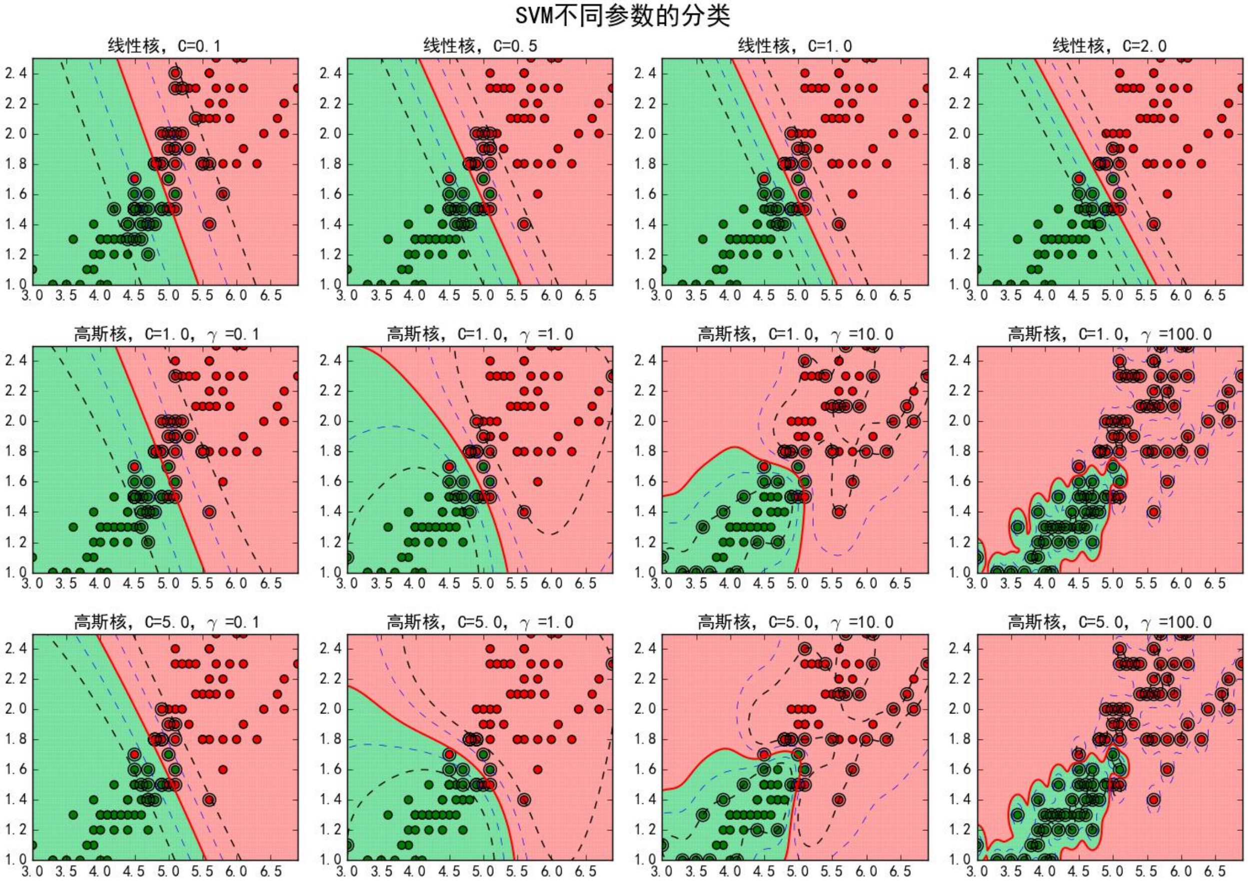
支持向量机



SVM不同参数的分类
线性核，C=0.1
线性核，C=0.5
线性核，C=1.0
线性核，C=2.0
高斯核，C=1.0，γ =0.1
高斯核，C=1.0，γ =1.0
高斯核，C=1.0，γ =10.0
高斯核，C=1.0，γ =100.0
高斯核，C=5.0，γ =0.1
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高斯核，C=5.0，γ =10.0
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主要内容和目标

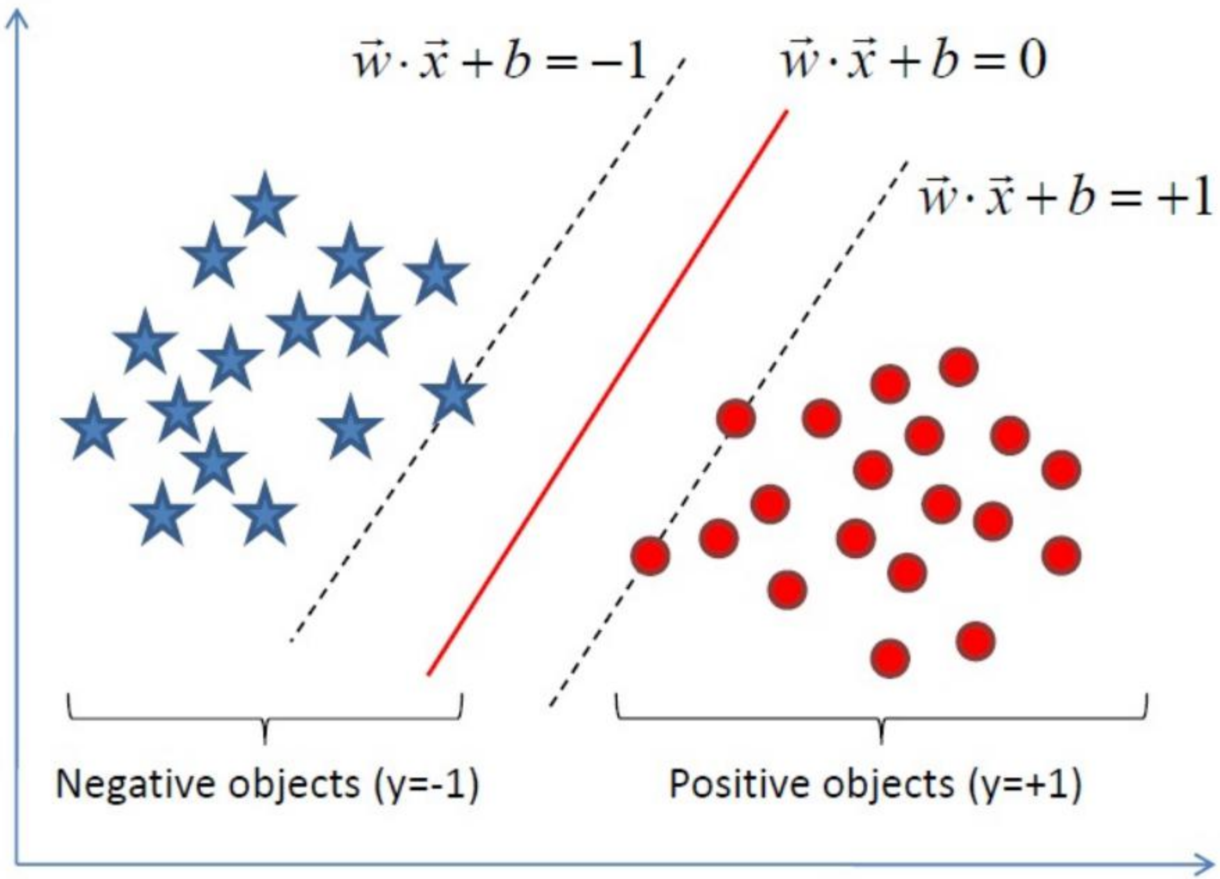
- 理解支持向量机SVM的原理和目标
- 掌握支持向量机的计算过程和算法步骤
- 理解软间隔最大化的含义
  - 对线性不可分的数据给出(略有错误)的分割面
  - 线性可分的数据需要使用“软间隔”目标函数吗?
- 了解核函数的思想
- 了解SMO算法的过程

各种概念

- 线性可分支持向量机
  - 硬间隔最大化hard margin maximization
  - 硬间隔支持向量机
- 线性支持向量机
  - 软间隔最大化soft margin maximization
  - 软间隔支持向量机
- 非线性支持向量机
  - 核函数kernel function

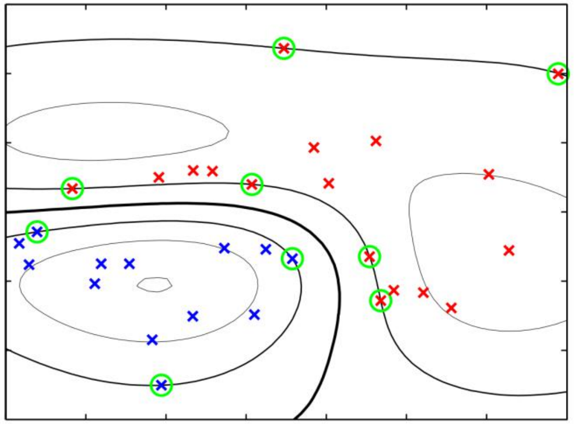
  - 注：以上概念的提法，各个文献并不十分统一。

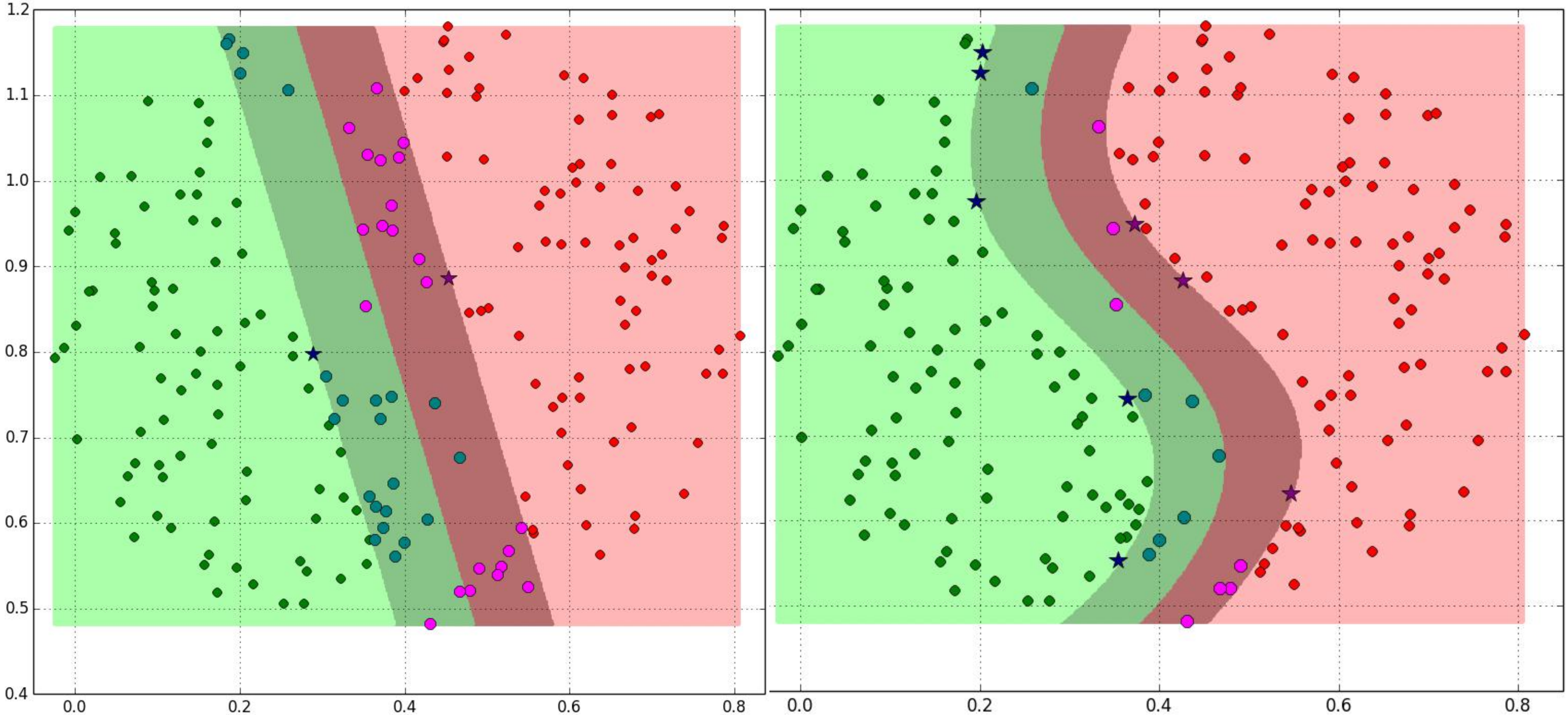
线性可分支持向量机

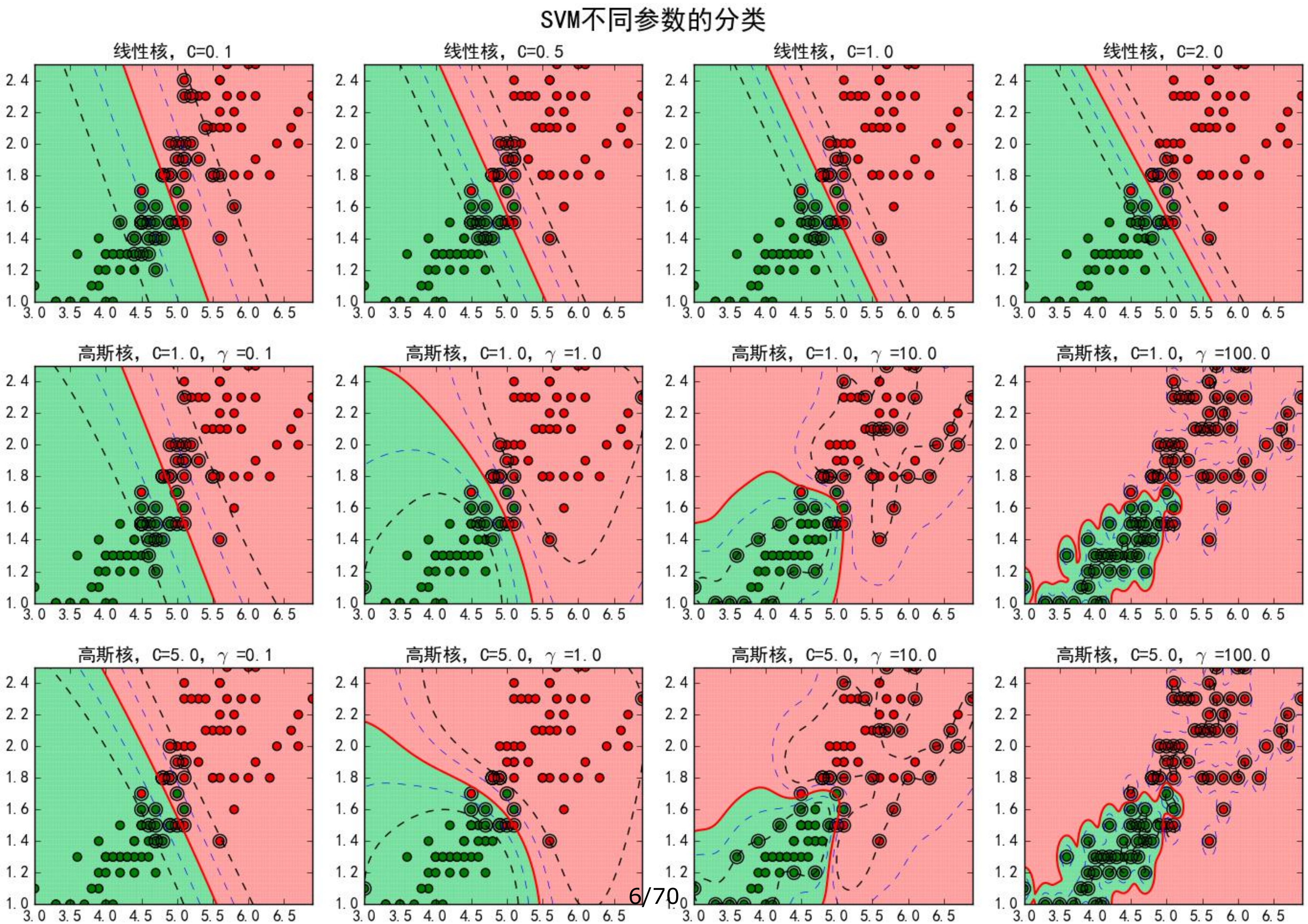


$\vec{w}\cdot\vec{x}+b=-1$
$\vec{w}\cdot\vec{x}+b=0$
$\vec{w}\cdot\vec{x}+b=+1$
Negative objects (y=-1)
Positive objects (y=+1)

使用核解决线性不可分



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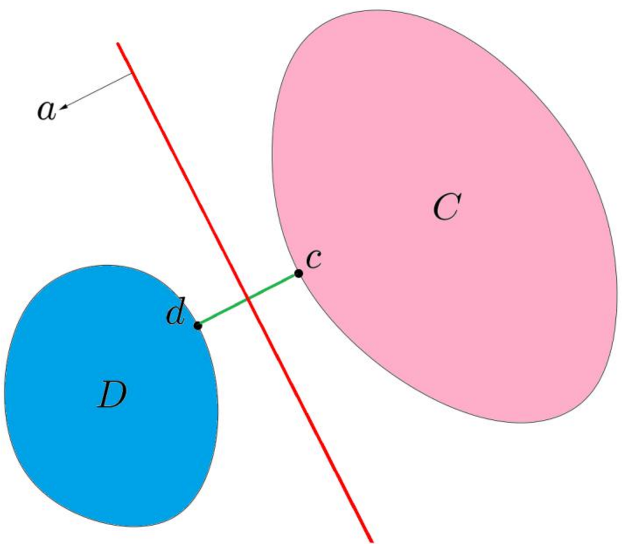
高斯核，C=5.0，γ =10.0
高斯核，C=5.0，γ =100.0

分割超平面

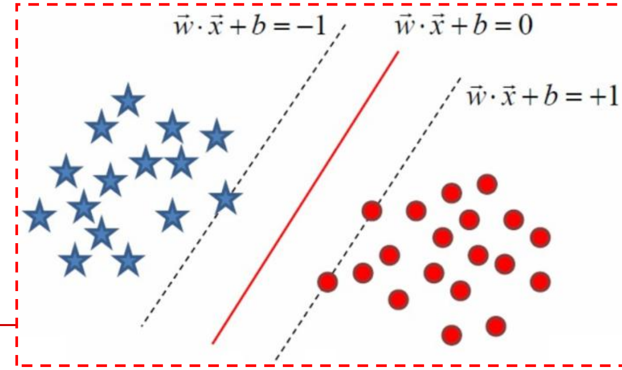
- 设C和D为两不相交的凸集，则存在超平面P，P可以将C和D分离。

$$\forall x \in C, a^T x \le b \text{且} \forall x \in D, a^T x \ge b$$

- 两个集合的距离，定义为两个集合间元素的最短距离。
- 做集合C和集合D最短线段的垂直平分线。

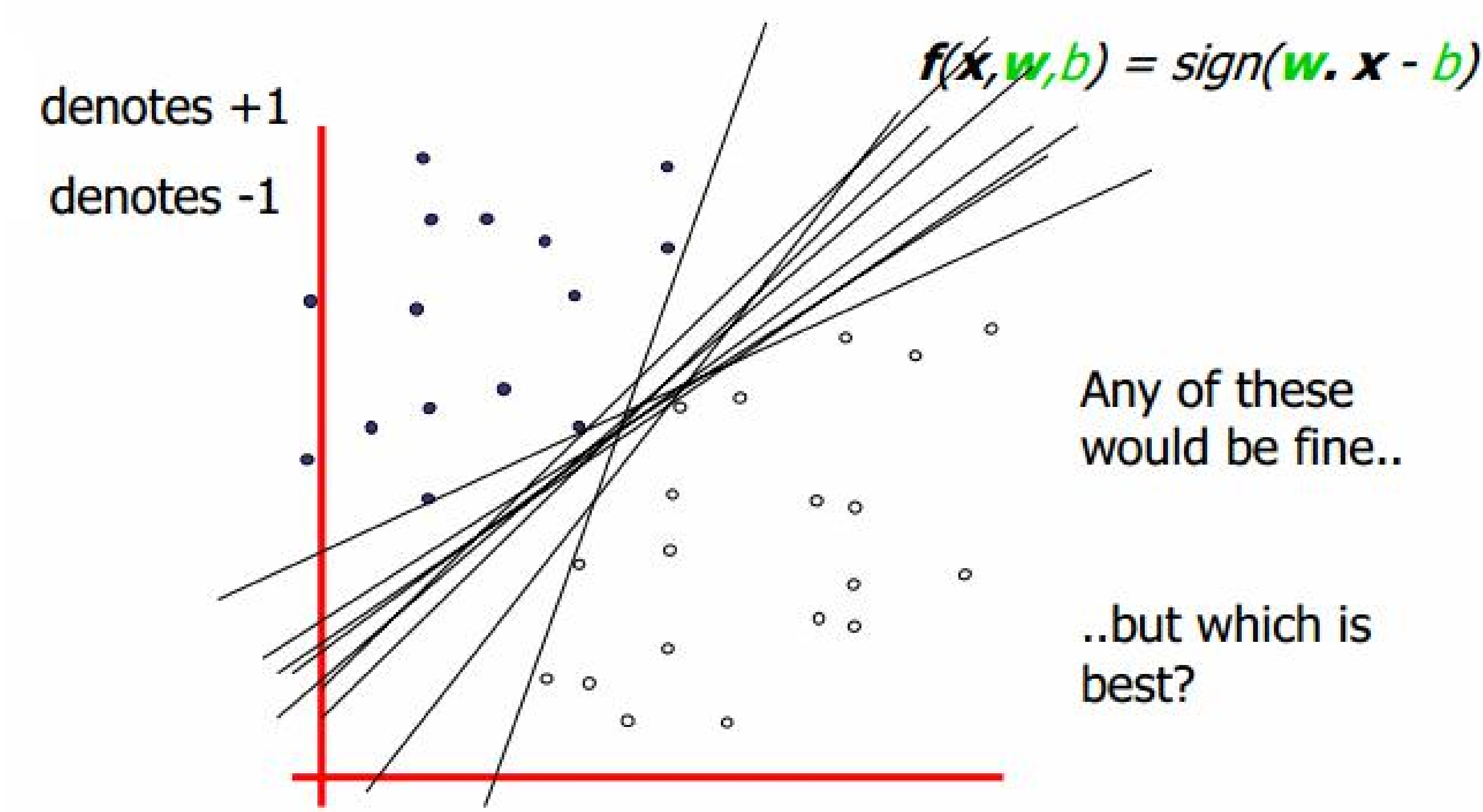


分割超平面的思考



- 如何定义两个集合的“最优”分割超平面？
  - 找到集合“边界”上的若干点，以这些点为“基础”计算超平面的方向；以两个集合边界上的这些点的平均作为超平面的“截距”
  - 支持向量：support vector
- 若两个集合有部分相交，如何定义超平面，使得两个集合“尽量”分开？

线性分类问题

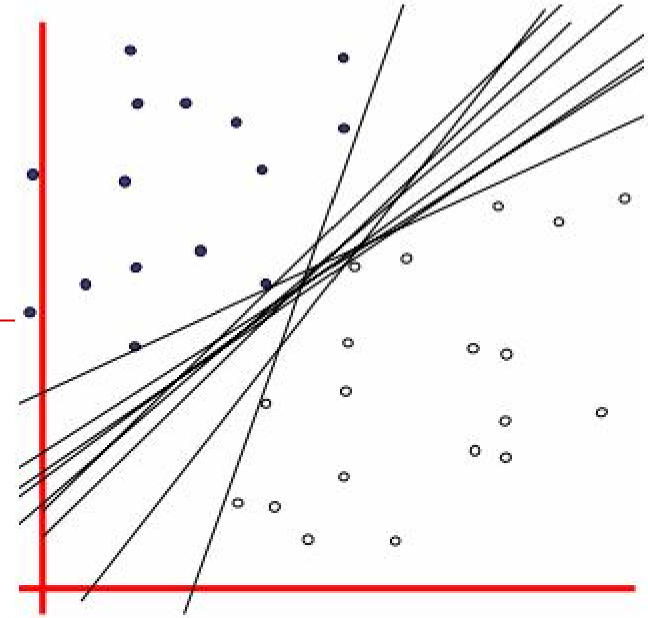


$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}.\ \mathbf{x} - b)$
denotes +1
denotes -1
Any of these would be fine..
..but which is best?

输入数据

- 假设给定一个特征空间上的训练数据集 $T=\{(\mathbf{x_1},y_1),(\mathbf{x_2},y_2)\ldots(\mathbf{x_N},y_N)\}$
  - 其中，$\mathbf{x_i}\in R^n$，$y_i\in\{+1,-1\}$，$i=1,2,\ldots N$。
- $\mathbf{x_i}$为第i个实例(若n>1，$\mathbf{x_i}$为向量)；
- y_i为$\mathbf{x_i}$的类标记；
  - 当$y_i=+1$时，称$\mathbf{x_i}$为正例；
  - 当$y_i=-1$时，称$\mathbf{x_i}$为负例；
- $(\mathbf{x_i},y_i)$称为样本点。

线性可分支持向量机



- 给定线性可分训练数据集，通过**间隔最大化**得到的分离超平面为

$$y(x)=w^T\Phi(x)+b$$

相应的分类决策函数 $f(x)=sign\left(w^T\Phi(x)+b\right)$

该决策函数称为线性可分支持向量机。

- φ(x)是某个确定的特征空间转换函数，它的作用是将x映射到(更高的)维度。
  - 最简单直接的：$\Phi(x)=x$
- 稍后会看到，求解分离超平面问题可以等价为求解相应的**凸二次规划问题**。

整理符号

- 分割平面：$w^T\Phi(x)+b=0$
- 训练集：$x_1, x_2, \cdots, x_n$
- 目标值：$y_1, y_2, \cdots, y_n$， $y_i \in \{-1, 1\}$
- 新数据的分类：

$$y(x)=w^T\Phi(x)+b$$

$$sign(y(x))$$

推导目标函数

- 根据题设 $y(x) = w^T \Phi(x) + b$
- 有：

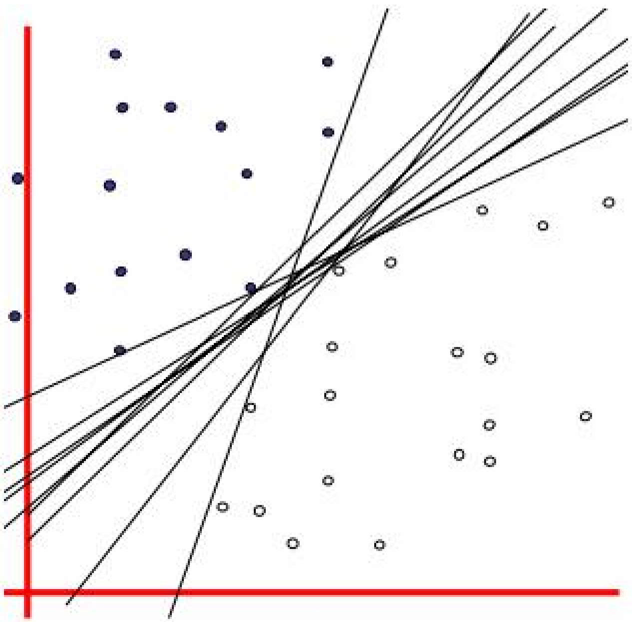
$$\begin{cases} y(x_i) > 0 \Leftrightarrow y_i = +1 \\ y(x_i) < 0 \Leftrightarrow y_i = -1 \end{cases} \Rightarrow y_i \cdot y(x_i) > 0$$

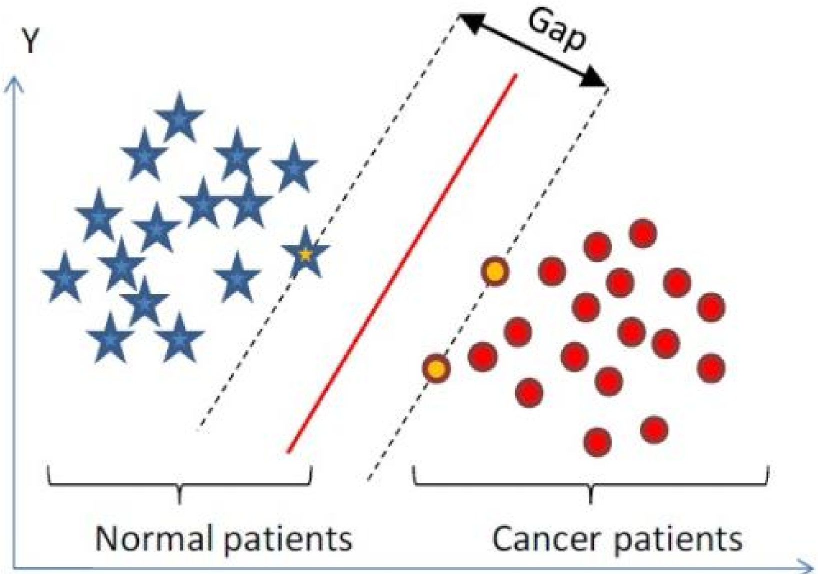
- **w**,b等比例缩放，则t*y的值同样缩放，从而：

$$\frac{y_i \cdot y(x_i)}{\|w\|} = \frac{y_i \cdot \left(w^T \cdot \Phi(x_i) + b\right)}{\|w\|}$$

最大间隔分离超平面 $\frac{y_i \cdot y(x_i)}{\|w\|} = \frac{y_i \cdot \left(w^T \cdot \Phi(x_i) + b\right)}{\|w\|}$

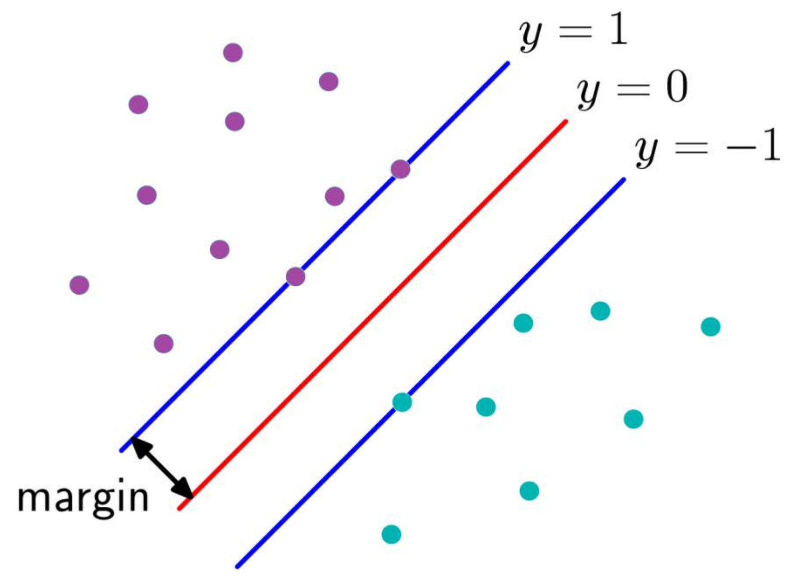
- 目标函数：$\underset{w,b}{\arg\max}\left\{\frac{1}{\|w\|}\min_i\left[y_i \cdot \left(w^T \cdot \Phi(x_i) + b\right)\right]\right\}$



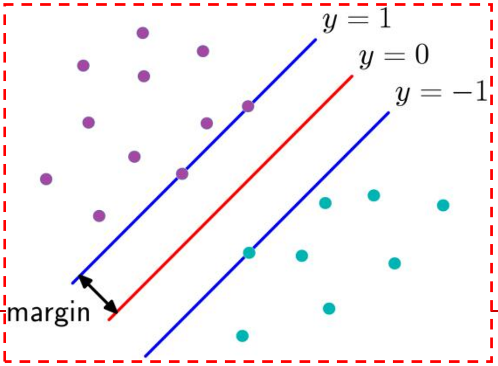


函数间隔和几何间隔 $\frac{w^T \cdot \Phi(x_i)+b}{\|w\|}$

- 分割平面：$y = w^T \cdot \Phi(x) + b$
- 总可以通过等比例缩放w的方法，使得两类点的函数值都满足$|\ y\ | \geq 1$



建立目标函数



- 总可以通过等比例缩放w的方法，使得两类点的函数值都满足$|y|\geq 1$
- 约束条件：$y_i \cdot \left(w^T \cdot \Phi(x_i) + b\right) \geq 1$
- 原目标函数：$$\arg\max_{w,b} \left\{ \frac{1}{\|w\|} \min_i \left[y_i \cdot \left(w^T \cdot \Phi(x_i) + b\right) \right] \right\}$$
- 新目标函数：$$\arg\max_{w,b} \frac{1}{\|w\|}$$

建立目标函数

$$\max_{w,b} \frac{1}{\|w\|}$$

$$s.t. \quad y_i\left(w^T \cdot \Phi\left(x_i\right)+b\right) \geq 1, \quad i=1,2,\cdots,n$$

$$\min_{w,b} \frac{1}{2}\|w\|^2$$

$$s.t. \quad y_i\left(w^T \cdot \Phi\left(x_i\right)+b\right) \geq 1, \quad i=1,2,\cdots,n$$

拉格朗日乘子法 $\min_{w,b}\frac{1}{2}\|w\|^2, s.t.\ y_i\left(w^T\cdot\Phi(x_i)+b\right)\geq 1, i=1,2\cdots N$

$$L(w,b,\alpha)=\frac{1}{2}\|w\|^2-\sum_{i=1}^{n}\alpha_i\left(y_i\left(w^T\cdot\Phi(x_i)+b\right)-1\right)$$

- 原问题是极小极大问题

$$\min_{w,b}\max_{\alpha}L(w,b,\alpha)$$

- 原始问题的对偶问题，是极大极小问题

$$\max_{\alpha}\min_{w,b}L(w,b,\alpha)$$

拉格朗日函数

- 将拉格朗日函数L(**w**,b,**a**)分别对**w**，b求偏导并令其为0：

$$\frac{\partial L}{\partial w}=0\Rightarrow w=\sum_{i=1}^{n}\alpha_i y_i\Phi\left(x_i\right)$$

$$\frac{\partial L}{\partial b}=0\Rightarrow 0=\sum_{i=1}^{n}\alpha_i y_i$$

计算拉格朗日函数的对偶函数

$$w = \sum_{i=1}^{n} \alpha_i y_i \Phi(x_n)$$

$$0 = \sum_{i=1}^{n} \alpha_i y_i$$

$$L(w,b,\alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(w^T \cdot \Phi(x_i) + b \right) - 1 \right)$$

$$= \frac{1}{2} w^T w - w^T \sum_{i=1}^{n} \alpha_i y_i \Phi(x_i) - b \sum_{i=1}^{n} \alpha_i y_i + \sum_{i=1}^{n} \alpha_i$$

$$= \frac{1}{2} w^T \sum_{i=1}^{n} \alpha_i y_i \Phi(x_i) - w^T \sum_{i=1}^{n} \alpha_i y_i \Phi(x_i) - b \cdot 0 + \sum_{i=1}^{n} \alpha_i$$

$$= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \left(\sum_{i=1}^{n} \alpha_i y_i \Phi(x_i) \right)^T \sum_{i=1}^{n} \alpha_i y_i \Phi(x_i)$$

$$= \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \Phi^T(x_i) \Phi(x_j)$$

$$a^* = \arg\max_{\alpha} \left(\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \Phi^T(x_i) \Phi(x_j) \right)$$

继续求$\min_{w,b} L(w,b,\alpha)$对α的极大

$$\max_{\alpha} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \left(\Phi(x_i) \cdot \Phi(x_j) \right)$$

$$s.t. \ \sum_{i=1}^{n} \alpha_i y_i = 0$$

$$\alpha_i \geq 0, \quad i = 1,2,\ldots,n$$

整理目标函数：添加负号

$$\min_{\alpha} \quad \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \left(\Phi\left(x_i\right)\cdot\Phi\left(x_j\right)\right)-\sum_{i=1}^{n}\alpha_i$$

$$s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$\alpha_i \geq 0, \quad i = 1,2,\ldots,n$$

线性可分支持向量机学习算法

- 构造并求解约束最优化问题

$$\min_{\alpha} \quad \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j\left(\Phi(x_i)\cdot\Phi(x_j)\right)-\sum_{i=1}^{n}\alpha_i$$

$$s.t. \quad \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$\alpha_i \geq 0, \quad i=1,2,\ldots,n$$

- 求得最优解α*

线性可分支持向量机学习算法

- 计算

$$w^* = \sum_{i=1}^{N} \alpha_i^* y_i \Phi(x_i)$$

$$b^* = y_i - \sum_{i=1}^{N} \alpha_i^* y_i \left(\Phi(x_i) \cdot \Phi(x_j)\right)$$

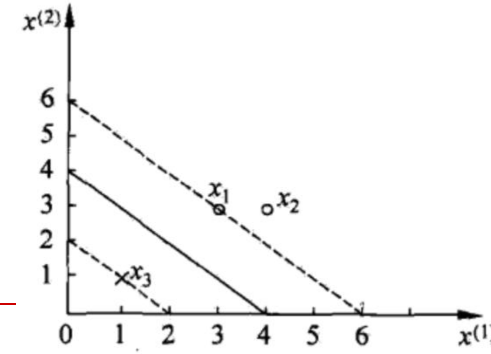
- 求得分离超平面

$$w^* \Phi(x) + b^* = 0$$

- 分类决策函数

$$f(x) = sign\left(w^* \Phi(x) + b^*\right)$$

举例



- 给定3个数据点：正例点$x_1=(3,3)^T$，$x_2=(4,3)^T$，负例点$x_3=(1,1)^T$，求线性可分支持向量机。
- 目标函数：

$$\min_{\alpha} \quad \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j\left(x_i \cdot x_j\right)-\sum_{i=1}^{n}\alpha_i$$

$$=\frac{1}{2}\left(18\alpha_1^2+25\alpha_2^2+2\alpha_3^2+42\alpha_1\alpha_2-12\alpha_1\alpha_3-14\alpha_2\alpha_3\right)-\alpha_1-\alpha_2-\alpha_3$$

$$s.t.\ \ \alpha_1+\alpha_2-\alpha_3=0$$

$$\alpha_i \geq 0, \quad i=1,2,3$$

将约束带入目标函数，化简计算

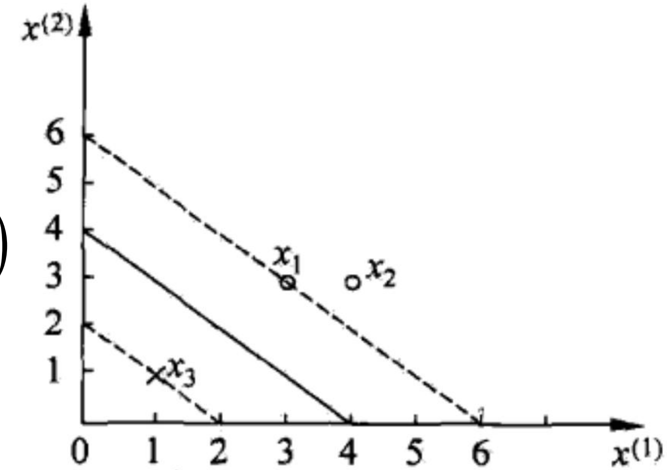
- 将 $\alpha_1+\alpha_2=\alpha_3$
- 带入目标函数，得到关于α_1，α_2的函数：

$$s(\alpha_1,\alpha_2)=4\alpha_1^2+\frac{13}{2}\alpha_2^2+10\alpha_1\alpha_2-2\alpha_1-2\alpha_2$$

- 对α_1，α_2求偏导并令其为0，易知$s(\alpha_1,\alpha_2)$在点(1.5,-1)处取极值。而该点不满足条件$\alpha_2\geq 0$，所以，最小值在边界上达到。
- 当$\alpha_1=0$时，最小值s(0,2/13)=-2/13=-0.1538
- 当$\alpha_2=0$时，最小值s(1/4,0)=-1/4=-0.25
- 于是，$s(\alpha_1,\alpha_2)$在$\alpha_1=1/4$，$\alpha_2=0$时达到最小，此时，$\alpha_3=\alpha_1+\alpha_2=1/4$

分离超平面

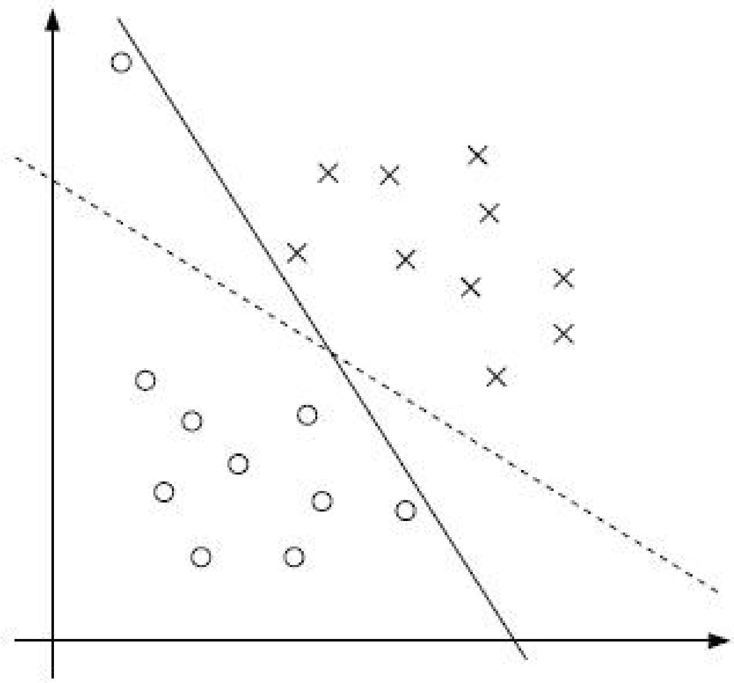
- $\alpha_1=\alpha_3=1/4$对应的点x_1,x_3是支持向量。
- 带入公式：$$w^*=\sum_{i=1}^{N}\alpha_i^* y_i \Phi(x_i)$$
$$b^*=y_i-\sum_{i=1}^{N}\alpha_i^* y_i \left(\Phi(x_i)\cdot\Phi(x_j)\right)$$



- 得到$w_1=w_2=0.5$，$b=-2$
- 因此，分离超平面为 $$\frac{1}{2}x_1+\frac{1}{2}x_2-2=0$$
- 分离决策函数为 $$f(x)=sign\left(\frac{1}{2}x_1+\frac{1}{2}x_2-2\right)$$

线性支持向量机

- 不一定分类完全正确的超平面就是最好的
- 样本数据本身线性不可分



线性支持向量机

- 若数据线性不可分，则增加松弛因子$\xi_i \geq 0$，使函数间隔加上松弛变量大于等于1。这样，约束条件变成

$$y_i(w \cdot x_i + b) \geq 1 - \xi_i$$

- 目标函数：

$$\min_{w,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\xi_i$$

线性SVM的目标函数

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\xi_i$$

$$s.t. \quad y_i\left(w\cdot x_i + b\right) \ge 1-\xi_i, \quad i=1,2,\cdots,n$$

$$\xi_i \ge 0, \quad i=1,2,\cdots,n$$

带松弛因子的SVM拉格朗日函数

- 拉格朗日函数

$$L(w,b,\xi,\alpha,\mu)\equiv\frac{1}{2}\|w\|^2+C\sum_{i=1}^{n}\xi_i-\sum_{i=1}^{n}\alpha_i\left(y_i\left(w\cdot x_i+b\right)-1+\xi_i\right)-\sum_{i=1}^{n}\mu_i\xi_i$$

- 对w,b,ξ求偏导

$$\frac{\partial L}{\partial w}=0\Rightarrow w=\sum_{i=1}^{n}\alpha_i y_i\phi(x_i)$$

$$\frac{\partial L}{\partial b}=0\Rightarrow 0=\sum_{i=1}^{n}\alpha_i y_i$$

$$\frac{\partial L}{\partial \xi_i}=0\Rightarrow C-\alpha_i-\mu_i=0$$

带入目标函数

- 将三式带入L中，得到

$$\min_{w,b,\xi} L(w,b,\xi,\alpha,\mu) = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j (x_i \cdot x_j) + \sum_{i=1}^{n}\alpha_i$$

- 对上式求关于α的极大，得到：

$$\max_{\alpha} \; -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j (x_i \cdot x_j) + \sum_{i=1}^{n}\alpha_i$$

$$
\begin{aligned}
s.t.\ & \sum_{i=1}^{n}\alpha_i y_i = 0 \\
& C - \alpha_i - \mu_i = 0 \\
& \alpha_i \ge 0 \\
& \mu_i \ge 0, \quad i = 1,2,\ldots,n
\end{aligned}
$$

$$0 \le \alpha_i \le C$$

最终的目标函数

- 整理，得到对偶问题：

$$\min_{\alpha} \ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \left(x_i \cdot x_j\right) - \sum_{i=1}^{n}\alpha_i$$

$$s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$0 \le \alpha_i \le C, \quad i = 1,2,\ldots,n$$

线性支持向量机学习算法

- 构造并求解约束最优化问题

$$\min_{\alpha} \quad \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \left(x_i \cdot x_j\right) - \sum_{i=1}^{n}\alpha_i$$

$$s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$0 \le \alpha_i \le C, \quad i = 1,2,\ldots,n$$

- 求得最优解α*

线性支持向量机学习算法

- 计算

$$w^{*}=\sum_{i=1}^{n}\alpha_{i}^{*}y_{i}x_{i}$$

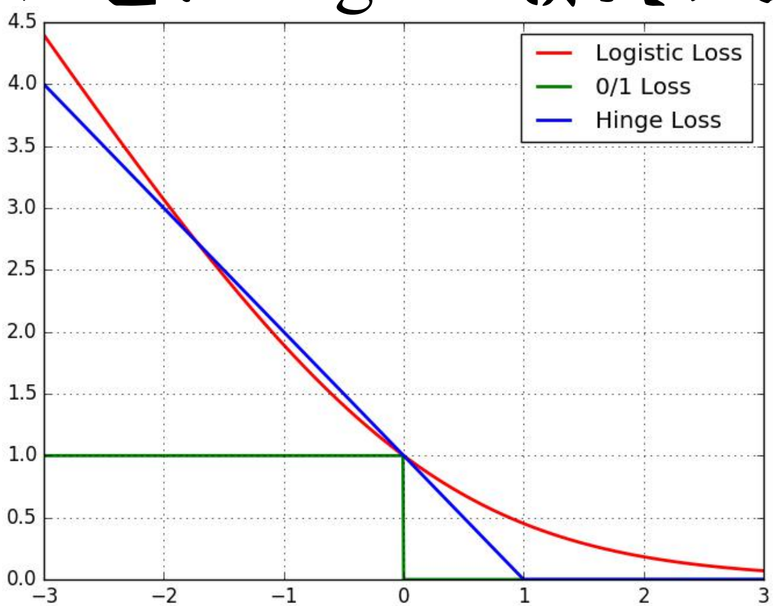
$$b^{*}=\frac{\max\limits_{i:\ y_{i}=-1} w^{*}\cdot x_{i}+\min\limits_{i:\ y_{i}=1} w^{*}\cdot x_{i}}{2}$$

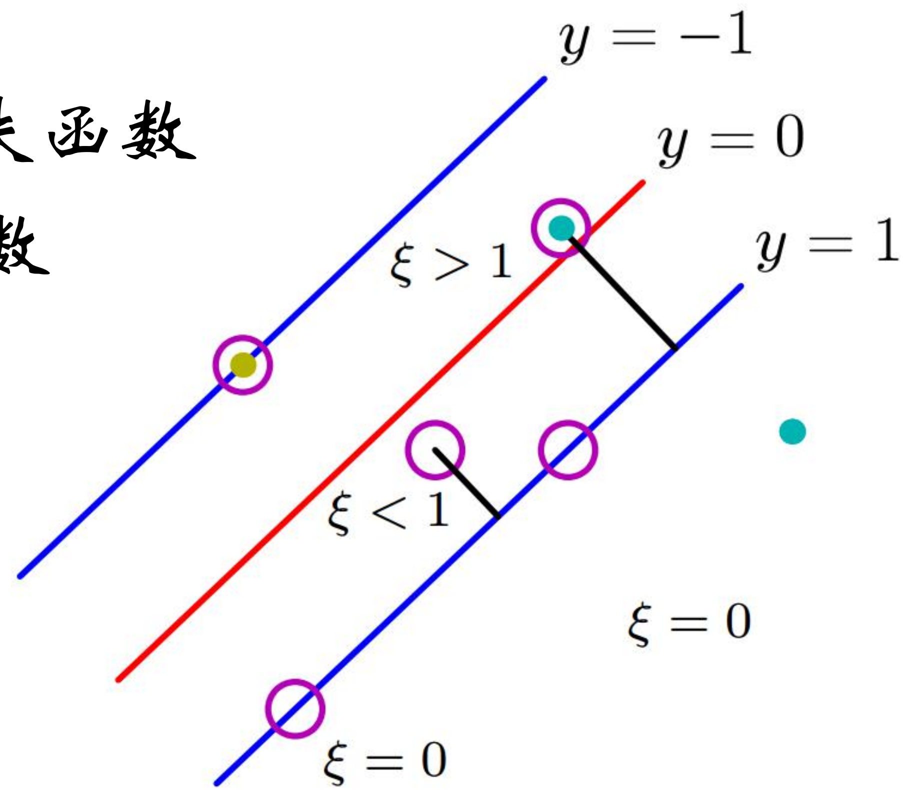
  - 注意：计算b*时，需要使用满足条件$0<\alpha_j<C$的向量
  - 实践中往往取支持向量的所有值取平均，作为b*
- 求得分离超平面 $w^{*}x+b^{*}=0$
- 分类决策函数

$$f(x)=sign(w^{*}x+b^{*})$$

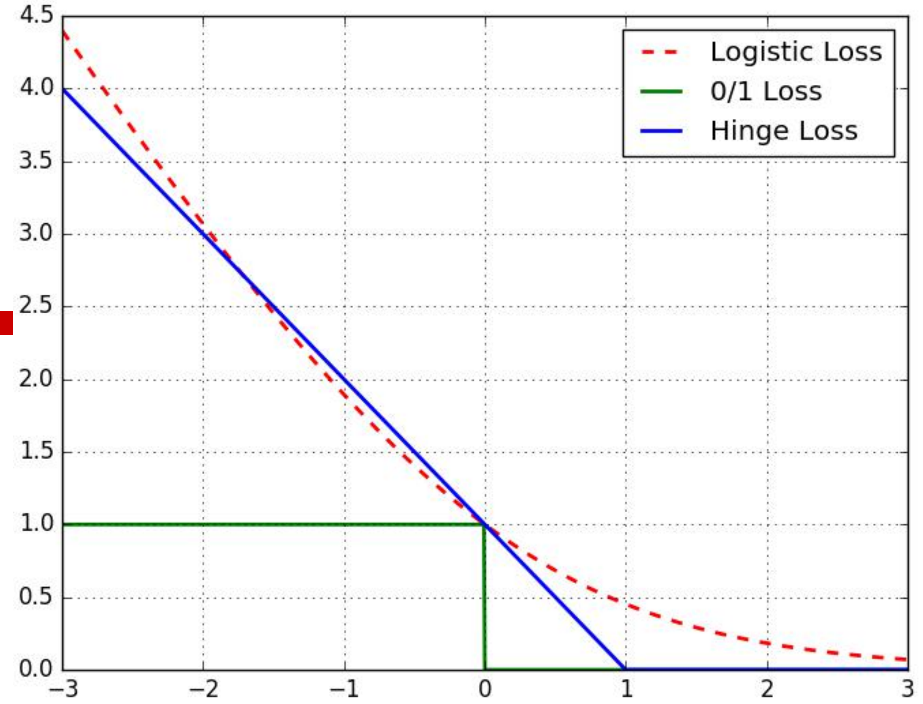
损失函数分析

- 绿色：0/1损失
- 蓝色： SVM Hinge损失函数
- 红色：Logistic损失函数





Code




```python
import math
import numpy as np
import matplotlib.pyplot as plt

if __name__ == "__main__":
    x = np.array(np.linspace(start=-3, stop=3, num=1001, dtype=np.float))
    y_logit = np.log(1 + np.exp(-x)) / math.log(2)
    y_01 = x < 0
    y_hinge = 1.0 - x
    y_hinge[y_hinge < 0] = 0
    plt.plot(x, y_logit, 'r--', label='Logistic Loss', linewidth=2)
    plt.plot(x, y_01, 'g-', label='0/1 Loss', linewidth=2)
    plt.plot(x, y_hinge, 'b-', label='Hinge Loss', linewidth=2)
    plt.grid()
    plt.legend(loc='upper right')
    plt.savefig('1.png')
    plt.show()
```

核函数

- 可以使用核函数，将原始输入空间映射到新的特征空间，从而，使得原本线性不可分的样本可能在核空间可分。
  - 多项式核函数： $\kappa(x_1, x_2) = (x_1 \cdot x_2 + c)^d$
  - 高斯核RBF函数： $\kappa(x_1, x_2) = \exp\left(-\gamma \cdot \|x_1 - x_2\|^2\right)$
  - Sigmoid核函数： $\kappa(x_1, x_2) = tanh(x_1 \cdot x_2 + c)$
- 在实际应用中，往往依赖先验领域知识/交叉验证等方案才能选择有效的核函数。
  - 没有更多先验信息，则使用高斯核函数

多项式核函数 $\kappa(\vec{x},\vec{y})=(\vec{x}\cdot\vec{y})^2$

$$\kappa(\vec{x},\vec{y})=(\vec{x}\cdot\vec{y})^2$$

$$\Rightarrow\left(\sum_{i=1}^{n}x_iy_i\right)^2 \qquad \Rightarrow \Phi(\vec{x})=vec(x_ix_j)\Big|_{i,j=1}^{n}$$

$$=\sum_{i=1}^{n}\sum_{j=1}^{n}x_ix_jy_iy_j$$

$$=\sum_{i=1}^{n}\sum_{j=1}^{n}(x_ix_j)(y_iy_j)$$

特殊的，若n=3，即：$\Phi(\vec{x})=\begin{pmatrix}x_1x_1\\x_1x_2\\x_1x_3\\x_2x_1\\x_2x_2\\x_2x_3\\x_3x_1\\x_3x_2\\x_3x_3\end{pmatrix}$

多项式核 $\kappa(\vec{x},\vec{y})=(\vec{x}\cdot\vec{y}+c)^2$

$$\kappa(\vec{x},\vec{y})=(\vec{x}\cdot\vec{y}+c)^2$$

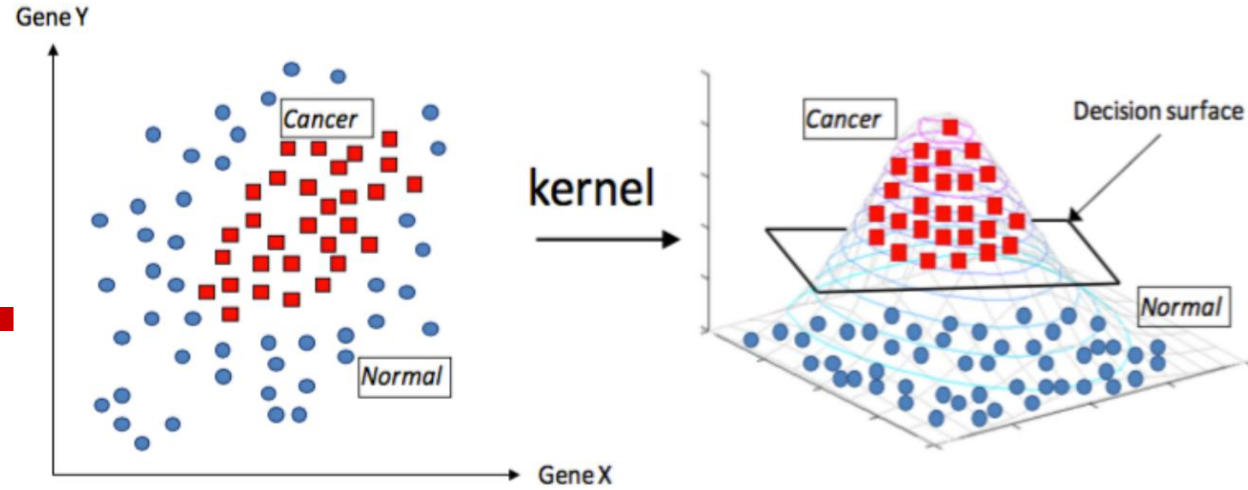
$$\Rightarrow(\vec{x}\cdot\vec{y})^2+2c\vec{x}\cdot\vec{y}+c^2$$

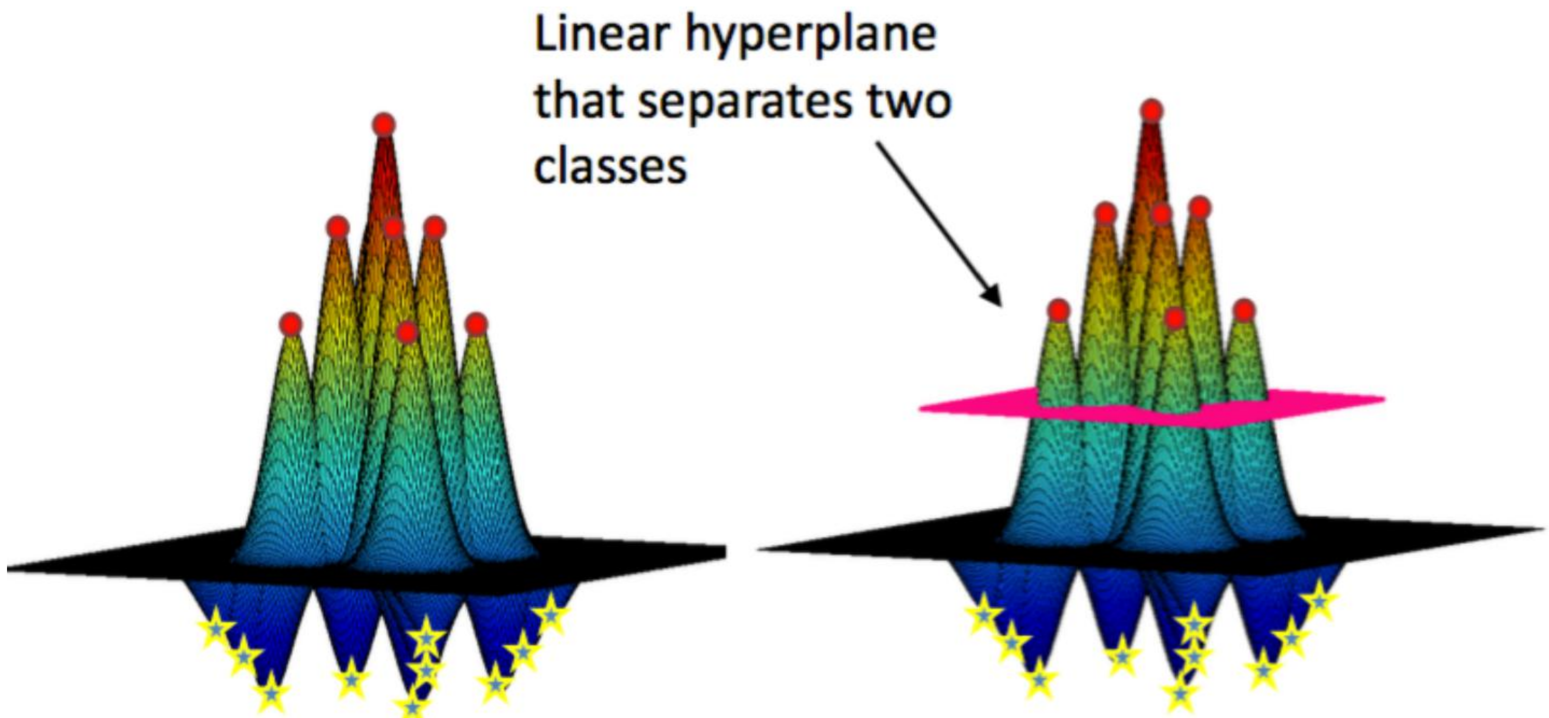
$$=\sum_{i=1}^{n}\sum_{j=1}^{n}\left(x_i x_j\right)\left(y_i y_j\right)+\sum_{i=1}^{n}\left(\sqrt{2c}x_i\cdot\sqrt{2c}x_j\right)+c^2$$

$$\Rightarrow\Phi(\vec{x})=\left(vec\left(x_i x_j\right)\Big|_{i,j=1}^{n},vec\left(\sqrt{2c}x_i\right)\Big|_{i=1}^{n},c\right)$$

特殊的，若n=3，即：$\Phi(\vec{x})=\begin{pmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \\ \sqrt{2c}x_1 \\ \sqrt{2c}x_2 \\ \sqrt{2c}x_3 \\ c \end{pmatrix}$

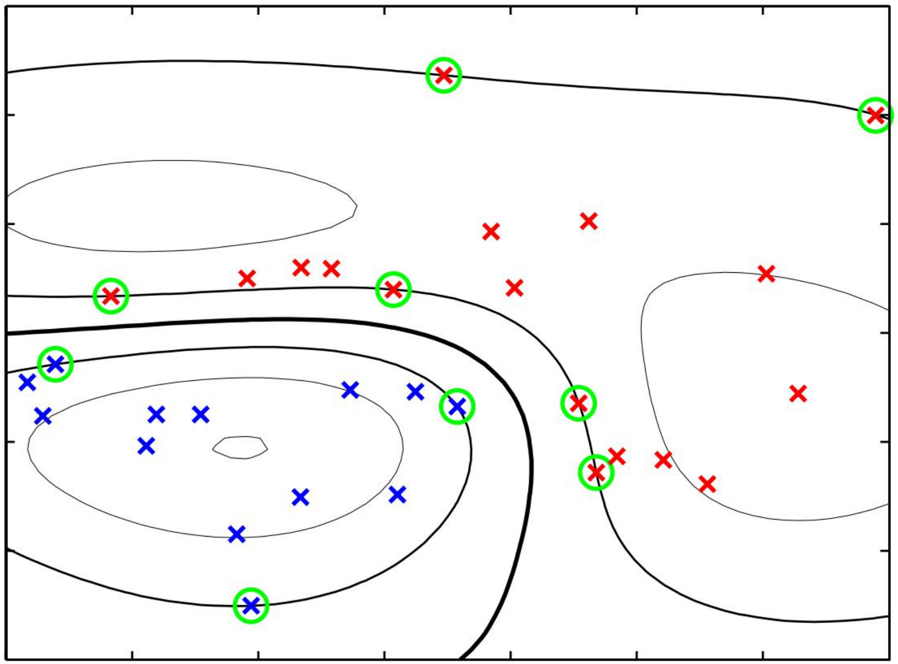
核函数映射


Gene Y
Cancer
Normal
Gene X
kernel
Cancer
Decision surface
Normal


Linear hyperplane
that separates two
classes

高斯核

- 粗线是分割超“平面”
- 其他线是y(x)的等高线
- 绿色圈点是支持向量点



高斯核是无穷维的 $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!} + R_n$

$$\kappa(x_1, x_2) = e^{-\frac{\|x_1 - x_2\|^2}{2\sigma^2}} = e^{-\frac{(x_1 - x_2)^2}{2\sigma^2}} = e^{-\frac{x_1^2 + x_2^2 - 2x_1x_2}{2\sigma^2}} = e^{-\frac{x_1^2 + x_2^2}{2\sigma^2}} \cdot e^{\frac{x_1x_2}{\sigma^2}}$$

$$= e^{-\frac{x_1^2 + x_2^2}{2\sigma^2}} \cdot \left(1 + \frac{1}{\sigma^2} \cdot \frac{x_1x_2}{1!} + \left(\frac{1}{\sigma^2}\right)^2 \cdot \frac{(x_1x_2)^2}{2!} + \left(\frac{1}{\sigma^2}\right)^3 \cdot \frac{(x_1x_2)^3}{3!} + \cdots + \left(\frac{1}{\sigma^2}\right)^n \cdot \frac{(x_1x_2)^n}{n!} + \cdots\right)$$

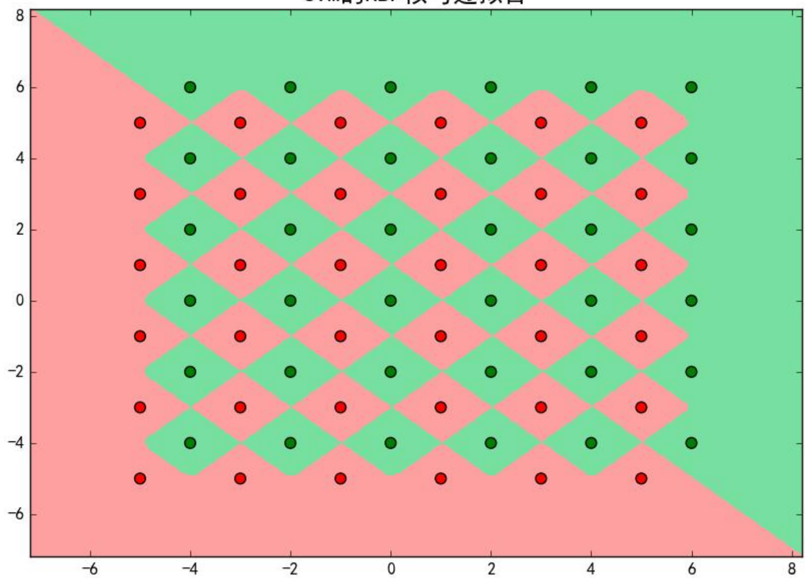
$$= e^{-\frac{x_1^2 + x_2^2}{2\sigma^2}} \cdot \left(1 \cdot 1 + \frac{1}{1!}\frac{x_1}{\sigma} \cdot \frac{x_2}{\sigma} + \frac{1}{2!} \cdot \frac{x_1^2}{\sigma^2} \cdot \frac{x_2^2}{\sigma^2} + \frac{1}{3!} \cdot \frac{x_1^3}{\sigma^3} \cdot \frac{x_2^3}{\sigma^3} + \cdots + \frac{1}{n!} \cdot \frac{x_1^n}{\sigma^n} \cdot \frac{x_2^n}{\sigma^n} + \cdots\right)$$

$$= \Phi(x_1)^T \cdot \Phi(x_2)$$

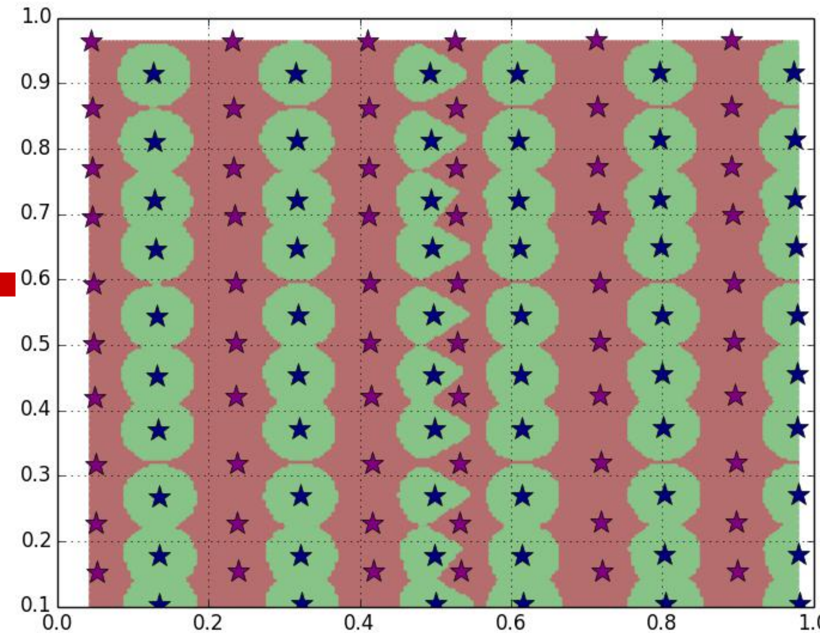
- 其中 $\Phi(x) = e^{-\frac{x^2}{2\sigma^2}} \left(1, \sqrt{\frac{1}{1!}}\frac{x}{\sigma}, \sqrt{\frac{1}{2!}}\frac{x^2}{\sigma^2}, \sqrt{\frac{1}{3!}}\frac{x^3}{\sigma^3}, \cdots, \sqrt{\frac{1}{n!}}\frac{x^n}{\sigma^n}, \cdots\right)$

高斯核的分类

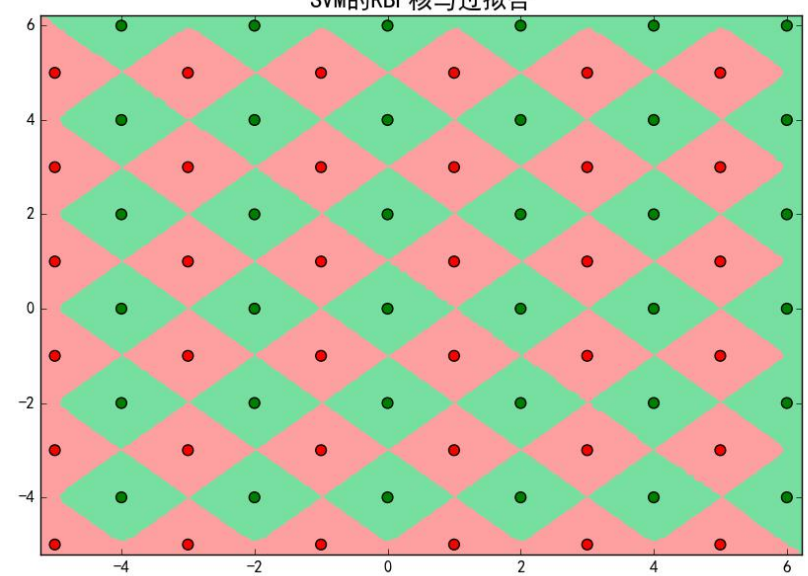
SVM的RBF核与过拟合



```python
def kernel(x1, x2):
    n = len(x2) - 1
    s = 0
    if kn == 0:  # 线性核
        for i in range(n):
            s += x1[i] * x2[i]
        return s
    for i in range(n):
        s += (x1[i] - x2[i]) ** 2
    k = math.exp(-s / (2 * sigma**2))
    return k
```



SVM的RBF核与过拟合



SVM中系数的求解：SMO

- 序列最小最优化
  - Sequential Minimal Optimization
- 有多个拉格朗日乘子
- 每次只选择其中两个乘子做优化，其他因子认为是常数。
  - 将N个解问题，转换成两个变量的求解问题：并且目标函数是凸的。

SMO：序列最小最优化

- 考察目标函数，假设α1和α2是变量，其他是定值：

$$\min_{\alpha} \ \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j K\left(x_i \cdot x_j\right)-\sum_{i=1}^{N}\alpha_i$$

$$s.t. \ \sum_{i=1}^{N}\alpha_i y_i = 0$$

$$0 \le \alpha_i \le C, \quad i = 1,2,\dots N$$

$$\min_{\alpha_1,\alpha_2} W\left(\alpha_1,\alpha_2\right)$$

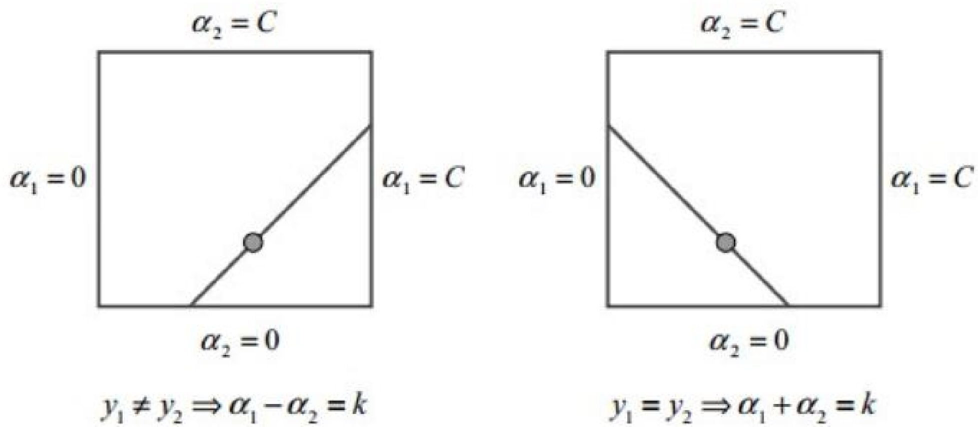
$$= \frac{1}{2}\kappa_{11}\alpha_1^2 + \frac{1}{2}\kappa_{22}\alpha_2^2 + y_1 y_2 \alpha_1\alpha_2\kappa_{12} - \left(\alpha_1 + \alpha_2\right)$$

$$+ y_1\alpha_1\sum_{i=3}^{N} y_i\alpha_i\kappa_{i1} + y_2\alpha_2\sum_{i=3}^{N} y_i\alpha_i\kappa_{i2}$$

$$s.t. \ \ \alpha_1 y_1 + \alpha_2 y_2 = -\sum_{i=3}^{N} y_i\alpha_i = \zeta$$

$$0 \le \alpha_i \le C$$

二变量优化问题



$$\begin{cases} L = \max\{0, \alpha_1 - \alpha_2\} \\ H = \min\{C, C + \alpha_1 - \alpha_2\} \end{cases}, \quad y_1 \neq y_2$$

$$\begin{cases} L = \max\{0, \alpha_1 + \alpha_2 - C\} \\ H = \min\{C, \alpha_1 + \alpha_2\} \end{cases}, \quad y_1 = y_2$$

SMO的迭代公式

- 迭代公式：

$$g(x)=\sum_{i=1}^{N} y_i\alpha_i\kappa(x_i,x)+b$$

$$\eta=\kappa(x_1,x_1)+\kappa(x_2,x_2)-2\kappa(x_1,x_2)=\left\|\Phi(x_1)-\Phi(x_2)\right\|^2$$

$$E_i=g(x_i)-y_i=\left(\sum_{j=1}^{N} y_j\alpha_j\kappa(x_j,x_i)+b\right)-y_i,\quad i=1,2$$

$$\alpha_j^{new}=\alpha_j^{old}+\frac{y_j(E_i-E_j)}{\eta}$$

退出条件

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

$$0 \le \alpha_i \le C, \quad i = 1,2,\ldots n$$

$$y_i \cdot g(x_i) = \begin{cases} \ge 1, & \{x_i | \alpha_i = 0\} // \text{落在边界外} \\ = 1, & \{x_i | 0 < \alpha_i < C\} // \text{落在边界上} \\ \le 1, & \{x_i | \alpha_i = C\} // \text{落在边界内} \end{cases}$$

$$g(x_i) = \sum_{j=1}^{n} y_j \alpha_j K(x_j, x_i) + b$$

Code

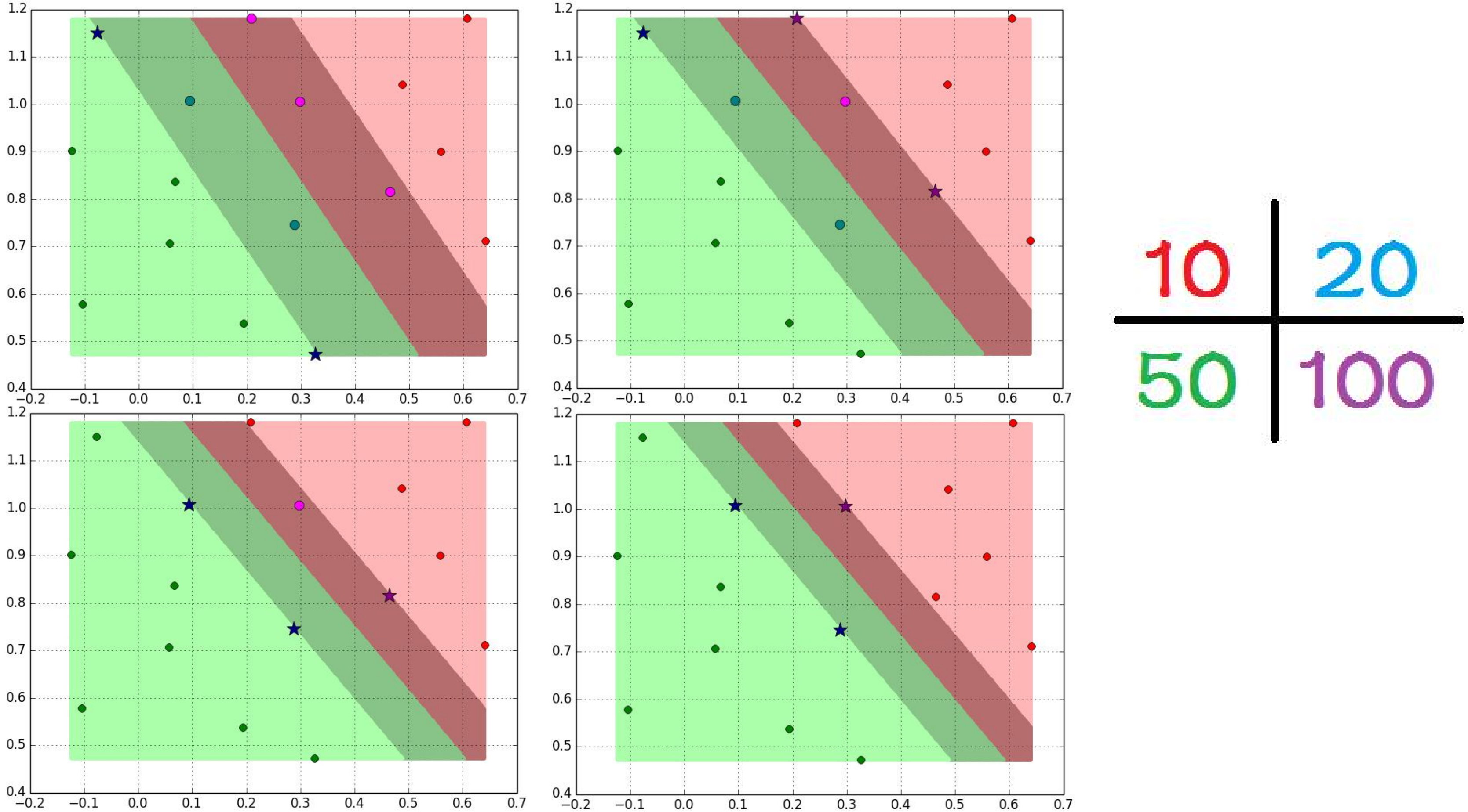
```python
def update(i, j, data):
    low = 0
    high = C
    if data[i][-1] == data[j][-1]:
        low = max(0, alpha[i]+alpha[j]-C)
        high = min(C, alpha[i]+alpha[j])
    else:
        low = max(0, alpha[j]-alpha[i])
        high = min(C, alpha[j]-alpha[i]+C)
    if low == high:
       return False
    eta = kernel(data[i], data[i]) + kernel(data[j], data[j])\
          - 2*kernel(data[i], data[j])
    if is_same(eta, 0):
        return False
    ei = predict(data[i], data) - data[i][-1]
    ej = predict(data[j], data) - data[j][-1]
    alpha_j = alpha[j] + data[j][-1] * (ei - ej) / eta
    if alpha_j == alpha[j]:
        return False
    if alpha_j > high:
        alpha_j = high
    elif alpha_j < low:
        alpha_j = low
    alpha[i] += (alpha[j] - alpha_j) * data[i][-1] * data[j][-1]
    alpha[j] = alpha_j
    return True
```

Code

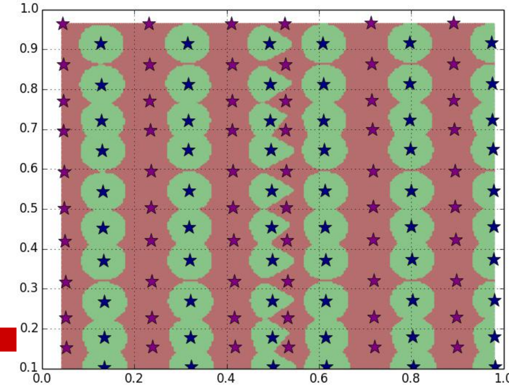
```
def update_b(i, j, data):
    global b
    bi = b + data[i][-1] - predict(data[i], data)
    bj = b + data[j][-1] - predict(data[j], data)
    if C > alpha[i] > 0:
        return bi
    elif C > alpha[j] > 0:
        return bj
    return (bi + bj) / 2


def smo(data):
    m = len(data)
    global b
    for time in range(5000):
        no_change = 0
        i = select_first(data)
        if i == -1:
            break
        j = select_second(i, m)
        if not update(i, j, data):
            no_change += 1
            continue
        b = update_b(i, j, data)
        print time, b
        if no_change > 100:
            break
```

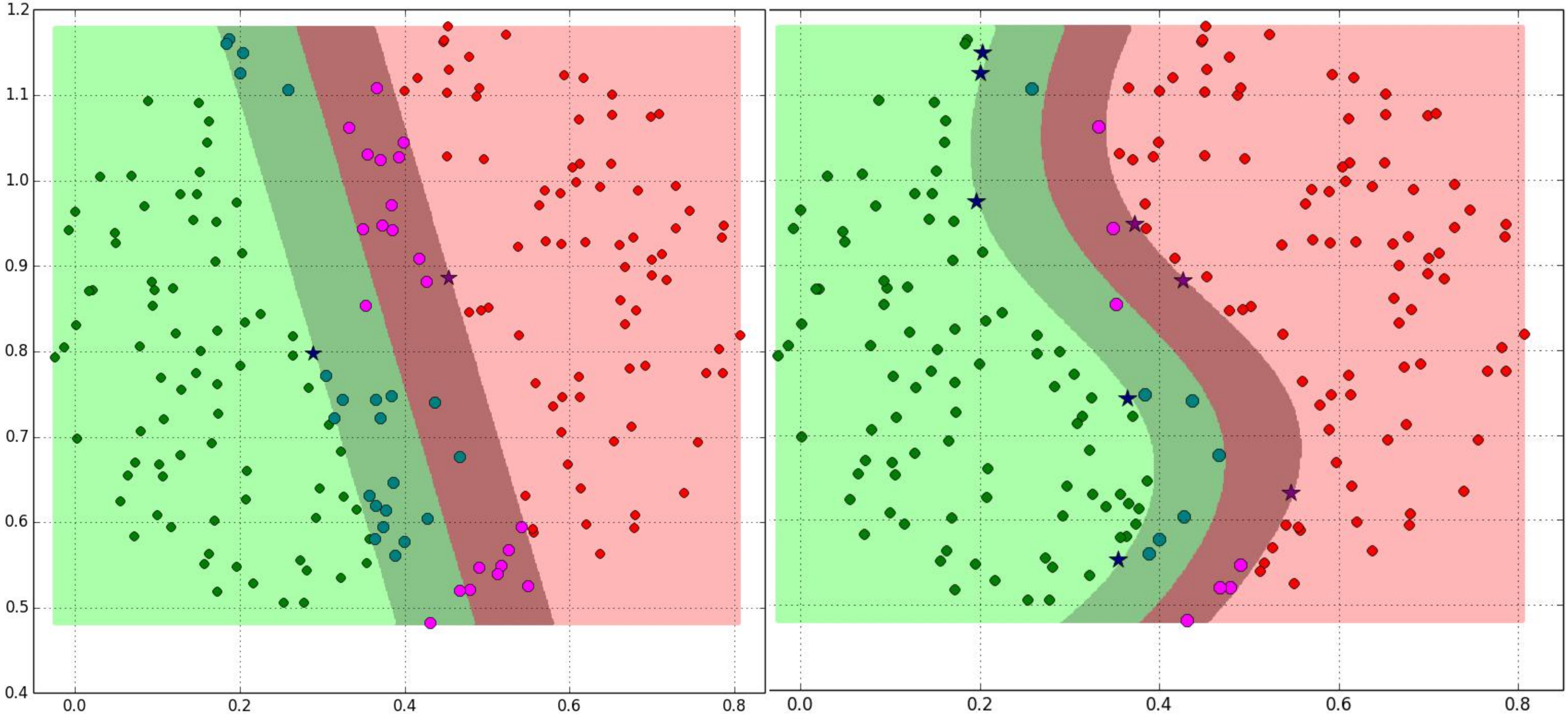
惩罚因子的影响



高斯核函数的影响

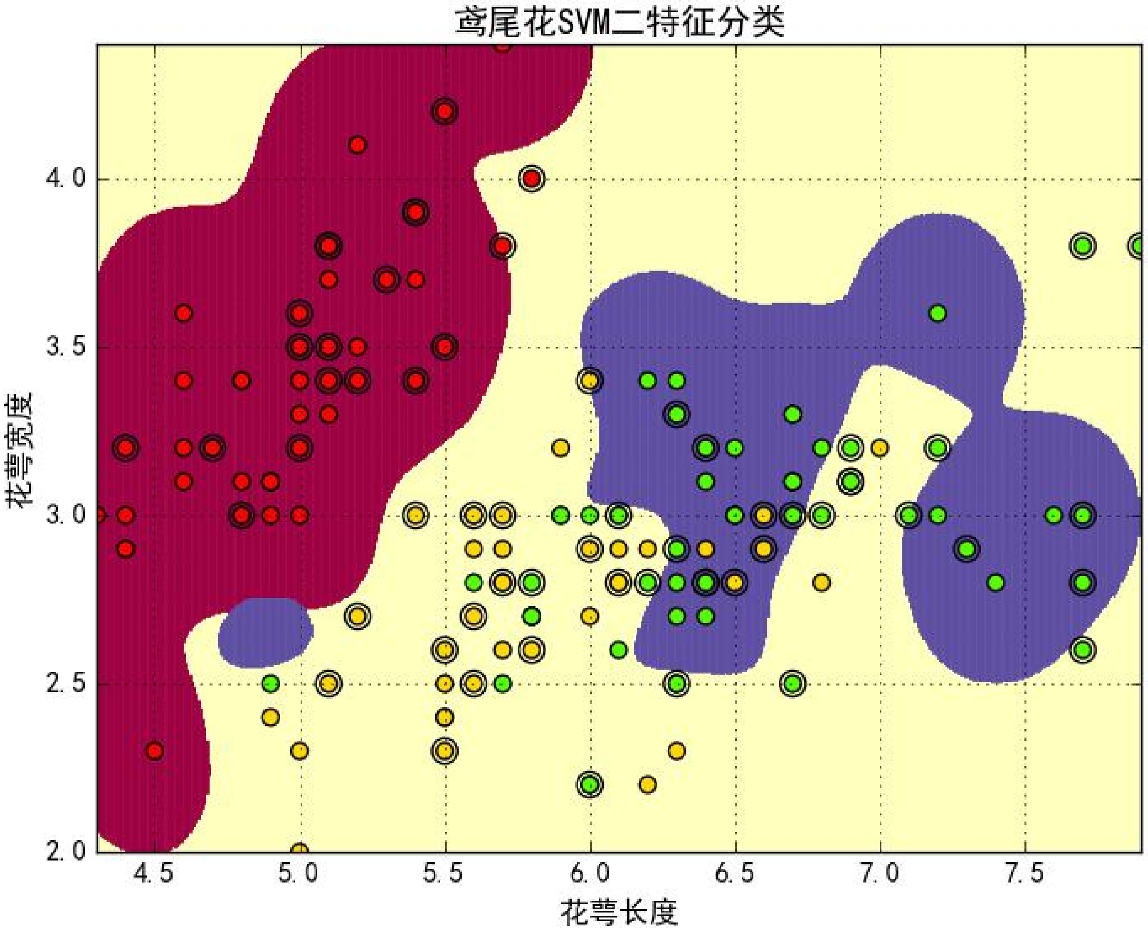


1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0 0.2 0.4 0.6 0.8 1.0

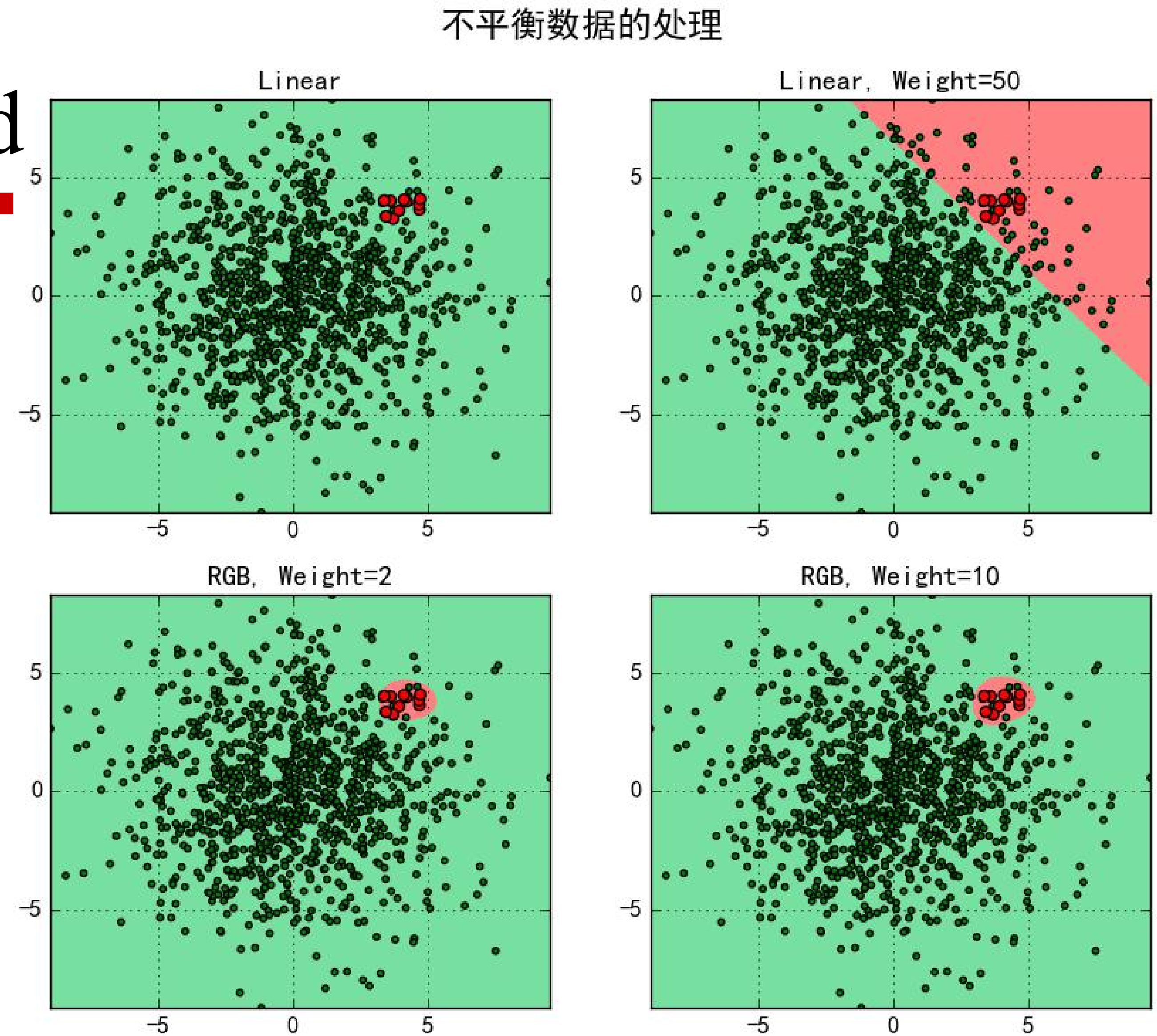


1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.0 0.2 0.4 0.6 0.8
0.0 0.2 0.4 0.6 0.8

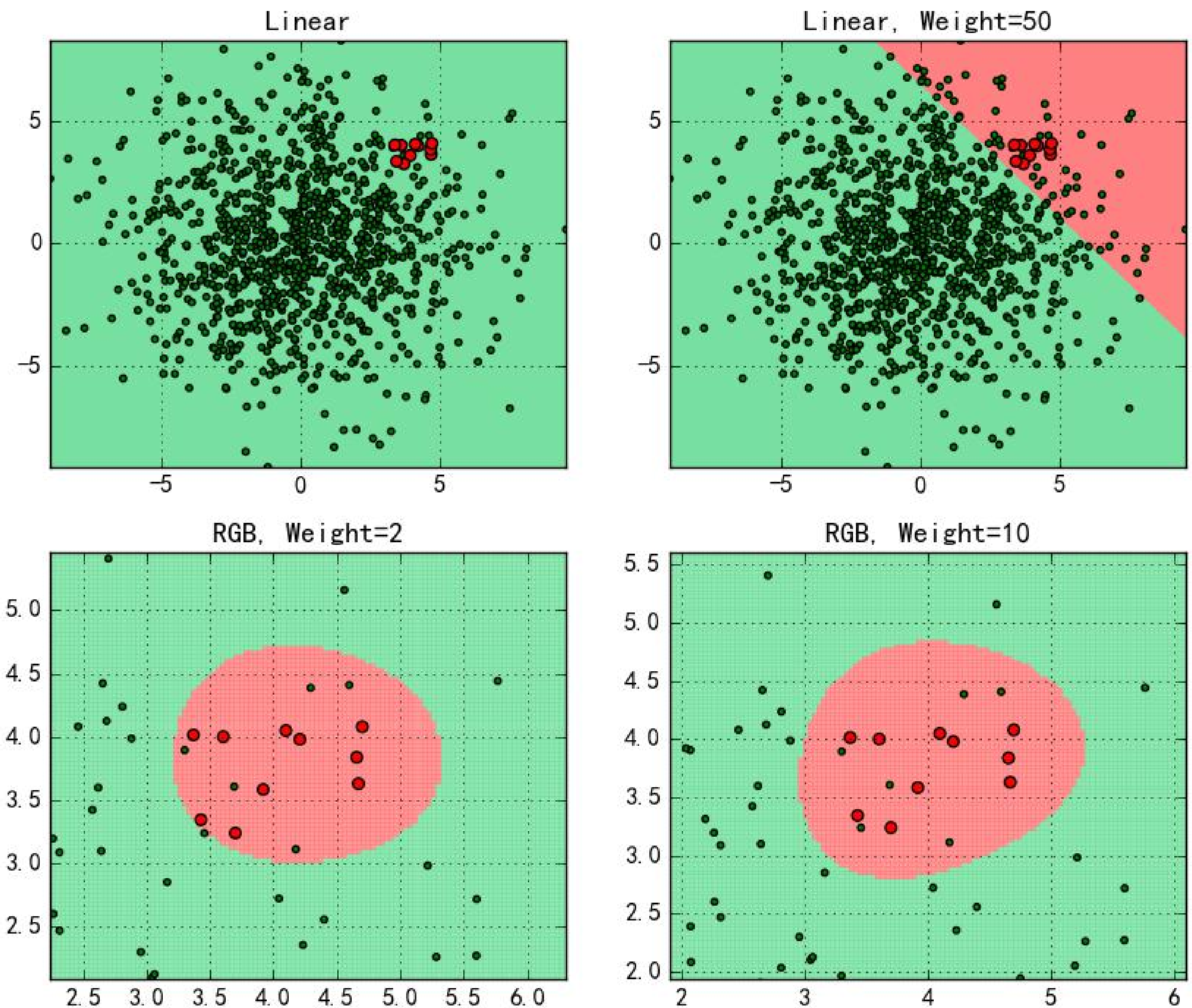
SVM分类



Unbalanced



放大

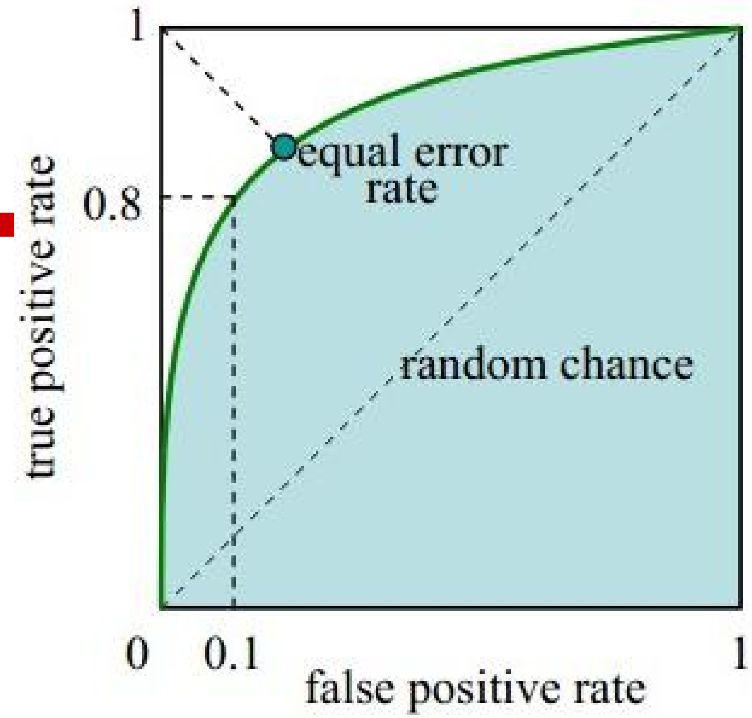


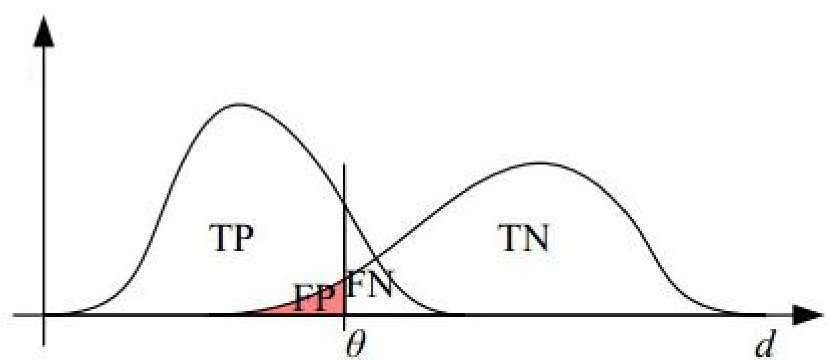
AUC

实际值 \ 预测值	Positive	Negtive
正	TP	FN
负	FP	TN

$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{FP + TN}$$





Receiver Operating Characteristic

Area Under Curve

分类器指标

$$accuracy = \frac{TP + TN}{TP + TN + FN + FP}$$

$$precision = \frac{TP}{TP + FP}$$

$$recall = \frac{TP}{TP + FN}$$

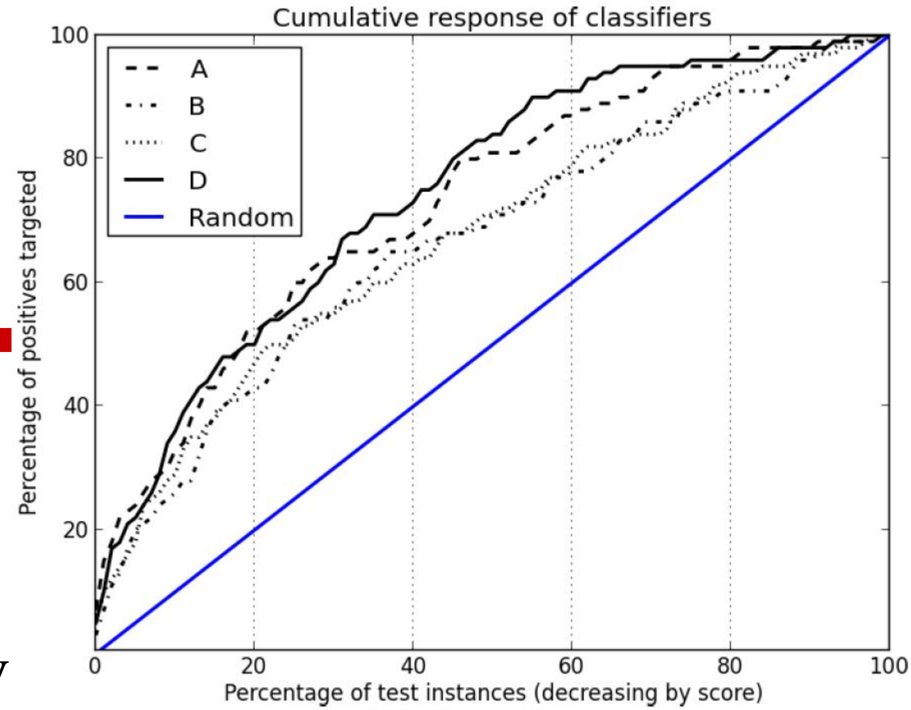
$$F_1 = \frac{2 \cdot precision \cdot recall}{precision + recall}$$

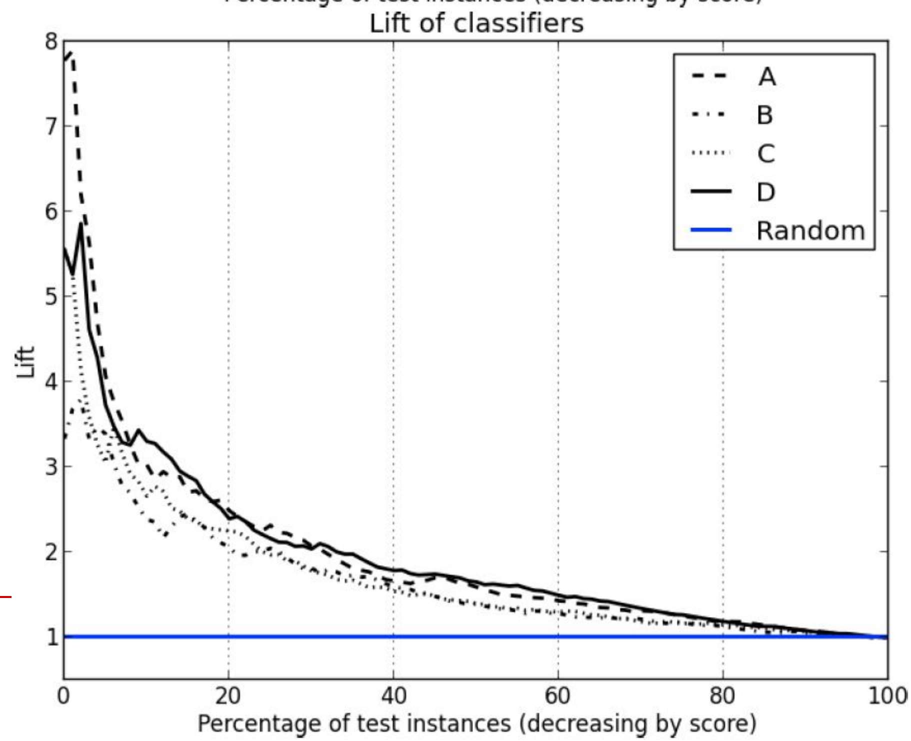
$$F_\beta = \frac{(1+\beta^2) \cdot precision \cdot recall}{\beta^2 \cdot precision + recall}$$

实际值 \ 预测值	Positive	Negtive
正	TP	FN
负	FP	TN

Lift Curve

- The cumulative response curve is sometimes called a lift curve, because one can see the increase over simply targeting randomly as how much the line representing the model performance is lifted up over the random performance diagonal.





计算

$$accuracy = \frac{TP + TN}{TP + TN + FN + FP}$$

$$precision = \frac{TP}{TP + FP}$$

$$recall = \frac{TP}{TP + FN}$$

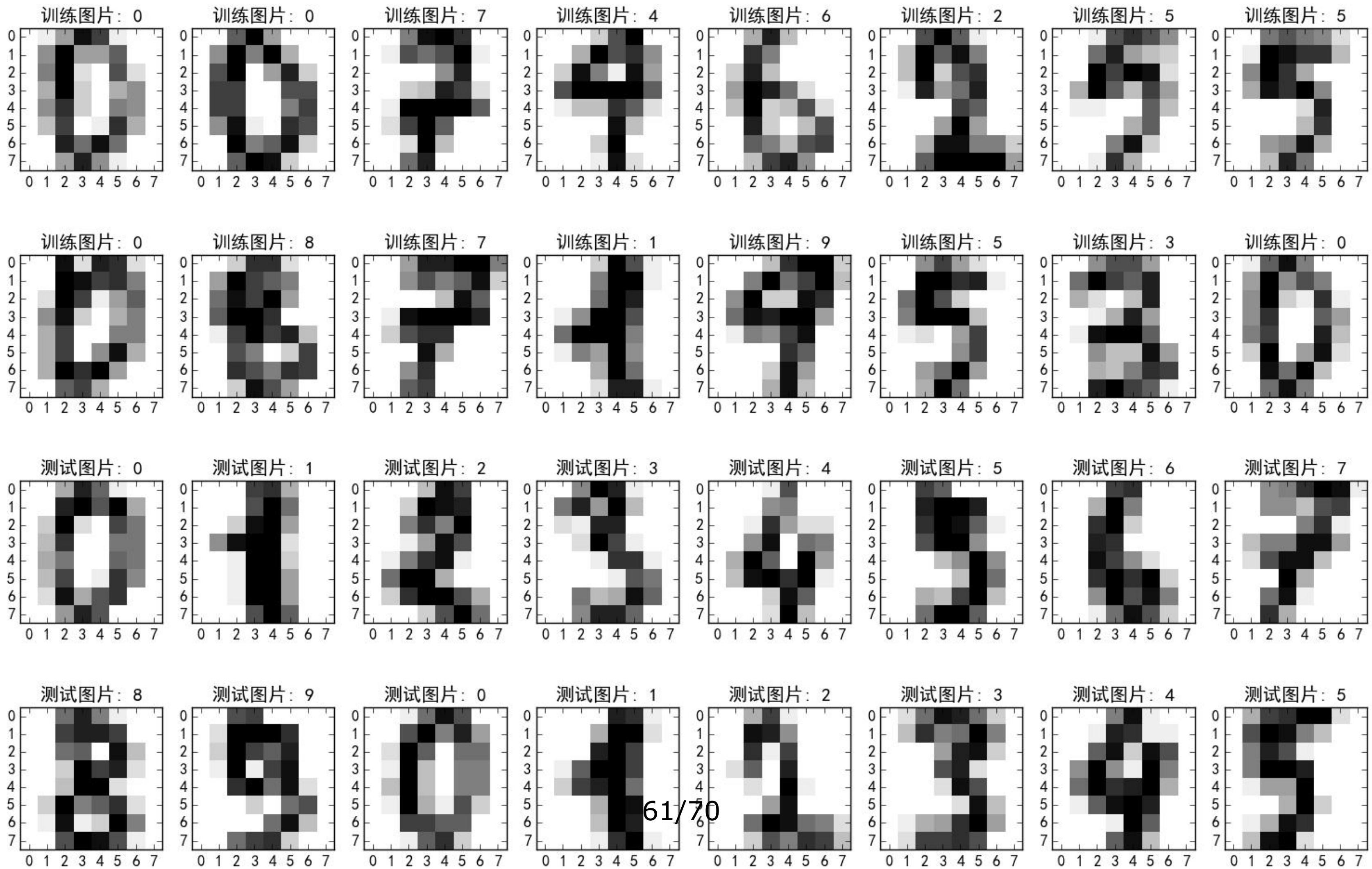
$$F_1 = \frac{2 \cdot precision \cdot recall}{precision + recall}$$

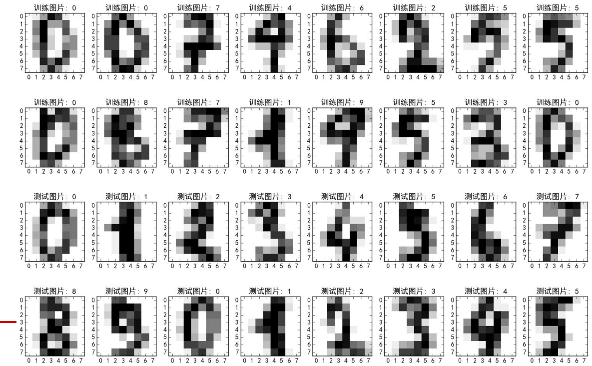
$$F_\beta = \frac{\left(1 + \beta^2\right) \cdot precision \cdot recall}{\beta^2 \cdot precision + recall}$$

```
y_true = np.array([1, 1, 1, 1, 0, 0])
y_hat  = np.array([1, 0, 1, 1, 1, 1])
```

```
ClassifierIndex
Accuracy:    0.5
Precision:   0.6
Recall:      0.75
f1 score:    0.666666666667
F-beta:
    beta=     0.001   F-beta=0.60000
    beta=     0.010   F-beta=0.60001
    beta=     0.100   F-beta=0.60119
    beta=     1.000   F-beta=0.66667
    beta=    10.000   F-beta=0.74815
    beta=   100.000   F-beta=0.74998
    beta=  1000.000   F-beta=0.75000
```

SVM用于手写图片识别

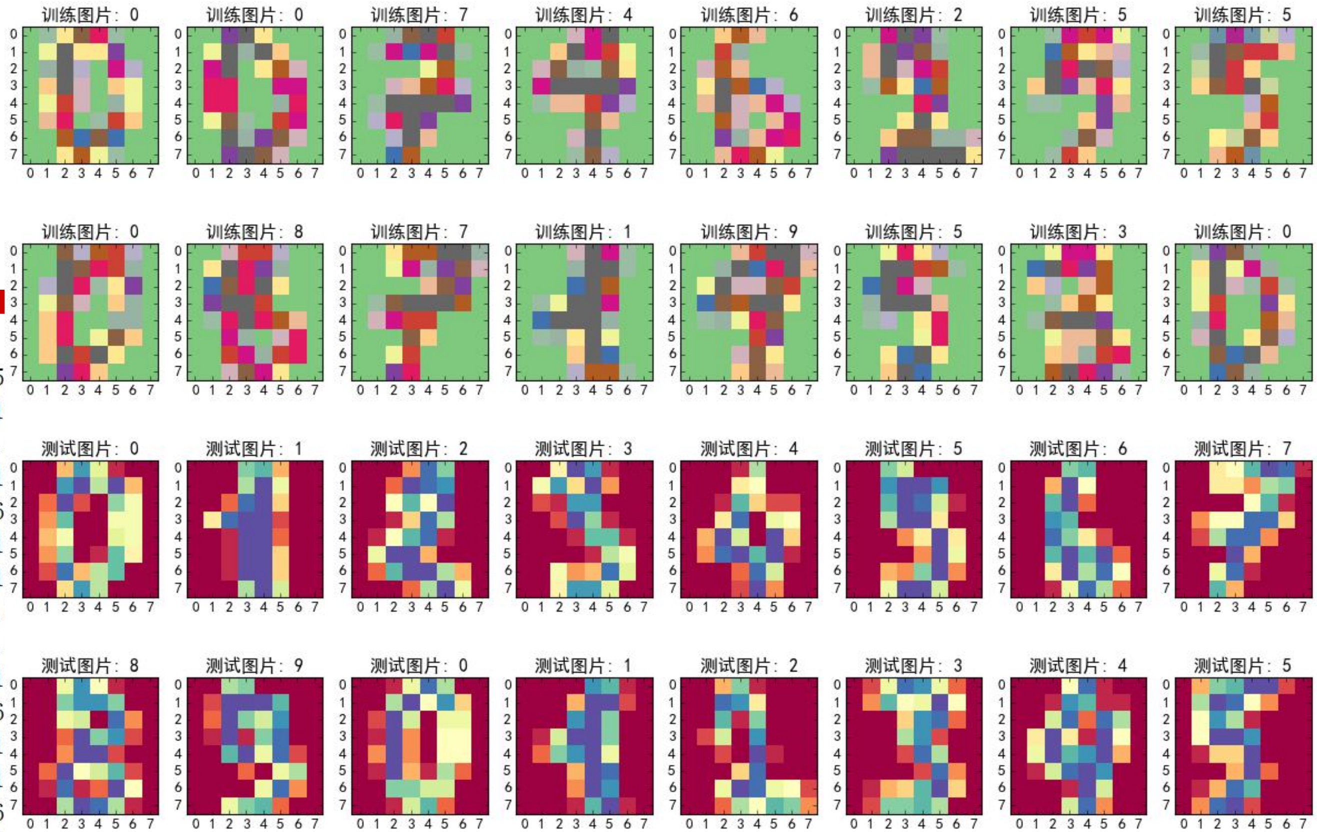




数据描述

- 该数据来自于43人的手写数字，其中30人用于训练，13人用于测试，训练集共3823个图片，测试集共1797个图片，每个图片为8×8的灰度图像，像素值从0到16，其中，16代表全黑，0代表全亮(与通常的像素亮度习惯正好相反)
- 该数据的下载地址为：
  - http://archive.ics.uci.edu/ml/datasets/Optical+Recognition+of+Handwritten+Digits

数据存取



0, 0, 5, 13, 9, 1, 0, 0, 0, 0, 13, 15, 10, 15, 5, 0, 0, 3, 15
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0, 0, 0, 4, 15, 12, 0, 0, 0, 0, 3, 16, 15, 14, 0, 0, 0, 0, 8,
0, 0, 7, 15, 13, 1, 0, 0, 0, 8, 13, 6, 15, 4, 0, 0, 0, 2, 1, 1
0, 0, 0, 1, 11, 0, 0, 0, 0, 0, 0, 7, 8, 0, 0, 0, 0, 0, 1, 13, 6
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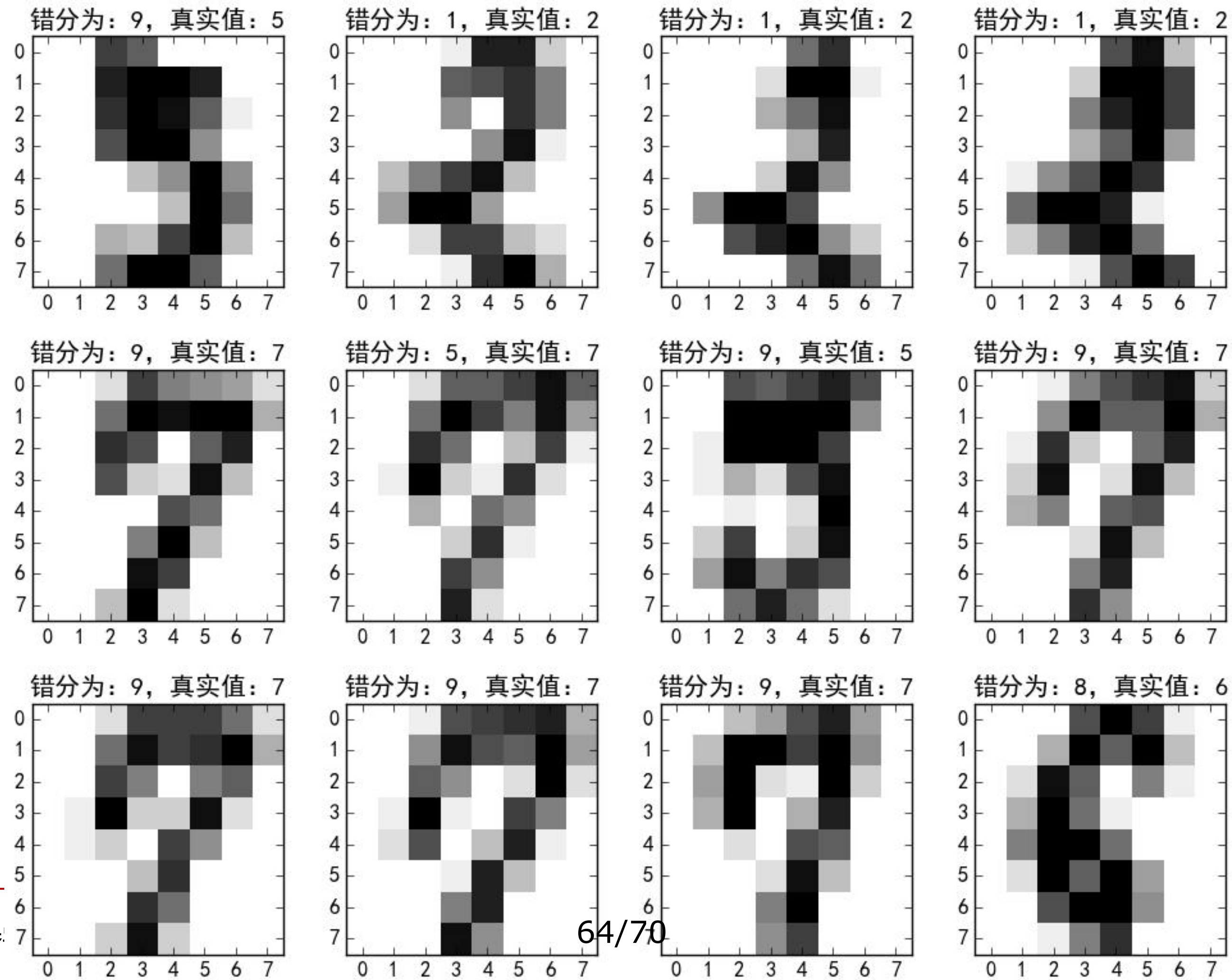
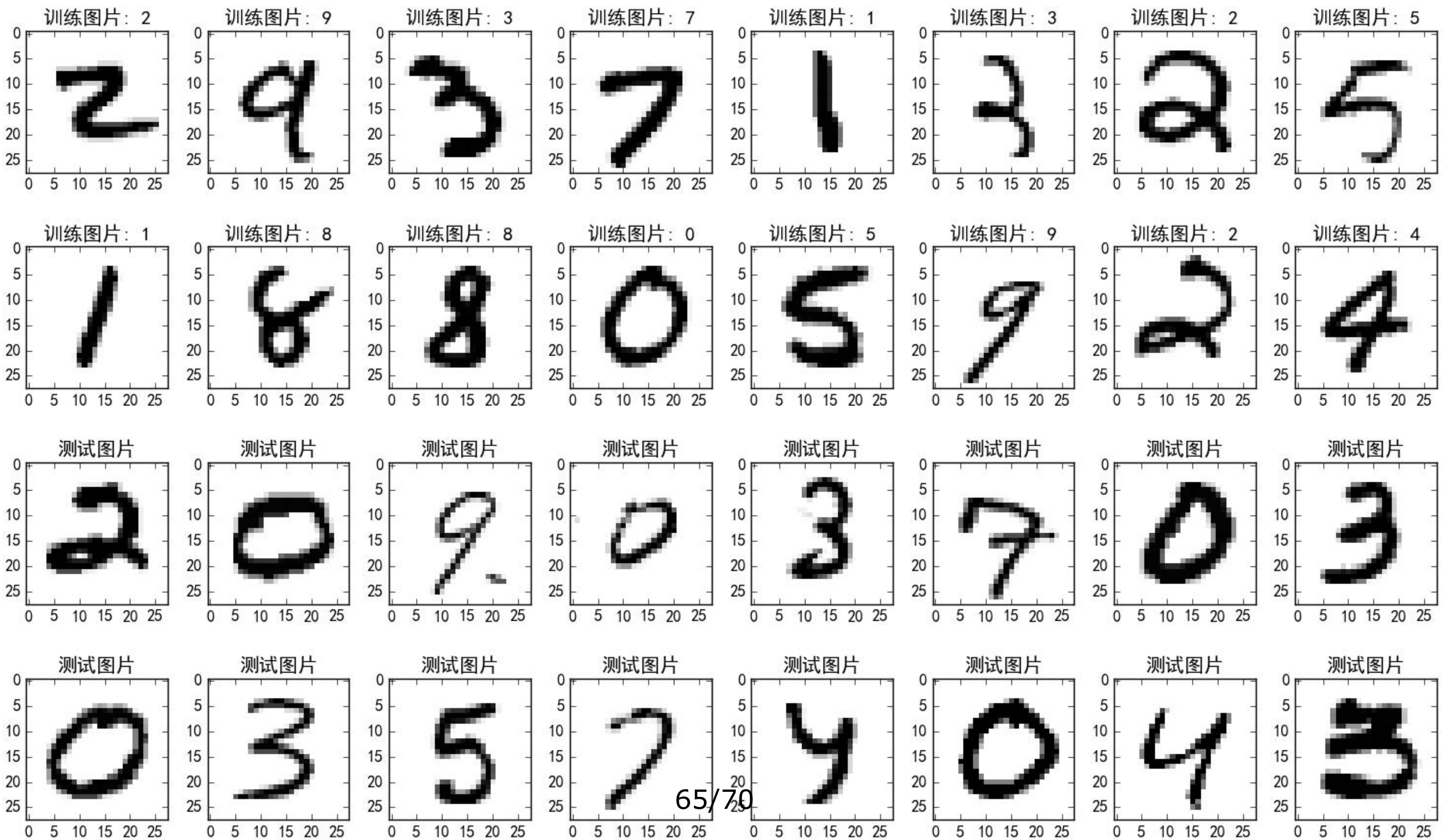
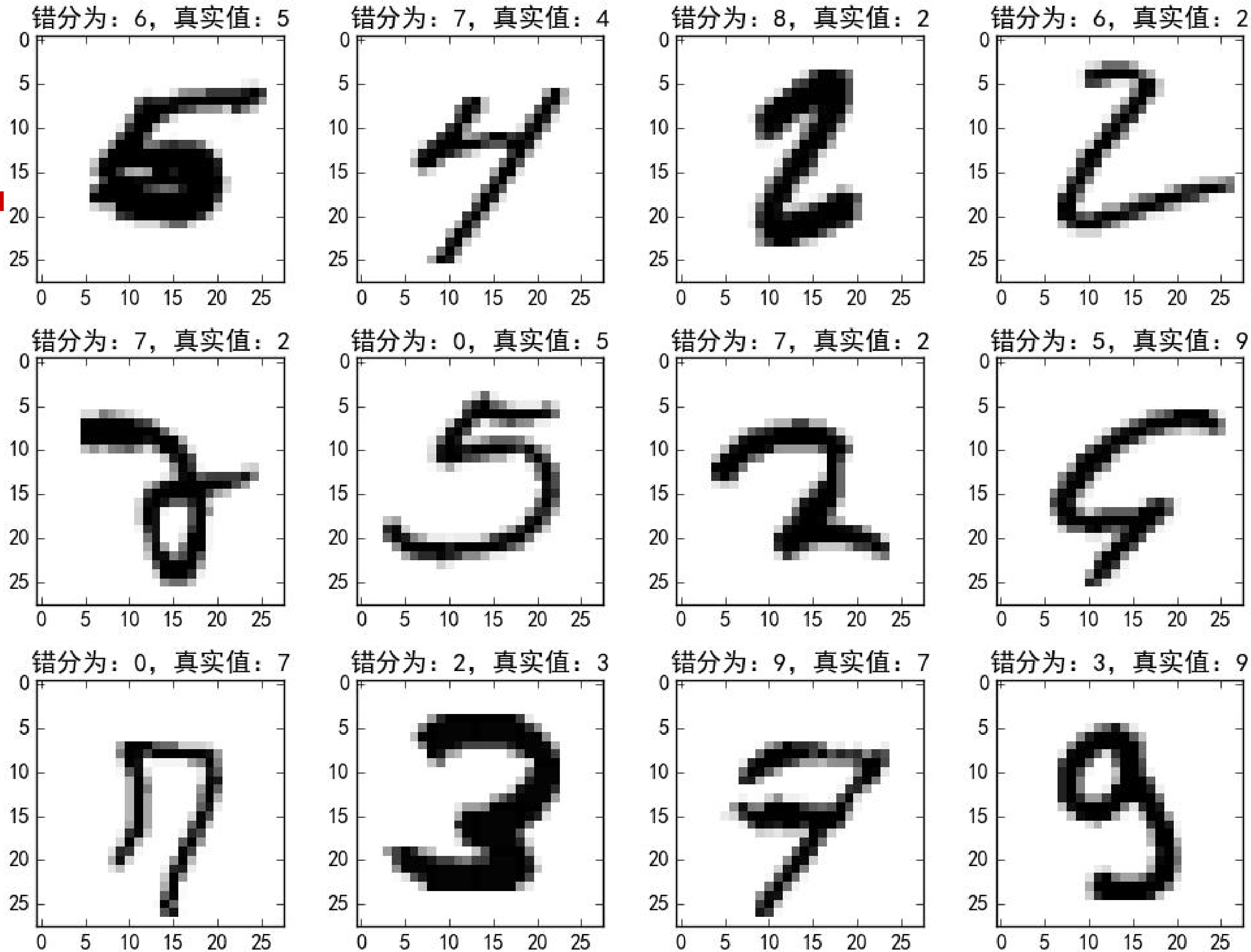
训练测试正确率：99.82% - 98.27%



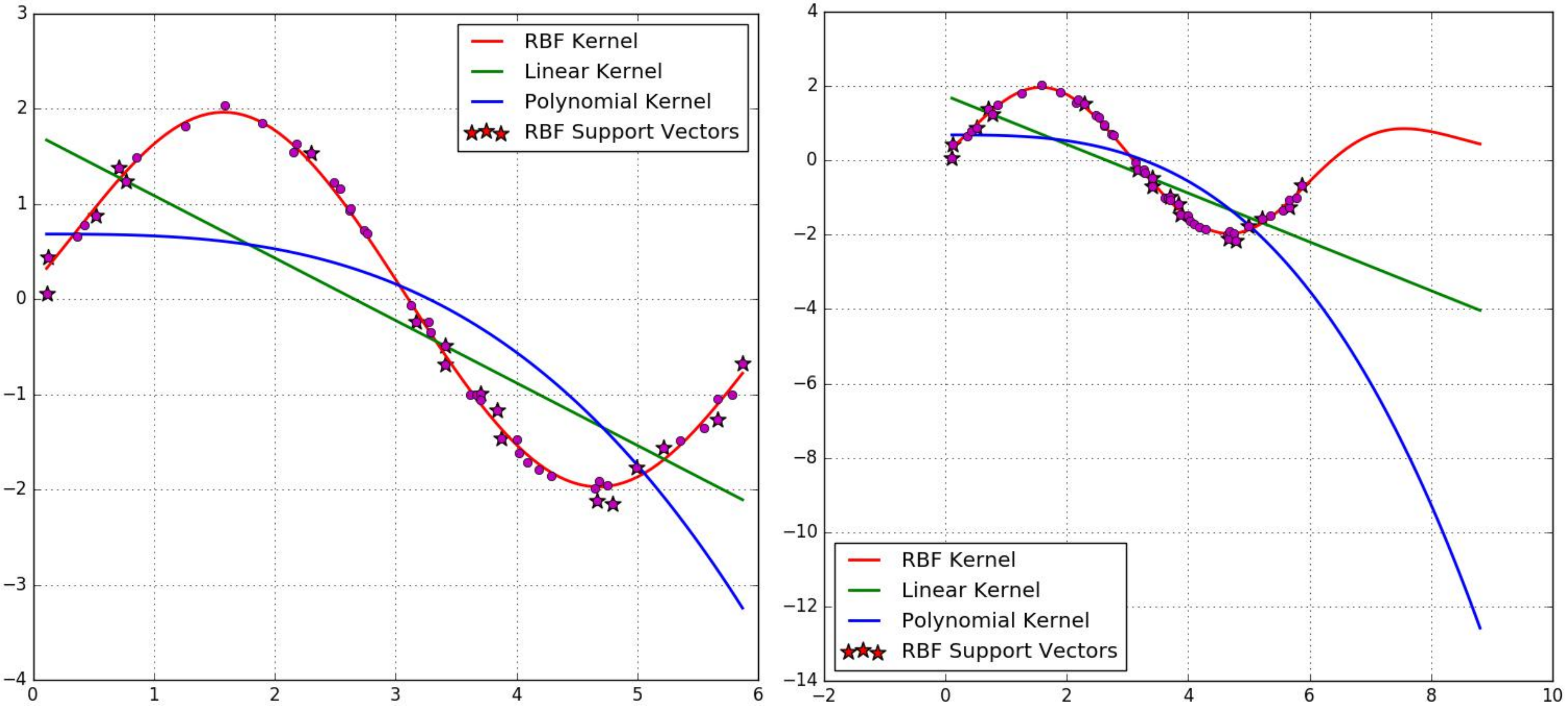
MNIST数字图片识别



数字图片手写体识别：分类器RF



SVR – 预测


RBF Kernel
Linear Kernel
Polynomial Kernel
RBF Support Vectors
RBF Kernel
Linear Kernel
Polynomial Kernel
RBF Support Vectors

总结与思考

- SVM可以用来划分多类别吗？
  - 直接多分类
  - 1 vs rest / 1 vs 1
- SVM和Logistic回归的比较
  - 经典的SVM，直接输出类别，不给出后验概率；
  - Logistic回归，会给出属于哪个类别的后验概率。
  - 重点：二者目标函数的异同
- SVM框架下引入Logistic函数：输出条件后验概率
- SVM用于回归问题：SVR；
- 体会SVM的目标函数的建立过程
  - 原始目标函数和Lagrange函数有什么联系？

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感谢大家！

恳请大家批评指正！