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## Outline

- Example of classification problems
- Formulating Support Vector Machines
- SVM Properties
- Soft-Margin SVMs
- Kernels and Nonlinear Data
- Regularization


## Example: Diabetes Diagnosis

| Patient <br> $\#$ | Plasma <br> gluc. | Diastolic BP Fold test <br> $(\mathbf{m m ~ H g})$ | 2-hr <br> $(\mathbf{m m})$ | BMI <br> Insulin <br> $\left(\mathbf{k g} / \mathbf{m}^{2}\right)$ | pedigree <br> function | Age <br> $(\mathbf{y r s})$ | diabetes <br> diagnosis |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 85 | 66 | 29 | 0 | 26.6 | 0.351 | 31 | no |
| 2 | 183 | 64 | 0 | 0 | 23.3 | 0.672 | 32 | yes |
| 3 | 89 | 66 | 23 | 94 | 28.1 | 0.167 | 21 | no |
| 4 | 137 | 40 | 35 | 168 | 43.1 | 2.288 | 33 | yes |
| 5 | 116 | 74 | 0 | 0 | 25.6 | 0.201 | 30 | no |
| 6 | 78 | 50 | 32 | 88 | 31 | 0.248 | 26 | yes |
| 7 | 197 | 70 | 45 | 543 | 30.5 | 0.158 | 53 | yes |
| $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |
| 768 | 166 | 72 | 19 | 175 | 25.8 | 0.587 | 51 | yes |

## Example: Diabetes Diagnosis

Do Not Have Diabetes
blood glucose $=30$ body mass index $=120 \mathrm{~kg} / \mathrm{m}^{2}$ body masindex $=160 \mathrm{~kg} / \mathrm{m}^{2}$ diastolic bp $=79 \mathrm{~mm} \mathrm{Hg}$ age $=32$ years



Have Diabetes

## Example: Diabetes Diagnosis



## Example: Diabetes Diagnosis



## Example: Diabetes Diagnosis

Do Not Have Diabetes
blood glucose $=30\}$ body mass index $=120 \mathrm{~kg} / \mathrm{m}^{2}$ diastolic bp $=79 \mathrm{~mm} \mathrm{Hg}$

Learn a classification function that can discriminate between the two classes


Have Diabetes

## Example: Credit Card Application

|  |  | Age <br> (yrs) | Income (\$) | Rent/Own? <br> (binary) | Monthly <br> Rent/Mort. | Manager's <br> Decision |
| :---: | :---: | :---: | :---: | :---: | ---: | :---: |
| 1 | Greg J. | 38 | 65,000 | rent | 1,050 | yes |
| 2 | James T. | 24 | 21,000 | rent | 350 | no |
| 3 | Hannah M. | 45 | 98,000 | own | 2,400 | no |
| 4 | Rashard K. | 19 | 19,500 | own | 400 | yes |
| 5 | Xavier N. | 29 | 75,000 | rent | 1,570 | no |
| 6 | Jillian A. | 29 | 39,000 | own | 1,000 | yes |
| 7 | Ramon H. | 35 | 103,000 | rent | 3,000 | yes |
| $\ldots$ | ... | $\ldots$. | $\ldots$ | $\ldots$ | $\ldots$ | ... |
| 2000 | Mary C. | 55 | 45,000 | rent | 1,200 | no |

Learn a classification function to determine who gets a credit card.

## Example: Handwritten Digit Recognition



## Goal of Classification: Generalization



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## Setting Up The SVM Problem

Do Not Have Diabetes
blood glucose $=30$ body mass index $=120 \mathrm{~kg} / \mathrm{m}$ diastolic bp $=79 \mathrm{~mm} \mathrm{Hg}$ age $=32$ years


Find a linear classification function (a hyperplane) $f(\boldsymbol{x})=\boldsymbol{w}^{\prime} \boldsymbol{x}-\boldsymbol{b}$ such that $\operatorname{sign}(f(x))=+1$, when diabetes $\operatorname{sign}(f(x))=-1$, when not diabetes


Have Diabetes

## The SVM Problem



## The Notion of Margin



## The Notion of Margin



## The Notion of Margin



## A Theoretical Digression

- When we have infinitely many solutions that reduce the error (variance), which one should we pick?
- We introduce a bias! Our bias is toward simpler solutions (minimal complexity).
- How do we measure complexity of hyperplanes with respect to data? Vapnik-Chervonenkis dimension


## A Theoretical Digression: VC Dimension

- Complexity for a class of functions $\boldsymbol{H}$ is measured by VC Dimension
- A given set of $\boldsymbol{\ell}$ points can be labeled in $\boldsymbol{2}^{\boldsymbol{\ell}}$ ways.
- If for each labeling, some function $\boldsymbol{f}$ from $\boldsymbol{H}$ can be found which correctly assigns those labels, we say that that set of points is shattered by H .
- The VC dimension for the set of functions H is defined as the maximum number of training points that can be shattered





## A Theoretical Digression: VC Dimension

Vladimir Vapnik showed that there is a connection between VC dimension and margin (Vapnik, 1995)


## Formulating the SVM



Distance of a point in Class to the margin is

$$
\frac{\left|\mathbf{w}^{\prime} \mathbf{x}-\alpha\right|}{\|\mathbf{w}\|}
$$

Distance of a point in
Class $O$ to the margin is $\frac{\left|\mathbf{w}^{\prime} \mathbf{x}-\beta\right|}{\|\mathbf{w}\|}$

## Formulating the SVM



## Formulating the SVM



## Formulating the SVM

We are given labeled data points

$$
\left(\mathbf{x}_{i}, y_{i}\right)_{i=1}^{\ell}
$$

We need to learn a hyperplane

$$
\mathbf{w}^{\prime} \mathbf{x}-b=0
$$

such that

1. all the points in class with labels $\mathbf{y}_{\mathrm{i}}=\boldsymbol{+ 1}$, lie above the margin, that is

$$
\mathbf{w}^{\prime} \mathbf{x}_{i}-b \geq 1
$$

2. all the points in class with labels $y_{i}=-\mathbf{1}$, lie below the margin, that is

$$
\mathbf{w}^{\prime} \mathbf{x}_{i}-b \leq-1
$$

3. the margin is maximized

$$
\gamma=\frac{2}{\|\mathbf{w}\|}
$$

## Formulating the SVM

Maximizing $\gamma=\frac{2}{\|\mathbf{w}\|}$ is equivalent to minimizing

$$
\frac{1}{2}\|\mathbf{w}\|^{2}
$$

with the constraints that

$$
\begin{aligned}
& \mathbf{w}^{\prime} \mathbf{x}_{i}-b \geq 1 \quad \text { when } y_{i}=+1 \\
& \mathbf{w}^{\prime} \mathbf{x}_{i}-b \leq-1 \text { when } y_{i}=-1
\end{aligned}
$$

Optimization problem for a support vector machine:
$\mathbf{w}^{\prime} \mathbf{x}-b=1^{\prime}$

s.t. $y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right) \geq 1 \quad \forall i=1 \ldots \ell$

$$
\begin{aligned}
& \text { Optimization problem for a support vector machine: } \\
& \text { min } \\
& \frac{1}{2}\|\mathbf{w}\|_{2}^{2} \\
& \text { s.t. } \\
& y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right) \geq 1 \quad \forall i=1 \ldots \ell
\end{aligned}
$$

- Convex, quadratic minimization problem called the primal problem. Guaranteed to have a global minimum.
- Further properties of the formulation can be studied by deriving the dual problem
- Introduce Lagrange multipliers, $\left\{\alpha_{i}\right\}_{i=1}^{\ell}$, one for each constraint (hence data point). These are the dual variables.
- Construct the Lagrangian function of primal and dual variables (note that by definition all $\alpha_{i} \geq 0$ )

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

Lagrangian function of a support vector machine

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

Differentiate the Lagrangian with respect to the primal variables

$$
\begin{array}{ll}
\nabla_{\mathbf{w}} L\left(\mathbf{w}, b, \alpha_{i}\right)=0: & \mathbf{w}=\sum_{i=1}^{\ell} \alpha_{i} y_{i} \mathbf{x}_{i} \\
\nabla_{b} L\left(\mathbf{w}, b, \alpha_{i}\right)=0: \quad \sum_{i=1}^{\ell} \alpha_{i} y_{i}=0
\end{array}
$$

These are the first order optimality conditions. We can now eliminate the primal variables by substituting the first order conditions into the Lagrangian.
support vector machine primal problem $\min \quad \frac{1}{2}\|\mathbf{w}\|_{2}^{2}$

$$
\text { s.t. } \quad y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right) \geq 1 \quad \forall i=1 \ldots \ell
$$

$$
\begin{array}{ll}
\text { support vector machine dual problem } \\
\max & -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{\prime} \mathbf{x}_{j}+\sum_{i=1}^{\ell} \alpha_{i} \\
\text { s.t. } & \sum_{i=1}^{\ell} \alpha_{i} y_{i}=0, \\
& \alpha_{i} \geq 0, \quad \forall i=1 \ldots \ell
\end{array}
$$

Why bother with the dual, and solving for $\alpha$ ?

- convex optimization problem. No duality gap
- Dual has fewer constraints. Easier to solve
- Dual solution is sparse. Easier to represent


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## Characteristics of the Solution

Recall the first order condition:

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

The final solution is a linear combination of the training data!

Additional optimality condition: complementarity slackness

$$
\begin{gathered}
0 \leq \alpha_{i} \perp y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}-b\right)-1 \geq 0 \\
\alpha_{i}=0 \quad \text { and } \quad y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right)>1 \quad \text { (point not on hyperplane) } \\
\alpha_{i}>0 \quad \text { and } \quad y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right)=1 \quad \text { (point on hyperplane) }
\end{gathered}
$$

## Characteristics of the Solution

Recall the first order condition:

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

The final solution is a sparse linear combination of the training data!
only support vectors have $\alpha_{i}>0$ (non-zero). All other vectors have $\alpha_{i}=0$, and this makes the solution sparse!
$\alpha_{i}=0 \quad$ and $\quad y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right)>1 \quad$ (point not on hypérplane)
or
$\alpha_{i}>0 \quad$ and $\quad y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right)=1 \quad$ (point on hyperplane)

## Characteristics of the Solution

Recall the first order condition:

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

The final solution is a sparse linear combination of the training data!

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## Linearly Inseparable Data



So far, assumed that the data is linearly separable. However, this assumption is not valid in most realworld applications.

Need to extend hard-margin support vector machines to be able to handle noisy data

This results in the soft-margin support vector machine

## Soft-margin Support Vector Machine

hard-margin support vector machine


## Soft-margin Support Vector Machine

hard-margin support vector machine


## Soft-margin Support Vector Machine



## Soft-margin Dual

hard-margin svm dual


## Some things to note about the Dual



Note that the regularization constant is set by the user.

This is an important parameter that can cause dramatically different behaviors on the same data set.

Note that the dual solution depends only on the inner products of the training data.

This is an important observation that allows us to extend linear SVMs to handle nonlinear data.

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## Nonlinear Data Sets



Naïve solution: Transform the input data into a higher dimension using the following nonlinear transformation:

$$
\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right] \rightarrow\left[\begin{array}{c}
x_{1}^{2} \\
\sqrt{2} x_{1} x_{2} \\
x_{2}^{2}
\end{array}\right]
$$




## Nonlinear Data Sets

 space, but a linear classifier can classify this nonlinear data in 3-d space!

Naïve solution: Transform the input data into a higher dimension using the following nonlinear transformation:

$$
\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right] \rightarrow\left[\begin{array}{c}
x_{1}^{2} \\
\sqrt{2} x_{1} x_{2} \\
x_{2}^{2}
\end{array}\right]
$$



## Nonlinear Data Sets



## Naïve Approach: Explicit Transformation



## Naïve Approach: Explicit Transformation

 products of the transformed data


## Inner Products in Feature Space




Let two points in the original input space be

$$
\begin{aligned}
\mathbf{x} & =\left(x_{1}, x_{2}\right) \\
\mathbf{z} & =\left(z_{1}, z_{2}\right)
\end{aligned}
$$

After transformation, in the high-dimensional feature space, they become

$$
\begin{aligned}
& \phi(\mathbf{x})=\left(x_{1}^{2}, \sqrt{2} x_{1} x_{2}, x_{2}^{2}\right) \\
& \phi(\mathbf{z})=\left(z_{1}^{2}, \sqrt{2} z_{1} z_{2}, z_{2}^{2}\right)
\end{aligned}
$$

What do inner products in this transformed feature space look like?

## The Kernel Trick




$$
\begin{aligned}
\langle\phi(\mathbf{x}), \phi(\mathbf{w})\rangle & =\left\langle\left(x_{1}^{2}, x_{2}^{2}, \sqrt{2} x_{1} x_{2}\right),\left(w_{1}^{2}, w_{2}^{2}, \sqrt{2} w_{1} w_{2}\right)\right\rangle \\
& =x_{1}^{2} w_{1}^{2}+x_{2}^{2} w_{2}^{2}+2 x_{1} w_{1} x_{2} w_{2} \\
& =\left(x_{1} w_{1}+x_{2} w_{2}\right)^{2} \\
& =\langle\mathbf{x}, \mathbf{w}\rangle^{2}
\end{aligned}
$$

## The Kernel Trick



## Better Approach: The Kernel Trick



## The Kernel Trick



Use a kernel function to directly learn a nonlinear classifier!

No need for explicit transformations

Can use existing approaches with slight modification!
linear support vector machine

$$
\begin{aligned}
\max & -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{\prime} \mathbf{x}_{j}+\sum_{i=1}^{\ell} \alpha_{i} \\
\text { s.t. } & \sum_{i=1}^{\ell} \alpha_{i} y_{i}=0 \\
& 0 \leq \alpha_{i} \leq C \quad \forall i=1 \ldots \ell
\end{aligned}
$$

kernel support vector machine

$$
\begin{aligned}
\max & -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_{i} \alpha_{j} y_{i} y_{j} \kappa\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)+\sum_{i=1}^{\ell} \alpha_{i} \\
\text { s.t. } & \sum_{i=1}^{\ell} \alpha_{i} y_{i}=0 \\
& 0 \leq \alpha_{i} \leq C \quad \forall i=1 \ldots \ell
\end{aligned}
$$

## Some Popular Kernels

Some popular kernels

- Linear kernel: $\kappa(\mathbf{x}, \mathbf{z})=\langle\mathbf{x}, \mathbf{z}\rangle$
- Polynomial kernel: $\kappa(\mathbf{x}, \mathbf{z})=(\langle\mathbf{x}, \mathbf{z}\rangle+c)^{d}, c, d \geq 0$
- Gaussian kernel: $\kappa(\mathbf{x}, \mathbf{z})=e^{-\frac{\|\mathbf{x}-\mathbf{z}\|^{2}}{\sigma}}, \sigma>0$
- Sigmoid kernel: $\kappa(\mathbf{x}, \mathbf{z})=\tanh ^{-1} \eta\langle\mathbf{x}, \mathbf{z}\rangle+\theta$

Kernels can also be constructed from other kernels:

- Conical (not linear) combinations, $\kappa(\mathbf{x}, \mathbf{z})=a_{1} \kappa_{1}(\mathbf{x}, \mathbf{z})+a_{2} \kappa_{2}(\mathbf{x}, \mathbf{z})$
- Products of kernels, $\kappa(\mathbf{x}, \mathbf{z})=\kappa_{1}(\mathbf{x}, \mathbf{z}) \kappa_{2}(\mathbf{x}, \mathbf{z})$
- Products of functions, $\kappa(\mathbf{x}, \mathbf{z})=f_{1}(\mathbf{x}) f_{2}(\mathbf{z}), f_{1}, f_{2}$ are real valued functions.


## Polynomial Kernels

$$
\kappa(\mathbf{x}, \mathbf{z})=(\langle\mathbf{x}, \mathbf{z}\rangle+1)^{d}
$$

Polynomial kernel, $p=3$


## Gaussian Kernels <br> $$
\kappa(\mathbf{x}, \mathbf{z})=\exp -\frac{\|\mathbf{x}-\mathbf{z}\|^{2}}{\sigma}
$$

Gaussian Kernel, gamma =



$$
\begin{aligned}
& \text { Gaussian Kernels } \\
& \kappa(\mathbf{x}, \mathbf{z})=\exp -\frac{\|\mathbf{x}-\mathbf{z}\|^{2}}{\sigma}
\end{aligned}
$$



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## Regularization and Over-fitting

## soft-margin support vector machine

 min
s.t. $\quad y_{i}\left(\mathbf{w}^{\prime} \mathbf{x}_{i}-b\right) \geq 1-\xi_{i} \quad \forall i=1 \ldots \ell$

$$
\xi \geq 0
$$

kernel support vector machine
$\max -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_{i} \alpha_{j} y_{i} y_{j} \kappa\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)+\sum_{i=1}^{\ell} \alpha_{i}$
s.t. $\quad \sum_{i=1}^{\ell} \alpha_{i} y_{i}=0$
$0 \leq \alpha_{i} \leq C \quad \forall i=1 \ldots \ell$

The regularization parameter, $\mathbf{C}$, is chosen a priori, defines the relative trade-off between norm (complexity / smoothness / capacity) and loss (error penalization)

We want to find classifiers that minimize (regularization $+C \cdot$ loss)

Regularization

- introduces inductive bias over solutions
- controls the complexity of the solution
- imposes smoothness restriction on solutions

As Cincreases, the effect of the regularization decreases and the SVM tends to overfit the data

## The Effect of C on Classification



$$
C=0.001
$$

## The Effect of C on Classification



$$
C=0.01
$$

## The Effect of C on Classification



## The Effect of C on Classification



## The Effect of C on Classification



$$
C=10
$$

## The Effect of C on Classification



$$
C=100
$$

## SVM Algorithms over the Years

- Earliest solution approaches: Quadratic Programming Solvers (CPLEX, LOQO, Matlab QP, SeDuMi)
- Decomposition methods: SVM chunking (Osuna et. al., 1997); implementation: SVMlight (Joachims, 1999)
- Sequential Minimization Optimization (Platt, 1999); implementation: LIBSVM (Chang et. al., 2000)
- Interior Point Methods (Munson and Ferris, 2006), Successive Over-relaxation (Mangasarian, 2004)
- Co-ordinate Descent Algorithms (Keerthi et. al., 2009), Bundle Methods (Teo et. al., 2010)

