Kernel Methods

Machine Learning

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Introduction

- In the last part, we have talked about linear methods for classification and regression.
- The methods we have covered so far are all *parametric*: a model is computed from the training data, then the training data is discarded, and only the model is used for further calculations.
- There are, however, methods where at least a part of the training data is kept.
- Some of them are based on simple comparison of test samples and training samples (e.g. the kNN classifier).
- Kernel methods are more sophisticated examples of this category.
- Kernel methods are linear methods in a feature space. Yet, they offer a different view of both linear models, and the concept of features.
- We will cover in detail the best-known kernel algorithm, the Support Vector Machine.

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Kernel Methods

Dual Representations

- Consider Linear Regression with training data $(\phi_n, t_n)_{n=1,\dots,N}$ with L_2 regularization, where $\phi_n = \phi(\mathbf{x}_n)$:

$$E(\mathbf{w}) = \sum_{n=1}^{N} \frac{1}{2}(\mathbf{w}^T\phi_n - t_n)^2 + \frac{\lambda}{2}||\mathbf{w}||_2^2$$

  (note that for easier calculation, this is the regularized squared error, not the *mean* squared error).
- The gradient of the right-hand side w.r.t. $\mathbf{w}$ is

$$\sum_{n=1}^{N}(\mathbf{w}^T\phi_n - t_n)\phi_n + \lambda\mathbf{w}$$

  and setting it to zero yields

$$\mathbf{w} = \sum_{n=1}^{N} \underbrace{-\frac{1}{\lambda}(\mathbf{w}^T\phi_n - t_n)}_{a_n}\phi_n$$

  with *scalars* a_n.

Dual Representations

- Using the design matrix Φ and writing the coefficients a_n as a vector $\mathbf{a}$, we get
$$\mathbf{w} = \Phi^T \mathbf{a}.$$
- Thus we see that not only the model is linear, but also that $\mathbf{w}$ is a linear combination of the (features of the) training data.
- Q: Do you think this is surprising?

Dual Representations

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- Thus we see that not only the model is linear, but also that $\mathbf{w}$ is a linear combination of the (features of the) training data.
- Q: Do you think this is surprising?
- The observation that $\mathbf{w}$ and the features Φ have such a simple relationship leads us to the idea of expressing the whole regression problem in terms of the training data points!
- Such a reformulation, called the dual representation, is possible for a variety of linear models.

Dual Representations

- Substituting $\mathbf{w} = \Phi^T \mathbf{a}$ into $E(\mathbf{w})$ yields the expression

$$E(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T \Phi\Phi^T \Phi\Phi^T \mathbf{a} - \mathbf{a}^T \Phi\Phi^T \mathcal{T} + \frac{1}{2}\mathcal{T}^T\mathcal{T} + \frac{\lambda}{2}\mathbf{a}^T\Phi\Phi^T\mathbf{a}$$

with the target vector $\mathcal{T} = (t_1, \ldots, t_N)^T$.

- We define the Kernel function

$$k(\mathbf{x}_n, \mathbf{x}_m) = \phi(\mathbf{x}_n)^T \phi(\mathbf{x}_m) = \langle \phi(\mathbf{x}_n), \phi(\mathbf{x}_m) \rangle$$

and the Gram matrix

$$\mathbf{K} = \Phi\Phi^T = (k(\mathbf{x}_n, \mathbf{x}_m))_{n,m=1,\ldots,N},$$

which allows us to express the error in the dual representation

$$E(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T \mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^T \mathbf{K}\mathcal{T} + \frac{1}{2}\mathcal{T}^T\mathcal{T} + \frac{\lambda}{2}\mathbf{a}^T\mathbf{K}\mathbf{a}.$$

Solving in Dual Representation

- Setting the gradient of

$$E(\mathbf{a}) = \frac{1}{2}\mathbf{a}^T\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^T\mathbf{K}\mathcal{T} + \frac{1}{2}\mathcal{T}^T\mathcal{T} + \frac{\lambda}{2}\mathbf{a}^T\mathbf{K}\mathbf{a}.$$

  w.r.t. **a** to zero, one obtains the following minimum of the error function:

$$\mathbf{a} = (\mathbf{K} + \lambda I_N)^{-1}\mathcal{T}.$$

  (I_N is the $N \times N$ unity matrix.)

- Plugging this solution into the original model, the prediction function is given by

$$y(\mathbf{x}) = \mathbf{k}(\mathbf{x})^T(\mathbf{K} + \lambda I_N)^{-1}\mathcal{T}$$

  with $\mathbf{k}(\mathbf{x}) = (k(\mathbf{x}_n, \mathbf{x}))_{n=1,\dots,N}$.

The Role of the Kernel

- The solution is found by inverting an $N \times N$ matrix, whereas in the original formulation, we have inverted an $M \times M$ matrix.
- (Here M is the number of features, and N is the number of training data points.)
- So what is the advantage of the dual formulation?

The Role of the Kernel

- The solution is found by inverting an $N \times N$ matrix, whereas in the original formulation, we have inverted an $M \times M$ matrix.
- (Here M is the number of features, and N is the number of training data points.)
- So what is the advantage of the dual formulation?
- We never use the feature vector ϕ directly!
- The input data appears only inside the kernel function $k(x, y)$.
- This allows us to **implicitly** use very high-dimensional (possibly infinite-dimensional) feature spaces!

Features and Kernels

- Let us consider a well-known feature, namely *quadratic features*: For $\mathbf{x} = (x^{(1)}, \ldots, x^{(K)})$, let

$$\phi(\mathbf{x}) = (1, \sqrt{2}x^{(1)}, \ldots, \sqrt{2}x^{(K)},$$
$$(x^{(1)})^2, \ldots, (x^{(K)})^2, \sqrt{2}x^{(1)}x^{(2)}, \ldots, \sqrt{2}x^{(K-1)}x^{(K)}).$$

- For larger dimensionalities K, it could take a lot of computing power to compute a) the feature itself, b) the scalar product $k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$ between two features?

Features and Kernels

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- For larger dimensionalities K, it could take a lot of computing power to compute a) the feature itself, b) the scalar product $k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$ between two features?
- **No**, since the kernel function is given by

$$k(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle = (\mathbf{x}^T \mathbf{y} + 1)^2 \qquad \text{(proof left as exercise)}$$

- The complex-looking kernel is thus actually very simple to compute! This is called the Kernel Trick.

Features and Kernels

- The feature space can even have an infinite number of dimensions!
- As an example, take the RBF (radial basis function) kernel

$$K(\mathbf{x},\mathbf{y}) = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}\right)$$

(with fixed σ).

- The exponential can be expanded as a power series, yielding a feature space of the form

$$\phi(\mathbf{x}) = \left[\exp\left(-\frac{1}{2}||\mathbf{x}||^2\right)\frac{x_1^{n_1}\cdot x_k^{n_k}}{\sqrt{(n_1!\cdot n_k!)}}\right]_{(n_1,\dots,n_k)\in\mathbb{N}^k}$$

which has an infinite number of dimensions.

- Still, we can use the kernel function to reason about linear regression (and other linear methods) in this infinite-dimensional space!

Features and Kernels

- The RBF kernel measures the closeness between two data points.
- This view can be extended to kernel functions in general:
  - As known from linear algebra, the scalar product measures the "alignment", i.e. the similarity, between two vectors.
  - Thus the kernel function likewise measures the alignment between data points!
- The feature which underlies a given kernel function determines what we consider "similar".
- Choosing a kernel is thus equivalent to choosing features, just that instead of searching for a good representation of the data, we search for a good representation of the *similarity* between data points!

Theory of Kernel Functions

- We aim to understand the properties of Kernel functions, and how to create new kernel functions.
- We have seen that the kernel function is defined as a scalar product in feature space:
$$k(\mathbf{x}_n, \mathbf{x}_m) = \phi(\mathbf{x}_n)^T \phi(\mathbf{x}_m)$$
- Clearly, the kernel function is symmetric, thus the Gram matrix is also symmetric. One can also show that the Gram matrix $\mathbf{K} = (k(\mathbf{x}_n, \mathbf{x}_m))_{n,m=1,\dots,N}$ is positive-semidefinite, i.e. for all vectors $\mathbf{c} \neq 0$, $\mathbf{c}^T \mathbf{K} \mathbf{c} \geq 0$:
$$\begin{aligned} \mathbf{c}^T \mathbf{K} \mathbf{c} &= \sum_i \sum_j c_i \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle c_j \\ &= \langle \sum_i c_i \phi(\mathbf{x}_i), \sum_j c_j \phi(\mathbf{x}_j) \rangle = \langle y, y \rangle \geq 0 \end{aligned}$$
for $y = \sum_i c_i \phi(\mathbf{x}_i)$.

Kernel Functions

- It is also possible to show the opposite: If for a function $k(\mathbf{x}_n, \mathbf{x}_m)$, the Gram matrix is positive-semidefinite for any finite data set $(\mathbf{x}_n)_{n=1,\dots,N}$, one can write k as a scalar product in some (possibly infinite-dimensional) feature space:

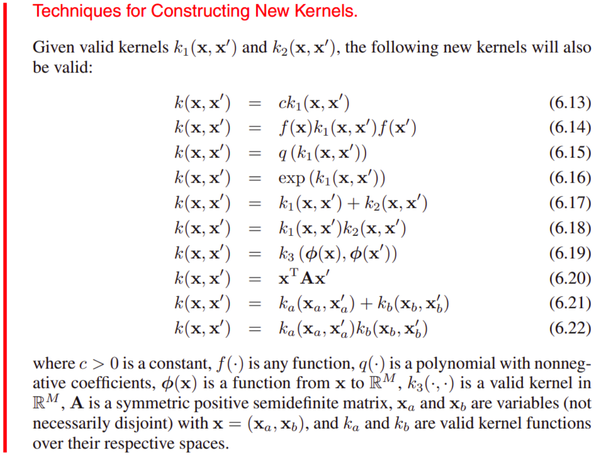
$$k(\mathbf{x}_n, \mathbf{x}_m) = \phi(\mathbf{x}_n)^T \phi(\mathbf{x}_m)$$

  for some mapping ϕ.
- In this case, the function k is called a valid kernel.
- Note that this does *not* mean that $k(\mathbf{x}_n, \mathbf{x}_m)$ must always be positive!
- We do not cover the proof in this lecture, as a reference, consider Taylor & Cristianini, *Kernel Methods for Pattern Analysis*, Cambridge University Press 2004.

Constructing Kernels

- In practice, kernels can be constructed using a set of transformations, starting from the linear kernel $k_{\text{lin}}(\mathbf{x}_n, \mathbf{x}_m) = \mathbf{x}_n^T \mathbf{x}_m$.
- Thus, one avoids to describe the feature space explicitly.
- A number of standard kernels has been described in literature, with the polynomial kernel and the RBF kernel among the most common choices.
- It is also possible to devise specific, application-dependent kernels. Note that these kernels may map *arbitrary objects* into the implicit feature space!

Constructing Kernels



Techniques for Constructing New Kernels.

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.22)
\end{aligned}
$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

From Bishop, p.296

Kernel Methods: Summary and Outlook

- We have seen that linear regression can be rewritten in *dual representation*, based only on the kernel function of the training data points.
- This reformulation allows to easily use high-dimensional or even infinite-dimensional feature spaces.
- Many linear methods can be *kernelized*, i.e. rewritten as kernel methods.
- However, this comes at the price of having to keep all training data points in memory. In particular, this can be a problem in the prediction phase.
- In the following section, we will get to know a specific kernel method for classification which avoids this problem by requiring only a small subset of the training data for classification: The Support Vector Machine (SVM).

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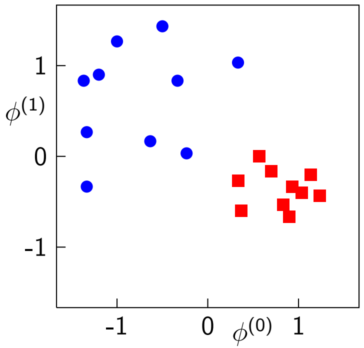
Support Vector Machines

Introduction

- Remember the two-class problem from the last lecture?
  - ➔ I again removed the outlier
  - ➔ Perfect solution(s) exist, the classes are *linearly separable*.



Introduction

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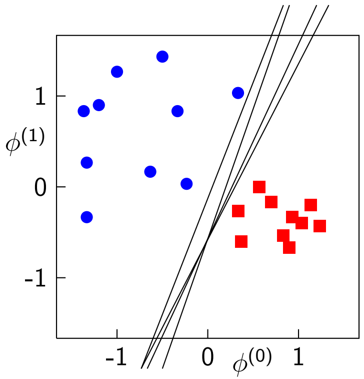
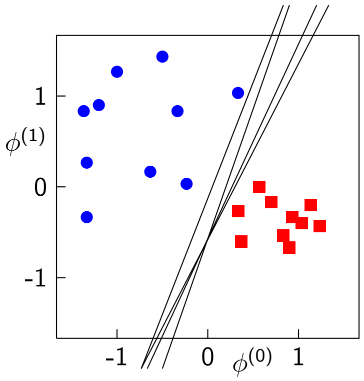


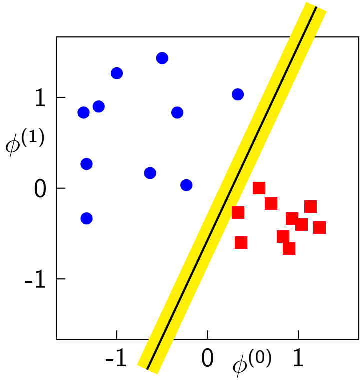
Introduction

- Remember the two-class problem from the last lecture?
  - → I again removed the outlier
  - → Perfect solution(s) exist, the classes are *linearly separable*.
- We do linear classification in feature space
  - → the classifier depends linearly on the features and the parameters
  - → the features themselves may be nonlinear.
- How can we choose an optimal hyperplane (here: a straight line) as decision boundary?



Definition of the Margin

- Assume that the classes are linearly separable.
- Define the *margin* of the linear classifier as twice the distance from the decision boundary to the nearest point (of either class).
- In the figure, the margin is indicated in yellow.



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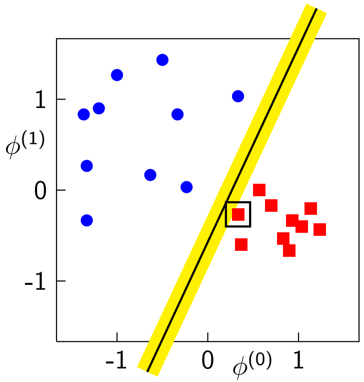
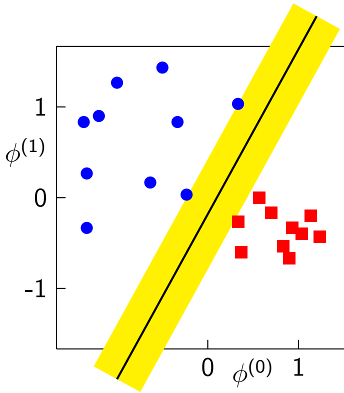


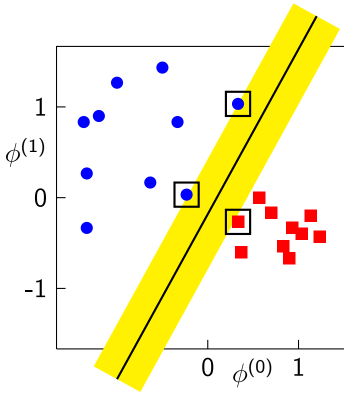
Maximum Margin

- Idea: We choose the decision boundary which *maximizes* the margin.



Maximum Margin

- Idea: We choose the decision boundary which *maximizes* the margin.
- Obviously, this means that we have at least one datapoint of each class which push against the margin.
- These data points are called the *support vectors*.



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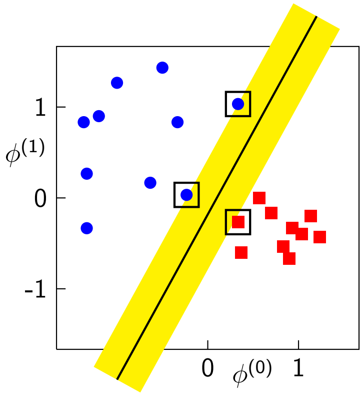

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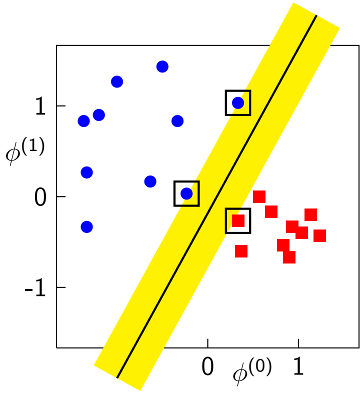
- This classifier is called the *Support Vector Machine*.
- There is always a unique solution.



Maximum Margin

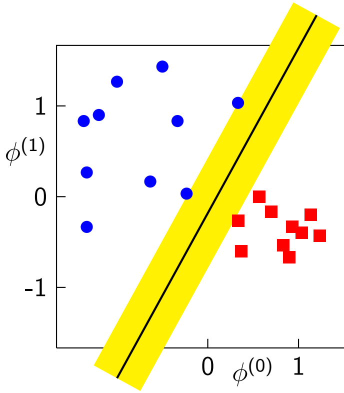
Why do we define our classifier this way?

- Intuitively this feels safest.
- If we have made a small error in the location of the boundary, this gives us least chance of causing a misclassification.
- The model is easy since it is depends only on the support vector datapoints (this also means that we do not need to save the training data points after fitting).
- There is some theory (using VC dimension) which indicates that maximizing the margin is a good thing.
- Empirically it works very very well (compared to other classifiers which are linear in parameter space).

Based on Andrew Moore's SVM tutorial slides.

Mathematical Formulation

- Training samples: $\mathbf{x}_1, \ldots, \mathbf{x}_N$, from which we get features $\phi_1, \ldots, \phi_N$.
- $y(\phi) = \mathbf{w}^T\phi + w_0$ is the discriminant function; determine $\mathbf{w}$ and w_0.
- ● if $y(\phi) > 0$, 🟥 if $y(\phi) < 0$ (equality does not occur since the classes are linearly separable).



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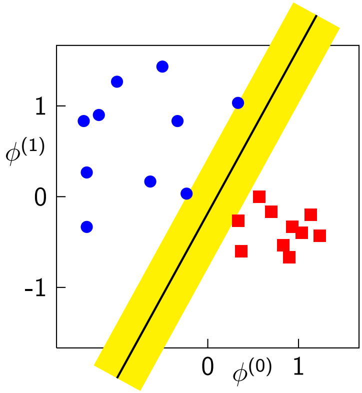

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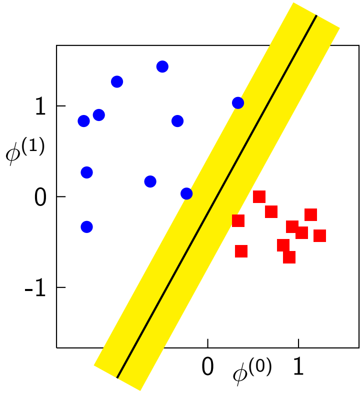

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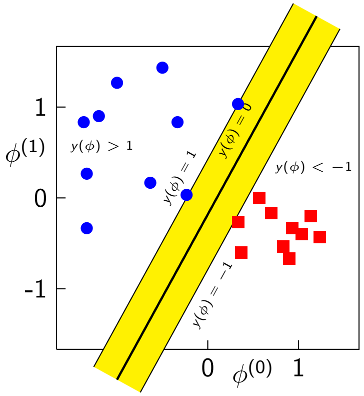
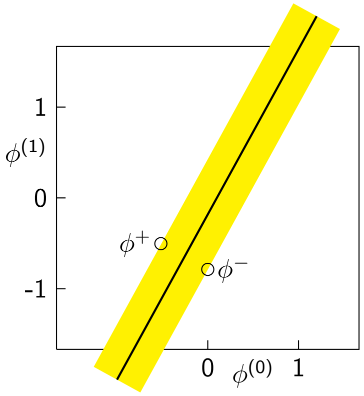


Mathematical Formulation

- We need an expression for the margin.
- Let ϕ^+ be a point (not necessarily a training data sample) on the "plus" margin, and ϕ^- the *closest* point to ϕ^+ on the "minus" margin.
- Then $\phi^+ = \phi^- + \lambda\mathbf{w}$ for a scalar λ. (Why?)



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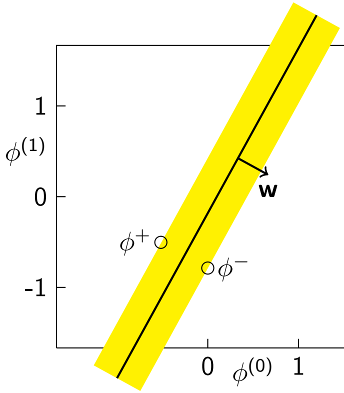

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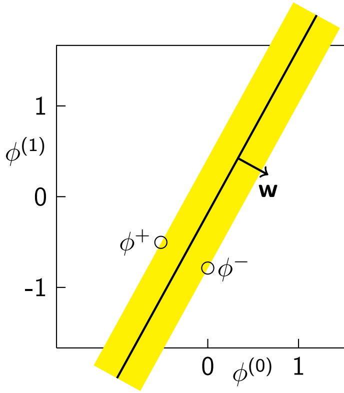
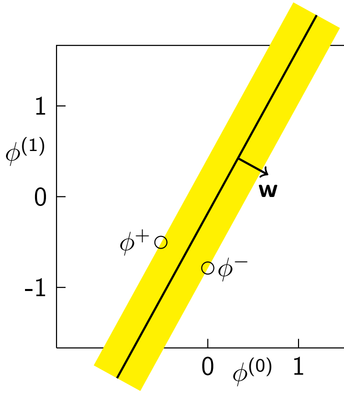
- Then $\phi^+ = \phi^- + \lambda \mathbf{w}$ for a scalar λ, since one finds the closest point on a plane by orthogonal projection, and $\mathbf{w}$ is orthogonal to the decision boundary and thus also to the margin planes.
- The margin width is thus $||\lambda \mathbf{w}||$.



Mathematical Formulation

- From
  - $\mathbf{w}^T\phi^+ + w_0 = 1$
  - $\mathbf{w}^T\phi^- + w_0 = -1$
  - $\phi^+ = \phi^- + \lambda\mathbf{w}$

  easily follows $\lambda = \frac{2}{\mathbf{w}^T\mathbf{w}}$.



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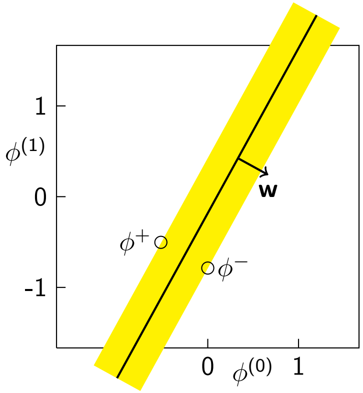
  - $\phi^+ = \phi^- + \lambda\mathbf{w}$

  easily follows $\lambda = \frac{2}{\mathbf{w}^T\mathbf{w}}$.
- Since the margin width is given by $M = ||\lambda\mathbf{w}||$, we finally obtain

$$M = ||\lambda\mathbf{w}|| = \lambda||\mathbf{w}|| = \lambda\sqrt{\mathbf{w}^T\mathbf{w}} = \frac{2\sqrt{\mathbf{w}^T\mathbf{w}}}{\mathbf{w}^T\mathbf{w}} = \frac{2}{\sqrt{\mathbf{w}^T\mathbf{w}}}.$$



Mathematical Formulation

Given a guess of $\mathbf{w}$ and w_0, we can

- check whether the resulting hyperplane separates the classes
- compute the margin width.

But how do we search through all possible solutions to find the best one (i.e. the one with maximal margin width)?

Mathematical Formulation

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But how do we search through all possible solutions to find the best one (i.e. the one with maximal margin width)?

The problem can be formulated as a **Quadratic programming** problem.

Quadratic Programming

A general quadratic programming problem is as follows:

- Minimize[1] (for fixed Q and $\mathbf{c}$)

$$\arg\min_{x} \frac{1}{2}\mathbf{x}^T Q\mathbf{x} + \mathbf{c}^T\mathbf{x}$$

- subject to the constraints

$$\begin{aligned} A_{\text{eq}}\mathbf{x} &= b_{\text{eq}} \\ A_{\text{ineq}}\mathbf{x} &\leq b_{\text{ineq}}, \end{aligned}$$

  where the two sets of linear equality and inequality constraints are written in matrix form.

- Such problems can be solved very efficiently and reliably with specialized algorithms (which we do not cover here).

[1] alternatively maximize

Margin Maximization by Quadratic Programming

- Remember the discriminant function with normalized $\mathbf{w}$:
  - ➔ ● if $\mathbf{w}^T\phi + w_0 \geq 1$; 🟥 if $\mathbf{w}^T\phi + w_0 \leq -1$.

  and the margin width
  - ➔ $M = \frac{2}{\sqrt{\mathbf{w}^T\mathbf{w}}}$.

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- From this, we get the setup for the Quadratic Programming problem:
  - Compute $\arg\min_{\mathbf{w}} \mathbf{w}^T\mathbf{w}$ (this amounts to maximizing M)

  under the set of constraints
  - $\mathbf{w}^T\phi + w_0 \leq -1$ for *all* samples ϕ of class ■
  - $\mathbf{w}^T\phi + w_0 \geq +1$ for *all* samples ϕ of class ● .

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- Define numerical targets $t_1, \ldots, t_N \in \{-1, +1\}$ for each sample $\phi_1, \ldots, \phi_N$ (🟥 $\equiv -1$, ● $\equiv +1$).

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- Define numerical targets $t_1, \ldots, t_N \in \{-1, +1\}$ for each sample $\phi_1, \ldots, \phi_N$ (🟥 $\equiv -1$, ● $\equiv +1$).
- Now we can write the constraints in a unified way
  - $t_n(\mathbf{w}^T\phi_n + w_0) \geq 1, n = 1, \ldots, N$

  and let a standard QP solver compute the solution.

Excurse: Lagrange Multipliers

- For the next step, we will briefly review a mathematical tool for constrained optimization, the *Lagrange Multipliers* and their generalization by Karush, Kuhn, and Tucker.
- For a simple start, assume we need to optimize a (two-dimensional) function as follows: Find

$$\arg\max_{x,y} f(x,y) \qquad \text{subject to} \qquad g(x,y) = 0$$

Excurse: Lagrange Multipliers

- Clearly, we cannot directly maximize f by setting the derivative to zero, since the resulting maximum (A) does not (generally) fulfill the constraint.
- At the constrained maximum B, the gradient of f is *not* zero.

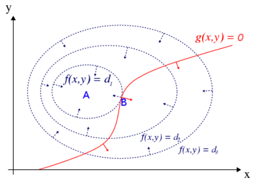


Image source: Wikipedia, Lagrange Multiplier, modified

- Of course, we could try to rewrite the constraint

$$g(x,y) = 0 \Leftrightarrow y = \tilde{g}(x)$$

- Then, eliminate y from f and solve the unconstrained problem

$$\arg\max_x f(x, \tilde{g}(x))$$

- But this is ugly, complicated, and often not even possible!

Excurse: Lagrange Multipliers

A better *intuitive* solution works like this:

- Walk along the constraint line $g(x, y) = 0$, looking for a maximum
- A maximum is reached when we just "touch" a contour line of f (a line where the value of f is constant)
- At a touching point, the tangents of the contour line and the constraint line must be parallel
- Since the gradient is orthogonal to the tangent, this means that the gradients of f and g must be parallel at such touching points

$\Rightarrow$ Necessary condition: $\nabla f + \lambda \nabla g = 0$ for some λ.

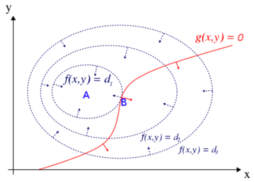


Image source: Wikipedia, Lagrange Multiplier, modified

Skipped some details (e.g. differentiability requirements, what happens when f or g has a plateau, how to check whether we really have a maximum, multiple variables and constraints, etc.). Never mind.

Excurse: Lagrange Multipliers

Task: Maximize[2] $f(\mathbf{x})$ (for a vector $\mathbf{x}$), subject to M constraints $g_m(\mathbf{x}) = 0, m = 1, \dots, M$.
Solution (without proof):

- Introduce the *Lagrangian*

$$L(\mathbf{x}, \lambda_1, \dots, \lambda_M) = f(\mathbf{x}) + \lambda_1 g_1(\mathbf{x}) + \dots + \lambda_M g_M(\mathbf{x})$$

- Solve (can also be done numerically)

$$\nabla_{(\mathbf{x}, \lambda_1, \dots, \lambda_M)} L(\mathbf{x}, \lambda_1, \dots, \lambda_M) = 0$$

  (note that the derivatives w.r.t. λ just yield the constraints)

- The resulting points (usually finitely many) are candidates for extrema. Check which ones suit your needs[3].

[2]or minimize

[3]there is a formal criterion, using a variant of the usual Hessian matrix, but even mathematicians say that's "more trouble than it's worth"

Karush-Kuhn-Tucker Conditions

- The idea can also be used when we have *inequality constraints* of the form $g(\mathbf{x}) \geq 0$.
- Consider a single constraint. Two cases are possible:
  - A constrained extremum $\mathbf{x}_E$ lies *within* the region described by $g(\mathbf{x}) \geq 0$, i.e. $g(\mathbf{x}_\mathbf{E}) > 0$. Then the constraint is *inactive*, and since a neighborhood of $\mathbf{x}_E$ is contained in the constraint zone $g(\mathbf{x}) > 0$, $\mathbf{x}_E$ must be a "true" extremum, the constraint is said to be *inactive*, and we have $\lambda = 0$ and $\nabla f(x_E) = 0$.
  - A constrained extremum $\mathbf{x}_E$ lies *on the border* of the region described by $g(\mathbf{x}) \geq 0$, i.e. $g(\mathbf{x}_\mathbf{E}) = 0$. This is the case we had before, the constraint is *active*.
- We again have the condition on the Lagrangian

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x}) = 0$$

here with a multiplier $\lambda \geq 0$ (the sign accounts for the inequality constraint).

Karush-Kuhn-Tucker Conditions

- In either case, $\lambda \cdot g(\mathbf{x}) = 0$ (for inactive constraints: $\lambda = 0$, for active constraints: $g(\mathbf{x}) = 0$).
- Thus we have to optimize the Lagrangian $L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda g(\mathbf{x})$ under the constraints

$$\begin{aligned} g(\mathbf{x}) &\geq 0 \\ \lambda &\geq 0 \\ \lambda g(\mathbf{x}) &= 0 \end{aligned}$$

- You will see that the last constraint ($\lambda g(\mathbf{x}) = 0$) plays a very important role for SVMs!
- Optimization is usually done numerically.

Dual Representation of the SVM

Let's go back to the SVM and use Lagrange multipliers to compute a solution!

- We have to minimize $\mathbf{w}^T\mathbf{w}$ with the constraints $t_n(\mathbf{w}^T\phi_n + w_0) \geq 1, n = 1, \ldots, N$.
- Introduce N Lagrange multipliers $\mathbf{a} = (a_n)_n, n = 1, \ldots, N$ with $a_n \geq 0$, to get the Lagrangian

$$L(\mathbf{w}, w_0, \mathbf{a}) = \frac{1}{2}||\mathbf{w}||^2 - \sum_{n=1}^{N} a_n(t_n(\mathbf{w}^T\phi_n + w_0) - 1)$$

- Setting the derivatives of L to zero yields the conditions

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi_n \qquad \text{and} \qquad 0 = \sum_{n=1}^{N} a_n t_n.$$

- Use these equations to simplify L by eliminating $\mathbf{w}$ and w_0.

Dual Representation of the SVM

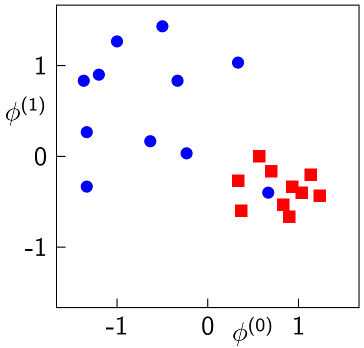
- We obtain the famous *dual representation* of the maximum margin problem

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m),$$

  where $k(\mathbf{x}_n, \mathbf{x}_m) = \phi_n^T \phi_m$ is the kernel function.
- $\tilde{L}$ needs to be optimized over $\mathbf{a}$ with the constraints $a_n \geq 0, n = 1, \ldots, N$, and $0 = \sum_{n=1}^{N} a_n t_n$.
- We need to optimize as many coefficients as there are training data points.
- This can again be solved by quadratic programming.
- Fundamental advantage of this formulation: the data samples only appear in the kernel function!

Overlapping Class Distributions

- What if the classes are *not* linearly separable in feature space?
- Introduce *slack variables* $\xi_n \geq 0$ for each training sample
  - ➔ $\xi_n = 0$ if the sample is correctly classified *and* outside the margin (i.e. $t_n(\mathbf{w}^T\phi_n + w_0) \geq 1$)
  - ➔ $\xi_n = |t_n - y(\phi_n)|$ otherwise
- Note that $\xi_n > 0$ does *not* mean the data point is misclassified (it could be correctly classified, but violate the margin)



Overlapping Class Distributions

- The classification constraints now become $t_n y(\phi_n) = t_n(\mathbf{w}^T \phi_n + w_0) \geq 1 - \xi_n$ with $\xi_n \geq 0$.
- Compute

$$\arg\min_{\mathbf{w}} \left(\frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n \right)$$

where the parameter C is the trade-off between margin width and margin/classification errors.

- The dual representation of the problem is as before

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m),$$

with new constraints $0 \leq a_n \leq C$, $n = 1, \ldots, N$, and $0 = \sum_{n=1}^{N} a_n t_n$.

Prediction

- If we used the original, direct SVM formulation, we would obtain optimized $\mathbf{w}$ and w_0.
- Prediction is as usual: $y(\phi) = \mathbf{w}^T\phi + w_0$, with the optimal values for $\mathbf{w}$ and w_0.
- If we use the dual representation, we have optimal parameters $\mathbf{a}$.
- The prediction can likewise be formulated using the kernel function (without proof):

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x_n}) + w_0$$

with

$$w_0 = \frac{1}{|\mathcal{S}|} \sum_{n\in\mathcal{S}} \left(t_n - \sum_{m\in\mathcal{S}} a_m t_m k(\mathbf{x_m}, \mathbf{x_n}) \right)$$

where $\mathcal{S}$ contains the indices of the support vectors.

Summary so far

We have

- defined a criterion for finding a linear classifier (in feature space): *maximum margin*
- outlined how to formulate this criterion
- derived the *dual* formulation, where the features only appear in the kernel function
- have described how to set up the task to be solved by standard *quadratic programming* algorithms
- seen how to trade-off in the case that a perfect solution is impossible.

Further reading: Bishop, *Pattern Recognition and Machine Learning*, Chapter 7 (contains many more details on mathematical derivation, dealing with multiple classes, obtaining probability estimates, etc.)
Now we consider properties of the resulting classifier, particularly regarding efficient computation!

Role of Sparsity

- Even with the kernel trick, the prediction

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x_n}) + w_0.$$

still requires computing a sum over all training data points?

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- **No**, because all a_n which do *not* belong to support vectors are *zero*!

⇒ Multiplication needs only to be done for support vectors.

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Thus the whole classifier depends only on the support vectors: The sparsity property of SVMs. This can also be considered a form of simplicity regularization.

SVM Example

Example of synthetic data from two classes in two dimensions showing contours of constant $y(\mathbf{x})$ obtained from a support vector machine having a Gaussian kernel function. Also shown are the decision boundary, the margin boundaries, and the support vectors.

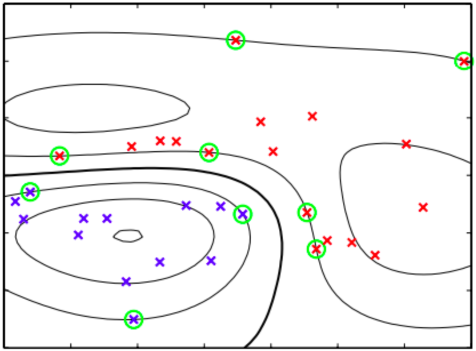

Image: Bishop, figure 7.2

Summary: SVM

- We have seen that the SVM is based on two fundamental concepts: *Kernel trick* (efficient dealing with nonlinearities) and *Sparsity* (data efficiency during testing).
- Thus, while the SVM is a classifier which is linear in feature space, the concept is different from the ordinary linear classification which we covered before:
  - ➔ we retain a (small) subset of the training samples (the support vectors) even during testing
  - ➔ we do not explicitly compute $\mathbf{w}$ (and neither the features).
- The specific properties of the dual formulation of the SVM make this possible.
- A variety of related algorithms exist, allowing to use the Support Vector framework e.g. for regression, or for probabilistic outputs, etc.

Conclusion

- In this lecture, we have taken the idea of linear models and pushed it forward quite a bit.
- We arrived at a reformulation of linear models which is quite different from the standard parametric model: Instead of using a parameter vector, prediction is performed on the basis of the training data points, which enter the calculation only via the kernel function.
- This allows us to easily reason about very high-dimensional, implicitly given feature spaces.
- The key ingredient for all kernel methods is the kernel function, which should reflect similarity between data points.
- We have covered a very important example of a kernel method, namely the SVM classifier.
- SVM keywords: max margin, kernel trick, sparsity