2019

最优化理论与方法

研究生学位课

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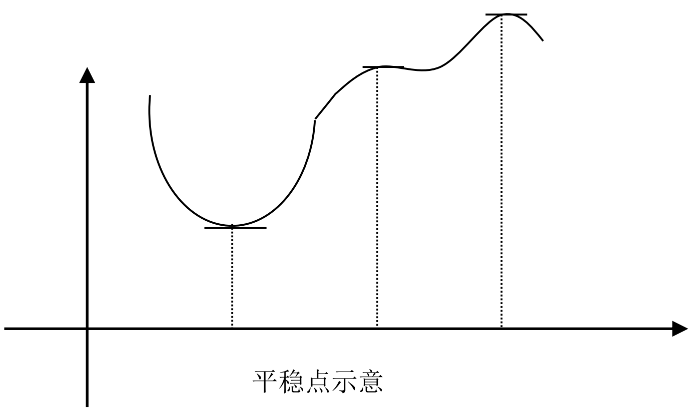
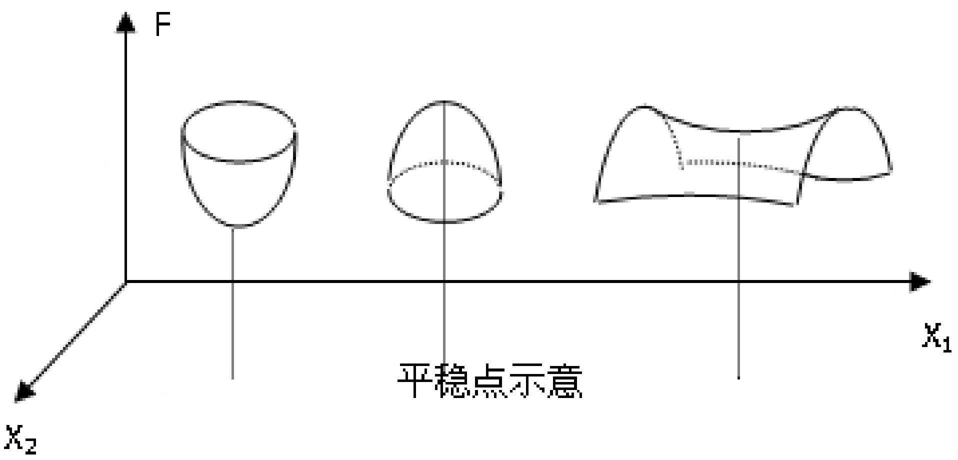
- **函数极值存在的条件**

- **等式约束的最优性条件（Lagrange条件）**

- **Kuhn-Tucker条件**

- NLP由于受约束条件的影响，目标函数的极值点不一定是规划的最优点，最优点也不一定是目标函数的极值点，那么什么情况下才存在最优极值点呢？
- 高等数学中函数极值存在的必要条件是 $f'(x) = 0$，是否可推广到N维空间？

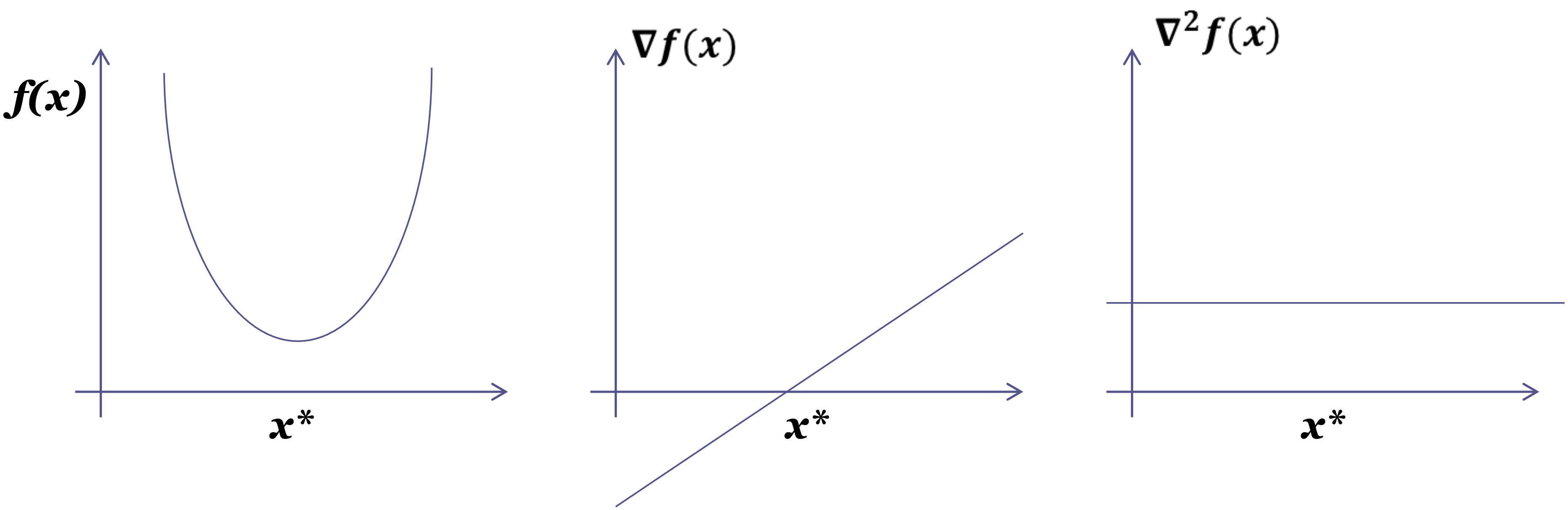

平稳点示意



平稳点示意

- **最优解的必要条件**
  - 第1序：$\nabla f(x^*) = 0$

    第2序：$\nabla^2 f(x^*) \geq 0$,f(x)需要连续二阶可导。



- **最优解的必要条件证明:**
  - For an arbitrary direction d and scalar $\alpha > 0$

    $f(x^* + \alpha d) = f(x^*) + \alpha \nabla f(x^*)' d + o(\alpha)$

    If $\nabla f(x^*) \neq 0$,

    Let $d = -\nabla f(x^*)$, then $f(x^* + \alpha d) < f(x^*)$

  So this is a contradiction and $\nabla f(x^*) = 0$

  Also, to have

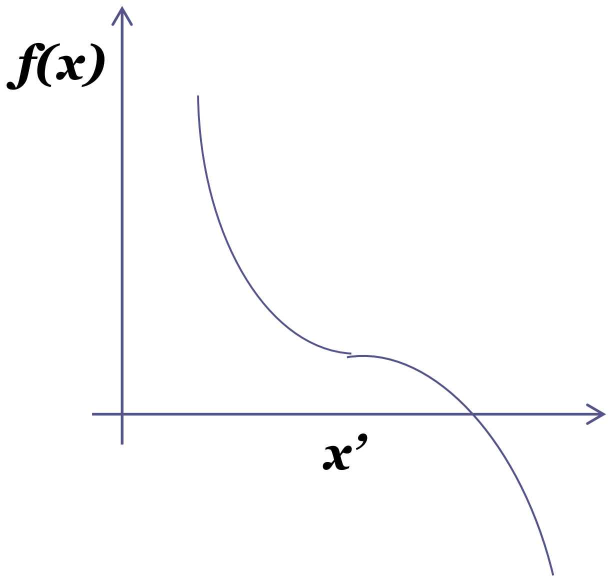
  $$f(x^* + \alpha d) = f(x^*) + \alpha \nabla f(x^*)' d + \frac{1}{2}\alpha^2 d^T \nabla^2 f(x^*) d + o(a^2)$$

  $$= f(x^*) + \frac{1}{2}\alpha^2 d^T \nabla^2 f(x^*) d + o(a^2) \geq f(x^*)$$

  We need $\nabla^2 f(x^*) \geq 0$

对于最优解为求极大，其必要条件是?

- **最优解的充分条件**
  - 若函数满足：$\nabla f(x^*) = 0$；$\nabla^2 f(x^*) \geq 0$,f(x)连续二阶可导。
  - 是否即为最优点？



最优解的充分条件

- f(x)连续二阶可导，定义域为开集。

若$\boldsymbol{x}^* \in \boldsymbol{S}$，满足：$\nabla \boldsymbol{f}(\boldsymbol{x}^*) = \boldsymbol{0}$，$\nabla^2 \boldsymbol{f}(\boldsymbol{x}^*) > \boldsymbol{0}$

那么$\boldsymbol{x}^*$为严格局部极小点。

证明：

$$\boldsymbol{f}(\boldsymbol{x}^* + \boldsymbol{d}) - \boldsymbol{f}(\boldsymbol{x}^*) = \nabla \boldsymbol{f}(\boldsymbol{x}^*)^T \boldsymbol{d} + \frac{1}{2} \boldsymbol{d}^T \nabla^2 \boldsymbol{f}(\boldsymbol{x}^*) \boldsymbol{d} + \boldsymbol{o}\left(\|\boldsymbol{d}\|^2\right) > \boldsymbol{0}$$

满足必要但不满足充分的点称为奇异点；

满足必要和充分的点称为非奇异点。

- **最优解的条件**
  - 对于**f(x)**，若为凸集，如定义域为开集。

    x^*为全局最优解的充要条件为：

    $$\nabla f(x^*) = 0$$

- **例3_1 求以下非线性凸规划问题**

$$Min\ f(x_1, x_2) = x_1^2 + 2x_2^2 + 2x_1 - x_1x_2$$

- 例3_1 求以下非线性凸规划问题

$$Min\ f(x_1,x_2)=x_1^2+2x_2^2+2x_1-x_1x_2$$

$$\frac{\partial f}{\partial x_1}=2x_1+2-x_2=0$$

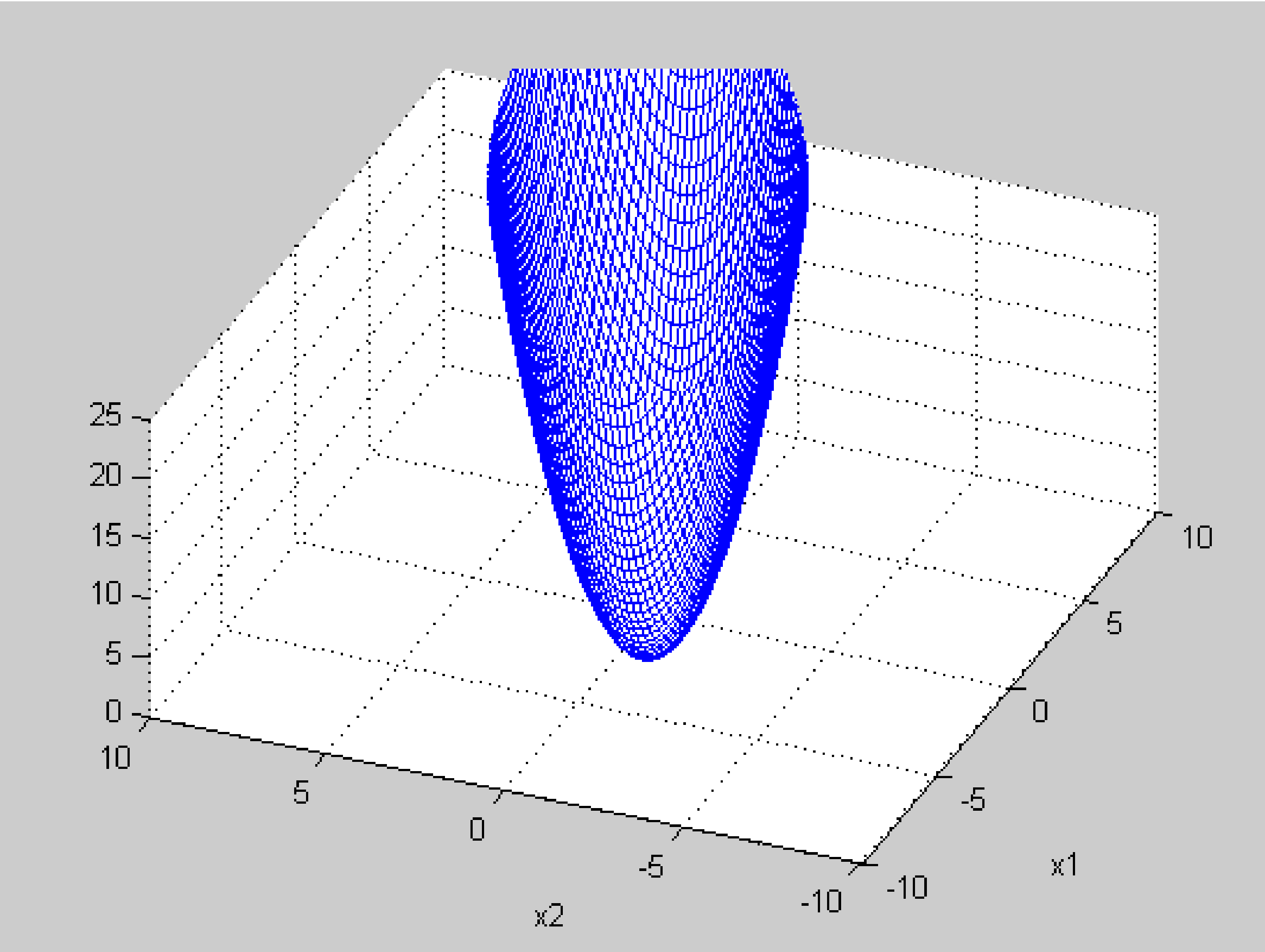
$$\frac{\partial f}{\partial x_2}=4x_2-x_2=0$$

$$\therefore x^*=\begin{pmatrix}-\frac{\frac{8}{7}}{\frac{2}{7}}\end{pmatrix}$$

$$\nabla^2 f=\begin{pmatrix}2 & -1\\ -1 & 4\end{pmatrix}>0$$

- **例3_1 求以下非线性凸规划问题**

$$Min\ f(x_1, x_2) = x_1^2 + 2x_2^2 + 2x_1 - x_1 x_2$$



- **例3_2**

讨论：$f(x) = x^3 - 4x^2$ 的极值点

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$$f'(x)=3x^2-8x$$

$$f''(x)=6x-8$$

$$f'(x)=0,x^*=0,\frac{8}{3}$$

$$f''(0)=-8<0,f''\left(\frac{8}{3}\right)=8>0$$

- **例3_3**

$$f(x) = \frac{1}{4}x^4 - 2x^3 + \frac{11}{2}x^2 - 6x + 1$$

$$s.t \quad 0 \le x \le 4$$

- **例3_3**

$$f(x) = \frac{1}{4}x^4 - 2x^3 + \frac{11}{2}x^2 - 6x + 1$$
$$s.t \quad 0 \le x \le 4$$

- **First-order information:**

$$f'(x) = x^3 - 6x^2 + 11x - 6 = (x-1)(x-2)(x-3)$$
$$f'(0) = -6, f'(1) = f'(2) = f'(3) = 0, f'(4) = 6$$

- **Second-order information:**

$$f''(x) = 3x^2 - 12x^2 + 11$$
$$f''(1) > 0, f''(2) < 0, f''(3) > 0$$

- **例3_4**

$$\min f(x_1, x_2) = x_1^2 - x_1 + x_2 + x_1 x_2$$
$$s.t \quad x_1, x_2 \geq 0$$

Check if $x^* = \left[\frac{1}{2}, 0\right]$ satisfies the necessary condition or not.

- **例3_4**

$$\min f(x_1,x_2) = x_1^2 - x_1 + x_2 + x_1 x_2$$
$$s.t \quad x_1, x_2 \geq 0$$

Check if $x^* = \left[\frac{1}{2}, 0\right]$ satisfies the first-order necessary condition or not.

- **First-order information:**

$$\nabla f(x)\Big|_{x^*} = [2x_1 - 1 + x_2, 1 + x_1]\Big|_{x_1=\frac{1}{2}, x_2=0} = [0, \frac{3}{2}]$$

$\rightarrow \nabla f(x^*)d \geq 0$ for all d with $d_2 \geq 0$ (feasible direction at x^*)

- **例3_4**

Check if $x^* = \left[\frac{1}{2}, 0\right]$ satisfies the second-order necessary condition or not.

$$\nabla f(x^*) = [0, \frac{3}{2}], \text{ Since } \nabla f(x^*)d = \frac{3}{2}d_2 = 0$$

$$\rightarrow d_2 = 0$$

$$\rightarrow d^T \nabla^2 f(x^*) d = [d_1, d_2]\begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = 2d_1^2 \geq 0$$

- **例3_5**

$f(x,y)=x^2-y^2$, **在点 (0,0) 的极值情况。**

- **二元函数的极值判别**

Theorem: If $\frac{\partial f}{\partial x}(x_0, y_0) = \frac{\partial f}{\partial y}(x_0, y_0) = 0$

$$\Delta = \left\{ \frac{\partial^2 f}{\partial x^2} \frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y} \right)^2 \right\}$$

Then:

1) (x_0, y_0) **is a local maximum if** $\Delta > 0$ **and** $\frac{\partial^2 f}{\partial x^2} |(x_0, y_0) < 0, \frac{\partial^2 f}{\partial y^2} |(x_0, y_0) < 0$

2) (x_0, y_0) **is a local minimum if** $\Delta > 0$ **and** $\frac{\partial^2 f}{\partial x^2} |(x_0, y_0) > 0, \frac{\partial^2 f}{\partial y^2} |(x_0, y_0) > 0$

3) (x_0, y_0) **is an saddle point if** $\Delta < 0$

4) If $\Delta = 0$**, need further discussion.**

- **最优解的存在性讨论**
  - 最优解总存在吗?

$$f(x)=\frac{1}{x}, f(x)=e^{x}$$

  - 什么条件下存在最优解（极小）？
  - **1**、如果**f(x)**是连续的且**X**是紧集（有界闭集），最优一定存在。
  - **2**、如果**f(x)**是连续的且**X**是闭集，且**f**强制函数（**coercive**）

- 等式约束的最优性条件（Lagrange条件）

$$\begin{cases} \min f(x) \\ h_j(x) = 0 \quad j = 1, \dots, q \end{cases}$$

- 不等式约束的最优性条件（KT条件）

$$\begin{aligned} h_j(x) &= 0 \quad j = 1, \dots, q \\ g_i(x) &\geq 0 \quad i = 1, \dots, l \end{aligned}$$