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Outline

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

Patient	Plasma	Diastolic BP	Fold test	2-hr	BMI	pedigree	Age	diabetes
#	gluc.	(mm Hg)	(mm)	Insulin	(kg/m ²)	function	(yrs)	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
•••	•••	•••		•••		•••		
768	166	72	19	175	25.8	0.587	51	yes









Example: Credit Card Application

		Age (yrs)	Income (\$)	Rent/Own? (binary)	Monthly Rent/Mort.	Manager's 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
•••	•••	•••	•••	•••		•••
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



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** *H* is measured by **VC Dimension**
- A given set of *e* points can be labeled in *2***^{***e***}** ways.
- If for each labeling, some function *f* from *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)

To minimize the VC dimension (and hence complexity), we have to maximize the margin!

 \mathbf{w} such that $|\mathbf{w}|$ ٦ $\mathbf{w'}\mathbf{x} - b =$ $\mathbf{w'}\mathbf{x} - b = 0$ $\mathbf{w}'\mathbf{x}_i - b = -1$

We are given labeled data points

$$(\mathbf{x}_i, y_i)_{i=1}^\ell$$

We need to learn a hyperplane

$$\mathbf{w}'\mathbf{x} - b = 0$$

 all the points in class with labels y_i = +1, lie above the margin, that is

 $\mathbf{w'}\mathbf{x}_i - b \ge 1$

2. all the points in class
with labels y_i = -1, lie below the margin, that is

$$\mathbf{w}'\mathbf{x}_i - b \leq -1$$

3. the margin is maximized

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

Optimization problem for a support vector machine: min $\frac{1}{2} ||\mathbf{w}||_2^2$ s.t. $y_i(\mathbf{w}'\mathbf{x}_i - b) \ge 1 \quad \forall i = 1 \dots \ell$

- 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, $\{\alpha_i\}_{i=1}^{\ell}$, 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 $\alpha_i \ge 0$)

$$L(\mathbf{w}, b, \alpha_i) = \frac{1}{2}\mathbf{w'w} - \sum_{i=1}^{\ell} \alpha_i \left[y_i(\mathbf{w'x}_i - b) - 1 \right]$$

Lagrangian function of a support vector machine $L(\mathbf{w}, b, \alpha_i) = \frac{1}{2}\mathbf{w'w} - \sum_{i=1}^{\ell} \alpha_i \left[y_i(\mathbf{w'x}_i - b) - 1 \right]$

Differentiate the Lagrangian with respect to the primal variables

$$egin{aligned}
abla_{\mathbf{w}} L(\mathbf{w},b,lpha_i) &= 0: & \mathbf{w} = \sum_{i=1}^\ell lpha_i y_i \mathbf{x}_i \
abla_b L(\mathbf{w},b,lpha_i) &= 0: & \sum_{i=1}^\ell lpha_i y_i = 0 \end{aligned}$$

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
$$\frac{1}{2} ||\mathbf{w}||_2^2$$

s.t. $y_i(\mathbf{w}'\mathbf{x}_i - b) \ge 1 \quad \forall i = 1 \dots \ell$

support vector machine **dual problem**
max
$$-\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_i \alpha_j y_i y_j \mathbf{x}'_i \mathbf{x}_j + \sum_{i=1}^{\ell} \alpha_i$$

s.t. $\sum_{i=1}^{\ell} \alpha_i y_i = 0,$
 $\alpha_i \ge 0, \quad \forall i = 1 \dots \ell$

Why bother with the dual, and solving for α ?

- 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

$$0 \le \alpha_i \perp y_i(\mathbf{w}'\mathbf{x} - b) - 1 \ge 0$$

 $lpha_i = 0$ and $y_i(\mathbf{w}'\mathbf{x}_i - b) > 1$ (point not on hyperplane) or

 $\alpha_i > 0$ and $y_i(\mathbf{w}'\mathbf{x}_i - b) = 1$ (point on hyperplane)

Characteristics of the Solution

Recall the first order condition:

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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!**

solution **does not change if** all other vectors with $\alpha_i = 0$ are **deleted!**

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Linearly Inseparable Data

XXX

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

Soft-margin Support Vector Machine

Soft-margin Support Vector Machine

Soft-margin Dual

Some things to note about the Dual

 $\begin{array}{ll} \max & -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_i \alpha_j y_i y_j \mathbf{x}'_i \mathbf{x}_j + \sum_{i=1}^{\ell} \alpha_i \\ \text{s.t.} & \sum_{i=1}^{\ell} \alpha_i y_i = 0 \\ 0 \leq \alpha_i \leq C, \quad \forall i = 1 \dots \ell \\ & \text{Note that the dual set} \end{array}$

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:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$$

Nonlinear Data Sets

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

$$\left[\begin{array}{c} x_1\\ x_2 \end{array}\right] \rightarrow \left[\begin{array}{c} x_1^2\\ \sqrt{2}x_1x_2\\ x_2^2 \end{array}\right]$$

No linear classifier exists in 2-d space, but a linear classifier can classify this nonlinear data in 3-d space!

Nonlinear Data Sets

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

$$\left[\begin{array}{c} x_1\\ x_2 \end{array}\right] \rightarrow \left[\begin{array}{c} x_1^2\\ \sqrt{2}x_1x_2\\ x_2^2 \end{array}\right]$$

Linear classifier in 3-d space becomes non-linear in 2-d space!

Naïve Approach: Explicit Transformation

Naïve Approach: Explicit Transformation

Let two points in the original input space be

$$\mathbf{x} = (x_1, x_2)$$

 $\mathbf{z} = (z_1, z_2)$

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

$$\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

$$\phi(\mathbf{z}) = (z_1^2, \sqrt{2}z_1z_2, z_2^2)$$

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

$$\begin{aligned} \langle \phi(\mathbf{x}), \phi(\mathbf{w}) \rangle &= \langle (x_1^2, x_2^2, \sqrt{2}x_1x_2), (w_1^2, w_2^2, \sqrt{2}w_1w_2) \rangle \\ &= x_1^2 w_1^2 + x_2^2 w_2^2 + 2x_1 w_1 x_2 w_2 \\ &= (x_1 w_1 + x_2 w_2)^2 \\ &= \langle \mathbf{x}, \mathbf{w} \rangle^2 \end{aligned}$$

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

$$\max \quad -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_i \alpha_j y_i y_j \mathbf{x}'_i \mathbf{x}_j + \sum_{i=1}^{\ell} \alpha_i$$
s.t.
$$\sum_{\substack{i=1\\0 \leq \alpha_i \leq C}}^{\ell} \alpha_i y_i = 0$$

kernel support vector machine

$$\max \quad -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) + \sum_{i=1}^{\ell} \alpha_i$$
s.t.
$$\sum_{\substack{i=1\\0 \le \alpha_i \le C}}^{\ell} \alpha_i y_i = 0$$

Some Popular Kernels

Some popular kernels

- Linear kernel: $\kappa(\mathbf{x}, \mathbf{z}) = \langle \mathbf{x}, \mathbf{z} \rangle$
- Polynomial kernel: $\kappa(\mathbf{x}, \mathbf{z}) = (\langle \mathbf{x}, \mathbf{z} \rangle + c)^d, c, d \ge 0$
- 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 kernel, p = 3

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

Gaussian Kernel, gamma =

Gaussian Kernel, gamma =

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

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Regularization and Over-fitting

soft-margin support vector machine
min
$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^{i=1} \xi$$

s.t. $y_i(\mathbf{w}'\mathbf{x}_i - b) \ge 1 - \xi_i \quad \forall i = 1 \dots k$
 $\xi \ge 0$

kernel support vector machine $\max \quad -\frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) + \sum_{i=1}^{\ell} \alpha_i$ s.t. $\sum_{\substack{i=1\\0 \leq \alpha_i \leq \mathbf{C}}}^{\ell} \forall i = 1 \dots \ell$

The **regularization parameter, 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 • loss)

Regularization

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

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

C = 0.001

C = 0.01

C = 0.1

C = 1

C = 10

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)