优化与深度学习

优化与估计

尽管优化方法可以最小化深度学习中的损失函数值，但本质上优化方法达到的目标与深度学习的目标并不相同。

- 优化方法目标：训练集损失函数值
- 深度学习目标：测试集损失函数值（泛化性）

In [1]:

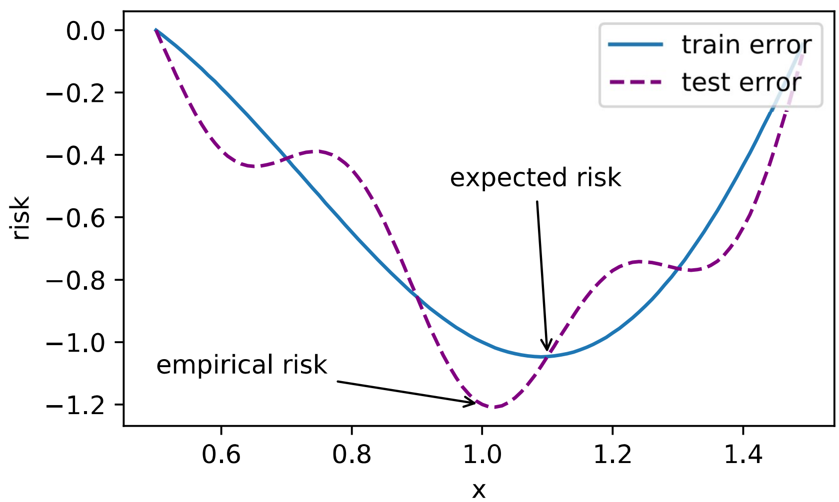
```
%matplotlib inline
import sys
sys.path.append('/home/kesci/input')
import d2lzh1981 as d2l
from mpl_toolkits import mplot3d # 三维画图
import numpy as np
```

In [2]:

```
def f(x): return x * np.cos(np.pi * x)
def g(x): return f(x) + 0.2 * np.cos(5 * np.pi * x)

d2l.set_figsize((5, 3))
x = np.arange(0.5, 1.5, 0.01)
fig_f, = d2l.plt.plot(x, f(x),label="train error")
fig_g, = d2l.plt.plot(x, g(x),'--', c='purple', label="test error")
fig_f.axes.annotate('empirical risk', (1.0, -1.2), (0.5, -1.1),arrowprops=dict(arrowsty
fig_g.axes.annotate('expected risk', (1.1, -1.05), (0.95, -0.5),arrowprops=dict(arrowst
d2l.plt.xlabel('x')
d2l.plt.ylabel('risk')
d2l.plt.legend(loc="upper right")
```

Out[2]:

```
<matplotlib.legend.Legend at 0x7f38a7692320>
```



优化在深度学习中的挑战

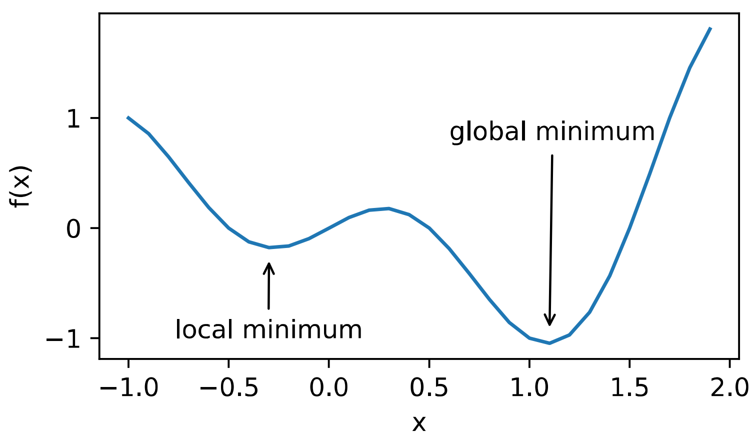
1. 局部最小值
2. 鞍点
3. 梯度消失

局部最小值

$$f(x) = x \cos \pi x$$

In [3]:

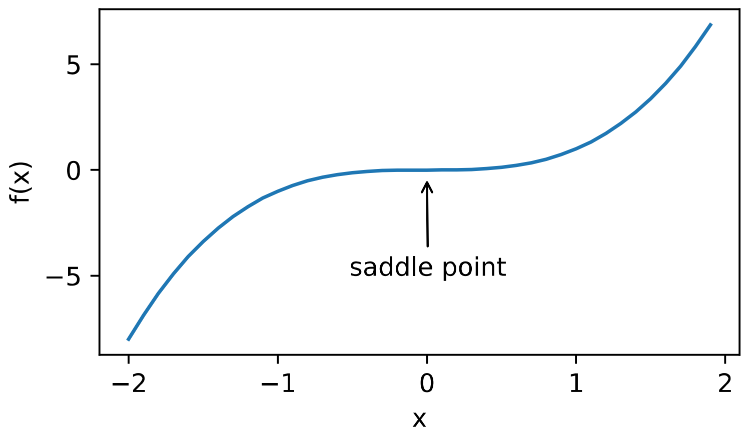
```
def f(x):
    return x * np.cos(np.pi * x)

d2l.set_figsize((4.5, 2.5))
x = np.arange(-1.0, 2.0, 0.1)
fig,  = d2l.plt.plot(x, f(x))
fig.axes.annotate('local minimum', xy=(-0.3, -0.25), xytext=(-0.77, -1.0),
                  arrowprops=dict(arrowstyle='->'))
fig.axes.annotate('global minimum', xy=(1.1, -0.95), xytext=(0.6, 0.8),
                  arrowprops=dict(arrowstyle='->'))
d2l.plt.xlabel('x')
d2l.plt.ylabel('f(x)');
```



鞍点 (一阶、二阶导均为0)

In [4]:

```
x = np.arange(-2.0, 2.0, 0.1)
fig, = d2l.plt.plot(x, x**3)
fig.axes.annotate('saddle point', xy=(0, -0.2), xytext=(-0.52, -5.0),
                  arrowprops=dict(arrowstyle='->'))
d2l.plt.xlabel('x')
d2l.plt.ylabel('f(x)');
```



$$A=\begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

海森矩阵

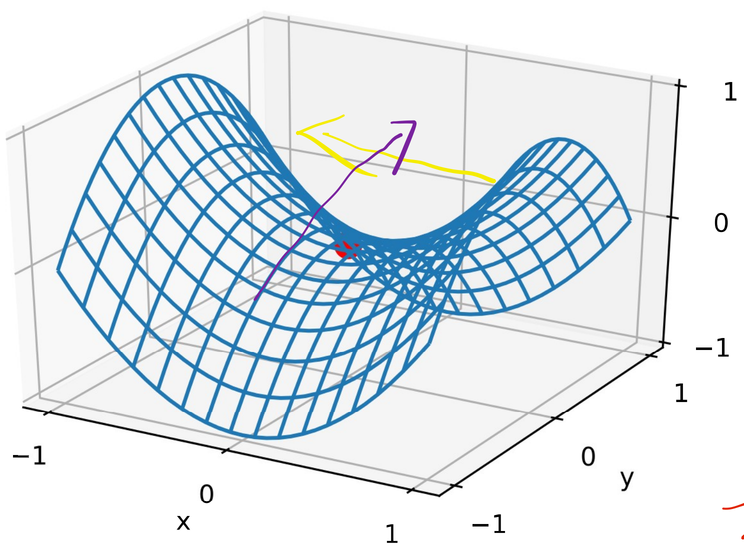
特征值均为正则为最小值点

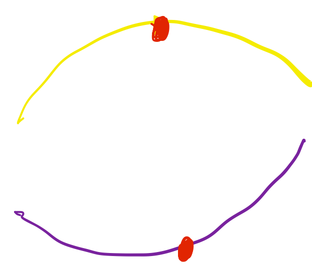
e.g.

有正有负为鞍点

In [4]:

```
x, y = np.mgrid[-1: 1: 31j, -1: 1: 31j]
z = x**2 - y**2

d2l.set_figsize((6, 4))
ax = d2l.plt.figure().add_subplot(111, projection='3d')
ax.plot_wireframe(x, y, z, **{'rstride': 2, 'cstride': 2})
ax.plot([0], [0], [0], 'ro', markersize=10)
ticks = [-1,  0, 1]
d2l.plt.xticks(ticks)
d2l.plt.yticks(ticks)
ax.set_zticks(ticks)
d2l.plt.xlabel('x')
d2l.plt.ylabel('y');
```





局部

黄色看是最大.

紫色方向看是局部最小.

故为鞍点

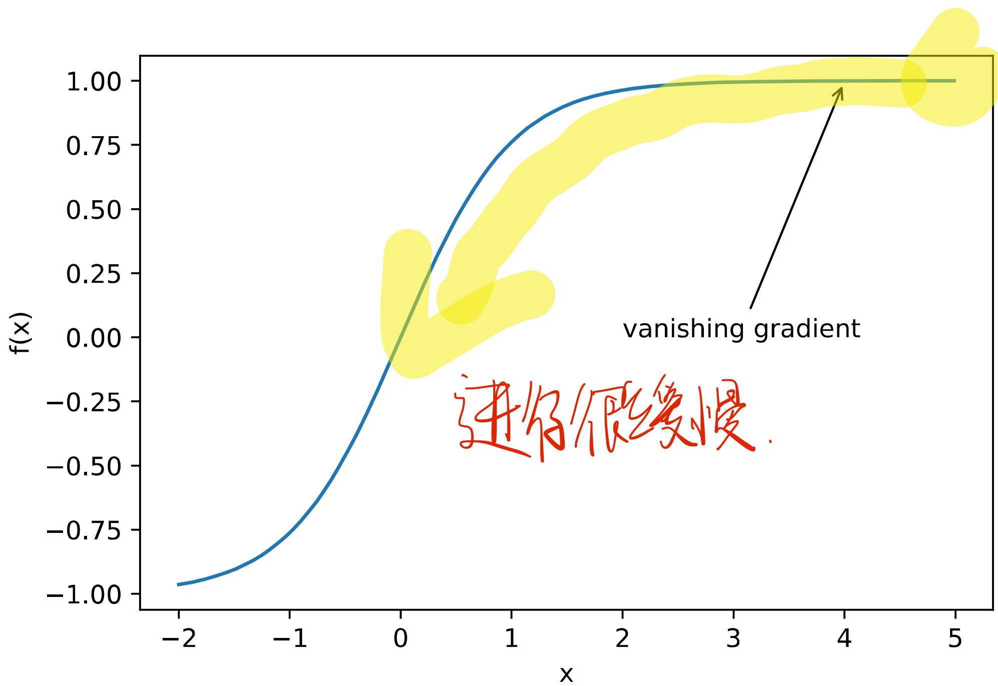
梯度消失

In [6]:

```
x = np.arange(-2.0, 5.0, 0.01)
fig, = d2l.plt.plot(x, np.tanh(x))
d2l.plt.xlabel('x')
d2l.plt.ylabel('f(x)')
fig.axes.annotate('vanishing gradient', (4, 1), (2, 0.0) ,arrowprops=dict(arrowstyle='-
```

Out[6]:

```
Text(2, 0.0, 'vanishing gradient')
```

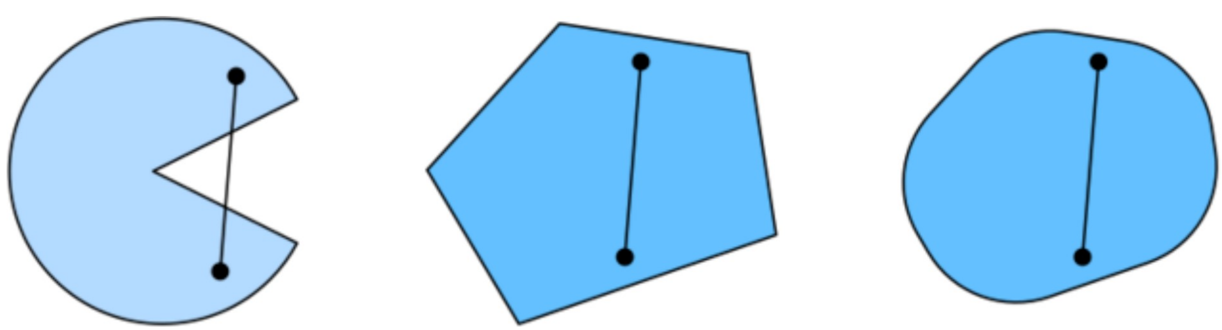


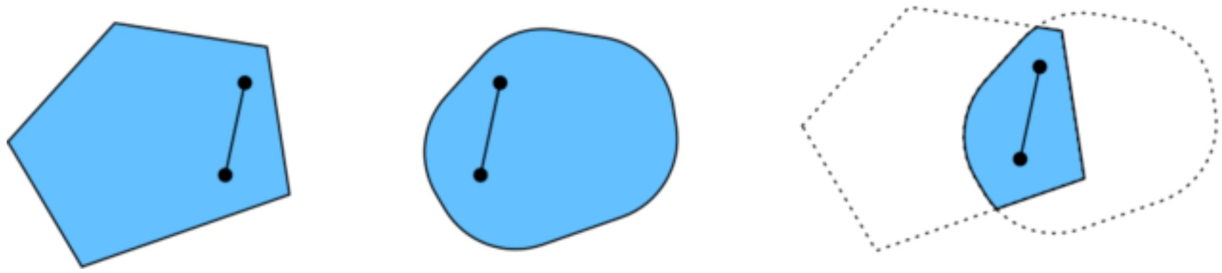
凸性 (Convexity) 凸函数

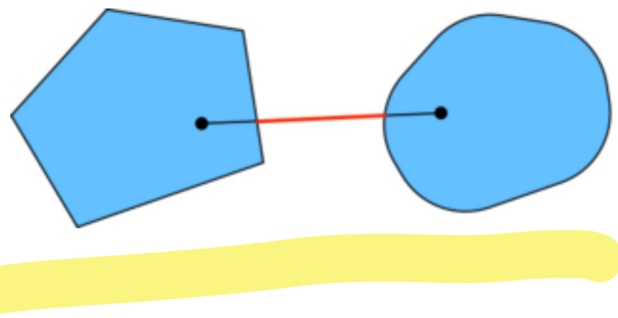
基础

集合

任意两点连线均在集合内 则为凸集合







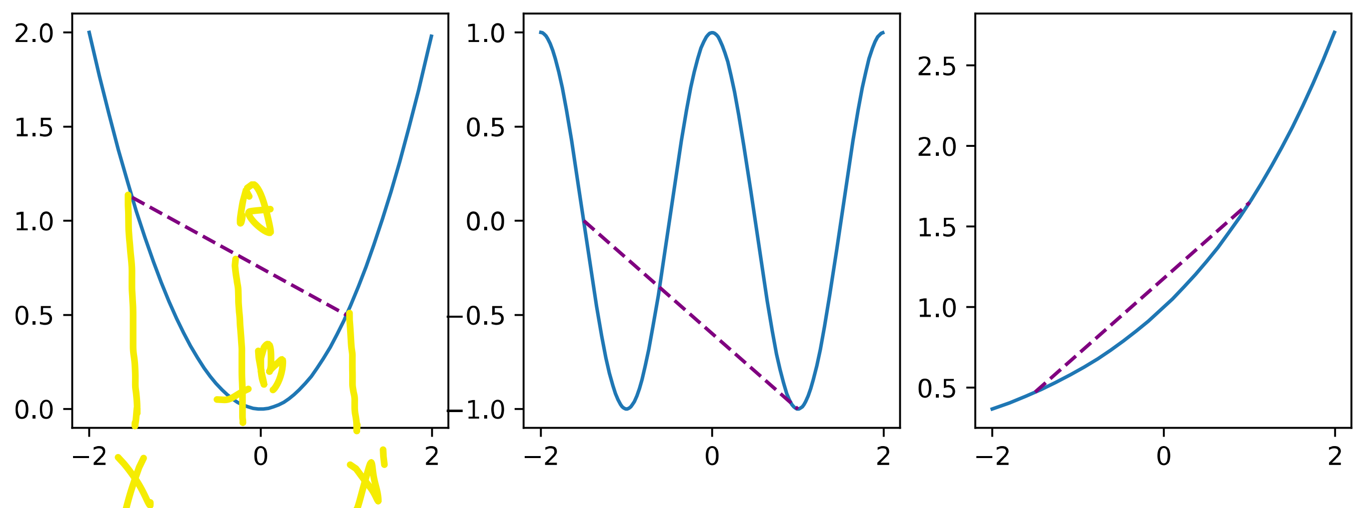
凸集的并不一定是凸集合.

函数

$$\lambda f(x)+(1-\lambda) f\left(x^{\prime}\right) \geq f\left(\lambda x+(1-\lambda) x^{\prime}\right)$$

In [10]:

```
def f(x):
    return 0.5 * x**2  # Convex

def g(x):
    return np.cos(np.pi * x)  # Nonconvex

def h(x):
    return np.exp(0.5 * x)  # Convex

x, segment = np.arange(-2, 2, 0.01), np.array([-1.5, 1])
d2l.use_svg_display()
_, axes = d2l.plt.subplots(1, 3, figsize=(9, 3))

for ax, func in zip(axes, [f, g, h]):
    ax.plot(x, func(x))
    ax.plot(segment, func(segment),'--', color="purple")
    # d2l.plt.plot([x, segment], [func(x), func(segment)], axes=ax)
```



Jensen 不等式

$$\sum_i \alpha_i f\left(x_i\right) \geq f\left(\sum_i \alpha_i x_i\right) \text{ and } E_x[f(x)] \geq f\left(E_x[x]\right)$$

性质 (凸函数的).

1. 无局部极小值

2. 与凸集的关系
3. 二阶条件

无局部最小值

证明：假设存在 $x \in X$ 是局部最小值，则存在全局最小值 $x' \in X$, 使得 $f(x) > f(x')$, 则对 $\lambda \in (0, 1]$:

$$f(x) > \lambda f(x) + (1 - \lambda) f(x') \geq f(\lambda x + (1 - \lambda) x')$$

凸函数定义

与凸集的关系

对于凸函数 $f(x)$，定义集合 $S_b := \{x | x \in X \text{ and } f(x) \leq b\}$，则集合 S_b 为凸集

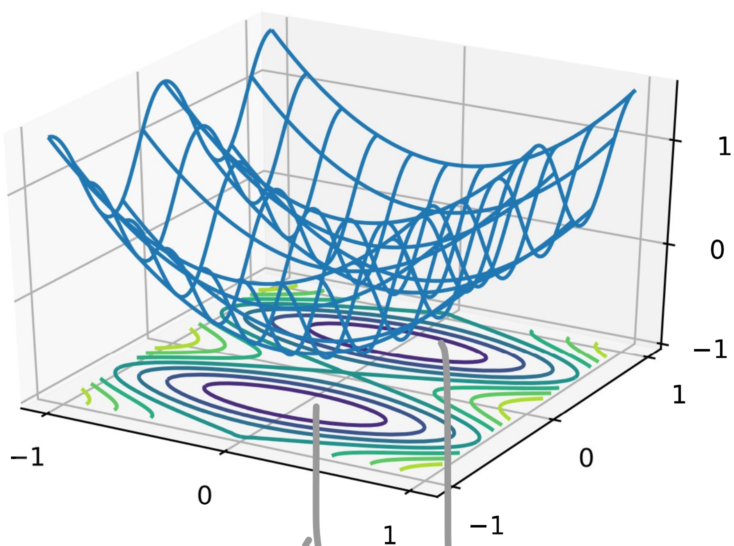
证明：对于点 $x, x' \in S_b$, 有 $f\left(\lambda x + (1 - \lambda) x'\right) \leq \lambda f(x) + (1 - \lambda) f\left(x'\right) \leq b$, 故 $\lambda x + (1 - \lambda) x' \in S_b$

$f(x) \leq b$ 且 $f'(x) \leq b$.

$f(x, y) = 0.5x^2 + \cos(2\pi y)$

In [12]:

```
x, y = np.meshgrid(np.linspace(-1, 1, 101), np.linspace(-1, 1, 101),
                   indexing='ij')

z = x**2 + 0.5 * np.cos(2 * np.pi * y)

# Plot the 3D surface
d2l.set_figsize((6, 4))
ax = d2l.plt.figure().add_subplot(111, projection='3d')
ax.plot_wireframe(x, y, z, **{'rstride': 10, 'cstride': 10})
ax.contour(x, y, z, offset=-1)
ax.set_zlim(-1, 1.5)

# Adjust labels
for func in [d2l.plt.xticks, d2l.plt.yticks, ax.set_zticks]:
    func([-1, 0, 1])
```



两个紫色圈组成的不是凸集.

凸函数与二阶导数

$f''(x) \geq 0 \Longleftrightarrow f(x)$ 是凸函数

必要性 ($\Leftarrow$):

对于凸函数:

$$\frac{1}{2}f(x+\epsilon)+\frac{1}{2}f(x-\epsilon) \geq f\left(\frac{x+\epsilon}{2}+\frac{x-\epsilon}{2}\right)=f(x)$$

故:

$$f''(x)=\lim_{\varepsilon\rightarrow 0}\frac{\frac{f(x+\epsilon)-f(x)}{\epsilon}-\frac{f(x)-f(x-\epsilon)}{\epsilon}}{\epsilon}$$
$$f''(x)=\lim_{\varepsilon\rightarrow 0}\frac{f(x+\epsilon)+f(x-\epsilon)-2f(x)}{\epsilon^2}\geq 0$$

充分性 (⇒):

令 $a<x<b$ 为 $f(x)$ 上的三个点，由拉格朗日中值定理:

$$\begin{array}{l}f(x)-f(a)=(x-a)f'(\alpha) \text{ for some } \alpha\in[a,x] \text{ and } \\ f(b)-f(x)=(b-x)f'(\beta) \text{ for some } \beta\in[x,b]\end{array}$$

根据单调性，有 $f'(\beta)\geq f'(\alpha)$, 故:

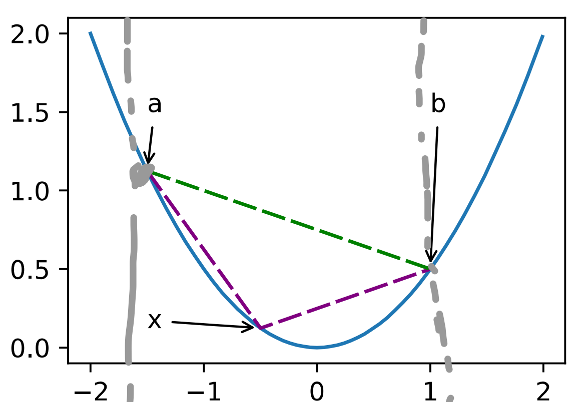
$$\begin{aligned}f(b)-f(a)&=f(b)-f(x)+f(x)-f(a)\\&=(b-x)f'(\beta)+(x-a)f'(\alpha)\\&\geq(b-a)f'(\alpha)\end{aligned}$$

In [13]:

```
def f(x):
    return 0.5 * x**2

x = np.arange(-2, 2, 0.01)
axb, ab = np.array([-1.5, -0.5, 1]), np.array([-1.5, 1])

d2l.set_figsize((3.5, 2.5))
fig_x, = d2l.plt.plot(x, f(x))
fig_axb, = d2l.plt.plot(axb, f(axb), '-.',color="purple")
fig_ab, = d2l.plt.plot(ab, f(ab),'g-.')

fig_x.axes.annotate('a', (-1.5, f(-1.5)), (-1.5, 1.5),arrowprops=dict(arrowstyle='->'))
fig_x.axes.annotate('b', (1, f(1)), (1, 1.5),arrowprops=dict(arrowstyle='->'))
fig_x.axes.annotate('x', (-0.5, f(-0.5)), (-1.5, f(-0.5)),arrowprops=dict(arrowstyle='-
```

Out[13]:

```
Text(-1.5, 0.125, 'x')
```



x只能在这个范围取.

限制条件

$$\begin{aligned} & \underset{\mathbf{x}}{\operatorname{minimize}} f(\mathbf{x}) \\ & \text{subject to } c_i(\mathbf{x}) \leq 0 \text{ for all } i \in \{1, \ldots, N\} \end{aligned}$$

1 拉格朗日乘子法

Boyd & Vandenberghe, 2004 (https://d2l.ai/chapter_references/zreferences.html#boyd-vandenberghe-2004)

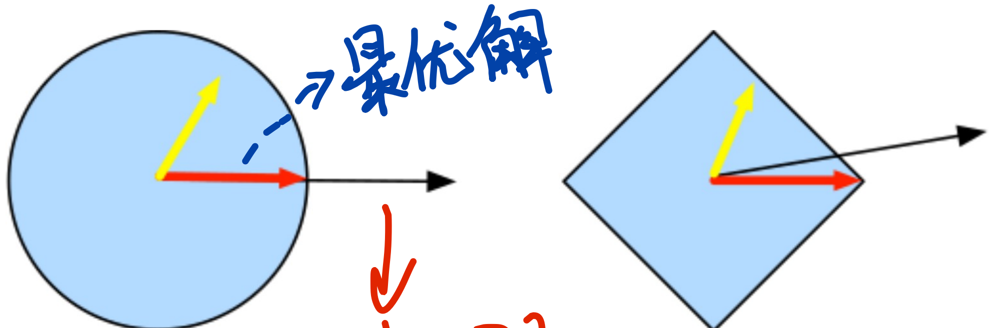
$$L(\mathbf{x}, \alpha) = f(\mathbf{x}) + \sum_i \alpha_i c_i(\mathbf{x}) \text{ where } \alpha_i \geq 0$$

2 惩罚项

欲使 $c_i(x) \leq 0$, 将项 $\alpha_i c_i(x)$ 加入目标函数，如多层感知机章节中的 $\frac{\lambda}{2}||w||^2$

3 投影

$$\operatorname{Proj}_X(\mathbf{x}) = \underset{\mathbf{x}' \in X}{\operatorname{argmin}} \|\mathbf{x} - \mathbf{x}'\|_2$$



最优解

优化问题

域.