# Lecture 5: More on Kernels. SVM regression and classification

- More on kernels: How to tell if a function is a kernel?
- SVM classification
- SVM regression

# The “kernel trick”

- Recall: kernel functions are ways of expressing dot-products in some feature space:

$$K(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x}) \cdot \phi(\mathbf{z})$$

- In many cases, $K$ can be computed in time that depends on the size of the inputs $\mathbf{x}$ not the size of the feature space $\phi(\mathbf{x})$
- If we work with a “dual” representation of the learning algorithm, we do not actually have to compute the feature mapping $\phi$. We just have to compute the similarity $K$.

# Polynomial kernels

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

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

- If we expanded the sum above in the obvious way, we get $n^d$ terms (i.e. feature expansion)
- Terms are monomials (products of $x_i$) with total power equal to $d$.
- *Curse of dimensionality:* it is very expensive both to optimize and to predict in primal form
- However, *evaluating the dot-product of any two feature vectors can be done using $K$ in $O(n)$*!

# 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 kernel:

$$K(\mathbf{x},\mathbf{z}) = \exp(-\|\mathbf{x}-\mathbf{z}\|^2/2\sigma^2)$$

  The kernel has an infinite-dimensional feature expansion, but dot-products can still be computed in $O(n)$!

- Sigmoidal kernel:

$$K(\mathbf{x},\mathbf{z}) = \tanh(c_1\mathbf{x}\cdot\mathbf{z}+c_2)$$

# Recall: Dual-view regression

- By re-writing the parameter vector as a linear combination of instances and solving, we get:

$$\mathbf{a} = (\mathbf{K} + \lambda \mathbf{I}_m)^{-1}\mathbf{y}$$

- The *feature mapping is not needed* either to learn or to make predictions!
- This approach is useful if the feature space is very large

# Making predictions in the dual view

- For a new input $\mathbf{x}$, the prediction is:

$$h(\mathbf{x}) = \mathbf{w}^\top \phi(\mathbf{x}) = \mathbf{a}^\top \mathbf{\Phi} \phi(\mathbf{x}) = \mathbf{k}(\mathbf{x})^\top (\mathbf{K} + \lambda \mathbf{I}_m)^{-1} \mathbf{y}$$

  where $\mathbf{k}(\mathbf{x})$ is an $m$-dimensional vector, with the $i$th element equal to $K(\mathbf{x}, \mathbf{x}_i)$

- That is, the $i$th element has the similarity of the input to the $i$th instance
- The features are not needed for this step either!
- This is a *non-parametric* representation - its size scales with the number of instances.

# Kernels

- A lot of current research has to do with defining new kernels functions, suitable to particular tasks / kinds of input objects
- Many kernels are available:
  - 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!

# Example: 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 $K : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$, 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 $\phi$?
- We want a general recipe, which does not require explicitly defining $\phi$ every time

# Kernel matrix

- Suppose we have an arbitrary set of input vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_m$
- The *kernel matrix (or Gram matrix)* $\mathbf{K}$ corresponding to kernel function $K$ is an $m \times m$ matrix such that $\mathbf{K}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ (notation is overloaded on purpose).
- What properties does the kernel matrix $\mathbf{K}$ have?
- Claims:
  1. $\mathbf{K}$ is symmetric
  2. $\mathbf{K}$ 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

$$\mathbf{K}_{ij} = \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) = \phi(\mathbf{x}_j) \cdot \phi(\mathbf{x}_i) = \mathbf{K}_{ji}$$

# Proving the second claim

If $K$ is a valid kernel, then the kernel matrix is positive semidefinite

Proof: Consider an arbitrary vector $\mathbf{z}$

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

# Mercer's theorem

- We have shown that if $K$ is a kernel function, then for any data set, the corresponding kernel matrix $\mathbf{K}$ defined by $\mathbf{K}_{ij} = K(\mathbf{x_i}, \mathbf{x_j})$ is symmetric and positive semidefinite
- Mercer's theorem states that the reverse is also true:

  Given a function $K : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$, *$K$ is a kernel if and only if, for any data set, the corresponding kernel matrix is symmetric and positive semidefinite*
- The reverse direction of the proof is much harder (see e.g. Vapnik's book for details)
- This result gives us a way to check if a given function is a kernel, by checking these two properties of its kernel matrix.
- Kernels can also be obtained by combining other kernels, or by learning from data
- Kernel learning may suffer from overfitting (kernel matrix close to diagonal)

# More on RKHS

- Mercer's theorem tells us that a function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel (i.e. it corresponds to the inner product in some feature space) if and only if it is positive semi-definite.
- The feature space is the reproducing kernel Hilbert space (RKHS)

$$\mathcal{H} = \left\{ \sum_j \alpha_j K(z_j, \cdot) \ : \ z_j \in \mathcal{X},\ \alpha_j \in \mathbb{R} \right\}$$

  with inner product $\langle K(z,\cdot), K(z',\cdot)\rangle_{\mathcal{H}} = K(z, z')$.
- The term reproducing comes from the reproducing property of the kernel function:

$$\forall f \in \mathcal{H},\ x \in \mathcal{X} \ : \quad f(x) = \langle f(\cdot), K(x,\cdot)\rangle_{\mathcal{H}}$$

- Recall that the solution of the regularized least square in the feature space associated to a kernel function $K$ has the form $h(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i K(\mathbf{x}_i, \mathbf{x})$. This is a particular case of the representer theorem...

# Representer Theorem

**Theorem 1.** *Let* $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *be a positive definite kernel and let* $\mathcal{H}$ *be the corresponding RKHS.*

*Then for any training sample* $\mathcal{S} = \{(x_i, y_i)\}_{i=1}^m \subset \mathcal{X} \times \mathbb{R}$*, any loss function* $\ell : (\mathcal{X} \times \mathbb{R} \times \mathbb{R})^m \to \mathbb{R}$ *and any real-valued non-decreasing function* $g$*, the solution of the optimization problem*

$$\arg\min_{f \in \mathcal{H}} \ell\left((x_1, y_1, f(x_1)), \cdots, (x_m, y_m, f(x_m))\right) + g(\|f\|_{\mathcal{H}})$$

*admits a representation of the form*

$$f^*(\cdot) = \sum_{i=1}^m \alpha_i K(\mathbf{x}_i, \cdot).$$

[Schlkopf, Herbrich and Smola. *A generalized representer Theorem.* COLT 2001.]

# Regularization in the dual view

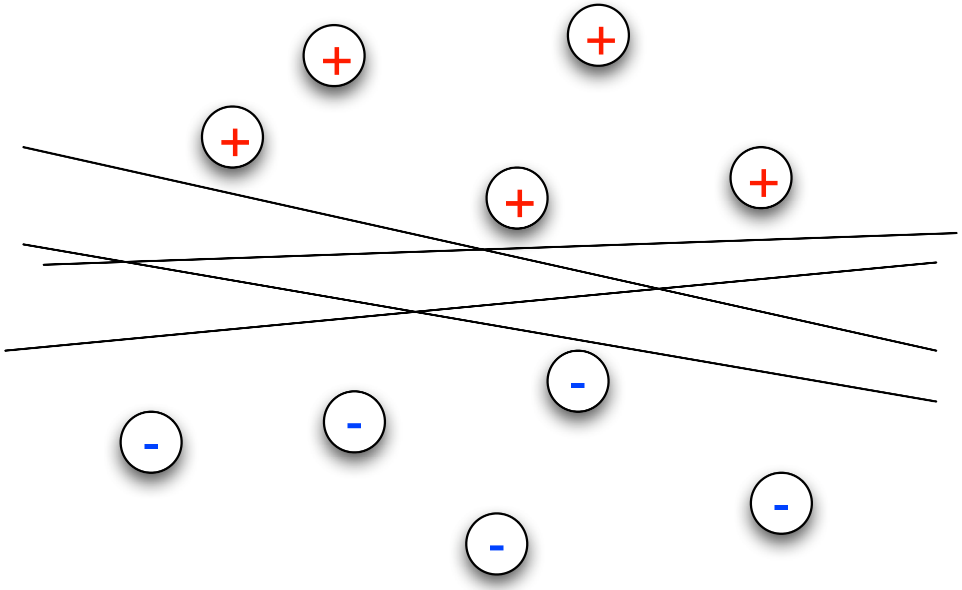
- We want to penalize the function we are trying to estimate (to keep it simple)
- Assume this is part of a reproducing kernel Hilbert space
- We want to minimize:

$$J(h) = \frac{1}{2}\sum_{i=1}^{n}(y_i - h(\mathbf{x}_i))^2 + \frac{\lambda}{2}||h||^2_{\mathcal{H}}$$

- If we put a Gaussian prior on $h$, and solve, we obtain *Gaussian process regression*

# Binary classification revisited

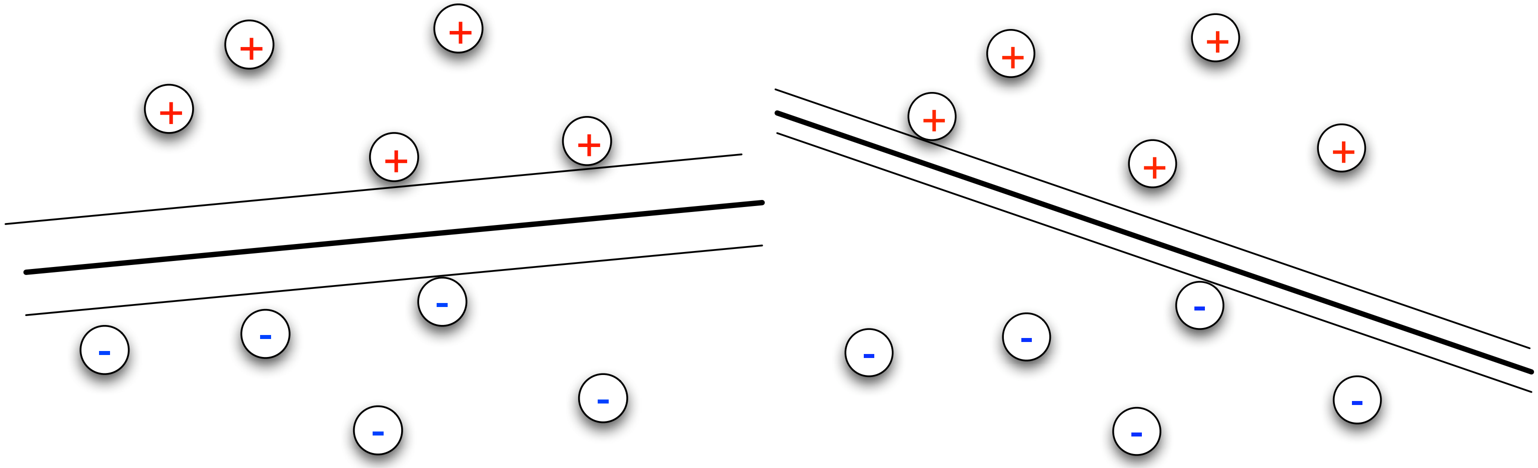
- Consider a linearly separable binary classification data set $\{\mathbf{x}_i, y_i\}_{i=1}^m$.
- There is an infinite number of hyperplanes that separate the classes:



- Which plane is best?
- Relatedly, for a given plane, for which points should we be most confident in the classification?

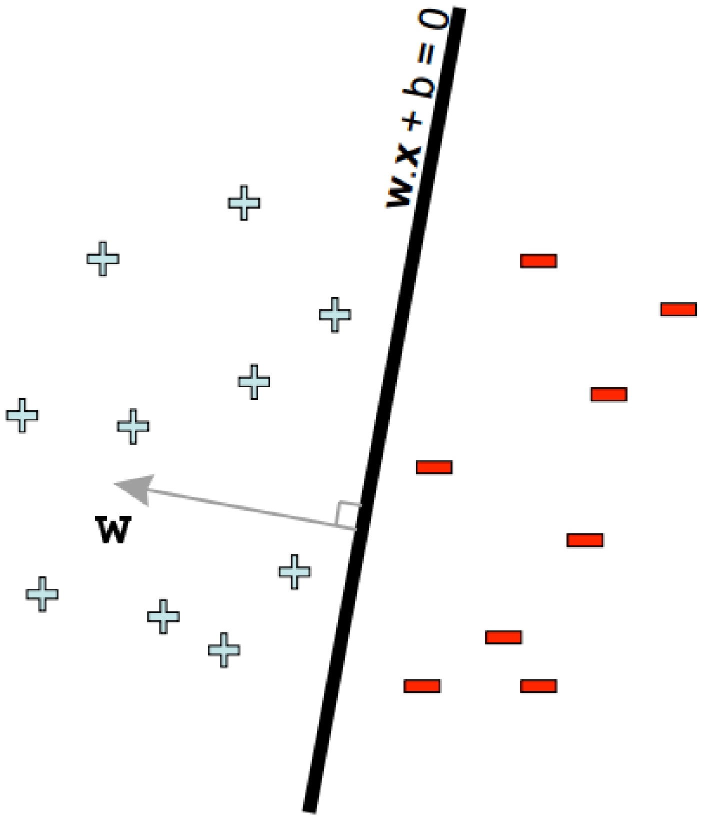
# The margin, and linear SVMs

- For a given separating hyperplane, the *margin* is two times the (Euclidean) distance from the hyperplane to the nearest training example.



- It is the width of the "strip" around the decision boundary containing no training examples.
- A linear SVM is a perceptron for which we choose $\mathbf{w}, w_0$ so that margin is maximized

# Hyperplanes and scale invariance

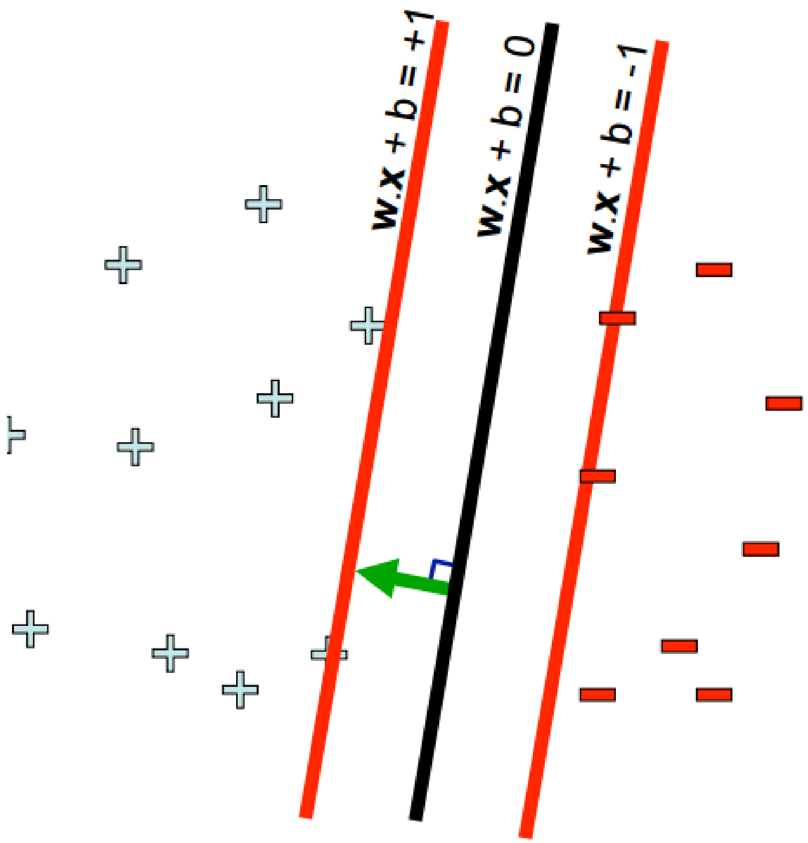


- Hyperplane: $\mathbf{w}^\top \mathbf{x} + b = 0$.

$\Rightarrow$ Scale invariance: $(\alpha \mathbf{w})^\top \mathbf{x} + \alpha b = 0$ define the same hyperplane for any scalar $\alpha \in \mathbb{R}$.

Figures taken form David Sontag's lecture slides:
`http://people.csail.mit.edu/dsontag/courses/ml13/slides/lecture3.pdf`

# Hyperplanes and scale invariance



- Hyperplane: $\mathbf{w}^\top \mathbf{x} + b = 0$.

⇒ Scale invariance: $\alpha \mathbf{w}^\top \mathbf{x} + \alpha b = 0 \ldots$

- Workaround: we set the scale by enforcing

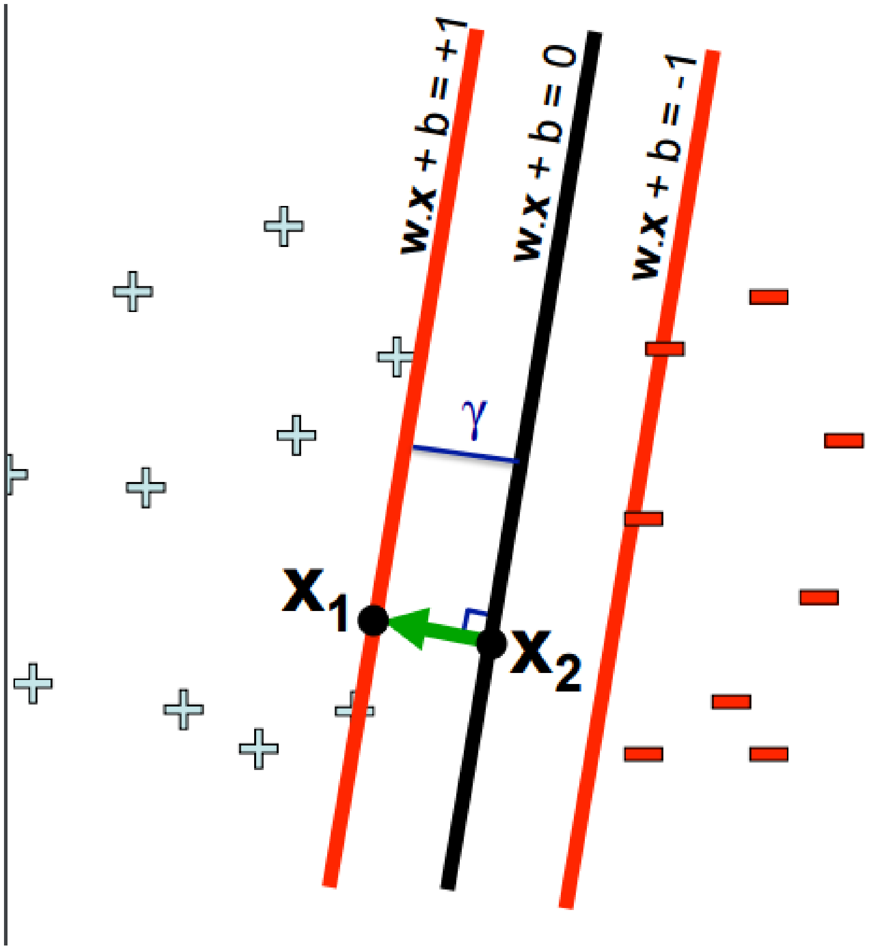
$$\begin{array}{ll} \mathbf{w}^\top \mathbf{x} + b \geq 1 & \text{for all positive examples} \\ \mathbf{w}^\top \mathbf{x} + b \leq -1 & \text{for all negative examples} \end{array}$$

→ equivalently, we want to satisfy the linear constraints

$$y_i(\mathbf{w}^\top \mathbf{x} + b) \geq 1$$

for all $i$ (here $\mathcal{Y} = \{-1, 1\}$).

# Margin as a function of the normal vector



- Let $\mathbf{x}_1$ be a point on the boundary and $\mathbf{x}_2$ its projection on the hyperplane:

$$\mathbf{w}^\top \mathbf{x}_1 + b = 1$$

$$\mathbf{w}^\top \mathbf{x}_2 + b = 0$$

  We get $\mathbf{w}^\top(\mathbf{x}_1 - \mathbf{x}_2) = 1$.

- But we also know that

$$\mathbf{x}_1 - \mathbf{x}_2 = \gamma \frac{\mathbf{w}}{\|\mathbf{w}\|}$$

- Hence $\gamma = \dfrac{1}{\|\mathbf{w}\|}$: maximizing the margin is equivalent to minimizing the norm of $\mathbf{w}$!

# SVM final formulation

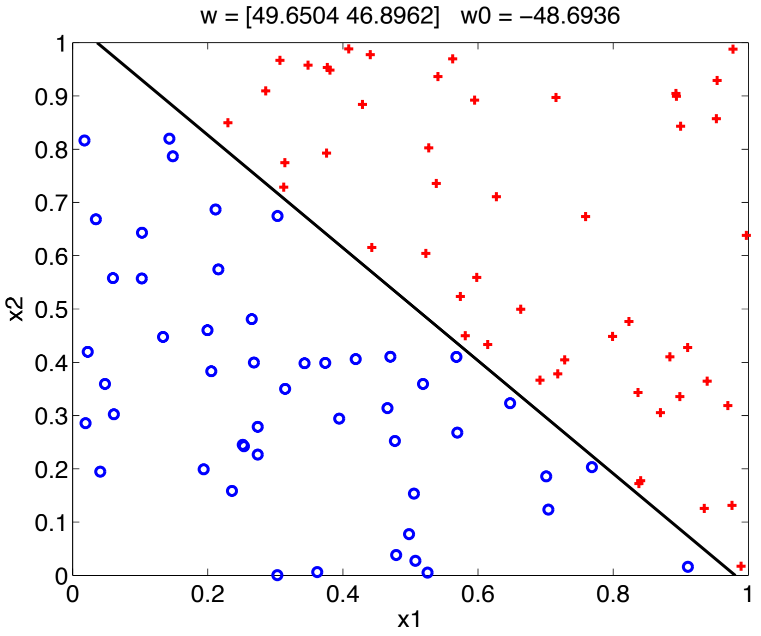
- Let's minimize $\|\mathbf{w}\|^2$ instead of $\|\mathbf{w}\|$.
(it will be easier and taking the square is a monotone transformation, as $\|\mathbf{w}\|$ is postive, so this doesn't change the optimal solution.)
- This gets us to:

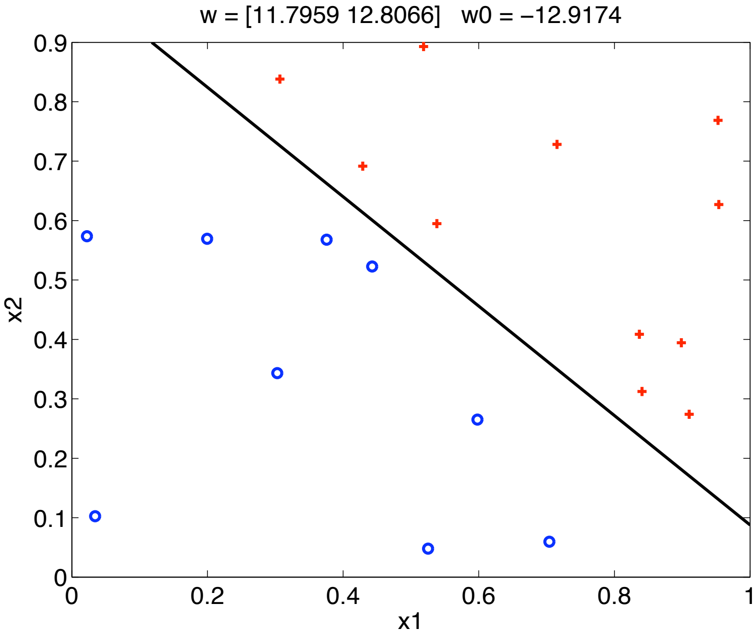
$$\begin{array}{rl} \text{min} & \|\mathbf{w}\|^2 \\ \text{w.r.t.} & \mathbf{w}, w_0 \\ \text{s.t.} & y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) \geq 1 \end{array}$$

- This we can solve! How?
  - It is a *quadratic programming* (QP) problem—a standard type of optimization problem[1] for which many efficient packages are available.
  - Better yet, it's a convex (positive semidefinite) QP

[1] optimization of a quadratic function of several variables subject to linear constraints on these variables.

# Example





We have a solution, but no support vectors yet...

# Lagrange multipliers for inequality constraints (revisited)

- Suppose we have the following optimization problem, called *primal*:

$$\min_{\mathbf{w}} f(\mathbf{w})$$

$$\text{such that } g_i(\mathbf{w}) \quad \leq \quad 0,\ i = 1 \ldots k$$

- We define the *Lagrangian*:

$$L(\mathbf{w}, \boldsymbol{\alpha}) = f(\mathbf{w}) + \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}), \tag{1}$$

where $\alpha_i,\ i = 1 \ldots k$ are the Lagrange multipliers.

# A different optimization problem

$$L(\mathbf{w}, \boldsymbol{\alpha}) = f(\mathbf{w}) + \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w})$$

- Consider $\mathcal{P}(\mathbf{w}) = \max_{\alpha:\alpha_i \geq 0} L(\mathbf{w}, \alpha)$
- Observe that the following is true:

$$\mathcal{P}(\mathbf{w}) = \begin{cases} f(\mathbf{w}) & \text{if all constraints are satisfied} \\ +\infty & \text{otherwise} \end{cases}$$

- Hence, instead of computing $\min_{\mathbf{w}} f(\mathbf{w})$ subject to the original constraints, we can compute:

$$p^* = \min_{\mathbf{w}} \mathcal{P}(\mathbf{w}) = \min_{\mathbf{w}} \max_{\alpha:\alpha_i \geq 0} L(\mathbf{w}, \alpha)$$

# Dual optimization problem

- We defined the primal problem:

$$p^* = \min_{\mathbf{w}} \max_{\alpha:\alpha_i \geq 0} L(\mathbf{w}, \alpha)$$

- The dual problem is obtained by swapping $\min$ and $\max$:

$$d^* = \max_{\alpha:\alpha_i \geq 0} \min_{\mathbf{w}} L(\mathbf{w}, \alpha)$$

- We can show that $d^* \leq p^*$:
  - Let $p^* = L(w^p, \alpha^p)$, let $d^* = L(w^d, \alpha^d)$.
  - Then $d^* = L(w^d, \alpha^d) \leq L(w^p, \alpha^d) \leq L(w^p, \alpha^p) = p^*$.
- The non-negative number $p^* - d^*$ is called the duality gap.

# Dual optimization problem (cont'd)

- Slater's condition: if $f$ (objective) and the $g_i$'s (constraints) are convex, and the $g_i$'s can all be satisfied simultaneously for some $\mathbf{w}$, then we have equality: $d^* = p^* = L(\mathbf{w}^*, \alpha^*)$.

→ Which means that the two problems are equivalent!

- Moreover $\mathbf{w}^*, \alpha^*$ solve the primal and dual if and only if they satisfy the following conditions (called Karush-Kunh-Tucker):

$$\begin{aligned}
\frac{\partial}{\partial w_i} L(\mathbf{w}^*, \alpha^*) &= 0, \; i = 1 \dots n \quad (2) \\
\alpha_i^* g_i(\mathbf{w}^*) &= 0, \; i = 1 \dots k \quad (3) \\
g_i(\mathbf{w}^*) &\leq 0, \; i = 1 \dots k \quad (4) \\
\alpha_i^* &\geq 0, \; i = 1 \dots k \quad (5)
\end{aligned}$$

# Back to maximum margin perceptron

- We wanted to solve (rewritten slightly):

$$\begin{array}{rl} \text{min} & \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{w.r.t.} & \mathbf{w}, w_0 \\ \text{s.t.} & 1 - y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) \leq 0 \end{array}$$

- The Lagrangian is:

$$L(\mathbf{w}, w_0, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 + \sum_i \alpha_i(1 - y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0))$$

- The primal problem is: $\min_{\mathbf{w},w_0} \max_{\alpha:\alpha_i\geq 0} L(\mathbf{w}, w_0, \alpha)$
- We will solve the dual problem: $\max_{\alpha:\alpha_i\geq 0} \min_{\mathbf{w},w_0} L(\mathbf{w}, w_0, \alpha)$
- In this case, the optimal solutions coincide, because we have a quadratic objective and linear constraints (both of which are convex).

# Solving the dual

- Lagrangian: $L(\mathbf{w}, w_0, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 + \sum_i \alpha_i(1 - y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0))$
- From KKT (2), the derivatives of $L(\mathbf{w}, w_0, \alpha)$ wrt $\mathbf{w}, w_0$ should be $0$:

$$\frac{\partial L}{\partial w_0} = -\sum_i \alpha_i y_i \quad \Rightarrow \quad \sum_i \alpha_i y_i = 0$$

$$\nabla_{\mathbf{w}} L = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i \quad \Rightarrow \quad \mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

- Observe that $\alpha_i > 0$ implies that the corresponding constraint is tight, i.e. $y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) = 1$, from which we obtain

$$w_0 = y_i - \mathbf{w} \cdot \mathbf{x}_i \qquad \text{for all } i \text{ such that } \alpha_i > 0.$$

⇒ Just like for the perceptron with zero initial weights, the optimal solution for $\mathbf{w}$ is a linear combination of the $\mathbf{x}_i$.

- The output is

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

⇒ Output depends on weighted dot product of input vector with training examples

# Solving the dual (cont'd)

- By plugging these back into the expression for $L$, we get:

$$\max_{\alpha} \sum_{i} \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

with constraints: $\alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$

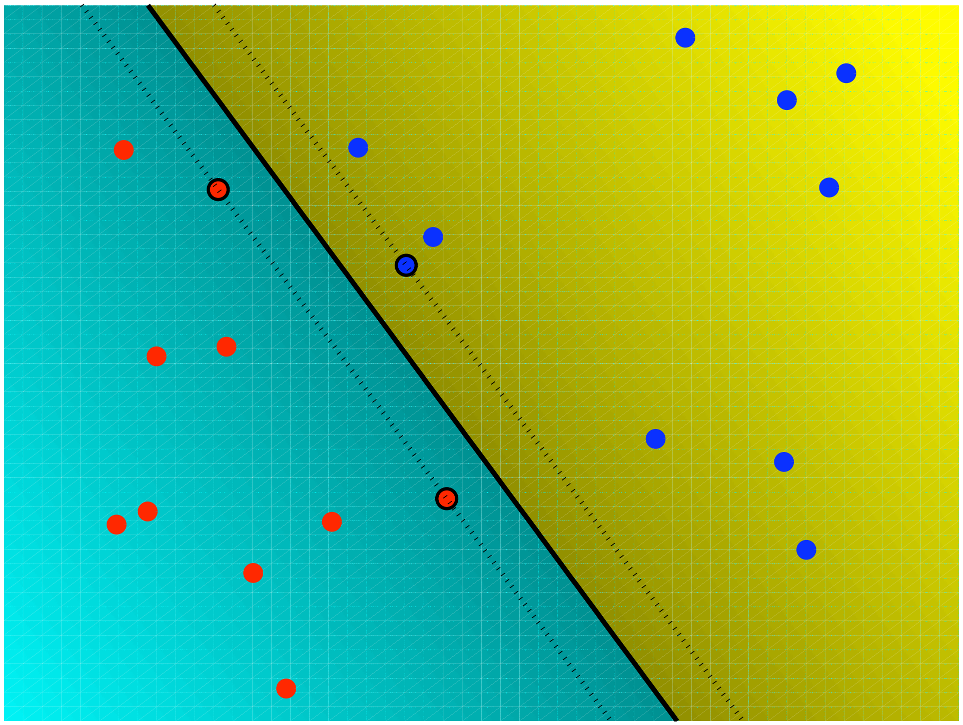
# The support vectors

- Suppose we find optimal $\alpha$s (e.g., using a standard QP package)
- The $\alpha_i$ will be $> 0$ only for the points for which $1 - y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) = 0$
- These are the points lying on the edge of the margin, and they are called *support vectors*, because they define the decision boundary
- The output of the classifier for query point $\mathbf{x}$ is computed as:

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

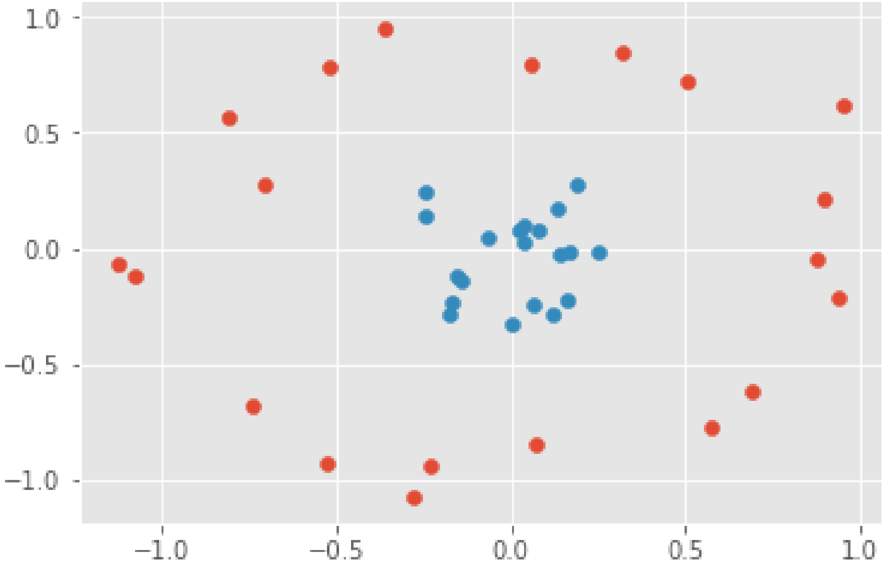
Hence, the output is determined by computing the *dot product of the point with the support vectors*!

# Example



Support vectors are in bold

# Non-linearly separable data



- A linear boundary might be too simple to capture the class structure.
- One way of getting a nonlinear decision boundary in the input space is to find a linear decision boundary in an expanded space (e.g., for polynomial regression.)
- Thus, $\mathbf{x}_i$ is replaced by $\phi(\mathbf{x}_i)$, where $\phi$ is called a *feature mapping*

# Margin optimization in feature space

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

$$\begin{array}{rl} \text{min} & \|\mathbf{w}\|^2 \\ \text{w.r.t.} & \mathbf{w}, w_0 \\ \text{s.t.} & y_i(\mathbf{w} \cdot \phi(\mathbf{x}_i) + w_0) \geq 1 \end{array}$$

- Dual form:

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

⇒ We just need to compute $\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$ for each $i, j$ to solve the dual problem, never need to compute the feature map explicitly...

# Feature space solution

- The optimal weights, in the expanded feature space, are given by

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \phi(\mathbf{x}_i) \quad \text{and} \quad w_0 = y_j - \sum_{i=1}^{m} \alpha_i y_i \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j)$$

  where $j$ is such that $\alpha_j > 0$.

- Classification of an input $\mathbf{x}$ is given by:

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

⇒ To solve the SVM optimization problem in dual form and to make a prediction, *we only need to compute dot-products of feature vectors*.

⇒ SVMs can straightforwardly be kernelized!

# The "kernel trick"

- If we work with the dual, we do not actually have to ever compute the feature mapping $\phi$. We just have to compute the similarity $K$.
- That is, we can solve the dual for the $\alpha_i$:

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

- The class of a new input $\mathbf{x}$ is computed as:

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

# Regularization with SVMs

- Kernels are a powerful tool for allowing non-linear, complex functions
- But now the number of parameters can be as high as the number of instances!
- With a very specific, non-linear kernel, each data point may be in its own partition
- With linear and logistic regression, we used regularization to avoid overfitting
- We need a method for allowing regularization with SVMs as well.

# Soft margin SVM

- Recall that in the linearly separable case, we compute the solution to the following optimization problem:

$$\begin{array}{rl} \text{min} & \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{w.r.t.} & \mathbf{w}, w_0 \\ \text{s.t.} & y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) \geq 1 \end{array}$$

- If we want to allow misclassifications, we can relax the constraints to:

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + w_0) \geq 1 - \xi_i$$

- If $\xi_i \in (0, 1)$, the data point is within the margin
- If $\xi_i \geq 1$, then the data point is misclassified
- We define the *soft error* as $\sum_i \xi_i$
- We will have to change the criterion to reflect the soft errors

# New problem formulation with soft errors

Instead of:

$$\begin{array}{rl} \text{min} & \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{w.r.t.} & \mathbf{w}, w_0 \\ \text{s.t.} & y_i(\mathbf{w}\cdot\mathbf{x}_i + w_0) \geq 1 \end{array}$$

we want to solve:

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

- Note that soft errors include points that are misclassified, as well as points within the margin
- There is a linear penalty for both categories
- The choice of the *constant $C$ controls overfitting*

# A built-in overfitting knob

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

- If $C$ is $0$, there is no penalty for soft errors, so the focus is on maximizing the margin, even if this means more mistakes
- If $C$ is very large, the emphasis on the soft errors will cause decreasing the margin, if this helps to classify more examples correctly.
- Internal cross-validation is a good way to choose $C$ appropriately

# Lagrangian for the new problem

- Like before, we can write a Lagrangian for the problem and then use the dual formulation to find the optimal parameters:

$$\begin{aligned} L(\mathbf{w}, w_0, \alpha, \xi, \mu) &= \frac{1}{2}||\mathbf{w}||^2 + C\sum_i \xi_i \\ &+ \sum_i \alpha_i \left(1 - \xi_i - y_i(\mathbf{w}_i \cdot \mathbf{x}_i + w_0)\right) + \sum_i \mu_i \xi_i \end{aligned}$$

- All the previously described machinery can be used to solve this problem
- Note that in addition to $\alpha_i$ we have coefficients $\mu_i$, which ensure that the errors are positive, but do not participate in the decision boundary

# Soft margin optimization with kernels

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

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

- Dual form and solution have similar forms to what we described last time, but in terms of kernels

# Getting SVMs to work in practice

- Two important choices:
  - Kernel (and kernel parameters)
  - Regularization parameter $C$
- The parameters may interact!

  E.g. for Gaussian kernel, the larger the width of the kernel, the more biased the classifier, so low $C$ is better
- Together, these control overfitting: always do an internal parameter search, using a validation set!
- Overfitting symptoms:
  - Low margin
  - Large fraction of instances are support vectors

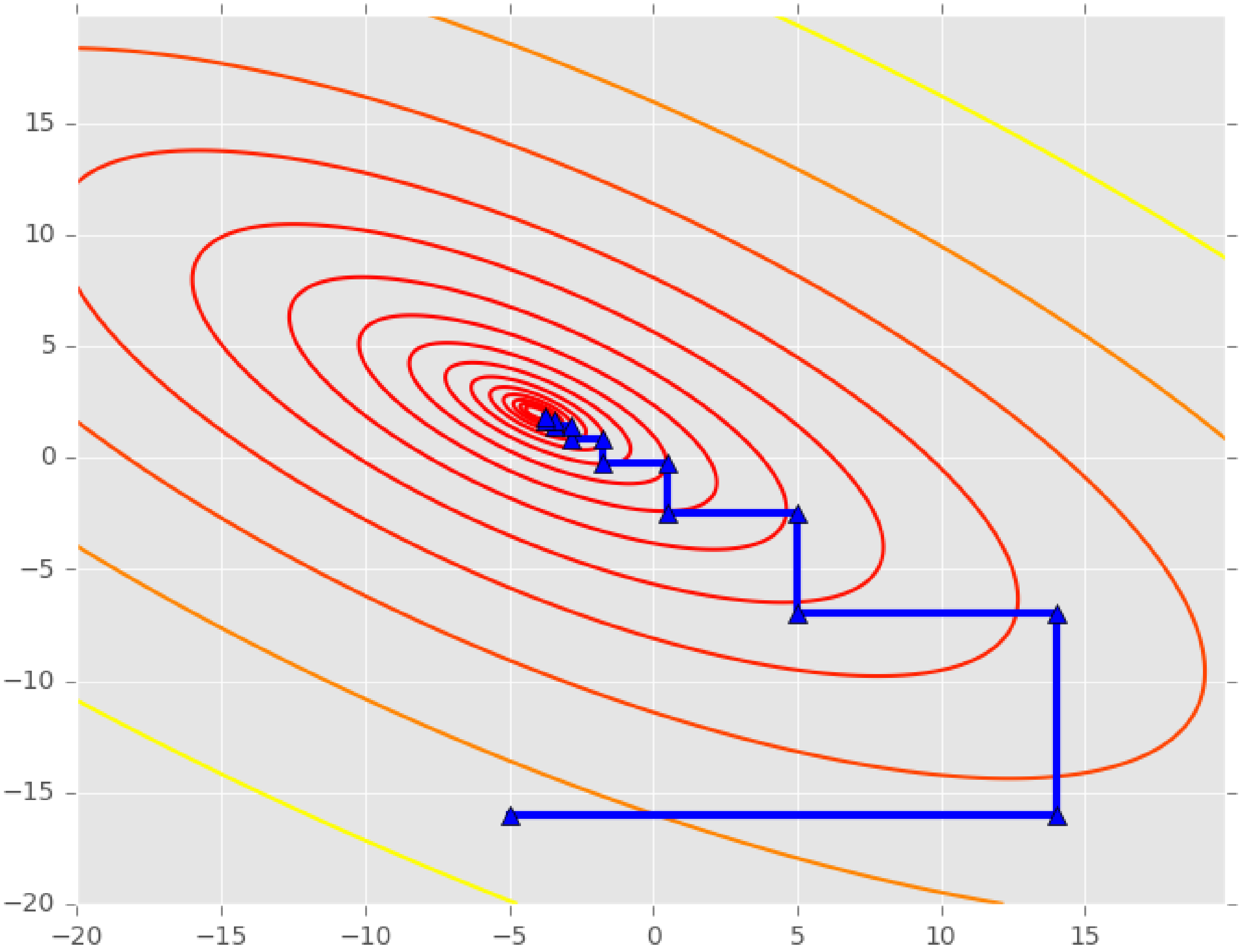
# Solving the quadratic optimization problem

- Many approaches exist
- Because we have constraints, gradient descent does not apply directly (the optimum might be outside of the feasible region)
- Platt's algorithm is the fastest current approach, based on *coordinate ascent*

# Coordinate ascent

- Suppose you want to find the maximum of some function $F(\alpha_1, \ldots \alpha_n)$ (the $\alpha_i$ could be scalars, vectors, matrices...)
- Coordinate ascent optimizes the function by repeatedly picking an $\alpha_i$ and optimizing it, while all other parameters are fixed:
  1. Initialize the $\alpha_i$'s
  2. Repeat until convergence (or stopping criterion):
     - Pick an $i$ (round-robin, random, ...)
     - Solve $\alpha_i \leftarrow \arg\min_{\alpha_i} F(\alpha_1, \cdots, \alpha_n)$
- There are different ways of looping through the parameters:
  - Round-robin
  - Repeatedly pick a parameter at random
  - Choose next the variable expected to make the largest improvement
  - ...

# Example



# Our optimization problem (dual form)

$$\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j))$$

with constraints: $0 \leq \alpha_i \leq C$ and $\sum_i \alpha_i y_i = 0$

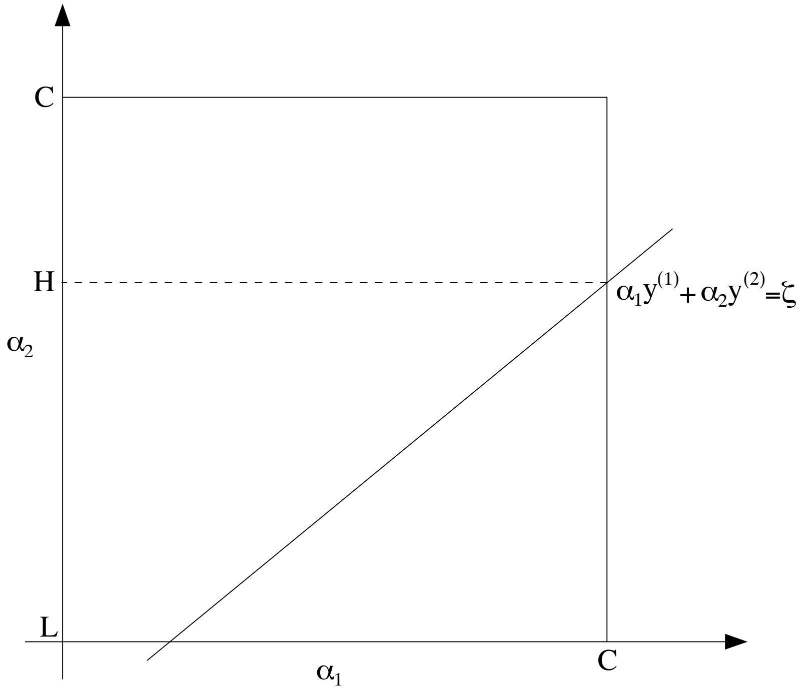
- Suppose we want to optimize for $\alpha_1$ while $\alpha_2, \ldots \alpha_n$ are fixed
- We cannot do it because $\alpha_1$ will be completely determined by the last constraint: $\alpha_1 = -y_1 \sum_{i=2}^{m} \alpha_i y_i$
- Instead, we have to optimize *pairs of parameters* $\alpha_i, \alpha_j$ together

# SMO

- Suppose that we want to optimize $\alpha_1$ and $\alpha_2$ together, while all other parameters are fixed.
- We know that $y_1\alpha_1 + y_2\alpha_2 = -\sum_{i=1}^{m} y_i\alpha_i = \xi$, where $\xi$ is a constant
- So $\alpha_1 = y_1(\xi - y_2\alpha_2)$ (because $y_1$ is either $+1$ or $-1$ so $y_1^2 = 1$)
- This defines a line, and any pair $\alpha_1, \alpha_2$ which is a solution has to be on the line

# SMO (II)

- We also know that $0 \leq \alpha_1 \leq C$ and $0 \leq \alpha_2 \leq C$, so the solution has to be on the line segment inside the rectangle below



# SMO(III)

- By plugging $\alpha_1$ back in the optimization criterion, we obtain a quadratic function of $\alpha_2$, whose optimum we can find exactly
- If the optimum is inside the rectangle, we take it.
- If not, we pick the closest intersection point of the line and the rectangle
- This procedure is very fast because all these are simple computations.

# Complexity

- Quadratic programming is expensive in the number of training examples
- Platt's SMO algorithm is quite fast though, and other fancy optimization approaches are available
- Best packages can handle $50,000+$ instances, but not more than $100,000$
- On the other hand, number of attributes can be very high (strength compared to neural nets)
- Evaluating a SVM is *slow if there are a lot of support vectors*.
- Dictionary methods attempt to select a subset of the data on which to train.

# Support Vector Regression

- In regression problems, so far we have been trying to minimize mean-squared error:

$$\sum_i (y_i - (\mathbf{w} \cdot \mathbf{x_i} + w_0))^2$$

- In SVM regression, we will be interested instead in minimizing absolute error:

$$\sum_i |y_i - (\mathbf{w} \cdot \mathbf{x_i} + w_0)|$$

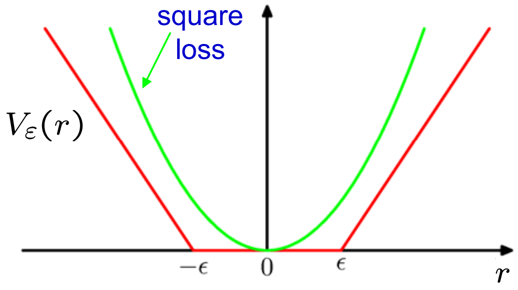
- This is more *robust to outliers* than the squared loss
- But we cannot require that all points be approximated correctly (overfitting!)

# Loss function for support vector regression

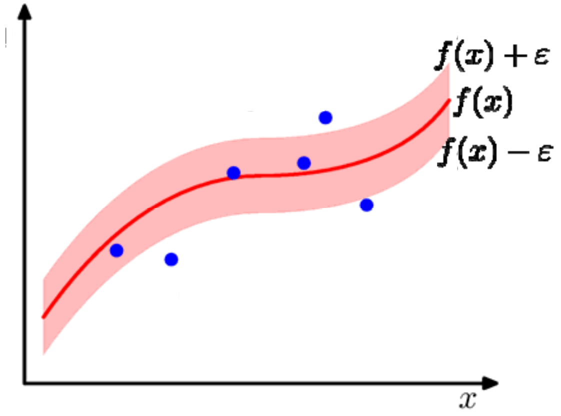
In order to allow for misclassifications in SVM regression (and have robustness to noise), we use the *$\varepsilon$-insensitive loss*:

$$J_\varepsilon = \sum_{i=1}^{m} J_\varepsilon(\mathbf{x_i}), \text{ where}$$

$$J_\varepsilon(\mathbf{x_i}) = \begin{cases} 0 & \text{if } |y_i - (\mathbf{w} \cdot \mathbf{x_i} + w_0)| \leq \varepsilon \\ |y_i - (\mathbf{w} \cdot \mathbf{x_i} + w_0)| - \varepsilon & \text{otherwise} \end{cases}$$



cost is zero inside epsilon "tube"



2

# Solving SVM regression

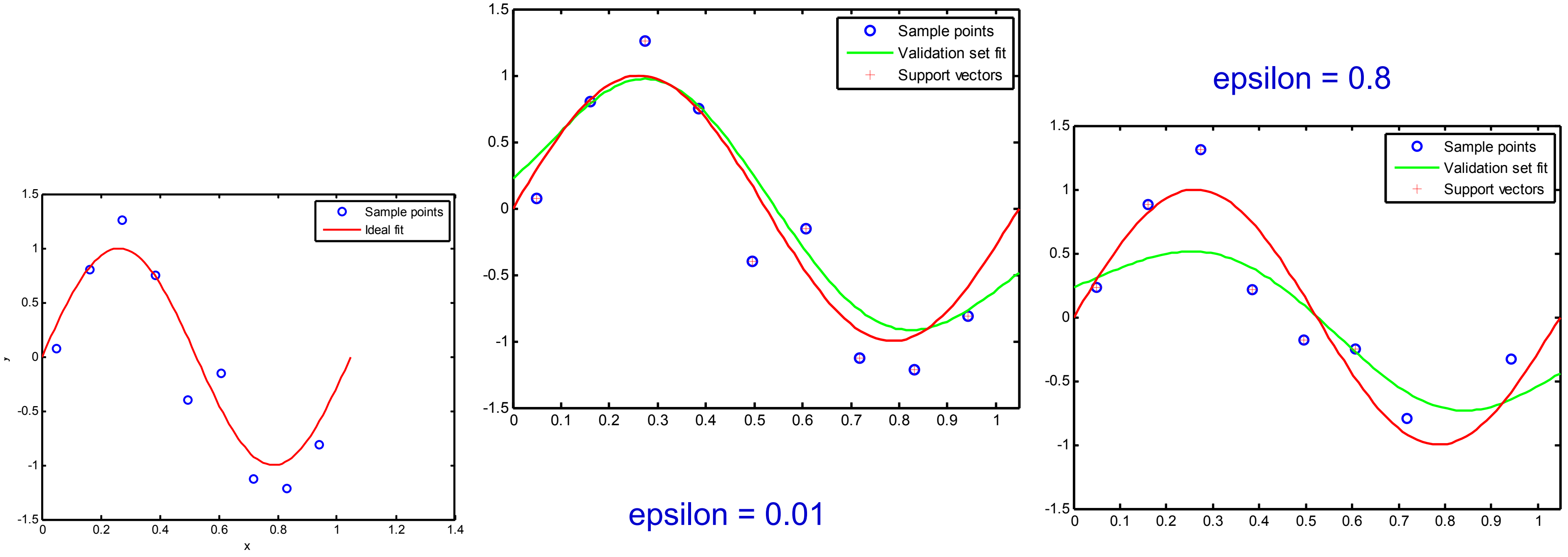
- We introduce slack variables, $\xi_i^+$, $\xi_i^-$ to account for errors outside the tolerance area
- We need two kinds of variables to account for both positive and negative errors

# The optimization problem

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

- Like before, we can write the Lagrangian and solve the dual form of the problem
- Kernels can be used as before to get non-linear functions

# Effect of $\varepsilon$



epsilon = 0.01

epsilon = 0.8

[3]

- As $\varepsilon$ increases, the function is allowed to move away from the data points, the number of support vectors decreases and the fit gets worse

[3] Zisserman course notes