to Step 1 unless Stopping Rules are satisfied

Stopping Rules
$\|\nabla f(\boldsymbol{x}^i)\| < \varepsilon$, $\|\boldsymbol{x}^n - \boldsymbol{x}^0\| < \varepsilon$

Example5.1

c5-Example-Powell-5.1.xlsx

$f(\boldsymbol{x}) = x_1^2 + 2x_2^2 \qquad \varepsilon = 0.03$

$\boldsymbol{x}^0 = [20,20]^T, \boldsymbol{d}^1 = [1,-1]^T, \boldsymbol{d}^2 = [1,1]^T$

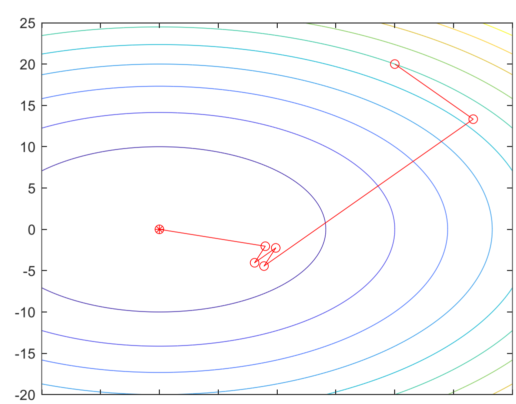
$$f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T Q \boldsymbol{x} - \boldsymbol{b}^T \boldsymbol{x}$$

$$Q = \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}, \boldsymbol{b} = \boldsymbol{0}$$

$$\boldsymbol{g}^i = \nabla f(\boldsymbol{x}^i) = Q\boldsymbol{x}^i - \boldsymbol{b}$$

$$\alpha_i = -\frac{\boldsymbol{g}^{i-1\,T} \boldsymbol{d}^i}{\boldsymbol{d}^{i\,T} Q \boldsymbol{d}^i}$$

$$\boldsymbol{x}^i = \boldsymbol{x}^{i-1} + \alpha_i \boldsymbol{d}^i$$



1st Iteration Step 1

i=1 $\boldsymbol{g}^0 = \nabla f(\boldsymbol{x}^0) = Q\boldsymbol{x}^0 - \boldsymbol{b} = \begin{bmatrix} 40 \\ 80 \end{bmatrix}$

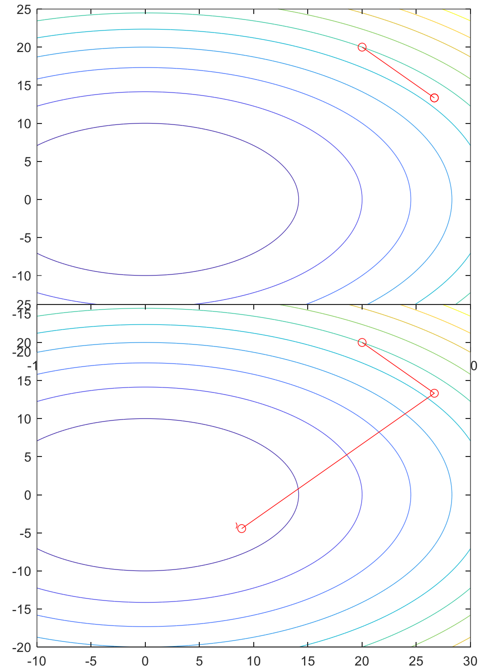
$$\alpha_1 = -\frac{\boldsymbol{g}^{0\,T}\boldsymbol{d}^1}{\boldsymbol{d}^{1\,T}Q\boldsymbol{d}^1} = -\frac{-40}{6} \approx 6.67$$

$$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \alpha_1\boldsymbol{d}^1 = \begin{bmatrix} 26.67 \\ 13.33 \end{bmatrix}$$

i=2 $\boldsymbol{g}^1 = \nabla f(\boldsymbol{x}^1) = Q\boldsymbol{x}^1 - \boldsymbol{b} \approx \begin{bmatrix} 53.34 \\ 53.34 \end{bmatrix}$

$$\alpha_2 = -\frac{\boldsymbol{g}^{1\,T}\boldsymbol{d}^2}{\boldsymbol{d}^{2\,T}Q\boldsymbol{d}^2} \approx -17.78$$

$$\boldsymbol{x}^2 = \boldsymbol{x}^1 + \alpha_2\boldsymbol{d}^2 = \begin{bmatrix} 8.89 \\ -4.44 \end{bmatrix}$$

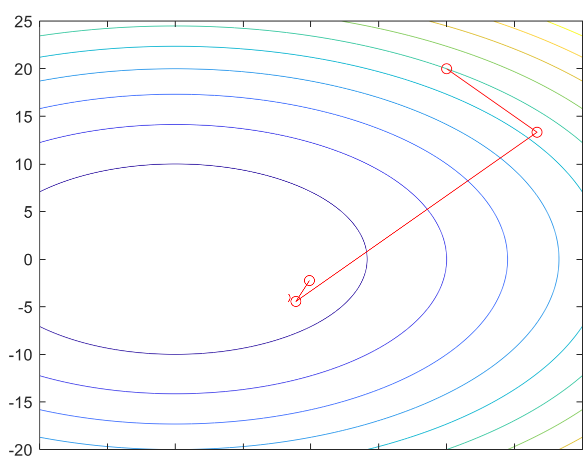


c5-Example-Powell-5.1.xlsx

Step 2

$$\boldsymbol{d}^1 = \boldsymbol{d}^2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\boldsymbol{d}^2 = \boldsymbol{x}^2 - \boldsymbol{x}^0 = \begin{bmatrix} -11.11 \\ -24.44 \end{bmatrix}$$



Step 3 $\boldsymbol{g}^2 = \nabla f(\boldsymbol{x}^2) = Q\boldsymbol{x}^2 - \boldsymbol{b} \approx \begin{bmatrix} 17.78 \\ -17.76 \end{bmatrix}$

$$\alpha_{0new} = -\frac{\boldsymbol{g}^{2\,T}\boldsymbol{d}^2}{\boldsymbol{d}^{2\,T}Q\boldsymbol{d}^2} \approx -0.09$$

$$\boldsymbol{x}^{0\,new} = \boldsymbol{x}^2 + \alpha_{0new}\boldsymbol{d}^2 \approx \begin{bmatrix} 9.89 \\ -2.25 \end{bmatrix}$$

$\|\boldsymbol{x}^{0\,new} - \boldsymbol{x}^0\| \approx 2.41 > \varepsilon$

$|f(\boldsymbol{x}^{0\,new}) - f(\boldsymbol{x}^0)| \approx 5.3 > \varepsilon$

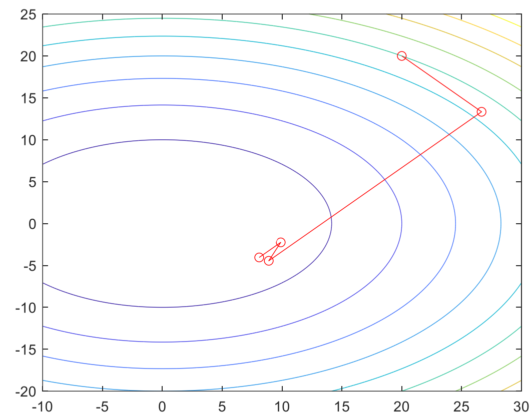
$\|\nabla f(\boldsymbol{x}^{0\,new})\| \approx 22$

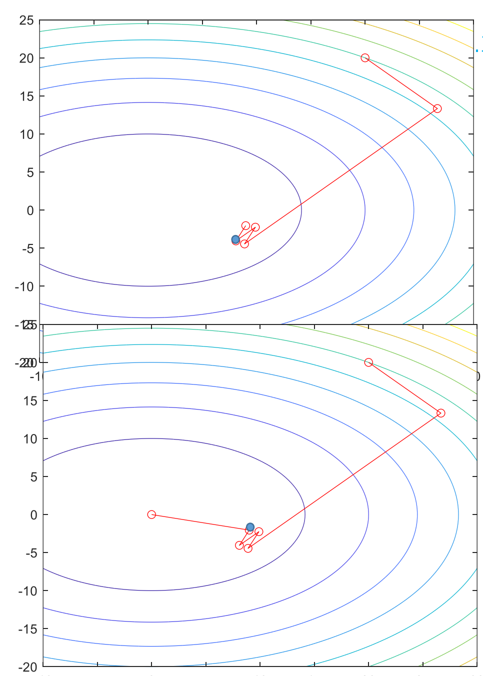
$\boldsymbol{x}^0 = \boldsymbol{x}^{0\,new}$

GoTo Step 1

$\varepsilon = 0.03$

Example_5_1_Powell_Algorithm.m





.1.xlsx

2nd Iteration $\boldsymbol{x}^0 = \begin{bmatrix} 9.89 \\ -2.25 \end{bmatrix}, \boldsymbol{d}^1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \boldsymbol{d}^2 = \begin{bmatrix} -11.11 \\ -24.44 \end{bmatrix}$

$$Q = \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}, \quad \boldsymbol{b} = \boldsymbol{0}$$

Step 1

i=1 $\boldsymbol{g}^0 = \nabla f(\boldsymbol{x}^0) = Q\boldsymbol{x}^0 - \boldsymbol{b} = \begin{bmatrix} 19.78 \\ -9 \end{bmatrix}$

$$\alpha_1 = -\frac{\boldsymbol{g}^{0\,T}\boldsymbol{d}^1}{\boldsymbol{d}^{1\,T}Q\boldsymbol{d}^1} \approx -1.80$$

$$\boldsymbol{x}^1 = \boldsymbol{x}^0 + \alpha_1\boldsymbol{d}^1 = \begin{bmatrix} 8.09 \\ -4.04 \end{bmatrix}$$

i=2 $\boldsymbol{g}^1 = \nabla f(\boldsymbol{x}^1) = Q\boldsymbol{x}^1 - \boldsymbol{b} \approx \begin{bmatrix} 16.18 \\ -16.16 \end{bmatrix}$

$$\alpha_2 = -\frac{\boldsymbol{g}^{1\,T}\boldsymbol{d}^2}{\boldsymbol{d}^{2\,T}Q\boldsymbol{d}^2} \approx -0.08$$

$$\boldsymbol{x}^2 = \boldsymbol{x}^1 + \alpha_2\boldsymbol{d}^2 = \begin{bmatrix} 9 \\ -2.05 \end{bmatrix}$$

c5-Example-Powell-5.1.xlsx

Step 2

$$\boldsymbol{d}^1 = \boldsymbol{d}^2 = \begin{bmatrix} -11.11 \\ -24.44 \end{bmatrix}$$

$$\boldsymbol{d^2} = \boldsymbol{x}^2 - \boldsymbol{x}^0 = \begin{bmatrix} -0.89 \\ 0.20 \end{bmatrix}$$

Step 3

$$\boldsymbol{g}^2 = \nabla f(\boldsymbol{x}^2) = Q\boldsymbol{x}^2 - \boldsymbol{b} \approx \begin{bmatrix} 18 \\ -8.2 \end{bmatrix}$$

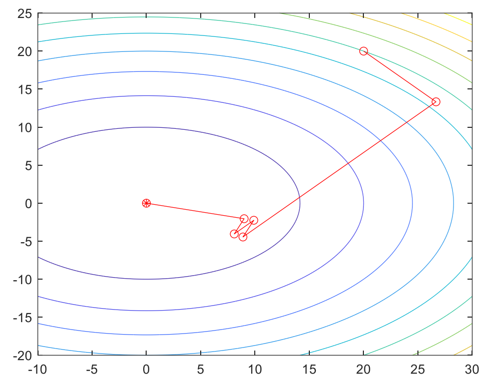
$$\alpha_{0new} = -\frac{\boldsymbol{g}^{2\,T}\boldsymbol{d}^2}{\boldsymbol{d}^{2\,T}Q\boldsymbol{d}^2} \approx 10.1$$

$$\boldsymbol{x}^{0\,new} = \boldsymbol{x}^2 + \alpha_{0new}\boldsymbol{d}^2 \approx \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$\|\boldsymbol{x}^{0\,new} - \boldsymbol{x}^0\| \approx 9.22 > \varepsilon$

$|f(\boldsymbol{x}^{0\,new}) - f(\boldsymbol{x}^0)| \approx 44.67 > \varepsilon$

$\varepsilon = 0.03$

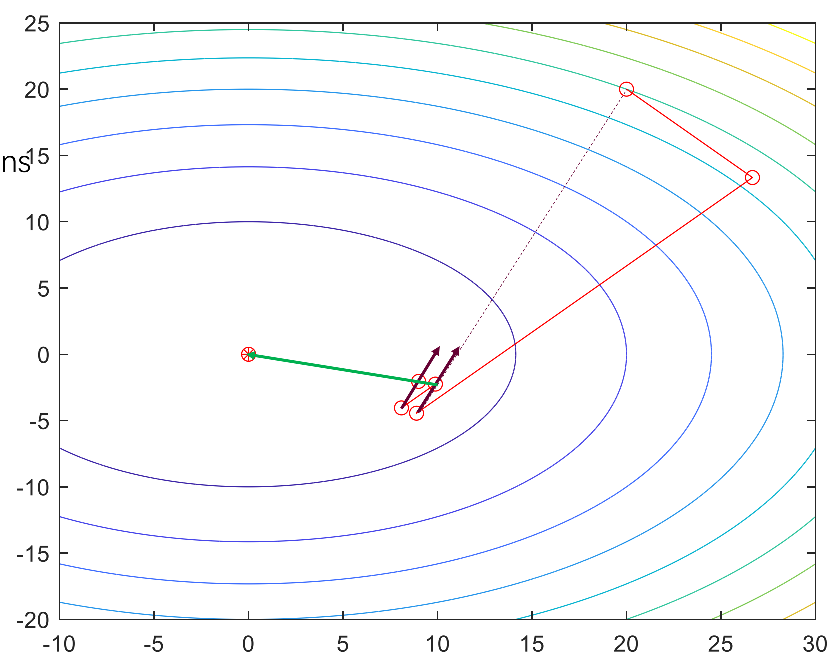


$\|\nabla f(\boldsymbol{x}^{0\,new})\| \approx 0$

Stop

$\boldsymbol{x}^* = \boldsymbol{x}^{0\,new}$

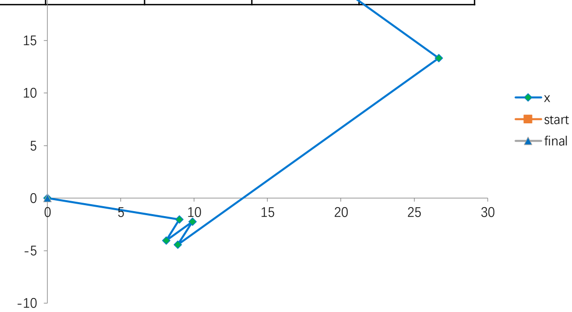
Q-Conjugate Directions



Powell's Algorithm - Example5.1

n	$\boldsymbol{x}$		Q				$\boldsymbol{g}$		$\boldsymbol{d}$		α	$\lVert\boldsymbol{g}\rVert$	$f(\boldsymbol{x})$
0	20	20	2	0	0	4	40	80	1	-1	6.6667	89.4427	1200
1	26.667	13.3333	2	0	0	4	53.3333	53.3333	1	1	-17.7778	75.4247	1066.667
2	8.8889	-4.4444	2	0	0	4	17.7778	-17.7778	-11.1111	-24.4444	-0.0899	25.1416	118.5185
0	9.8876	-2.2472	2	0	0	4	19.7753	-8.9888	1	1	-1.7978	21.7223	107.8652
1	8.0899	-4.0449	2	0	0	4	16.1798	-16.1798	-11.1111	-24.4444	-0.0818	22.8817	98.1694
2	8.9989	-2.0452	2	0	0	4	17.9977	-8.1808	-0.8888	0.2020	10.125	19.7698	89.3452
0	0	4.88E-15	2	0	0	4	0	1.95E-14				1.95E-14	4.77E-29

c5-Example-Powell-5.1.xlsx



Powell's Algorithm - Disadvantage

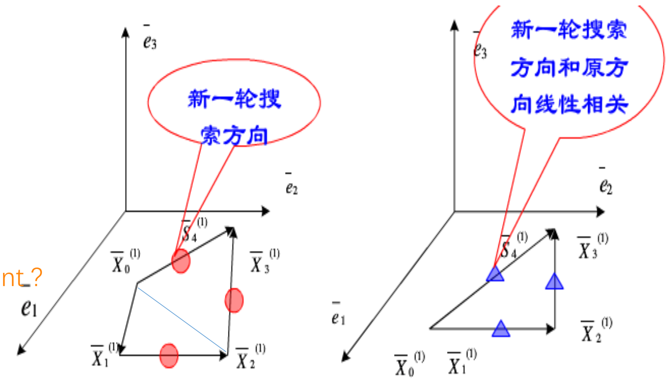
After the new displacement vector becomes a new search vector and is added to the end of the search vector list, the vectors may become linearly dependent and not produce *n*-dimensional space.

$$\boldsymbol{x}^i = \boldsymbol{x}^{i-1} + \alpha_i \boldsymbol{d}^i, i = 1, \cdots, n$$

$$\boldsymbol{x}^n = \boldsymbol{x}^{n-1} + \alpha_n \boldsymbol{d}^n$$

$$= \boldsymbol{x}^{n-2} + \alpha_{n-1} \boldsymbol{d}^{n-1} + \alpha_n \boldsymbol{d}^n$$

$$= \boldsymbol{x}^0 + \underbrace{\alpha_1 \boldsymbol{d}^1 + \cdots + \alpha_n \boldsymbol{d}^n}_{\text{linearly independent or dependent?}}$$



Introduce an **Improved Powell's algorithm**

• Improved Powell's algorithm

1. Determine whether the original search direction set is available for next iteration ?
   If available, just use it; else go to 2.
2. Determine in which direction the function value decrease the largest, and then use the new search vector to replace it.

For kth iteration, denote

$$f_1 = f(\boldsymbol{x}_0^k), f_2 = f(\boldsymbol{x}_n^k), f_3 = f(\boldsymbol{x}_{n+1}^k)$$
$$\Delta_m^k = \max_i\{\Delta_i^k, i = 1,2,\dots,n\}$$
$$\Delta_i^k = f(\boldsymbol{x}_{i-1}^k) - f(\boldsymbol{x}_i^k), \qquad i = 1,2,\dots,n$$
$$\boldsymbol{s}_m^k = \boldsymbol{x}_m^k - \boldsymbol{x}_{m-1}^k$$
$$\boldsymbol{s}^k = \boldsymbol{x}_n^k - \boldsymbol{x}_0^k$$

the reflection point

$$\boldsymbol{x}_{n+1}^k = \boldsymbol{x}^k = 2\boldsymbol{x}_n^k - \boldsymbol{x}_0^k$$

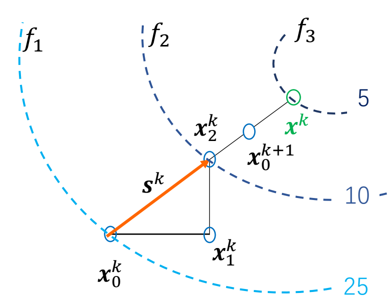
The search vector $\boldsymbol{s}_m^k$ corresponds to Δ_m^k for the function value $f(\boldsymbol{x}_m^k)$ decreases largest of all.

Reflection Point $\quad n = 2, \quad \boldsymbol{x} \in \mathcal{R}^2$

$$\boldsymbol{x}^k = 2\boldsymbol{x}_2^k - \boldsymbol{x}_0^k$$

$$\boldsymbol{x}^k - \boldsymbol{x}_2^k = \boldsymbol{x}_2^k - \boldsymbol{x}_0^k$$

$$f_1 = f(\boldsymbol{x}_0^k), f_2 = f(\boldsymbol{x}_2^k), f_3 = f(\boldsymbol{x}^k)$$
$$\Delta_m^k = \max_{i=1,2}\{\Delta_i^k\}$$
$$\Delta_i^k = f(\boldsymbol{x}_{i-1}^k) - f(\boldsymbol{x}_i^k), \qquad i = 1,2$$
$$\boldsymbol{s}_m^k = \boldsymbol{x}_m^k - \boldsymbol{x}_{m-1}^k$$
$$\boldsymbol{s}^k = \boldsymbol{x}_2^k - \boldsymbol{x}_0^k$$



$$f_1 = 25,\ f_2 = 10,\ f_3 = 5$$
$$\Delta_1^k = 25 - 10 = 15 > \Delta_2^k = 5$$

$$\Delta_1^k > \Delta_2^k, \quad m = 1$$
$$\boldsymbol{s}_1^k = \boldsymbol{x}_2^k - \boldsymbol{x}_0^k \xleftarrow{\text{Replace by}} \boldsymbol{s}^k$$

Powell's condition

$$\text{If} \begin{cases} f_3 < f_1 & \text{Cond}_{\text{PWL 1}} \\ (f_1 - 2f_2 + f_3)\left(f_1 - f_2 - \Delta_m^k\right)^2 < \frac{1}{2}\Delta_m^k (f_1 - f_3)^2 & \text{Cond}_{\text{PWL 2}} \end{cases}$$

then $\boldsymbol{s}_m^k = \boldsymbol{s}^k$ and others $\boldsymbol{s}_i^k, i = 1,2,\dots,m-1,m+1,\dots n$

else $\boldsymbol{s}_i^k, i = 1,2,\dots,m-1,m,m+1,\dots n$ (NO Change)

Improved Powell's algorithm

1. Let, the number of iteration $k = 1$,
   initial point $\boldsymbol{x}_0^1 = \boldsymbol{x}_0$, accuracy $\varepsilon_1, \varepsilon_2$
   initial direction set $\boldsymbol{s}_i^1 = \boldsymbol{e}_i,\ i = 1,2,\dots,n$

$$\lambda^* = -\frac{(\boldsymbol{Q}\boldsymbol{x} - \boldsymbol{b})^{\mathrm{T}} \boldsymbol{s}}{\boldsymbol{s}^{\mathrm{T}} \boldsymbol{Q} \boldsymbol{s}}$$

2. For i=1,2,…,n, from the point $\boldsymbol{x}_{i-1}^k$ along the search vector $\boldsymbol{s}_i^k$

$$\begin{cases} \lambda_i^* = \underset{\lambda_i}{\operatorname{argmin}} f\left(\boldsymbol{x}_{i-1}^k + \lambda_i \boldsymbol{s}_i^k\right) \\ \boldsymbol{x}_i^k = \boldsymbol{x}_{i-1}^k + \lambda_i^* \boldsymbol{s}_i^k \end{cases}$$

   and let $\boldsymbol{s}^k = \boldsymbol{x}_n^k - \boldsymbol{x}_0^k$

   1st search

   If $\|\boldsymbol{s}^k\| = \|\boldsymbol{x}_n^k - \boldsymbol{x}_0^k\| > \varepsilon$

$$\text{then} \begin{cases} \lambda^* = \underset{\lambda}{\operatorname{argmin}} f\left(\boldsymbol{x}_n^k + \lambda \boldsymbol{s}^k\right) \\ \boldsymbol{x}_{n+1}^k = \boldsymbol{x}_n^k + \lambda^* \boldsymbol{s}^k \end{cases}$$

   else $\boldsymbol{x}^* = \boldsymbol{x}_n^k,\ \ f^* = f(\boldsymbol{x}^*)$, STOP

   from the point $\boldsymbol{x}_n^k$ along the search vector $\boldsymbol{s}^k$

   2nd search

3. Stopping rule $\|\boldsymbol{x}_{n+1}^k - \boldsymbol{x}_0^k\| \le \varepsilon_1$ or $|f(\boldsymbol{x}_{n+1}^k) - f(\boldsymbol{x}_0^k)| \le \varepsilon_2 |f(\boldsymbol{x}_{n+1}^k)|$
   If Stopping rule is satisfied, we get $\boldsymbol{x}^* = \boldsymbol{x}_{n+1}^k$, $f^* = f(\boldsymbol{x}^*)$
   Else go to 4.

4. Calculate $f(\boldsymbol{x}_i^k)$, $i = 1,2,\dots,n$
   $\Delta_m^k = \max_{i=1,2,\dots,n} \{\Delta_i^k = f(\boldsymbol{x}_{i-1}^k) - f(\boldsymbol{x}_i^k)\}$
   Decrease largest along $\boldsymbol{s}_m^k = \boldsymbol{x}_m^k - \boldsymbol{x}_{m-1}^k$

5. Let $\boldsymbol{x}^k = 2\boldsymbol{x}_n^k - \boldsymbol{x}_0^k$, $f_1 = f(\boldsymbol{x}_0^k), f_2 = f(\boldsymbol{x}_n^k), f_3 = f(\boldsymbol{x}^k)$

$$\text{If}\begin{cases} f_3 < f_1 & \text{Cond}_{\text{PWL 1}} \\ (f_1 - 2f_2 + f_3)(f_1 - f_2 - \Delta_m^k)^2 < \frac{1}{2}\Delta_m^k (f_1 - f_3)^2 & \text{Cond}_{\text{PWL 2}} \end{cases}$$

   then GO TO 6
   else GO TO 7

6. $\boldsymbol{x}_0^{k+1} = \boldsymbol{x}_{n+1}^k$
   $s_i^{k+1} = s_i^k, i = 1,\dots,m-1; s_i^{k+1} = s_{i+1}^k, i = m,\dots,n-1; s_n^{k+1} = s^k$
   $k = k+1$
   GO TO 2

$$[s_1^{k+1}, s_2^{k+1}, \dots, s_n^{k+1}] \Leftarrow [s_1^k, \dots, s_{m-1}^k, s_{m+1}^k, s_n^k, \dots, s^k]$$

7. If $f_2 < f_3$, then $x_0^{k+1} = x_n^k$ else $x_0^{k+1} = x^k$
   $s_i^{k+1} = s_i^k, i = 1,\dots,n$
   $k = k+1$
   GO TO 2

OR

6. $\boldsymbol{x}_0^{k+1} = \boldsymbol{x}^k$
   $s_m^{k+1} = s^k$ and others $s_i^{k+1} = s_i^k, i = 1, \ldots, n$ and $i \neq m$
   $k = k + 1$
   GO TO 2

$$\left[s_1^{k+1}, s_2^{k+1}, \ldots, s_n^{k+1}\right] \Longleftarrow \left[s_1^k, \ldots, s_{m-1}^k, s^k, s_{m+1}^k, \ldots, s_n^k\right]$$

7. If $f_2 < f_3$, then $x_0^{k+1} = x_n^k$ else $x_0^{k+1} = x^k$
   $s_i^{k+1} = s_i^k, i = 1, \ldots, n$
   $k = k + 1$
   GO TO 2