GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 11: SUPPORT VECTOR MACHINES

LAST TIME:

- DECISION TREES
- PRUNING TREES
- CLASSIFICATION PERFORMANCE

I. DISCRIMINATIVE VS GENERATIVE CLASSIFICATION
II. SUPPORT VECTOR MACHINES
III. MAXIMUM MARGIN HYPERPLANES
IV. SLACK VARIABLES
V. NONLINEAR CLASSIFICATION

EXERCISE: SVM IN SKLEARN

I. DISCRIMINATIVE VS GENERATIVE ALGORITHMS

*Review: What what does it mean for an algorithm to be **discriminative vs generative**?*

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Discriminative: $P(C \mid D)$

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Discriminative: $P(C \mid D)$

Pragmatic: focuses on distinguishing. Can only classify

Generative: $P(D \mid C), P(C)$

Deeper understanding: modeling classes. Can generate data.

Review: Which is which?

Logistic Regression:

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Logistic Regression: *Discriminative*

KNN:

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Decision Trees:

Review: Which is which?

Logistic Regression: *Discriminative*

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Naíve Bayes: *Generative*

Decision Trees: *Discriminative*

SVM: ?

II. 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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recall:

binary classifier – *solves two-class problem*

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

Q: How is the decision boundary derived?

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A: Using geometric reasoning.

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In 3 dimensions, it's a 2D plane:

$$w_1x_1 + w_2x_2 + w_3x_3 + w_0 = 0$$

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.*

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Margins provide the largest impact: even moving ***one point*** *along the margin can completely change the decision boundary!*

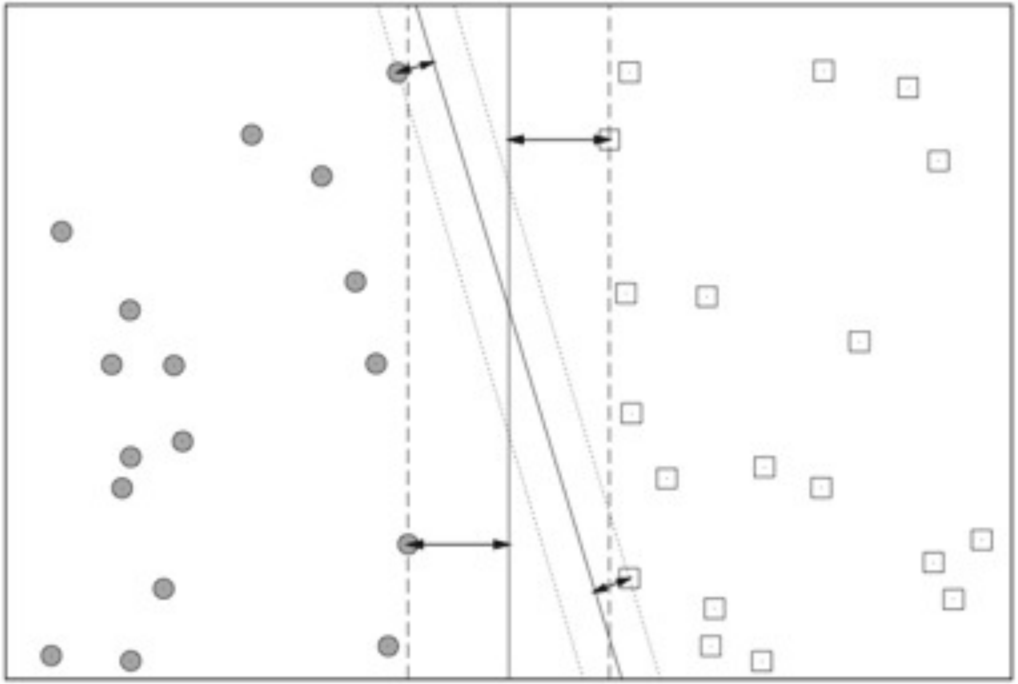

FIGURE 18-4. Two decision boundaries and their margins. Note that the vertical decision boundary has a wider margin than the other one. The arrows indicate the distance between the respective support vectors and the decision boundary.

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

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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 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!

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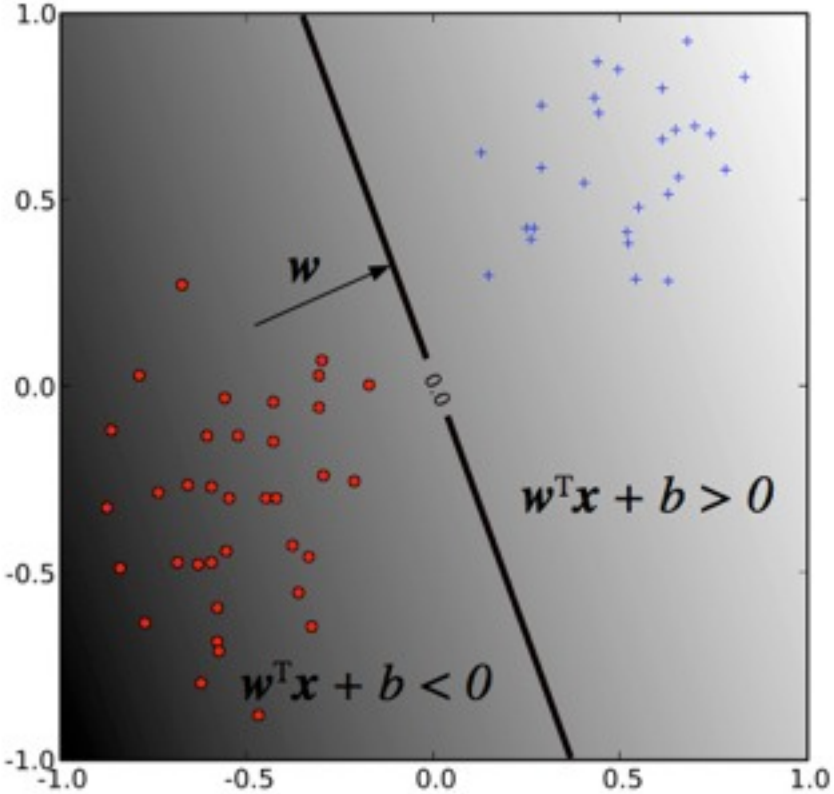
such that w is the weight vector and b is the bias.

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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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.

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NOTE

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

Q: Why are these the same thing?

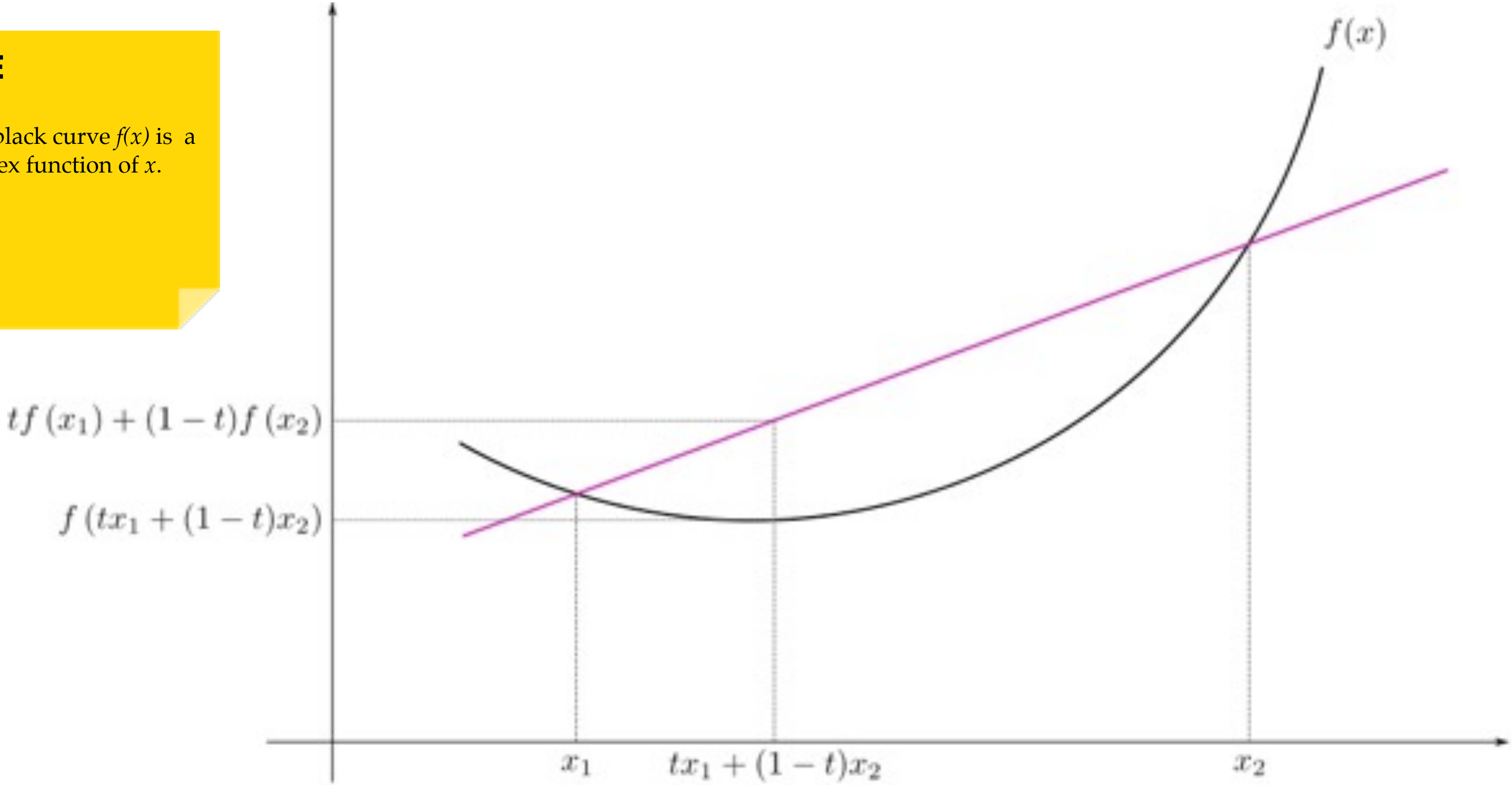
A: Because using the mmh as the decision boundary minimizes the probability that a small perturbation in the position of a point produces a classification error.

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.*

NOTE

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



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

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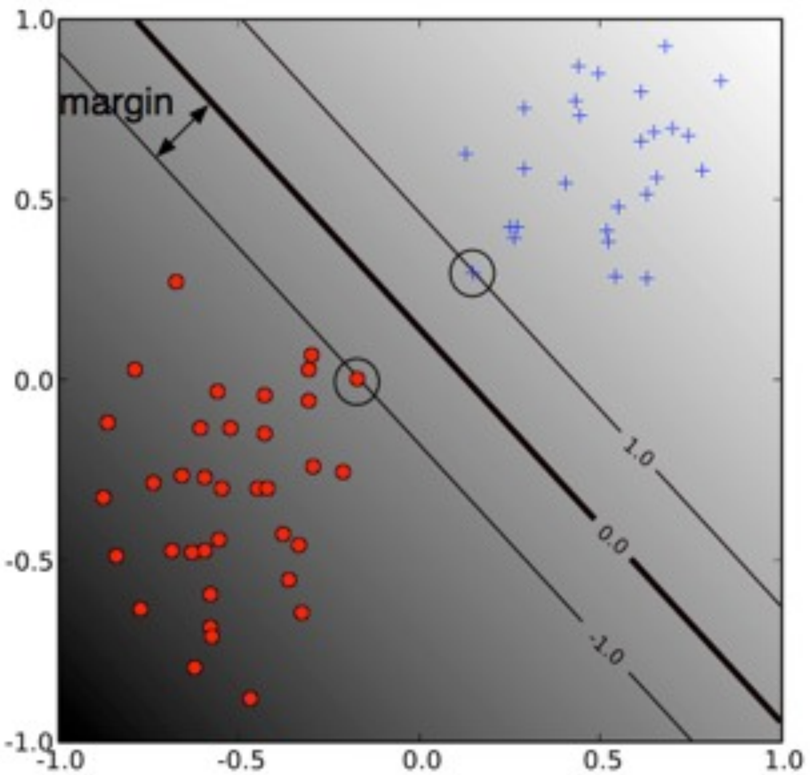
Notice that the margin depends only on a subset of the training data; namely, those points that are nearest to the decision boundary.

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!

All of the decision boundaries we've seen so far have split the data perfectly; eg, the data are **linearly separable**, *and therefore the training error is 0.*

We are always solving for one optimum (global, instead of the local optimum).

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The optimization problem that this SVM solves is:

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

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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 VARABLES

Recall that in building the hard margin classifier, we assumed that our data was **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:*

$$\begin{array}{ll} \underset{\mathbf{w},b}{\text{minimize}} & \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i \\ \text{subject to:} & y_i(\mathbf{w}^\top\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0. \end{array}$$

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This an example of bias-variance tradeoff.

Translated, this means that soft margins create a “zone” for potential error, allowing the algorithm to potentially pick out “better” support vectors.

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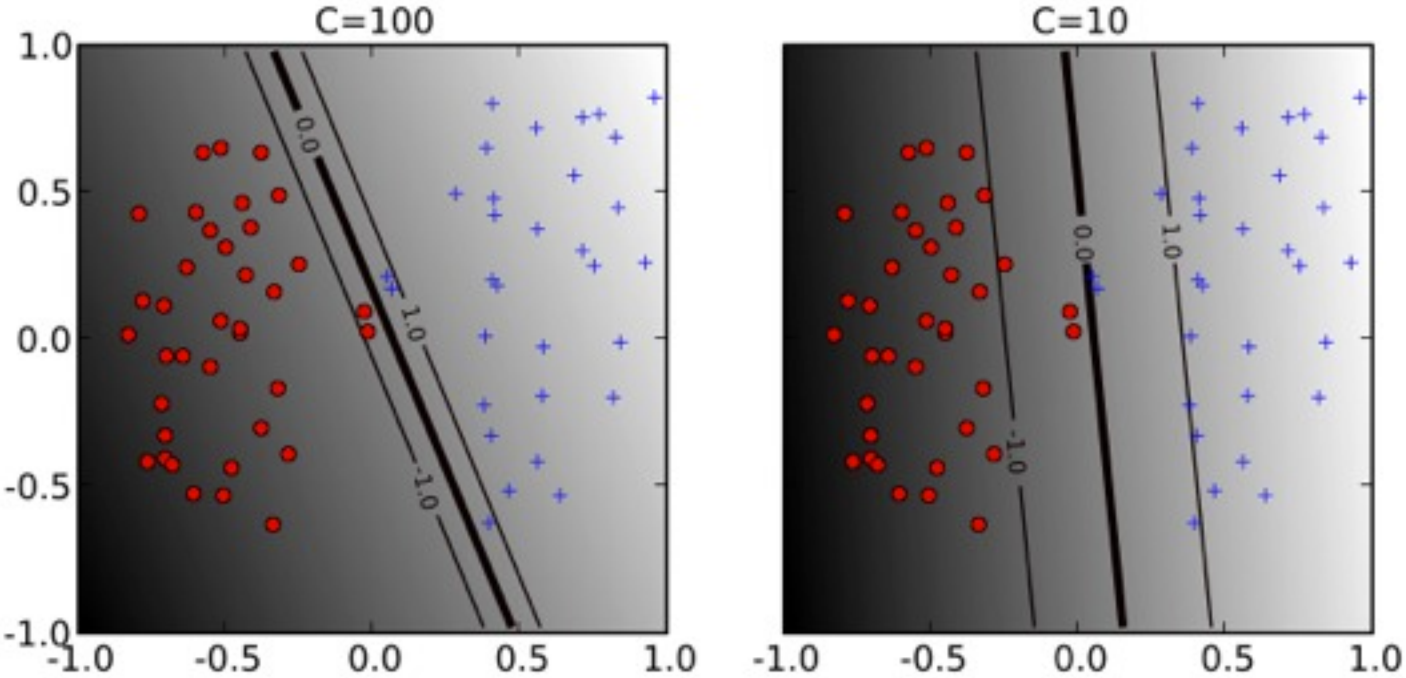
*By removing the **bias** error from the hard margin, we introduce **variance** error (and thus, generalization error) into our model*

SLACK VARIABLES – SOFT MARGIN CONSTANT



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The soft-margin optimization problem can be rewritten as:

$$\begin{aligned} \underset{\alpha}{\text{maximize}} \quad & \textstyle\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^\top \mathbf{x}_j \\ \text{subject to:} \quad & \textstyle\sum_{i=1}^{n} y_i \alpha_i = 0, \quad 0 \leq \alpha_i \leq C. \end{aligned}$$

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NOTE

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

(reached via Lagrange multipliers)

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$$
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\text{subject to:} & \sum_{i=1}^{n} y_i \alpha_i = 0, \quad 0 \leq \alpha_i \leq C.
\end{array}
$$

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

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

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Higher values of C = higher accuracy in model

Lower values of C = training error and better generalization

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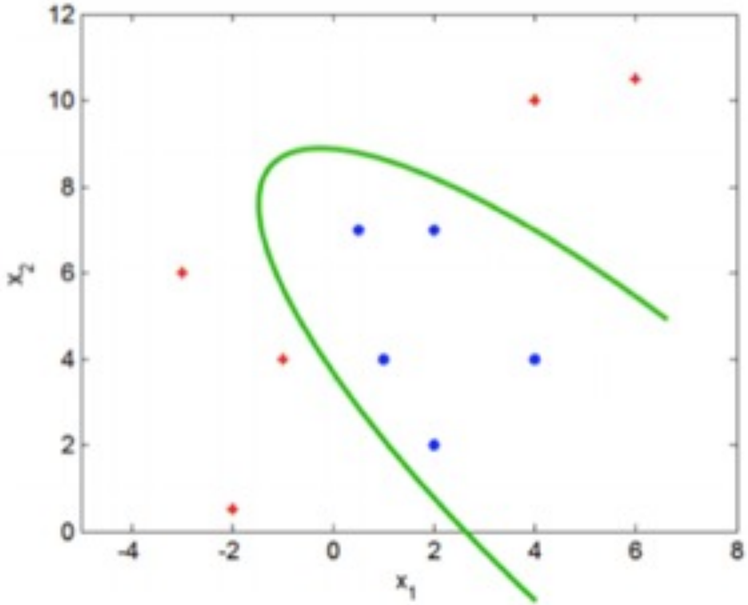
The fact that we we can rewrite the optimization problem in terms of the inner product means that we don't actually have to do any calculations in the feature space K.

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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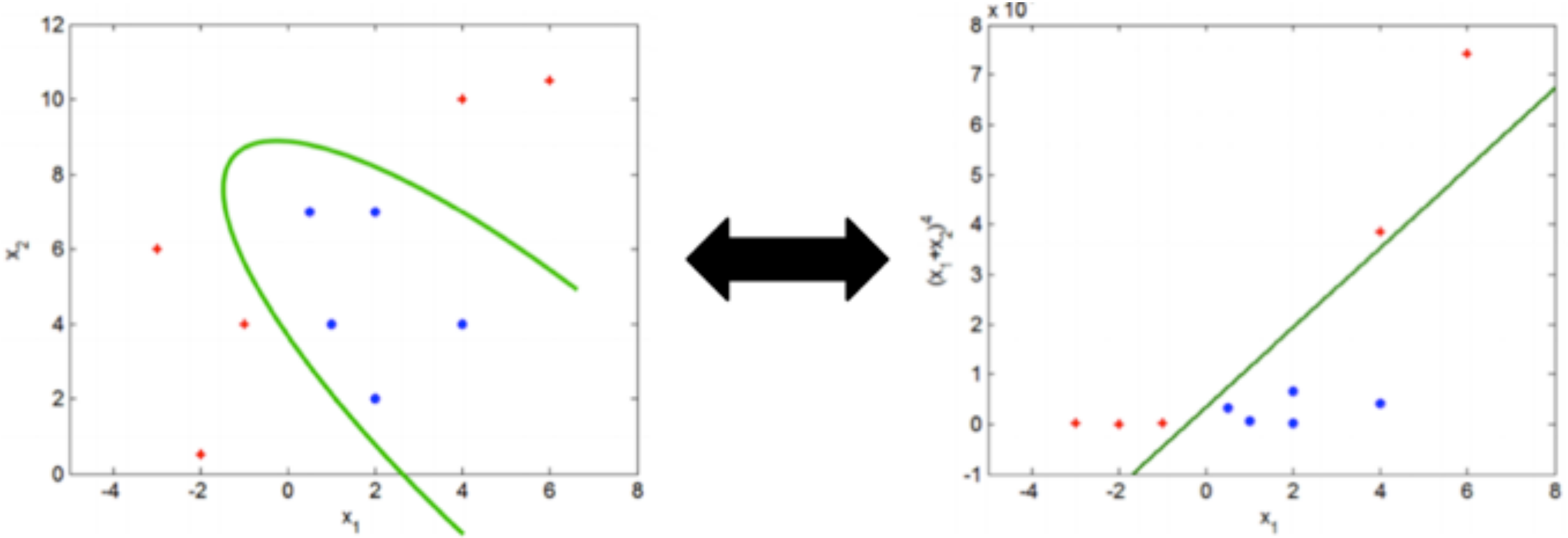
One possibility is to add nonlinear combinations of features to the data, and then to create a linear decision boundary in the enhanced (higher-dimensional) feature space.

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



original feature space K

higher-dim feature space K'

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- Does not scale well: requires many high-dimensional calculations.

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- Does not scale well: requires many high-dimensional calculations.
- Leads to more complexity (both modeling complexity and computational complexity) than we want.

Let’s hang on to the logic of the previous example, namely:

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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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Let's hang on to the logic of the previous example, namely:

- *remap the feature vectors* x_i *into a higher-dimensional space* K'
- *create a linear decision boundary in* K'
- *back out the nonlinear decision boundary in* K *from the result*

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 $x^T x$:

$$\begin{aligned} &\underset{\alpha}{\text{maximize}} \quad \textstyle\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^\mathsf{T} \mathbf{x}_j \\ &\text{subject to:} \qquad \textstyle\sum_{i=1}^{n} y_i \alpha_i = 0, \quad 0 \le \alpha_i \le C. \end{aligned}$$

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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.

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

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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* $\mathbb{R}$ *.*

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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.

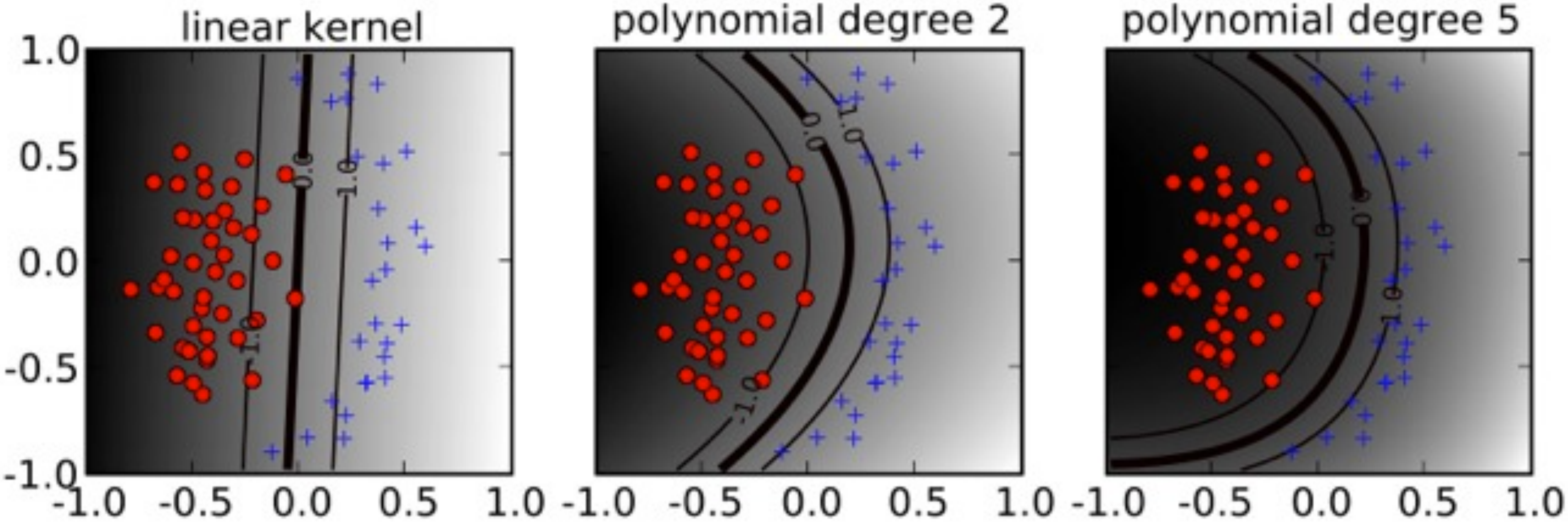
some popular kernels:

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

polynomial kernel $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\mathsf{T}\mathbf{x}' + 1)^d$

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

NONLINEAR CLASSIFICATION – POLYNOMIAL KERNEL



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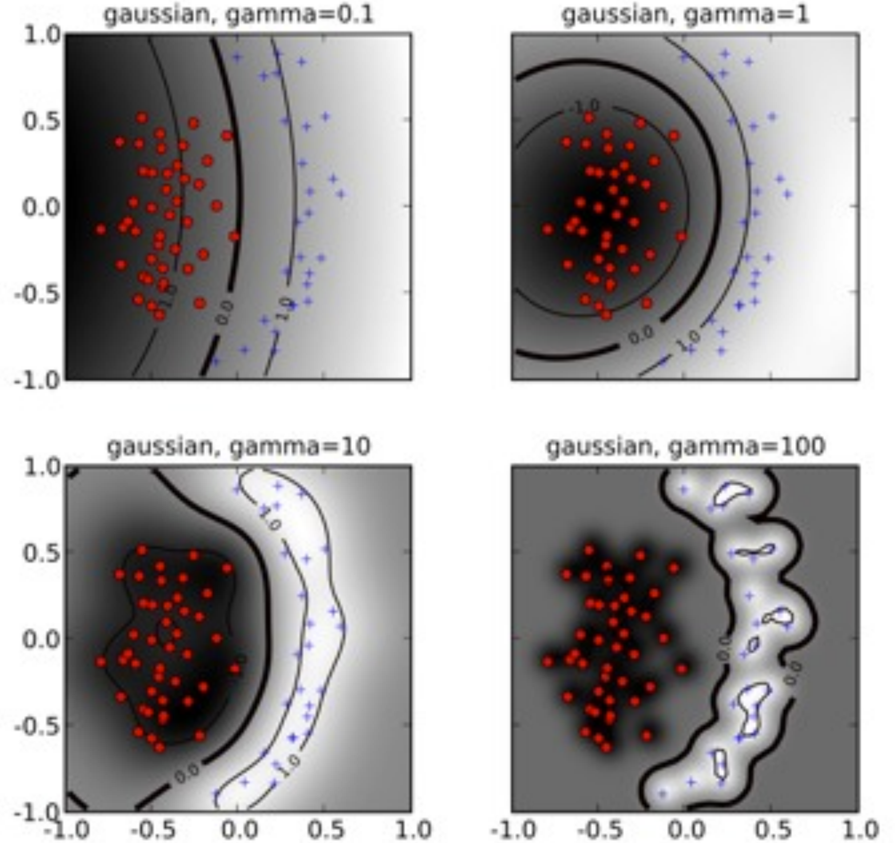
NONLINEAR CLASSIFICATION – GAUSSIAN KERNEL



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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: SVMS AND KERNELS