GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 13: SUPPORT VECTOR MACHINES

I. DECISION TREES
II. FITTING DECISION TREES
III. OBJECTIVE FUNCTIONS
IV. REGULARIZATION
V. ENSEMBLE METHODS

BAGGING BOOSTING RANDOM FORESTS

Questions?

- DATA EXPLORATION
- SUPERVISED LEARNING: REGRESSION
- **SUPERVISED LEARNING: CLASSIFICATION**
- UNSUPERVISED LEARNING
- VARIOUS TOPICS

- LOGISTIC REGRESSION
- NAIVE BAYES
- RANDOM FORESTS
- **SUPPORT VECTOR MACHINES**
- COMPETITION

Final outlines for your project are due next lesson

I. SUPPORT VECTOR MACHINES

II. REGULARIZATION

III. KERNELS

- DESCRIBE WHAT THE SVM'S OBJECTIVE IS
- DESCRIBE THE EFFECT OF REGULARIZATION
- DESCRIBE WHAT KERNELS ARE
- APPLY SVMS IN SKLEARN

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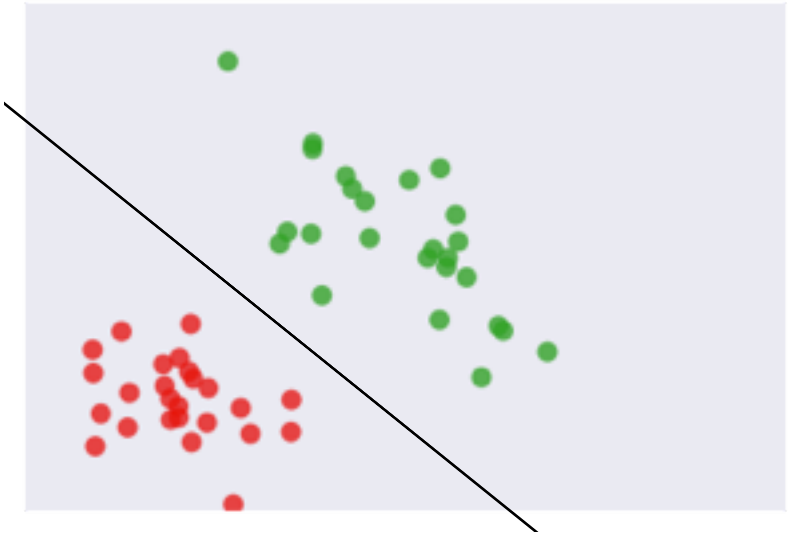
WE WON'T DIVE INTO THE MATHEMATICAL DETAILS TODAY
BUT THERE ARE LINKS IN THE REPO IF YOU'RE INTERESTED

I. SUPPORT VECTORS

Suppose we have data with binary labels, which we would like to classify



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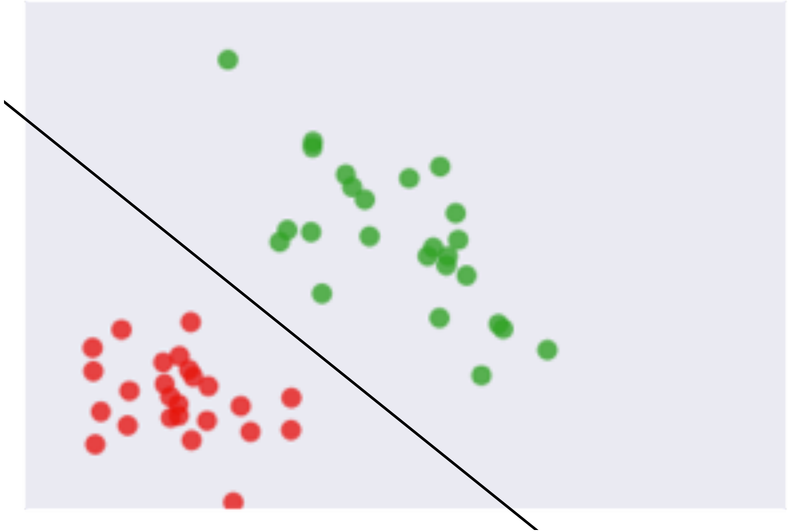
Recall that after fitting a classifier, we can draw the **decision boundary** *which separates the two classes*



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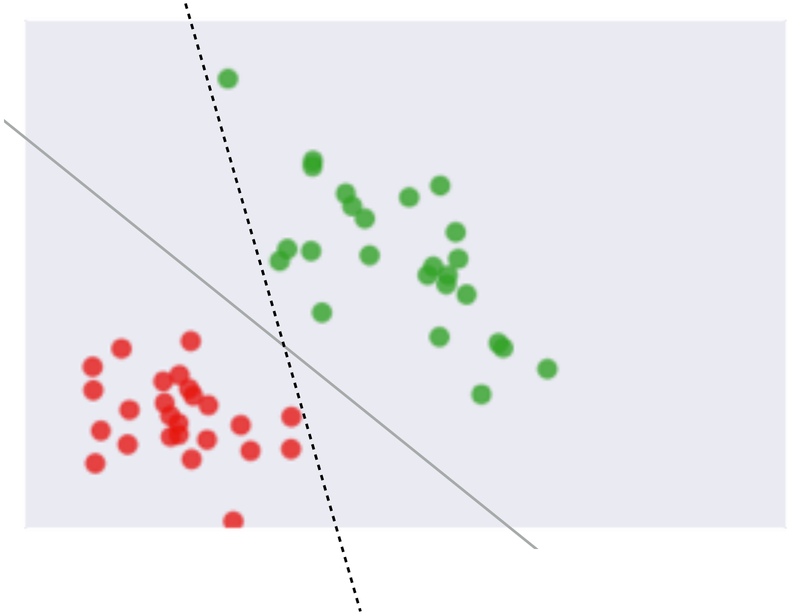

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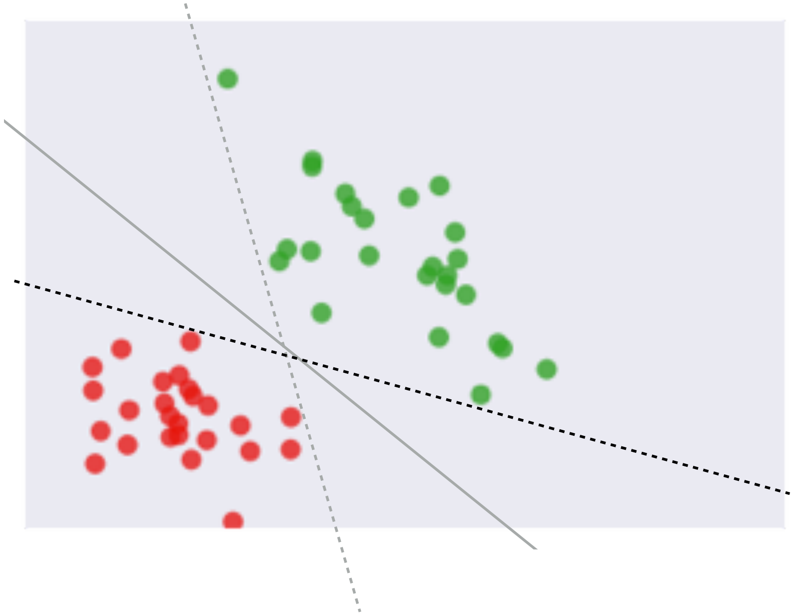

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NOTE

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

Familiarity with more than one leads to deeper understanding!

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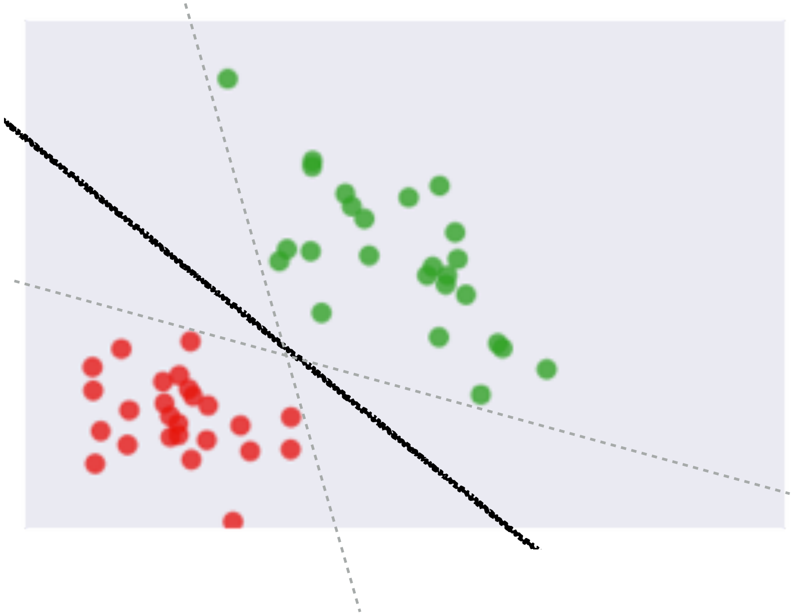
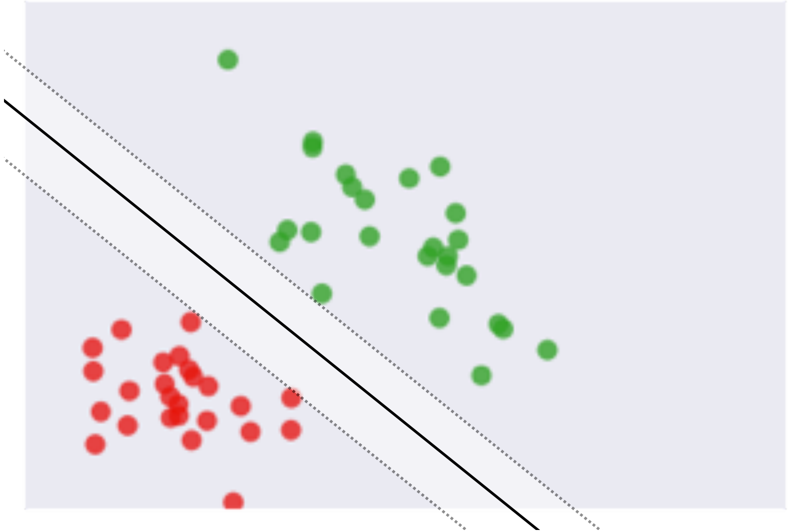


Support Vector Machines is a classifier that explicitly constructs a decision boundary that geometrically "makes the most sense"



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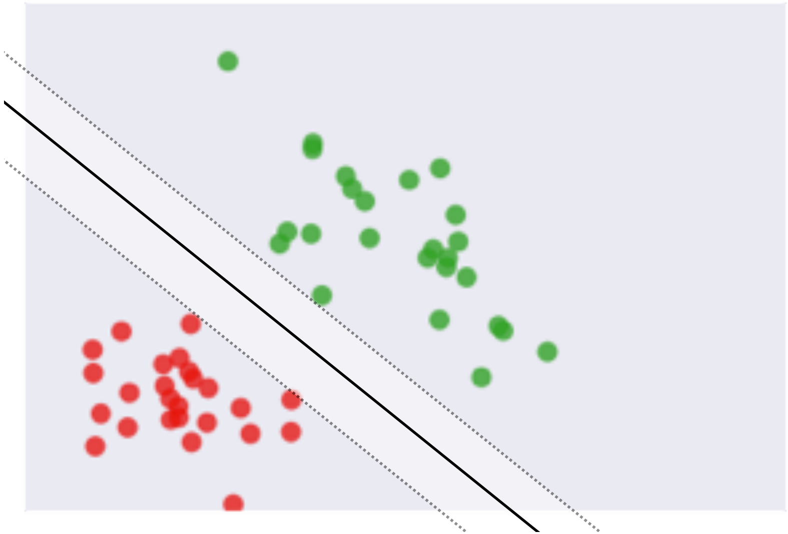
The generalization error is equated with the geometric concept of **margin**, *which is the region along the boundary that is free of points.*



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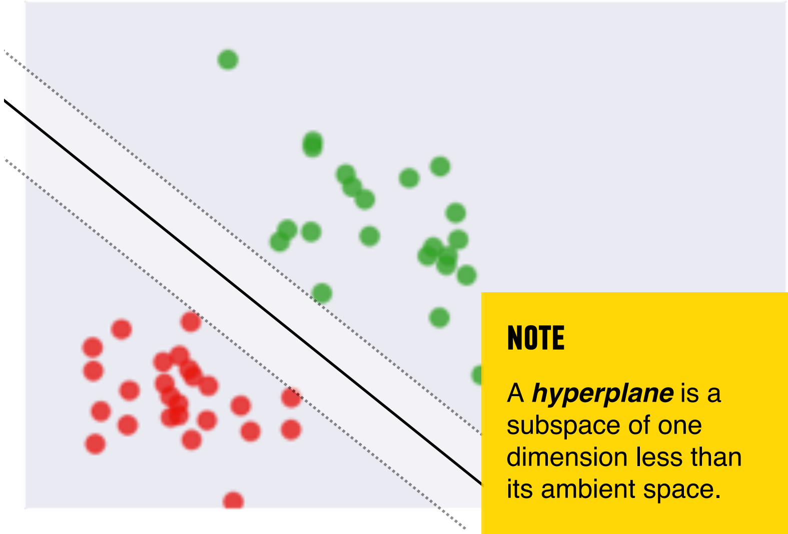
The generalization error is equated with the geometric concept of **margin***, which is the region along the boundary that is free of points.*

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



NOTE

A ***hyperplane*** is a subspace of one dimension less than its ambient space.

In this 2D example, it is a line, and in a 3D space it is an ordinary plane.

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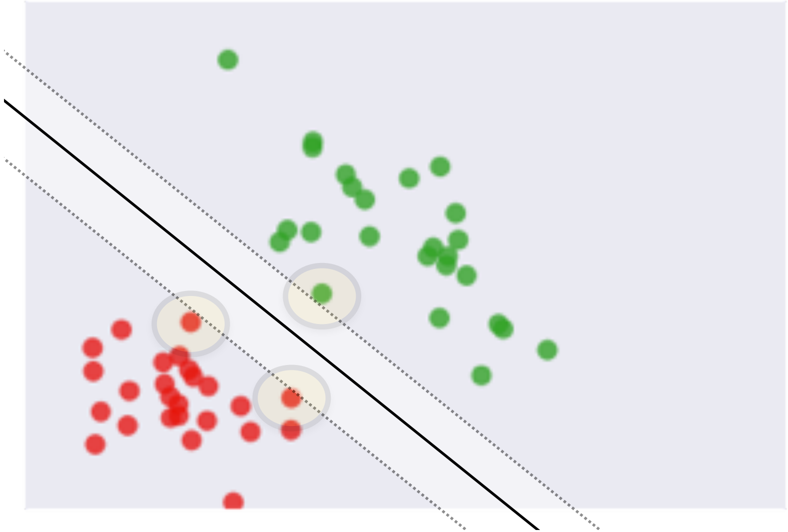
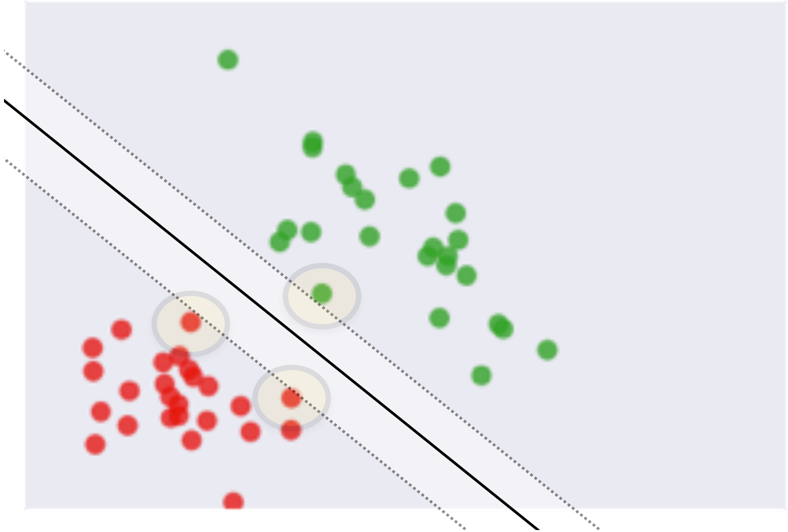
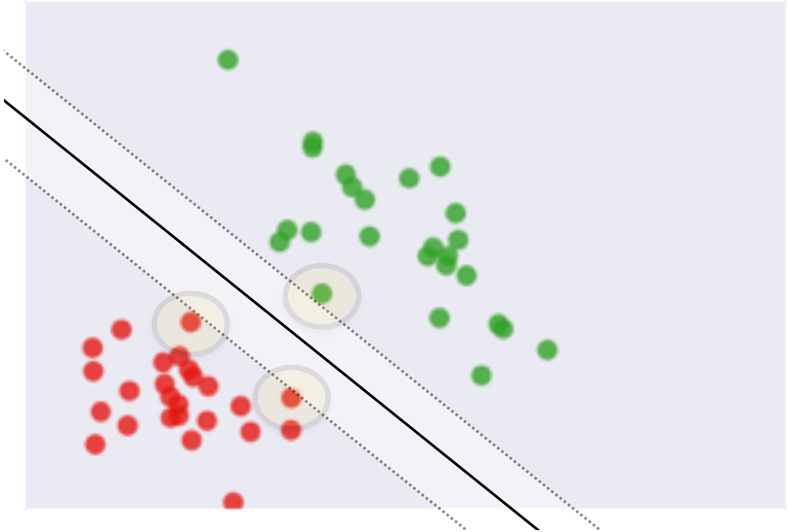


Notice that the margin depends only on a subset of the training data – the points nearest to the decision boundary.



Notice that the margin depends only on a subset of the training data – the points nearest to the decision boundary.

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



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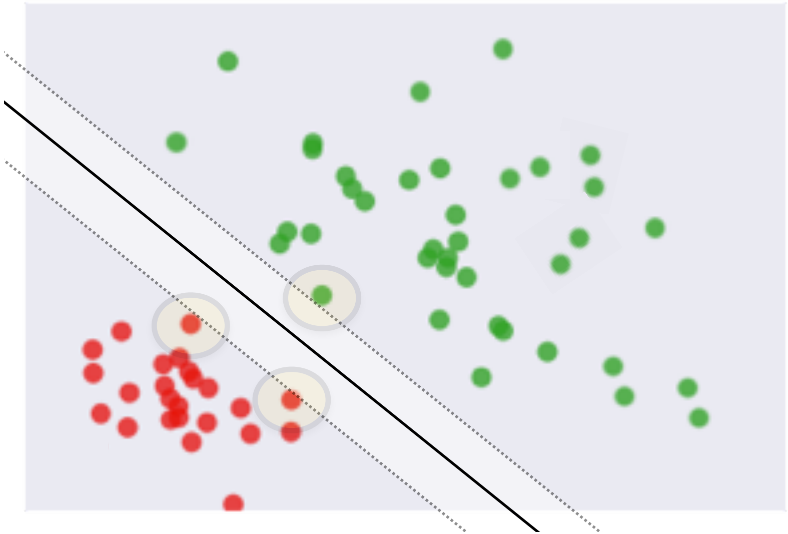

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In short, this requires the optimization of a **convex** *objective function.*

Convex optimization are guaranteed to give **global optima.**

So to summarize, what is a support vector machine?

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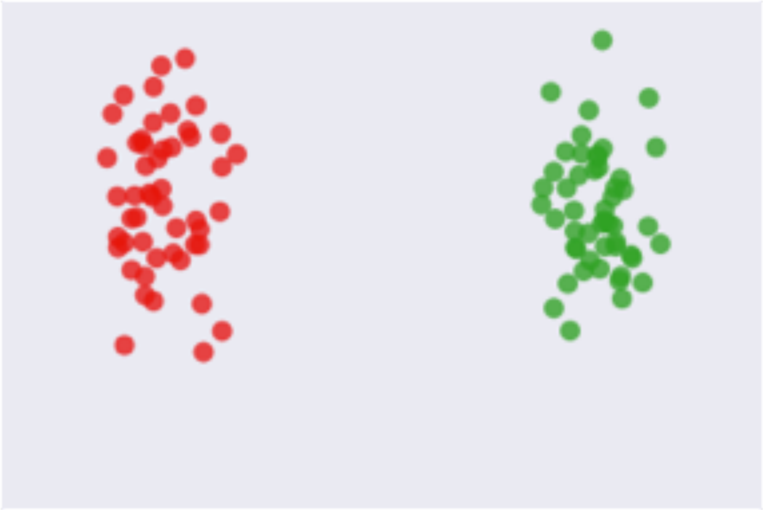
An SVM is a binary linear classifier whose decision boundary is explicitly constructed to minimize generalization error.

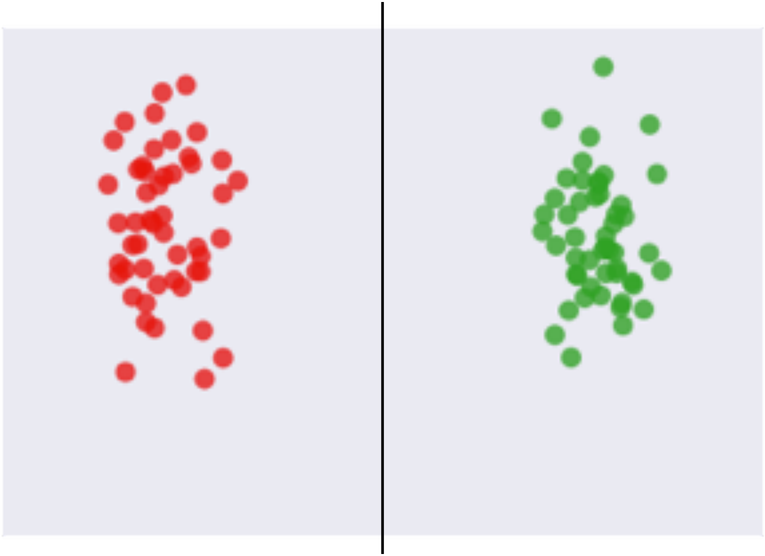
recall:

- **binary classifier** – *solves two-class problem*
- **linear classifier** – *creates linear decision boundary*

II. REGULARIZATION

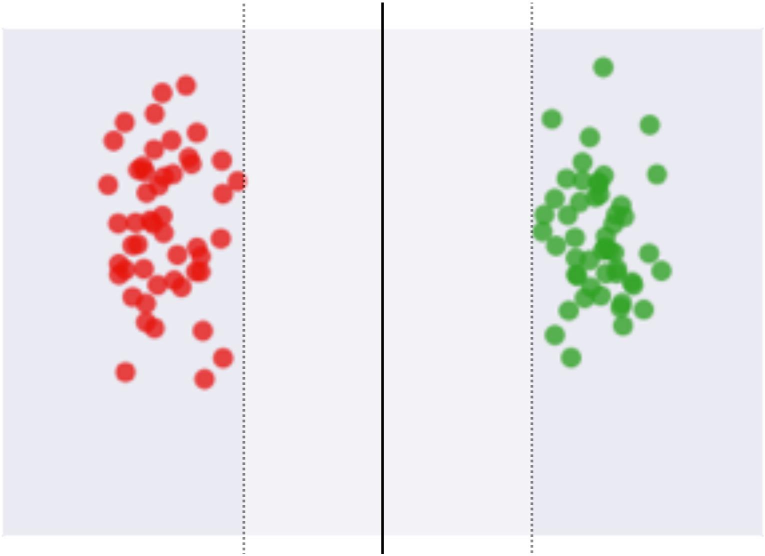
Let's apply a SVM to the dataset on the left





Let's apply a SVM to the dataset on the left.

If the data are **linearly separable**, *the training error is zero.*



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The **margin** *is nice and wide.*

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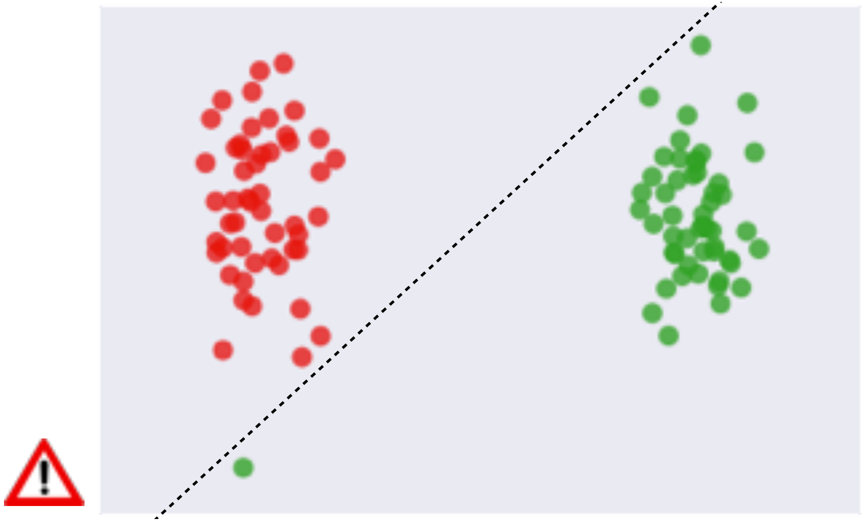

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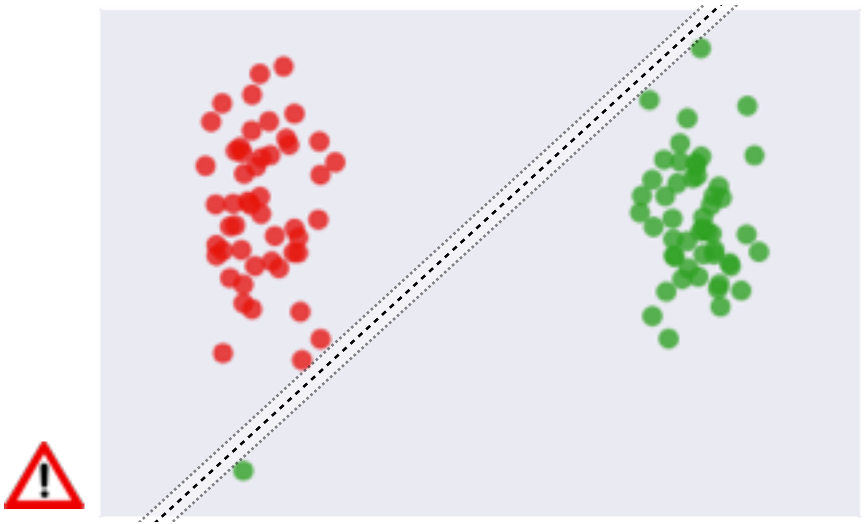
This will disproportionally impact the result, since the SVM tries to linearly separate **all** *data.*



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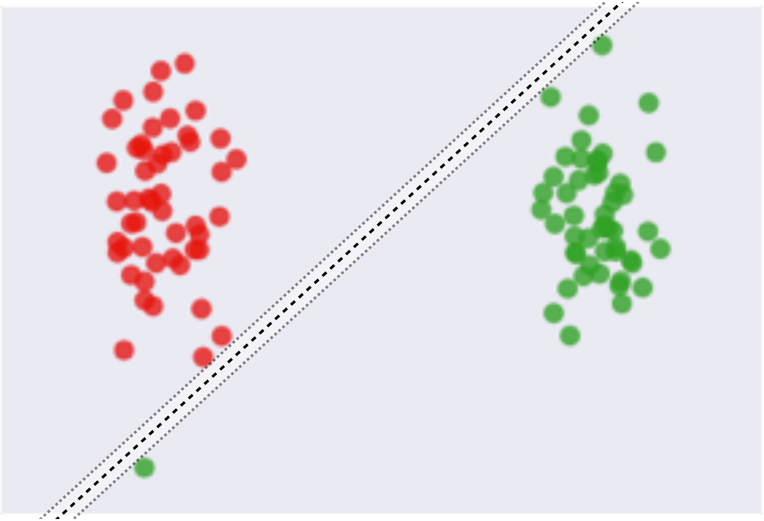
If the data are **linearly separable**, *the training error is zero.*

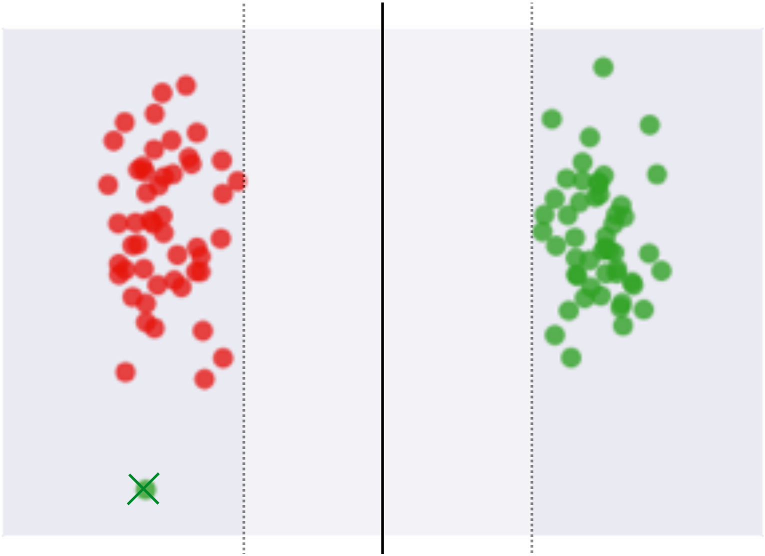
But what if our data has a single outlier?

This will disproportionally impact the result, since the SVM tries to linearly separate **all** *data.*

The **margin** *is very small.*

Again, we'll need some sort of regularization.





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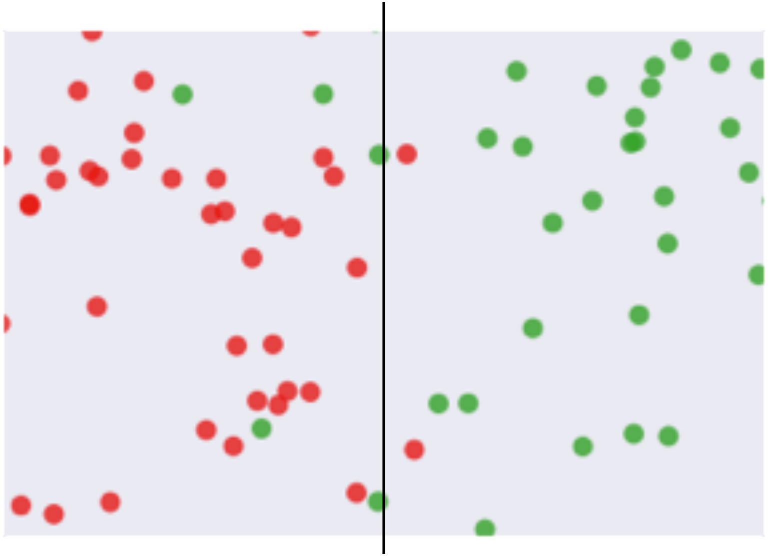
We want a **tradeoff** *of the width of the margin and the number of misclassifications.*



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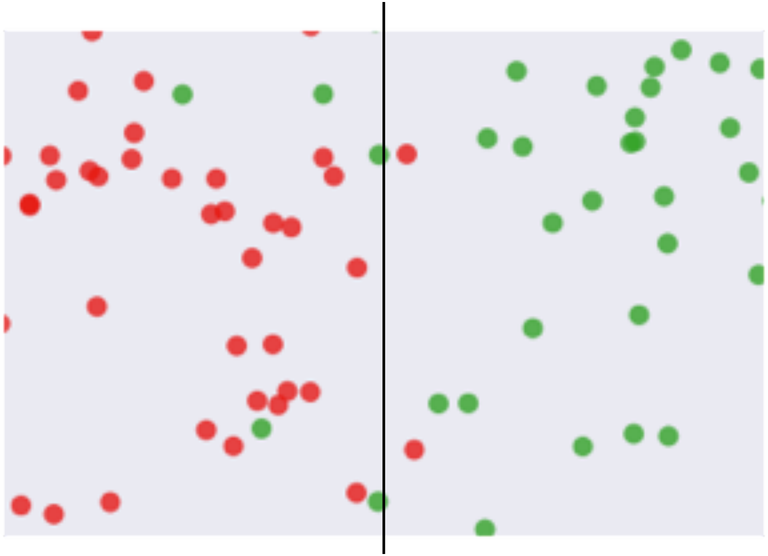

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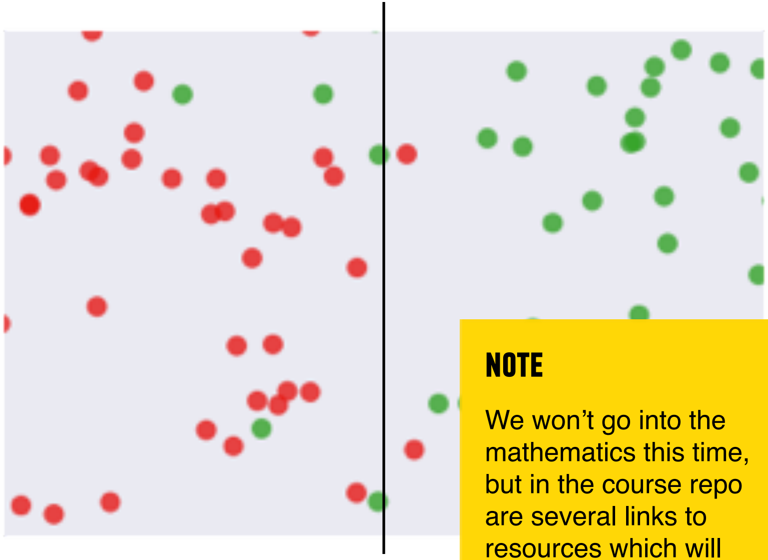
This is again a bias-variance tradeoff, which is done by **slack variables***.*



NOTE

We won't go into the mathematics this time, but in the course repo are several links to resources which will explain this if you're interested.

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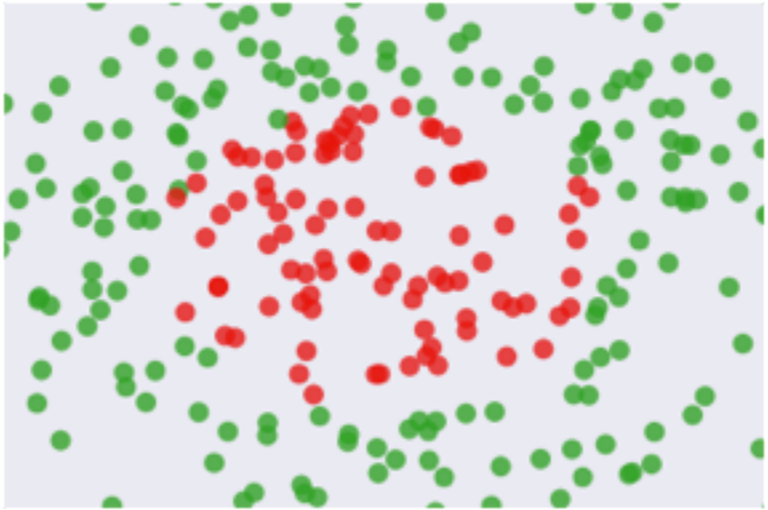
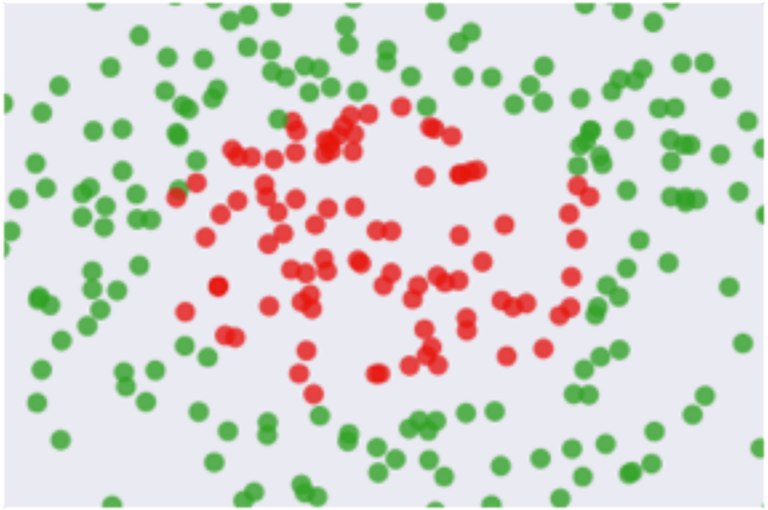
III. KERNELS

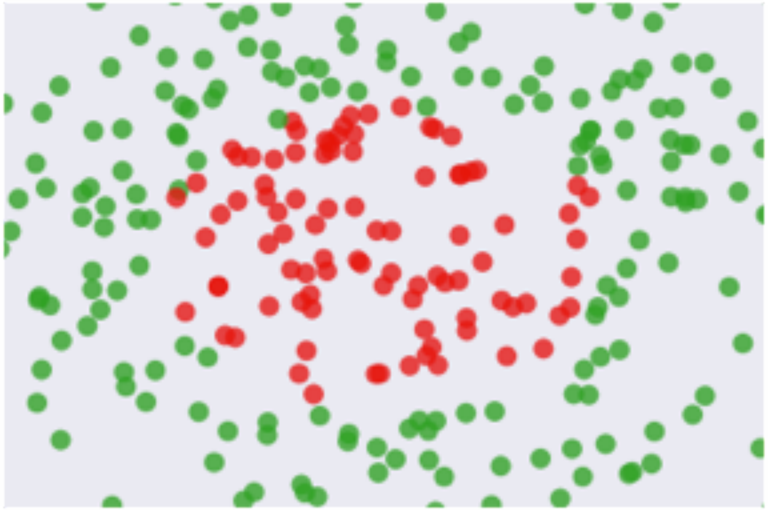
What if our data is not linearly separable at all?





What if our data is not linearly separable at all?

Again, we could add polynomial features. (This might be computationally expensive.)



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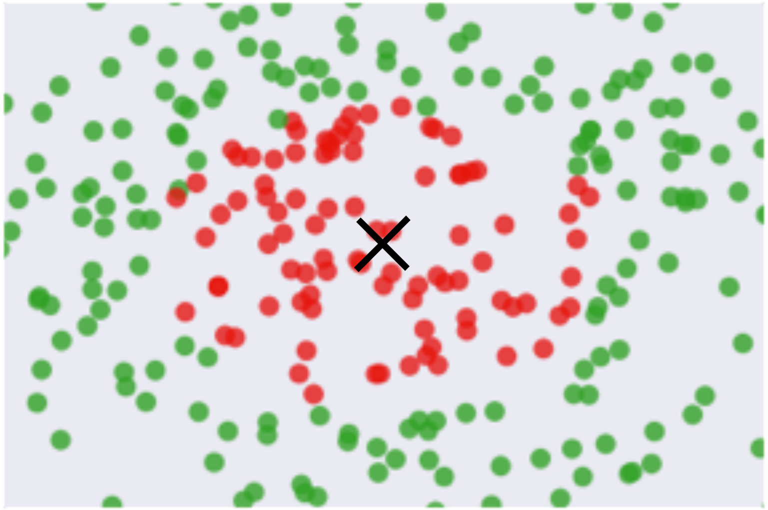
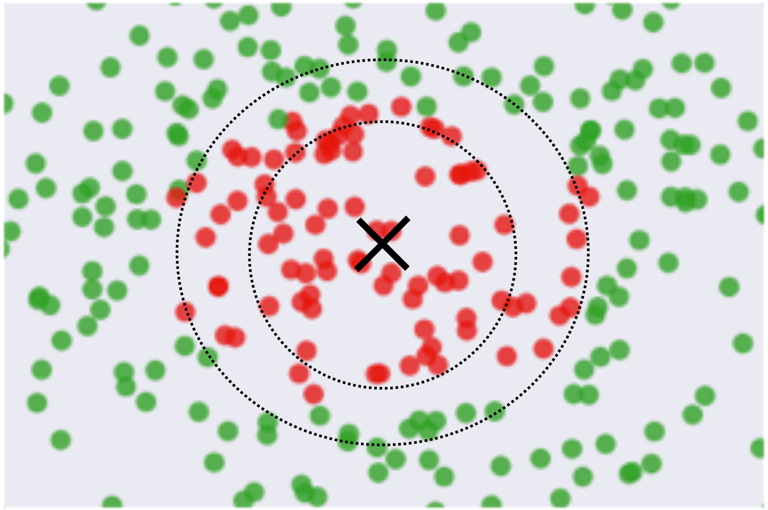
Again, we could add polynomial features. (This might be computationally expensive.)

We could also use ***kernels****.*

Add a **landmark** *to the feature space.*





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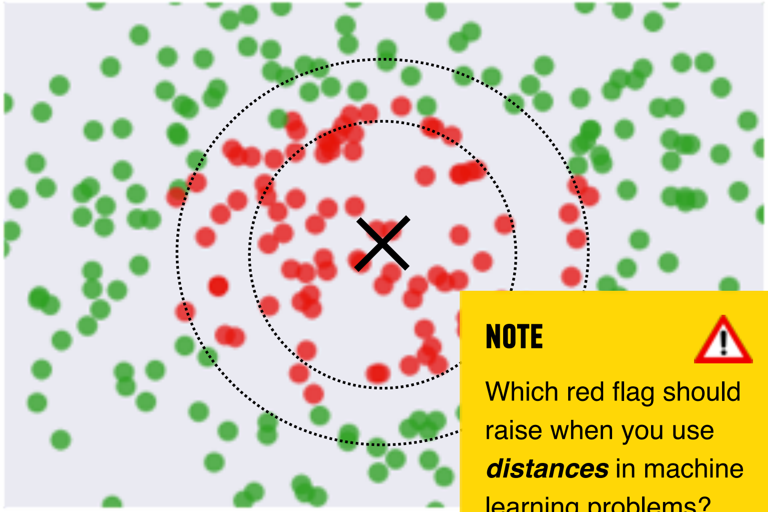

NOTE

Which red flag should raise when you use ***distances*** in machine learning problems?

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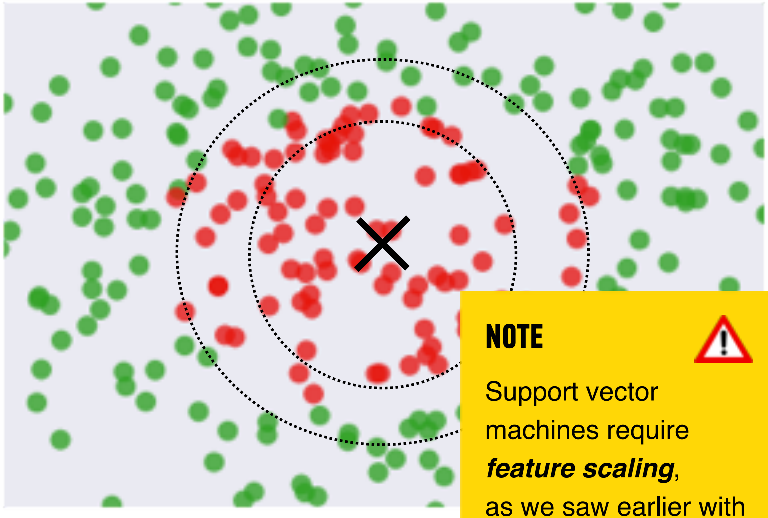

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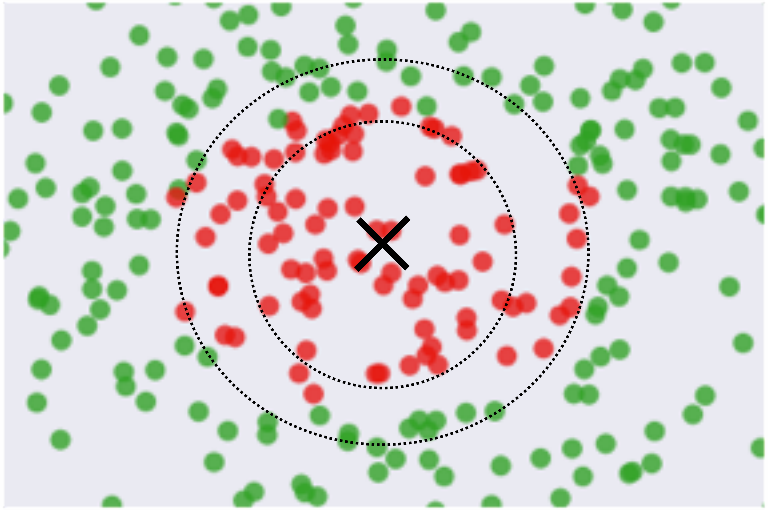
NOTE

Support vector machines require ***feature scaling***, as we saw earlier with k-nearest neighbors.



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Then define the similarity as the **radius basis function (rbf)**

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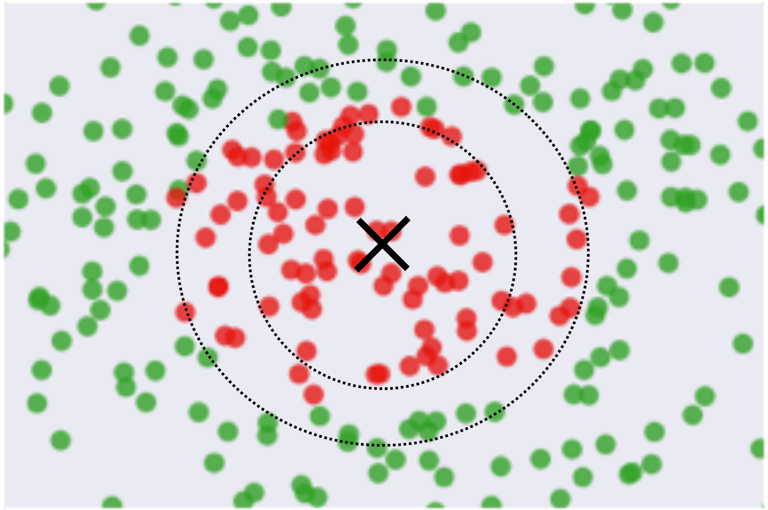

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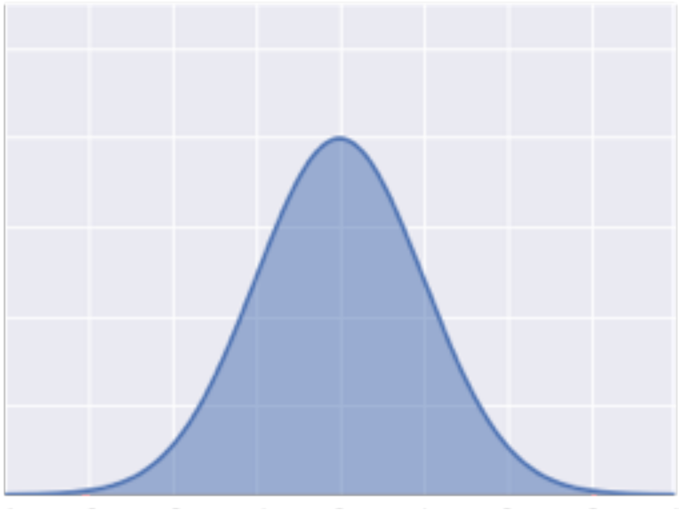

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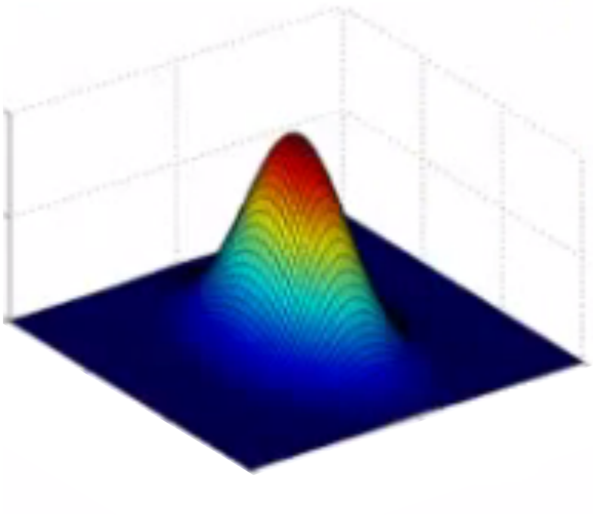

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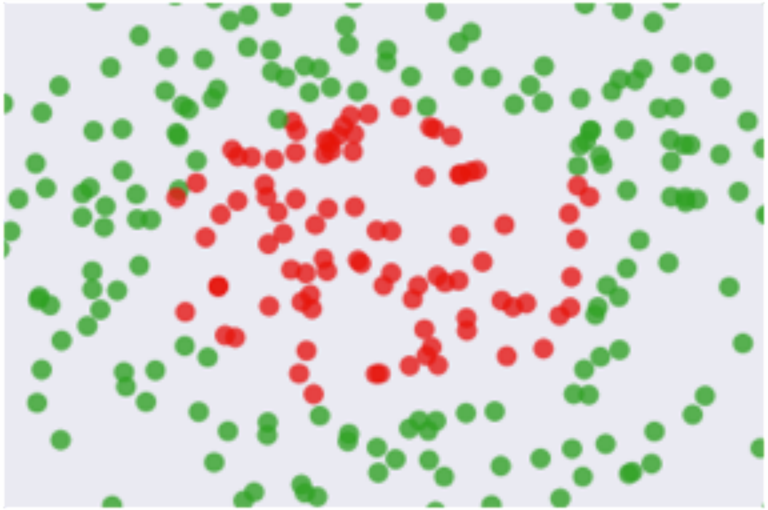

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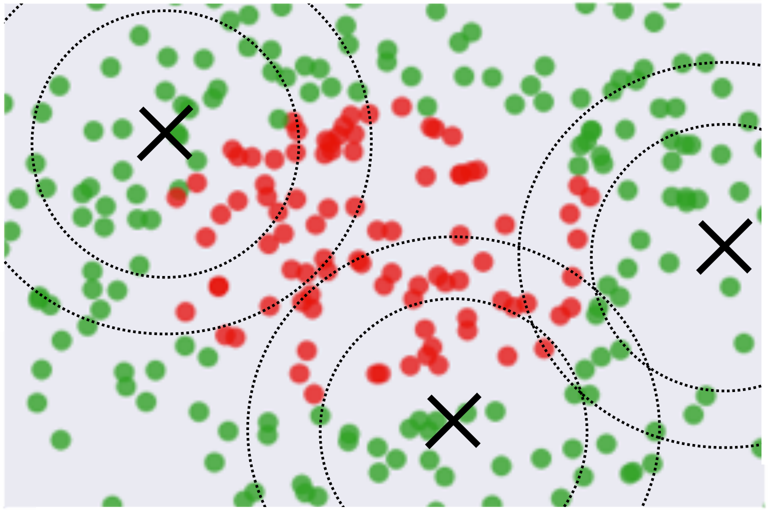

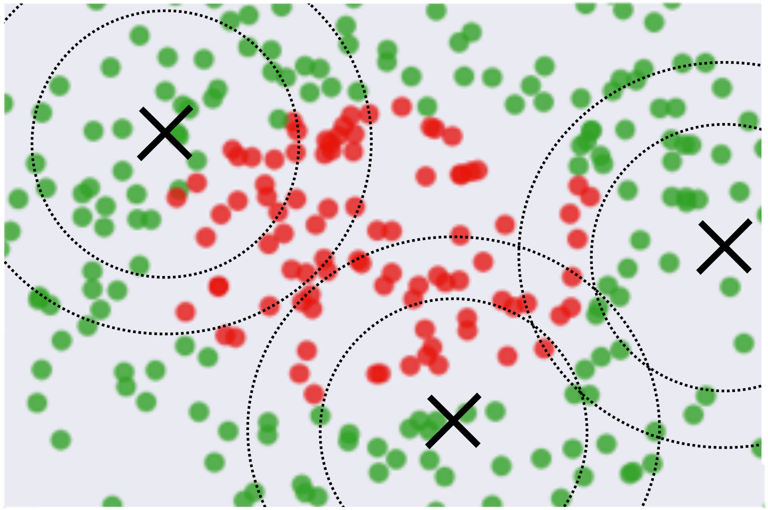

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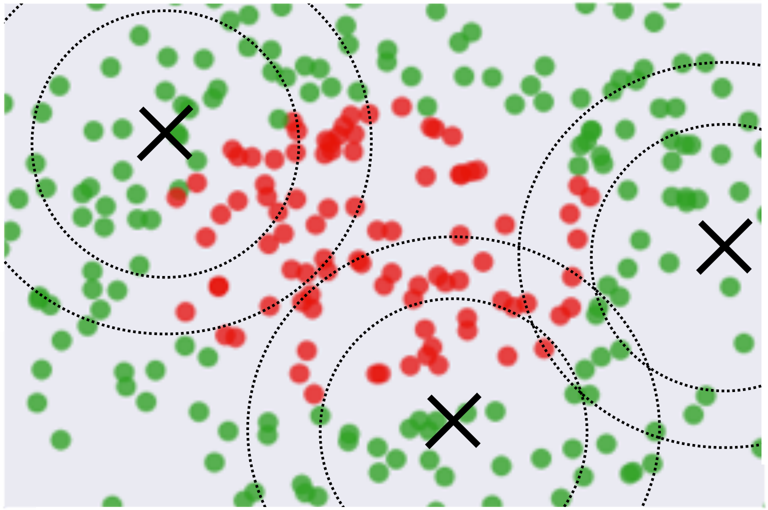

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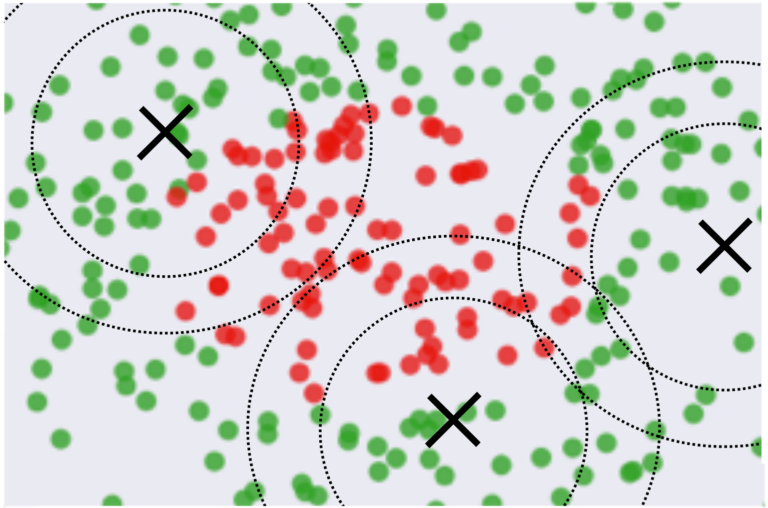
Choose each sample as a landmark.

Then replace all samples with the kernel values.



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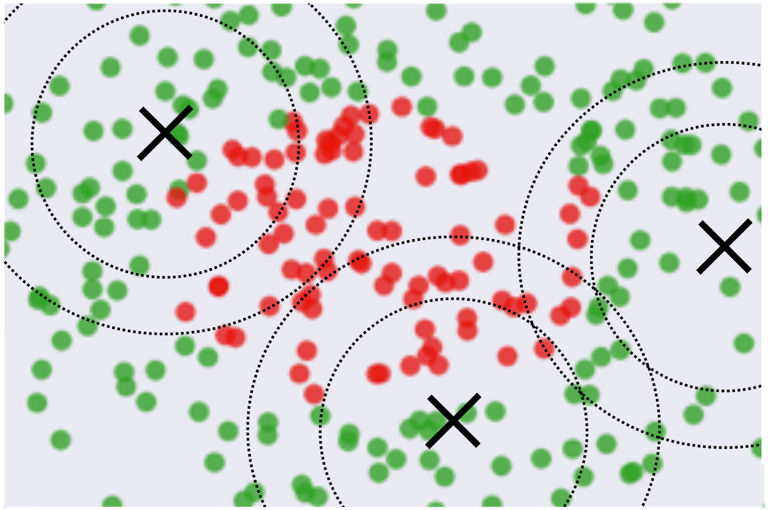
This will (non-linearly) transform your feature matrix ***X*** *from an N×n matrix to an N×N matrix.*



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*This will (non-linearly) transform your feature matrix **X** from an N×n matrix to an N×N matrix.*

On the diagonal we have ones (each sample compared with itself).

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Nonlinear classification is then obtained by creating a linear decision boundary in the higher-dimensional space

NOTE

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

Kernels can be used as preprocessing step at other models as well.

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However, they tend to be very computationally expensive.

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The SVM is far more efficient, so using kernels is more practical.

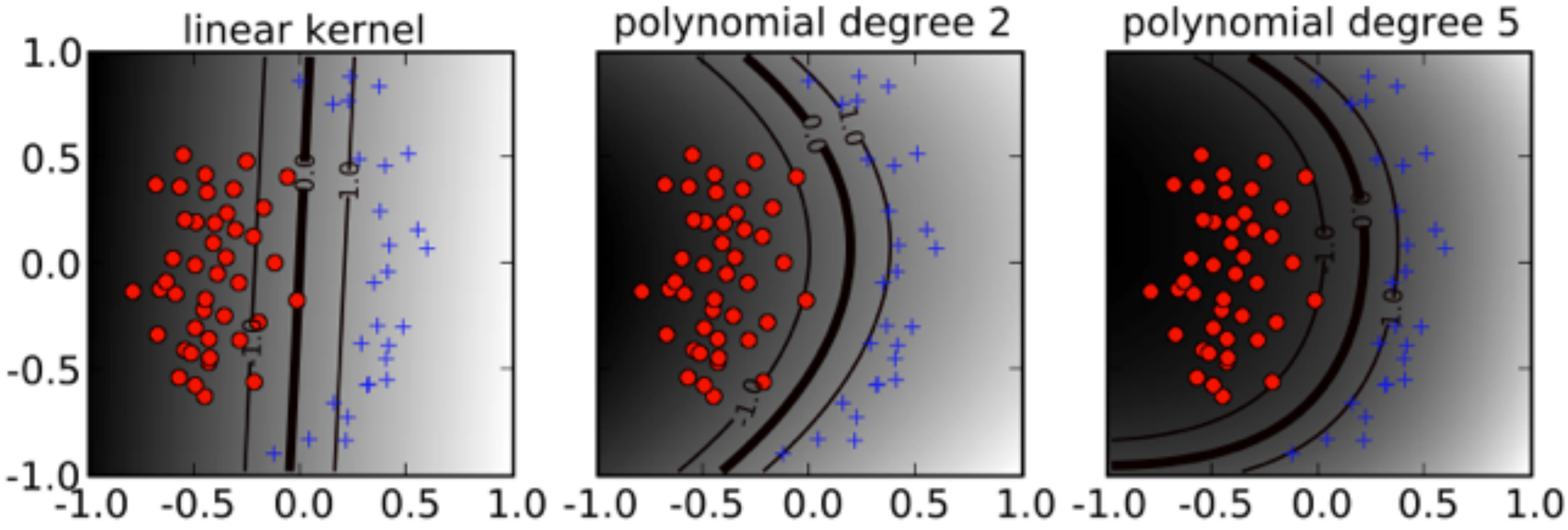
Some popular kernels

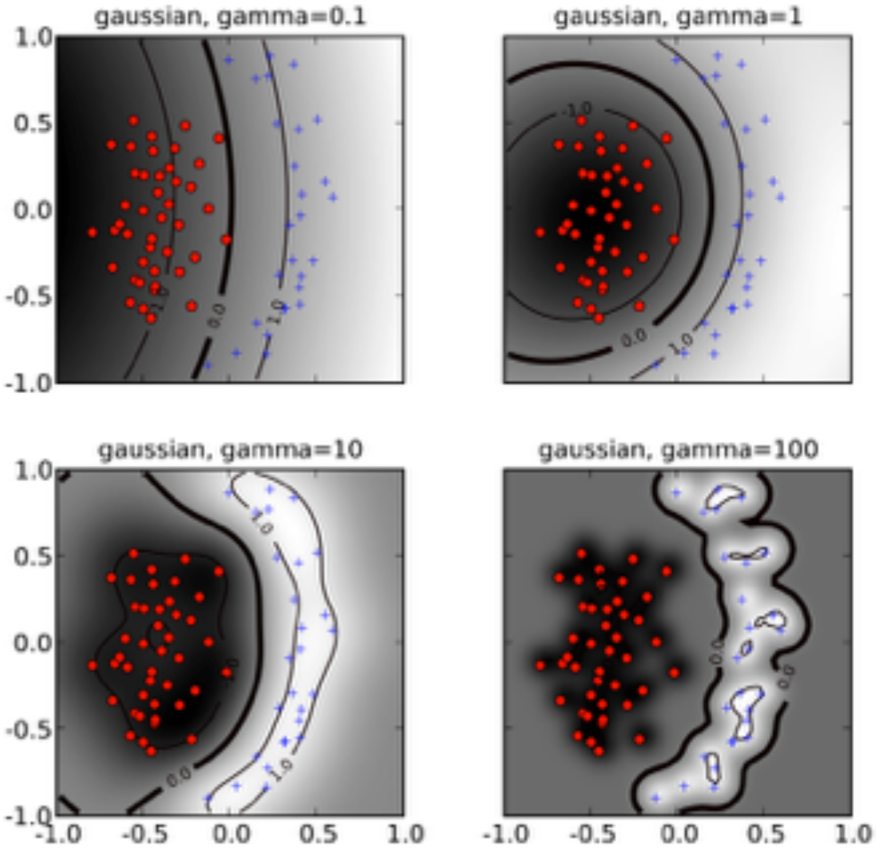
linear kernel $k(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$

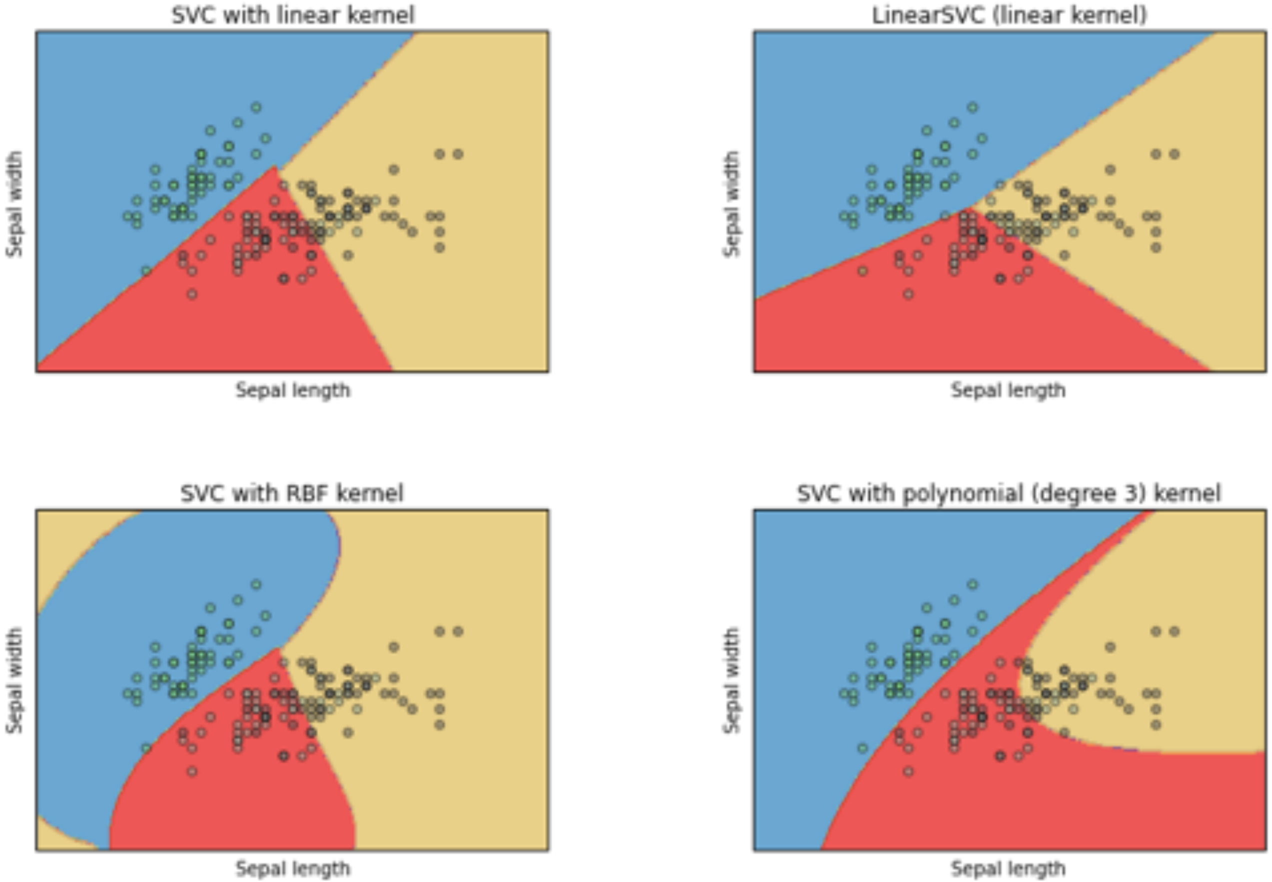
polynomial kernel $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + 1)^d$

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

The **hyperparameters** *d and γ affect the flexibility of the dec. boundary*


linear kernel
polynomial degree 2
polynomial degree 5
1.0
0.5
0.0
-0.5
-1.0
-1.0
-0.5
0.0
0.5
1.0


gaussian, gamma=0.1
gaussian, gamma=1
gaussian, gamma=10
gaussian, gamma=100
1.0
0.5
0.0
-0.5
-1.0
-1.0
-0.5
0.0
0.5
1.0


SVC with linear kernel
LinearSVC (linear kernel)
SVC with RBF kernel
SVC with polynomial (degree 3) kernel
Sepal width
Sepal length

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The main disadvantage of SVMs is the lack of intuition they produce.

These models are truly black boxes!

DISCUSSION