INTRODUCTION TO DATA SCIENCE

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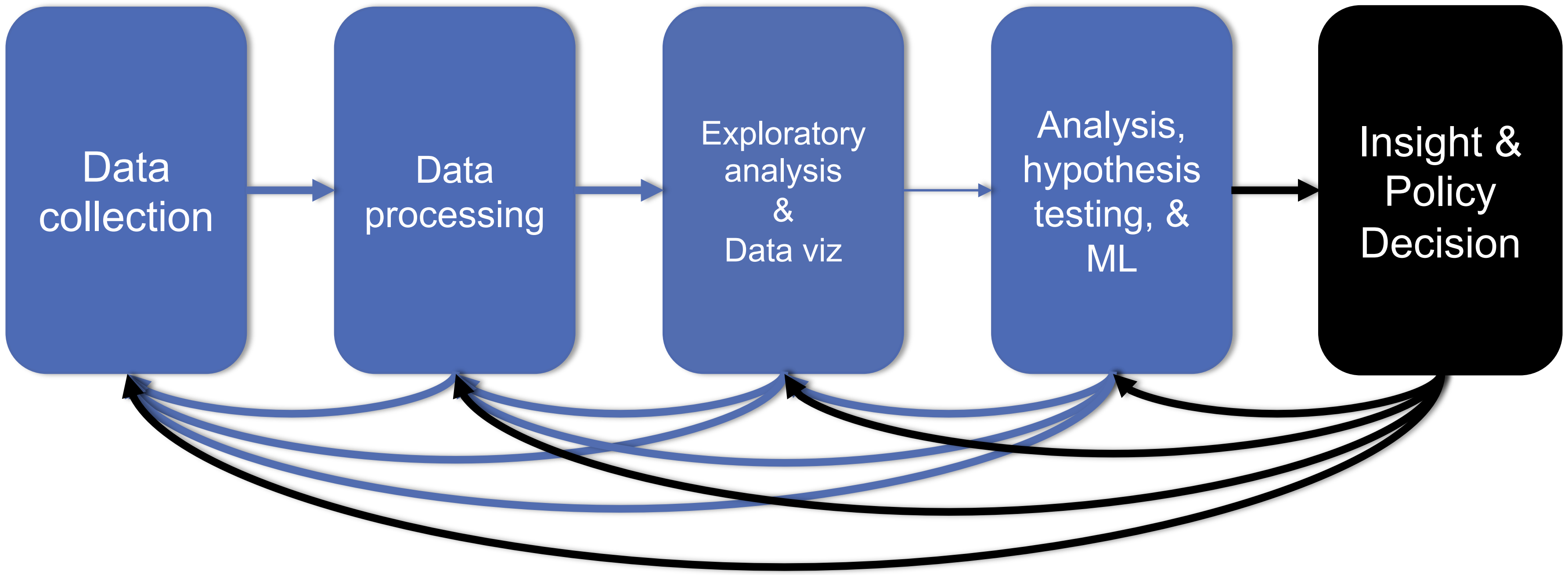
Lecture #21 – 11/5/2019

CMSC320
Tuesdays & Thursdays
5:00pm – 6:15pm

COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

TODAY'S LECTURE

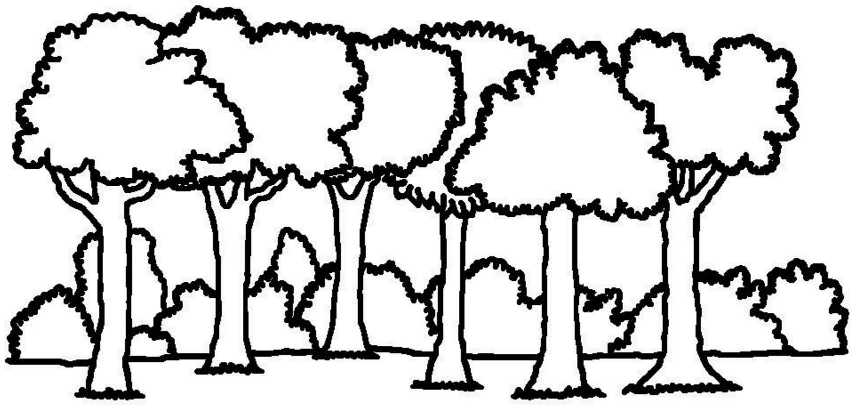

Data collection
Data processing
Exploratory analysis & Data viz
Analysis, hypothesis testing, & ML
Insight & Policy Decision

TODAY'S LECTURE

More nonlinear classification/regression methods

- Decision trees & random forests in Scikit-Learn
- K-Nearest Neighbors (KNN)
- Support Vector Machines (SVMs)

Thanks to: Hector Corrada Bravo (UMD), Panagiotis Tsaparas (U of I), Oliver Schulte (SFU)



DECISION TREES IN SCIKIT

```
from sklearn.datasets import load_iris
from sklearn import tree

# Load a common dataset, fit a decision tree to it
iris = load_iris()
clf = tree.DecisionTreeClassifier()
clf = clf.fit(iris.data, iris.target)
```

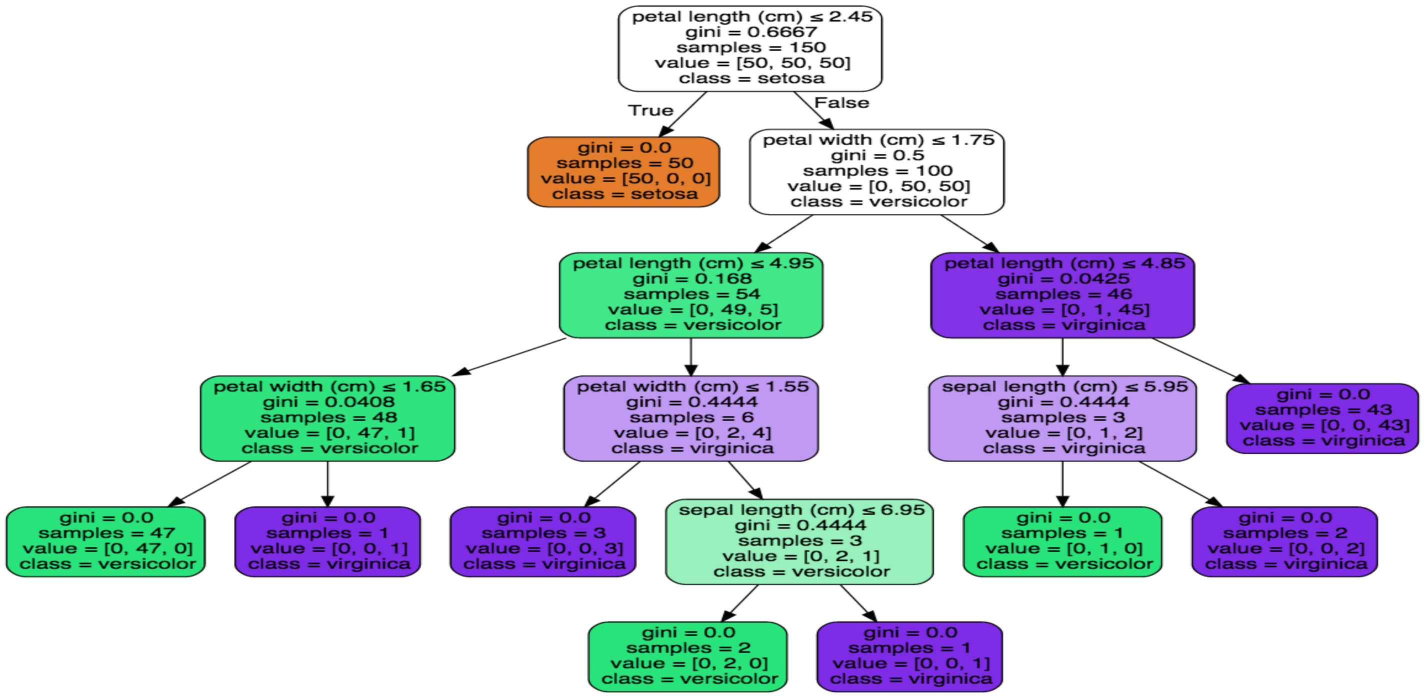
Trains a decision tree using default hyperparameters (attribute chosen to split on either Gini or entropy, no max depth, etc)

```
# Predict most likely class
clf.predict([[2., 2.]])
```

```
# Predict PDF over classes (%training samples in leaf)
clf.predict_proba([[2., 2.]])
```

VISUALIZING A DECISION TREE

```
from IPython.display import Image
dot_data = tree.export_graphviz(clf,
              out_file=None,
              feature_names=iris.feature_names,
              class_names=iris.target_names,
              filled=True, rounded=True)
graph = pydotplus.graph_from_dot_data(dot_data)
Image(graph.create_png())
```



RANDOM FORESTS

Decision trees are very interpretable, but may be brittle to changes in the training data, as well as noise

Random forests are an ensemble method that:

- Resamples the training data;
- Builds many decision trees; and
- Averages predictions of trees to classify.

This is done through bagging and random feature selection

BAGGING

Bagging: Bootstrap aggregation

Resampling a training set of size n via the bootstrap:

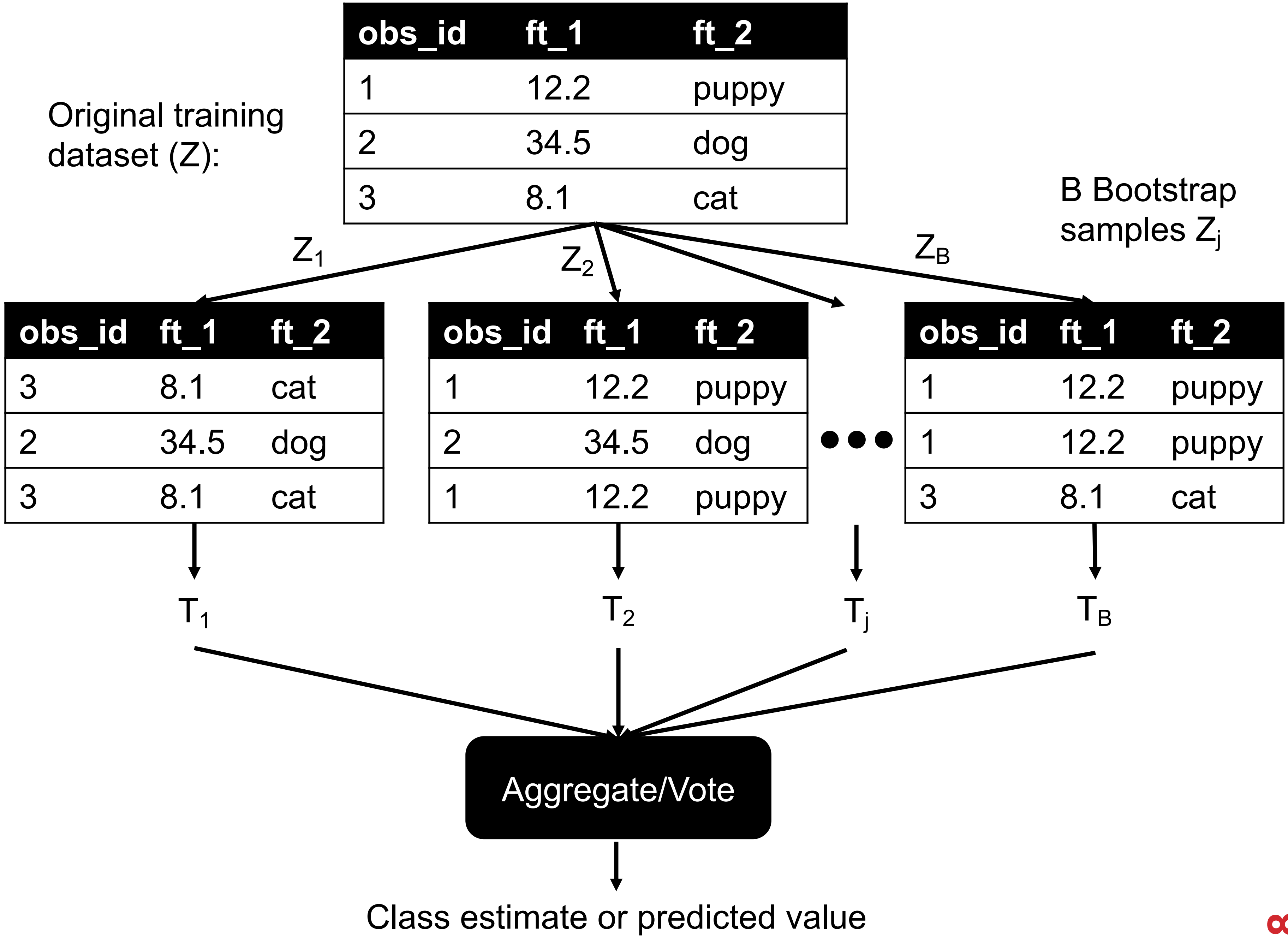
- Sample with replacement n elements

General scheme for random forests:

1. Create B bootstrap samples, $\{Z_1, Z_2, \ldots, Z_B\}$
2. Build B decision trees, $\{T_1, T_2, \ldots, T_B\}$, from $\{Z_1, Z_2, \ldots, Z_B\}$

Classification/Regression:

1. Each tree T_j predicts class/value y_j
2. Return average $1/B\ \Sigma_{j=\{1,\ldots,B\}}\ y_j$ for regression,
   or majority vote for classification


Original training dataset (Z):
B Bootstrap samples Z_j
Z_1
Z_2
Z_B
T_1
T_2
T_j
T_B
Aggregate/Vote
Class estimate or predicted value

Original training dataset (Z):

obs_id	ft_1	ft_2
1	12.2	puppy
2	34.5	dog
3	8.1	cat

Z_1

obs_id	ft_1	ft_2
3	8.1	cat
2	34.5	dog
3	8.1	cat

Z_2

obs_id	ft_1	ft_2
1	12.2	puppy
2	34.5	dog
1	12.2	puppy

Z_B

obs_id	ft_1	ft_2
1	12.2	puppy
1	12.2	puppy
3	8.1	cat

RANDOM ATTRIBUTE SELECTION

We get some randomness via bootstrapping

- We like this! Randomness increases the bias of the forest slightly at a huge decrease in variance (due to averaging)

We can further reduce correlation between trees by:

1. **For each tree, at every split point …**
2. **… choose a random subset of attributes …**
3. **… then split on the "best" (entropy, Gini) within only that subset**

RANDOM FORESTS IN SCIKIT-LEARN

```
from sklearn.ensemble import RandomForestClassifier

# Train a random forest of 10 default decision trees
X = [[0, 0], [1, 1]]
Y = [0, 1]
clf = RandomForestClassifier(n_estimators=10)
clf = clf.fit(X, Y)
```

Can we get even more random?!

Extremely randomized trees (`ExtraTreesClassifier`) **do bagging, random attribute selection, but also:**

1. **At each split point, choose random splits**
2. **Pick the best of those random splits**

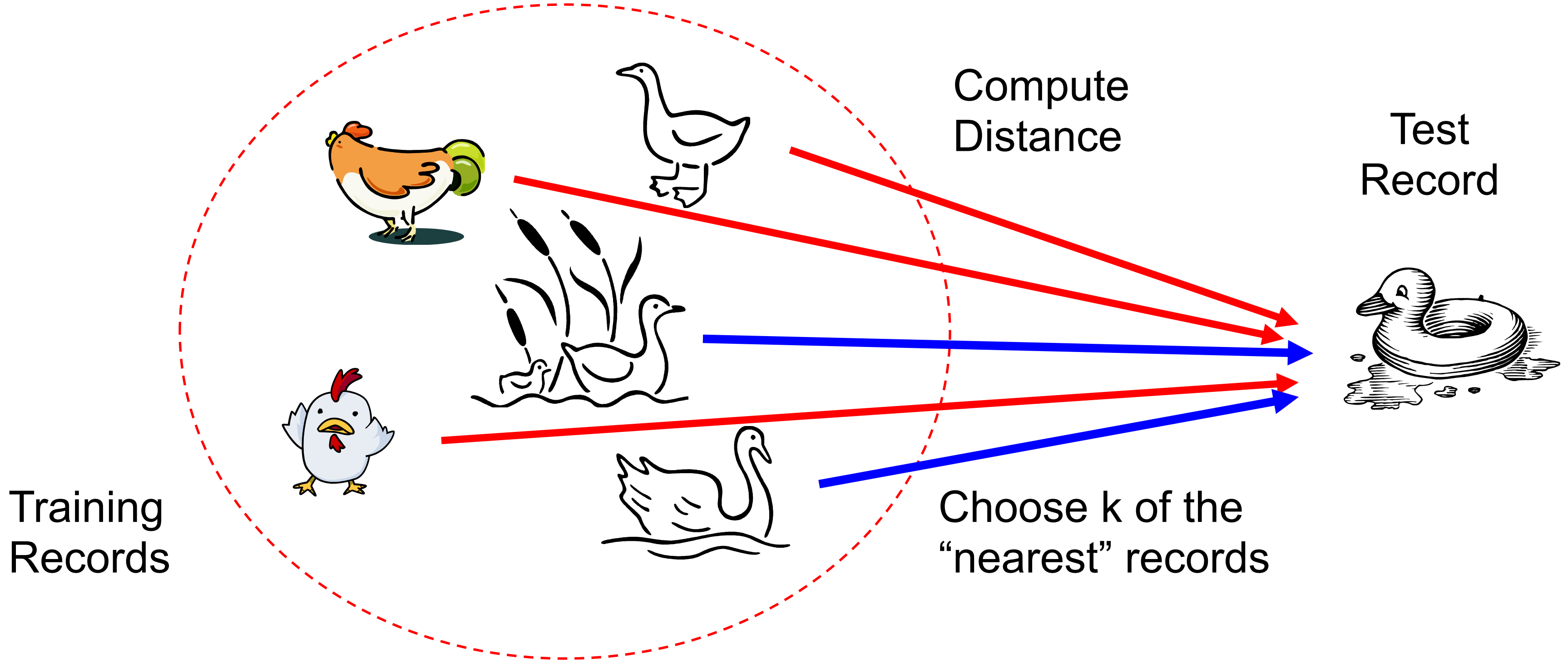
Similar bias/variance performance to RFs, but can be faster computationally

K-NEAREST NEIGHBORS

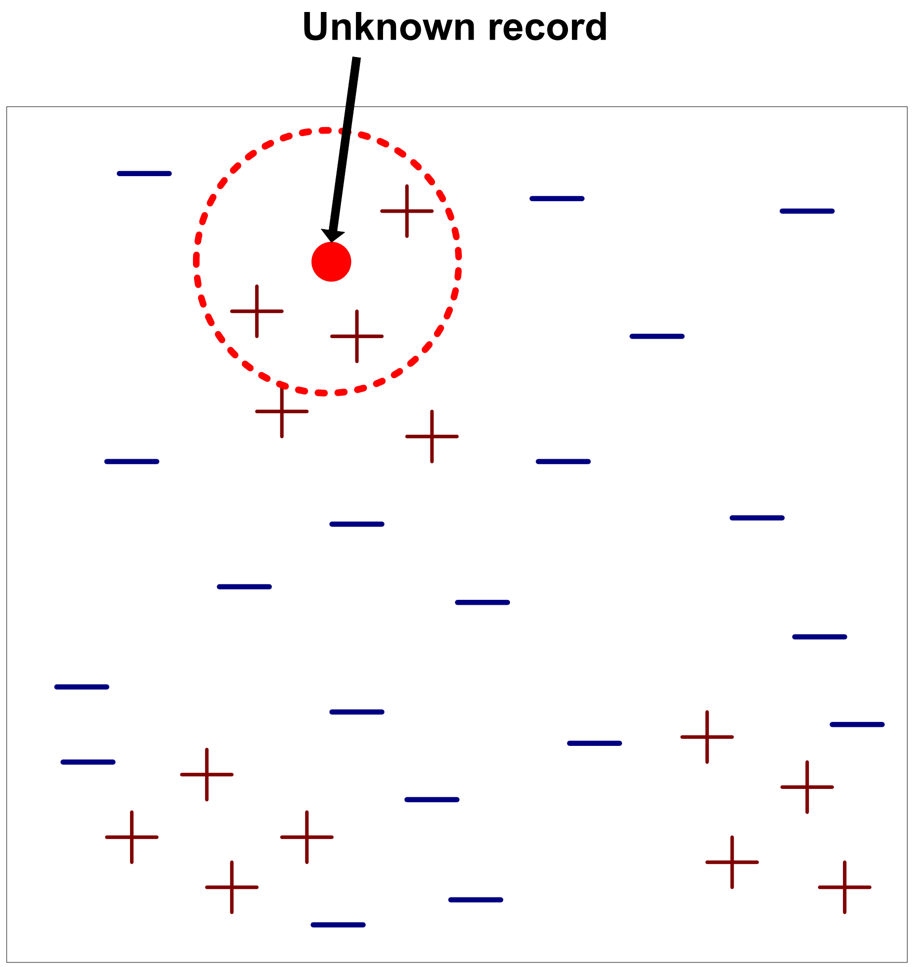
NEAREST NEIGHBOR CLASSIFIERS

Basic idea:

- If it walks like a duck, quacks like a duck, then it's probably a duck



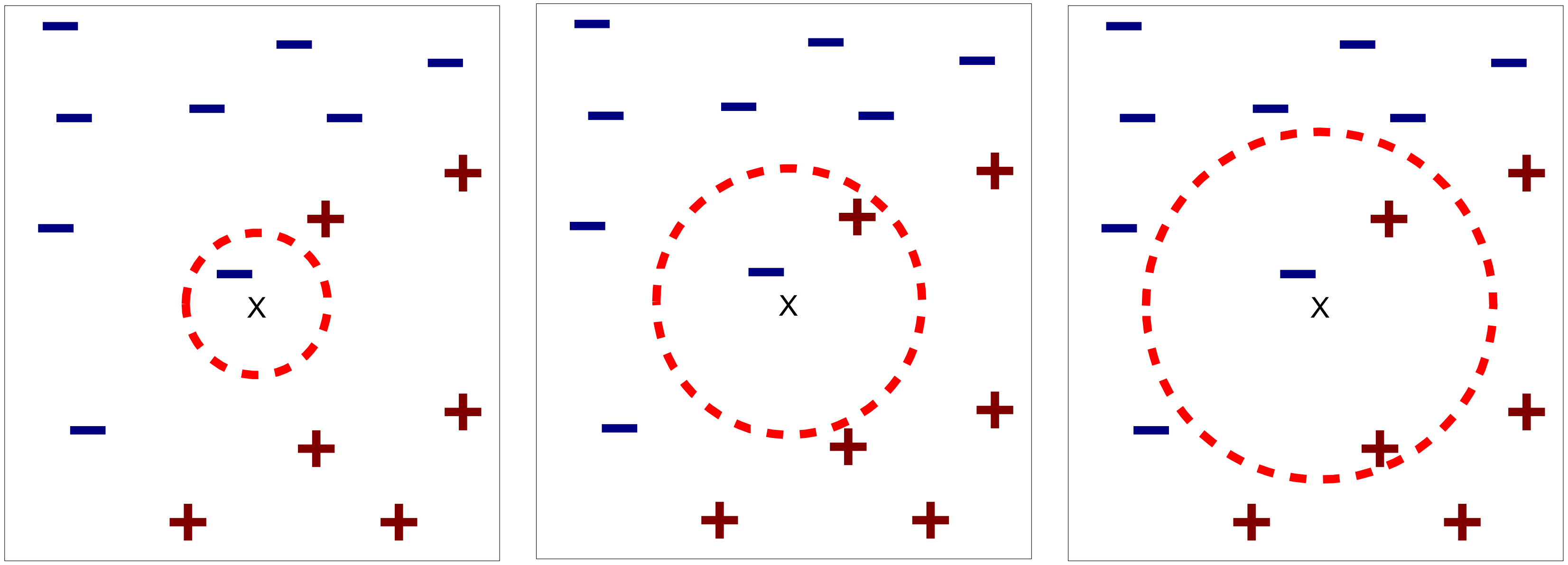
NEAREST-NEIGHBOR CLASSIFIERS



- Requires three things
  - The set of stored records
  - Distance Metric to compute distance between records
  - The value of *k*, the number of nearest neighbors to retrieve

- To classify an unknown record:
  - Compute distance to other training records
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

DEFINITION OF NEAREST NEIGHBOR

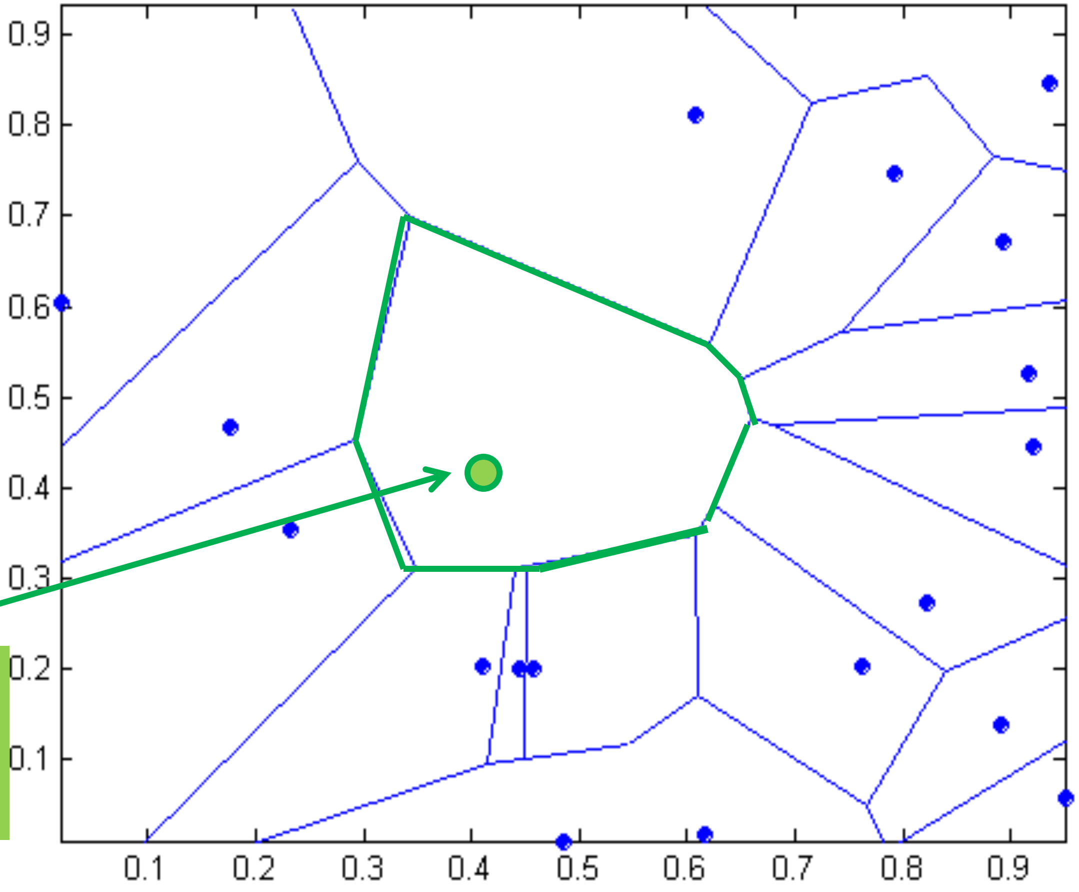


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distances to x

1-NEAREST NEIGHBOR

Voronoi Diagram defines the classification boundary



The area takes the class of the green point

NEAREST NEIGHBOR CLASSIFICATION

Compute distance between two points:

- Euclidean distance

$$d(p,q) = \sqrt{\sum_i (p_i - q_i)^2}$$

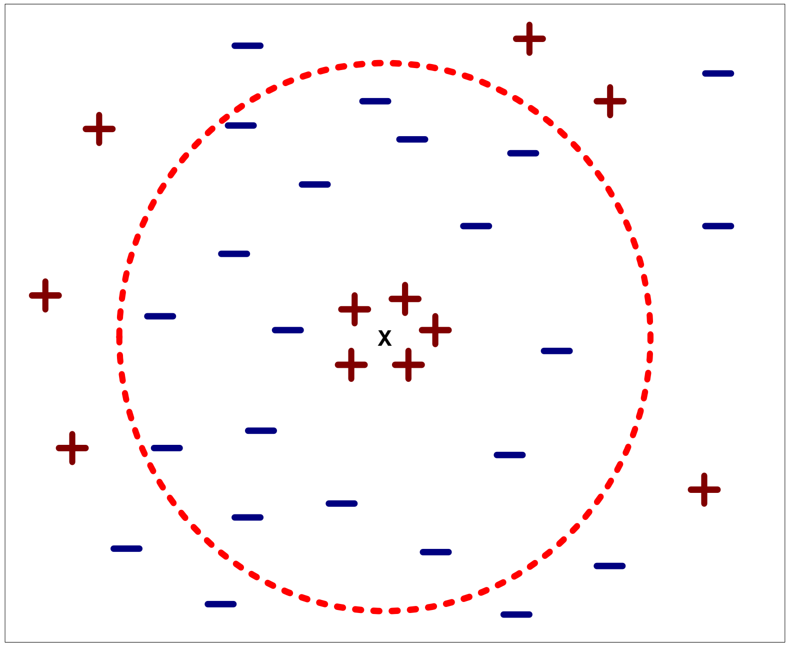
Determine the class from nearest neighbor list

- Take the majority vote of class labels among the k-nearest neighbors
- Weight the vote according to distance
  - E.g., weight factor w = $1/d^2$

NEAREST NEIGHBOR CLASSIFICATION…

Choosing the value of k:

- If k is too small, sensitive to noise points
- If k is too large, neighborhood may include points from other classes



NEAREST NEIGHBOR CLASSIFICATION…

Scaling issues

- **Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes**
- **Example:**
  - height of a person may vary from 1.5m to 1.8m
  - weight of a person may vary from 90lb to 300lb
  - income of a person may vary from $10K to $1M

Standardize variables, like in Mini-Project #2.

NEAREST NEIGHBOR CLASSIFICATION…

Problem with Euclidean measure:

- **High dimensional data**
  - The curse of dimensionality – data becomes sparse relative to the total volume of the space, distance metrics “lose meaning”
- **Can produce counter-intuitive results**

1 1 1 1 1 1 1 1 1 1 1 0	vs	1 0 0 0 0 0 0 0 0 0 0 0
0 1 1 1 1 1 1 1 1 1 1 1		0 0 0 0 0 0 0 0 0 0 0 1
d = 1.4142		d = 1.4142

Solution: Normalize the vectors to unit length

NEAREST NEIGHBOR CLASSIFICATION…

k-NN classifiers are lazy learners

- It does not build models explicitly
- Unlike eager learners such as decision tree induction and rule-based systems

Classifying unknown records are relatively expensive

- Naïve algorithm: O(n)
- Need for structures to retrieve nearest neighbors fast
  - The Nearest Neighbor Search problem
- CMSC420 covers spatial data structures extensively

NEAREST NEIGHBOR SEARCH

Two-dimensional kd-trees:

- A data structure for answering nearest neighbor queries in R^2

kd-tree construction algorithm

- Select the x or y dimension (alternating between the two)
- Partition the space into two with a line passing from the median point
- Repeat recursively in the two partitions as long as there are enough points
- Can quickly query the tree for nearest neighbors by finding an incumbent best and pruning large chunks of the tree away

K-NN: ADVANTAGES

Simple technique that is easily implemented

Building model is cheap

Extremely flexible classification scheme

Well suited for:

- Multi-modal classes
- Records with multiple class labels

Can sometimes be the best method

- Michihiro Kuramochi and George Karypis, Gene Classification using Expression Profiles: A Feasibility Study, International Journal on Artificial Intelligence Tools. Vol. 14, No. 4, pp. 641-660, 2005
- K nearest neighbor outperformed SVM for protein function prediction using expression profiles

K-NN: DISADVANTAGES

Classifying unknown records are relatively expensive

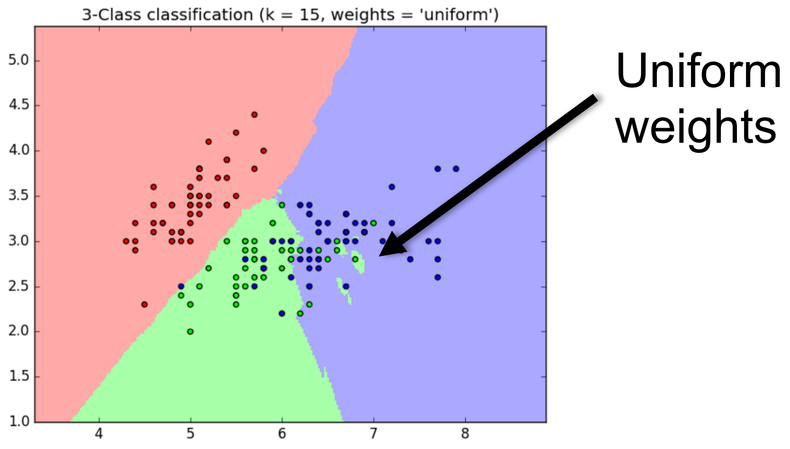
- Requires distance computation of k-nearest neighbors
- Computationally intensive, especially when the size of the training set grows

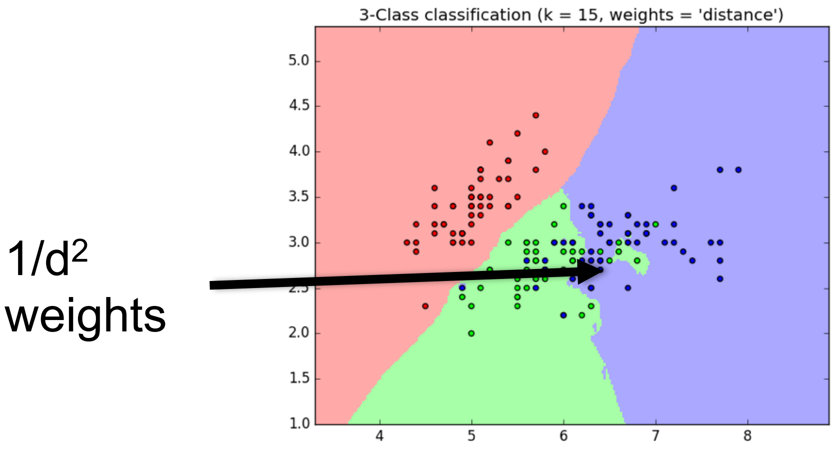
Accuracy can be severely degraded by the presence of:

- Noisy or irrelevant features
- High-dimensional space
- Choosing the wrong distance metric
- Choosing the wrong *k*

KNN CLASSIFICATION IN SCIKIT-LEARN

```
from sklearn import neighbors, datasets

# Load a common dataset, fit a 15-NN classifier to it
iris = datasets.load_iris()
X = iris.data[:, :2]  # take the first two features
y = iris.target

clf = neighbors.KNeighborsClassifier(
                    15, weights='uniform')
clf.fit(X, y)
```

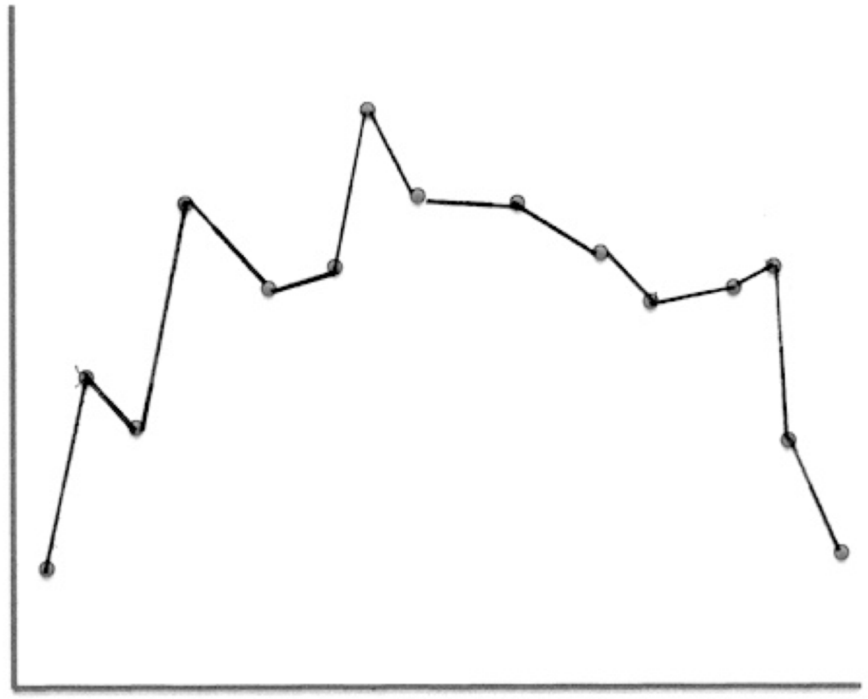




LOCAL REGRESSION

Basic Idea: To predict a target value y for data point x, apply interpolation/regression to the neighborhood of x.

Simplest version: connect the dots.

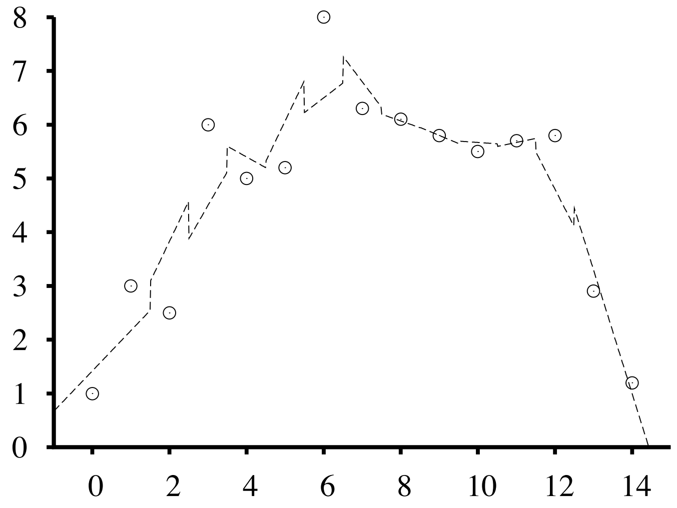


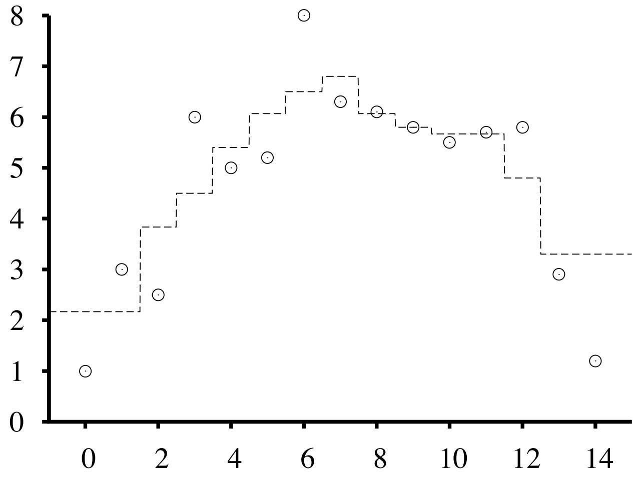
K-NEAREST NEIGHBOR REGRESSION

Connect the dots uses k = 2, fits a line.

Ideas for k =5.

- Fit a line using linear regression.
- Predict the average target value of the k points.





LOCAL REGRESSION WITH KERNELS

Spikes in regression prediction come from in-or-out nature of neighborhood

Instead, weight examples as function of the distance

A homogenous kernel function maps the distance between two vectors to a number, usually in a nonlinear way.
k(x,x’) = k(distance(x,x’))

Example: The quadratic kernel

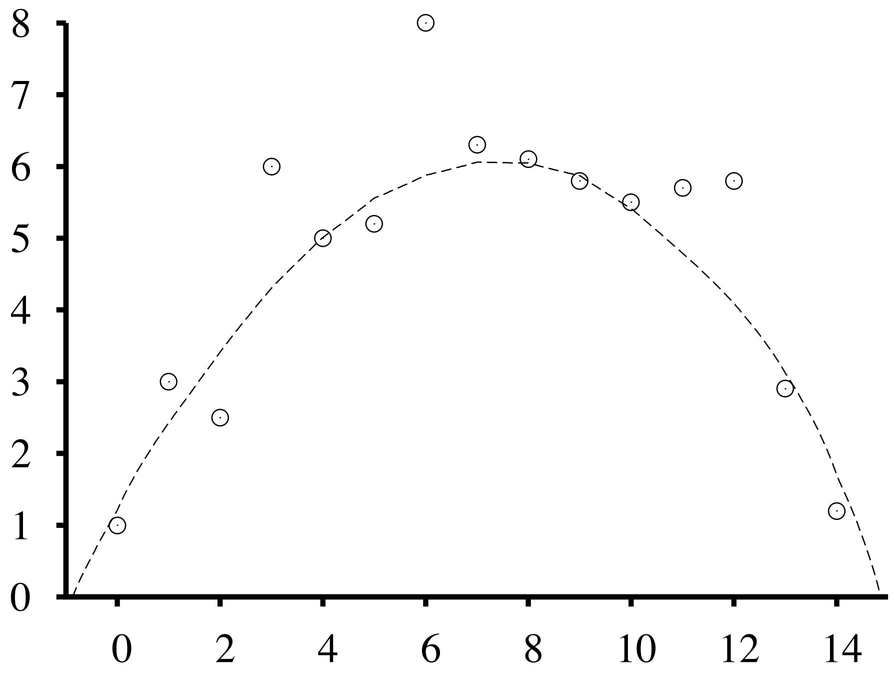
KERNEL REGRESSION

For each query point $\mathbf{x}_q$, prediction is made as weighted linear sum:

$$y(\mathbf{x}_q) = \mathbf{w} \bullet \mathbf{x}_q.$$

To find weights, solve the following regression on the k-nearest neighbors:

$$w^* = \underset{w}{\operatorname{argmin}} \sum_j k(dist(\mathbf{x}_q, \mathbf{x}_j))(t_j - \mathbf{w} \bullet \mathbf{x}_j)^2$$



KNN REGRESSION IN SCIKIT-LEARN

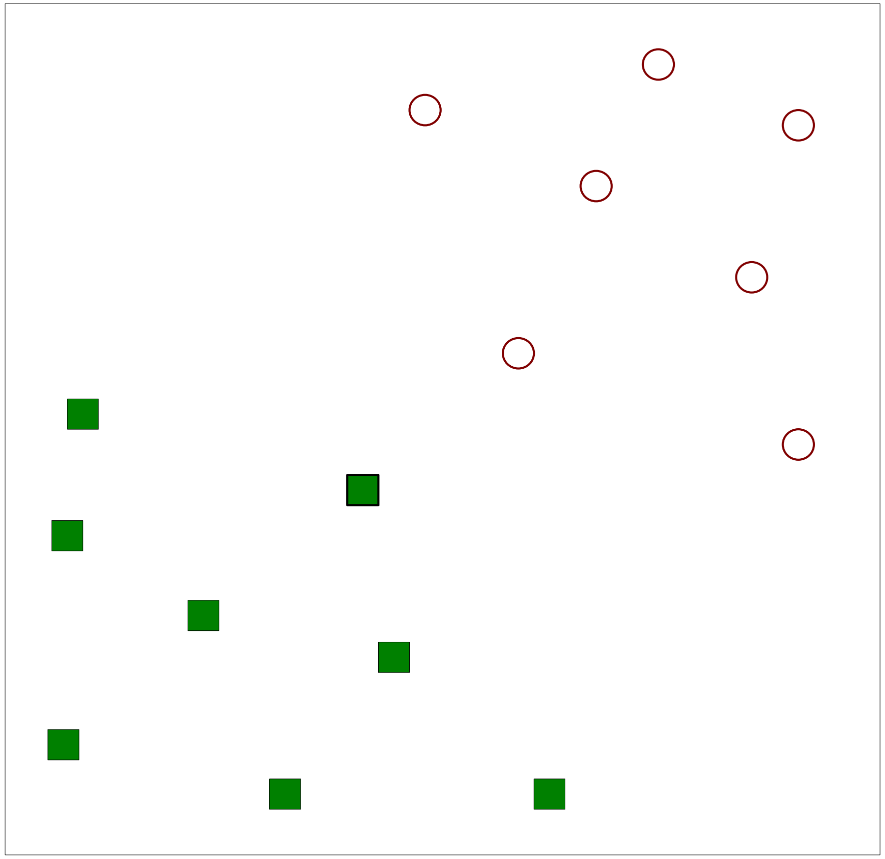
```
from sklearn.neighbors import KNeighborsRegressor

# Basic KNN regression in Scikit (interpolation)
X = [[0], [1], [2], [3]]
y = [0, 0, 1, 1]

neigh = KNeighborsRegressor( n_neighbors=2 )
neigh.fit(X, y)

print(neigh.predict([[1.5]]))
```

```
[ 0.5]
```

Also provides a variety of distance metrics, backing algorithms to find nearest neighbors, weight functions (down-weight points based on distance), etc.

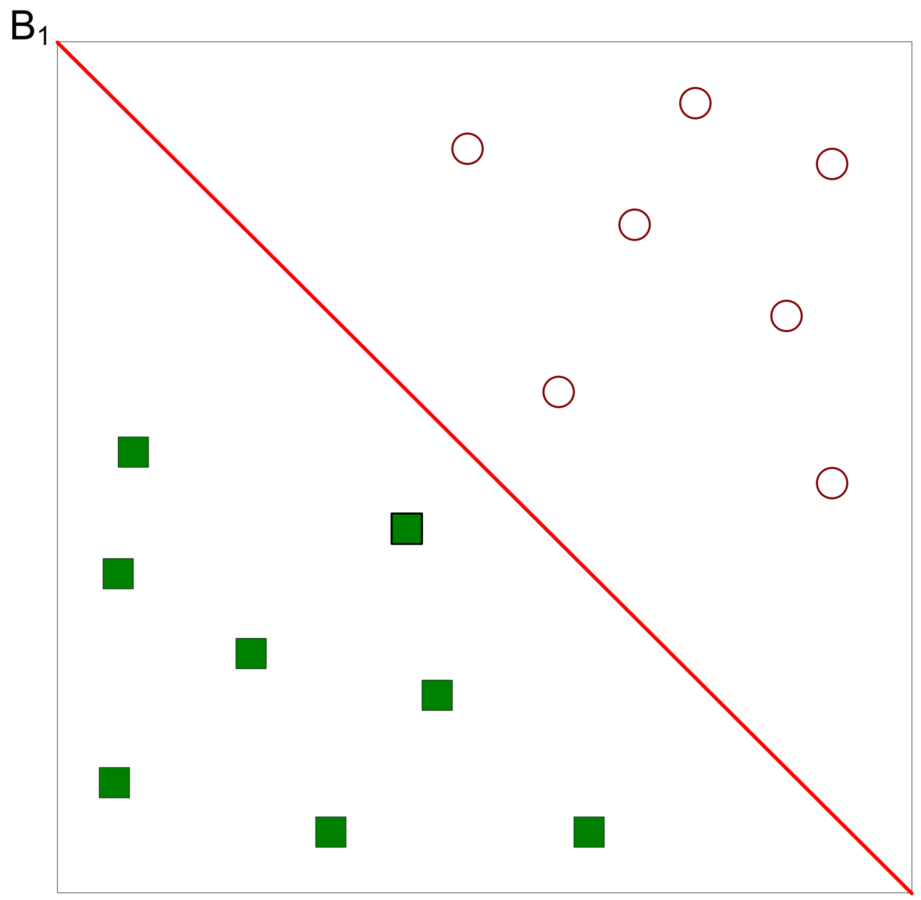
SUPPORT VECTOR MACHINES

SUPPORT VECTOR MACHINES (SVM)



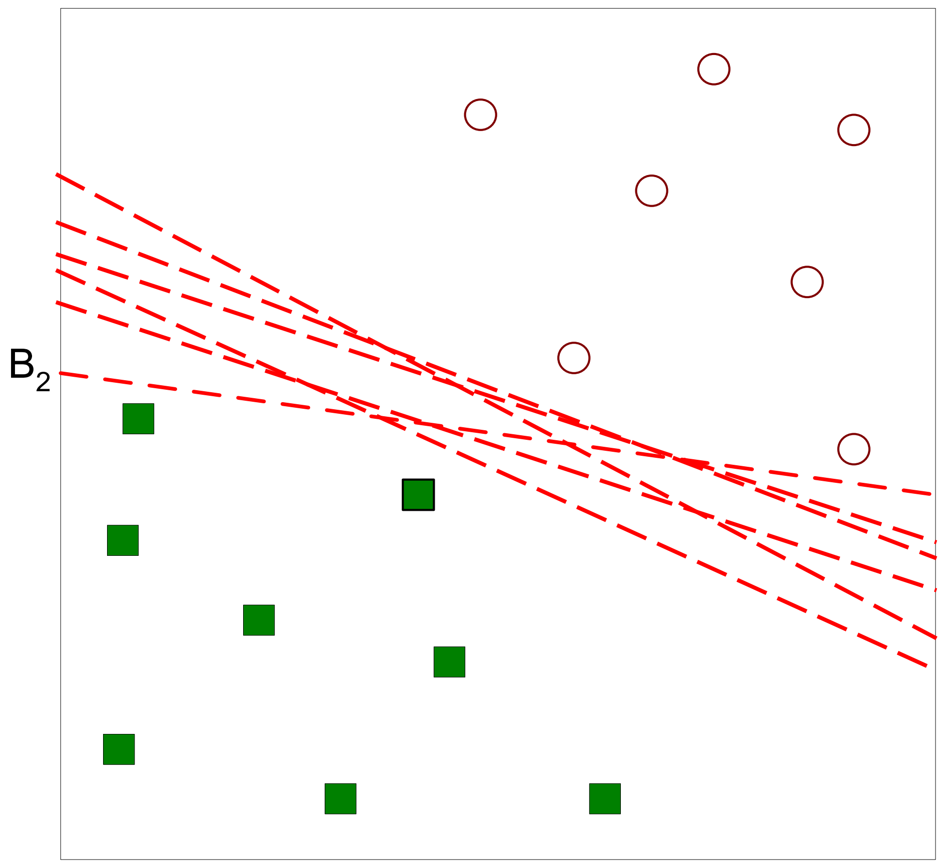
Find a linear hyperplane (decision boundary) that will separate the data

SUPPORT VECTOR MACHINES



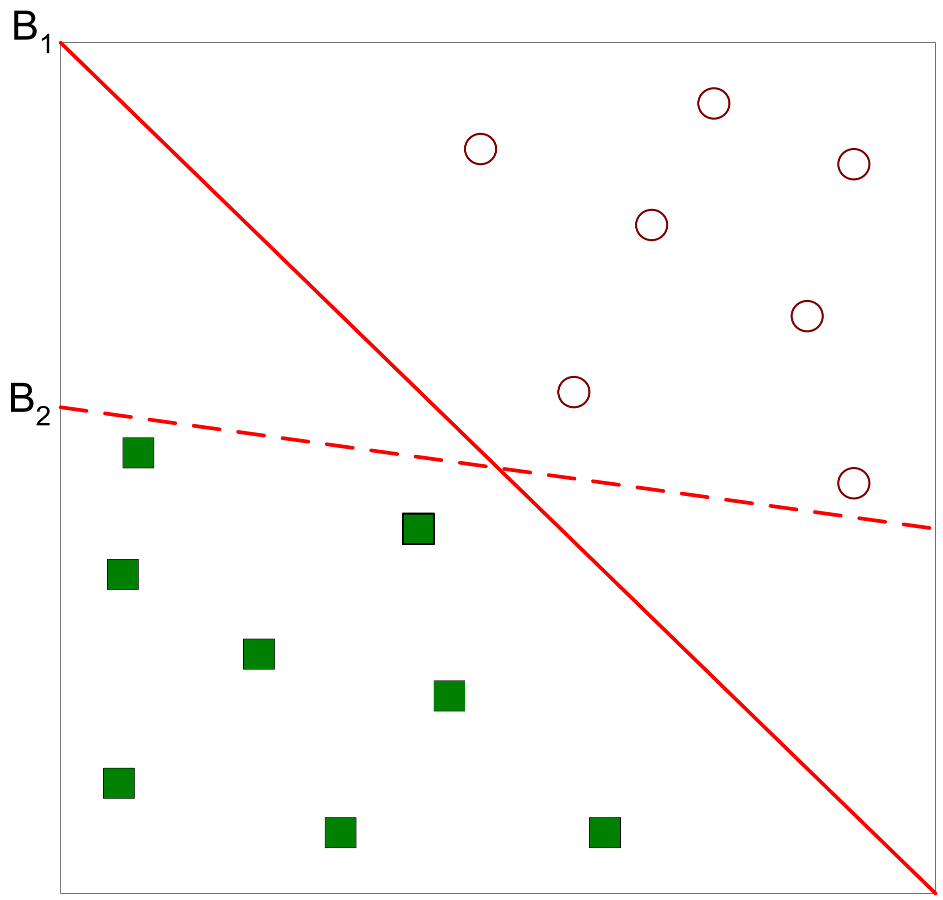
One possible solution

SUPPORT VECTOR MACHINES



Other possible solutions

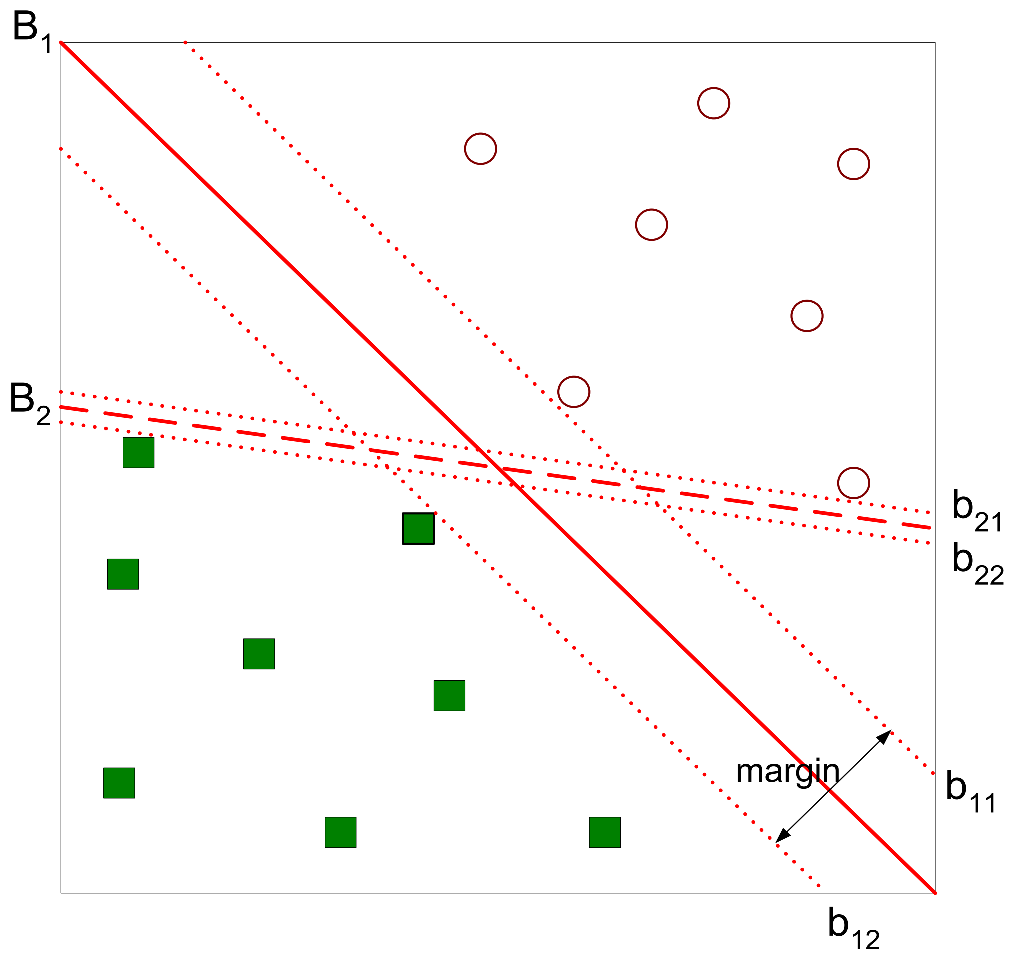
SUPPORT VECTOR MACHINES



Which one is better? B_1 or B_2?   ??????????

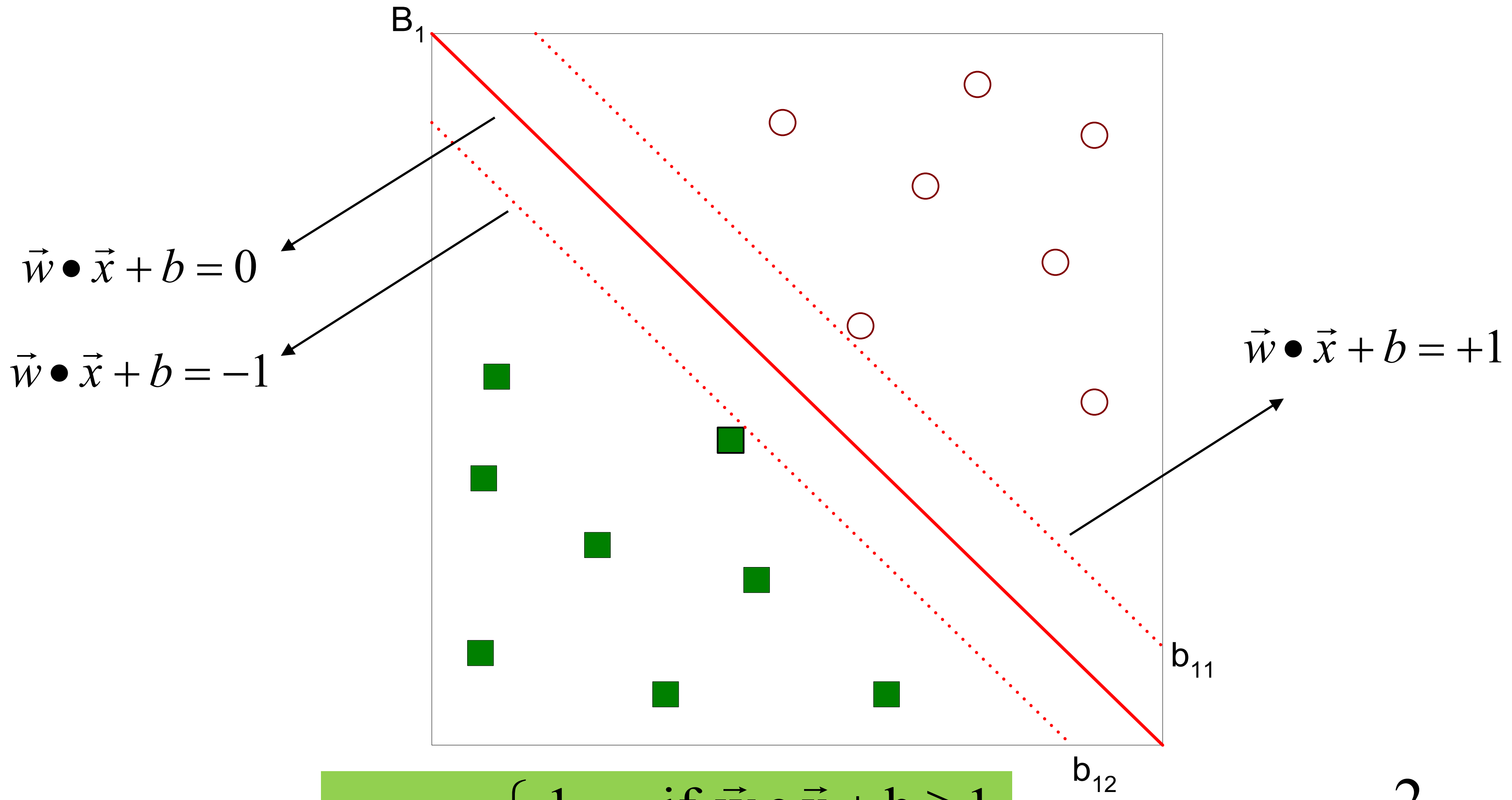
How do you define better?   ??????????

SUPPORT VECTOR MACHINES



Find hyperplane <span>maximizes</span> the margin → B_1 is better than B_2

SUPPORT VECTOR MACHINES



B_1
$\vec{w} \bullet \vec{x} + b = 0$
$\vec{w} \bullet \vec{x} + b = -1$
$\vec{w} \bullet \vec{x} + b = +1$
b_{11}
b_{12}

$$f(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \bullet \vec{x} + b \geq 1 \\ -1 & \text{if } \vec{w} \bullet \vec{x} + b \leq -1 \end{cases}$$

$$\text{Margin} = \frac{2}{\| \vec{w} \|^2}$$

SUPPORT VECTOR MACHINES

We want to maximize: $\text{Margin} = \frac{2}{\|\vec{w}\|^2}$

Which is equivalent to minimizing: $L(w) = \frac{\|\vec{w}\|^2}{2}$

But subject to the following constraints:

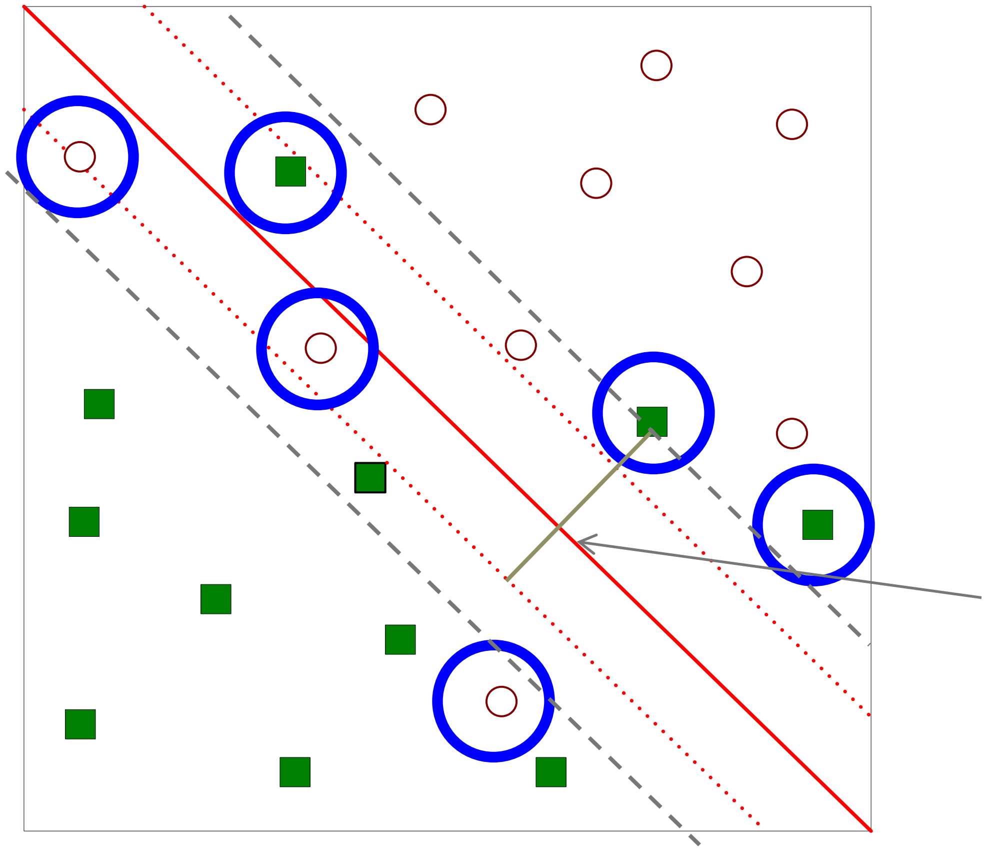
$$\vec{w} \cdot \vec{x_i} + b \geq 1 \text{ if } y_i = 1$$
$$\vec{w} \cdot \vec{x_i} + b \leq -1 \text{ if } y_i = -1$$

This is a constrained optimization problem

- Numerical approaches to solve it (e.g., quadratic programming)

SUPPORT VECTOR MACHINES

What if the problem is not linearly separable?



Apply some sort of penalty

$$\frac{\xi_i}{\|w\|}$$

SUPPORT VECTOR MACHINES

What if the problem is not linearly separable?

- Introduce slack variables
- Need to minimize:

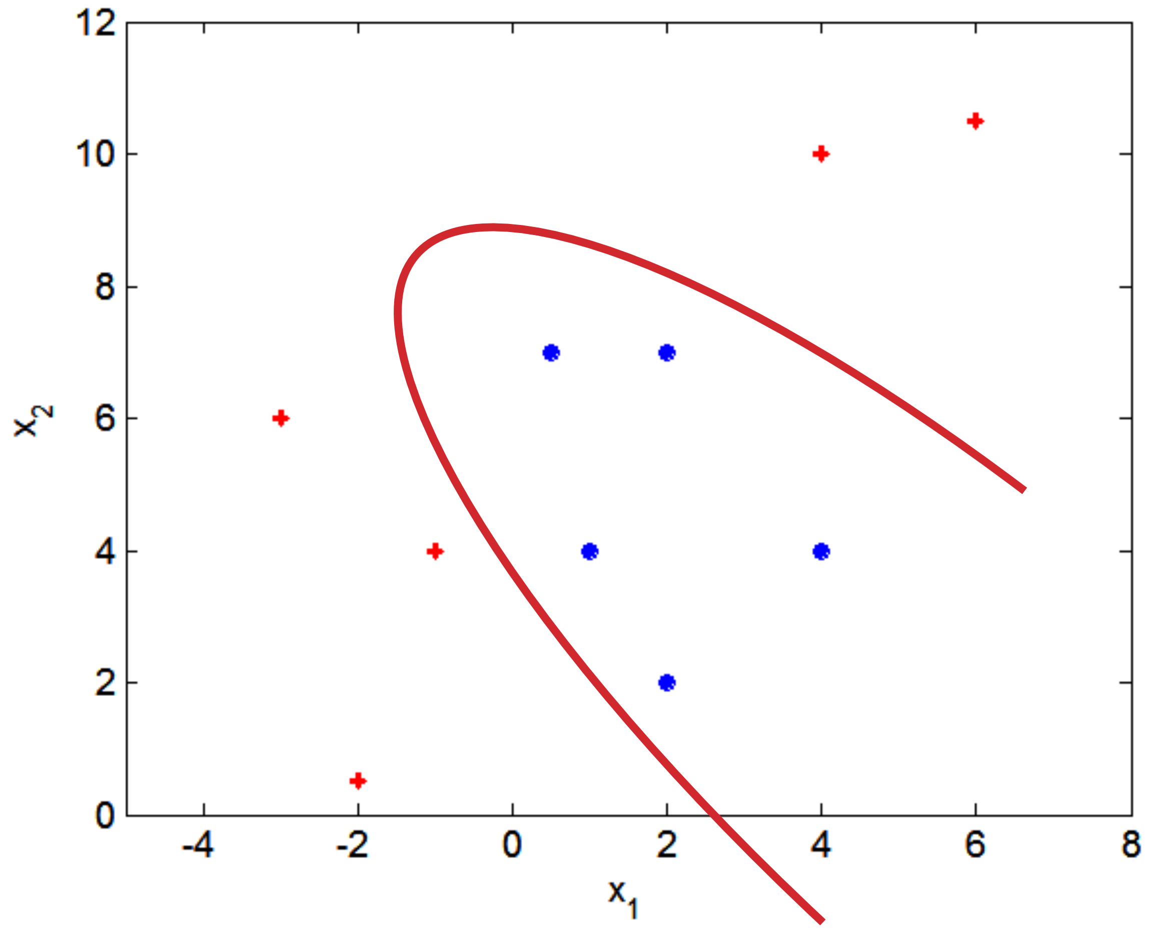
$$L(w) = \frac{\| \vec{w} \|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k\right)$$

- Subject to:

$$\vec{w} \cdot \vec{x_i} + b \geq 1 - \xi_i \text{ if } y_i = 1$$
$$\vec{w} \cdot \vec{x_i} + b \leq -1 + \xi_i \text{if } y_i = -1$$

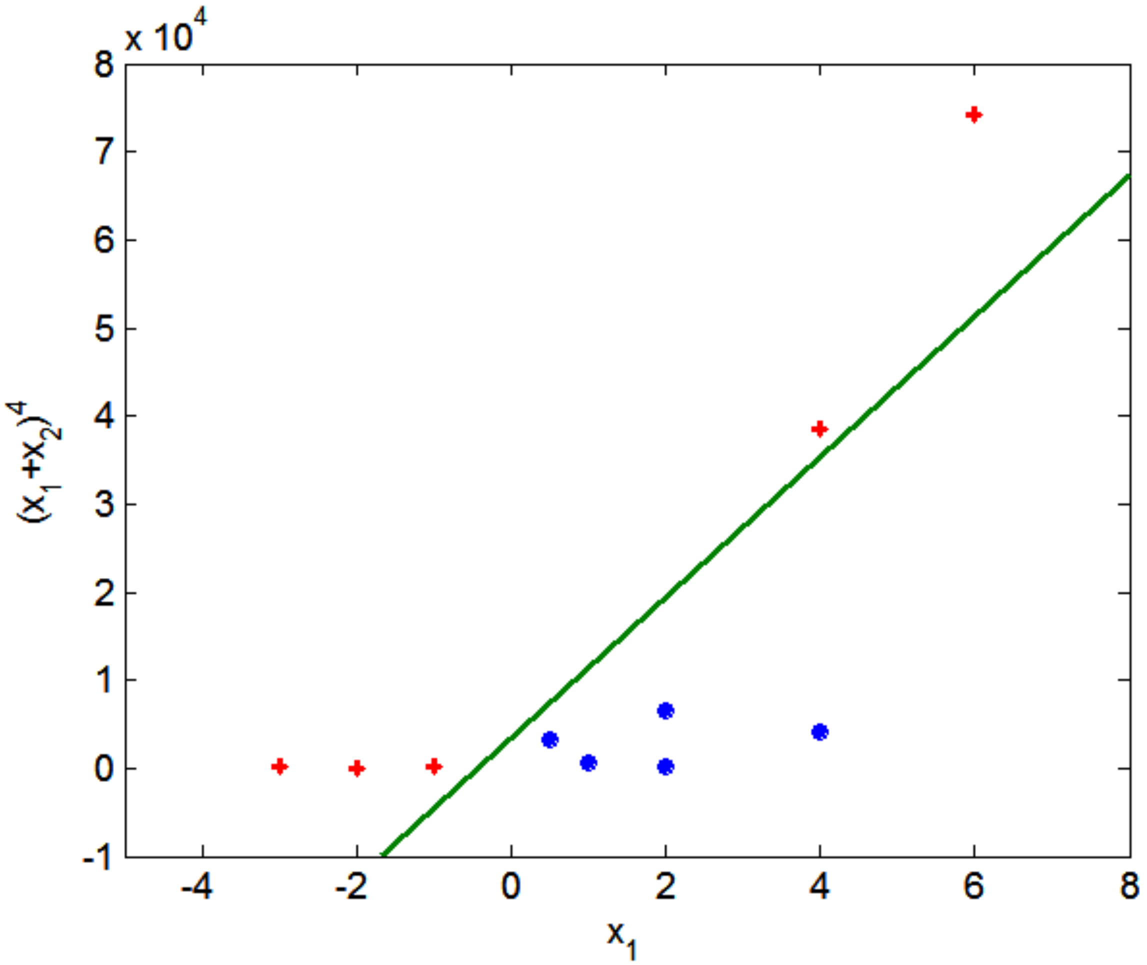
NONLINEAR SUPPORT VECTOR MACHINES

What if the decision boundary is not linear?



NONLINEAR SUPPORT VECTOR MACHINES

Transform data into higher dimensional space



SVMS IN SCIKIT-LEARN

```
from sklearn import svm

# Fit a default SVM classifier to fake data
X = [[0, 0], [1, 1]]
y = [0, 1]
clf = svm.SVC()
clf.fit(X, y)
```

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
decision_function_shape=None, degree=3, gamma='auto',
kernel='rbf', max_iter=-1, probability=False,
random_state=None, shrinking=True, tol=0.001,
verbose=False)
```

Lots of defaults used for hyperparameters – can use cross validation to search for good ones

MODEL SELECTION IN SCIKIT-LEARN

```
from sklearn.model_selection import train_test_split
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import classification_report

# ... Load some raw data into X and y ...
# Split the dataset in two equal parts
X_train, X_test, y_train, y_test = \
    train_test_split(X, y, test_size=0.5, random_state=0)
```

```
# Pick values of hyperparameters you want to consider
tuned_parameters = [{'kernel': ['rbf'],
                     'gamma': [1e-3, 1e-4],
                     'C': [1, 10, 100, 1000]},
                   {'kernel': ['linear'],
                     'C': [1, 10, 100, 1000]}
                   ]
```

MODEL SELECTION IN SCIKIT-LEARN

```
# Perform a complete grid search + cross validation
# for each of the hyperparameter vectors
clf = GridSearchCV(SVC(C=1),
                   tuned_parameters,
                   cv=5,
                   scoring=‘precision’)
clf.fit(X_train, y_train)
```

```
# Now that you’ve selected good hyperparameters via CV,
# and trained a model on your training data, get an
# estimate of the “true error” on your test set
y_true, y_pred = y_test, clf.predict(X_test)
print(classification_report(y_true, y_pred))
```