迭代点附近的等值面

f(x)的二次近似

- 思想：二阶**Taylor**展开

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}^{(k)}) + \nabla f(\boldsymbol{x}^{(k)})^T (\boldsymbol{x} - \boldsymbol{x}^{(k)}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^{(k)})^T \nabla^2 f(\boldsymbol{x}^{(k)})(\boldsymbol{x} - \boldsymbol{x}^{(k)})$$

$$\Longrightarrow \quad f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^T \boldsymbol{x} + c$$

记为 $\boldsymbol{A} = \nabla^2 f(\boldsymbol{x}^{(k)})$ 二次函数时，**A**为确定值

$$\boldsymbol{b} = \nabla f(\boldsymbol{x}^{(k)}) - \nabla^2 f(\boldsymbol{x}^{(k)})\boldsymbol{x}^{(k)}$$

$$c = f(\boldsymbol{x}^{(k)}) + \nabla f(\boldsymbol{x}^{(k)})^T \boldsymbol{x}^{(k)} + \frac{1}{2}\boldsymbol{x}^{(k)T}\nabla^2 f(\boldsymbol{x}^{(k)})\boldsymbol{x}^{(k)}$$

二次函数

- 设A为对称矩阵，二次函数等值面

$$f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^T \boldsymbol{x} + c$$

驻点方程： $\nabla f(\overline{\boldsymbol{x}}) = \boldsymbol{A}\overline{\boldsymbol{x}} + \boldsymbol{b} = 0$

- 驻点方程有解： $rank\boldsymbol{A} = rank[\boldsymbol{A}\ \boldsymbol{b}]$

$$f(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x} - \overline{\boldsymbol{x}})^T \boldsymbol{A}(\boldsymbol{x} - \overline{\boldsymbol{x}}) + \overline{c} \qquad \overline{c} = c - \frac{1}{2}\overline{\boldsymbol{x}}^T \overline{\boldsymbol{x}}$$

- 驻点方程无解： $rank\boldsymbol{A} \neq rank[\boldsymbol{A}\ \boldsymbol{b}]$ $\quad rank\boldsymbol{A} < n$

如抛物面 $x_2 + f_0 - c = x_1^2$ $\quad$ ***f*(*x*)**无极小值

二次型函数分析

- 设**A**为对称矩阵，二次型函数

$$f(\boldsymbol{x})=\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}=\boldsymbol{x}^T\boldsymbol{T}^T\boldsymbol{\Lambda}\boldsymbol{T}\boldsymbol{x}=\tilde{\boldsymbol{x}}^T\boldsymbol{\Lambda}\tilde{\boldsymbol{x}}=\sum_{i=1}^{n}\lambda_i\tilde{x}_i^2$$

其中 $\boldsymbol{\Lambda}=diag[\lambda_1,\lambda_2,\cdots,\lambda_n]$特征值构成的对角阵

$\boldsymbol{T}^T\boldsymbol{T}=\mathbf{I}$　旋转矩阵，为正交矩阵

A有正定、半正定、负定、半负定和满秩不定、不满秩不定**6**种情况

A>0： f(x) ≥ 0 椭球面

$$f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{T}^T \boldsymbol{\Lambda}\boldsymbol{T}\boldsymbol{x} = \tilde{\boldsymbol{x}}^T \boldsymbol{\Lambda}\tilde{\boldsymbol{x}} = \sum_{i=1}^{n} \lambda_i \tilde{x}_i^2$$

A>0 $\lambda_i > 0 \qquad i = 1, \cdots, n$

等值面： $f(\boldsymbol{x}) = \sum_{i=1}^{n} \lambda_i \tilde{x}_i^2 = c \qquad c \geq 0$

椭圆方程： $\sum_{i=1}^{n} \frac{\tilde{x}_i^2}{a_i^2} = 1 \qquad a_i = \sqrt{\frac{\mathrm{c}}{\lambda_i}}$

唯一极小值点， **x*=0, f(x*)=0**

A≥0： f(x) ≥ 0椭圆柱面

$$f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{T}^T \boldsymbol{\Lambda}\boldsymbol{T}\boldsymbol{x} = \tilde{\boldsymbol{x}}^T \boldsymbol{\Lambda}\tilde{\boldsymbol{x}} = \sum_{i=1}^{n} \lambda_i \tilde{x}_i^2$$

A>0 $\quad \lambda_i > 0 \quad i = 1, \cdots, m \quad \lambda_i = 0 \quad i = m+1, \cdots, n$

等值面： $f(\boldsymbol{x}) = \sum_{i=1}^{m} \lambda_i \tilde{x}_i^2 = c \qquad c \geq 0$

椭圆柱面： $\sum_{i=1}^{m} \frac{\tilde{x}_i^2}{a_i^2} = 1 \qquad a_i = \sqrt{\frac{\mathrm{c}}{\lambda_i}}$

平行超平面： $\frac{\tilde{x}_1^2}{a_1^2} = 1 \qquad \tilde{x}_1 = \pm a_1 \qquad$ **m=1**

无穷多个极小值点，**x*=[0, …,0,x$_{m+1}$, …,x$_n$]^T, f(x*)=0**

A<0： $f(x) \le 0$椭球面

$$f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{T}^T \boldsymbol{\Lambda}\boldsymbol{T}\boldsymbol{x} = \tilde{\boldsymbol{x}}^T \boldsymbol{\Lambda}\tilde{\boldsymbol{x}} = \sum_{i=1}^{n} \lambda_i \tilde{x}_i^2$$

A>0 $\quad \lambda_i < 0 \qquad i = 1, \cdots, n$

等值面： $f(\boldsymbol{x}) = \sum_{i=1}^{n} \lambda_i \tilde{x}_i^2 = c \qquad c \le 0$

椭圆方程： $\sum_{i=1}^{n} \frac{\tilde{x}_i^2}{a_i^2} = 1 \qquad a_i = \sqrt{\frac{\mathrm{c}}{\lambda_i}}$

唯一极大值点，**x*=0, f(x*)=0**

A≤0：椭圆柱面

$$f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{T}^T \boldsymbol{\Lambda}\boldsymbol{T}\boldsymbol{x} = \tilde{\boldsymbol{x}}^T \boldsymbol{\Lambda}\tilde{\boldsymbol{x}} = \sum_{i=1}^{n} \lambda_i \tilde{x}_i^2$$

A>0 $\lambda_i < 0 \quad i = 1, \cdots, m \quad \lambda_i = 0 \quad i = m+1, \cdots, n$

等值面： $f(\boldsymbol{x}) = \sum_{i=1}^{m} \lambda_i \tilde{x}_i^2 = c$ $c \le 0$

椭圆柱面： $\sum_{i=1}^{m} \frac{\tilde{x}_i^2}{a_i^2} = 1$ $a_i = \sqrt{\frac{\mathrm{c}}{\lambda_i}}$

平行超平面： $\frac{\tilde{x}_1^2}{a_1^2} = 1$ $\tilde{x}_1 = \pm a_1$ **m=1**

无穷多个极大值点，**$x^* = [0, \ldots, 0, x_{m+1}, \ldots, x_n]^T$, $f(x^*) = 0$**

A不定：双曲面

$$f(\boldsymbol{x})=\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}=\boldsymbol{x}^T\boldsymbol{T}^T\boldsymbol{\Lambda}\boldsymbol{T}\boldsymbol{x}=\tilde{\boldsymbol{x}}^T\boldsymbol{\Lambda}\tilde{\boldsymbol{x}}=\sum_{i=1}^{n}\lambda_i\tilde{x}_i^2$$

A不定 $\lambda_i>0 \quad i=1,\cdots,m \quad \lambda_i<0 \quad i=m+1,\cdots,n$

等值面： $f(\boldsymbol{x})=\sum_{i=1}^{n}\lambda_i\tilde{x}_i^2=c$

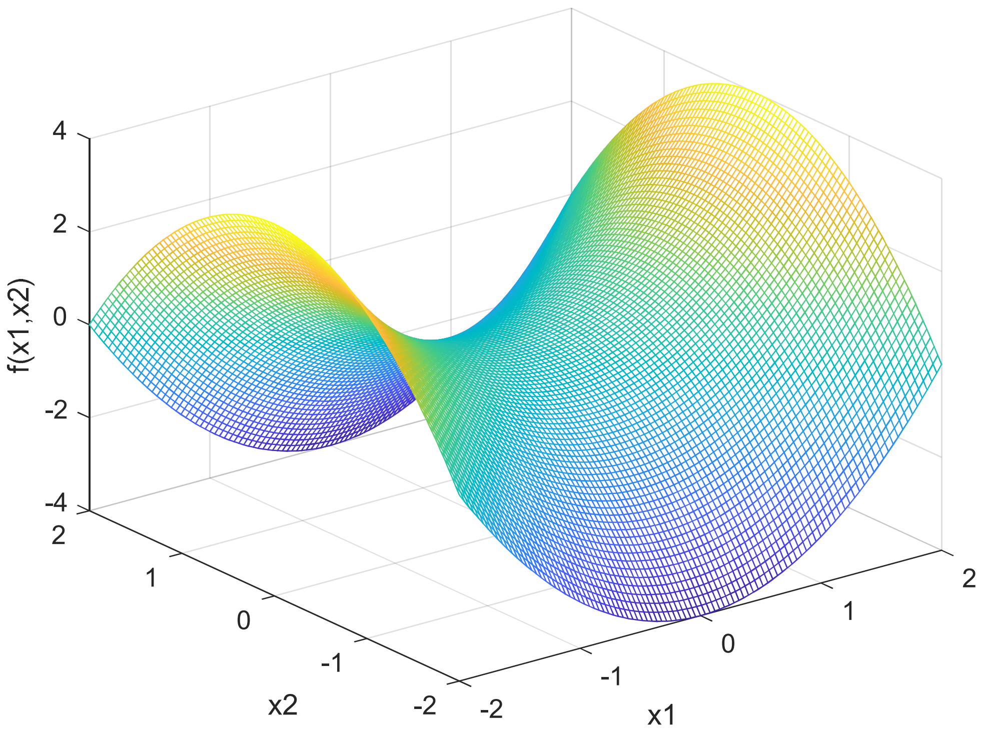
双曲面： $\sum_{i=1}^{m}\pm\frac{\tilde{x}_i^2}{a_i^2}\mp\sum_{i=m}^{n}\frac{\tilde{x}_i^2}{a_i^2}=1 \qquad a_i=\sqrt{\left|\frac{\mathrm{c}}{\lambda_i}\right|}$

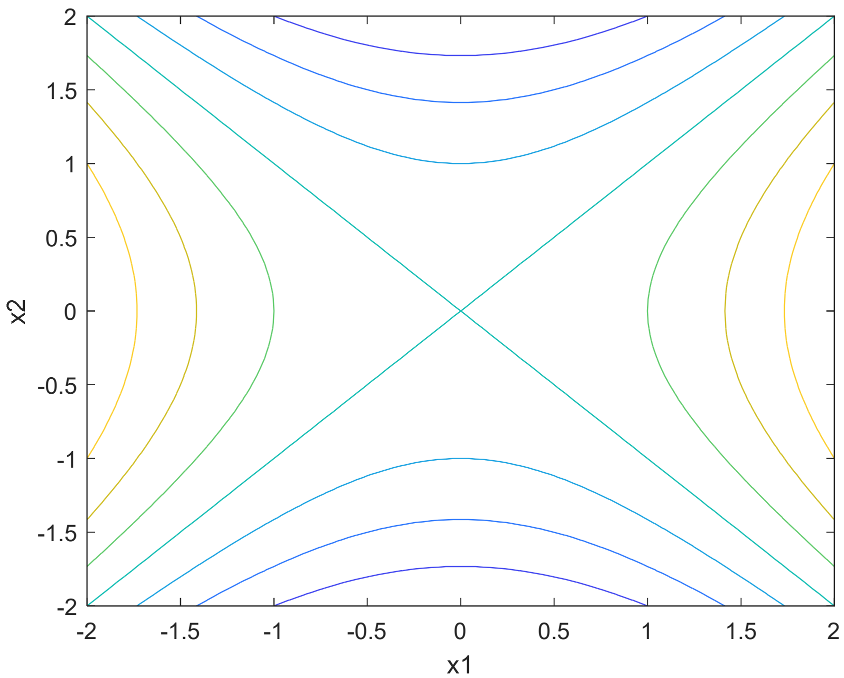
存在**0**特征值时为双曲柱面

有驻点，无极小值

马鞍面

等值面： $f(\boldsymbol{x}) = x_1^2 - x_2^2 = c$



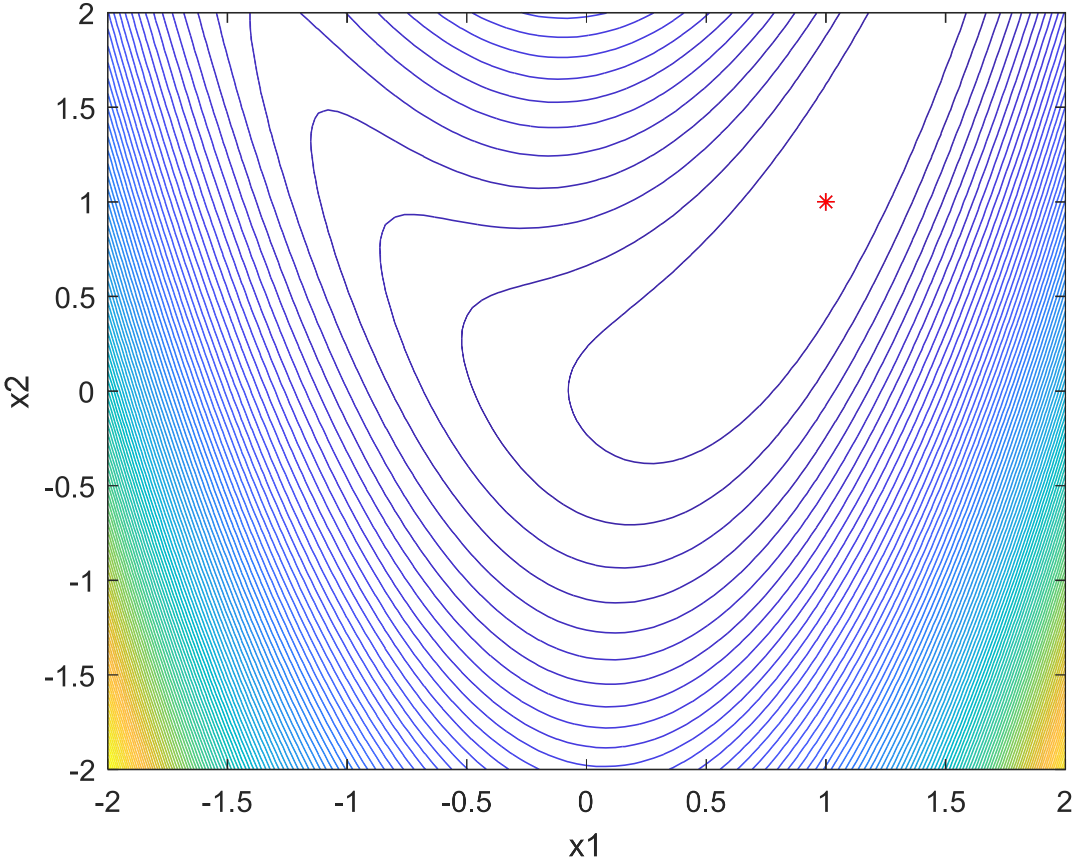


Rosenbrock香蕉函数

$$f(\boldsymbol{x}) = (a - x_1)^2 + b(x_2 - x_1^2)^2$$

***a*=1, *b*=3**

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} -2(a-x_1) - 4b(x_2 - x_1^2)x_1 \\ 2b(x_2 - x_1^2) \end{bmatrix}$$



$$\boldsymbol{x}^* = \begin{bmatrix} a \\ a^2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\nabla^2 f(\boldsymbol{x}) = \begin{bmatrix} 2 + 12bx_1^2 - 4bx_2 & -4bx_1 \\ -4bx_1 & 2b \end{bmatrix}$$

$$\nabla^2 f(\boldsymbol{x}^*) = \begin{bmatrix} 26 & -12 \\ -12 & 6 \end{bmatrix} > 0$$