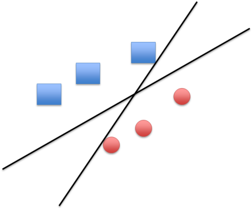
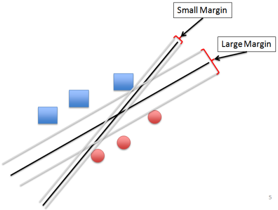
Kernel methods



- Perceptron (and other linear classifiers) can lead to many equally valid choices for the decision boundary
- Are these really equally valid ?
- How can we pick which is best?



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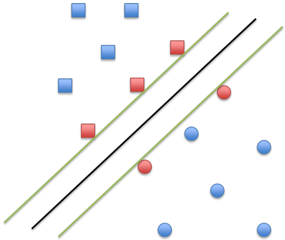
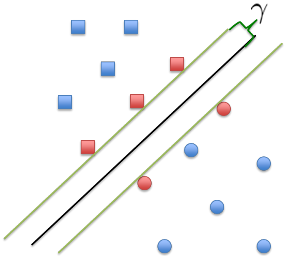
  $\rightarrow$ Maximize the size of the margin



- Support Vectors are those input points (vectors) closest to the decision boundary
- decision problem: $w^T x + b = 0$

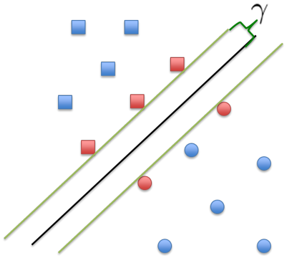


Notations

- x_i: data ; $y_i \in \{-1, 1\}$: labels
- decision hyperplane: $w^T x + b = 0$
- decision function : $f(x) = Sign(w^T x + b)$
- Margin hyperplanes: $w^T x + b = \pm\gamma$
- Scale invariance: $\lambda w^T x + \lambda b = 0$.

Scaling

This scaling does not change the decision hyperplane, or the support vector hyperplanes. $\Rightarrow$ Margin hyperplanes: $w^T x + b = \pm 1$



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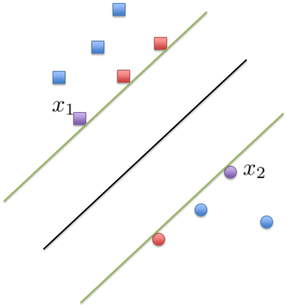


Size of the margin

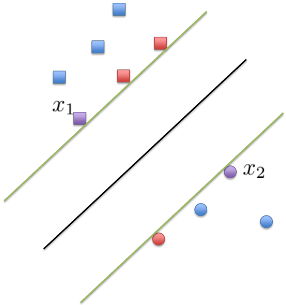
represented in terms of w.

1. identification of a decision boundary
2. maximization of the margin

Relation margin $\leftrightarrow w$

At least one point that lies on each support hyperplanes. $w^T x_1 + b = 1$ and $w^T x_2 + b = -1$ $\Rightarrow w^T(x_1 - x_2) = 2$

WHAT ARE WE OPTIMIZING ?



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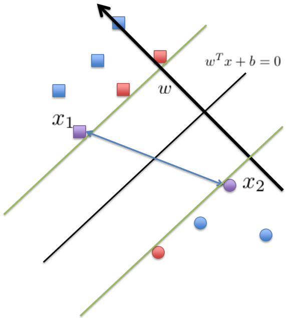

$w^T(x_1 - x_2) = 2$

1. w: orthogonal to the decision hyperplane
2. margin: projection of $x_1 - x_2$ onto w,

Projection

$w^T(x_1 - x_2) = 2$

Projection: $\frac{w^T(x_1 - x_2)}{||w||} w$

Size of the margin: $\frac{2}{||w||}$

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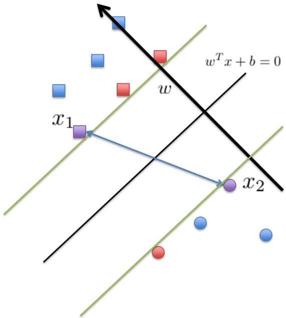

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Maximizing the margin

Maximization

$Max \frac{2}{\|w\|}$
subject to $\forall i \quad y_i(w^T x_i + b) \geq 1$

Minimization

$Min \|w\|$
subject to $\forall i \quad y_i(w^T x_i + b) \geq 1$

Lagrangian relaxation

$$L(w,b) = \frac{1}{2} w^T w - \sum_{i=1}^{N} \alpha_i \left[y_i(w^T x_i + b) - 1 \right]$$

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$$L(w, b) = \frac{1}{2} w^T w - \sum_{i=1}^{N} \alpha_i \left[y_i(w^T x_i + b) - 1 \right]$$

Max Margin Loss Function

Primal problem

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\frac{\partial L}{\partial w} = 0 \Rightarrow w - \sum_{i=1}^{N} \alpha_i y_i x_i = 0$$

DUAL PROBLEM

DUAL PROBLEM

Now have to find α_i: substitute back to the loss function

$$L(w,b) = \frac{1}{2} w^T w - \sum_{i=1}^{N} \alpha_i \left[y_i (w^T x_i + b) - 1 \right]$$

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

$$W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

where $\alpha_i \geq 0$ and $\sum_{i=1}^{N} \alpha_i y_i = 0$

Dual formulation of the error

Primal problem

Optimize this quadratic program to identify the lagrange multipliers and thus the weights

$$W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

where $\alpha_i \geq 0$

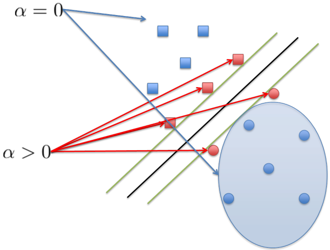
Support Vector Expansion

$$
\begin{aligned}
f(x) &= Sign(w^T x + b) \\
&= Sign\left(\left[\sum_{i=1}^{N} \alpha_i y_i x_i\right]^T x + b\right) \\
&= Sign\left(\left[\sum_{i=1}^{N} \alpha_i y_i x_i^T x\right] + b\right)
\end{aligned}
$$

- When α_i is non-zero then x_i is a support vector
- When α_i is zero x_i is not a support vector

Remark: $w = \sum_{i=1}^{N} \alpha_i y_i x_i$ Independent of the dimension of x_i

Kuhn-Tucker Conditions



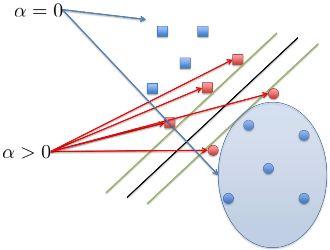
At the optimal solution

$$\alpha_i(1 - y_i(w^T x_i + b)) = 0$$

If $\alpha_i \neq 0$: $y_i(w^T x_i + b) = 1$

$\Rightarrow$ Only points on the decision boundary contribute to the solution.

KUHN-TUCKER CONDITIONS



AT THE OPTIMAL SOLUTION

$$\alpha_i(1 - y_i(w^T x_i + b)) = 0$$

If $\alpha_i \neq 0 : y_i(w^T x_i + b) = 1$

$\Rightarrow$ Only points on the decision boundary contribute to the solution.

Interpretability of SVM parameters

- α_i large $\Rightarrow$ the associated data point is quite important.
- It's either an outlier, or incredibly important

But this only gives us the best solution for linearly separable data sets

```
from sklearn.svm import LinearSVC
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
X, y = ...
svm = make_pipeline(StandardScaler(),LinearSVC(random_state=0, tol=1e-5))
svm.fit(X, y)
```

Learning Theory bases of SVMs

Bounds

Theoretical bounds on testing error:

→ The upper bound doesn't depend on the dim of the space
→ The lower bound is maximized by maximizing the margin associated with the decision boundary

Properties of SVM

→ Good generalization capability
→ Decision boundary is based on the data in the form of the support vectors → easy to interpret
→ Principled bounds on testing error from Learning Theory (VC dimension)

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Soft margin classification

Outliers

- There can be outliers on the other side of the decision boundary, or leading to a small margin.
- ⇒ Introduce a penalty term to the constraint function

New function

$$Min \frac{1}{2} w^T w + C \sum_{i=1}^{N} \xi_i$$

s.c.

$$\begin{aligned} y_i(w^T x_i + b) &\geq 1 - \xi_i \\ \xi_i &\geq 0 \end{aligned}$$

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Lagrangian

$$L(w,b) = \frac{1}{2}w^T w + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i\left[y_i(w^T x_i + b) + \xi_i - 1\right]$$

Soft margin classification

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$Min \frac{1}{2} w^T w + C \sum_{i=1}^{N} \xi_i$

s.c.

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Soft margin classification

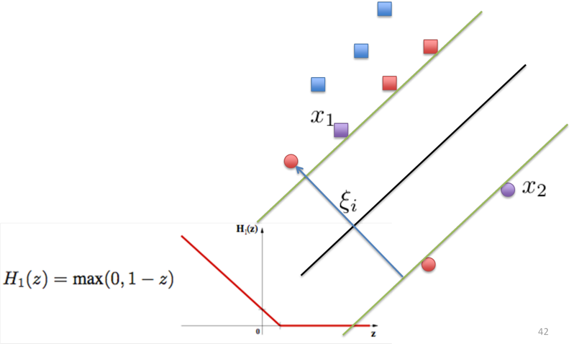
Still quadratic programming

$$W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j x_i^T x_j$$

where $0 \leq \alpha_i \leq C$

$\sum_{i=1}^{N} \alpha_i y_i = 0$

Soft margin Example



H_1: hinge loss

```
from sklearn.svm import SVC
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
X, y = ...
svm = make_pipeline(StandardScaler(),SVC(random_state=0, tol=1e-5))
svm.fit(X, y)
```

Multiclass

So far, binary classification problem. What about multiclass ?

Key ideas

- Decompose into multiple binary classification problems
- Make a final decision based on these binary classifiers

Two strategies

- One versus all
- One versus one

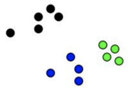
One vs all

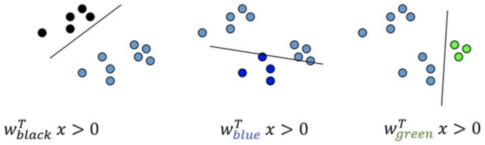
For C classes, decompose into C binary classification problems
For problem c:

- positive examples: x_i such that $y_i = c$
- negative examples: all others elements.

Inference: Winner takes all: for an example x

$$\hat{c} = arg \max_{c \in [\![1,c]\!]} w_c^T x$$



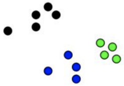


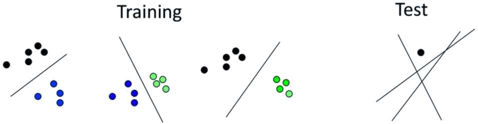
One vs one

For C classes, decompose into $C(C+1)/2$ binary classification problems
For each class pair (k,l):

- positive examples: x_i such that $y_i = k$
- negative examples: x_i such that $y_i = l$.

Inference: Majority.





One vs all

- Assumption: each class individually separable from the others
- No theoretical justification
- Easy to implement
- Unbalanced classes
- Works well in practice

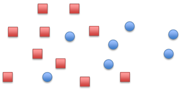
One vs one

- If class sizes are small, possible overfitting
- Need large memory to store models

These methods are applicable to any binary classifier.

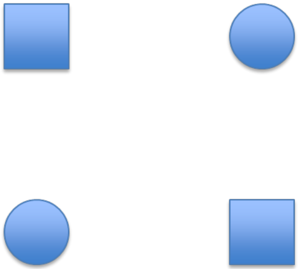
```
from sklearn.model_selection import train_test_split
from sklearn.multiclass import OneVsOneClassifier
from sklearn.multiclass import OneVsRestClassifier
from sklearn.svm import LinearSVC
X, y = ...
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, shuffle=True, random_state=0)
ovo = OneVsOneClassifier(LinearSVC(random_state=0)).fit(X_train, y_train)
ovo.predict(X_test)

ova = OneVsRestClassifier(LinearSVC(random_state=0)).fit(X_train, y_train)
ova.predict(X_test)
```

SVM: non linearly separable case



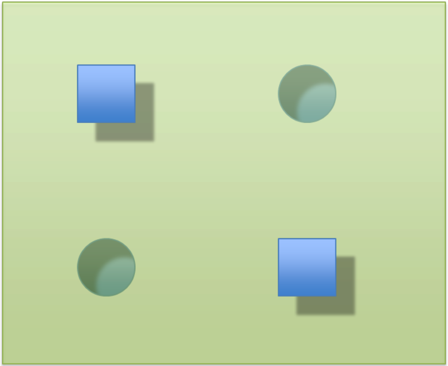
→ So far, support vector machines can only handle linearly separable data
→ But most data isn't.
→ We already see how to deal with this problem: soft margin
→ Now: another solution...

SVM: NON LINEARLY SEPARABLE CASE



→ Points that are not linearly separable in 2 dimension ..

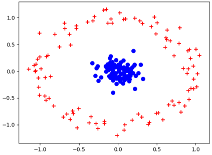
SVM: non linearly separable case



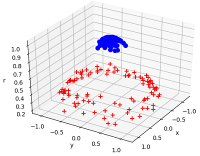
→ Points that are not linearly separable in 2 dimension, might be linearly separable in 3.

SVM: NON LINEARLY SEPARABLE CASE

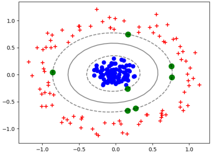
Another example



(a) Data.



(b) 3D Mapping (RBF).



(c) Classification.

Basis of Kernel Methods

Recall...

$$W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^T x_j \quad w = \sum_{i=1}^{N} \alpha_i y_i x_i$$

And then...

- → The decision process doesn't depend on the dimensionality of the data.
- → We can map to a higher dimensionality of the data space.
- → data points only appear within a dot product.
- → The error is based on the dot product of data points, not the data points themselves.

Basis of Kernel Methods

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Basis of Kernel Methods

And so...

How to add dimensionality to the data in order to make it linearly separable ?

- Extreme case: construct a dimension for each data point ⇒ overfitting
- Mapping: $x_i^T x_j \leftrightarrow \phi(x_i)^T \phi(x_j)$

$$W(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \phi(x_i)^T \phi(x_j)$$

Why Dual formulation ?

Untractable example

$$\phi(x_0, x_1) = (x_0^2, x_0 x_1, x_1 x_0, x_1^2)$$

applied to a 20x30 image of 600 pixels $\approx$ 180000 dimensions ! Would be computationally infeasible to work in this space

Dual problem

- α_i: dual variables
- Since any component orthogonal to the space spanned by the training data has no effect, general result that weight vectors have dual representation: the representer theorem.
- can reformulate algorithms to learn dual variables rather than weight vector directly

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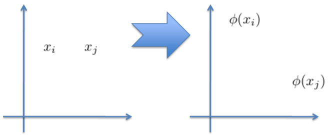
Kernel

Kernels

1. We can represent this dot product as a Kernel (Kernel Function, Kernel Matrix)
2. Finite (if large) dimensionality of $K(x_i, x_j)$ unrelated to dimensionality of x

Remember the dual



Kernels are a mapping

$$x_i^T x_j \leftrightarrow \phi(x_i)^T \phi(x_j)$$

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

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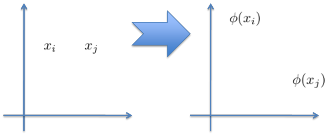

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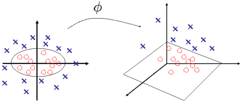
$$x_i^T x_j \leftrightarrow \phi(x_i)^T \phi(x_j)$$

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

Kernel

Gram Matrix: $K_{ij} = K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

First example



with

$$\phi(y) = (y_0^2, \sqrt{2} y_0 y_1, y_1^2)$$

$$\begin{aligned} K(x,z) &= (x^T z)^2 \\ &= (x_0 z_0 + x_1 z_1)^2 \\ &= x_0^2 z_0^2 + 2 x_0 z_0 x_1 z_1 + x_1^2 z_1^2 \\ &= (x_0^2, \sqrt{2} x_0 x_1, x_1^2)^T (z_0^2, \sqrt{2} z_0 z_1, z_1^2) \\ &= \phi(x)^T \phi(z) \end{aligned}$$

Gram Matrix: $K_{ij} = K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

Second example

$\phi : x \in X \rightarrow \phi(x) \in \mathcal{F}$
$(x, y) \mapsto (x_0^2, x_0 x_1, x_1 x_0, x_1^2)$
Linear equation in $\mathcal{F}$ $ax_0^2 + bx_1^2 = c \rightarrow$ ellipse (non linear shape) in X

Capacity of feature spaces

The capacity is proportional to the dimension

Theorem

Given $m+1$ examples in general position in a m-dimensional space, every possible classification can be generated with a thresholded linear function

Extension: Cover's theorem

- Capacity may easily become too large and lead to over-fitting: being able to realise every classifier means unlikely to generalise well
- Computational costs involved in dealing with large vectors

Kernel

Kernels

- In general: don't need to know the form of ϕ.
- Just specifying the kernel function is sufficient.
- A good kernel: Computing K_{ij} is cheaper than $\phi(x_i)$

Valid Kernels

- Symmetric
- Must be decomposable into ϕ functions
- Harder to show.
  - Gram matrix is positive semi-definite
  - Positive entries are definitely positive semi-definite.
  - Negative entries may still be positive semi-definite

$$x^T K x \geq 0$$

Kernel

Kernels

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- Just specifying the kernel function is sufficient.
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- Must be decomposable into ϕ functions
- Harder to show.
  - Gram matrix is positive semi-definite
  - Positive entries are definitely positive semi-definite.
  - Negative entries may still be positive semi-definite

$$x^T K x \geq 0$$

Kernel

Examples

K, K' Kernel $\Rightarrow \quad cK, K+K', K.K', exp(K)...$
Examples: Polynomial kernels, RBF, String kernels, graph kernels
Note: a SVM model using a sigmoid kernel function is equivalent to a two-layer, perceptron neural network.

Incorporating Kernels in SVMs

$$
\begin{aligned}
W(\alpha) &= \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \phi(x_i)^T \phi(x_j) \\
&= \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j K(x_i, x_j)
\end{aligned}
$$

- optimize the α_i and b w.r.t. K
- decision function $f(x) = sign\left[\sum_{i=1}^{N} \alpha_i y_i K(x, x_i) + b\right]$

Examples

Polynomial Kernels

$K(x,z) = (x^T z + \theta)^d \quad \theta \geq 0$

- dot product: polynomial power of the original dot product.
- c large $\Rightarrow$ focus on linear terms
- c small $\Rightarrow$ focus on higher order terms
- Very fast to calculate

RBF

$K(x,z) = e^{\frac{\|x-z\|^2}{2\sigma^2}}$

- dot product: related to the distance in space between the two points.
- Placing a bump on each point

```
from sklearn.svm import SVC
X, y = ...
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, shuffle=True, random_state=0)
rbf=SVC(kernel="rbf", gamma=0.1, C=100).fit(X_train, y_train)
poly = SVC(kernel="poly", degree=4, coef0=0.5, C=5).fit(X_train, y_train)
```

Examples

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Examples

String kernels

Not a gaussian, but still a legitimate Kernel

- $K(s, s')$ = difference in length,count of different letters, minimum edit distance
- allow for infinite dimensional inputs
- don't need to manually encode the input

Examples

Graph Kernels

- Define the kernel function based on graph properties
- must be computable in poly-time (paths, spanning trees, cycles, bag of paths...)
- Possible incorporation of knowledge about the input without direct feature extraction

To conclude: kernel Trick

To conclude (Kernel trick) : a kernel can be applied where a dot product is used in an optimization:

- Kernel PCA
- Kernel perceptron
- unsupervised clustering (similarity $\approx$ distance $\leftrightarrow$ dot product)