Support Vector Machines

INFO-4604, Applied Machine Learning

University of Colorado Boulder

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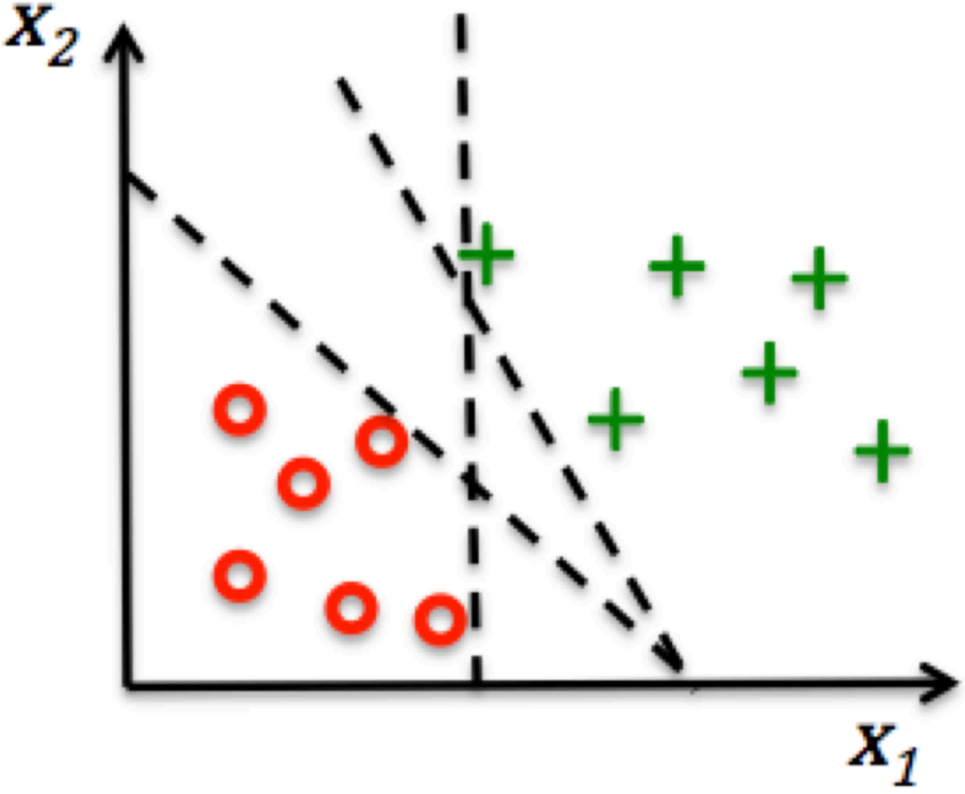
Today

Three important concepts:

- SVMs
- Margins
- Kernels

Large Margin Classification



Which hyperplane?

Linear Predictions

Perceptron:

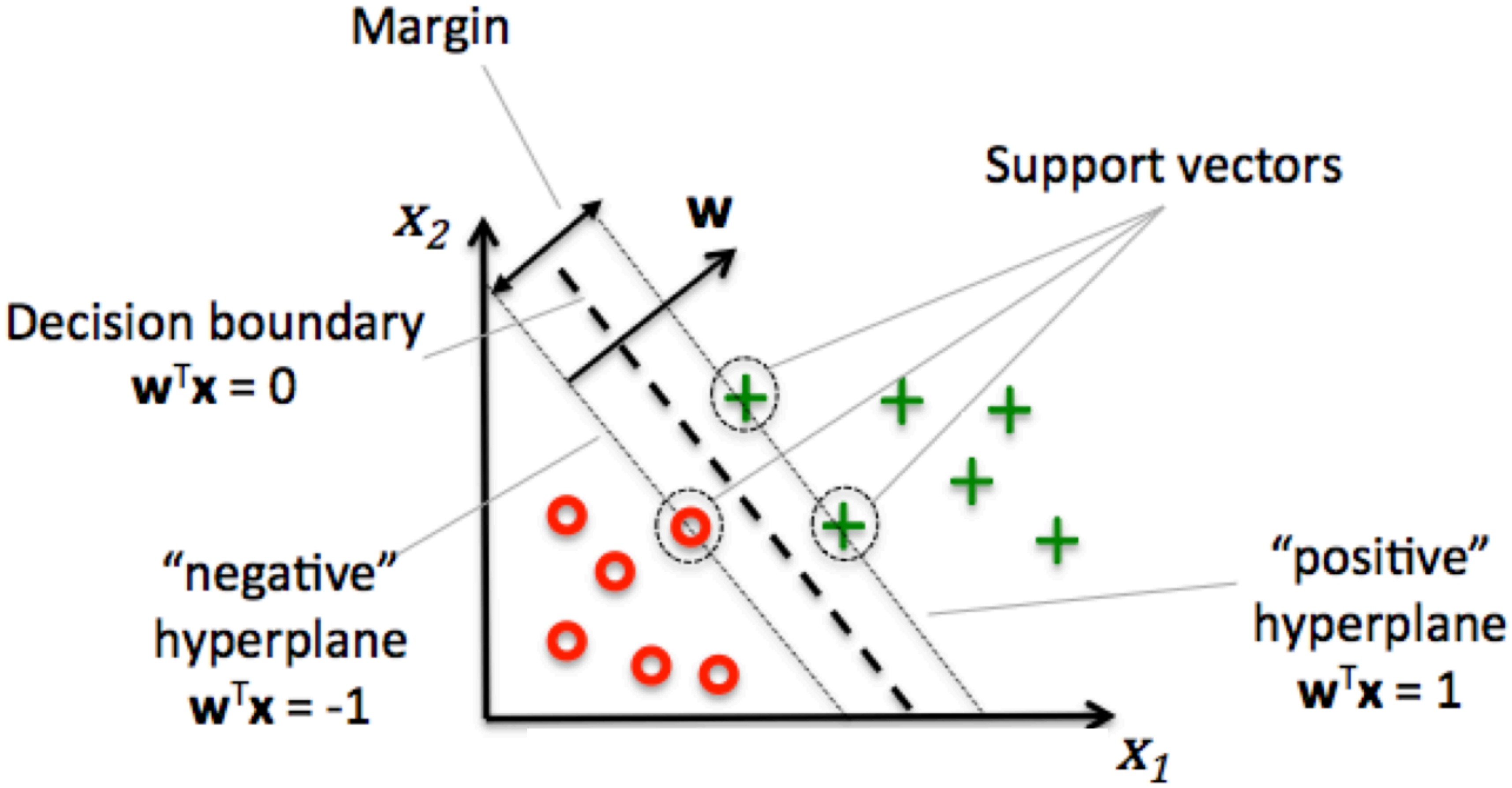
$$f(\mathbf{x}) = \begin{cases} 1, & \mathbf{w}^T\mathbf{x} \geq 0 \\ -1, & \mathbf{w}^T\mathbf{x} < 0 \end{cases}$$

SVM:

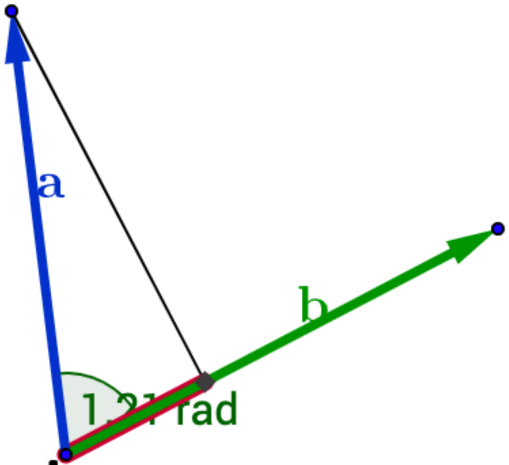
$$f(\mathbf{x}) = \begin{cases} 1, & \mathbf{w}_1^T\mathbf{x} \geq 1 \\ -1, & \mathbf{w}_2^T\mathbf{x} \leq -1 \end{cases}$$

Two different boundaries
for positive vs negative

Large Margin Classification



Dot product intuition



$$\frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{b}\|} = 1.27$$

https://mathinsight.org/dot_product

Large Margin Classification

The **margin** is the distance between the two boundaries.

The **support vectors** are the instances at the boundaries (when $\mathbf{w}^T\mathbf{x} = 1$ or -1)

- Or within the boundaries, if not linearly separable

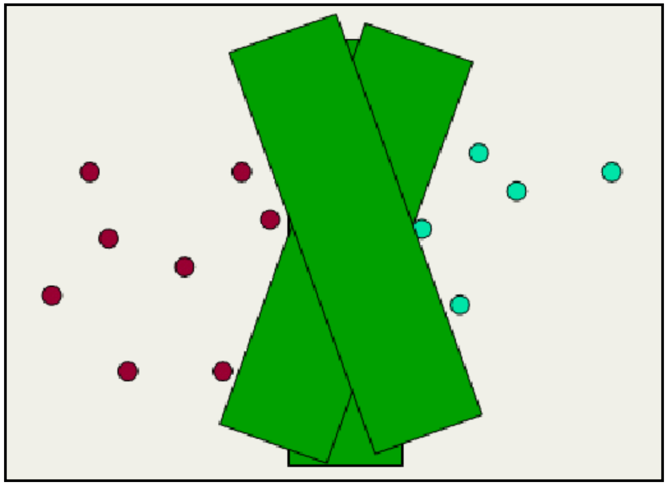
The goal of SVMs is to learn the boundaries to make the margin as large as possible (while still correctly classifying the instances)

- *maximum margin* classification

Large margin intuition

- If a point is right at a decision boundary, a classifier is unsure
  - So good to have lots of distance between decision boundaries

- Large margins limit what a model can learn, and prevent overfitting



Large Margin Classification

The size of the margin is: 2 / ll**w**ll

- Recall: ll**w**ll is the *L2 norm* of the weight vector
- It turns out that smaller weights → larger margin
    - Explanations
        - https://nlp.stanford.edu/IR-book/html/htmledition/support-vector-machines-the-linearly-separable-case-1.html
        - Also Chapter 3 of PML

Large Margin Classification

The size of the margin is: 2 / ll**w**ll

- Recall: ll**w**ll is the *L2 norm* of the weight vector
- Smaller weights → larger margin

Learning goal:

- Maximize 2 / ll**w**ll, subject to the constraints that all instances are correctly classified
- Turn it into minimization problem by taking the inverse: ½ ll**w**ll

Large Margin Classification

The size of the margin is: 2 / ll**w**ll

- Recall: ll**w**ll is the *L2 norm* of the weight vector
- Smaller weights → larger margin

Learning goal:

- Minimize: $\frac{1}{2}\|\boldsymbol{w}\|^2$
- Subject to the constraints:

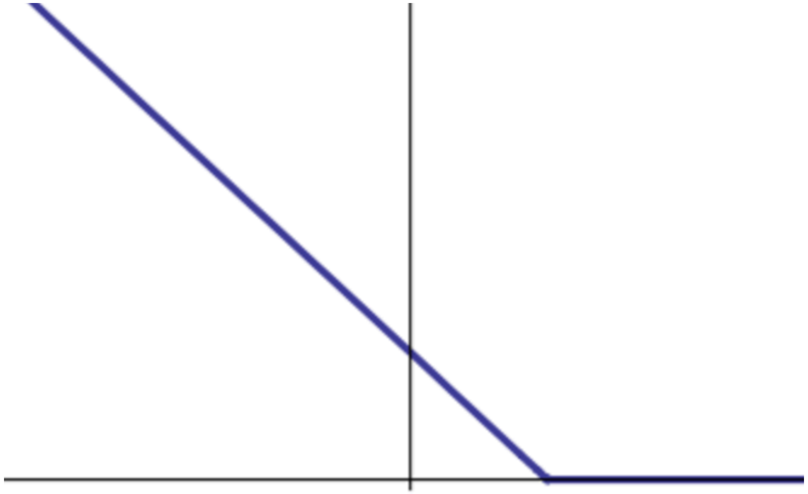
$$y^{(i)}\left(w_0 + \boldsymbol{w}^T \boldsymbol{x}^{(i)}\right) \geq 1 \ \forall_i$$

Only possible to satisfy these constraints if the instances are linearly separable!

Large Margin Classification

In the general case, SVM uses this loss function:

$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\,(\mathbf{w}^T\mathbf{x_i}) \geq 1 \\ -\,y_i\,(\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$



Same as perceptron, but $y_i\,(\mathbf{w}^T\mathbf{x_i}) \geq 1$ instead of $y_i\,(\mathbf{w}^T\mathbf{x_i}) \geq 0$

Large Margin Classification

In the general case, SVM uses this loss function:

$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\ (\mathbf{w}^T\mathbf{x_i}) \geq 1 \\ -\ y_i\ (\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$

The learning goal of SVMs when the data are not linearly separable is to minimize:

$$\underbrace{½\ ||\mathbf{w}||^2}_{\text{inverse margin}} + C\ \underbrace{L(\mathbf{w})}_{\text{training loss}}$$

SVMs also use L2 regularization

- *C* is like λ from before, but larger *C* → lower loss

Large Margin Classification

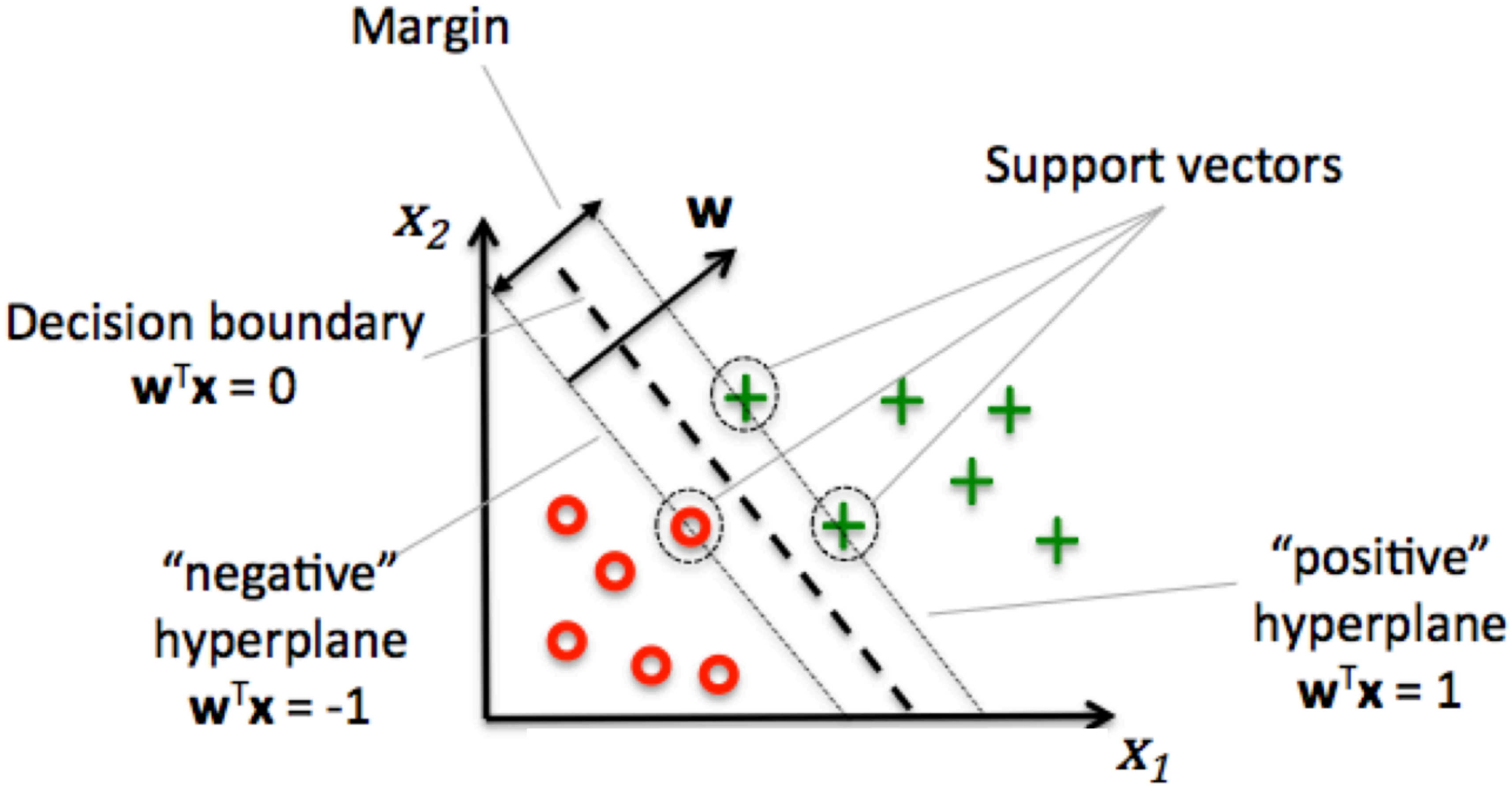
Like perceptron, the SVM function can be minimized using stochastic (sub)gradient descent

- With sklearn’s `SGDClassifier` class, SVM can be implemented by setting `loss='hinge’`

Other implementations (usually using different optimization algorithms than SGD)

- Liblinear and LIBSVM (both used by sklearn)
- SVM-light

Large Margins: Summary



Large Margins: Summary

Classifiers with large margins are more likely to have better generalization, less overfitting

- Hyperparameter *C* controls the tradeoff between margin size and classification error

The large margin principle is another justification for L2 regularization that we saw earlier

- Since the size of the margin is inversely proportional to the L2 norm of the weight vector

The Kernel Trick

Kernel Trick

It turns out that the optimal solution for **w** is equivalent to:

$$\sum_i \alpha_i \mathbf{x_i}$$

Combination of each training instance's feature vector, weighted by α

So in the loss function and prediction functions, we can replace $\mathbf{w}^T\mathbf{x}$ with $\sum_i \alpha_i \mathbf{x_i}^T\mathbf{x}$

α_i is only nonzero for support vectors

- This summation can therefore skip over all other instances, making this calculation more efficient.

Kernel Trick

In the loss function and prediction functions, we can replace $\mathbf{w}^T\mathbf{x}$ with $\sum_i \alpha_i \mathbf{x_i}^T\mathbf{x}$

Now this looks similar to weighted nearest neighbor classification, where the “similarity” between an instance $\mathbf{x}$ and another instance $\mathbf{x_i}$ is $\mathbf{x_i}^T\mathbf{x}$ and this is additionally weighted by α_i

Learning goal is now to learn $\boldsymbol{\alpha}$ instead of $\mathbf{w}$

- How? More complex than before…

Kernel Functions

Loosely, a kernel function is a similarity function between two instances

General kernel trick:
Replace $\mathbf{w}^T\mathbf{x}$ with $\sum_i \alpha_i k(\mathbf{x_i}, \mathbf{x})$

The **linear kernel** function for an SVM is:

$$k(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i}^T\mathbf{x_j}$$

Kernel Functions

What happens if we define the kernel function in some other way?

Then it won't be true that $\sum_i \alpha_i \mathrm{k}(\mathbf{x_i}, \mathbf{x}) = \mathbf{w}^\mathrm{T}\mathbf{x}$

But: kernels can be defined so that,

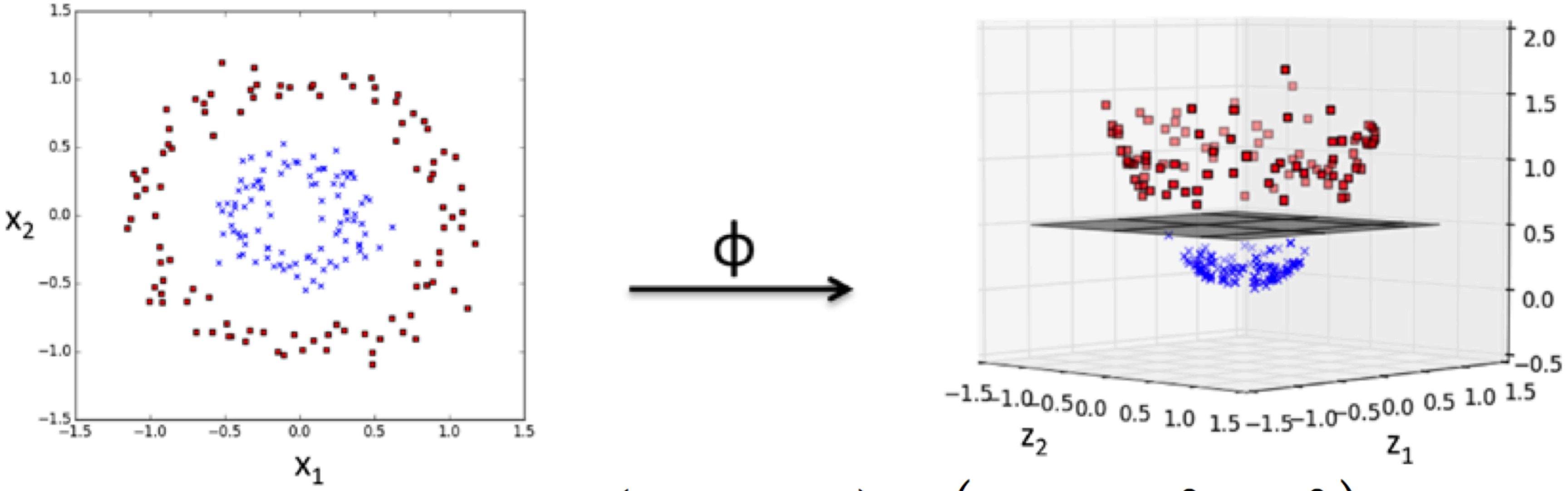
$$\sum_i \alpha_i \mathrm{k}(\mathbf{x_i}, \mathbf{x}) = \mathbf{w}^\mathrm{T}\phi(\mathbf{x}),$$

where $\phi(\mathbf{x})$ is some other feature representation.

Kernel Functions

In general, the kernel trick can create new features as nonlinear combinations of the old features

- Data that are not linearly separable in the original feature space might be separable in the new space



$$\phi(x_1, x_2) = (z_1, z_2, z_3) = \left(x_1, x_2, x_1^2 + x_2^2\right)$$

Kernel Functions: Polynomial

A **polynomial kernel** function is defined as:

$$k(\mathbf{x_i}, \mathbf{x_j}) = (\mathbf{x_i}^T\mathbf{x_j} + c)^d$$

If d=2 (quadratic kernel), then it turns out that

$$\textstyle\sum_i \alpha_i \, k(\mathbf{x_i}, \mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x})$$

where

$$\varphi(x) = \langle x_n^2, \ldots, x_1^2, \sqrt{2}x_n x_{n-1}, \ldots, \sqrt{2}x_n x_1, \sqrt{2}x_{n-1}x_{n-2},$$

$$\ldots, \sqrt{2}x_{n-1}x_1, \ldots, \sqrt{2}x_2 x_1, \sqrt{2c}x_n, \ldots, \sqrt{2c}x_1, c\rangle$$

Kernel Functions: Polynomial

In other words, using a quadratic kernel is equivalent to using a standard SVM where you’ve expanded the feature vectors to include:

- Each original feature value (times a constant)
- Each feature value squared
- The product of each pair of feature values (times a constant)
    - This can be especially useful, since it can capture *interactions* between features

Without the kernel trick, this large feature set would be computationally expensive to work with.

Kernel Functions: RBF

The **radial basis function** (RBF kernel) is:

$$k(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\gamma \underbrace{||\mathbf{x_i} - \mathbf{x_j}||^2}_{\text{squared Euclidean distance}})$$

- One of the most popular SVM kernels
- Related to the Gaussian/normal distribution
- Interpretation as expanded feature vector?
  - It actually maps to a feature vector with infinitely many features… so technically equivalent, but impossible to implement without using the kernel trick.

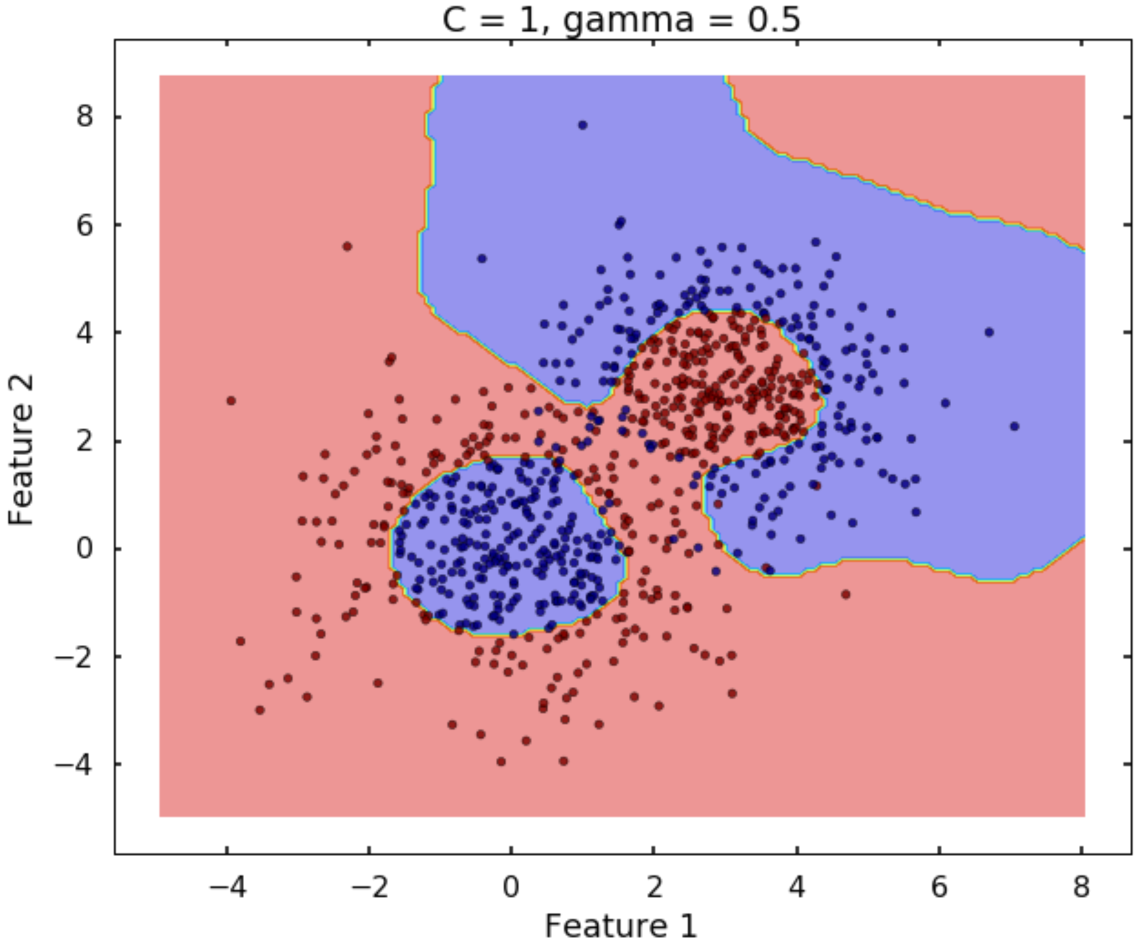
Kernel Functions: RBF

The **radial basis function** (RBF kernel) is:

$$k(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\gamma\ ||\mathbf{x_i} - \mathbf{x_j}||^2\ )$$

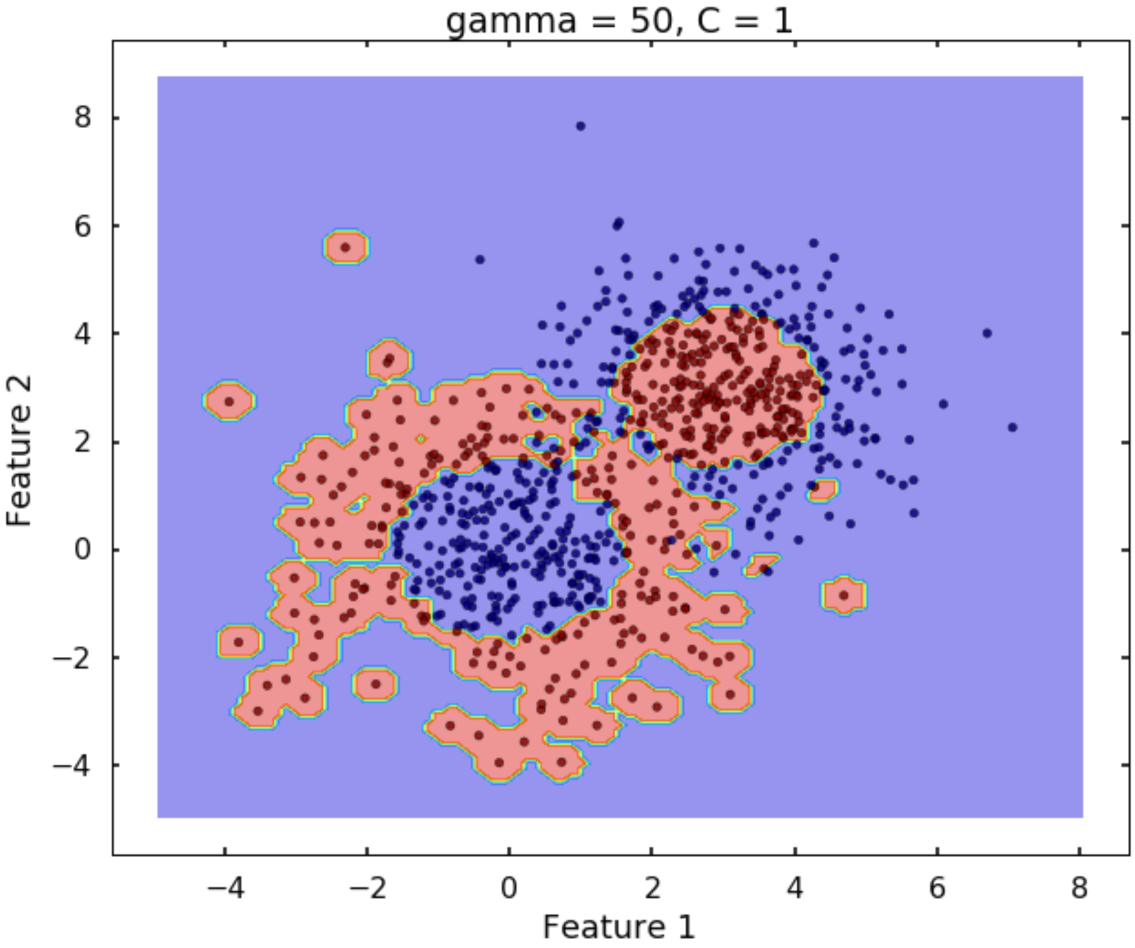
- In addition to *C*, γ also affects overfitting
- Large γ → small differences in distance between $\mathbf{x_i}$ and $\mathbf{x_j}$ are magnified
    - This will cause the classifier to fit the training data better, but may do worse on future data

Kernel Functions: RBF



From: http://qingkaikong.blogspot.com/2016/12/machine-learning-8-support-vector.html

Kernel Functions: RBF



From: http://qingkaikong.blogspot.com/2016/12/machine-learning-8-support-vector.html

Kernel Methods: Summary (1)

- Kernel SVM is a reformulation of SVM that uses similarity between instances
  - To make a prediction for a new instance, need to calculate kernel function for the new instance and all training instances that are the support vectors
- Kernel SVM is equivalent to an SVM with a expanded feature set
  - Sometimes there is an intuitive interpretation of what the “new” features mean; sometimes not
- Kernel SVM with a linear kernel is equivalent to a standard SVM

Kernel Methods: Summary (2)

- Kernels can be useful when your data has a small number of features and/or when the dataset is not linearly separable
- Some kernels are prone to overfitting
  - High degree polynomial; RBF with high scaling parameter
- Kernel SVM has additional hyperparameters you have to choose
  - Type of kernel
  - Parameters of kernel (e.g., d in polynomial, γ in RBF)

Kernel Methods: Summary (3)

Also be aware that:

- Kernel methods not unique to SVM (invented long before, for perceptron), but popularized by it.
- Lots of other kernel functions not shown here, but these are the most common.
  - Specialized kernels exist for certain types of data (e.g., biological sequences, syntax trees)