COMP 652: Machine Learning

Lecture 13

Today

- Nonseparable data
- Feature expansions and the kernel trick

Recall one version of the linear SVM problem

- Recall, we formulated the quadratic program (QP) for finding the maximum-margin perceptron (a.k.a. linear SVM) as:

$$\begin{aligned} \text{min} \quad & \|\mathbf{w}\|^2 \\ \text{w.r.t.} \quad & \mathbf{w}, w_0 \\ \text{s.t.} \quad & y_i(\mathbf{w} \cdot \mathbf{x_i} + w_0) \geq 1 \end{aligned}$$

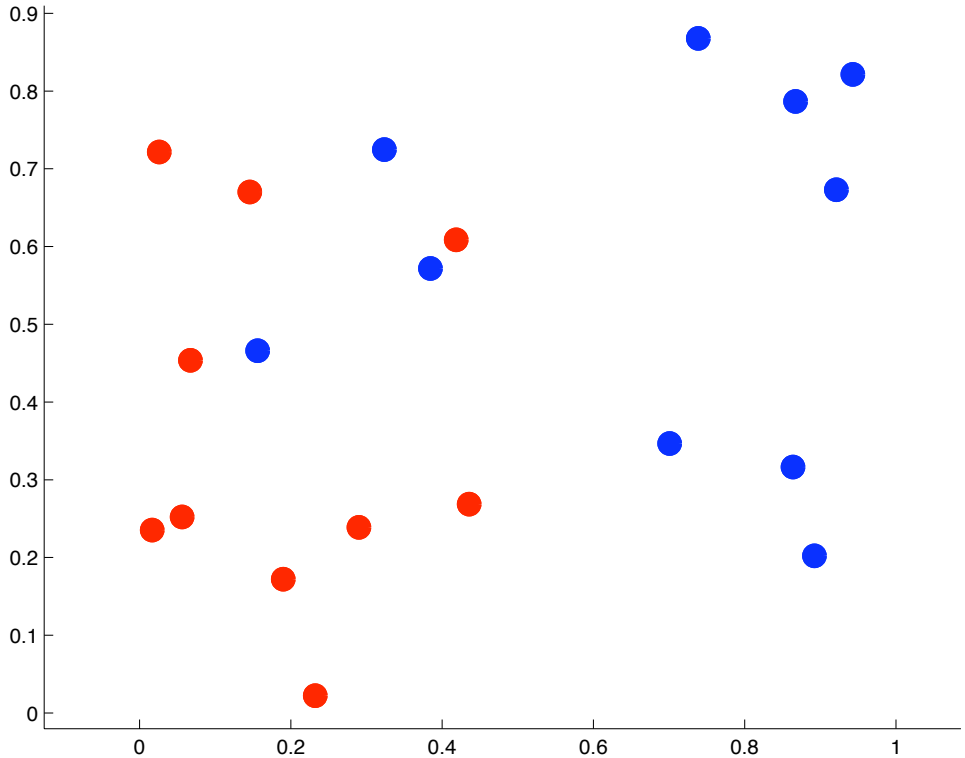
- The margin is $2M$ where $M = 1/\|\mathbf{w}\|$.

- The constraints, $y_i(\mathbf{w} \cdot \mathbf{x_i} + w_0) \geq 1$, ensure that each example is on the right side of the decision boundary at distance at least M.

- What if the data is not linearly separable?

Non-linearly separable data

- For example, consider this data set:



- If we try to use the previous formulation of the problem, the optimization package will tell us something like "no feasible solution". That is, the constraint cannot all be satisfied.

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- Recall, we formulated the quadratic program (QP) for finding the maximum-margin perceptron (a.k.a. linear SVM) as:

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- What if the data is not linearly separable?
  - Relax the constraints somehow
  - Try a different feature space, in which the data may be separable. (Maybe better for generalization too.)

Relaxing the constraints

- Given $\mathbf{w}, w_0$, an example $(\mathbf{x_i}, y_i)$ as at least distance $M = 1/\|\mathbf{w}\|$ on the right side of the margin if:

$$y_i(\mathbf{w} \cdot \mathbf{x_i} + w_0) \geq 1$$

- If we can't achieve that, suppose we require:

$$y_i(\mathbf{w} \cdot \mathbf{x_i} + w_0) \geq 1 - \zeta_i$$

  where $\zeta_i \geq 0$.

- How can we interpret ζ_i?
  - If $\zeta_i = 0$, then the original distance constraint is satisfied.
  - If $\zeta_i \in (0, 1)$, then the point is on the correct side of the decision boundary, but not as far as it should be.
  - If $\zeta_i = 1$, then the point is on the decision boundary.
  - If $\zeta_i > 1$ then the point is on the wrong side of the decision boundary.

Reformulating the problem

- Such constraints can always be satisfied – but we must penalize the ζ_i in order to encourage satisfaction of the original constraints.
- This suggests the optimization problem:

$$\begin{array}{rl} \text{min} & \|\mathbf{w}\|^2 + C \sum_i \zeta_i \\ \text{w.r.t.} & \mathbf{w}, w_0, \zeta_i \\ \text{s.t.} & y_i(\mathbf{w} \cdot \mathbf{x_i} + w_0) \geq (1 - \zeta_i) \\ & \zeta_i \geq 0 \end{array}$$

  where $C > 0$ is a user-chosen cost associated with constraint violation.
- Intuitively, this formulation tries to maximize the margin without violating the constraints too much.
- This formulation can also be solved by quadratic programming.

Solution

- As in the separable case, the solution for $\mathbf{w}$ is of the form

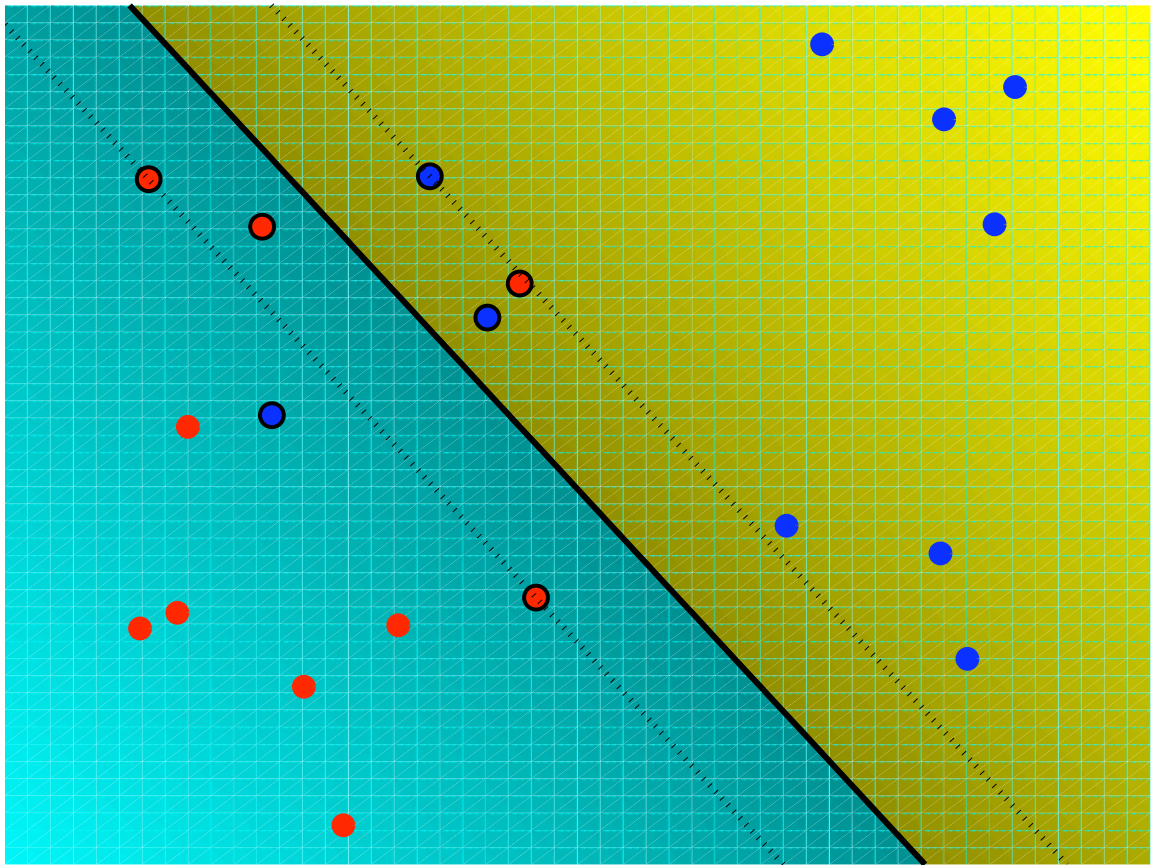
$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x_i}$$

  where the α_i are non-negative weighting factors. Thus,

$$h_{\mathbf{w},w_0}(\mathbf{x}) = \text{sgn}\left(\sum_{i=1}^{m} \alpha_i y_i \mathbf{x_i} \cdot \mathbf{x} + w_0\right)$$

- α_i is positive if and only if $\mathbf{x_i}$ lies on the edge of the margin *or* on the wrong side of the margin. That is, if $y_i(\mathbf{w} \cdot \mathbf{x_i} + w_0) \leq 1$.
- Such an $\mathbf{x_i}$ is a *support vector*.

Example



Feature expansions and nonlinear decision boundaries

- Linear SVMs always produce a decision boundary that is a hyperplane. For some data this is not appropriate.
- One way of getting a nonlinear decision boundary in the input space is to find a linear decision boundary in an expanded space. (As we've seen, e.g., for polynomial regression.)
- Thus, $\mathbf{x_i}$ is replaced by $\phi(\mathbf{x_i})$, where ϕ is called a "feature mapping"

- What's the big deal?

Feature-expanded optimization problem

Replacing $\mathbf{x_i}$ with $\phi(\mathbf{x_i})$, the optimization problem to find $\mathbf{w}$ and w_0 becomes:

$$\begin{array}{rl} \text{min} & \|\mathbf{w}\|^2 + C\sum_i \zeta_i \\ \text{w.r.t.} & \mathbf{w}, w_0, \zeta_i \\ \text{s.t.} & y_i(\mathbf{w}\cdot\phi(\mathbf{x_i}) + w_0) \geq (1-\zeta_i) \\ & \zeta_i \geq 0 \end{array}$$

or in dual form:

$$\begin{array}{rl} \text{max} & \sum_{i=1}^m \alpha_i - \frac{1}{2}\sum_{i,j=1}^m y_i y_j \alpha_i \alpha_j \phi(\mathbf{x_i})\cdot\phi(\mathbf{x_j}) \\ \text{w.r.t.} & \alpha_i \\ \text{s.t.} & 0 \leq \alpha_i \leq C \\ & \sum_{i=1}^m \alpha_i y_i = 0 \end{array}$$

Feature-expanded solution

- The optimal weights, in the expanded feature space, are $\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \phi(\mathbf{x_i})$.
- Classification is by the rule:

$$h_{\mathbf{w},w_0}(\mathbf{x}) = \text{sgn}\left(\sum_{i=1}^{m} \alpha_i y_i \phi(\mathbf{x_i}) \cdot \phi(\mathbf{x}) + w_0\right)$$

$\Rightarrow$ Observation: to solve the fitting problem in dual form and to make a classification prediction, we only ever need to computed dot-products of feature-expanded vectors.

Kernel functions

- Whenever a learning algorithm (such as SVMs) can be written in terms of dot-products, it can be generalized to kernels.
- A *kernel* is any function $K : \Re^n \times \Re^n \mapsto \Re$ which corresponds to a dot product for some feature mapping ϕ. That is, $K(\mathbf{x}_1, \mathbf{x}_2) = \phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2)$ for some ϕ.
- Conversely, by choosing feature mapping ϕ, we are implicitly choosing a Kernel function
- Recalling that $\phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2) = \cos A \|\mathbf{x}_1\| \|\mathbf{x}_2\|$ where A is the angle between the vectors, a Kernel function can be thought of as a notion of *similarity*.

$\Rightarrow$ We can substitute other notions of similarity (as long as they are Kernel functions)

Example: Quadratic kernel

- Let $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^2$.
- Is this a Kernel? Yes:

$$K(\mathbf{x}, \mathbf{z}) = \left(\sum_{i=1}^{n} x_i z_i\right)\left(\sum_{j=1}^{n} x_j z_j\right) = \sum_{i,j \in \{1 \ldots n\}} x_i z_i x_j z_j = \sum_{i,j \in \{1 \ldots n\}} (x_i x_j)(z_i z_j)$$

- Hence, it is a kernel, with feature mapping:

$$\phi(\mathbf{x}) = \langle x_1^2,\ x_1 x_2,\ \ldots,\ x_1 x_n,\ x_2 x_1,\ x_2^2,\ \ldots,\ x_n^2 \rangle$$

- The feature vector includes all squares of elements and all cross terms.
- Note some redundancy among the features – that's OK.
- Fitting the SVM puts a weight on each of these features.

Polynomial kernels

- More generally, $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^d$ is a Kernel, for any positive integer d.

$$K(\mathbf{x}, \mathbf{z}) = \left(\sum_{i=1}^{n} \mathbf{x}_i \mathbf{z}_i \right)^d$$

- If we expanded the sum above in the obvious way, we get n^d terms.
- Thus, this K is a kernel with a length n^d feature expansion.
- Terms are monomials (products of x_i) with total power equal to d.
- E.g., if $n = 2$ and $d = 3$, the (most direct) feature mapping is

$$\phi(\mathbf{x}) = \langle x_1^3, x_1^2 x_2, x_1^2 x_2, x_1 x_2^2, x_1^2 x_2, x_1 x_2^2, x_1 x_2^2, x_2^3 \rangle$$

A "curse of dimensionality"

- Suppose we want to use a polynomial Kernel $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^d = \phi(\mathbf{x}) \cdot \phi(\mathbf{z})$ to fit an SVM.
- If we try to solve the SVM in primal form, we have to work with some very big feature vectors:

$$\begin{array}{rl} \text{min} & \|\mathbf{w}\|^2 + C \sum_i \zeta_i \\ \text{w.r.t.} & \mathbf{w}, w_0, \zeta_i \\ \text{s.t.} & y_i(\mathbf{w} \cdot \phi(\mathbf{x_i}) + w_0) \geq (1 - \zeta_i) \\ & \zeta_i \geq 0 \end{array}$$

- Even making a prediction is computationally intensive:

$$h_{\mathbf{w}, w_0}(\mathbf{x}) = \text{sgn}(\mathbf{w} \cdot \phi(\mathbf{x}) + w_0)$$

The "kernel trick"

- If we work with the dual, we don't actually have to ever compute the feature mapping ϕ. We just have to compute the similarity K.
- That is, we can solve the dual for the α_i:

$$\begin{array}{rl} \text{max} & \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m y_i y_j \alpha_i \alpha_j K(\mathbf{x_i}, \mathbf{x_j}) \\ \text{w.r.t.} & \alpha_i \\ \text{s.t.} & 0 \leq \alpha_i \leq C \\ & \sum_{i=1}^m \alpha_i y_i = 0 \end{array}$$

- Keeping in mind that the optimal weights are of the form $\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \phi(\mathbf{x_i})$, we can make predictions as:

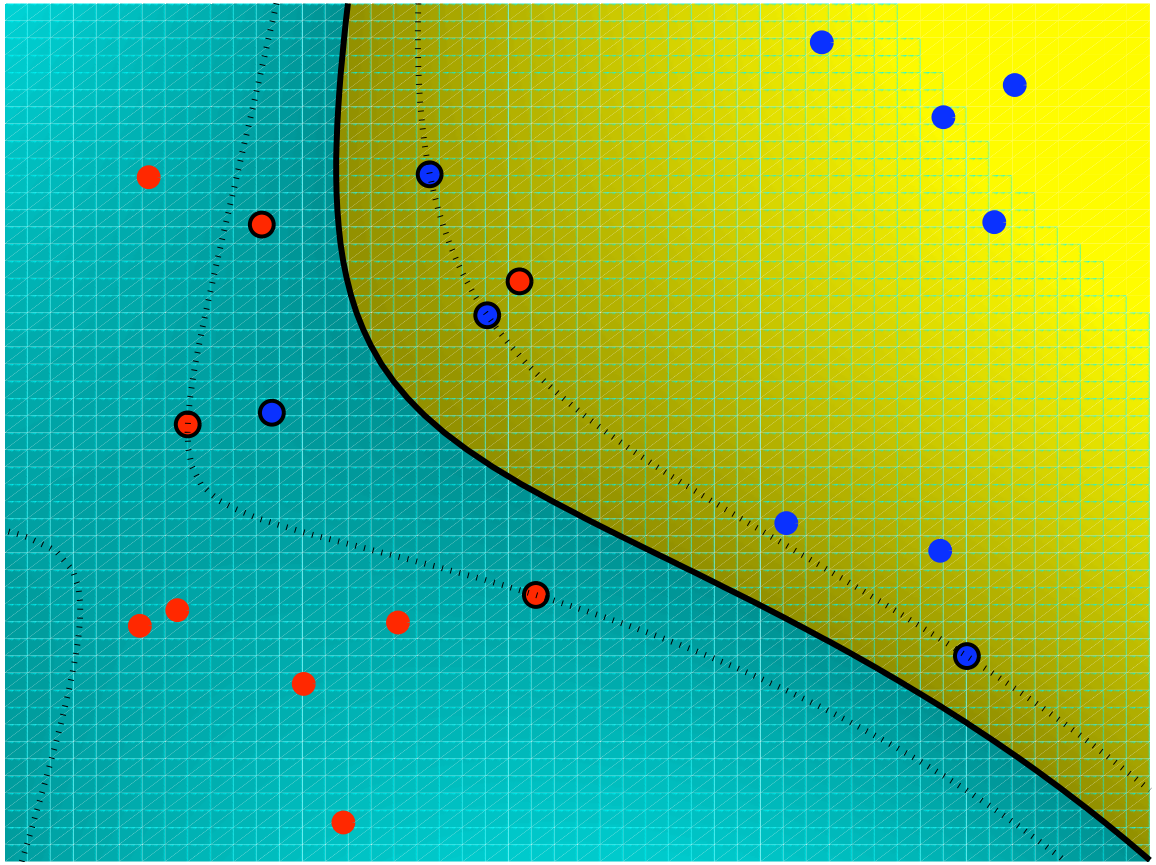
$$\begin{aligned} h_{\mathbf{w},w_0}(\mathbf{x}) &= \text{sgn}\left(\left(\sum_{i=1}^m \alpha_i y_i \phi(\mathbf{x_i})\right) \cdot \phi(\mathbf{x}) + w_0\right) \\ &= \text{sgn}\left(\sum_{i=1}^m \alpha_i y_i K(\mathbf{x_i}, \mathbf{x}) + w_0\right) \end{aligned}$$

- Often, $K(\cdot, \cdot)$ can be evaluated in $O(n)$ time—a big savings!

Some other (fairly generic) Kernel functions

- $K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^d$ – feature expansion has all monomial terms of $\leq d$ total power.
- Radial basis/Gaussian $K(\mathbf{x}, \mathbf{z}) = \exp(-\|\mathbf{x} - \mathbf{z}\|^2/s)$ – has infinite-dimensional feature expansion!
- Sigmoidal $K(\mathbf{x}, \mathbf{z}) = \tanh(c_1 \mathbf{x} \cdot \mathbf{z} + c_2)$

Example: Gaussian kernel



Application: Text classification

(Joachims, 1998)

- Evaluated several methods, including SVMs, on a suite of text classification problems
- Words were stemmed (e.g. learn, learning, learned $\rightarrow$ learn)
- Nondiscriminative stopwords and words occurring < 3 times ignored
- Of remaining words, considered a binary presence-absence feature
- 1000 features with greatest information gain retained, others discarded
- Each feature scaled by "inverse document frequency":

$$\log \frac{\#\text{ docs}}{\#\text{ docs with word } i}$$

Results

					SVM (poly) $d =$					SVM (rbf) $\gamma =$			
	Bayes	Rocchio	C4.5	k-NN	1	2	3	4	5	0.6	0.8	1.0	1.2
earn	95.9	96.1	96.1	97.3	98.2	98.4	**98.5**	98.4	98.3	**98.5**	98.5	98.4	98.3
acq	91.5	92.1	85.3	92.0	92.6	94.6	**95.2**	95.2	95.3	95.0	95.3	95.3	**95.4**
money-fx	62.9	67.6	69.4	78.2	66.9	72.5	75.4	74.9	**76.2**	74.0	75.4	**76.3**	75.9
grain	72.5	79.5	89.1	82.2	91.3	93.1	**92.4**	91.3	89.9	**93.1**	91.9	91.9	90.6
crude	81.0	81.5	75.5	85.7	86.0	87.3	88.6	**88.9**	87.8	**88.9**	89.0	88.9	88.2
trade	50.0	77.4	59.2	77.4	69.2	75.5	76.6	77.3	**77.1**	76.9	78.0	**77.8**	76.8
interest	58.0	72.5	49.1	74.0	69.8	63.3	67.9	73.1	**76.2**	74.4	75.0	**76.2**	76.1
ship	78.7	83.1	80.9	79.2	82.0	85.4	86.0	**86.5**	86.0	**85.4**	86.5	87.6	87.1
wheat	60.6	79.4	85.5	76.6	83.1	84.5	85.2	**85.9**	83.8	**85.2**	85.9	85.9	85.9
corn	47.3	62.2	87.7	77.9	86.0	86.5	85.3	**85.7**	83.9	**85.1**	85.7	85.7	84.5
microavg.	**72.0**	**79.9**	**79.4**	**82.3**	84.2	85.1	85.9	86.2	85.9	86.4	86.5	86.3	86.2
					combined: **86.0**					combined: **86.4**			

Figure 4: Precision/recall-breakeven point on the ten most frequent Reuters categories and microaveraged performance over all Reuters categories. k-NN, Rocchio, and C4.5 achieve highest performance at 1000 features (with $k = 30$ for k-NN and $\beta = 1.0$ for Rocchio). Naive Bayes performs best using all features.

Kernels for everyone!

A lot of SVM research has to do with defining new kernels functions, suitable to particular tasks / kinds of input objects, plus proving that they are indeed kernels.

- Information diffusion kernels (Lafferty and Lebanon, 2002)
- Diffusion kernels on graphs (Kondor and Jebara 2003)
- String kernels for text classification (Lodhi et al, 2002)
- String kernels for protein classification (e.g., Leslie et al, 2002)
- ... and others!

String kernels

- Very important for DNA matching, text classification, ...
- Example: in DNA matching, we use a sliding window of length k over the two strings that we want to compare
- The window is of a given size, and inside we can do various things:
  - Count exact matches
  - Weigh mismatches based on how bad they are
  - Count certain markers, e.g. AGT
- The kernel is the sum of these similarities over the two sequences
- How do we prove this is a kernel?

Establishing "kernelhood"

- Suppose someone hands you a function K. How do you know that it is a kernel?
- More precisely, given a function $K : \Re^n \times \Re^n \rightarrow \Re$, under what conditions can $K(\mathbf{x}, \mathbf{z})$ be written as a dot product $\phi(\mathbf{x}) \cdot \phi(\mathbf{z})$ for some feature mapping ϕ?

Kernel matrix

- Suppose we have an arbitrary set of input vectors $\mathbf{x_1}, \mathbf{x_2}, \ldots \mathbf{x_m}$
- The **kernel matrix** K corresponding to kernel function K is an $m \times m$ matrix such that $K_{ij} = K(\mathbf{x_i}, \mathbf{x_j})$ (notation is overloaded on purpose).
- What properties does the kernel matrix K have?
- Claims:

  1. K is symmetric
  2. K is positive semidefinite

- Note that these claims are consistent with the intuition that K is a "similarity" measure (and will be true regardless of the data)

Proving the first claim

If K is a valid kernel, then the kernel matrix is symmetric

$$K_{ij} = \phi(\mathbf{x_i}) \cdot \phi(\mathbf{x_j}) = \phi(\mathbf{x_j}) \cdot \phi(\mathbf{x_i}) = K_{ji}$$

Proving the second claim

If K is a valid kernel, then the kernel matrix is positive semidefinite
Proof: Consider an arbitrary vector $\mathbf{z}$

$$\begin{aligned}
\mathbf{z}^T K \mathbf{z} &= \sum_i \sum_j z_i K_{ij} z_j = \sum_i \sum_j z_i \left(\phi(\mathbf{x_i}) \cdot \phi(\mathbf{x_j})\right) z_j \\
&= \sum_i \sum_j z_i \left(\sum_k \phi_k(\mathbf{x_i}) \phi_k(\mathbf{x_j}) \right) z_j \\
&= \sum_k \sum_i \sum_j z_i \phi_k(\mathbf{x_i}) \phi_k(\mathbf{x_j}) z_j \\
&= \sum_k \left(\sum_i z_i \phi_k(\mathbf{x_i}) \right)^2 \geq 0
\end{aligned}$$

Mercer's theorem

- We have shown that if K is a kernel function, then for any data set, the corresponding kernel matrix K defined such that $K_{ij} = K(\mathbf{x_i}, \mathbf{x_j})$ is symmetric and positive semidefinite
- Mercer's theorem states that the reverse is also true!
  Given a function $K : \Re^n \times \Re^n \rightarrow \Re$, K is a kernel *if and only if*, for any data set, the corresponding kernel matrix is positive and semidefinite
- The reverse direction of the proof is much harder
- This result gives us a way to *check* is a given function is a kernel, by checking these two properties of its kernel matrix.

Symptoms of overfitting in SVMs

- Low margin
- Large number of support vectors
- If you look at the kernel matrix (also called Gram matrix) it is almost diagonal
  - This means each point is only similar to itself
  - So the kernel used is not really adequate (it does not generalize over the data

Getting this to work in practice

- Choice of kernel
- Choice of regularization parameter
- These control the overfitting: always check the margin/number of support vectors or do cross-validation

Interpretability

- More interpretable than neural nets if you look at the machine and the misclassifications
- E.g. Ovarian cancer data (Haussler) - 31 tissue samples of 3 classes, misclassified examples wronlgy labelled
- *No* biological plausibility

Complexity

- Quadratic programming is expensive in the number of training examples
- Platt's algorithm is quite fast though
- Best packages can handle 10,000-20,000 instances, not more
- On the other hand, number of attributes can be very high (strength compared to neural nets)
- Evaluating a SVM requires taking the dot product of an instance with the support vectors, which is *slow if there are a lot of support vectors*.
- Dictionary methods attempt to select data points and/or support vectors

Applications of SVMs

- The biggest strength of SVMs is dealing with large numbers of features (which relies on the kernel trick and the control of overfitting)
- Many successful applications in:
  - Text classification (e.g. Joachims, 1998)
  - Object detection (e.g. Osuna, Freund and Girosi, 1997)
  - Object recognition (e.g. Pontil and Verri, 1998)
  - Bioinformatics (e.g. lee et al, 2002)
- SVMs are considered by many the state-of-the art approach to classification
- Experimentally, SVMs and neural nets are roughly tied based on evidence to date, each has its own preferred applications

Summary of Perceptrons & Support vector machines

- A perceptron is basically just a linear decision boundary
- For linearly separable data, the gradient-like perceptron training rule can find weights that separate the data
- A linear support vector machine maximizes the margin of the decision boundary
- We can modify the SVM optimization to allow for misclassified examples
- We can define other notions of similarity — Kernels — the allow nonlinear decision boundaries (in the original space)
- The kernel trick allows us to work efficiently with Kernels even if they have large feature expansions — because we only ever need to compute the Kernel, not the actual features