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]:

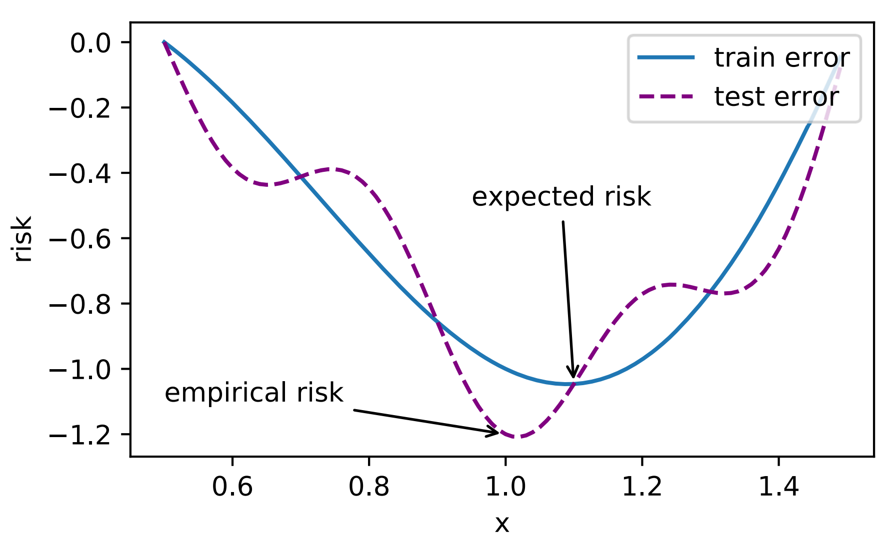
```
%matplotlib inline
import sys
sys.path.append('/home/kesci/input')
import d2lzh4910 as d2l
from mpl_toolkits import mplot3d # 三维画图
import numpy as np
```

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(arrowstyle='->'))
fig_g.axes.annotate('expected risk', (1.1, -1.05), (0.95, -0.5),arrowprops=dict(arrowstyle='->'))
d2l.plt.xlabel('x')
d2l.plt.ylabel('risk')
d2l.plt.legend(loc="upper right")
```

Out[2]:

```
<matplotlib.legend.Legend at 0x7fe869390828>
```



优化在深度学习中的挑战

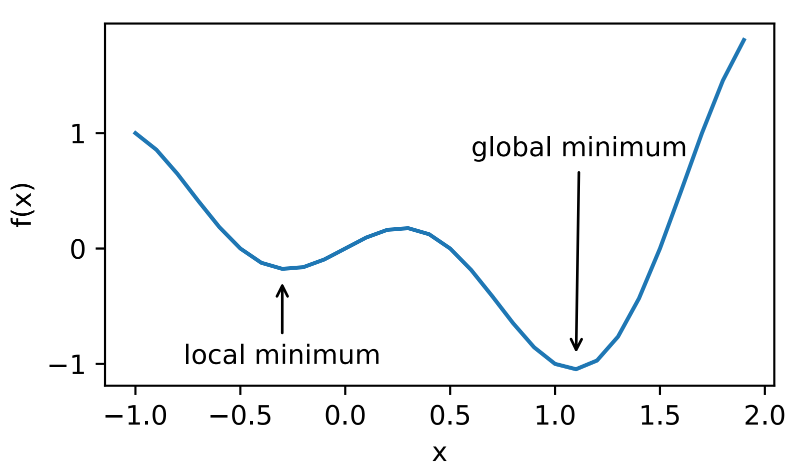
1. 局部最小值
2. 鞍点
3. 梯度消失

局部最小值

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

In [3]:

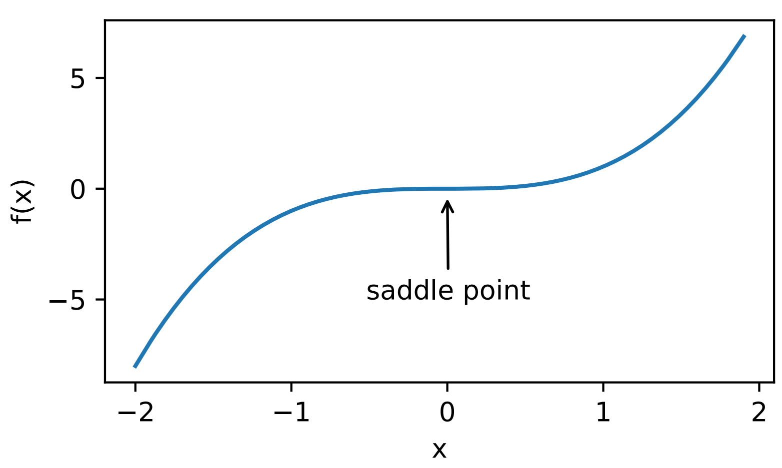
```
def f(x):
    return x * np.cos(np.pi * x)

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

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)');
```

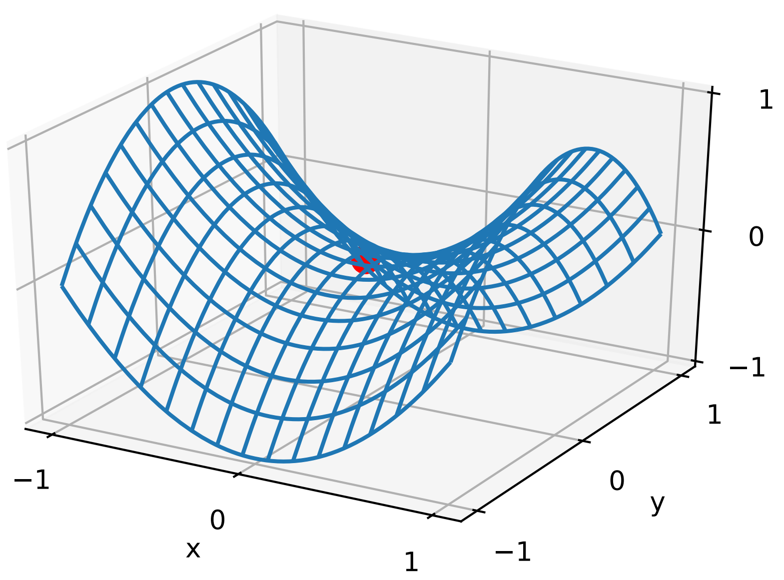


$$A=\begin{bmatrix}\frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial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

e.g.

In [5]:

```
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');
```



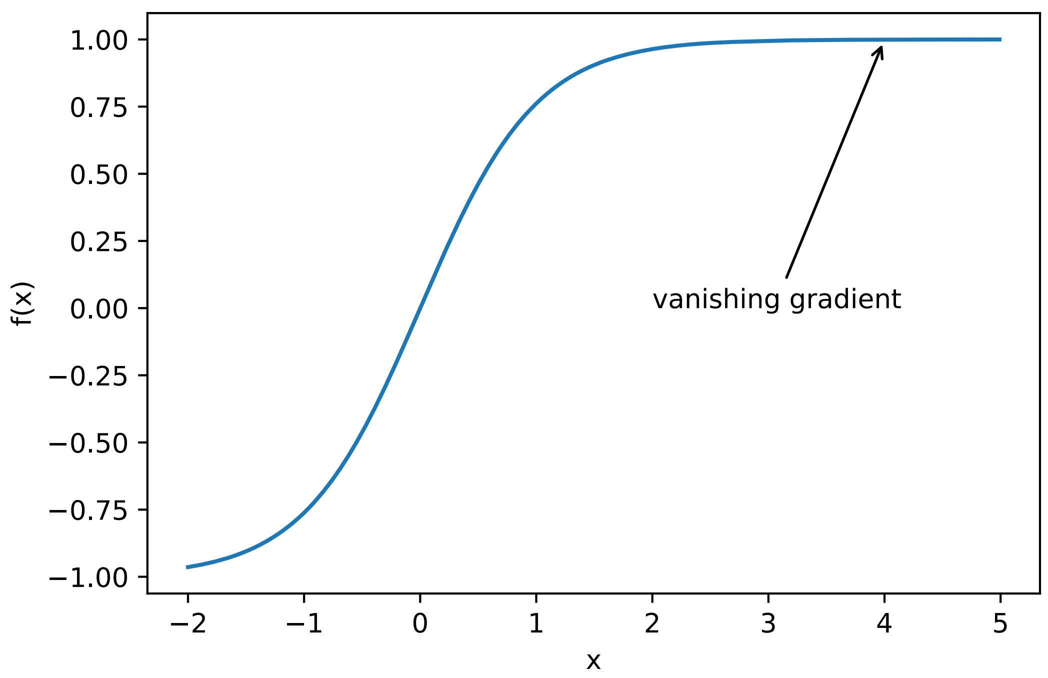
梯度消失

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]:

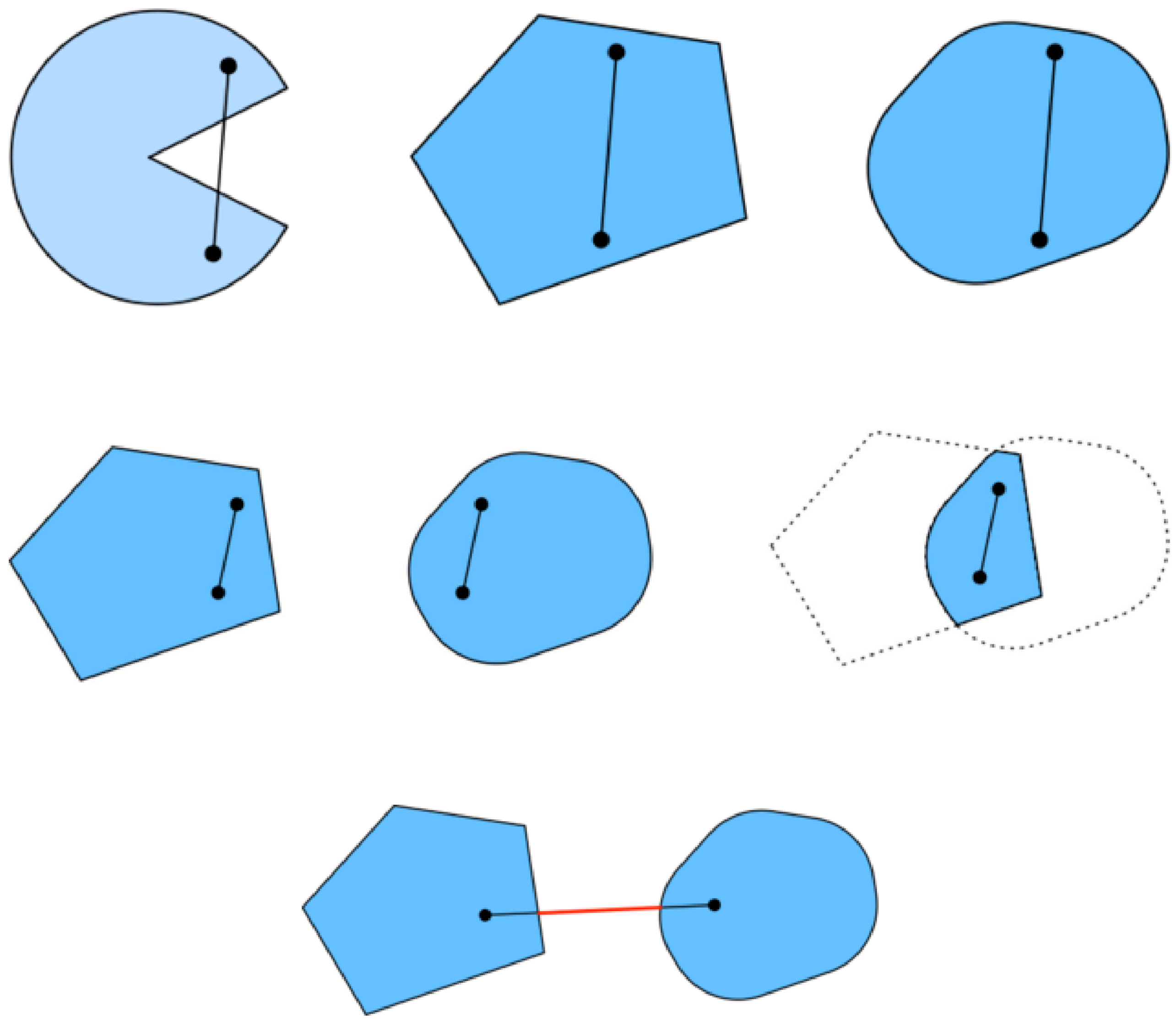
```
Text(2, 0.0, 'vanishing gradient')
```



凸性 (Convexity)

基础

集合

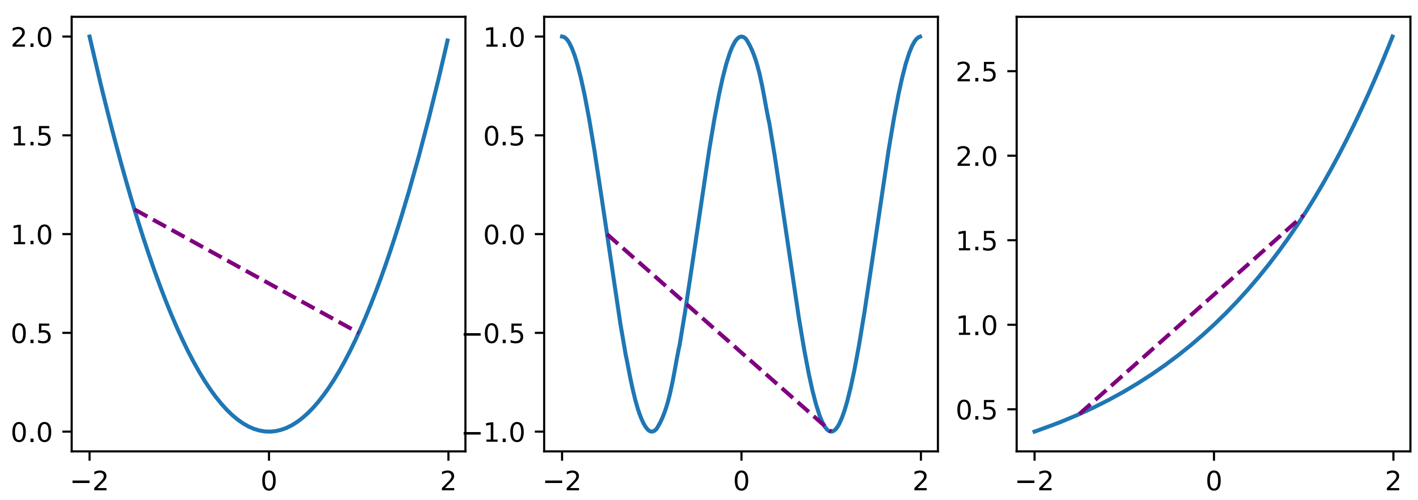


函数

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

In [7]:

```
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

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 $x^{\prime} \in X$, 使得 $f(x)>f\left(x^{\prime}\right)$, 则对 $\lambda \in(0,1]$:

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

与凸集的关系

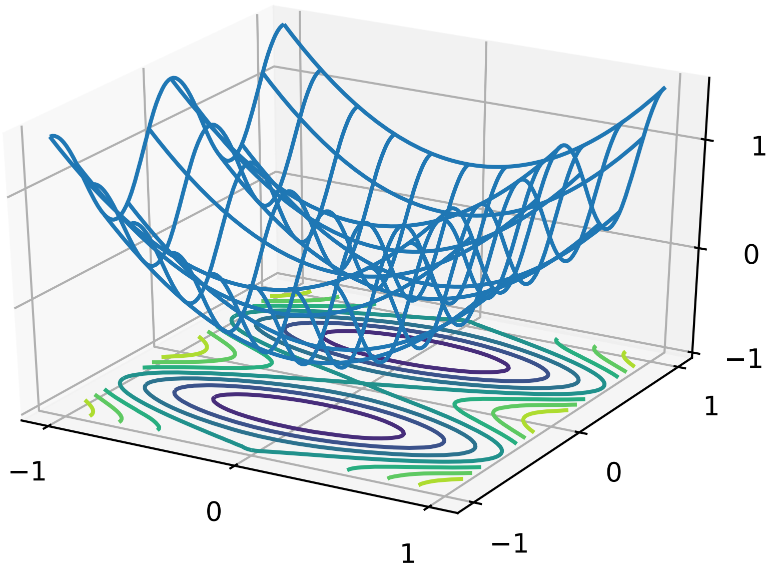
对于凸函数 $f(x)$，定义集合 $S_{b}:=\{x | x \in X \text { and } f(x) \leq b\}$，则集合 S_{b} 为凸集

证明：对于点 $x, x^{\prime} \in S_{b}$, 有 $f\left(\lambda x+(1-\lambda) x^{\prime}\right) \leq \lambda f(x)+(1-\lambda) f\left(x^{\prime}\right) \leq b$, 故 $\lambda x+(1-\lambda) x^{\prime} \in S_{b}$

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

In [8]:

```
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])
```



凸函数与二阶导数

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

必要性 (⇐):

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:

$$f^{\prime \prime}(x)=\lim _{\varepsilon \rightarrow 0} \frac{\frac{f(x+\epsilon)-f(x)}{\epsilon}-\frac{f(x)-f(x-\epsilon)}{\epsilon}}{\epsilon}$$
$$f^{\prime \prime}(x)=\lim _{\varepsilon \rightarrow 0} \frac{f(x+\epsilon)+f(x-\epsilon)-2 f(x)}{\epsilon^{2}} \geq 0$$

充分性 (⇒):

令 $a<x<b$ 为 $f(x)$ 上的三个点，由拉格朗日中值定理:

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

根据单调性，有 $f^{\prime}(\beta) \geq f^{\prime}(\alpha)$, 故:

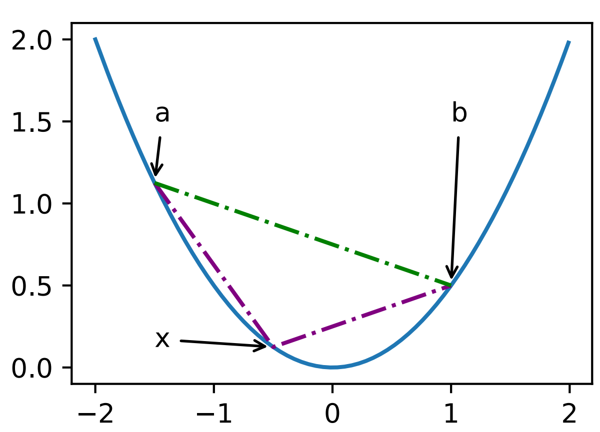
$$\begin{aligned} f(b)-f(a) &=f(b)-f(x)+f(x)-f(a) \\ &=(b-x) f^{\prime}(\beta)+(x-a) f^{\prime}(\alpha) \\ & \geq(b-a) f^{\prime}(\alpha) \end{aligned}$$

In [9]:

```
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[9]:

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



限制条件

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

拉格朗日乘子法

Boyd & Vandenberghe, 2004

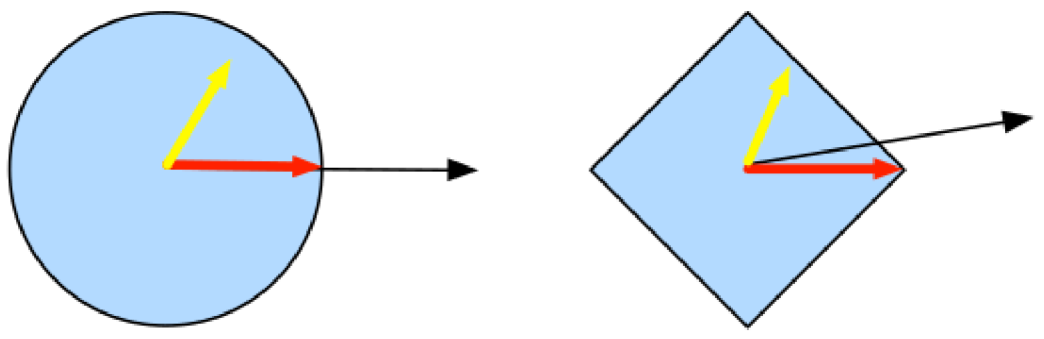
$$L(\mathbf{x}, \alpha) = f(\mathbf{x}) + \sum_i \alpha_i c_i(\mathbf{x}) \text{ where } \alpha_i \geq 0$$

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 $\frac{\lambda}{2} ||w||^2$

投影

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



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