Support Vector Machines (SVM)

Objectives

1. Gain an intuition about the *purpose* and *power* of SVMs.
2. Explore (some) of the mathematics behind SVMs.
3. Supercharge SVMs with kernels and soft margins.
4. Gain an intuition about the Bias-Variance tradeoff while using SVMs.

Support Vector Machines

A rough history

loosely referred as SVM

Maximum Margin Classifier: (morning lecture)
1963: Vapnik, Chervonenkis

or SVC

the real SVM

Soft Margins and the "Kernel Trick": (afternoon lecture)
1992-1995: Vapnik, Boser, Guyon, Cortes
This is the modern Support Vector Machine (SVM).

Outline

Supervised Learning

High level: What is supervised learning?

Learn an unknown function from a set of **labeled** training data.

- Our training data is limited and finite. A useful algorithm must generalize well to "unseen" data.
- Example: Children learning colors.
- Support Vector Machines (SVMs) are a *supervised* learning algorithm.

Outline

Notation

Goal:

Learn a model of a function $F : X \to Y$ from a training set D.

$D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$, where

- $x^{(j)} \in X$ is often called the "input".
- $y^{(j)} \in Y$ is often called the "label" or "target".

Notation (cont.)

$F : X \to Y$

- Often, $X = \mathbb{R}^n$
- Often, Y is a finite set (i.e. a classification task)

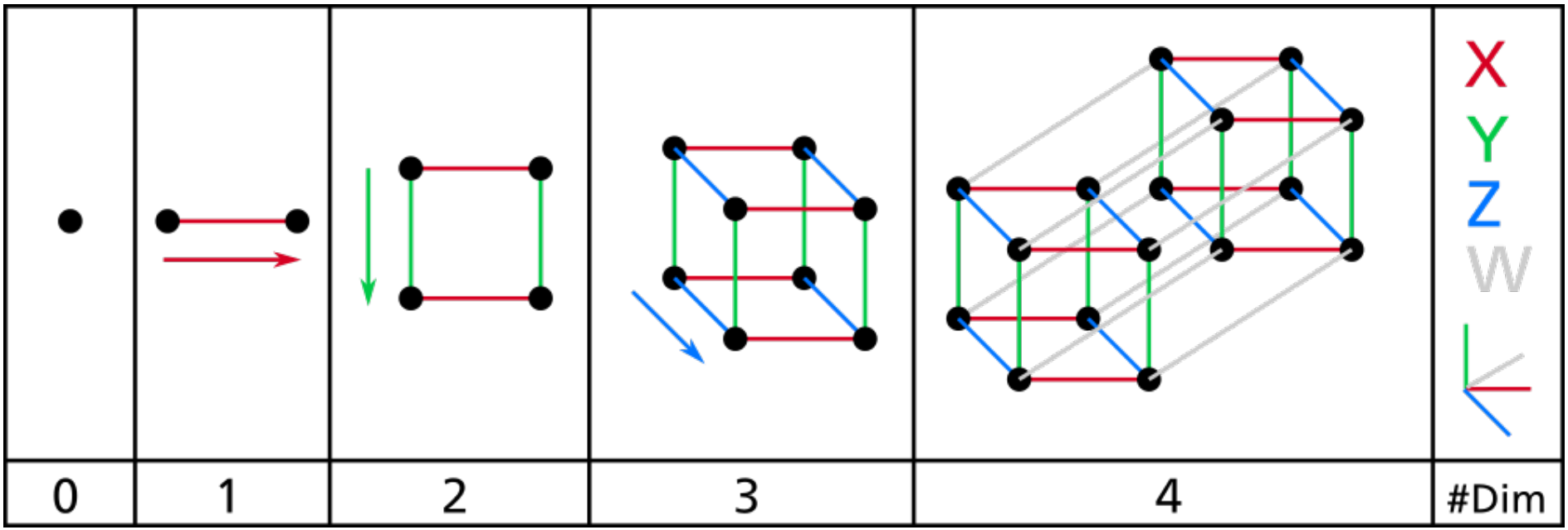
We want our learned model to *generalize* well.

Generalization error is a measure of the model's performance on all possible "unseen" data.

Outline

Dimensions

Basic stuff, I know...



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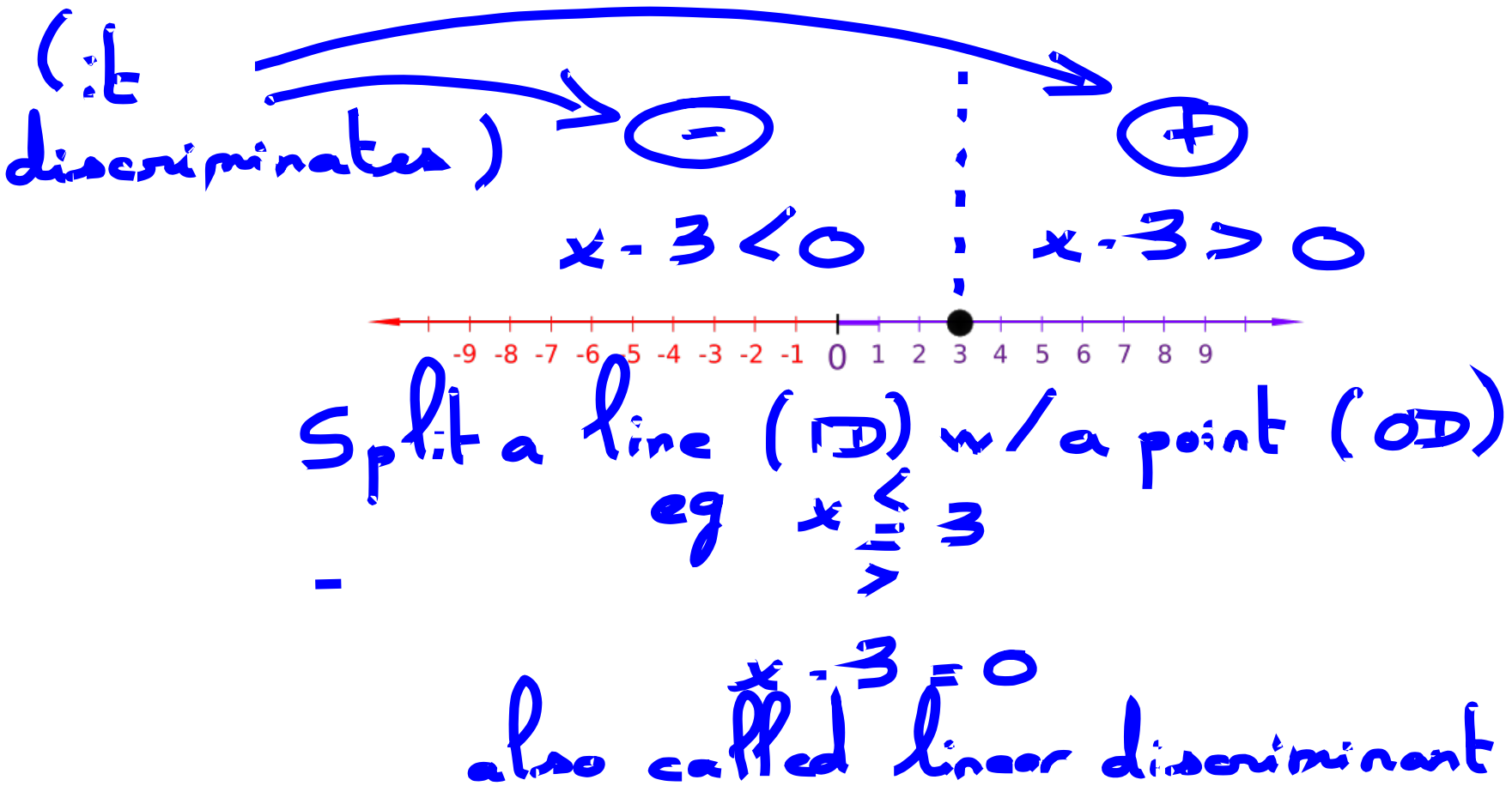
1D

How do you split this space?



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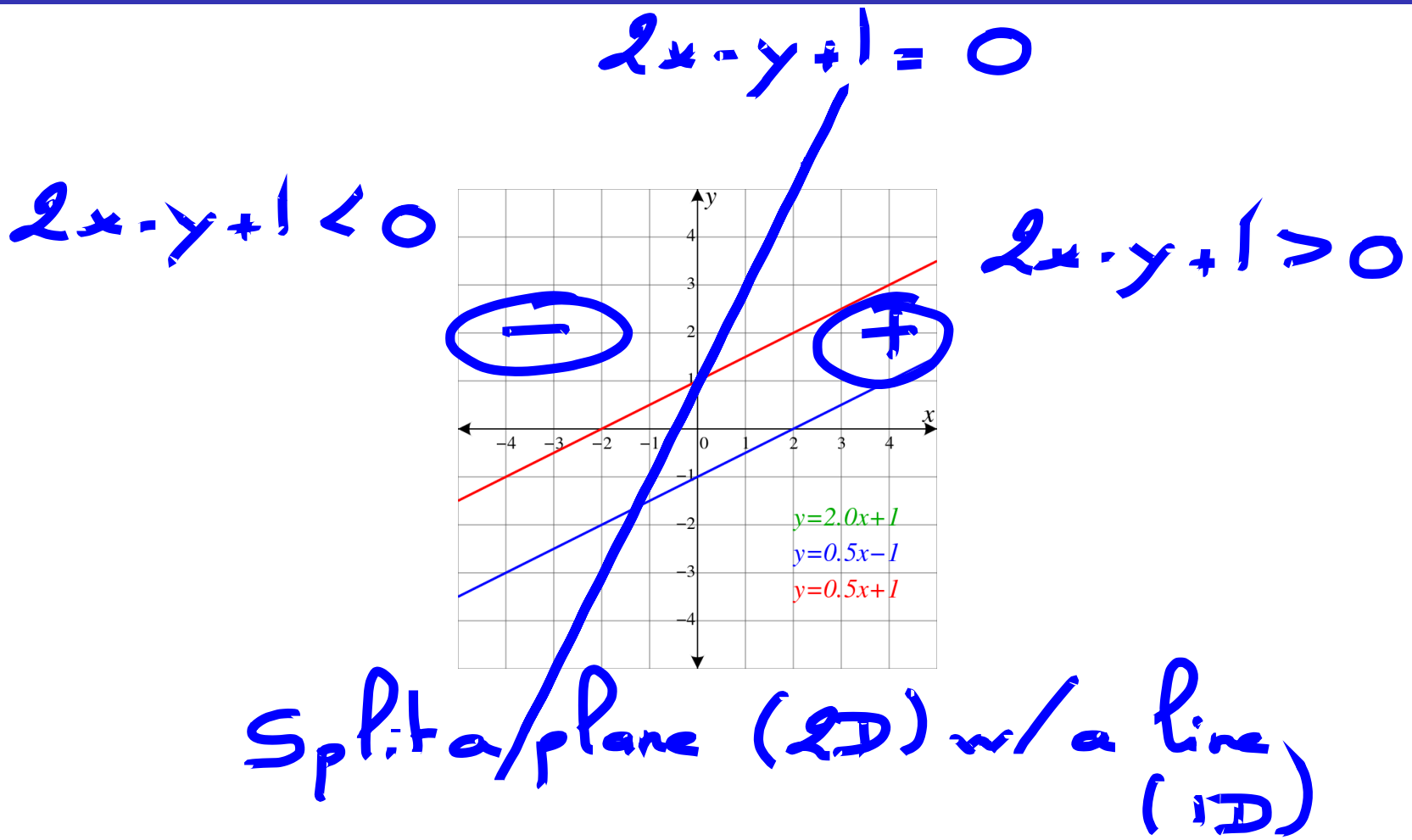
2D

How do you split this space?



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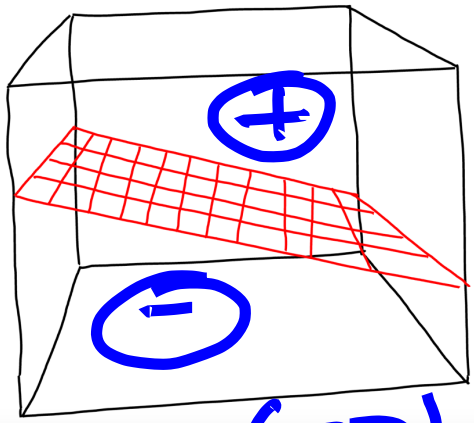
3D

How do you split this space?



Split a space (3D) w/ a plane (2D)

hyperspace/plane is of the form

$$\alpha x + \beta y + \gamma z = 0$$

4D, 5D, etc...

Hard to visualize... :/

In general, an n-dimensional space can be separated by an $(n-1)$-dimensional *hyperplane*.

In an n-dimensional space any hyperplane can be defined by $w \in \mathbb{R}^n$ and $b \in \mathbb{R}$. The hyperplane includes all $x \in \mathbb{R}^n$ where:

$$w_0 x_0 + w_1 x_1 + \ldots + w_{n-1} x_{n-1} - b = 0$$

usually written: changed notation here

in matrix/vector form: $w \cdot x - b = 0$

How to interpret w and b

So, w and b define a hyperplane. Is there an interpretation of w and b that can help us visualize this hyperplane?

How to interpret w and b

So, w and b define a hyperplane. Is there an interpretation of w and b that can help us visualize this hyperplane?

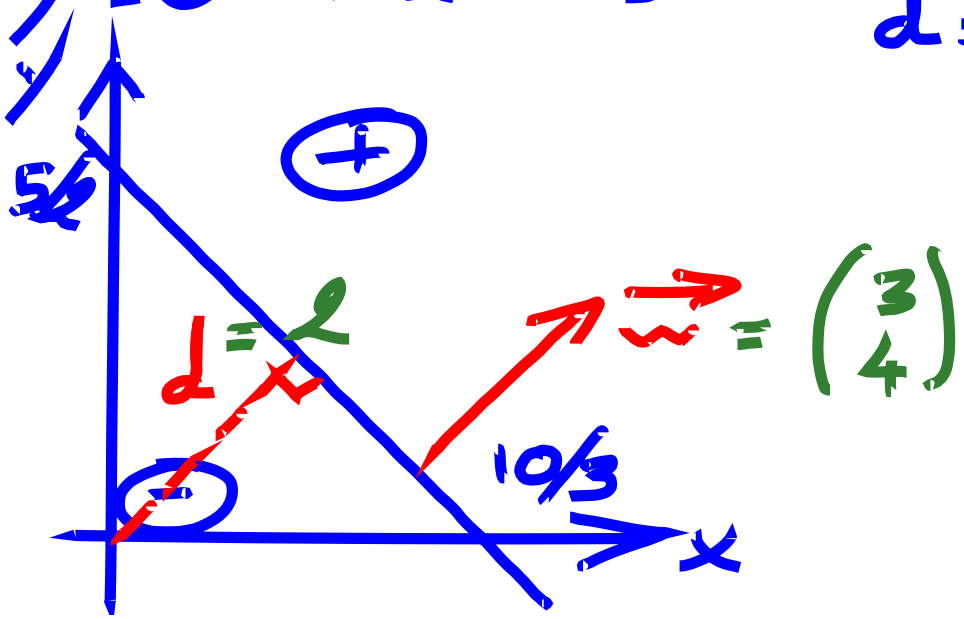
- $\frac{w}{||w||}$ is the hyperplane's normal vector.
- $\frac{b}{||w||}$ is the hyperplane's distance from the origin.

Example in 2D

$3x + 4y - 10 = 0 \quad \vec{w} = \begin{pmatrix} 3 \\ 4 \end{pmatrix} \quad b = 10$

$x = 0 \rightarrow y = 5/2$

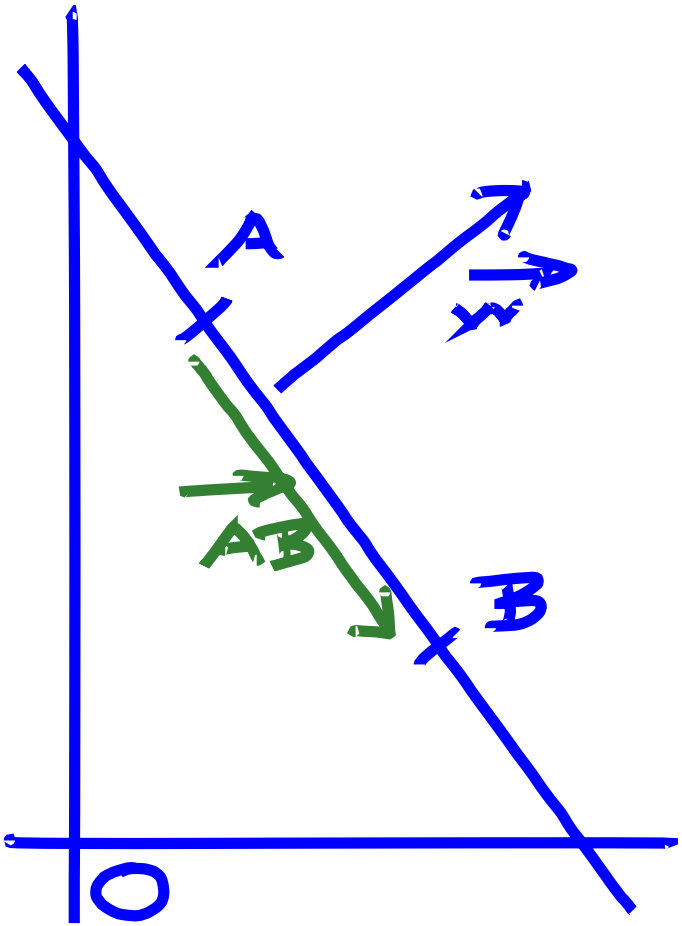
$y = 0 \rightarrow x = 10/3$



$d = \frac{b}{\|\vec{w}\|} = \frac{10}{\sqrt{3^2 + 4^2}} = \frac{10}{\sqrt{25}}$

$= \frac{10}{5} = 2$

$\frac{w}{\|w\|}$ is the hyperplane's normal vector



$\vec{w} \cdot \vec{x_1} - b = 0$ (1) ($A \in$ hyperplane)

$\vec{w} \cdot \vec{x_2} - b = 0$ (2) ($B \in$ hyperplane)

(2) - (1) : $\vec{w} \cdot \vec{OB} - b - \vec{w} \cdot \vec{OA} + b = 0$

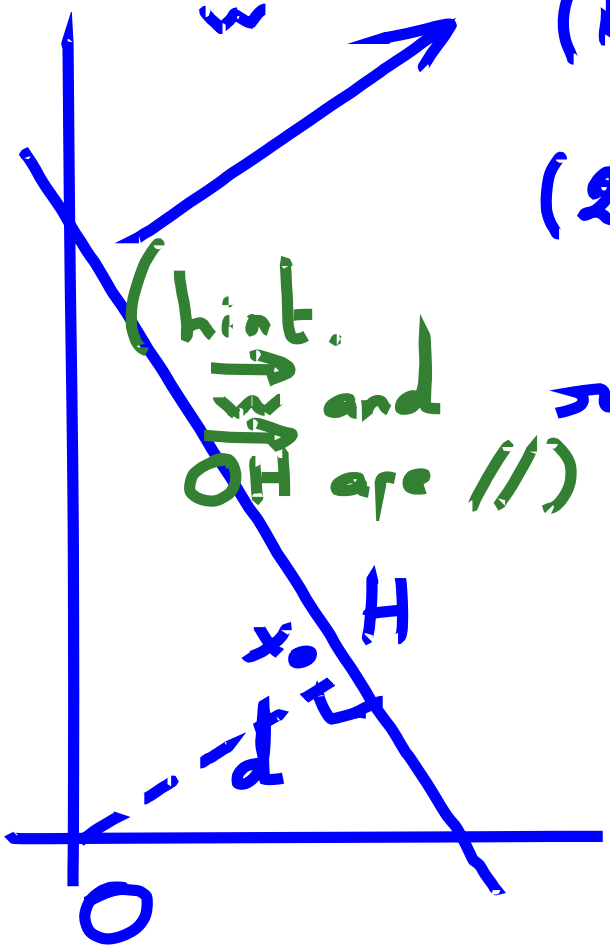
$\vec{w} \cdot (\vec{OB} - \vec{OA}) = 0$

$\vec{AO} + \vec{OB} = \vec{AB}$

$\vec{w} \cdot \vec{AB} = 0 \quad \forall A, B \in$ hyperplane

$\vec{w}$ is normal to the hyperplane

$\frac{b}{\|w\|}$ is the hyperplane's distance from the origin



(1) $\vec{w} \cdot \vec{x_0} - b = 0$ (H ∈ hyperplane)

(2) $\vec{x_0} = d \frac{\vec{w}}{\|\vec{w}\|}$ ($\vec{OH}$ // $\vec{w}$, $\|\vec{OH}\| = d$)

$\vec{x_0}$ projection of O

replace $\vec{x_0}$ (2) in (1):

$\vec{w} \cdot \left(d \frac{\vec{w}}{\|\vec{w}\|} \right) - b = 0$

est

$\|\vec{w}\|^2 = \vec{w} \cdot \vec{w}$

$d \frac{\vec{w} \cdot \vec{w}}{\|\vec{w}\|} - b = 0$

$d \frac{\|\vec{w}\|^2}{\|\vec{w}\|} - b = 0$

- so $d\|\vec{w}\| - b = 0 \iff$ $\boxed{d = \frac{b}{\|\vec{w}\|}}$

Outline

Binary Classification

A supervised learning problem

Recall, we're trying to learn $F : X \to Y$.

- Let, $X = \mathbb{R}^n$
- For binary classification, $Y = \{0, 1\}$

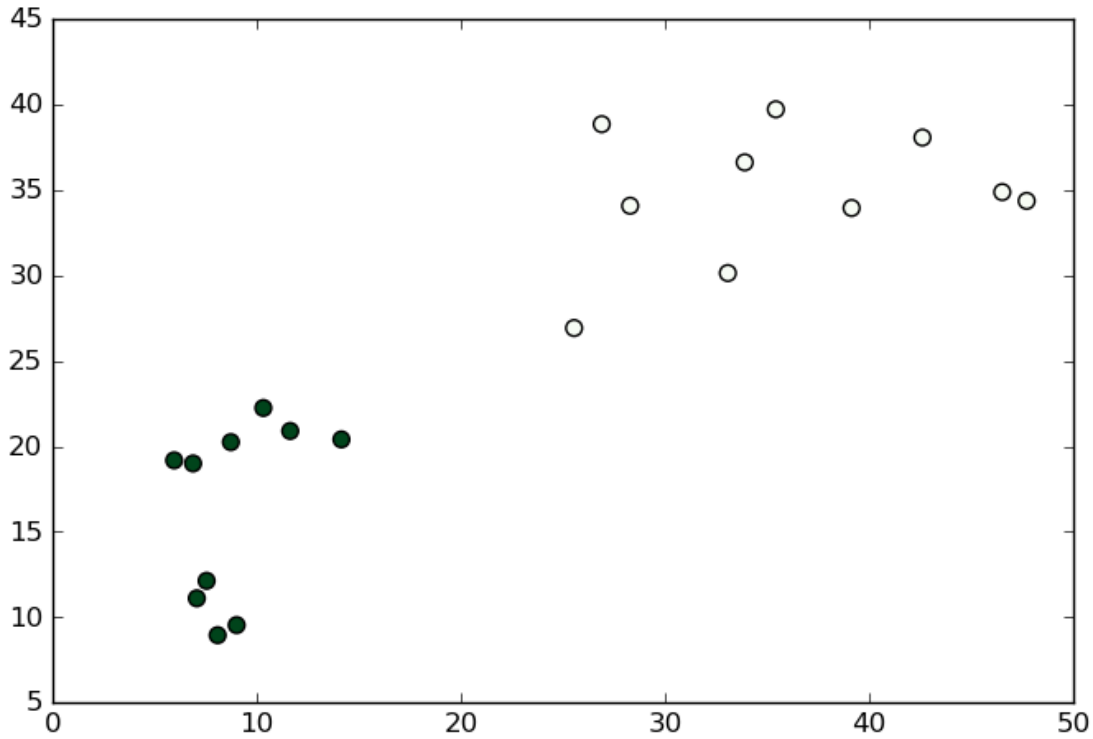
-1

We'll be using -1 instead of 0 for (future) convenience

Big idea: Let's have our model find a hyperplane that splits our n-dimensional data X into the set where $y = -1$ and the set where $y = 1$.

Binary Classification: Example

How many ways can we use a hyperplane to classify this dataset correctly?

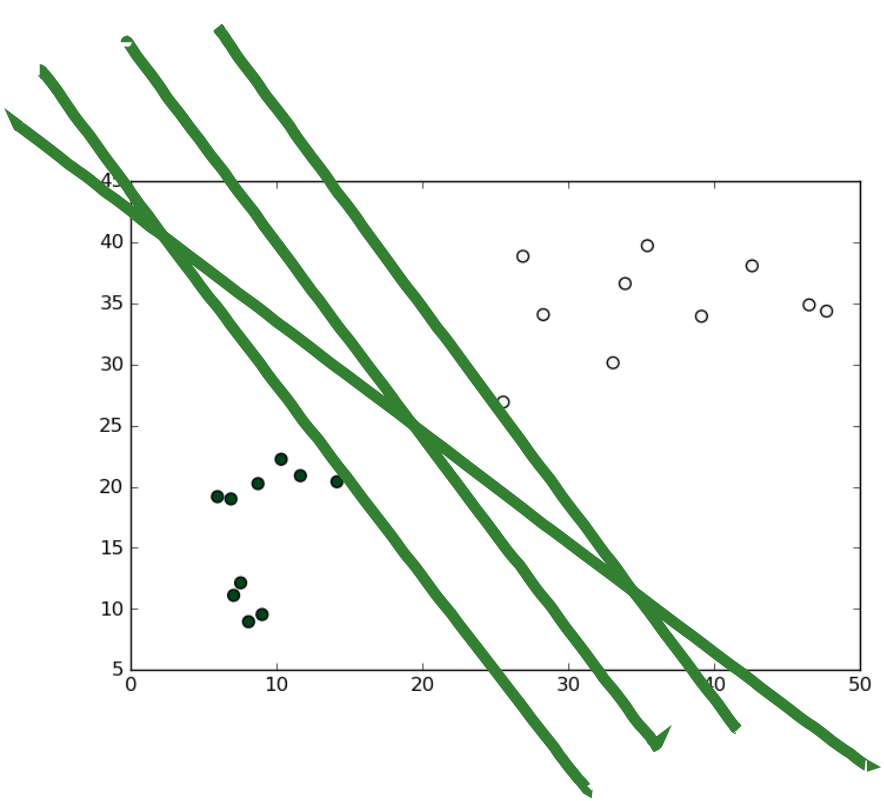


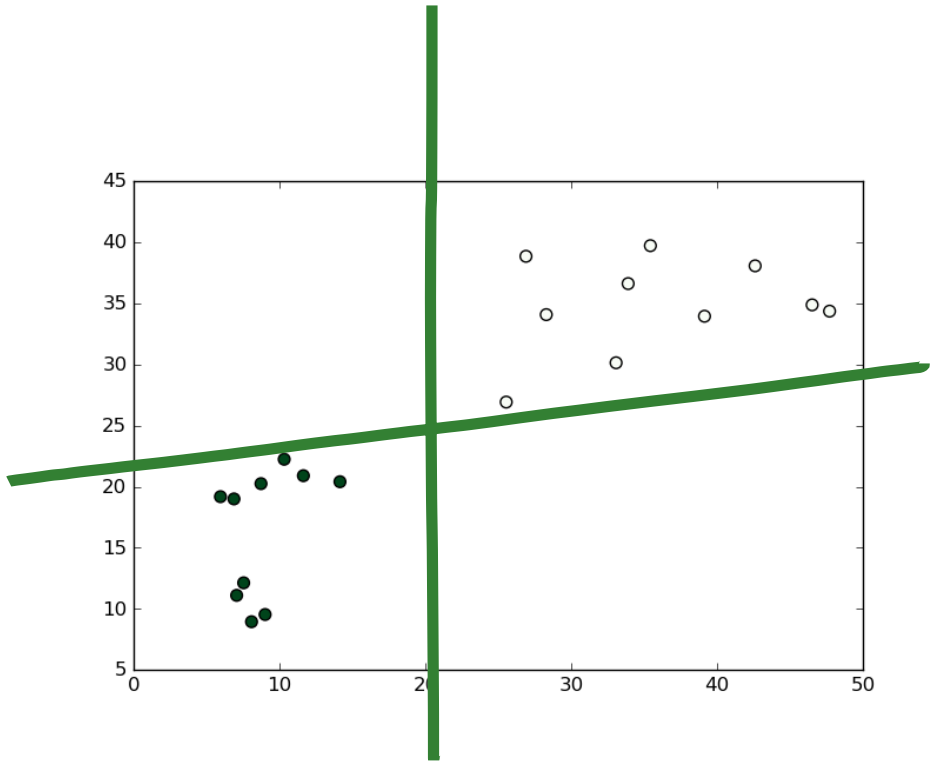
$$X = \mathbb{R}^2$$

$$Y = \{-1, 1\}$$

Binary Classification: Example

Two Example Solutions



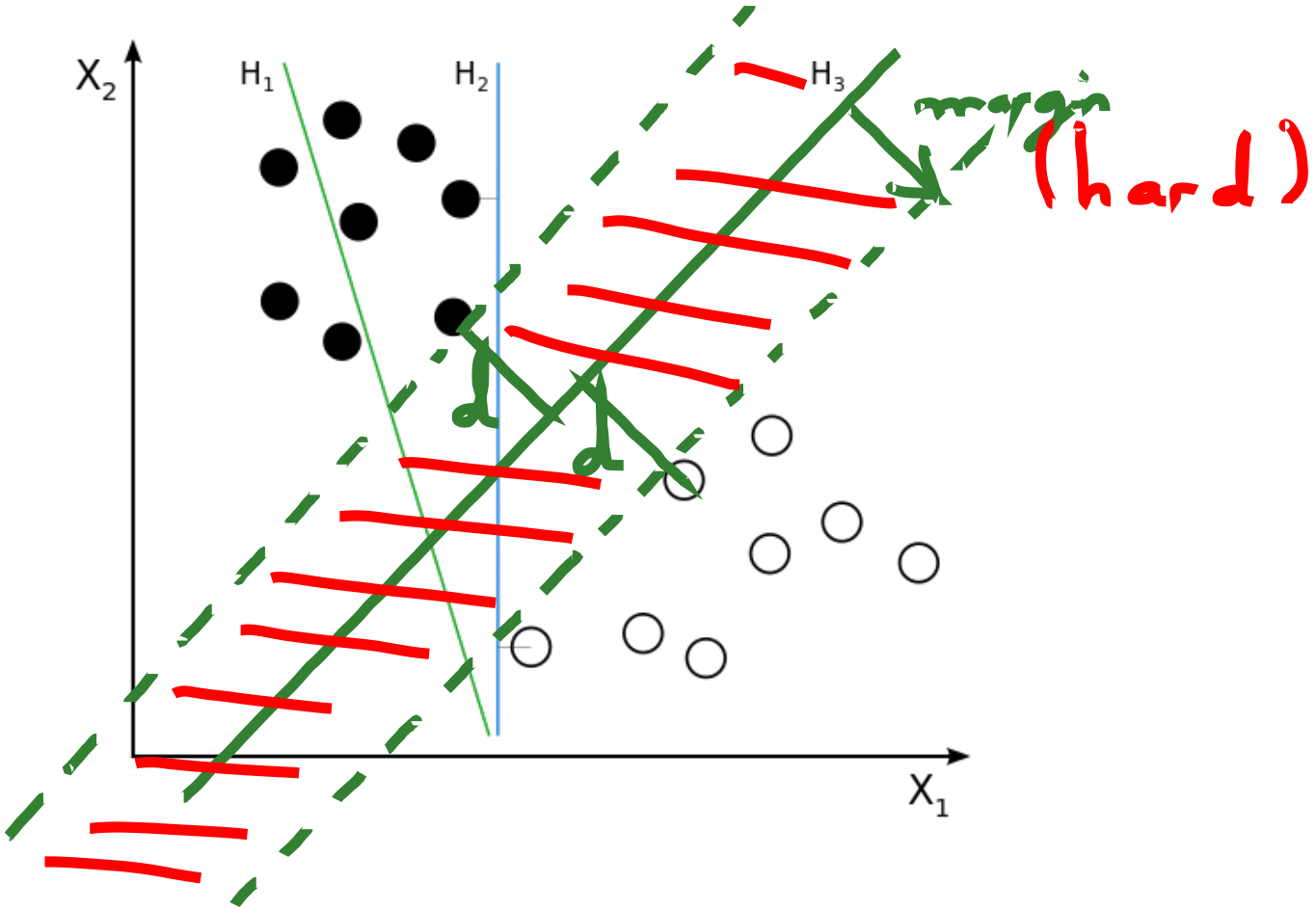


Which is better?

Outline

Defining Margin

The distance from the hyperplane to the nearest training-data point.



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Why Maximize the Margin?

Our goal is to train a model that generalizes to "unseen" data.

Large margin means better generalization.

Intuitively, this makes sense (see previous slide)

Outline

Maximum Margin Classifier

Goal

Goal: Calculate w and b of the hyperplane:

$$w \cdot x - b = 0$$

... such that the classes are split correctly and the margin is maximized.

Maximum Margin Classifier

Goal (cont.)

First, some house cleaning: What happens to the hyperplane when we scale w and b by some factor c?

$\vec{w}' = c\vec{w}$

$b' = cb$

$\vec{w}' \cdot \vec{x} - b' = (c\vec{w}) \cdot \vec{x} - (cb)$

$= c\vec{w} \cdot \vec{x} - cb$

$= c(\vec{w} \cdot \vec{x} - b)$

$= 0$

cst

If $f(\vec{w}, b)$ defines an hyperplane, then $(c\vec{w}, cb)$ $(c \neq 0)$ define the same hyperplane (that's too many!)

Maximum Margin Classifier

Setup

We need to define a "canonical" w and b. This will help later.

Let

$$|w \cdot x^{(i)} - b| = 1$$

where $x^{(i)}$ is the closest point to the hyperplane.

There will be a unique scaled w and b to achieve this.

Now, if $x^{(i)}$ is the closest point to the hyperplane, then the distance from $x^{(i)}$ to the hyperplane (at point x_0) is our margin. What is that distance?

Our equations are:

$\|\vec{x}^{(i)} - \vec{x}_0\| = d$ (1) (by definition)

$\langle \vec{w}, \vec{x}_0 \rangle - b = 0$ (2) ($x_0 \in$ hyperplane) (: projection of x)

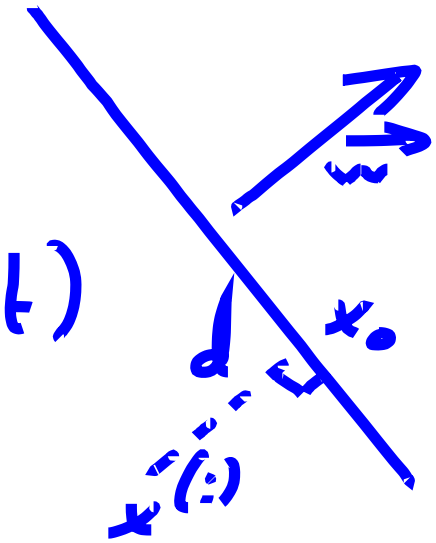
$|\langle \vec{w}, \vec{x}^{(i)} \rangle - b| = 1$ (3) (canonical constraint)

$\left\| \frac{\vec{w}}{\|\vec{w}\|} \cdot (\vec{x}^{(i)} - \vec{x}_0) \right\| = ?$ 2 ways

distribute

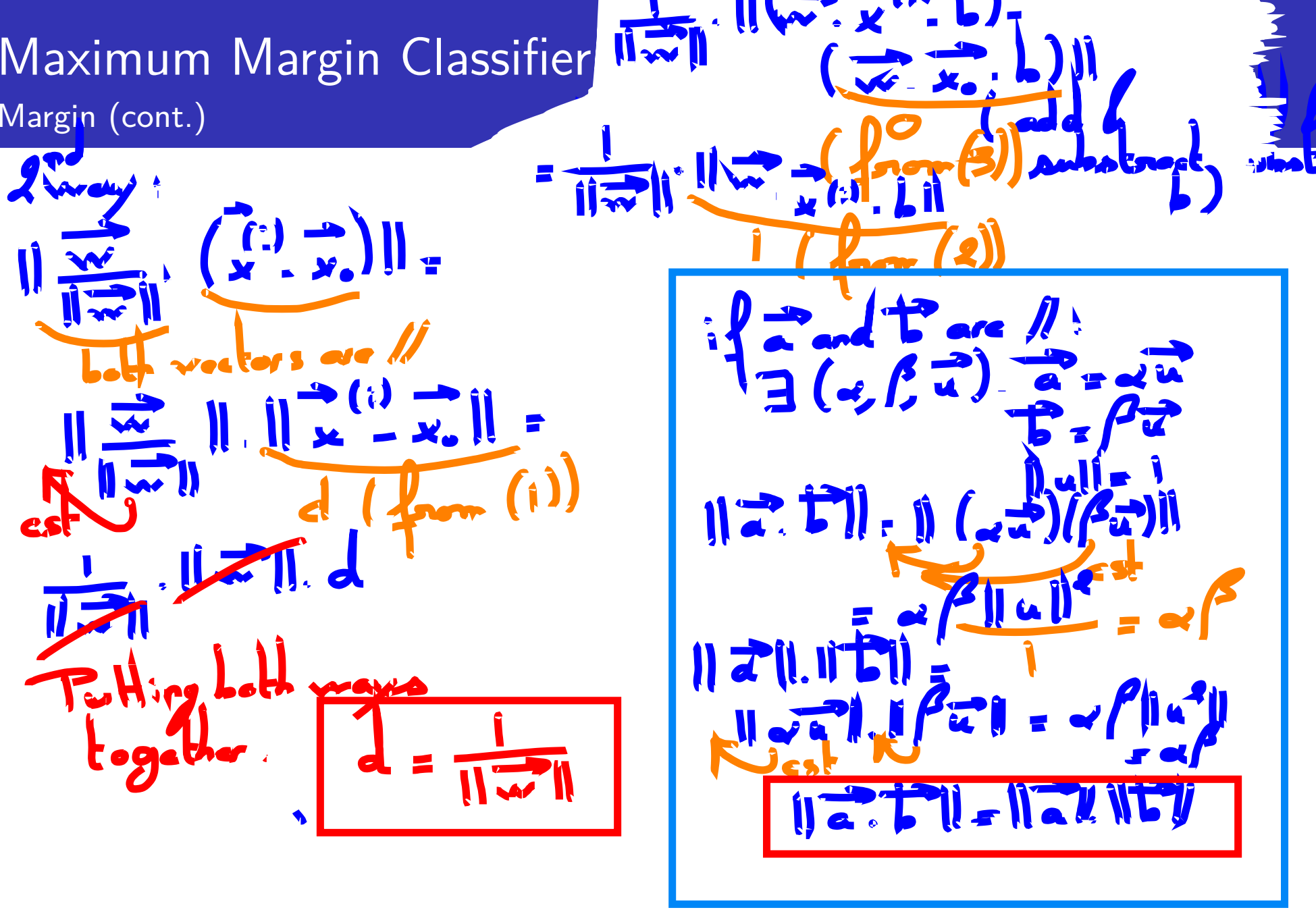
1st way: $\left\| \frac{\vec{w}}{\|\vec{w}\|} \right\| \cdot \|\vec{x}^{(i)} - \vec{x}_0\| = \frac{1}{\|\vec{w}\|} \|\vec{w}^{(:)} \cdot (\vec{x}^{(i)} - \vec{x}_0)\|$

est



Maximum Margin Classifier

Margin (cont.)



Maximum Margin Classifier

First Attempt

Maximize $\frac{1}{||w||}$

subject to:

$$|w \cdot x^{(i)} - b| \geq 1,$$

for all $x^{(i)} \in D$

... but we don't know how to solve this optimization problem. Let's reformulate.

Maximum Margin Classifier

Reformulated

Minimize $||w||^2$

details of optimization outside of class ...

subject to:

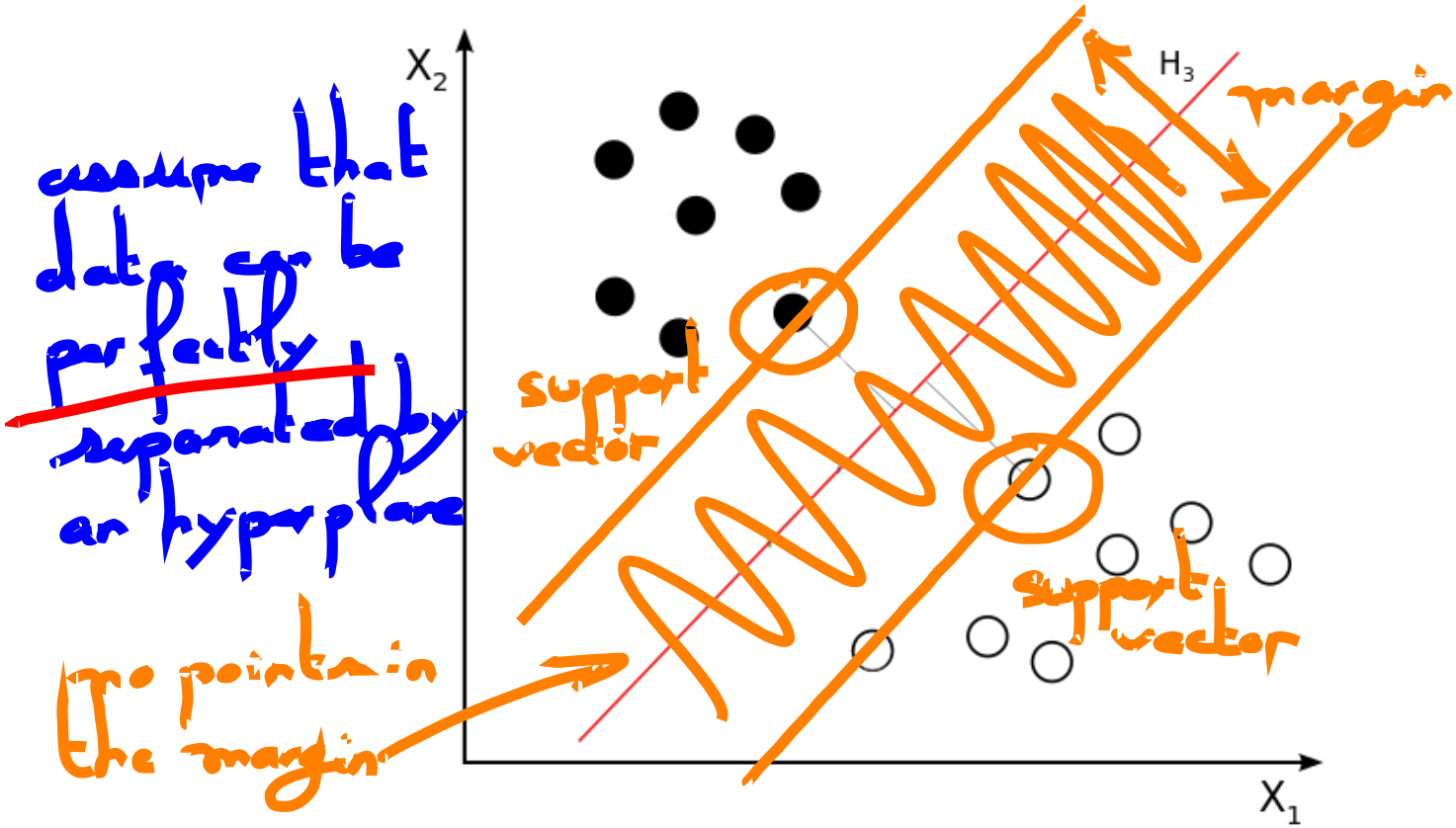
$$y^{(i)}(w \cdot x^{(i)} - b) \geq 1,$$

for all $(y^{(i)}, x^{(i)}) \in D$

... plus more steps... and we eventually get a quadratic programming formulation.

Support Vectors

The maximum margin hyperplane is defined only by the points that touch the margin. These are called the "support vectors".



LogisticRegression:

▸ Link

SVC:

▸ Link

(end of morning lecture)

Outline

Soft Margin Motivation

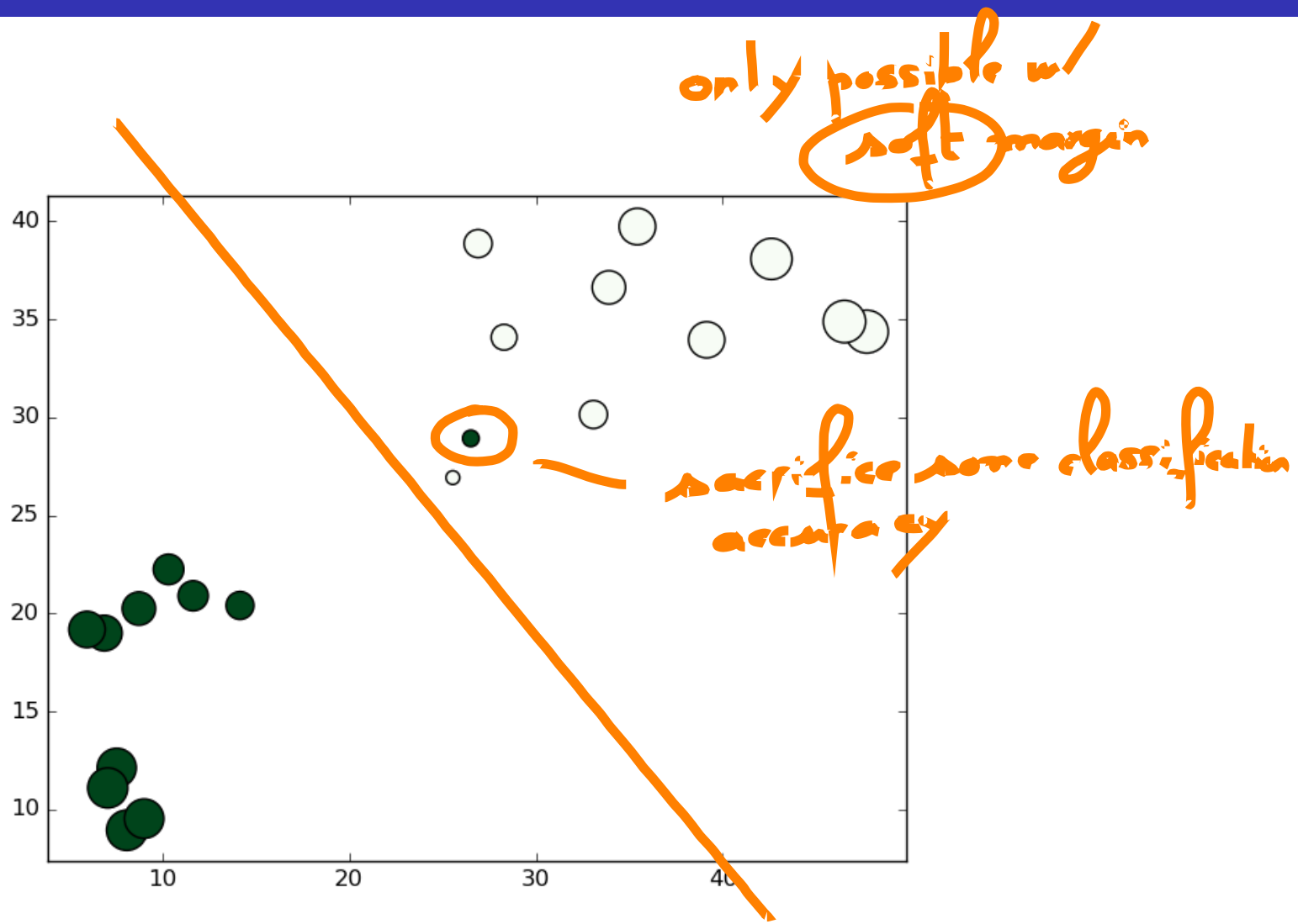
What if:

1. Your data isn't linearly separable?
2. Your data is noisy/has outliers?

Soft Margins address these problems.

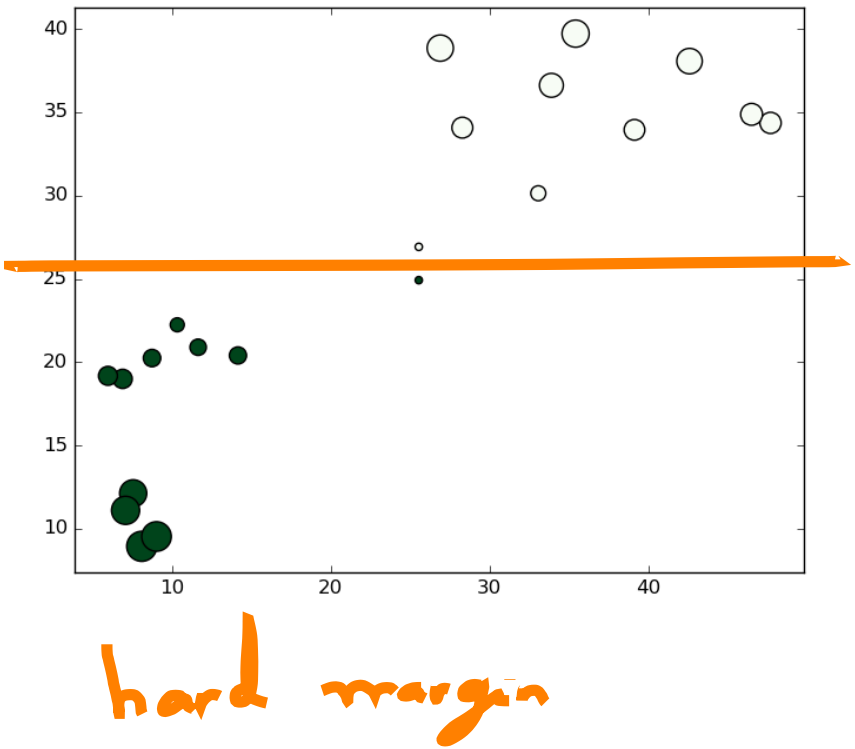
Soft Margins

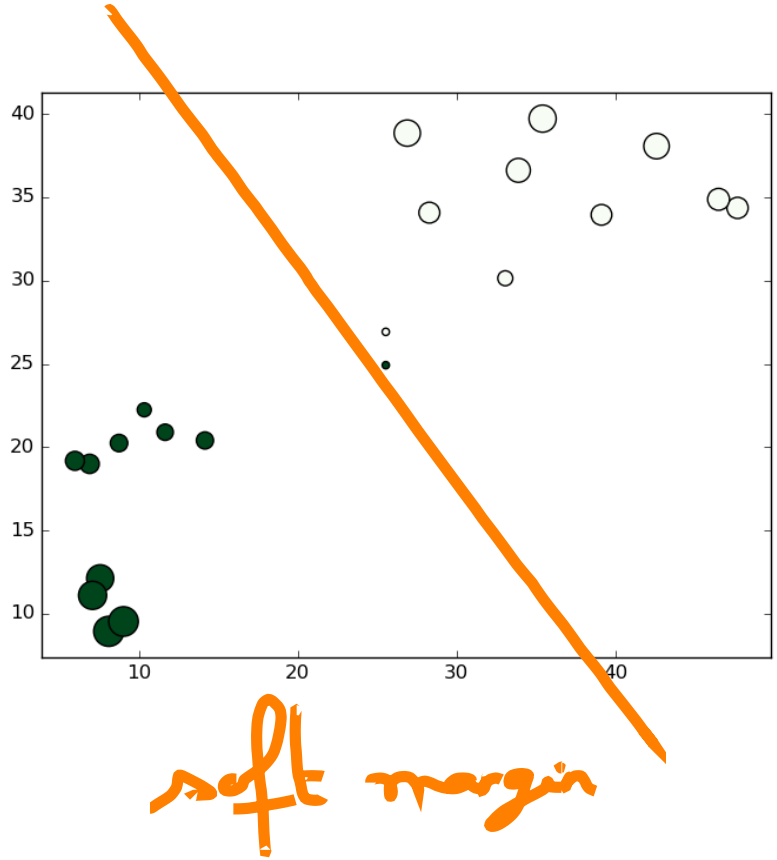
Inseparable Data



Soft Margins

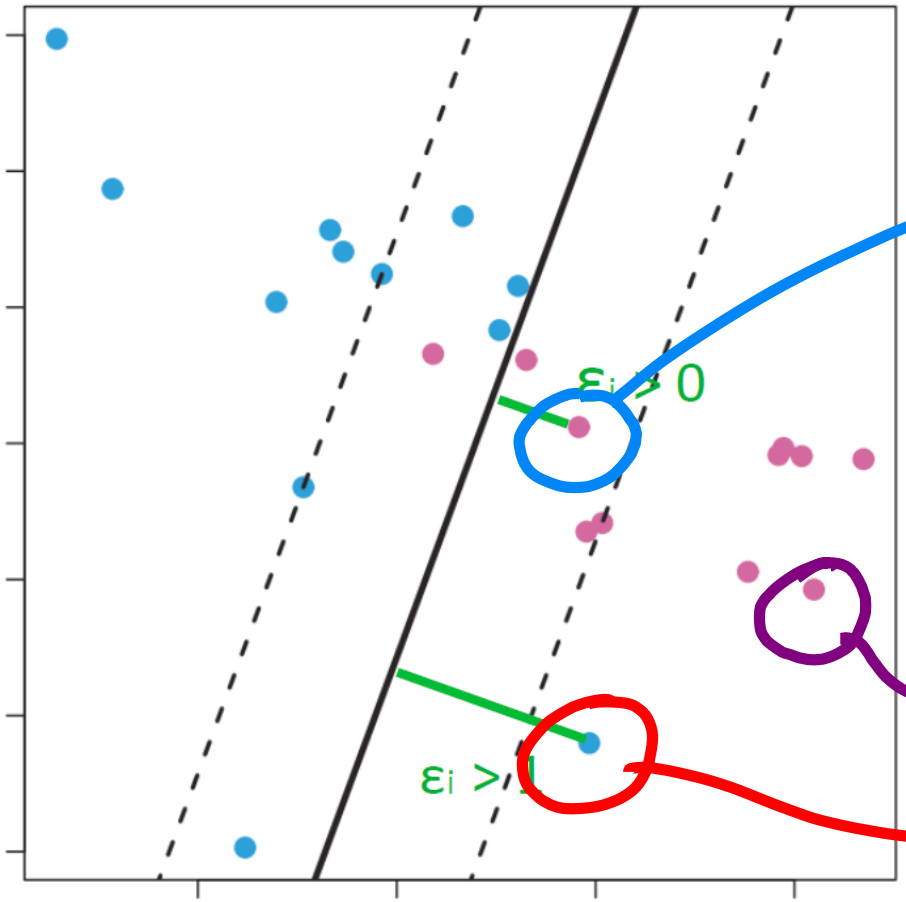
Outliers in Data





Soft Margins

We need some sort of slack/budget



right side of hyperplane but violate margin $\varepsilon_i > 0$

$\varepsilon_i = 0$ for being on correct side of margin

$\varepsilon_i > 0$ for violating the margin

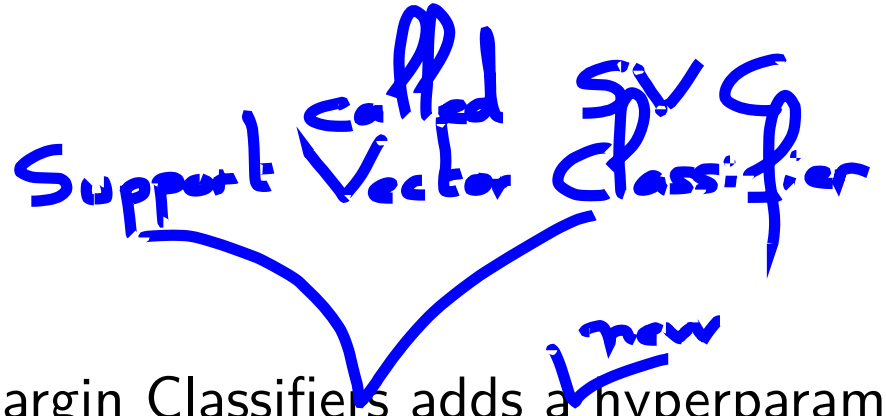
$\varepsilon_i > 1$ for being on wrong side of hyperplane

right side of margin $\varepsilon_i = 0$

wrong side of hyperplane $\varepsilon_i > 1$

Soft Margin

The C hyperparameter



An extension to Maximum Margin Classifiers adds a hyperparameter C to control the misclassification error penalty/margin tradeoff.

SVC = Maximum Margin Classifier
+ soft-margin

Support Vector Classifier

The C hyperparameter

Minimize $||w||^2$

subject to:

- $y^{(i)}(w \cdot x^{(i)} - b) \geq 1 - \varepsilon^{(i)}$

  for all $(y^{(i)}, x^{(i)}) \in D$

- $\varepsilon^{(i)} \geq 0 \ \forall i$
- $\sum_i \varepsilon^{(i)} \leq 1/C$

slack from each point

some textbooks/ software package use $C \leftrightarrow 1/C$

Budget we can tune

sk-learn convention

Support Vector Classifier

The C hyperparameter

Support Vector Classifier (SVC) extends Maximum Margin Classifiers by adding a hyperparameter C to control the misclassification error penalty/margin tradeoff.

Large C**:** Harder margins: value classification accuracy over a large margin

small $1/C$ → low margin

Small C**:** Softer margins: value a large margin over classification accuracy

large $1/C$ → large margin

Soft Margins

scikit-learn code

```
from sklearn.svm import SVC
...
svc = SVC(C=1.0, kernel='linear')
svc.fit(x, y)
```

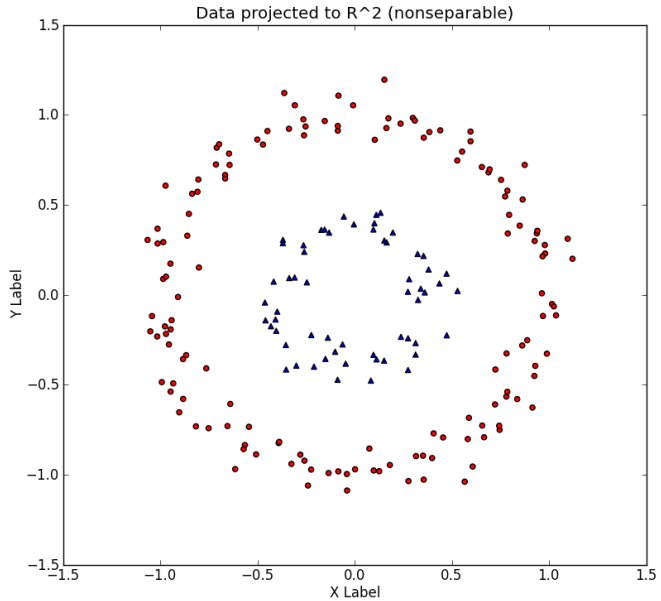
SVC supports the C parameter as the soft-margin hyperparameter.

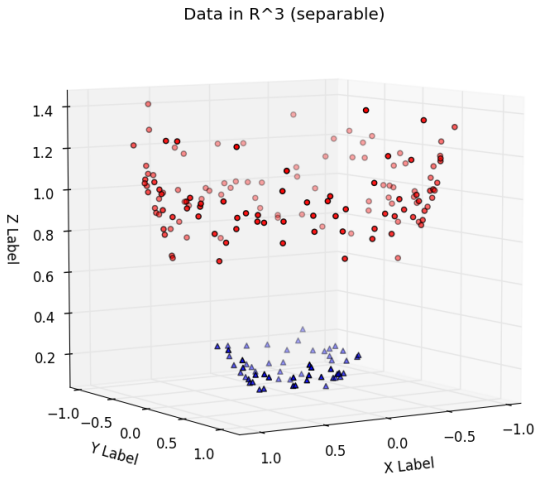
Outline

The "Kernel Trick"

The idea...

Idea: If data is inseparable in its input space, maybe it will be separable in a higher-dimensional space.





[1] Unknown source

The "Kernel Trick"

Back to some math...

We have not discussed exactly how the SVC is computed but it turns out that the optimization problem to maximize the margin involves only the *dot products* of the observations (as opposed to the observations themselves):

$$\mathcal{L}(\alpha) = \sum_{i=1}^{m} \alpha^{(i)} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} y^{(i)} y^{(j)} \alpha^{(i)} \alpha^{(j)} (x^{(i)} \cdot x^{(j)})$$

dot/inner product

The "Kernel Trick"

Creating a kernel...

What if we never took the dot product, but we instead replaced it with a generalization of the dot product of the form (a "kernel function")?

$$x^{(i)} . x^{(j)} \rightarrow K(x^{(i)}, x^{(j)})$$

The "Kernel Trick"

Why is this so cool?

SVM = SVC + "kernels"

$$\mathcal{L}(\alpha) = \sum_{i=1}^{m} \alpha^{(i)} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} y^{(i)} y^{(j)} \alpha^{(i)} \alpha^{(j)} (K(x^{(i)}, x^{(j)}))$$

- Saves some computation.
- Opens new possibilities. A kernel can operate in infinite dimensions!

The Linear Kernel

$$K(x^{(i)}, x^{(j)}) = x^{(i)} \cdot x^{(j)}$$

(basically SVC)

The Polynomial Kernel

expand feature space by adding new features

$$K(x^{(i)}, x^{(j)}) = (1 + x^{(i)} \cdot x^{(j)})^d$$

kernels are a powerful way to accomodate non-linear class boundaries

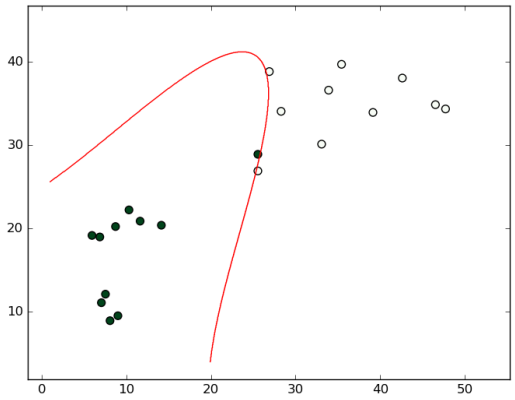
- Equivalent to the dot product in the d-order ϕ space
- Requires an extra hyper-parameter, d, for "degree"

$d = 2$

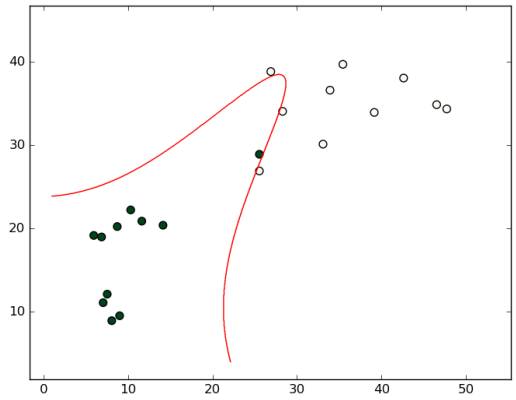
$K(x^{(i)}, x^{(j)}) = 1 + 2 x^{(i)} x^{(j)} + (x^{(i)})^2 (x^{(j)})^2$

The Polynomial Kernel

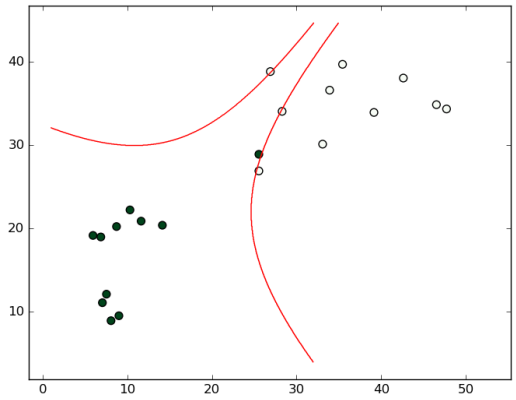
Example



svc = SVC(C=10000.0, kernel='poly', degree=3)



svc = SVC(C=10000.0, kernel='poly', degree=5)



svc = SVC(C=10000.0, kernel='poly', degree=10)

The RBF Kernel ("Gaussian")

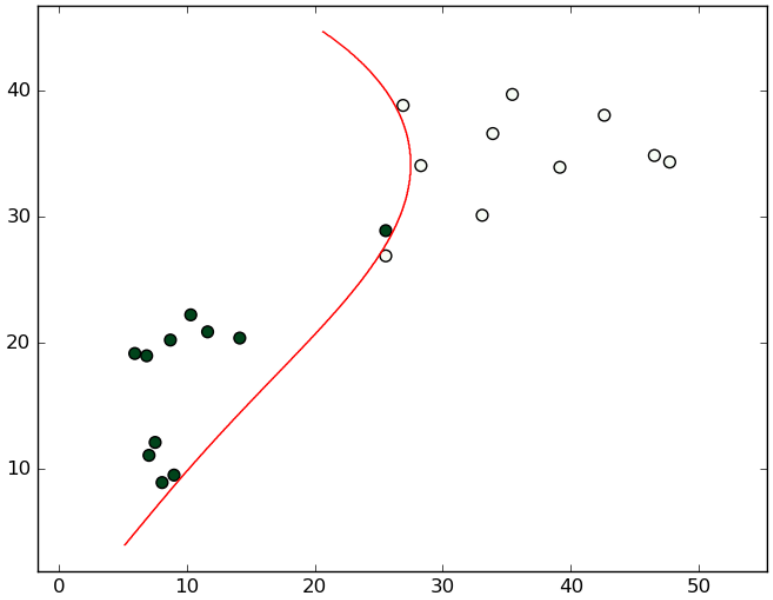
(Radial Basis Function)

$$K(x^{(i)}, x^{(j)}) = \exp\left(-\gamma ||x^{(i)} - x^{(j)}||^2\right)$$

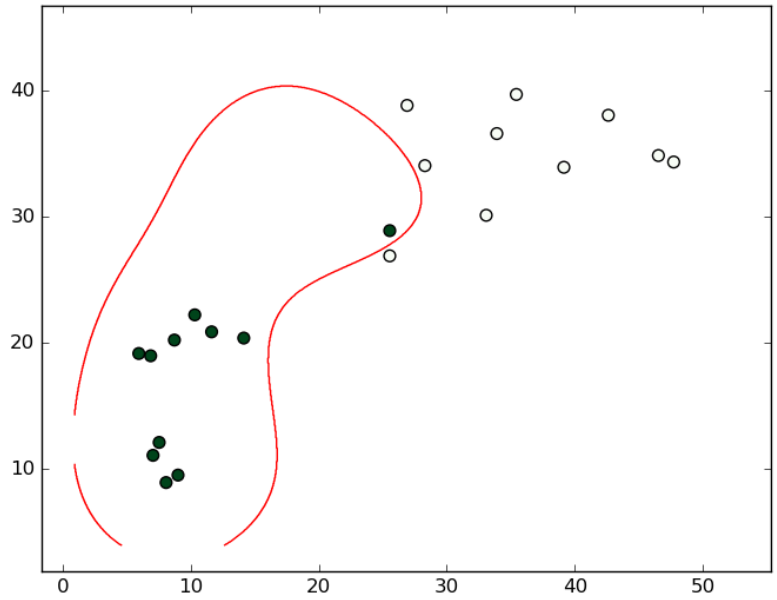
- Equivalent to the dot product in the Hilbert space of infinite dimensions
- Requires an extra hyper-parameter, γ, "gamma"

The RBF Kernel

Examples



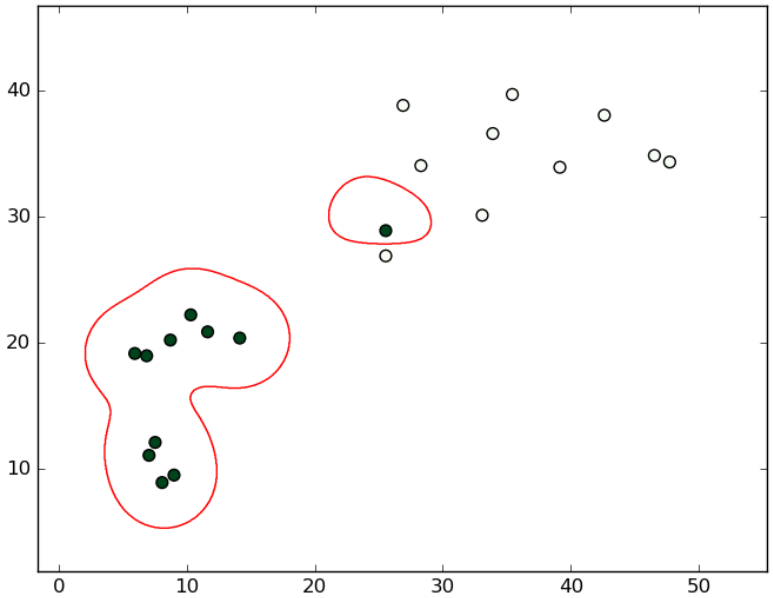
svc = SVC(C=10000.0, kernel='rbf', gamma=0.001)



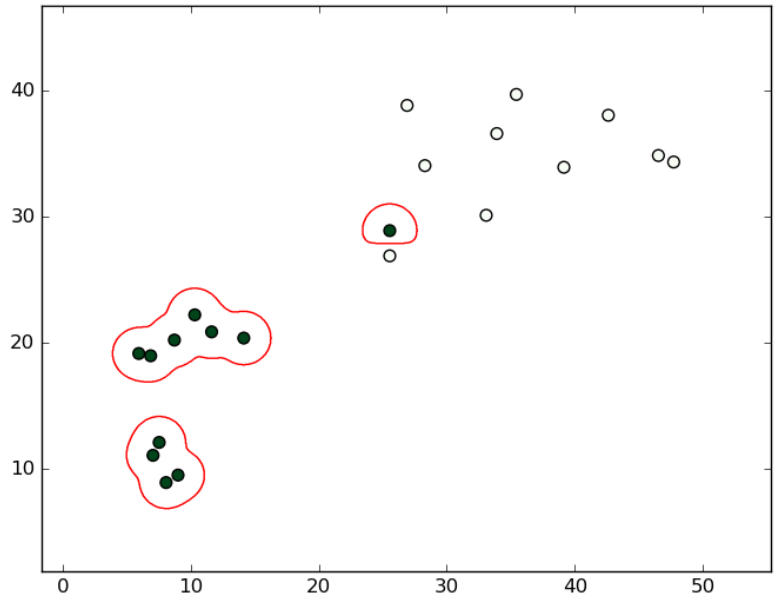
svc = SVC(C=10000.0, kernel='rbf', gamma=0.01)

The RBF Kernel

More Examples



svc = SVC(C=10000.0, kernel='rbf', gamma=0.1)



svc = SVC(C=10000.0, kernel='rbf', gamma=1.0)

Revisiting the Bias-Variance Tradeoff with SVM...

High-Bias Models

Makes many assumptions and prefers to solve problems a certain way.

E.g. A linear SVM looks for dividing hyperplanes in the input space *only*.

For complex data, high-bias models often *underfit* the data.

High-Variance Models

Makes fewer assumptions and has more representational power.

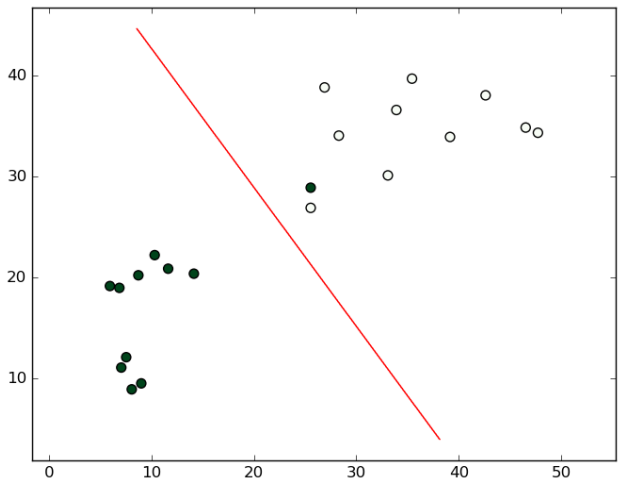
E.g. An RBF SVM looks for dividing hyperplanes in an infinite-dimensional space.

For simple data, high-variance models often *overfit* the data.

Bias-Variance Tradeoff

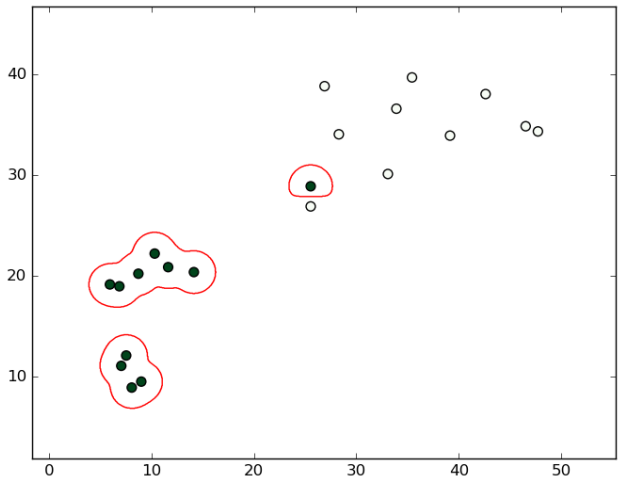
Example

low variance / higher bias



svc = SVC(C=0.01, kernel="linear")

low bias / high variance



svc = SVC(C=10000.0, kernel='rbf', gamma=1.0)

Outline

SVMs vs Logistic Regression

(some rules of thumb)

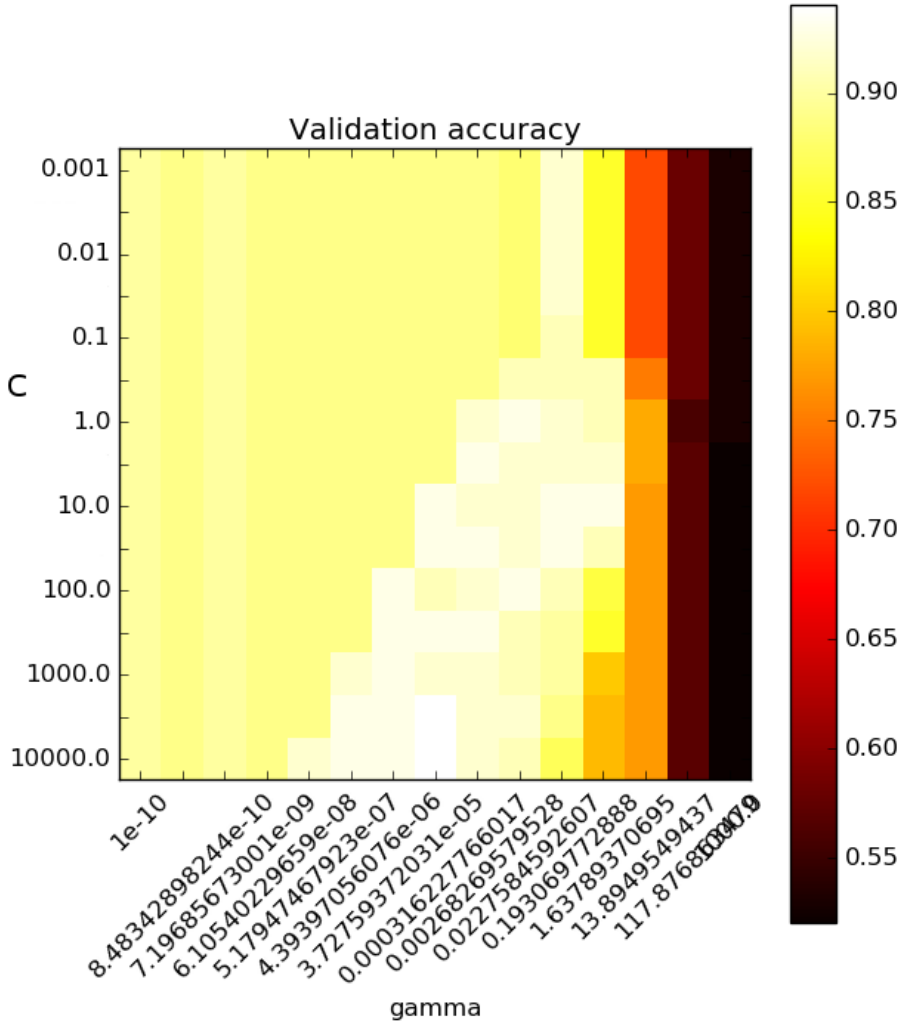
1. Logistic Regression maximizes the *Binomial Log Likelihood* function. SVMs maximize the *margin*.
2. When classes are nearly separable, SVMs tends to do better than Logistic Regression. Otherwise, Logistic Regression (with Ridge) and SVMs are similar.
3. If you want to estimate probabilities however, Logistic Regression is the better choice.
4. With kernels, SVMs work well. Logistic Regression works fine with kernels but can get computationally too expensive.

Grid Search

Hyperparameter Tuning

Let's find C and γ by searching through values we expect might work well.

Use cross-validation accuracy to determine which values are best.



Grid Search

code

```
svc_rbf = SVC(kernel='rbf')

param_space = {'C':     np.logspace(-3, 4, 15),
               'gamma': np.logspace(-10, 3, 15)}

grid_search = GridSearchCV(svc_rbf, param_space,
                           scoring='accuracy', cv=10)
grid_search.fit(x, y)

print grid_search.grid_scores_
print grid_search.best_params_
print grid_search.best_score_
print grid_search.best_estimator_
```