支持向量机与核算法

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Content

1. 线性分类
2. 支持向量机
3. 总结

分类：日常生活中的例子

- 信用卡申请Credit card application
- 垃圾邮件过滤
- 网络入侵检测
- …

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- 信用卡申请Credit card application
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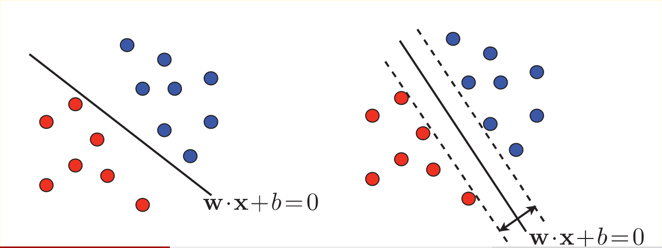
示例



基本符号

- $\mathcal{X} \subseteq \mathbb{R}^d$: 输入空间
- $\mathcal{Y} = \{-1, +1\}$: 输出空间
- $f : \mathcal{X} \mapsto \mathcal{Y}$: 未知的目标函数

- $\mathcal{S} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$，其中$y_i = f(\mathbf{x}_i)$，$\{\mathbf{x}_i\}_{i=1}^n$从输入空间$\mathcal{X}$中依据某个分布$\mathcal{D}$采集得到：训练集合
- $\mathcal{H} = \{\mathbf{x} \mapsto \mathrm{sgn}(\boldsymbol{\omega}^\top \mathbf{x} + b) : \boldsymbol{\omega} \in \mathbb{R}^d, b \in \mathbb{R}\}$: 假说集合
- $R_{\mathcal{S}}(h) = \frac{1}{n} \sum_{i=1}^n [h(\mathbf{x}_i) \neq f(\mathbf{x}_i)]$ with $h \in \mathcal{H}$: 经验误差
- $R_{\mathcal{D}}(h) = \Pr_{\mathbf{x} \sim \mathcal{D}} [h(\mathbf{x}) \neq f(\mathbf{x})]$ with $h \in \mathcal{H}$: 泛化误差

二分类问题形式化定义

给定训练样本集合 $\mathcal{S} = \{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)\}$，其中$\{\mathbf{x}_i\}_{i=1}^n \subseteq \mathcal{X}^n$ 独立同分布，$y_i = f(\mathbf{x}_i) \in \mathcal{Y} \, (\forall i = 1, \cdots, n)$。二分类问题的目标是基于数据 $\mathcal{S}$，从假说集合 $\mathcal{H}$ 中选择一个假说 h，以使得期望误差

$$\mathrm{E}_{\mathbf{x}\sim\mathcal{D}} \left[h(\mathbf{x}) \neq f(\mathbf{x}) \right] \tag{1}$$

最小。

二分类问题形式化定义

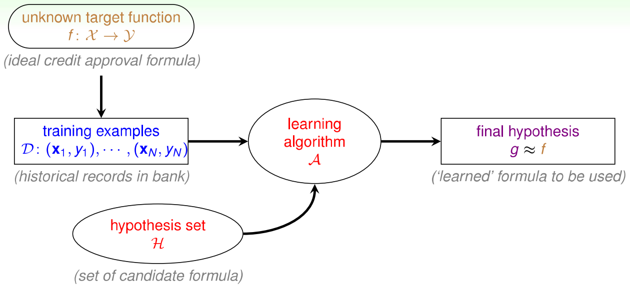
给定训练样本集合 $\mathcal{S} = \{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)\}$，其中$\{\mathbf{x}_i\}_{i=1}^n \subseteq \mathcal{X}^n$ 独立同分布，$y_i = f(\mathbf{x}_i) \in \mathcal{Y}\ (\forall i = 1, \cdots, n)$。二分类问题的目标是基于数据 $\mathcal{S}$，从假说集合 $\mathcal{H}$ 中选择一个假说 h，以使得期望误差

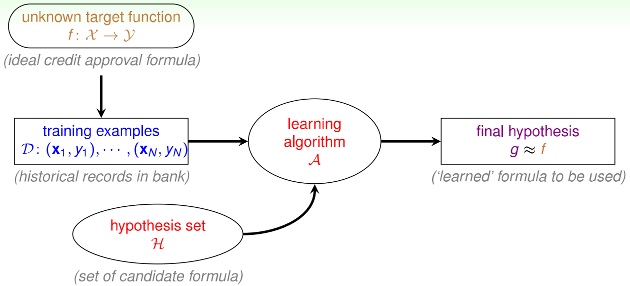
$$\mathrm{E}_{\mathbf{x}\sim\mathcal{D}}\left[h(\mathbf{x}) \neq f(\mathbf{x})\right] \tag{1}$$

最小。

$$\begin{aligned}\mathrm{E}_{\mathbf{x}\sim\mathcal{D}}\left[h(\mathbf{x}) \neq f(\mathbf{x})\right] &= 1 \cdot \Pr_{\mathbf{x}\sim\mathcal{D}}(h(\mathbf{x}) \neq f(\mathbf{x})) + 0 \cdot \Pr_{\mathbf{x}\sim\mathcal{D}}(h(\mathbf{x}) = f(\mathbf{x})) \\ &= \Pr_{\mathbf{x}\sim\mathcal{D}}(h(\mathbf{x}) \neq f(\mathbf{x}))\end{aligned} \tag{2}$$

学习一个分类器

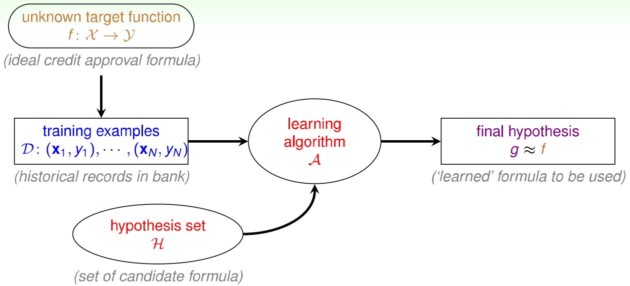

unknown target function
$f\colon \mathcal{X} \to \mathcal{Y}$
(ideal credit approval formula)
training examples
$\mathcal{D}\colon (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$
(historical records in bank)
learning
algorithm
$\mathcal{A}$
final hypothesis
$g \approx f$
('learned' formula to be used)
hypothesis set
$\mathcal{H}$
(set of candidate formula)



假说集(线性)

$$\mathcal{H} = \{\mathbf{x} \mapsto \operatorname{sgn}(\boldsymbol{\omega}^\top \mathbf{x} + b) : \boldsymbol{\omega} \in \mathbb{R}^d, b \in \mathbb{R}\}.$$

学习一个分类器



假说集(线性)

$$\mathcal{H} = \{\mathbf{x} \mapsto \operatorname{sgn}(\boldsymbol{\omega}^\top \mathbf{x} + b) : \boldsymbol{\omega} \in \mathbb{R}^d, b \in \mathbb{R}\}.$$

学习算法

$\mathcal{A}$: 支持向量机（Support Vector Machines，SVMs）

假说集

$\mathcal{H} = \{\mathbf{x} \mapsto \text{sgn}[\boldsymbol{\omega}^\top \mathbf{x} + b] : \boldsymbol{\omega} \in \mathbb{R}^d, b \in \mathbb{R}\}.$

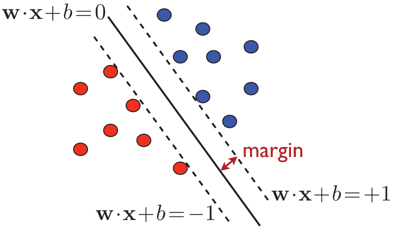
- 假说集 $h \in \mathcal{H} : \mathbf{x} \in \mathcal{X} \mapsto \{-1, +1\}.$
- 决策函数 $h' : \mathbf{x} \in \mathcal{X} \mapsto \boldsymbol{\omega}^\top \mathbf{x} + b \in \mathbf{R}.$
- $h(x) = \text{sgn}\,[h'(x)]$。因为假说$h$由$h'$确定，$h'$是我们研究关注的重点，因此我们通常直接称它为分类器。
- 线性分类器: h'是线性的.

Content

1 线性分类

2 支持向量机
- 线性可分
- Non-Separable Case
- 实现
- 选择正则化参数C

3 总结



(a) 支持向量机

- 考虑超平面$\boldsymbol{\omega}^\top \mathbf{x} + b = 0$
- 给定$a > 0$，我们要求该超平面
  - 对于正类样本(即$y_i = 1$)
    $$\boldsymbol{\omega}^\top \mathbf{x}_i + b \geq a$$
  - 对于负类样本(即$y_i = -1$)
    $$\boldsymbol{\omega}^\top \mathbf{x}_i + b \leq -a$$
  - 即$\boxed{y_i \left(\boldsymbol{\omega}^\top \mathbf{x}_i + b\right) \geq a \, \forall i}$

样本$\mathbf{x}_i$到超平面$\boldsymbol{\omega}^\top \mathbf{x} + b = 0$的距离：$\frac{|\boldsymbol{\omega}^\top \mathbf{x}_i + b|}{\|\boldsymbol{\omega}\|} = \frac{y_i\left(\boldsymbol{\omega}^\top \mathbf{x}_i + b\right)}{\|\boldsymbol{\omega}\|}$

样本集$\mathcal{S}$到超平面$\boldsymbol{\omega}^\top \mathbf{x} + b = 0$的距离$\rho$被定义为：

$$\rho = \min_{(\mathbf{x}_i, y_i) \in \mathcal{S}} \frac{y_i \left(\boldsymbol{\omega}^\top \mathbf{x}_i + b\right)}{\|\boldsymbol{\omega}\|} = \frac{a}{\|\boldsymbol{\omega}\|} \tag{3}$$

优化目标

$$\max_{\boldsymbol{\omega},b} \quad \frac{a}{\|\boldsymbol{\omega}\|} \quad s.t. \quad y_i\left(\boldsymbol{\omega}^\top \mathbf{x}_i + b\right) \geq a, \ \forall i \tag{4}$$

优化目标

$$\max_{\omega,b} \quad \frac{a}{\|\omega\|} \quad s.t. \;\; y_i\left(\omega^\top \mathbf{x}_i + b\right) \geq a, \; \forall i \tag{4}$$

定义$\hat{\omega} = \frac{\omega}{a}$和$\hat{b} = \frac{b}{a}$，EQ.(4)可以等价地写成

优化目标–等价形式

$$\max_{\hat{\omega},\hat{b}} \quad \frac{1}{\|\hat{\omega}\|} \quad s.t. \quad y_i\left(\hat{\omega}^\top \mathbf{x}_i + \hat{b}\right) \geq 1, \; \forall i \tag{5}$$

这种变换($(\omega, b) \Rightarrow (\hat{\omega}, \hat{b})$)会不会影响分类器的预测性能？

优化目标

$$\max_{\boldsymbol{\omega},b} \quad \frac{a}{\|\boldsymbol{\omega}\|} \quad s.t. \;\; y_i\left(\boldsymbol{\omega}^\top \mathbf{x}_i + b\right) \geq a, \; \forall i \tag{4}$$

定义$\hat{\boldsymbol{\omega}} = \frac{\boldsymbol{\omega}}{a}$和$\hat{b} = \frac{b}{a}$，EQ.(4)可以等价地写成

优化目标–等价形式

$$\max_{\hat{\boldsymbol{\omega}},\hat{b}} \quad \frac{1}{\|\hat{\boldsymbol{\omega}}\|} \quad s.t. \quad y_i\left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b}\right) \geq 1, \; \forall i \tag{5}$$

这种变换$((\boldsymbol{\omega}, b) \Rightarrow (\hat{\boldsymbol{\omega}}, \hat{b}))$会不会影响分类器的预测性能？

$h(\mathbf{x}) = \mathrm{sgn}(\boldsymbol{\omega}^\top \mathbf{x} + b) = \mathrm{sgn}\left(a\hat{\boldsymbol{\omega}}^\top \mathbf{x} + a\hat{b}\right) = \mathrm{sgn}\left(\hat{\boldsymbol{\omega}}^\top \mathbf{x} + \hat{b}\right) \triangleq \hat{h}(\mathbf{x}) \; (a > 0)$

优化目标—概念上等价

$$\begin{aligned}\min_{\hat{\omega},\hat{b}} \quad & \frac{1}{2}\|\hat{\omega}\|^2 \\ s.t. \quad & y_i\left(\hat{\omega}^\top \mathbf{x}_i + \hat{b}\right) \geq 1, \ \forall i\end{aligned} \tag{6}$$

- 优化目标是严格正定的（Hessian矩阵）
- 所有的约束都是线性的
- EQ.(6)中的优化问题是具有线性约束的二次规划—典型的凸优化问题。
- 最优解存在且唯一

Lagrange函数

$$\mathcal{L}(\hat{\boldsymbol{\omega}}, \hat{b}; \boldsymbol{\alpha}) = \frac{1}{2}\|\hat{\boldsymbol{\omega}}\|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b} \right) - 1 \right) \tag{7}$$

其中$\boldsymbol{\alpha} = [\alpha_1, \cdots, \alpha_n]^\top$, $\alpha_i \geq 0\,(\forall i)$ 为Lagrange乘子。

KKT条件

$$\begin{cases} \nabla_{\hat{\boldsymbol{\omega}}}\mathcal{L} = \hat{\boldsymbol{\omega}} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 & \Longrightarrow \hat{\boldsymbol{\omega}} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \\ \nabla_{\hat{b}}\mathcal{L} = -\sum_{i=1}^{n} \alpha_i y_i = 0 & \Longrightarrow \sum_{i=1}^{n} \alpha_i y_i = 0 \\ \forall i \;\; \alpha_i \left(y_i \left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b} \right) - 1 \right) = 0 & \Longrightarrow \alpha_i \vee y_i \left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b} \right) = 1 \end{cases} \tag{8}$$

对偶问题

$$
\begin{aligned}
&\min_{\boldsymbol{\alpha}} \ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j\left(\mathbf{x}_i^\top\mathbf{x}_j\right) - \sum_{i=1}^{n}\alpha_i \\
&s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0,\ \alpha_i \geq 0,\ \forall i.
\end{aligned}
\tag{9}
$$

上式是一个标准的带约束二次规划问题。

- 支持向量(Support Vectors): 对应$\alpha_i \geq 0\,(\forall i)$的样本
- 怎样计算$\hat{b}$?

对偶问题

$$\min_{\boldsymbol{\alpha}} \ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \left(\mathbf{x}_i^\top \mathbf{x}_j\right) - \sum_{i=1}^{n}\alpha_i$$
$$s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0, \ \alpha_i \geq 0, \ \forall i. \tag{9}$$

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- 支持向量(Support Vectors): 对应$\alpha_i \geq 0\ (\forall i)$的样本
- 怎样计算$\hat{b}$? $\hat{b} = y_i - \sum_{j=1}^{n}\alpha_j y_j \left(\mathbf{x}_j^\top \mathbf{x}_i\right)\ (\alpha_i > 0)$

对偶问题

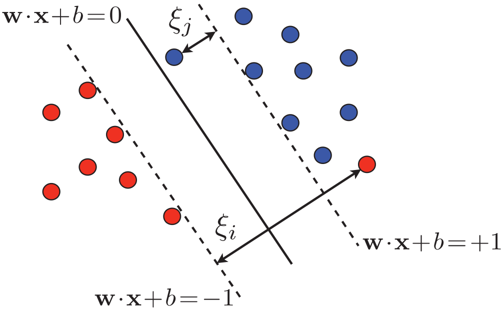
$$\min_{\boldsymbol{\alpha}} \ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \left(\mathbf{x}_i^\top \mathbf{x}_j\right) - \sum_{i=1}^{n}\alpha_i$$
$$s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0, \ \alpha_i \geq 0, \ \forall i. \tag{9}$$

上式是一个标准的带约束二次规划问题。

- 支持向量(Support Vectors): 对应$\alpha_i \geq 0 \ (\forall i)$的样本
- 怎样计算$\hat{b}$? $\hat{b} = y_i - \sum_{j=1}^{n}\alpha_j y_j \left(\mathbf{x}_j^\top \mathbf{x}_i\right) \ (\alpha_i > 0)$
- 预测函数：$\hat{h}(\mathbf{x}) = \operatorname{sgn}\left(\hat{\boldsymbol{\omega}}^\top \mathbf{x} + \hat{b}\right) = \operatorname{sgn}\left(\sum_{j=1}^{n}\alpha_j y_j \left(\mathbf{x}_j^\top \mathbf{x}\right) + \hat{b}\right)$
- 样本总是成对出现

- 在绝大多数应用中，训练数据并非线性可分，即对任意超平面 $\boldsymbol{\omega}^\top \mathbf{x} + b = 0$，存在$\mathbf{x}_i \in \mathcal{S}$，使得

$$y_i \left(\boldsymbol{\omega}^\top \mathbf{x}_i + b \right) \ngeq 1 \tag{10}$$



超平面$\boldsymbol{\omega}^\top \mathbf{x} + b = 0$: i)错误地分类$\mathbf{x}_i$; ii)正确地分类$\mathbf{x}_j$，但是间隔小于1

非线性可分—优化目标

考虑如下两个相互矛盾的因素

- 间距最大化
- 训练误差最小化

考虑如下两个相互矛盾的因素

- 间距最大化
- 训练误差最小化

优化目标—松弛变量

$$\min_{\hat{\omega},\hat{b},\boldsymbol{\xi}} \quad \frac{1}{2}\|\hat{\omega}\|^2 + C\sum_{i=1}^{n}\xi_i \quad s.t. \quad y_i\left(\hat{\omega}^\top \mathbf{x}_i + \hat{b}\right) \geq 1 - \xi_i,\ \xi_i \geq 0,\ \forall i \tag{11}$$

- 允许训练过程中有误差
- C为正则化参数—调节模型复杂度与训练误差

$$\begin{aligned}\mathcal{L}(\hat{\boldsymbol{\omega}}, \hat{b}, \boldsymbol{\xi}; \boldsymbol{\alpha}, \boldsymbol{\beta}) &= \frac{1}{2}\|\hat{\boldsymbol{\omega}}\|^2 + C\sum_{i=1}^{n}\xi_i \\ &\quad - \sum_{i=1}^{n}\alpha_i\left(y_i\left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b}\right) - 1 + \xi_i\right) - \sum_{i=1}^{n}\beta_i\xi_i\end{aligned} \tag{12}$$

其中$\boldsymbol{\alpha} = [\alpha_1, \cdots, \alpha_n]^\top$, $\boldsymbol{\beta} = [\beta_1, \cdots, \beta_n]^\top$ 为Lagrange乘子。

KKT条件

$$\begin{cases} \nabla_{\hat{\boldsymbol{\omega}}}\mathcal{L} = \hat{\boldsymbol{\omega}} - \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i = 0 & \Longrightarrow \hat{\boldsymbol{\omega}} = \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i \\ \nabla_{\hat{b}}\mathcal{L} = -\sum_{i=1}^{n}\alpha_i y_i = 0 & \Longrightarrow \sum_{i=1}^{n}\alpha_i y_i = 0 \\ \nabla_{\xi_i}\mathcal{L} = C - \alpha_i - \beta_i & \Longrightarrow \alpha_i + \beta_i = C \\ \forall i \;\; \alpha_i\left(y_i\left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b}\right) - 1 + \xi_i\right) = 0 & \Longrightarrow \alpha_i \vee y_i\left(\hat{\boldsymbol{\omega}}^\top \mathbf{x}_i + \hat{b}\right) = 1 - \xi_i \\ \forall i \;\; \beta_i\xi_i = 0 & \Longrightarrow \beta_i = 0 \vee \xi_i = 0 \end{cases} \tag{13}$$

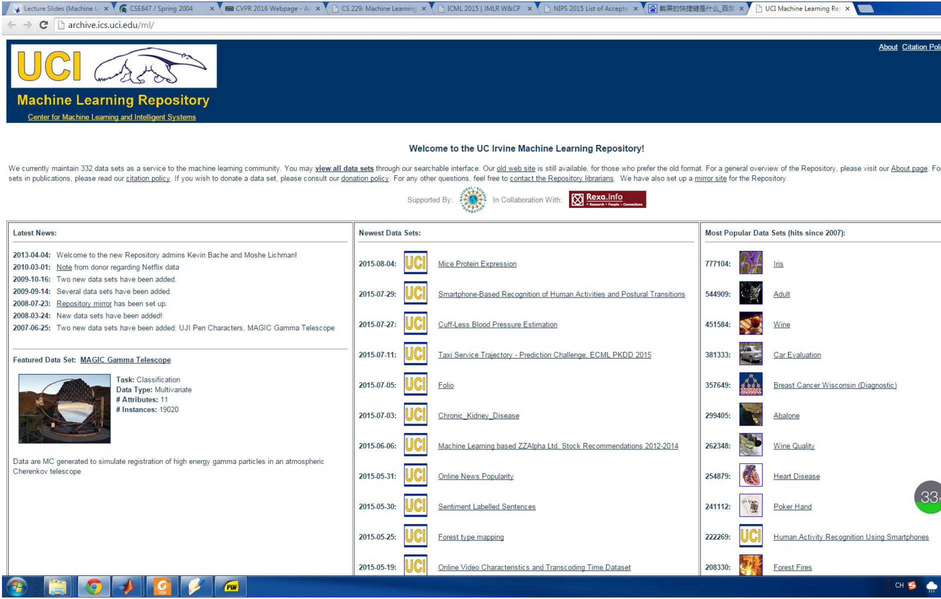
对偶问题

$$
\begin{aligned}
&\min_{\boldsymbol{\alpha}} \ \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \left(\mathbf{x}_i^\top \mathbf{x}_j\right) - \sum_{i=1}^{n}\alpha_i \\
&s.t. \ \sum_{i=1}^{n}\alpha_i y_i = 0, \ C \geq \alpha_i \geq 0, \ \forall i.
\end{aligned}
\tag{14}
$$

```
function [w,d,pos,obj]=mySVMclass(y,c,X)

if min(y) ~= -1
    error(' y must coded: 1 for class one and -1 for class two')
end
%-------------------------------------------------------------------
%      monqp(H,b,c) solves the quadratic programming problem:
%
%    min 0.5*x'Hx - d'x   subject to:  A'x = b  and  0 <= x <= c
%     x
%-------------------------------------------------------------------
K = X*X';
KY = sparse(y*y');
H = K.*KY;
e = ones(size(y));
A = y;
b = 0;
[alpha,lambda0, pos] = mymonqp(H,e,A,b,c);
alphaall=zeros(size(e));
alphaall(pos)=alpha;
obj=-0.5*alphaall'*H*alphaall +e'*alphaall;
ysup = y(pos);
w = (alpha.*ysup);
d = lambda0;
```

UCI数据集



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Latest News:
2013-04-04: Welcome to the new Repository admins Kevin Bache and Moshe Lichman!
2010-03-01: Note from donor regarding Netflix data
2009-10-16: Two new data sets have been added.
2009-09-14: Several data sets have been added.
2008-07-23: Repository mirror has been set up.
2008-03-24: New data sets have been added!
2007-06-25: Two new data sets have been added: UJI Pen Characters, MAGIC Gamma Telescope
Featured Data Set: MAGIC Gamma Telescope
Task: Classification
Data Type: Multivariate
Attributes: 11
Instances: 19020
Data are MC generated to simulate registration of high energy gamma particles in an atmospheric Cherenkov telescope
Newest Data Sets:
2015-08-04: Mice Protein Expression
2015-07-29: Smartphone-Based Recognition of Human Activities and Postural Transitions
2015-07-27: Cuff-Less Blood Pressure Estimation
2015-07-11: Taxi Service Trajectory - Prediction Challenge, ECML PKDD 2015
2015-07-05: Folio
2015-07-03: Chronic_Kidney_Disease
2015-06-06: Machine Learning based ZZAlpha Ltd. Stock Recommendations 2012-2014
2015-05-31: Online News Popularity
2015-05-30: Sentiment Labelled Sentences
2015-05-25: Forest type mapping
2015-05-19: Online Video Characteristics and Transcoding Time Dataset
Most Popular Data Sets (hits since 2007):
777104: Iris
544909: Adult
451584: Wine
381333: Car Evaluation
357649: Breast Cancer Wisconsin (Diagnostic)
299405: Abalone
262348: Wine Quality
254879: Heart Disease
241112: Poker Hand
222269: Human Activity Recognition Using Smartphones
208330: Forest Fires

留一法（Leave-One-Out，LOO）

- Training set $\mathcal{S} = \{(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)\}$
- Approach: Repeatedly leave one example out for testing.

Train	Test
$\{(\mathbf{x}_2, y_2), (\mathbf{x}_3, y_3), \cdots, (\mathbf{x}_n, y_n)\}$	$(\mathbf{x}_1, y_1)$
$\{(\mathbf{x}_1, y_1), (\mathbf{x}_3, y_3), \cdots, (\mathbf{x}_n, y_n)\}$	$(\mathbf{x}_2, y_2)$
$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_n, y_n)\}$	$(\mathbf{x}_3, y_3)$
$\ldots$	$\ldots$
$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_{n-1}, y_{n-1})\}$	$(\mathbf{x}_n, y_n)$

- Performance Evaluation: $\mathrm{Err}_{loo}(\mathcal{A}, C) = \frac{1}{n}\sum_{i=1}^{n}\left[h_{\mathcal{S}-\{\mathbf{x}_i\}}(\mathbf{x}_i) \neq y_i\right]$

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3. 总结

总结

- 支持向量机推导
- 优化算法
- Matlab实现
- 参数选择

总结

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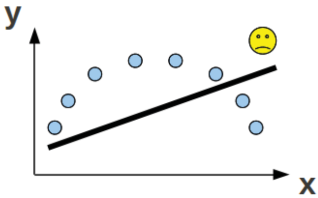
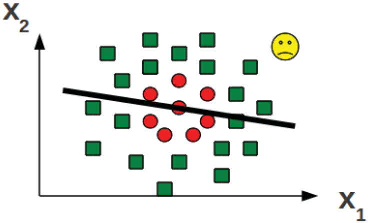
Homework 2：实现线性支持向量机算法

支持向量机(线性)优缺点

1. 优点：
   - 算法简单、直观、可理解性强
2. 缺点：表达能力有限，无法捕获数据间的非线性模式。
   - 输入—输出不再是线性关系;
   - 类与类之间不能通过线性边界来划分。





3. Next: Kernel Methods