GA GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 13: SUPPORT VECTOR MACHINES

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DAT5 SF // April 21, 2014

RECAP

LAST TIME:

- DECISION TREES
- RANDOM FORESTS
- DECISION TREES IN SCIKIT-LEARN
- DEMO OF BIGML

AGENDA

I. SUPPORT VECTOR MACHINES

II. MAXIMUM MARGIN HYPERPLANES

III. SLACK VARIABLES

IV. NONLINEAR CLASSIFICATION

EXERCISE:

V. SVM IN SCIKIT-LEARN

I. SUPPORT VECTOR MACHINES

Q: What is a support vector machine?

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A: A binary linear classifier whose decision boundary is explicitly constructed to minimize generalization error.

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Quick review – who can define one of the underlined terms for us…?

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A: A binary linear classifier whose decision boundary is explicitly constructed to minimize generalization error.

recall:

binary classifier – *solves two-class problem*

linear classifier – *creates linear decision boundary (in 2d)*

	continuous	*categorical*
supervised	???	???
unsupervised	???	???

	continuous	categorical
supervised	regression	classification
unsupervised	dimension reduction	clustering

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NOTE

These are two different ways of looking at the same problem.

Familiarity with both leads to deeper understanding!

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A: Using geometric reasoning (as opposed to the algebraic reasoning we've used to derive other classifiers).

The generalization error is equated with the geometric concept of **margin***, which is the region along the decision boundary that is free of data points.*

SUPPORT VECTOR MACHINES

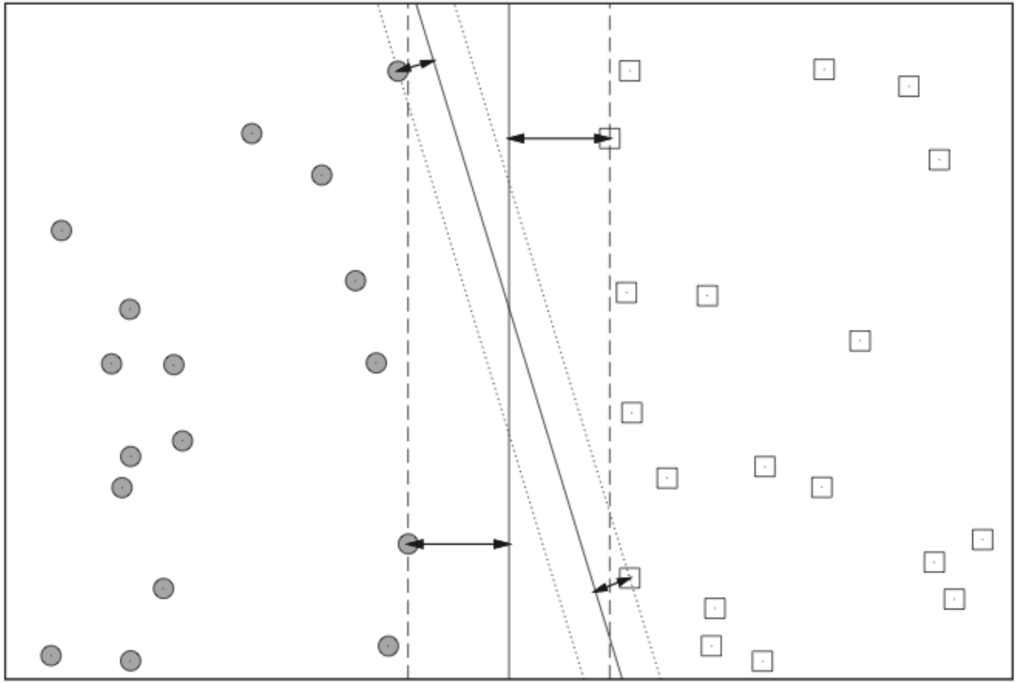

FIGURE 18-4. Two decision boundaries and their margins. Note that the vertical decision boundary has a wider margin than the other one. The arrows indicate the distance between the respective support vectors and the decision boundary.

source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

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The goal of an SVM is to create the linear decision boundary with the largest margin. This is commonly called the **maximum margin hyperplane**.

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NOTE

A *hyperplane* is just a high-dimensional generalization of a line.

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A: Using a clever maneuver called the **kernel trick***.*

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Nonlinear applications of SVM rely on an implicit (nonlinear) mapping that sends vectors from the original feature space K into a higher-dimensional feature space K'.

Nonlinear classification in K is then obtained by creating a linear decision boundary in K'.

In practice, this involves no computations in the higher dimensional space!

II. MAXIMUM MARGIN HYPERPLANES

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$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b.$$

such that w is the weight vector and b is the bias.

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A: By the **discriminant function**,

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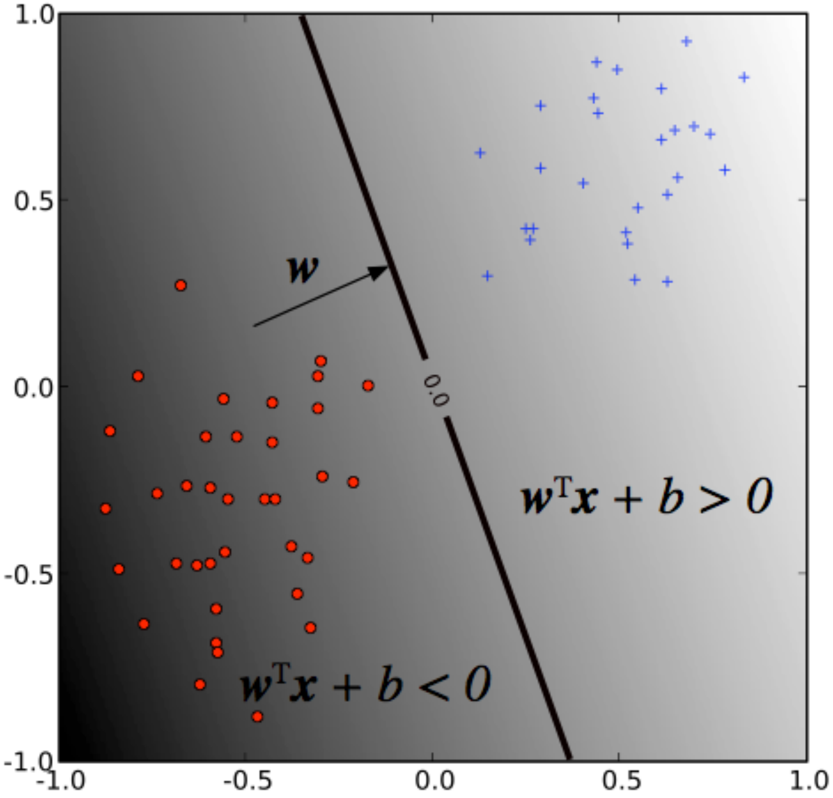
The sign of f(x) determines the (binary) class label of a record x.

MAXIMUM MARGIN HYPERPLANES



source: http://pyml.sourceforge.net/doc/howto.pdf

NOTE

The weight vector determines the *orientation* of the decision boundary.

The bias determines its *translation* from the origin.

As we said before, SVM solves for the decision boundary that minimizes generalization error, or equivalently, that has the maximum margin.

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Q: Why are these the same thing?

A: Because using the MMH as the decision boundary minimizes the probability that a small perturbation in the position of a point produces a classification error.

NOTE

Intuitively, the wider the margin, the clearer the distinction between classes.

Selecting the MMH is a straightforward exercise in analytic geometry (we won't go through the details here).

In particular, this task reduces to the optimization of a **convex** *objective function.*

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Remember what convex means in this context…?

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This is nice because convex optimization problems are guaranteed to give **global optima** *(and they're easy to solve numerically too).*

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NOTE

The heuristic techniques we've discussed (eg greedy algorithms) are not necessary with convex optimization!

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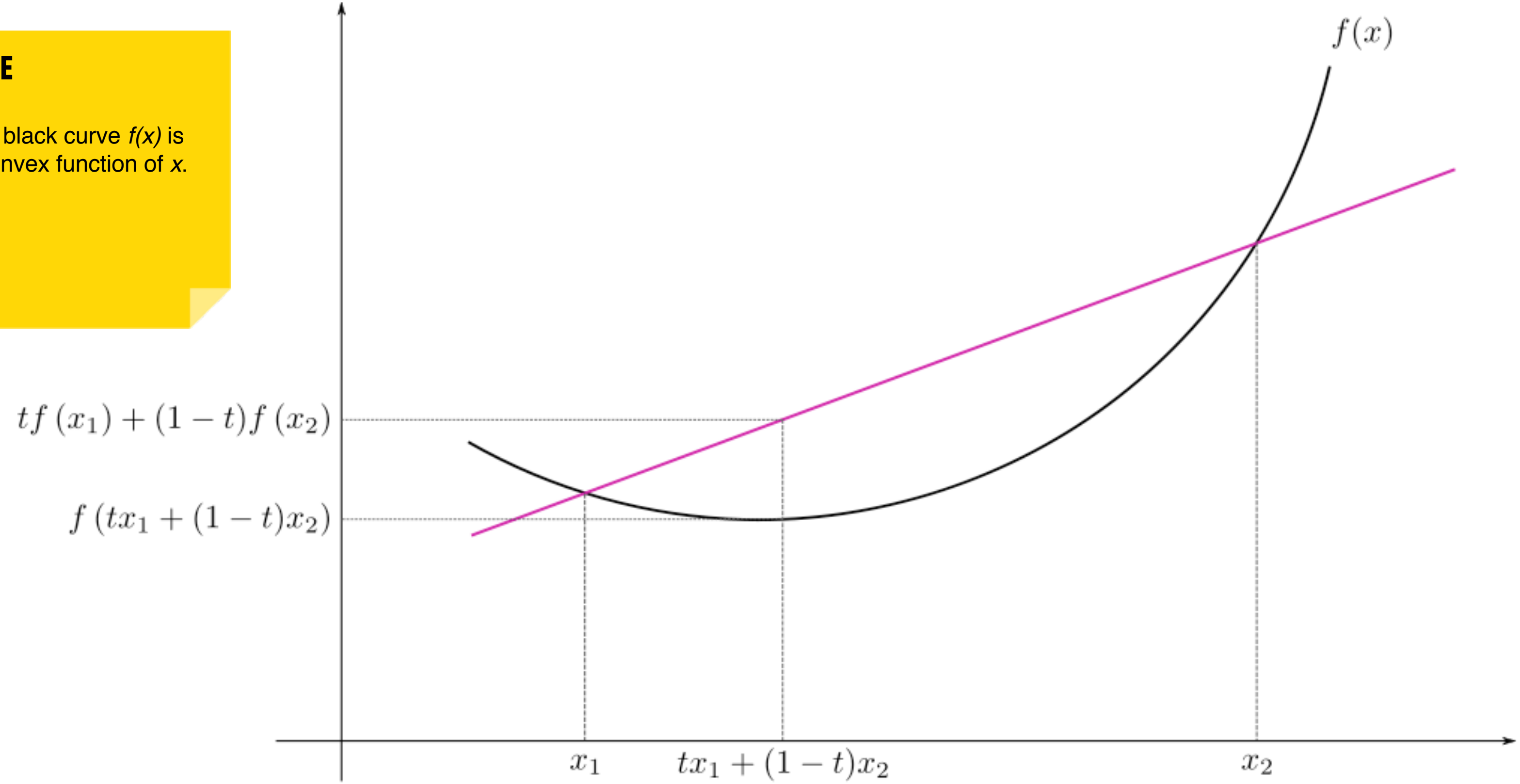
CONVEX FUNCTIONS

NOTE

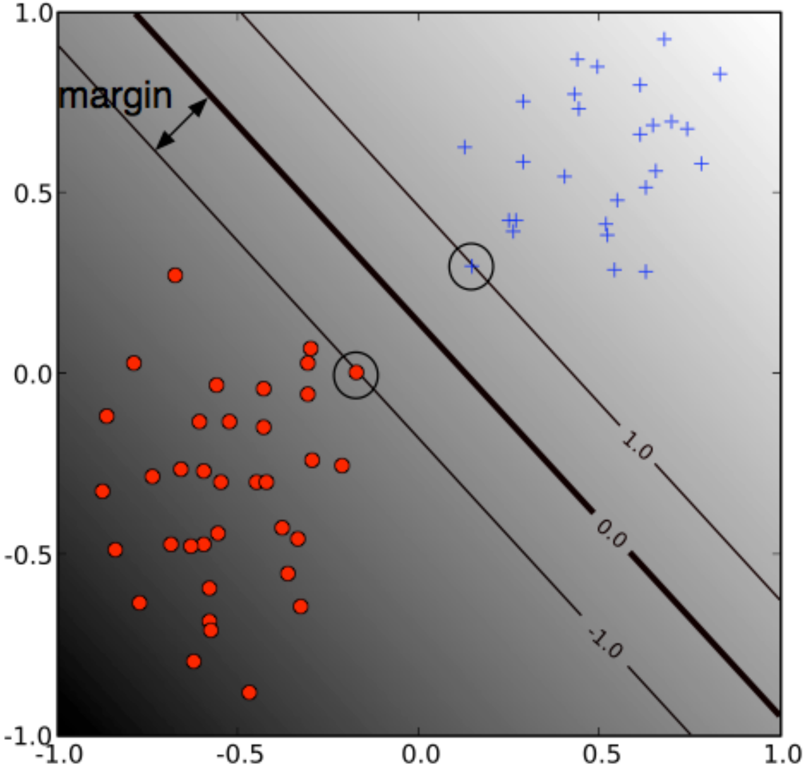
The black curve *f(x)* is a convex function of *x*.



source: http://en.wikipedia.org/wiki/File:ConvexFunction.svg

Notice that the margin depends only on a subset of the training data; namely, those points that are nearest to the decision boundary.

MAXIMUM MARGIN HYPERPLANES



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These points are called the **support vectors***.*

The other points (far from the decision boundary) don't affect the construction of the MMH at all! However, the global (convex) nature of the algorithm means that for those support vectors, the optimal MMH will be found!

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The optimization problem that this SVM solves is:

$$\begin{aligned} \underset{\mathbf{w},b}{\text{minimize}} \quad & \tfrac{1}{2}||\mathbf{w}||^2 \\ \text{subject to:} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad i = 1, \ldots, n\,. \end{aligned}$$

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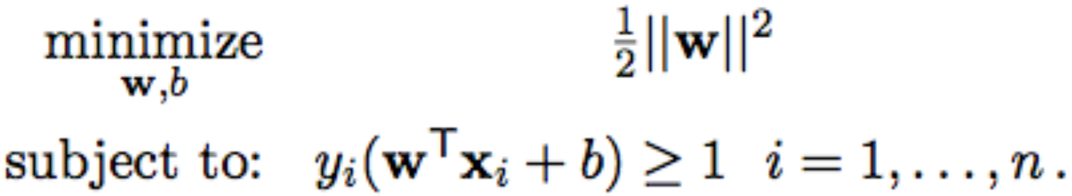

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NOTE

This type of optimization problem is called a *quadratic program*.

The result of this qp is the *hard margin classifier* we've been discussing.

III. SLACK VARIABLES

Recall that in building the hard margin classifier, we assumed that our data was (perfectly) **linearly separable** *(eg, that we could perfectly classify each record with a linear decision boundary).*

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This can be done using by introducing **slack variables.**

Slack variables ξ_i *generalize the optimization problem to permit some misclassified training records (which come at a cost* C*).*

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The resulting **soft margin classifier** *is given by:*

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\underset{\mathbf{w},b}{\text{minimize}} & \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i \\
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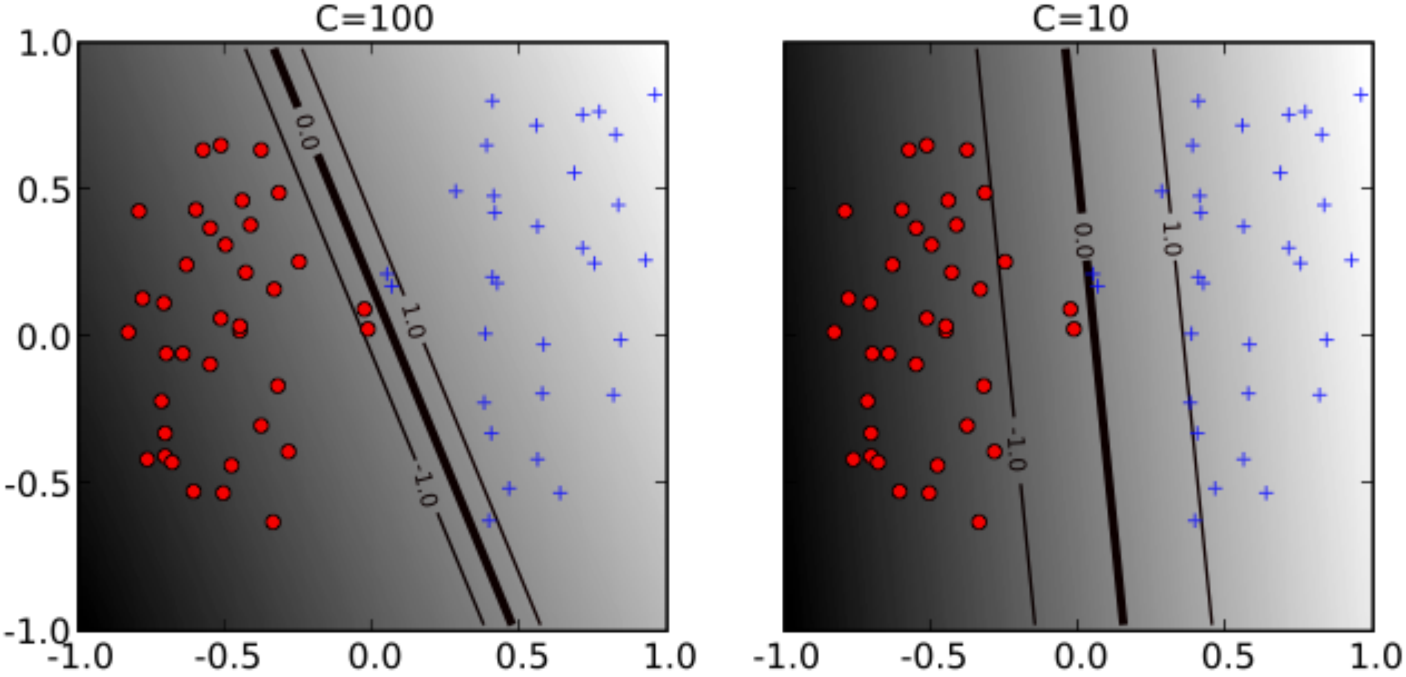
This an example of bias-variance tradeoff.

SLACK VARIABLES – SOFT MARGIN CONSTANT



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The soft-margin optimization problem can be rewritten as:

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NOTE

This is called the *dual formulation* of the optimization problem.

(reached via Lagrange multipliers)

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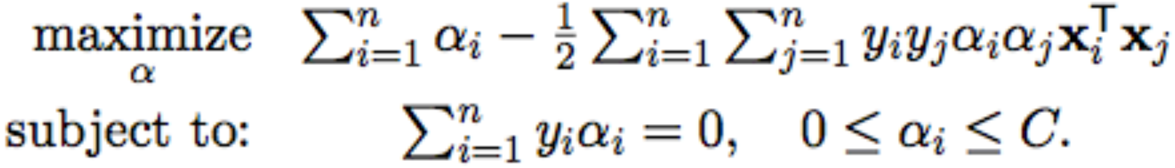

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Notice that this expression depends on the features x_i only via the **inner product**

$$<x_i, x_j> = x_i^T x_j$$

The inner product is an operation that takes two vectors and returns a real number.

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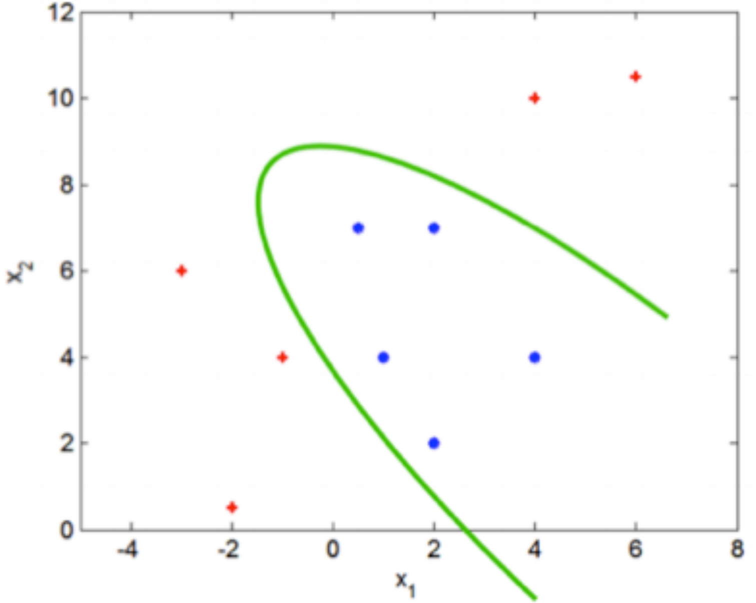
The fact that we we can rewrite the optimization problem in terms of the inner product means that we don't actually have to do any calculations in the feature space K*.*

In particular, we can easily change K *to be some other space* K'*.*

IV. NONLINEAR CLASSIFICATION

Suppose we need a more complex classifier than a linear decision boundary allows.



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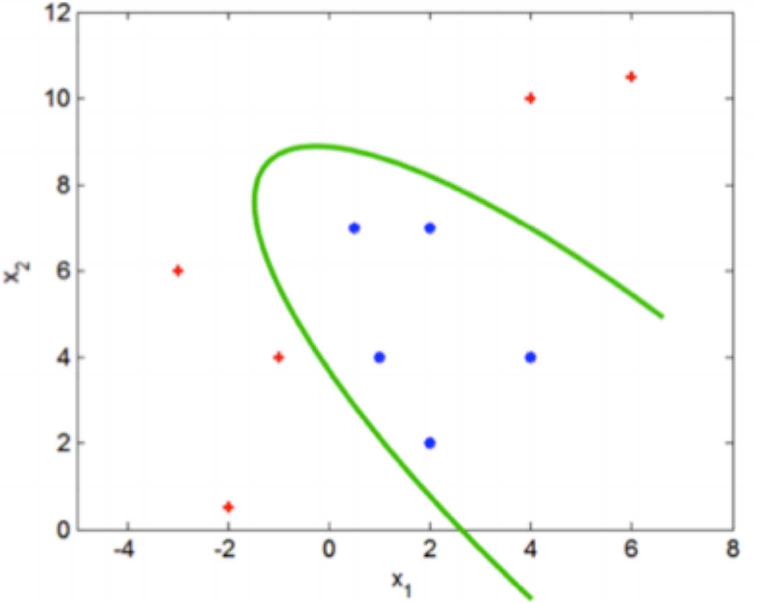
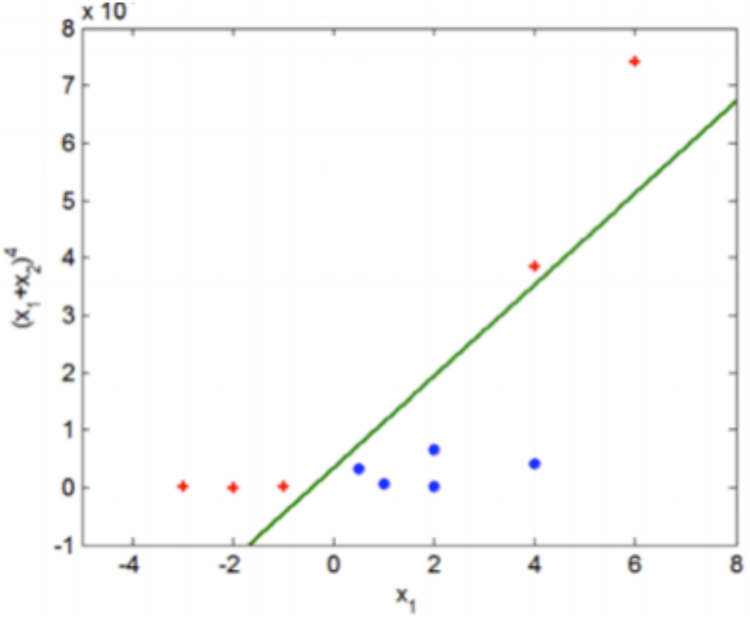
This linear decision boundary will be mapped to a nonlinear decision boundary in the original feature space.

NONLINEAR CLASSIFICATION



original feature space *K*



higher-dim feature space *K’*

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In particular, this will not scale well, since it requires many high-dimensional calculations.

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In particular, this will not scale well, since it requires many high-dimensional calculations.

It will likely lead to more complexity (both modeling complexity and computational complexity) than we want.

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- remap the feature vectors x_i into a higher-dimensional space K'

- create a linear decision boundary in K'

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But we want to save ourselves the trouble of doing a lot of additional high-dimensional calculations. How can we do this?

Recall that our optimization problem depends on the features only through the inner product $x^T x$:

$$
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\underset{\alpha}{\text{maximize}} & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^{\mathsf{T}} \mathbf{x}_j \\
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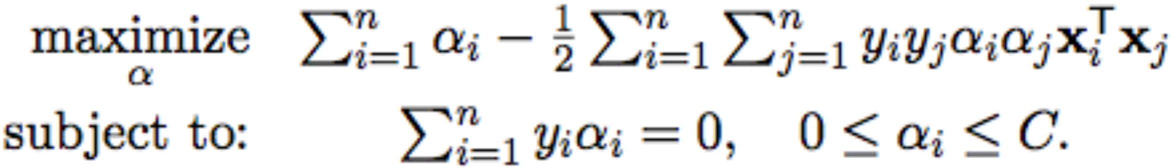

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We can replace this inner product with a more general function that has the same type of output as the inner product.

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Formally, we can think of the inner product as a map that sends two vectors in the feature space K into the real line $\mathbb{R}$ *.*

We can replace this with a generalization of the inner product called a **kernel function** *that maps two vectors in a higher-dimensional feature space K' into* $\mathbb{R}$ *.*

The upshot is that we can use a kernel function to implicitly train our model in a higher-dimensional feature space, without incurring additional computational complexity!

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NOTE

These conditions are contained in a result called *Mercer's theorem*.

The upshot is that we can use a kernel function to implicitly train our model in a higher-dimensional feature space, without incurring additional computational complexity!

As long as the kernel function satisfies certain conditions, our conclusions above regarding the mmh continue to hold.

In other words, no algorithmic changes are necessary, and all the benefits of a linear SVM are maintained.

some popular kernels:

linear kernel $k(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$

polynomial kernel $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + 1)^d$

Gaussian kernel $k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma ||\mathbf{x} - \mathbf{x}'||^2)$

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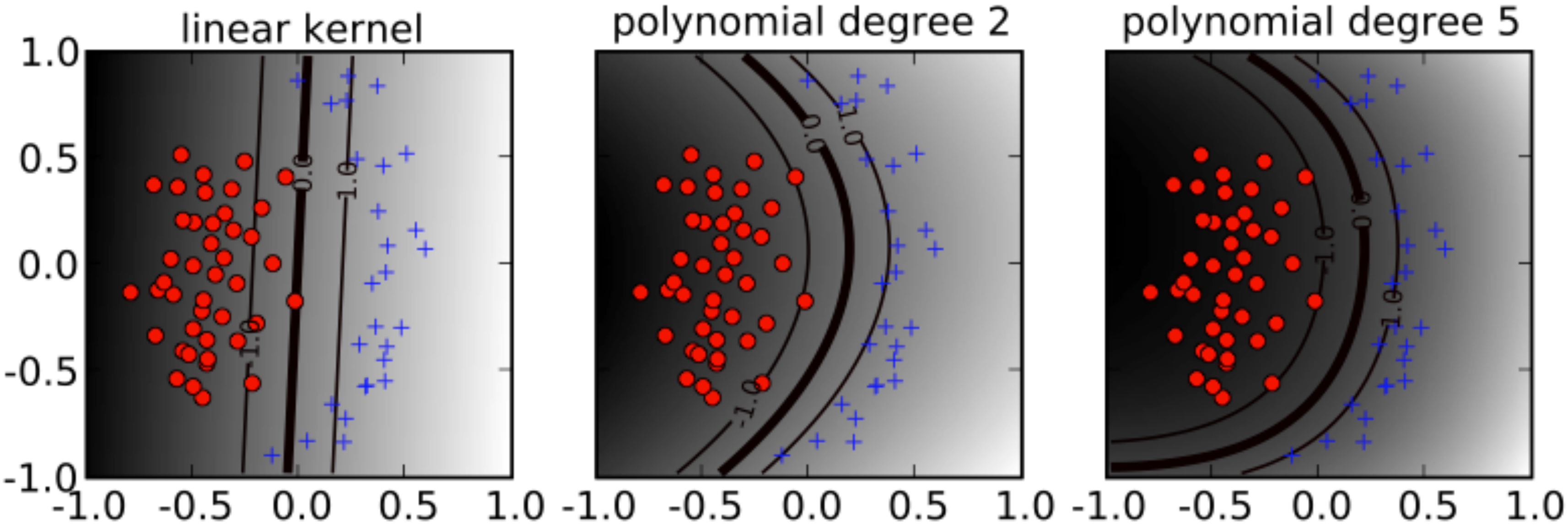
The **hyperparameters** *d, γ affect the flexibility of the decision bdy.*

NONLINEAR CLASSIFICATION – POLYNOMIAL KERNEL



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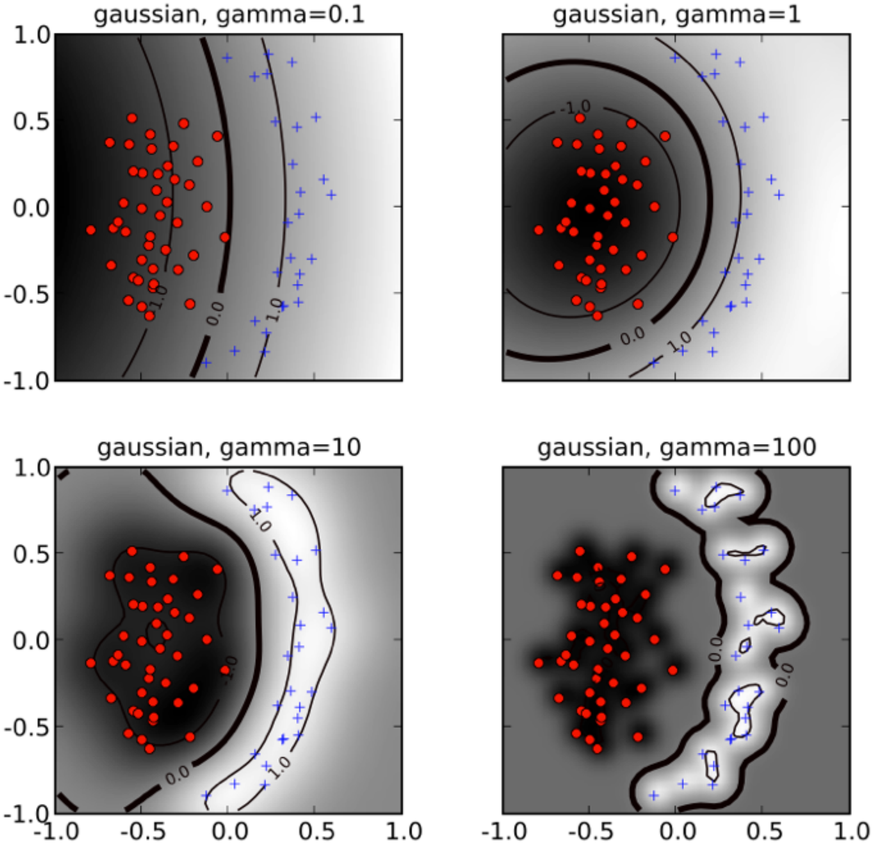
NONLINEAR CLASSIFICATION – GAUSSIAN KERNEL



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SVMs (and **kernel methods** *in general) are versatile, powerful, and popular techniques that can produce accurate results for a wide array of classification problems.*

The main disadvantage of SVMs is the lack of intuition they produce. These models are truly black boxes!

EX: SVM IN SCIKIT-LEARN