## Support Vector Machines支持向量机

## Supervised learning

Supervised learning

- An agent or machine is given $N$ sensory inputs $D=\left\{x_{1}, x_{2} \ldots, x_{N}\right\}$, as well as the desired outputs $y_{1}, y_{2}, \ldots y_{N}$, its goal is to learn to produce the correct output given a new input.
- Given $D$ what can we say about $\mathrm{x}_{\mathrm{N}+1}$ ?

Classification: $\mathrm{y}_{1}, \mathrm{y}_{2}, \ldots \mathrm{y}_{\mathrm{N}}$ are discrete class labels, learn a labeling function $f(\mathbf{x}) \mapsto y$

- Naïve bayes
- Decision tree
- K nearest neighbor
- Least squares classification


## Classification

## Classification

= learning from labeled data. Dominant problem in Machine Learning


## Linear Classifiers

Binary classification can be viewed as the task of separating classes in feature space（特征空间）：


## Linear Classification

Which of the linear separators is optimal?


## Classification Margin (间距)

- Geometry of linear classification
- Discriminant function

$$
\hat{y}(\mathbf{x})=\mathbf{w}^{\top} \mathbf{x}+b
$$

- Important: the distance does not change if we scale

$$
\mathbf{w} \rightarrow a \mathbf{w}, b \rightarrow a \cdot b
$$



## Classification Margin（间距）

Distance from example $\mathbf{x}_{i}$ to the separator is $r=\frac{\left|\mathbf{w}^{T} \mathbf{x}_{i}+b\right|}{\|\mathbf{w}\|}$
Define the margin of a linear classifier as the width that the boundary could be increased by before hitting a data point
Examples closest to the hyperplane（超平面）are support vectors（支持向量）．
Margin $m$ of the separator is the distance between support vectors．


## Maximum Margin Classification

最大间距分类Maximizing the margin is good according to intuition and PAC theory．
Implies that only support vectors matter；other training examples are ignorable．


## Maximum Margin Classification

最大间距分类Maximizing the margin is good according to intuition and PAC theory．
Implies that only support vectors matter；other training examples are ignorable．


## Maximum Margin Classification Mathematically

Let training set $\left\{\left(\mathbf{x}_{i}, y_{i}\right)\right\}_{i=1 . . N^{N}}, \mathbf{x}_{i} \in \mathbf{R}^{d}, y_{i} \in\{-1,1\}$ be separated by a hyperplane with margin $m$. Then for each training example ( $\mathbf{x}_{i}, y_{i}$ ):

$$
\begin{aligned}
& \mathbf{w}^{\top} \mathbf{x}_{i}+b \leq-c \quad \text { if } y_{i}=-1 \\
& \mathbf{w}^{\top} \mathbf{x}_{i}+b \geq c \quad \text { if } y_{i}=1
\end{aligned} \quad \Leftrightarrow \quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq c
$$

For every support vector $\mathbf{x}_{s}$ the above inequality is an equality. $y_{s}\left(\mathbf{w}^{\top} \mathbf{x}_{s}+b\right)=c$

In the equality, we obtain that distance between each $\mathbf{x}_{s}$ and the hyperplane is

$$
r=\frac{\left|\mathbf{w}^{T} \mathbf{x}_{s}+b\right|}{\|\mathbf{w}\|}=\frac{\mathbf{y}_{s}\left(\mathbf{w}^{T} \mathbf{x}_{s}+b\right)}{\|\mathbf{w}\|}=\frac{c}{\|\mathbf{w}\|}
$$



## Maximum Margin Classification Mathematically

Then the margin can be expressed through $\mathbf{w}$ and b ：

$$
m=2 r=\frac{2 c}{\|\mathbf{w}\|}
$$

Here is our Maximum Margin Classification problem：

$$
\begin{array}{lll}
\max _{\mathbf{w}, b} \frac{2 c}{\|\mathbf{w}\|} & \text { subject to } & y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq c, \forall i \\
\max _{\mathbf{w}, b} \frac{c}{\|\mathbf{w}\|} & \text { subject to } & y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq c, \forall i
\end{array}
$$

Note that the magnitude（大小）of $c$ merely scales $\mathbf{w}$ and b ，and does not change the classification boundary at all！

So we have a cleaner problem：

$$
\max _{\mathbf{w}, b} \frac{1}{\|\mathbf{w}\|} \text { subject to } y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1, \forall i
$$

This leads to the famous Support Vector Machines 支持向量机 — believed by many to be the best＂off－the－shelf＂supervised learning algorithm

## Learning as Optimization

Parameter Learning


## Support Vector Machine

－A convex quadratic programming（凸二次规划） problem with linear constraints：

$$
\max _{\mathbf{w}, b} \frac{1}{\|\mathbf{w}\|} \quad \text { subject to } \quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1, \forall i
$$

－The attained margin is now given by $\frac{1}{\|\mathbf{W}\|}$

－Only a few of the classification constraints are relevant $\rightarrow$ support vectors
－Constrained optimization（约束优化）
－We can directly solve this using commercial quadratic programming （QP）code
－But we want to take a more careful investigation of Lagrange duality （对偶性），and the solution of the above in its dual form．
－deeper insight：support vectors，kernels（核）．．．

## Quadratic Programming

Minimize（with respect to x ）

$$
g(\mathbf{x})=\frac{1}{2} \mathbf{x}^{\top} Q \mathbf{x}+\mathbf{c}^{\top} \mathbf{x}
$$

Subject to one or more constraints of the form：

$$
\begin{array}{lc}
A \mathbf{x} \leq \mathbf{b} & \text { (inequality constraint) } \\
E \mathbf{x}=\mathbf{d} & \text { (equality constraint) }
\end{array}
$$



If $Q \succeq 0$ ，then $g(\boldsymbol{x})$ is a convex function（凸函数）：In this case the quadratic program has a global minimizer

Quadratic program of support vector machine：

$$
\min _{\mathbf{W}, b} \mathbf{w}^{\top} \mathbf{w} \quad \text { subject to } \quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1, \forall i
$$

## Solving Maximum Margin Classifier

Our optimization problem:

$$
\begin{equation*}
\min _{\mathbf{w}, b} \mathbf{w}^{\top} \mathbf{w} \quad \text { subject to } \quad 1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \leq 0, \forall i \tag{1}
\end{equation*}
$$

The Lagrangian:

$$
\begin{aligned}
L(\mathbf{w}, b, \alpha) & =\frac{1}{2} \mathbf{w}^{\top} \mathbf{w}-\sum_{i=1}^{n} \alpha_{i}\left[y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)-1\right] \\
& =\frac{1}{2} \mathbf{w}^{\top} \mathbf{w}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)\right]
\end{aligned}
$$

Consider each constraint:

$$
\begin{aligned}
\max _{\alpha_{i} \geq 0} \alpha_{i}\left[1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)\right] & =0 & & \text { if } \mathbf{w}, \mathrm{b} \text { satisfies primal constraints } \\
& =\infty & & \text { otherwise }
\end{aligned}
$$

## Solving Maximum Margin Classifier

Our optimization problem：

$$
\begin{equation*}
\min _{\mathbf{w}, b} \mathbf{w}^{\top} \mathbf{w} \quad \text { subject to } \quad 1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \leq 0, \forall i \tag{1}
\end{equation*}
$$

The Lagrangian：

$$
L(\mathbf{w}, b, \alpha)=\frac{1}{2} \mathbf{w}^{\top} \mathbf{w}-\sum_{i=1}^{n} \alpha_{i}\left[y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)-1\right]
$$

Lemma：

$$
\begin{aligned}
\max _{\alpha \geq 0} L(\mathbf{w}, b, \alpha) & =\frac{1}{2} \mathbf{w}^{\top} \mathbf{w} & & \text { if } \mathbf{w}, \mathrm{b} \text { satisfies primal constraints } \\
& =\infty & & \text { otherwise }
\end{aligned}
$$

（1）can be reformulated as $\quad \min _{\mathbf{w}, b} \max _{\alpha \geq 0} L(\mathbf{w}, b, \alpha)$
The dual problem（对偶问题）： $\max _{\alpha \geq 0} \min _{\mathbf{w}, b} L(\mathbf{w}, b, \alpha)$

## The Dual Problem（对偶问题）

$$
\max _{\alpha \geq 0} \min _{\mathbf{w}, b} L(\mathbf{w}, b, \alpha)
$$

We minimize $L$ with respect to $\mathbf{w}$ and $b$ first：

$$
\begin{gather*}
\frac{\partial L}{\partial \mathbf{w}} L(\mathbf{w}, b, \alpha)=\mathbf{w}^{\top}-\sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i}^{\top}=0  \tag{2}\\
\frac{\partial L}{\partial \mathbf{b}} L(\mathbf{w}, b, \alpha)=-\sum_{i=1}^{n} \alpha_{i} y_{i}=0 \tag{3}
\end{gather*}
$$

Note：$d(\mathbf{A x}+\mathbf{b})^{T}(\mathbf{A x}+\mathbf{b})=\left(2(\mathbf{A x}+\mathbf{b})^{T} \mathbf{A}\right) d \mathbf{x}$

$$
d\left(\mathbf{x}^{T} \mathbf{a}\right)=d\left(\mathbf{a}^{T} \mathbf{x}\right)=\mathbf{a}^{T} d \mathbf{x}
$$

Note that the bias term b dropped out but had produced a ＂global＂constraint on $\alpha$

## The Dual Problem（对偶问题）

$$
\max _{\alpha \geq 0} \min _{\mathbf{w}, b} L(\mathbf{w}, b, \alpha)
$$

We minimize $L$ with respect to $\mathbf{w}$ and $b$ first：

$$
\begin{gather*}
\frac{\partial L}{\partial \mathbf{w}} L(\mathbf{w}, b, \alpha)=\mathbf{w}^{\top}-\sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i}^{\top}=0  \tag{2}\\
\frac{\partial L}{\partial \mathbf{b}} L(\mathbf{w}, b, \alpha)=-\sum_{i=1}^{n} \alpha_{i} y_{i}=0 \tag{3}
\end{gather*}
$$

Note that（2）implies

$$
\begin{equation*}
\mathbf{w}=\sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i} \tag{4}
\end{equation*}
$$

Plug（4）back to L，and using（3），we have

$$
L(\mathbf{w}, b, \alpha)=\sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j}\left(\mathbf{x}_{i}^{\top} \mathbf{x}_{j}\right)
$$

## The Dual Problem（对偶问题）

Now we have the following dual optimization problem：

$$
\begin{array}{rc}
\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j}\left(\mathbf{x}_{i}^{\top} \mathbf{x}_{j}\right) & \text { subject to } \\
\alpha_{i} \geq 0, \forall i \\
\sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{array}
$$

This is a quadratic programming problem again
－A global maximum can always be found

But what＇s the big deal？
1． w can be recovered by $\mathbf{w}=\sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i}$
2． b can be recovered by $\quad b=y_{i}-\mathbf{w}^{\top} \mathbf{x}_{i}$ for any it that $\alpha_{i} \neq 0$
3．The＂kernel＂一核 $\mathbf{x}_{i}^{\top} \mathbf{x}_{j}$ more later．．．

## Support Vectors

If a point $\mathbf{x}_{\mathbf{i}}$ satisfies $y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)>1$

Due to the fact that

$$
\begin{aligned}
\max _{\alpha_{i} \geq 0} \alpha_{i}\left[1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)\right] & =0 \quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1 \\
& =\infty \quad \text { otherwise }
\end{aligned}
$$

We have $\alpha^{*}=0 ; \mathbf{x}_{i}$ not a support vector
$\mathbf{w}$ is decided by the points with non-zero $\alpha$ 's

$$
\mathbf{w}=\sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i}
$$

## Support Vectors

## only a few $\alpha_{i}$ 's can be nonzero!!



## Support Vector Machines

Once we have the Lagrange multipliers $\alpha_{i}$, we can reconstruct the parameter vector $\mathbf{w}$ as a weighted combination of the training examples:

$$
\mathbf{w}=\sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i}=\sum_{i \in S V} \alpha_{i} y_{i} \mathbf{x}_{i}
$$

For testing with a new data $\mathbf{x}^{\prime}$
Compute $\mathbf{w}^{\top} \mathbf{x}^{\prime}+b=\sum_{i \in S V} \alpha_{i} y_{i}\left(\mathbf{x}_{i}^{\top} \mathbf{x}^{\mathbf{\prime}}\right)+b$
and classify $\mathbf{x}^{\prime}$ as class 1 if the sum is positive, and class 2 otherwise

Note: w need not be formed explicitly

## Interpretation（解释）of support vector machines

－The optimal $\mathbf{w}$ is a linear combination of a small number of data points．This＂sparse稀疏＂representation can be viewed as data compression（数据压缩）as in the construction of kNN classifier
－To compute the weights $\alpha_{i}$ ，and to use support vector machines we need to specify only the inner products内积（or kernel）between the examples $\mathbf{x}_{i}^{\top} \mathbf{x}_{j}$
－We make decisions by comparing each new example $\mathbf{x}^{\prime}$ with only the support vectors：

$$
y^{*}=\operatorname{sign}\left(\sum_{i \in S V} \alpha_{i} y_{i}\left(\mathbf{x}_{i}^{\top} \mathbf{x}^{\prime}\right)+b\right)
$$

## Soft Margin Classification

What if the training set is not linearly separable？
Slack variables（松弛变量）$\xi_{i}$ can be added to allow misclassification of difficult or noisy examples，resulting margin called soft．


## Soft Margin Classification Mathematically

＂Hard＂margin QP：

$$
\min _{\mathbf{w}, b} \mathbf{w}^{\top} \mathbf{w} \quad \text { subject to } \quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1, \forall i
$$

Soft margin QP：

$$
\begin{array}{r}
\min _{\mathbf{w}, b} \frac{1}{2} \mathbf{w}^{\top} \mathbf{w}+C \sum_{i} \xi_{i} \quad \text { subject to } \quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1-\xi_{i}, \forall i \\
\xi_{i} \geq 0, \forall i
\end{array}
$$

$>$ Note that $\xi_{i}=0$ if there is no error for $\mathbf{x}_{\mathbf{i}}$
$>\xi_{i}$ is an upper bound of the number of errors
$>$ Parameter C can be viewed as a way to control＂softness＂：it ＂trades off（折衷，权衡）＂the relative importance of maximizing the margin and fitting the training data（minimizing the error）．
－Larger C $\rightarrow$ more reluctant to make mistakes

## The Optimization Problem

The dual of this new constrained optimization problem is

$$
\begin{aligned}
\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j}\left(\mathbf{x}_{i}^{\top} \mathbf{x}_{j}\right) \quad \text { subject to } & 0 \leq \alpha_{i} \leq C, \forall i \\
& \sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{aligned}
$$

This is very similar to the optimization problem in the linear separable case, except that there is an upper bound $C$ on $\alpha_{i}$ now

Once again, a QP solver can be used to find $\alpha_{i}$

## Roadmap

SVM<br>Prediction



## Loss in SVM

$\min _{\mathbf{W}, b, \xi} \frac{1}{2} \mathbf{w}^{\top} \mathbf{w}+C \sum_{i} \xi_{i}$ subject to $\quad y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right) \geq 1-\xi_{i}, \forall i$

$$
\xi_{i} \geq 0, \forall i
$$

Loss is measured as

$$
\xi_{i}=\max \left(0,1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)\right)=\left[1-y_{i}\left(\mathbf{w}^{\top} \mathbf{x}_{i}+b\right)\right]_{+}
$$

This loss is known as hinge loss
$\min _{\mathbf{w}, b} \frac{1}{2 C} \mathbf{w}^{\top} \mathbf{w}+\sum_{i}$ hingeloss $_{i}$


## Loss functions

- Regression
- Squared loss $\mathrm{L}_{2}$
- Absolute loss $L_{1}$
- Binary classification
- Zero/one loss $L_{0 / 1}$ (no good algorithm)
- Squared loss $L_{2}$
- Absolute loss $L_{1}$
- Hinge loss (Support vector machines)
- Logistic loss (Logistic regression)


## Linear SVMs: Overview

The classifier is a separating hyperplane.

Most "important" training points are support vectors; they define the hyperplane.

Quadratic optimization algorithms can identify which training points $\mathbf{x}_{i}$ are support vectors with non-zero Lagrangian multipliers $\alpha_{i}$.

Both in the dual formulation of the problem and in the solution training points appear only inside inner products:

```
Find }\mp@subsup{\alpha}{1}{\ldots.. \mp@subsup{\alpha}{N}{}}\mathrm{ such that
```



```
(1) }\sum\mp@subsup{\alpha}{i}{}\mp@subsup{y}{i}{}=
(2)}0\leq\mp@subsup{\alpha}{i}{}\leqC\mathrm{ for all }\mp@subsup{\alpha}{i}{
```

$f(\mathbf{x})=\sum \alpha_{i} y_{i} \mathbf{x}_{i}^{\top} \mathbf{x}+b$

## Non-linearity: example

- Input x:
- Patient information and vital signs
- Output y:
- Health (positive is good)


## Features in linear space

- Philosophy: extract any features that might be relevant.
- Features for medical diagnosis: height, weight, body temperature, blood pressure, etc.
- Three problems: non-monotonicity, nonlinearity, interactions between features


## Non-monotonicity

- Features: $\phi(x)=(1 ;$ temperature $(x))$
- Output: health y
- Problem: favor extremes; true relationship is non-monotonic


## Non-monotonicity

- Solution: transform inputs
- $\phi(x)=\left(1 ;(\text { temperature }(x)-37)^{2}\right)$
- Disadvantage: requires manually-specied domain knowledge


## Non-monotonicity

- $\phi(x)=\left(1\right.$; temperature $(x)$; temperature $\left.(x)^{2}\right)$
- General: features should be simple building blocks to be pieced together


## Interaction between features

- $\phi(x)=($ height $(x) ;$ weight $(x))$
- Output: health y
- Problem: can't capture relationship between height and weight


## Interaction between features

- $\phi(x)=(\text { height }(x)-\text { weight }(x))^{2}$
- Solution: define features that combine inputs
- Disadvantage: requires manually-specified domain knowledge


## Interaction between features

- $\phi(x)=\left[\right.$ height $(x)^{2} ;$ weight $(x)^{2}$; height $(x)$ weight $\left.(x)\right]$
cross term
- Solution: add features involving multiple measurements


## Linear in what?

Prediction driven by score: w $\cdot \phi(x)$

- Linear in w? Yes
- Linear in $\phi(x)$ ? Yes
- Linear in $x$ ? No!

Key idea: non-linearity

- Predictors $f_{w}(x)$ can be expressive non-linear functions and decision boundaries of $x$.
- Score w $\cdot \phi(x)$ is linear function of $w$ and $\phi(x)$


## Non-linear SVMs

Datasets that are linearly separable with some noise work out great:


But what are we going to do if the dataset is just too hard?


How about... mapping data to a higher-dimensional space:


## Non-linear SVMs: Feature spaces

General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:


## The "Kernel Trick"

Recall the SVM optimization problem

$$
\begin{aligned}
\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j}\left(\mathbf{x}_{i}^{\top} \mathbf{x}_{j}\right) \quad \text { subject to } \quad & 0 \leq \alpha_{i} \leq C, \forall i \\
& \sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{aligned}
$$

The data points only appear as inner product

- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Many common geometric operations (angles, distances) can be expressed by inner products

Define the kernel function $K$ by $K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\phi\left(\mathbf{x}_{i}\right)^{\mathbf{T}} \phi\left(\mathbf{x}_{j}\right)$

## Kernel methods

- Features viewpoint: construct and work with $\phi(\mathbf{x})$ (think in terms of properties of inputs)
- Kernel viewpoint: construct and work with $K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)$ (think in terms of similarity between inputs)


## An Example for feature mapping and kernels

- Consider an input $\mathbf{x}=\left[x_{1}, x_{2}\right]$
- Suppose $\phi($.$) is given as follows$

$$
\phi\left(\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]\right)=1, \sqrt{2} x_{1}, \sqrt{2} x_{2}, x_{1}^{2}, x_{2}^{2}, \sqrt{2} x_{1} x_{2}
$$

- An inner product in the feature space is

$$
\left\langle\phi\left(\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]\right), \phi\left(\left[\begin{array}{l}
x_{1}^{\prime} \\
x_{2}^{\prime}
\end{array}\right]\right)\right\rangle=
$$

- So, if we define the kernel function as follows, there is no need to carry out $\phi($.$) explicitly$

$$
K\left(\mathbf{x}, \mathbf{x}^{\prime}\right)=\left(1+\mathbf{x}^{T} \mathbf{x}^{\prime}\right)^{2}
$$

## More Examples of Kernel Functions

－Linear：$K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\mathbf{x}_{i}{ }^{\mathbf{T}} \mathbf{x}_{j}$
－Mapping $\Phi: \mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$ ，where $\varphi(\mathbf{x})$ is $\mathbf{x}$ itself

- Polynomial（多项式）of power $p: K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\left(1+\mathbf{x}_{i}{ }^{\mathbf{T}} \mathbf{x}_{j}\right)^{p}$
- Gaussian（radial－basis function径向基函数）：$K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=e^{-\frac{\left\|\mathbf{x}_{i}-\mathbf{x}_{\mathbf{i}}\right\|^{2}}{\sigma^{2}}}$
－Mapping $\Phi: \mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$ ，where $\varphi(\mathbf{x})$ is infinite－dimensional
－Higher－dimensional space still has intrinsic dimensionality d， but linear separators in it correspond to non－linear separators in original space．


## Kernel matrix

Suppose for now that $K$ is indeed a valid kernel corresponding to some feature mapping $\phi$ ，then for $\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{n}}$ ，we can compute an $n \times n$ matrix $\left\{K_{i, j}\right\}$ where $K_{i, j}=\boldsymbol{\varphi}\left(\mathbf{x}_{i}\right)^{\mathbf{T}} \boldsymbol{\varphi}\left(\mathbf{x}_{j}\right)$

This is called a kernel matrix！

Now，if a kernel function is indeed a valid kernel，and its elements are dot－product in the transformed feature space，it must satisfy：
－Symmetry $K=K^{T}$
－Positive－semidefinite（半正定） $\mathbf{z}^{\top} K \mathbf{z} \geq 0, \quad \forall \mathbf{z} \in R^{n}$

## Matrix formulation

$$
\begin{array}{rc} 
& \max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) \\
= & \max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i, j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} K_{i, j} \\
= & \max _{\alpha} \alpha^{\top} \mathbf{e}-\frac{1}{2} \alpha^{\top}\left(\mathbf{y y}^{\top} \circ K\right) \alpha \\
\text { subject to } & 0 \leq \alpha_{i} \leq C, \forall i \\
\sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{array}
$$

## Nonlinear SVMs - RBF Kernel



## Summary: Support Vector Machines

Linearly separable case $\rightarrow$ Hard margin SVM

- Primal quadratic programming
- Dual quadratic programming

Not linearly separable? $\rightarrow$ Soft margin SVM

Non-linear SVMs

- Kernel trick



## Summary：Support Vector Machines

SVM training：build a kernel matrix K using training data
－Linear：$K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=\mathbf{x}_{i}{ }^{\mathbf{T}} \mathbf{x}_{j}$
－Gaussian（radial－basis function径向基函数）：$K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)=e^{-\frac{\| \mathbf{x}_{i}-\left.\mathbf{x}_{j}\right|^{2}}{\sigma^{2}}}$
solve the following quadratic program

$$
\begin{array}{cc}
\max _{\alpha} \alpha^{\top} \mathbf{e}-\frac{1}{2} \alpha^{\top}\left(\mathbf{y y}^{\top} \circ K\right) \alpha \\
\text { subject to } & 0 \leq \alpha_{i} \leq C, \forall i \\
\sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{array}
$$

SVM testing：now with $\alpha_{i}$ ，recover $b$ ，

$$
b=y_{i}-\sum_{j=1}^{n} \alpha_{j} y_{j} K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) \quad \text { for any i that } \alpha_{i} \neq 0
$$

we can predict new data points by：

$$
y^{*}=\operatorname{sign}\left(\sum_{i \in S V} \alpha_{i} y_{i} K\left(\mathbf{x}_{i}, \mathbf{x}^{\prime}\right)+b\right)
$$

## 作业

－已知正例点 $x_{1}=(1,2)^{\mathrm{T}}, x_{2}=(2,3)^{\mathrm{T}}, x_{3}=(3,3)^{\mathrm{T}}$ ，
负例点 $x_{4}=(2,1)^{\mathrm{T}}, x_{5}=(3,2)^{\mathrm{T}}$ ，试求Hard Margin SVM的最大间隔分离超平面和分类决策函数，并在图上画出分离超平面，间隔边界及支十卉

