MACHINE LEARNING

Slides: James Hays, Brown
Isabelle Guyon,
Erik Sudderth,
Mark Johnson,
Derek Hoiem,
Lana Lazebnik

What is Learning?

- Herbert Simon: "Learning is any process by which a system improves performance from experience."
- What is the task?
  - Classification
  - Categorization/clustering
  - Problem solving / planning / control
  - Prediction
  - others

Types of training

- Supervised learning: uses a series of labelled examples with direct feedback
- Unsupervised/clustering learning: no feedback
- Semi-supervised: using both labelled and unlabelled data
- Reinforcement learning: indirect feedback, after many examples

UNSUPERVISED LEARNING

K-Means

- Assumes documents are real-valued vectors.
- Clusters based on *centroids* (aka the *center of gravity* or mean) of points in a cluster, *c*:

$$\vec{\mu}(\mathrm{c}) = \frac{1}{|c|} \sum_{\vec{x} \in c} \vec{x}$$

- Reassignment of instances to clusters is based on distance to the current cluster centroids.
  - (Or one can equivalently phrase it in terms of similarities)

K-Means Algorithm

Select K random docs $\{s_1, s_2, \ldots s_K\}$ as seeds.

Until clustering *converges* (or other stopping criterion):

For each doc d_i:

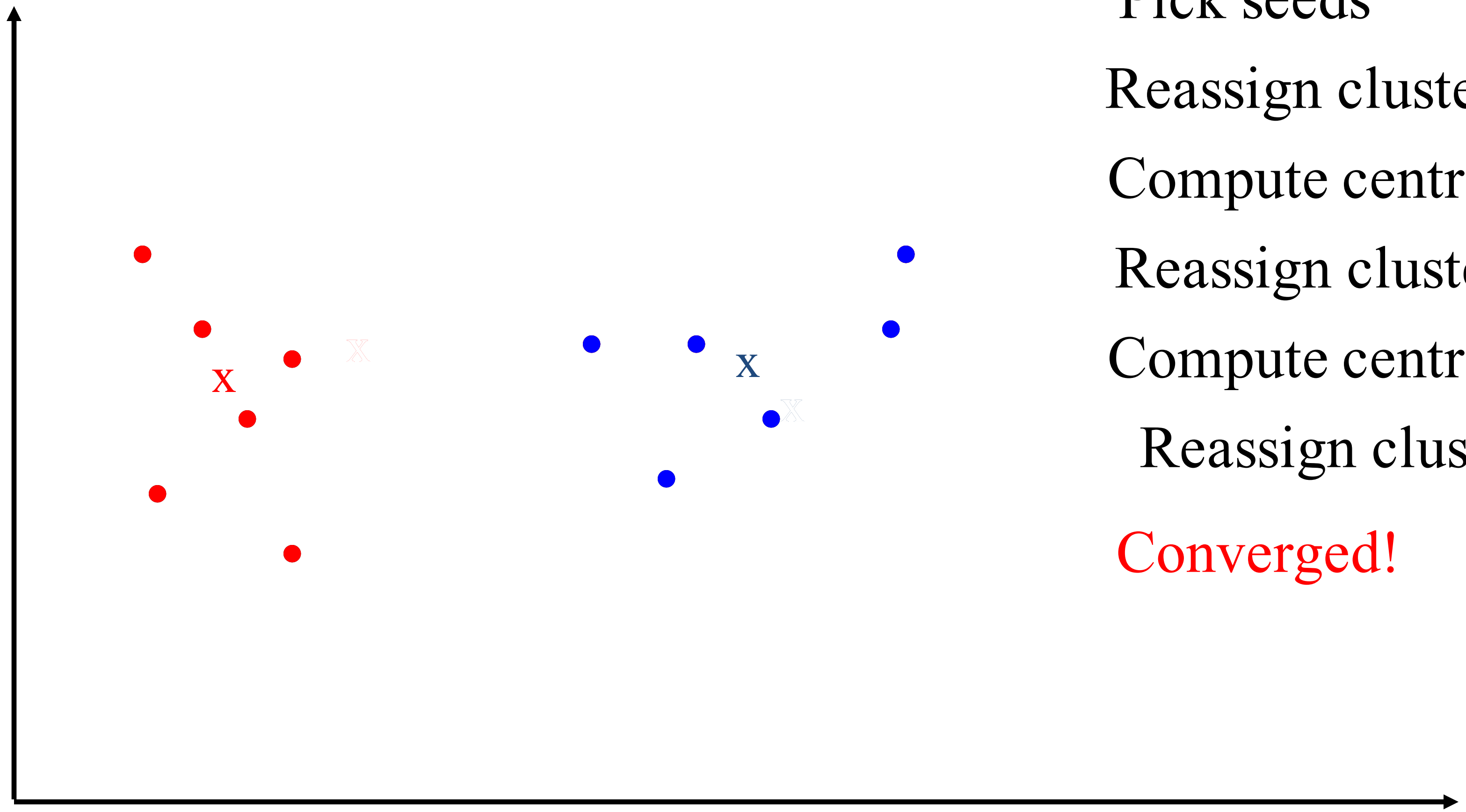
Assign d_i to the cluster c_j such that $dist(x_i, s_j)$ is minimal.

(*Next, update the seeds to the centroid of each cluster*)

For each cluster c_j

$s_j = \mu(c_j)$

K Means Example (*K*=2)



Pick seeds

Reassign clusters

Compute centroids

Reassign clusters

Compute centroids

Reassign clusters

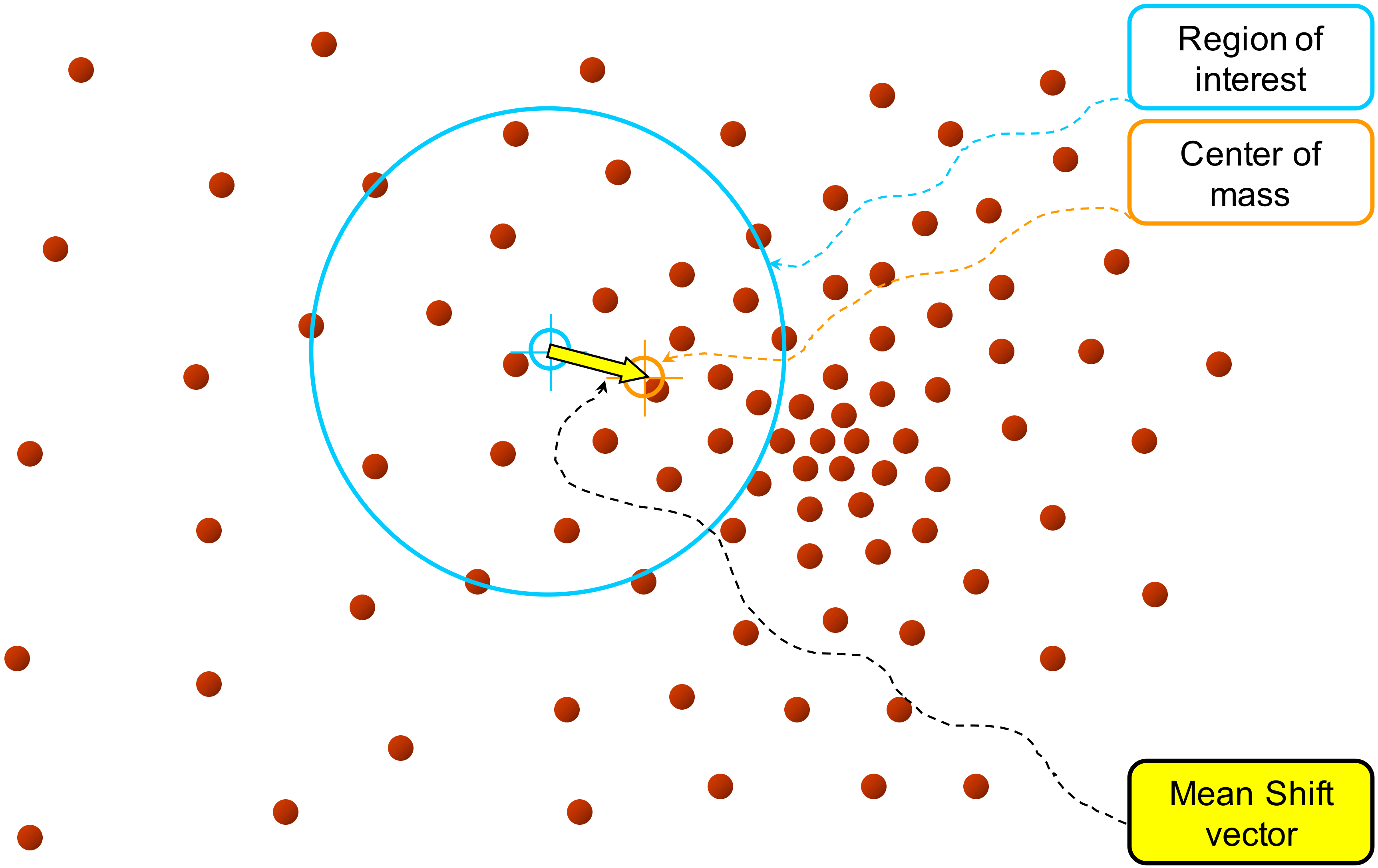
Converged!

Termination conditions

- Several possibilities, e.g.,
  - A fixed number of iterations.
  - Doc partition unchanged.
  - Centroid positions don’t change.

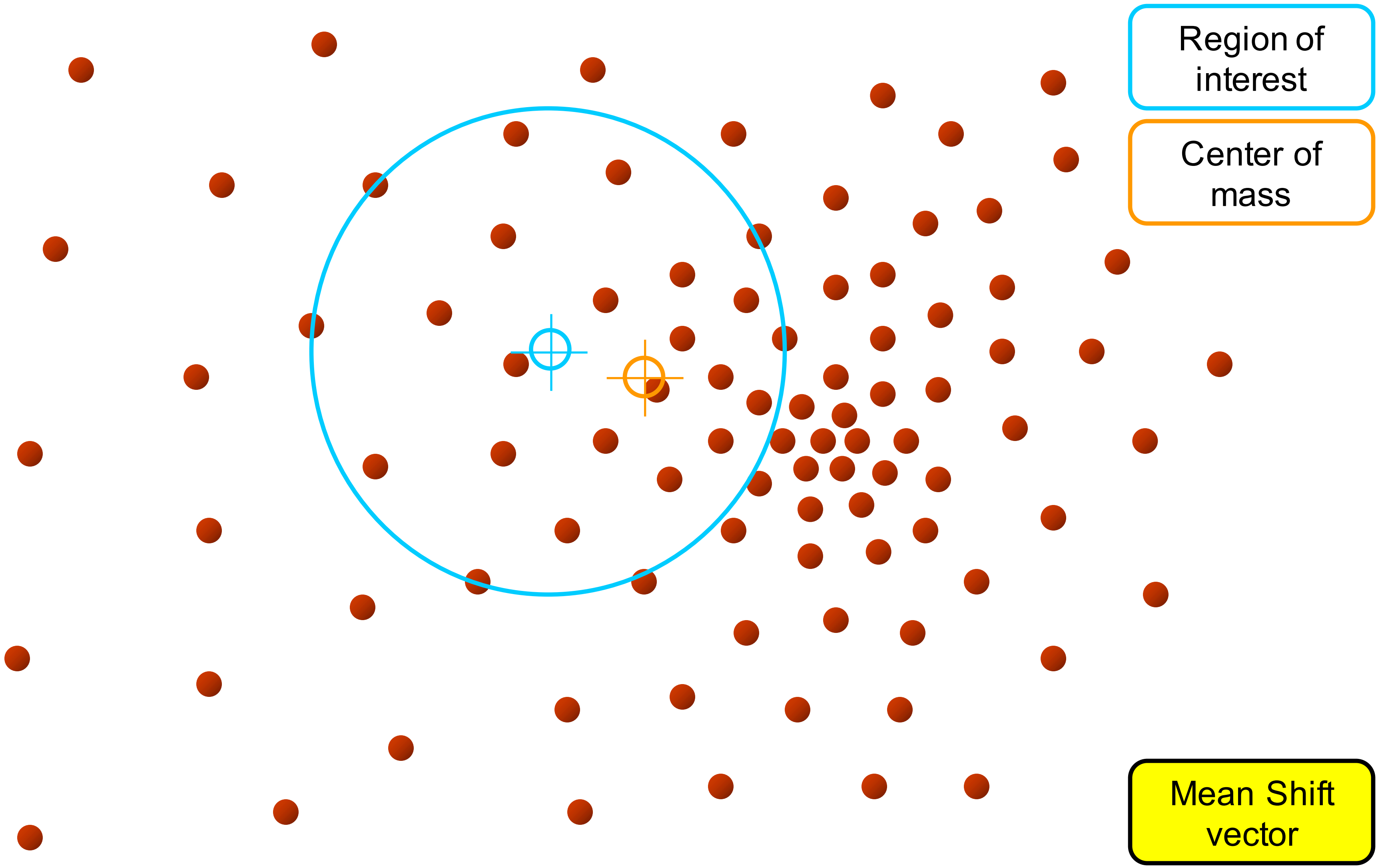
Does this mean that the docs in a cluster are unchanged?

Mean shift



Slide by Y. Ukrainitz & B. Sarel

Mean shift



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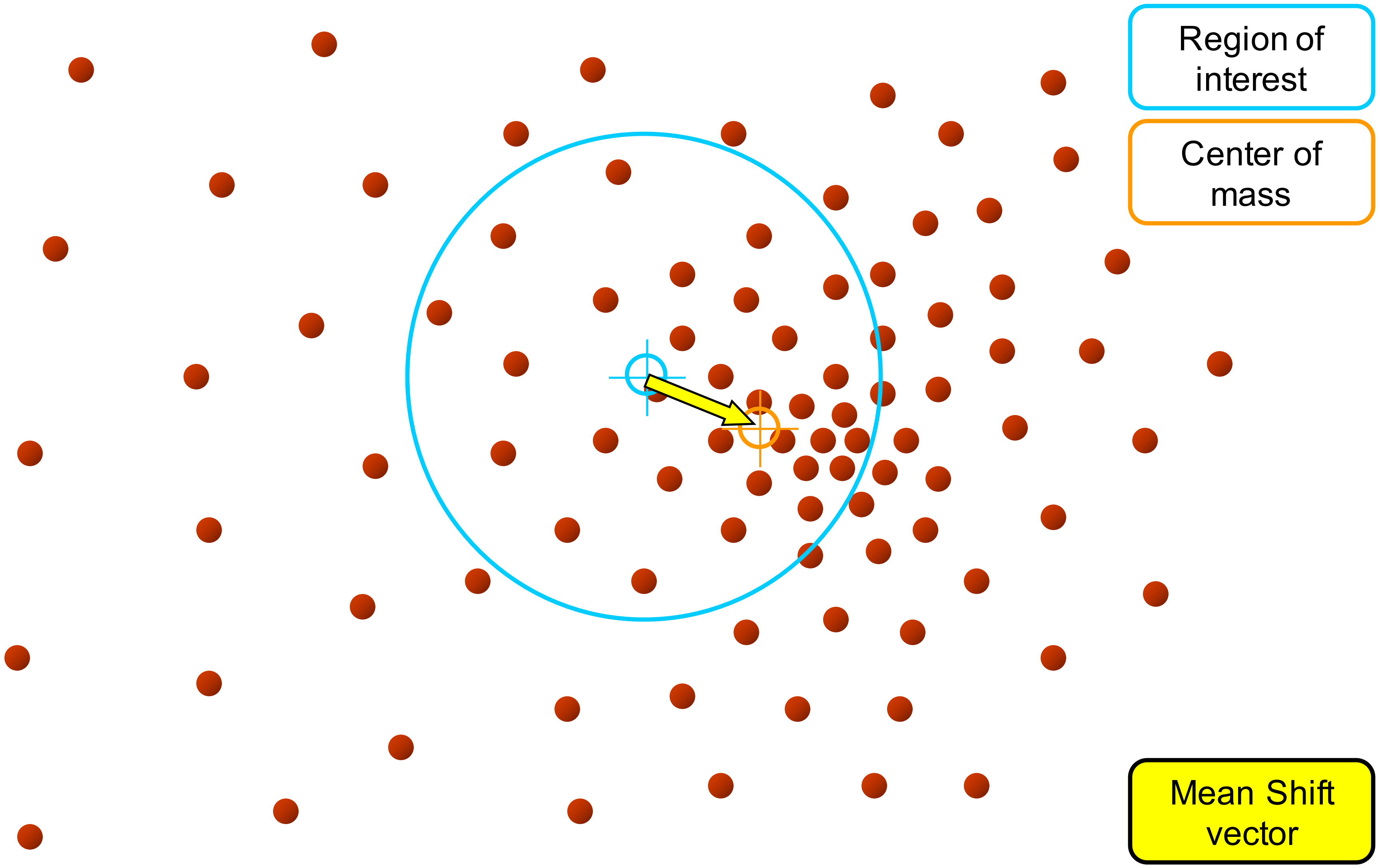
Mean shift



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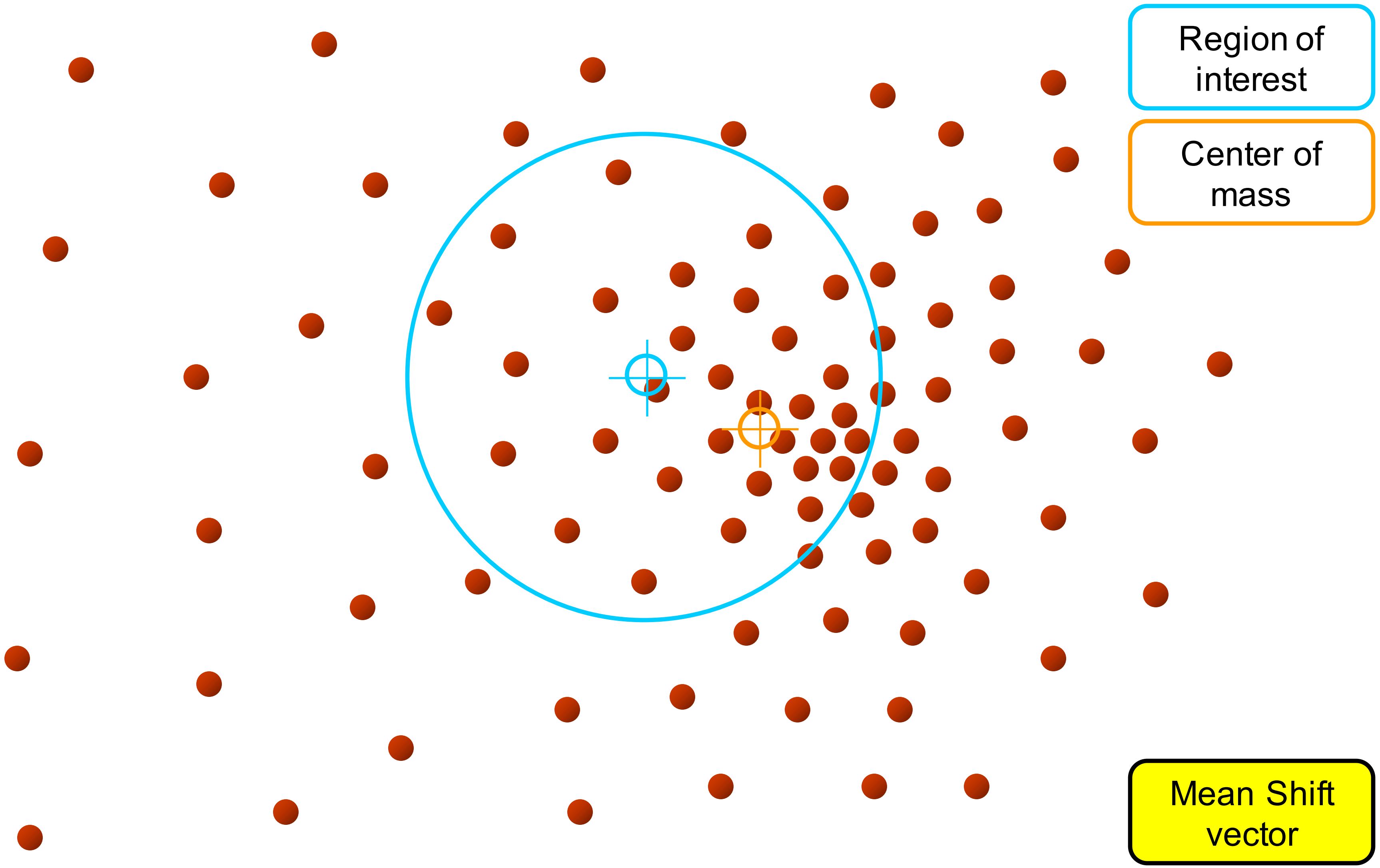
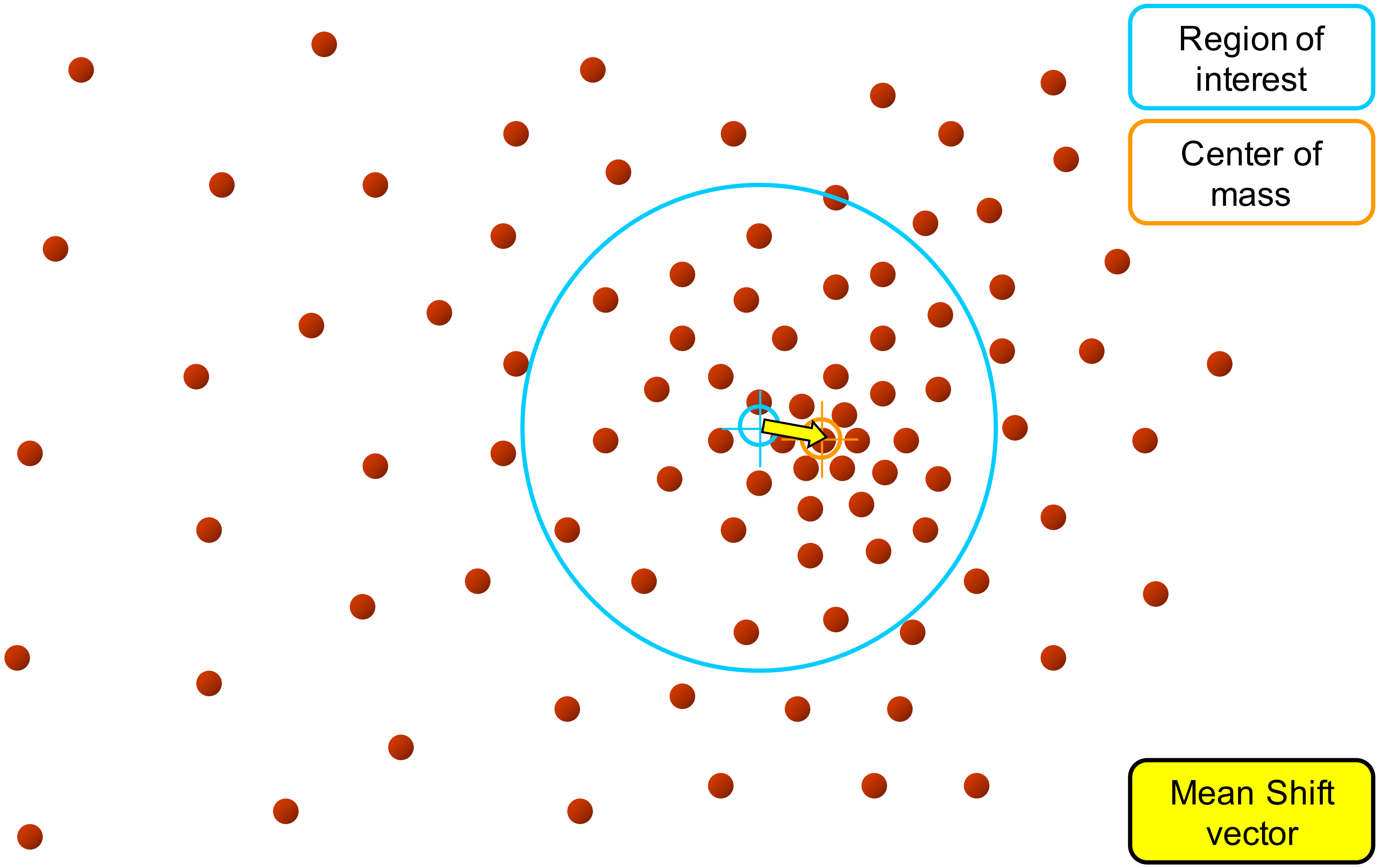
Mean shift



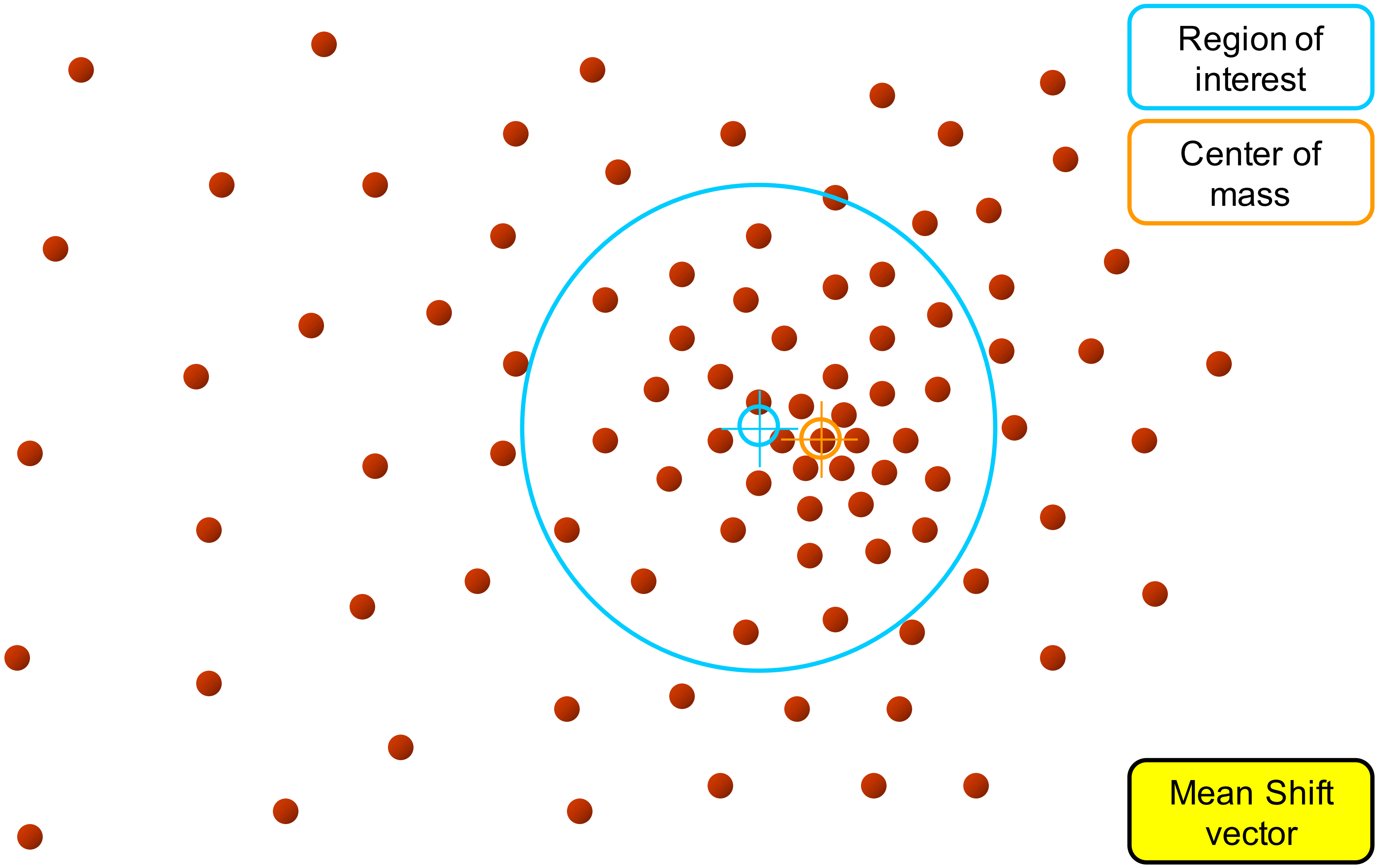
Slide by Y. Ukrainitz & B. Sarel

Mean shift



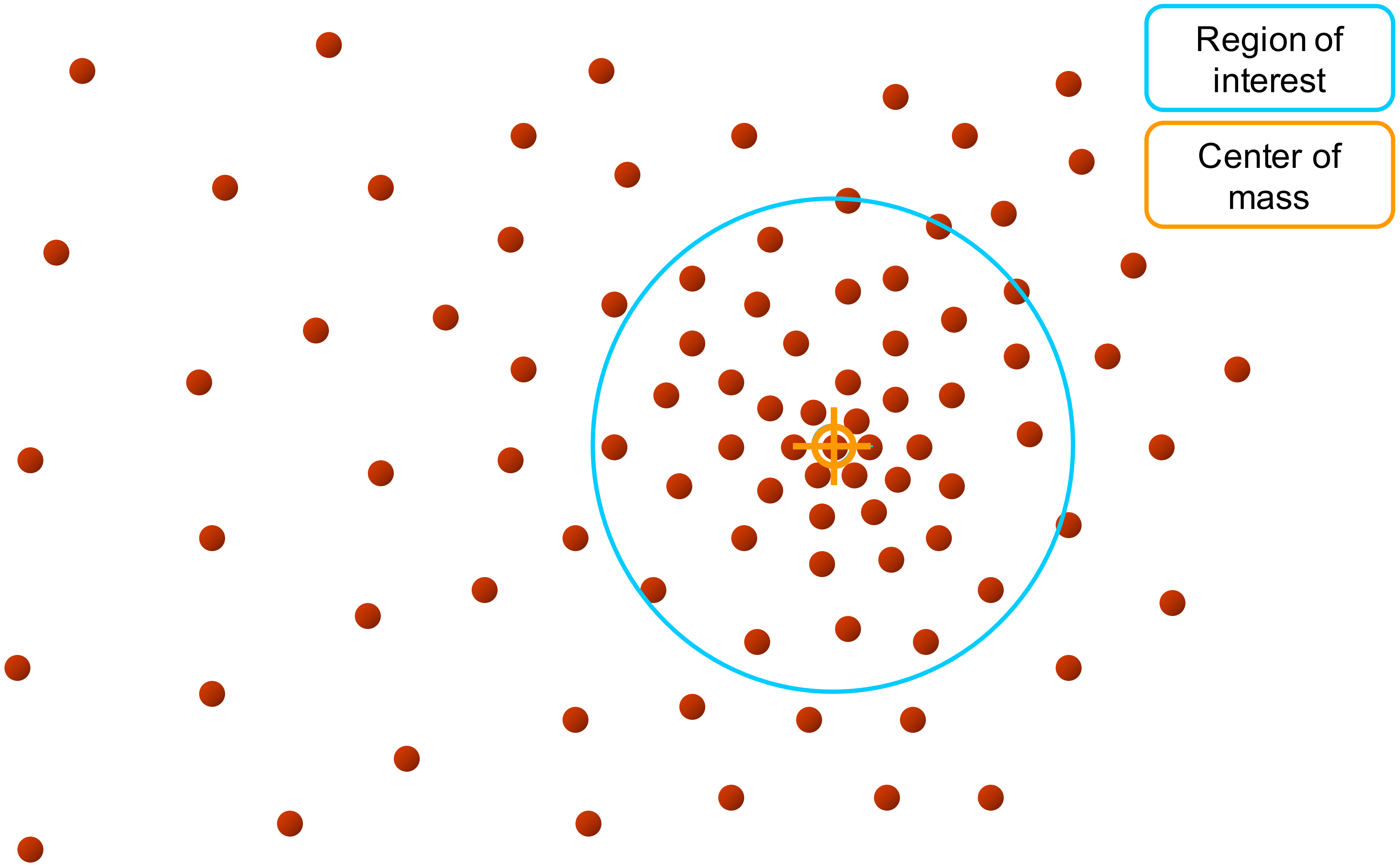
Slide by Y. Ukrainitz & B. Sarel

Mean shift



Slide by Y. Ukrainitz & B. Sarel

Mean shift



Slide by Y. Ukrainitz & B. Sarel

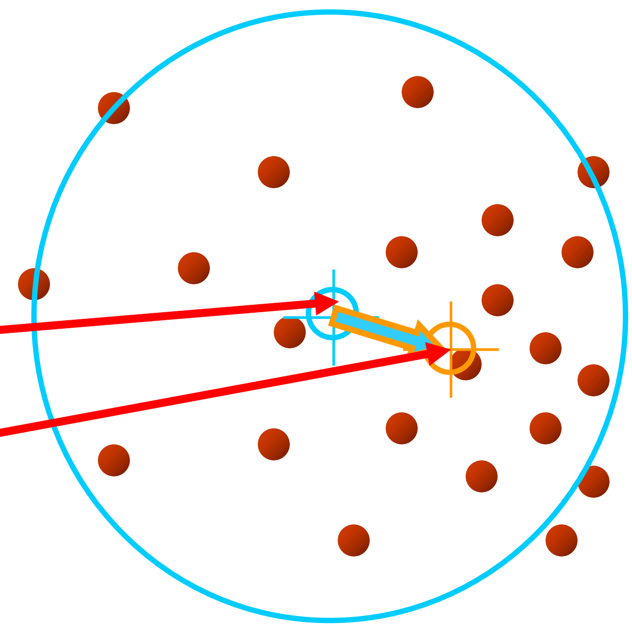
Computing the Mean Shift

<u>Simple Mean Shift procedure</u>:

• Compute mean shift vector

•Translate the Kernel window by **m(x)**

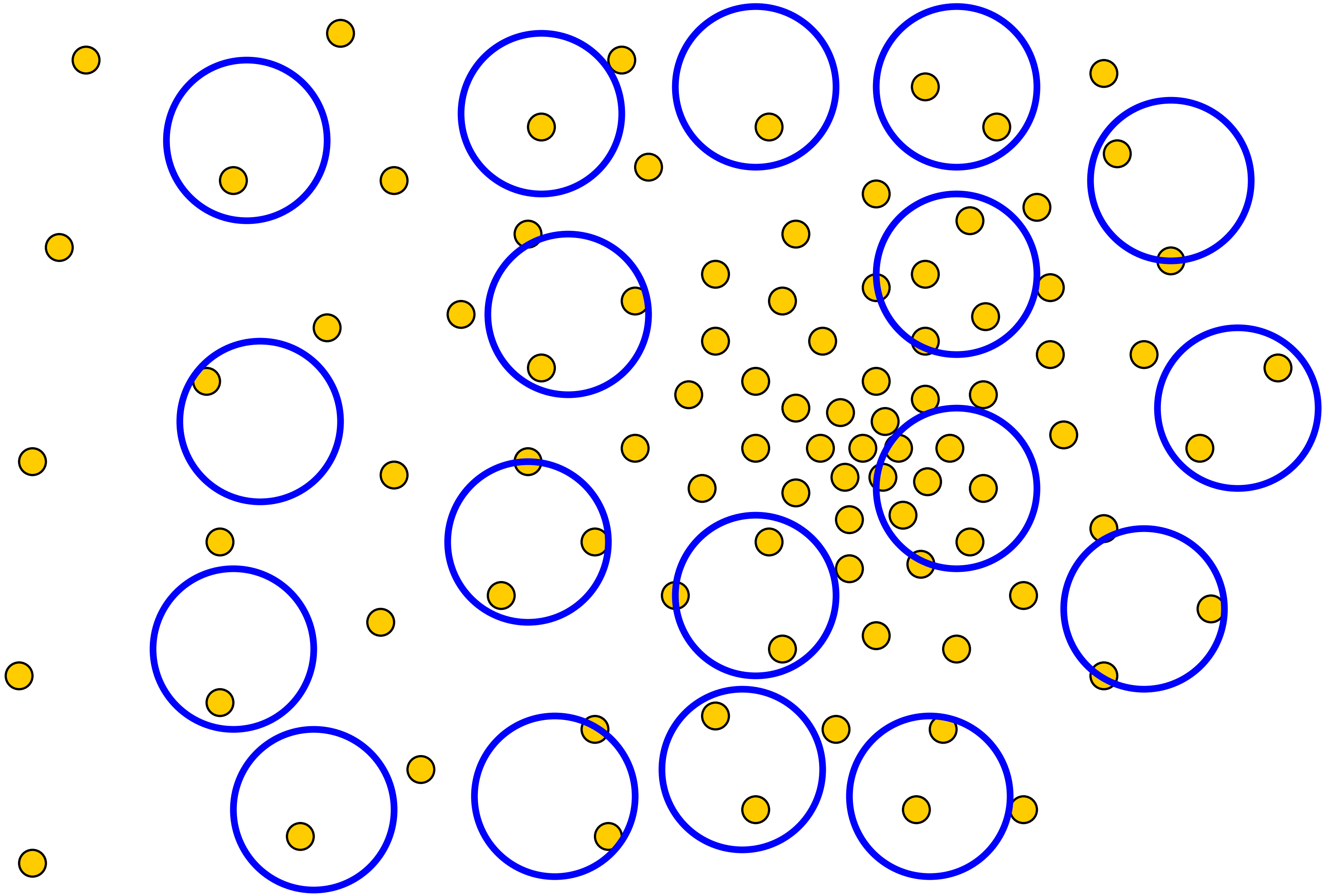
$$\mathbf{m}(\mathbf{x}) = \left[\boxed{\frac{\sum_{i=1}^{n} \mathbf{x}_i g\left(\frac{\left\| \mathbf{x} - \mathbf{x}_i \right\|^2}{h} \right)}{\sum_{i=1}^{n} g\left(\frac{\left\| \mathbf{x} - \mathbf{x}_i \right\|^2}{h} \right)}} - \boxed{\mathbf{x}} \right]$$



$g(\mathbf{x}) = -k'(\mathbf{x})$

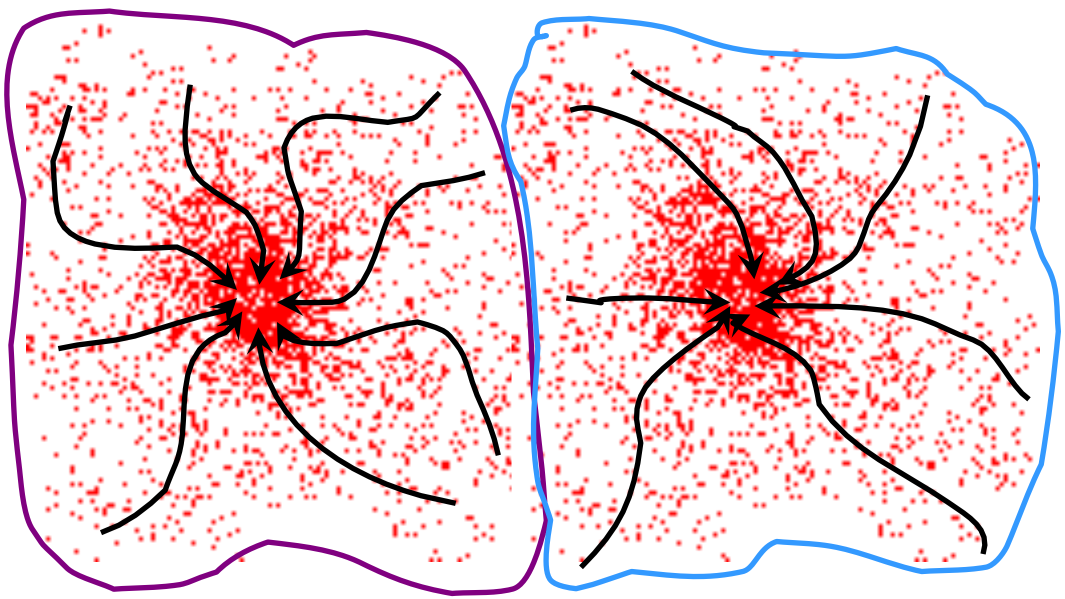
Slide by Y. Ukrainitz & B. Sarel

Real Modality Analysis



Attraction basin

- Attraction basin: the region for which all trajectories lead to the same mode
- Cluster: all data points in the attraction basin of a mode



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Mean shift clustering

- The mean shift algorithm seeks *modes* of the given set of points
  1. Choose kernel and bandwidth
  2. For each point:
     a) Center a window on that point
     b) Compute the mean of the data in the search window
     c) Center the search window at the new mean location
     d) Repeat (b,c) until convergence
  3. Assign points that lead to nearby modes to the same cluster

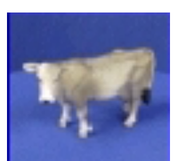
SUPERVISED LEARNING

The machine learning framework

- Apply a prediction function to a feature representation of the image to get the desired output:

f() = “apple”

f() = “tomato”

f() = “cow”

Slide credit: L. Lazebnik

The machine learning framework

$$\mathbf{y} = f(\mathbf{x})$$

output

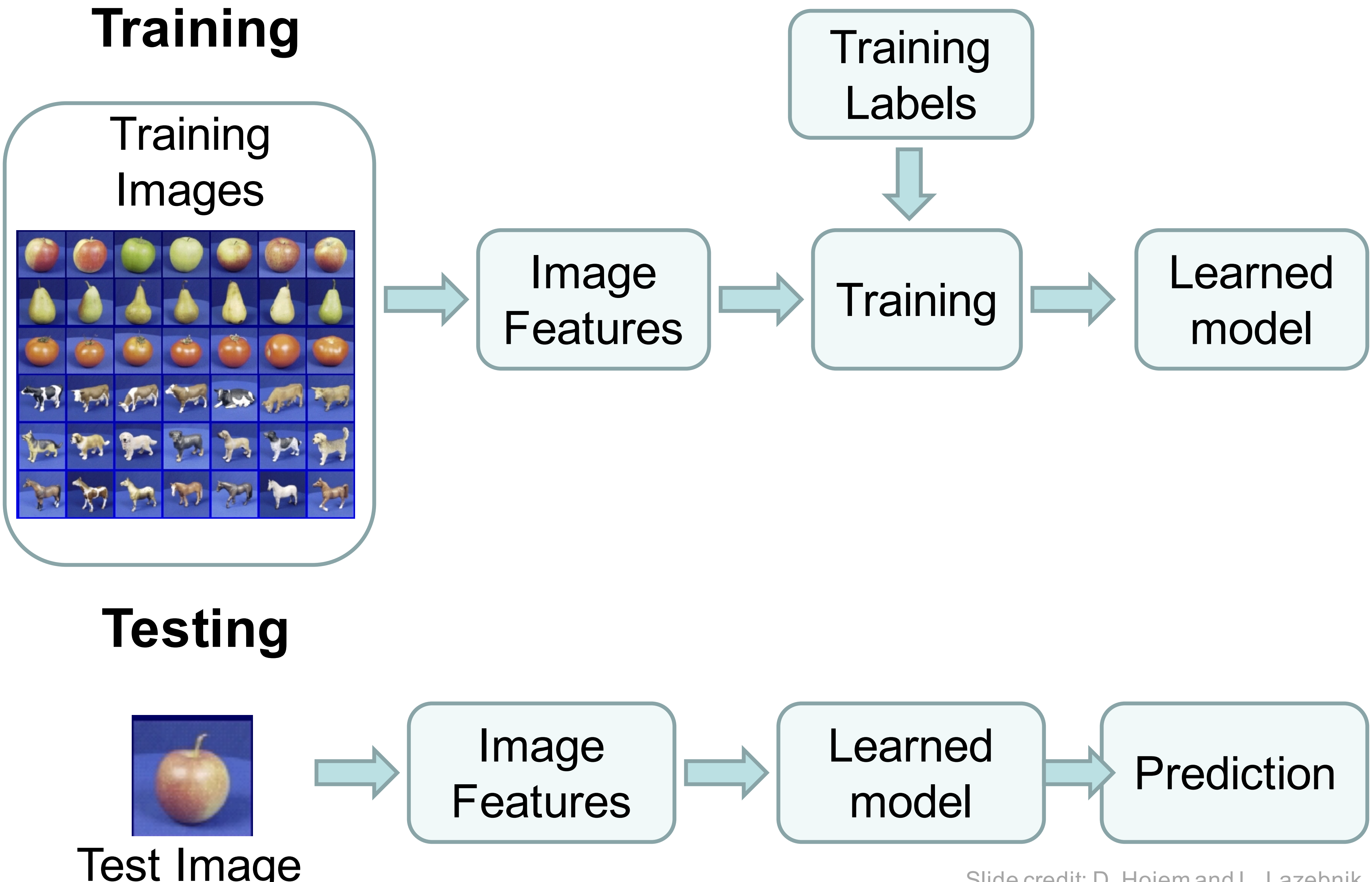
prediction function

Image feature

- **Training:** given a *training set* of labeled examples $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$, estimate the prediction function f by minimizing the prediction error on the training set
- **Testing:** apply f to a never before seen *test example* $\mathbf{x}$ and output the predicted value $y = f(\mathbf{x})$

Slide credit: L. Lazebnik

Steps

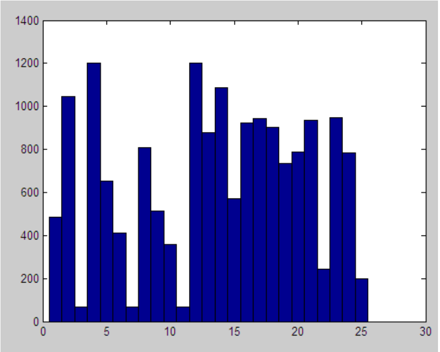


Slide credit: D. Hoiem and L. Lazebnik

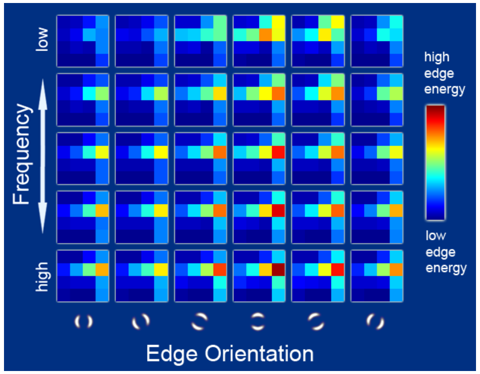
Features

- Raw pixels

- Histograms



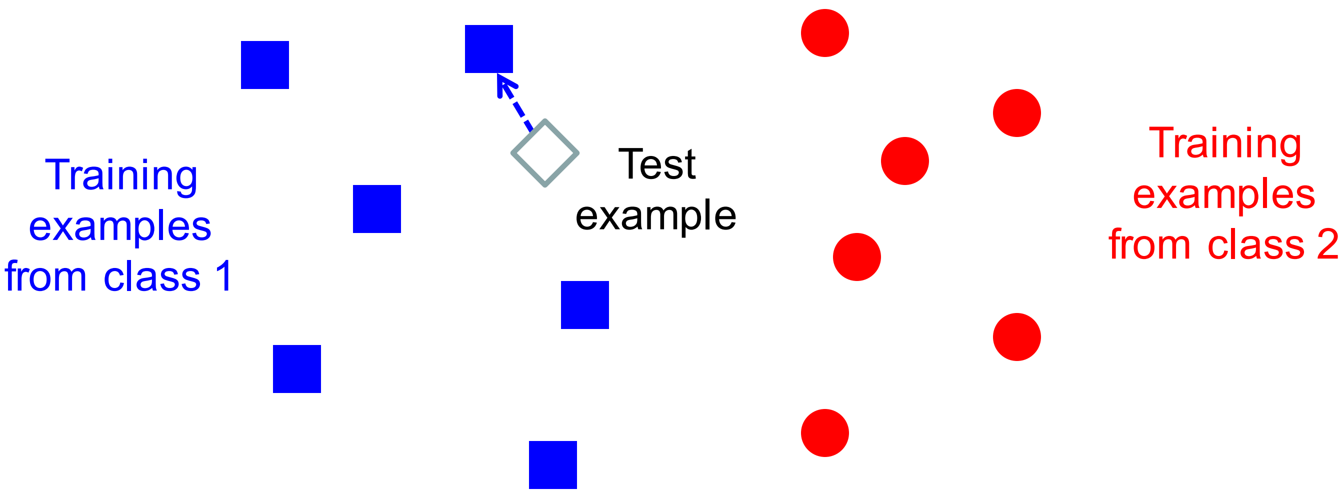
- GIST descriptors



- ...

Slide credit: L. Lazebnik

Classifiers: Nearest neighbor

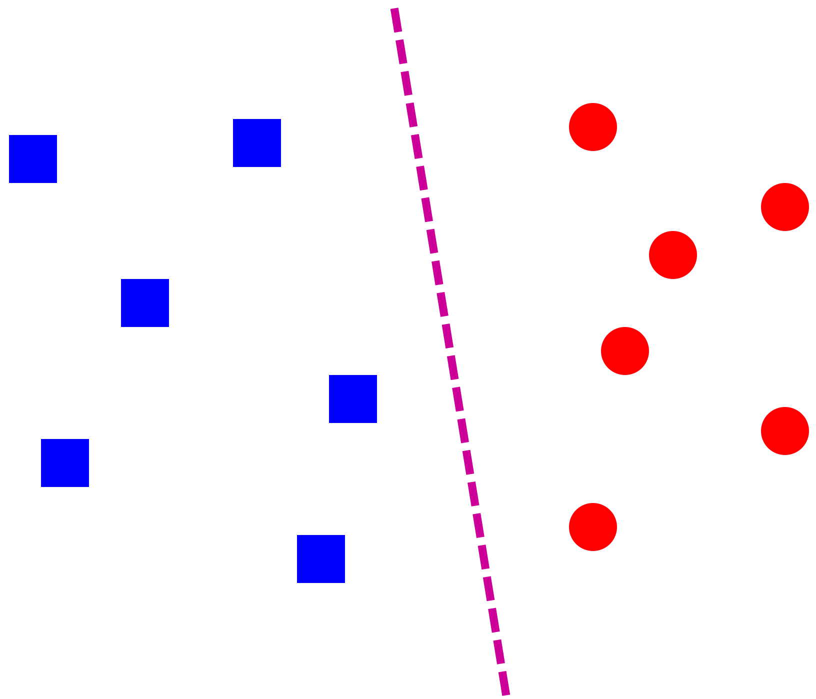


f(**x**) = label of the training example nearest to **x**

- All we need is a distance function for our inputs
- No training required!

Slide credit: L. Lazebnik

Classifiers: Linear



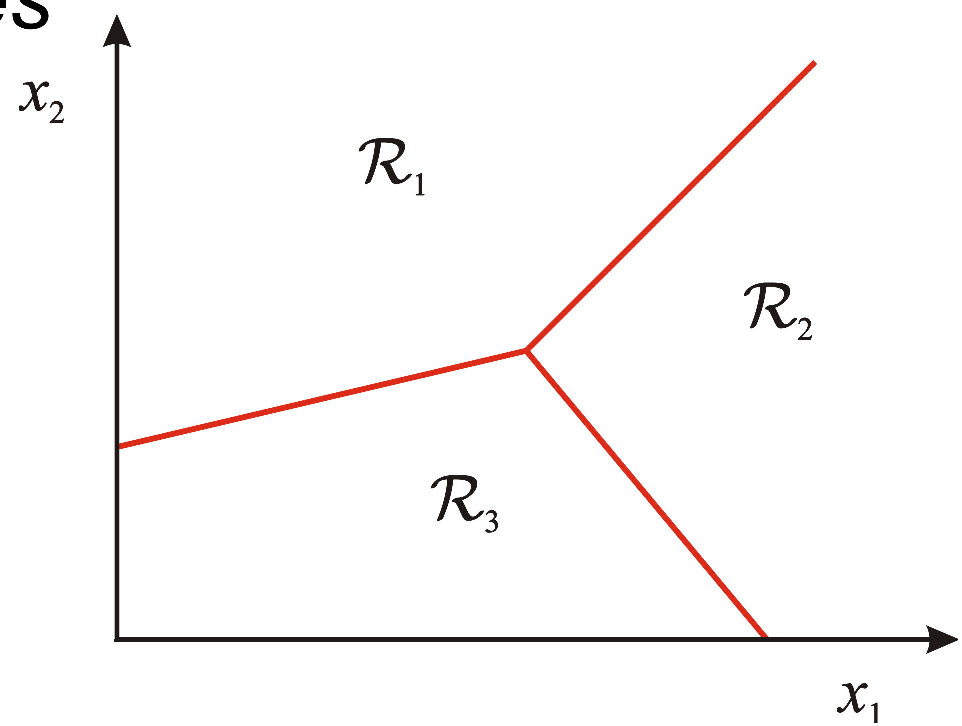
- Find a *linear function* to separate the classes:

$$f(\mathbf{x}) = \text{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$$

Slide credit: L. Lazebnik

Classification

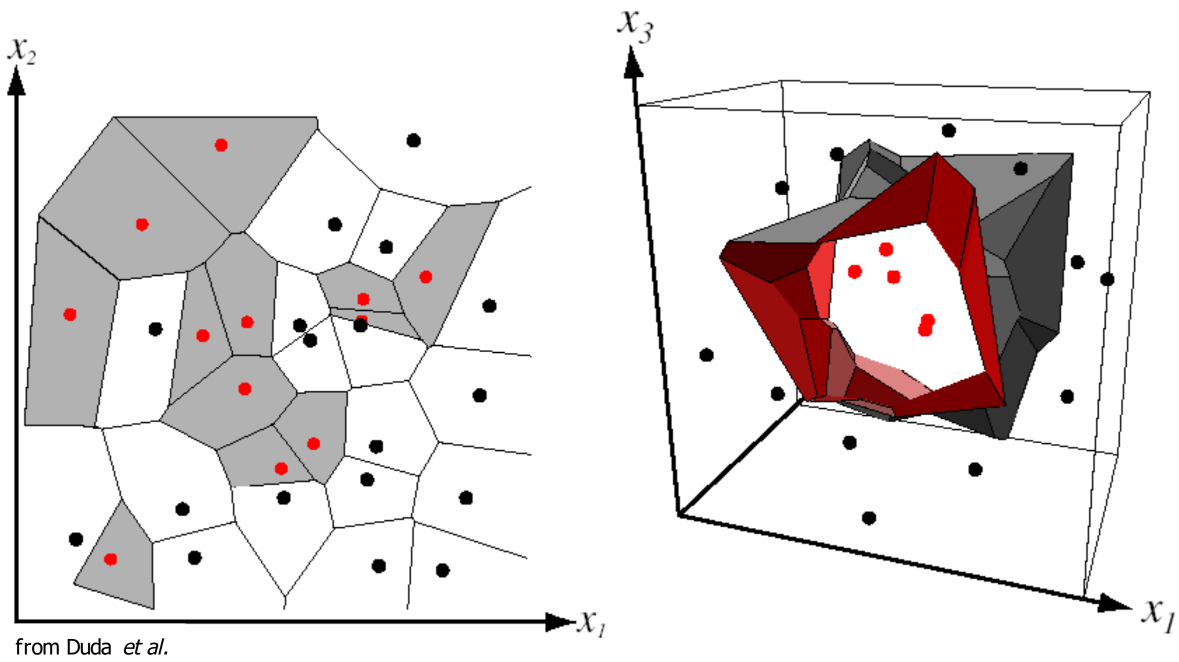
- Assign input vector to one of two or more classes
- Any decision rule divides input space into *decision regions* separated by *decision boundaries*



Slide credit: L. Lazebnik

Nearest Neighbor Classifier

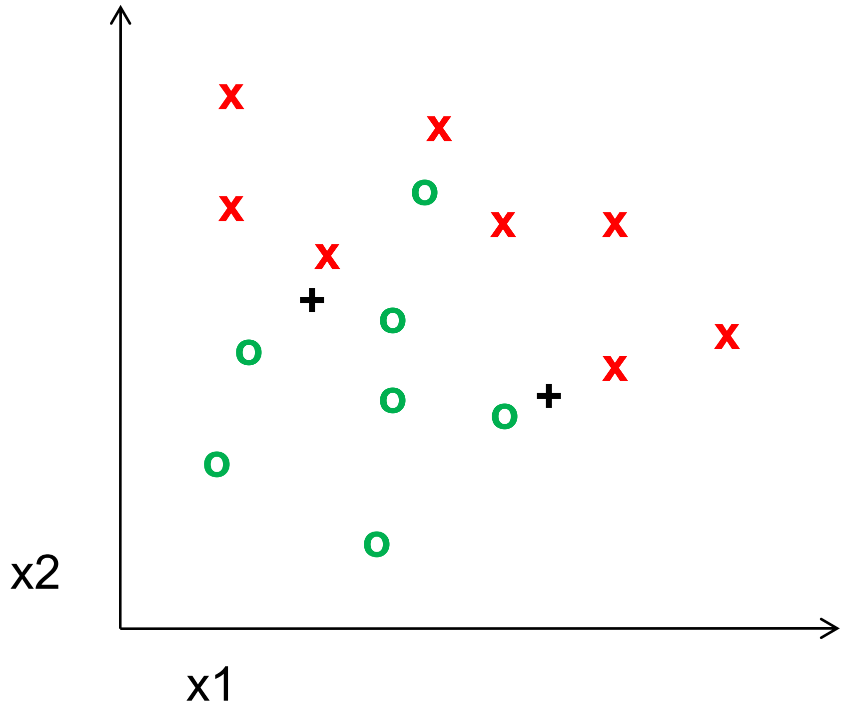
- Assign label of nearest training data point to each test data point



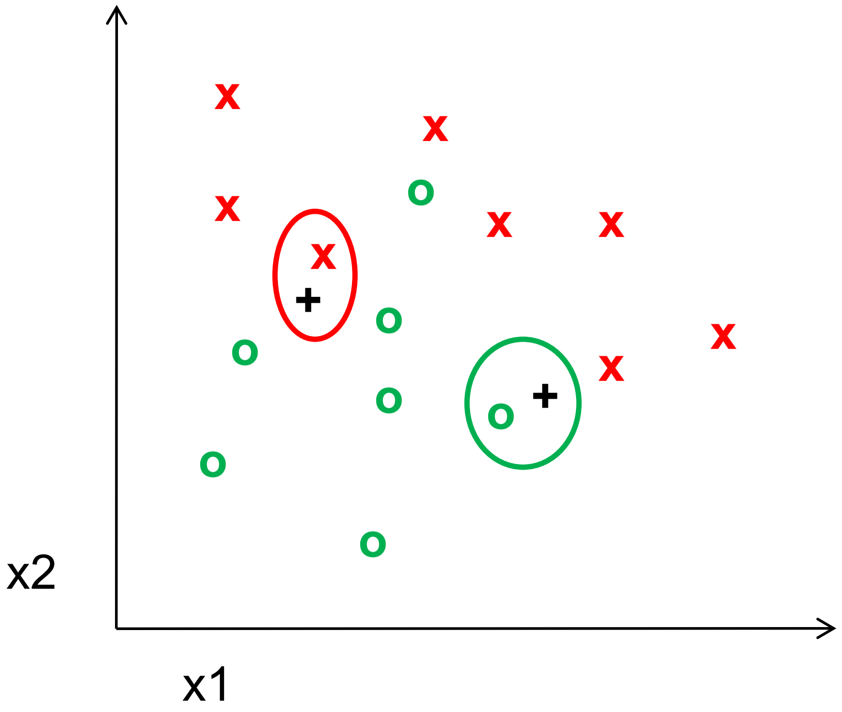
Voronoi partitioning of feature space
for two-category 2D and 3D data

Source: D. Lowe

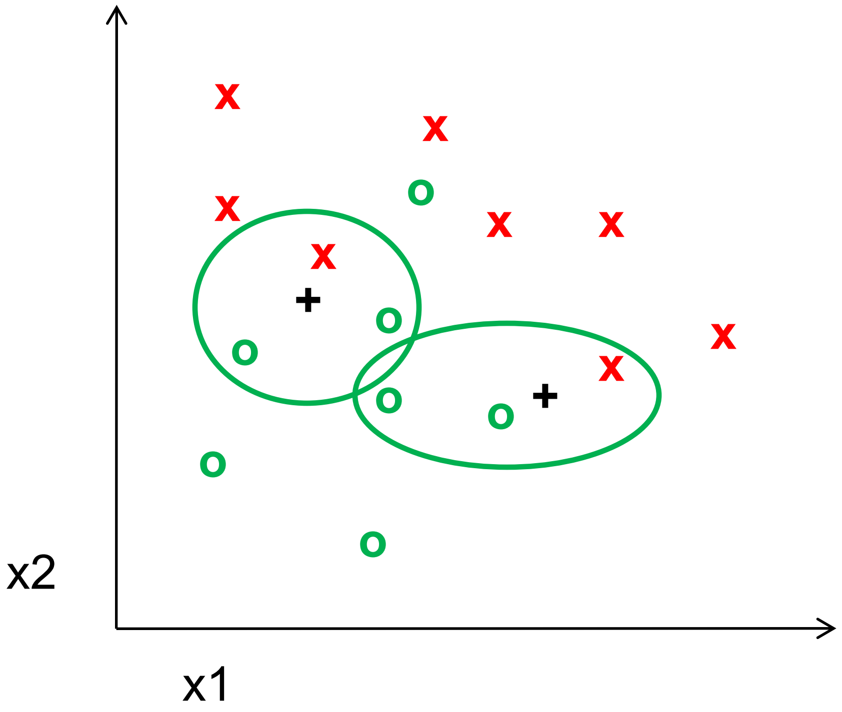
K-nearest neighbor



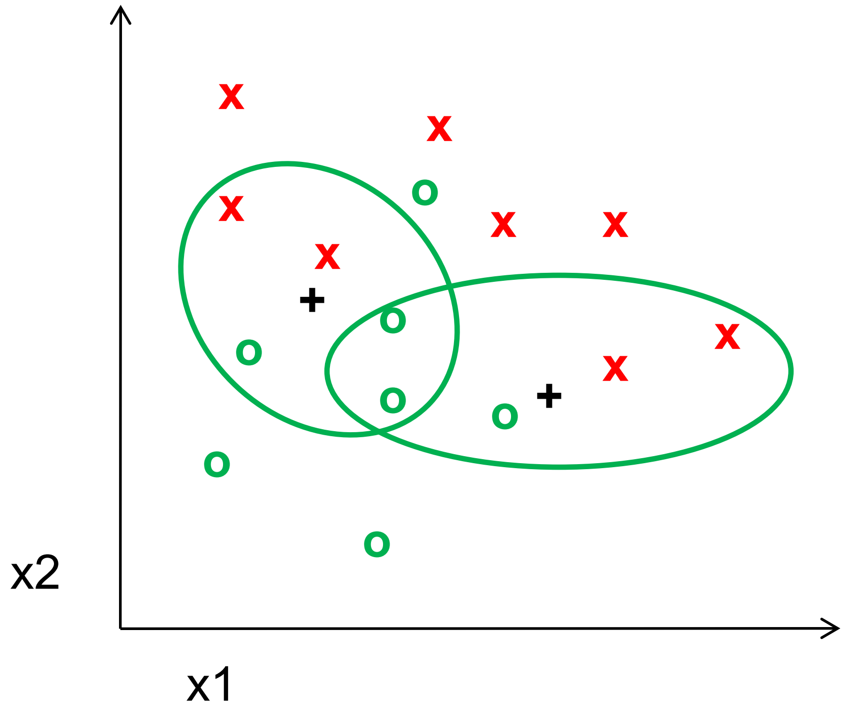
1-nearest neighbor



3-nearest neighbor



5-nearest neighbor



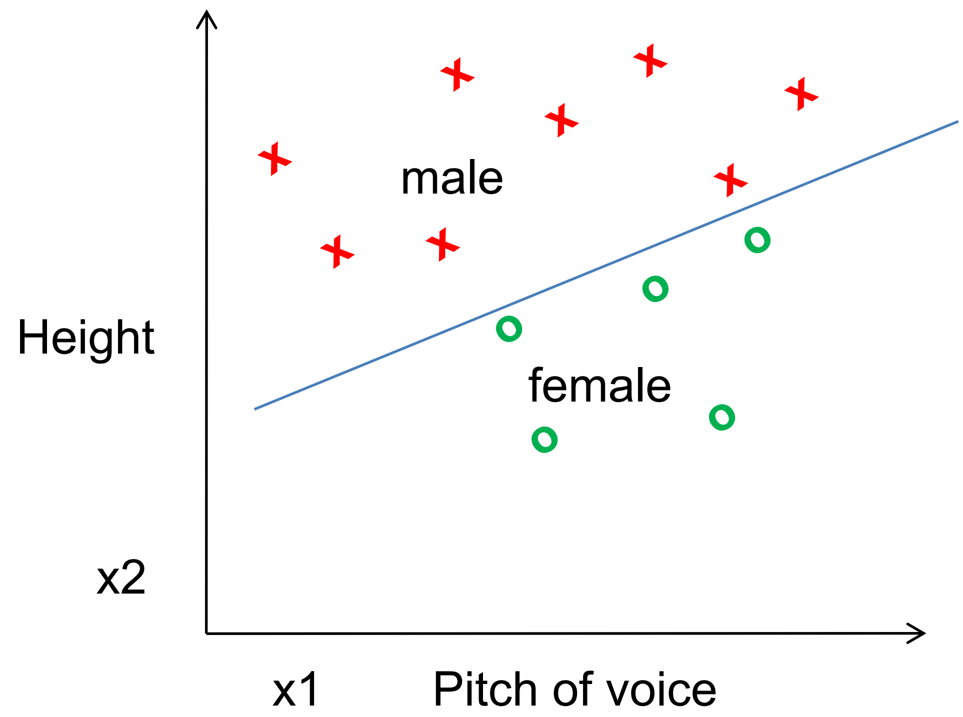
Using K-NN

- Simple, a good one to try first

- With infinite examples, 1-NN provably has error that is at most twice Bayes optimal error

Classifiers: Logistic Regression

Maximize likelihood of label given data, assuming a log-linear model



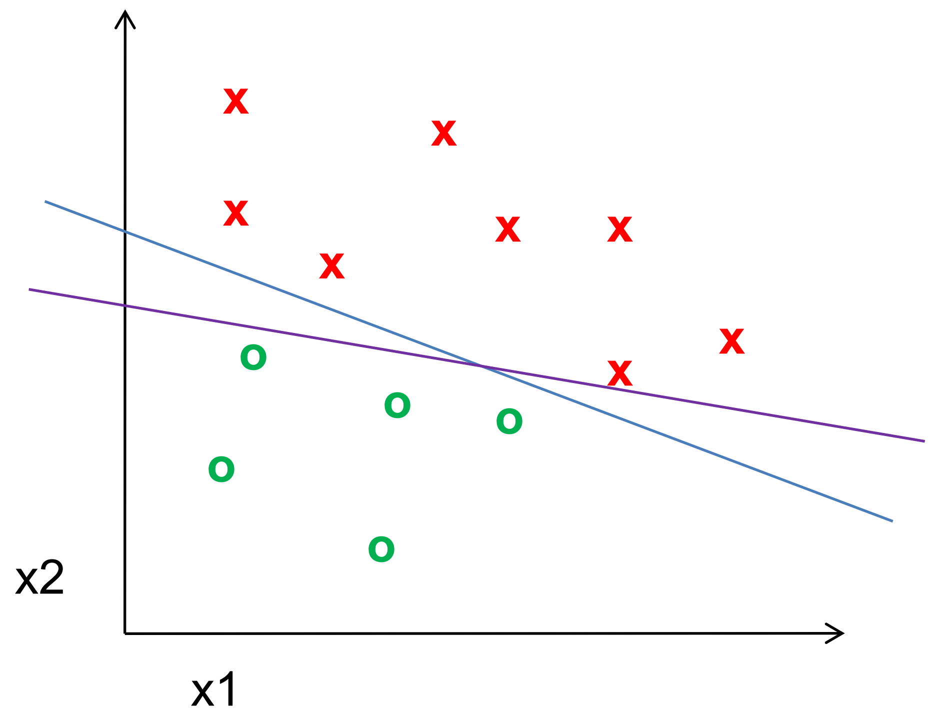
$$\log \frac{P(x_1, x_2 \mid y = 1)}{P(x_1, x_2 \mid y = -1)} = \mathbf{w}^T \mathbf{x}$$

$$P(y = 1 \mid x_1, x_2) = 1 / \left(1 + \exp\left(-\mathbf{w}^T \mathbf{x}\right)\right)$$

Using Logistic Regression

- Quick, simple classifier (try it first)
- Outputs a probabilistic label confidence
- Use L2 or L1 regularization
  - L1 does feature selection and is robust to irrelevant features but slower to train

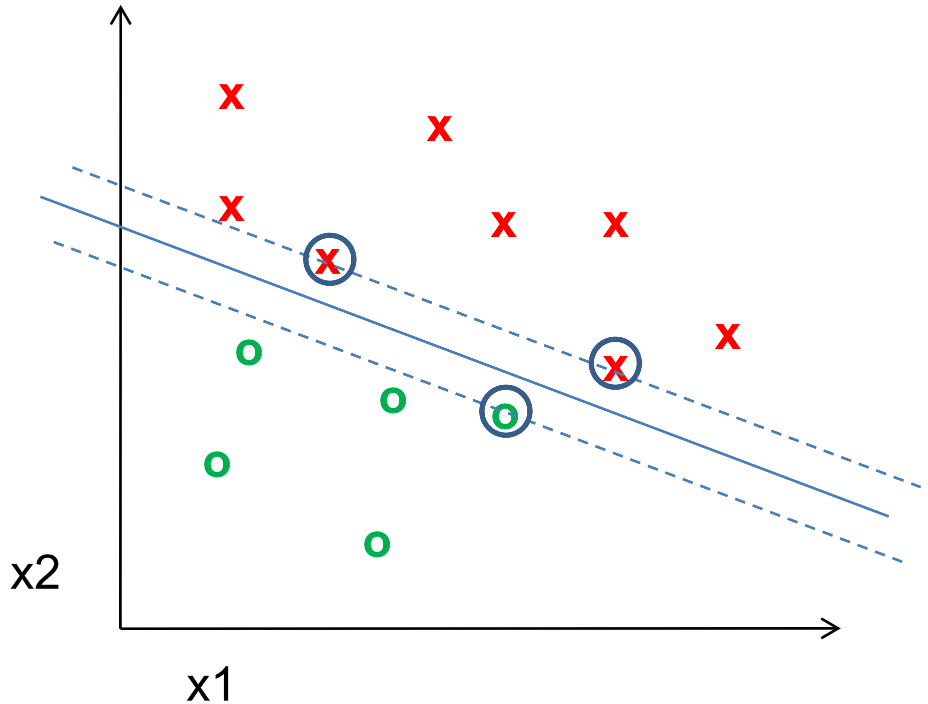
Classifiers: Linear SVM



- Find a *linear function* to separate the classes:

$$f(\mathbf{x}) = \text{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$$

Classifiers: Linear SVM



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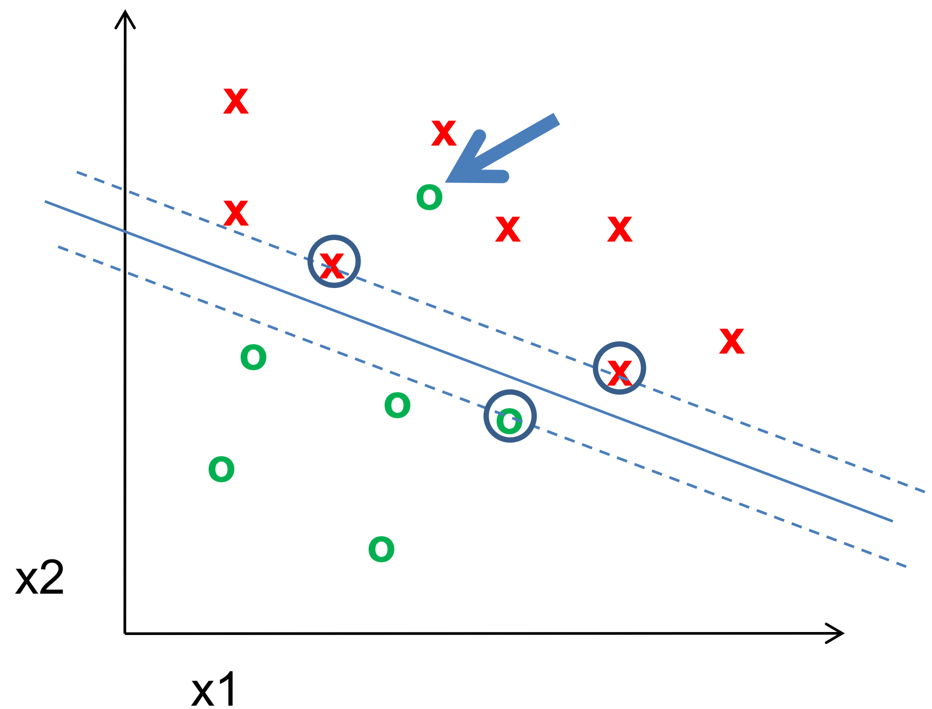
Classifiers: Linear SVM

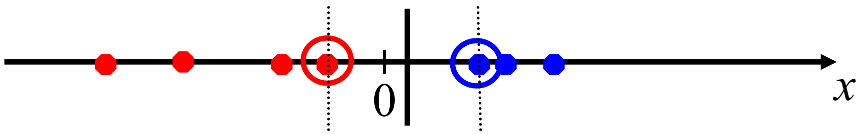


- Find a *linear function* to separate the classes:

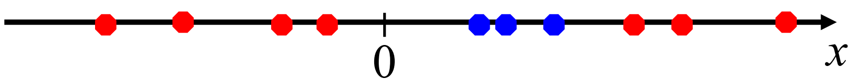
$$f(\mathbf{x}) = \mathrm{sgn}(\mathbf{w} \cdot \mathbf{x} + b)$$

Nonlinear SVMs

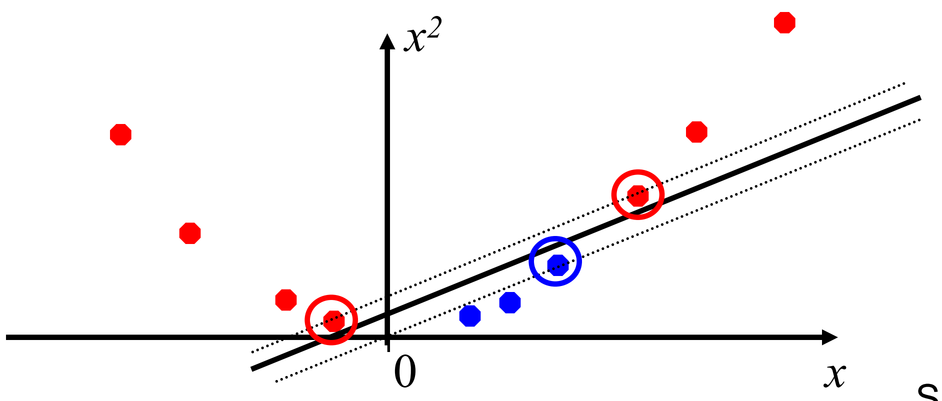
- Datasets that are linearly separable work out great:



- But what if the dataset is just too hard?



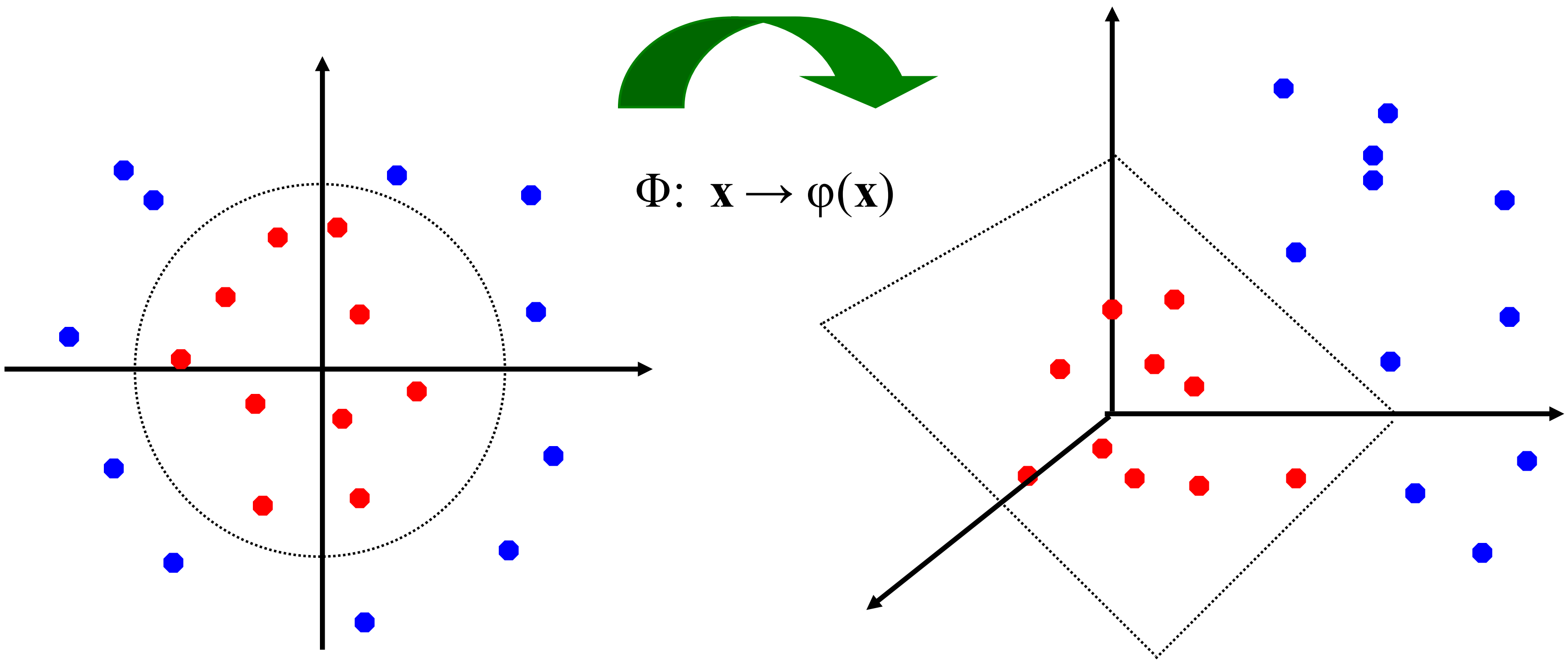
- We can map it to a higher-dimensional space:



Slide credit: Andrew Moore

Nonlinear SVMs

- General idea: the original input space can always be mapped to some higher-dimensional feature space where the training set is separable:



Slide credit: Andrew Moore

Nonlinear SVMs

- *The kernel trick*: instead of explicitly computing the lifting transformation $\varphi(\mathbf{x})$, define a kernel function K such that

$$K(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$$

  (to be valid, the kernel function must satisfy *Mercer's condition*)

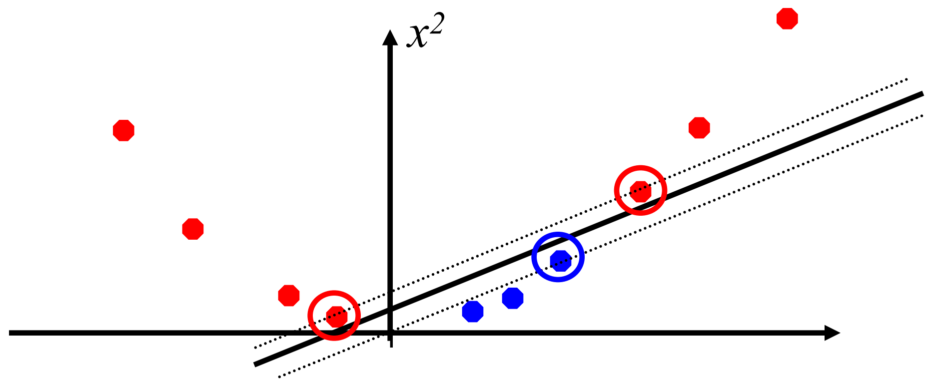
- This gives a nonlinear decision boundary in the original feature space:

$$\sum_i \alpha_i y_i \varphi(\boldsymbol{x}_i) \cdot \varphi(\boldsymbol{x}) + b = \sum_i \alpha_i y_i K(\boldsymbol{x}_i, \boldsymbol{x}) + b$$

C. Burges, A Tutorial on Support Vector Machines for Pattern Recognition, Data Mining and Knowledge Discovery, 1998

Nonlinear kernel: Example

- Consider the mapping $\varphi(x) = (x, x^2)$



$$\varphi(x) \cdot \varphi(y) = (x, x^2) \cdot (y, y^2) = xy + x^2 y^2$$

$$K(x, y) = xy + x^2 y^2$$

Kernels for bags of features

- Histogram intersection kernel:

$$I(h_1, h_2) = \sum_{i=1}^{N} \min(h_1(i), h_2(i))$$

- Generalized Gaussian kernel:

$$K(h_1, h_2) = \exp\left(-\frac{1}{A} D(h_1, h_2)^2 \right)$$

- *D* can be (inverse) L1 distance, Euclidean distance, χ^2 distance, etc.

J. Zhang, M. Marszalek, S. Lazebnik, and C. Schmid, Local Features and Kernels for Classifcation of Texture and Object Categories: A Comprehensive Study, IJCV 2007

Summary: SVMs for image classification

1. Pick an image representation (in our case, bag of features)
2. Pick a kernel function for that representation
3. Compute the matrix of kernel values between every pair of training examples
4. Feed the kernel matrix into your favorite SVM solver to obtain support vectors and weights
5. At test time: compute kernel values for your test example and each support vector, and combine them with the learned weights to get the value of the decision function

Slide credit: L. Lazebnik

What about multi-class SVMs?

- Unfortunately, there is no "definitive" multi-class SVM formulation
- In practice, we have to obtain a multi-class SVM by combining multiple two-class SVMs
- One vs. others
  - Traning: learn an SVM for each class vs. the others
  - Testing: apply each SVM to test example and assign to it the class of the SVM that returns the highest decision value
- One vs. one
  - Training: learn an SVM for each pair of classes
  - Testing: each learned SVM "votes" for a class to assign to the test example

Slide credit: L. Lazebnik

SVMs: Pros and cons

- Pros
  - Many publicly available SVM packages: http://www.kernel-machines.org/software
  - Kernel-based framework is very powerful, flexible
  - SVMs work very well in practice, even with very small training sample sizes

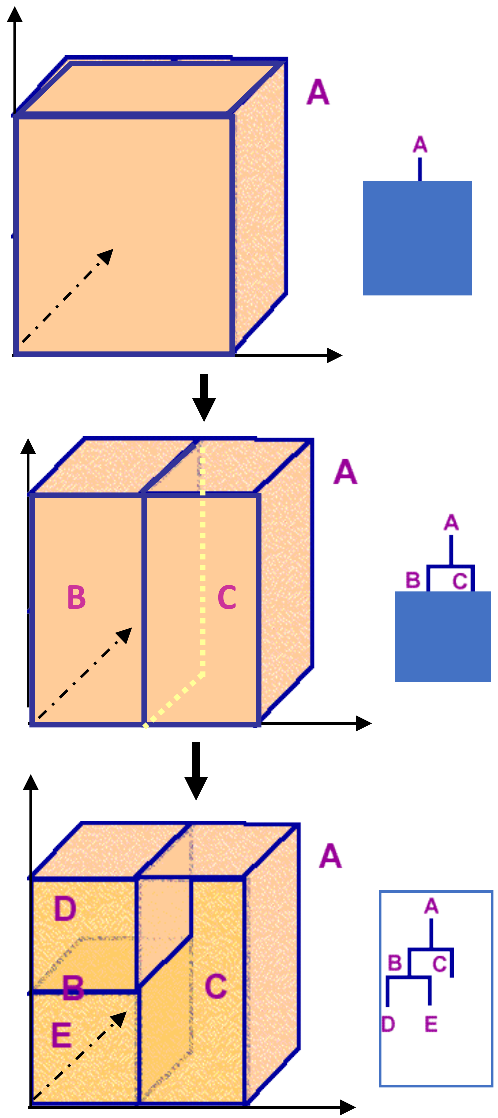
- Cons
  - No “direct” multi-class SVM, must combine two-class SVMs
  - Computation, memory
    - During training time, must compute matrix of kernel values for every pair of examples
    - Learning can take a very long time for large-scale problems

Decision Tree

- Classification Models: Many
- Why decision?
  - Relatively fast compared to other classification models
  - Obtain similar and sometimes better accuracy compared to other models
  - Simple and easy to understand
  - Can be converted into simple and easy to understand classification rules

Decision trees
-Binary decision trees

- Since each inequality that is used to split the input space is only based on one input variable.
- Each node draws a boundary that can be geometrically interpreted as a hyperplane perpendicular to the axis.

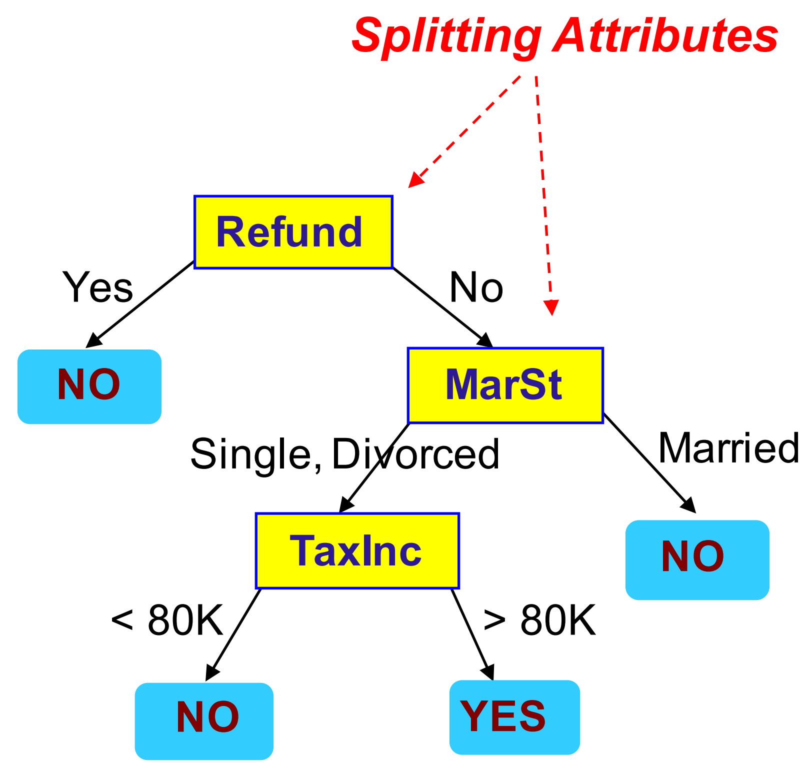


Model by Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Another Example of Decision Tree

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
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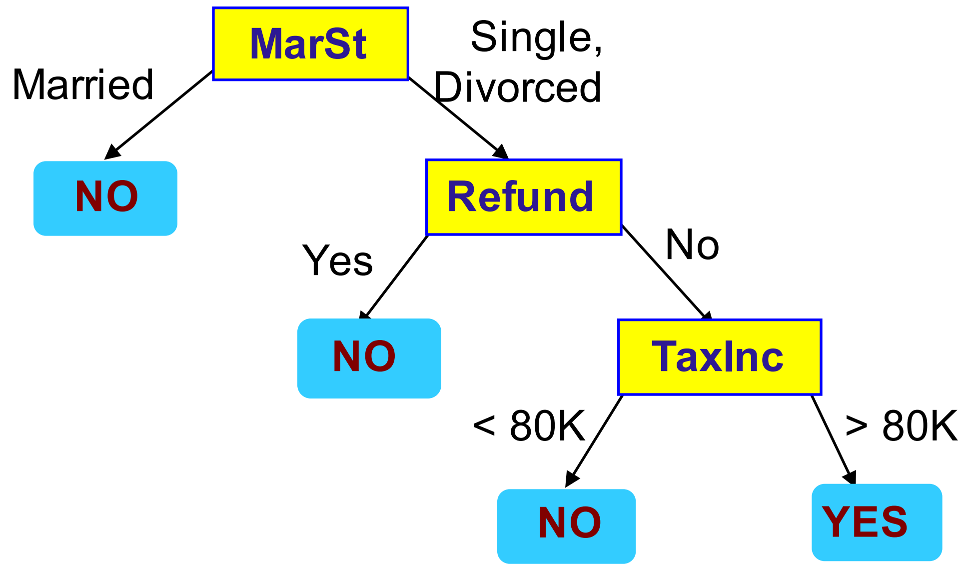
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

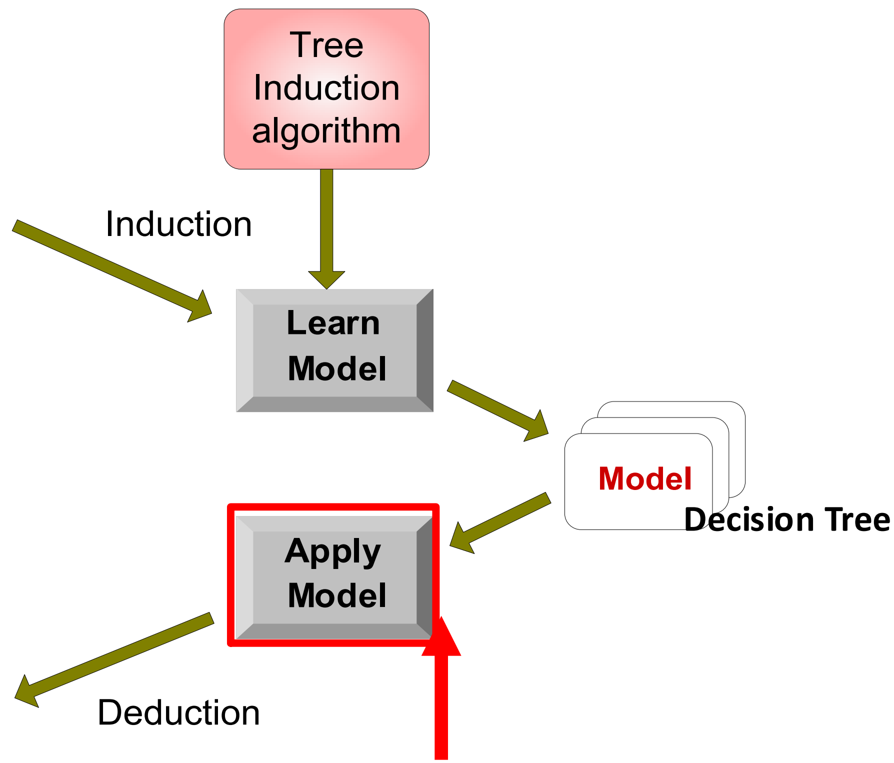


There could be more than one tree that fits the same data!

Decision Tree Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

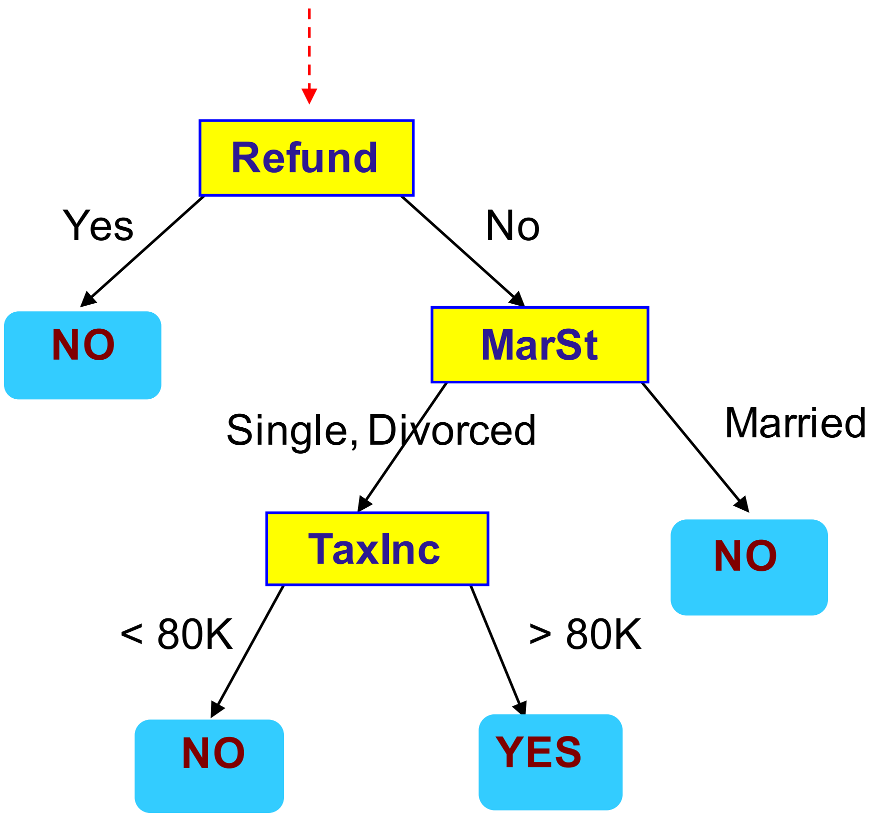


Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Apply Model to Test Data

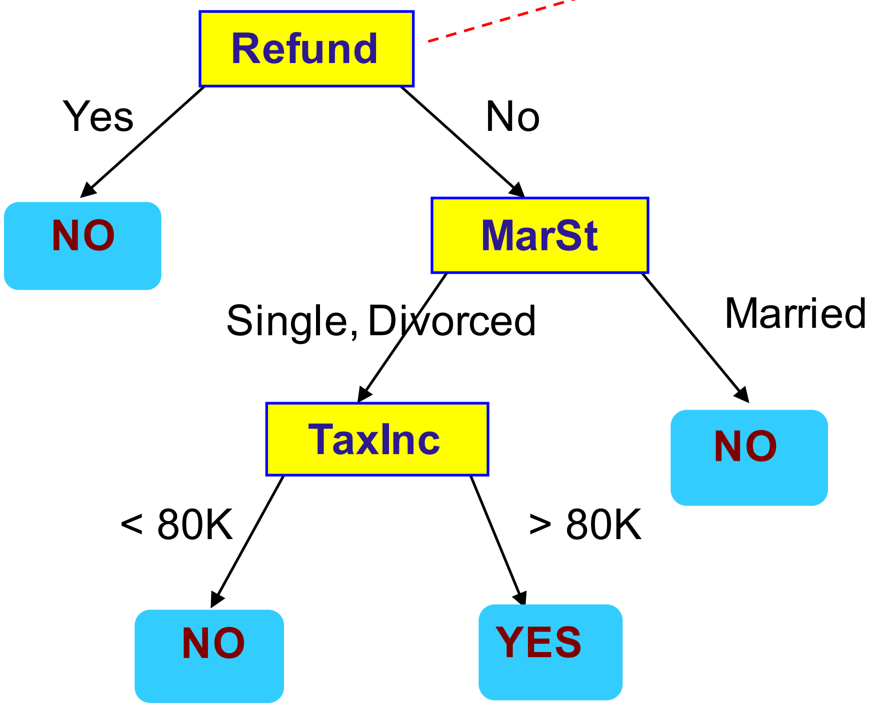
Start from the root of tree.



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



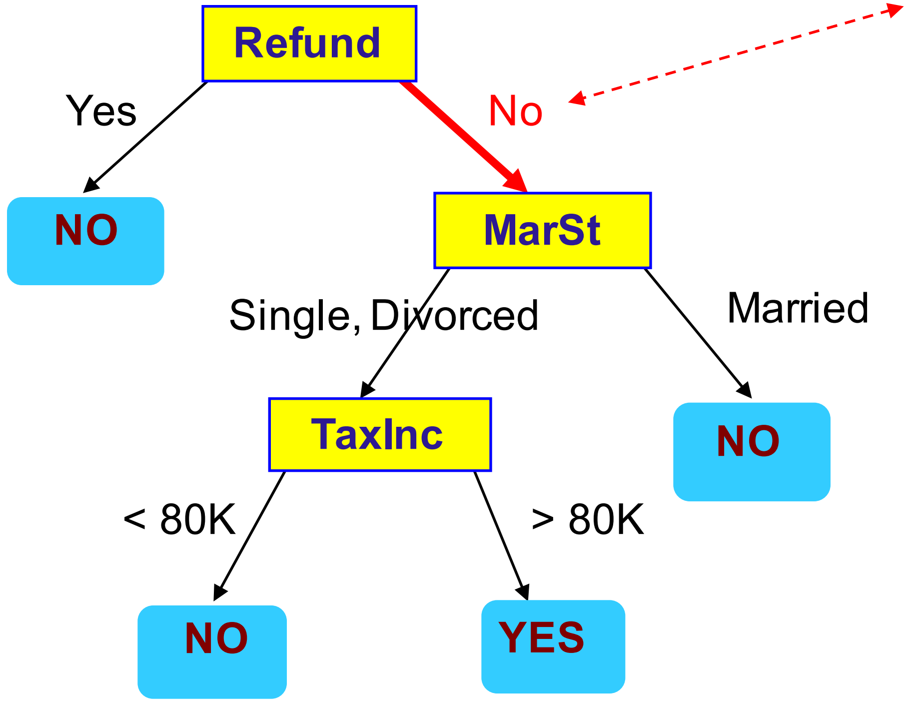
Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

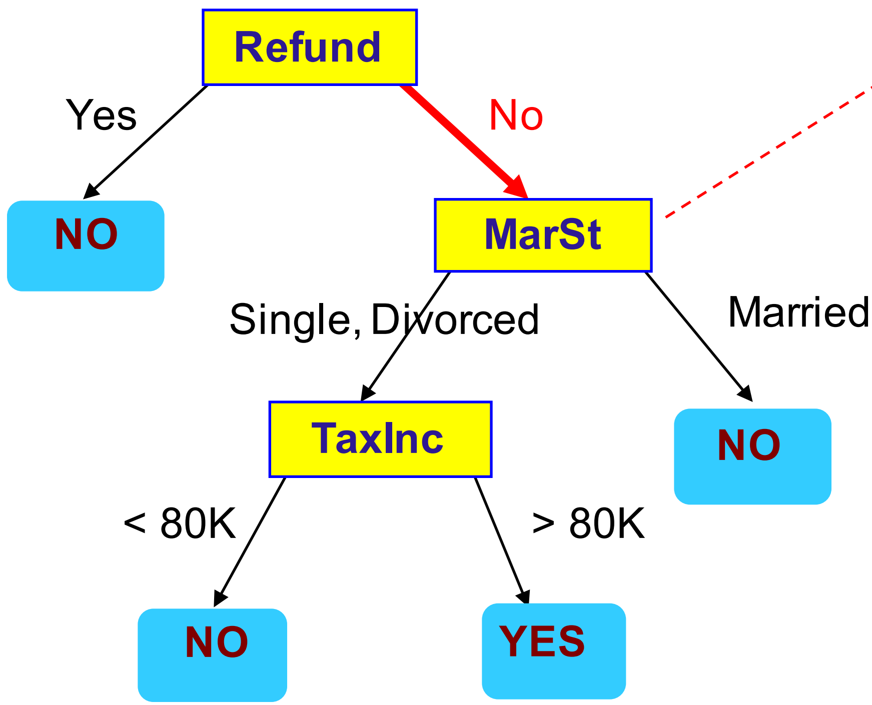
Apply Model to Test Data

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



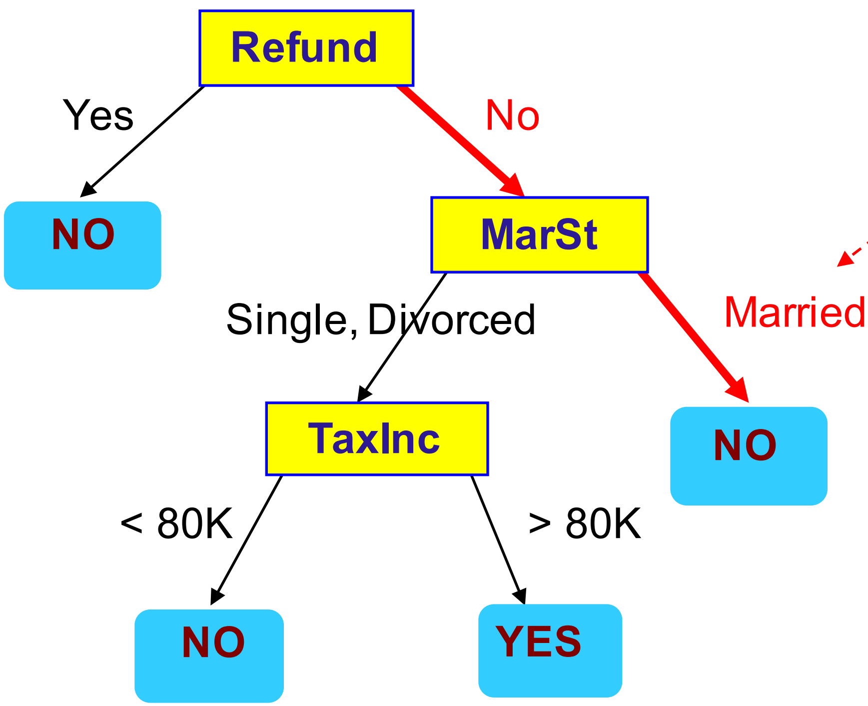
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

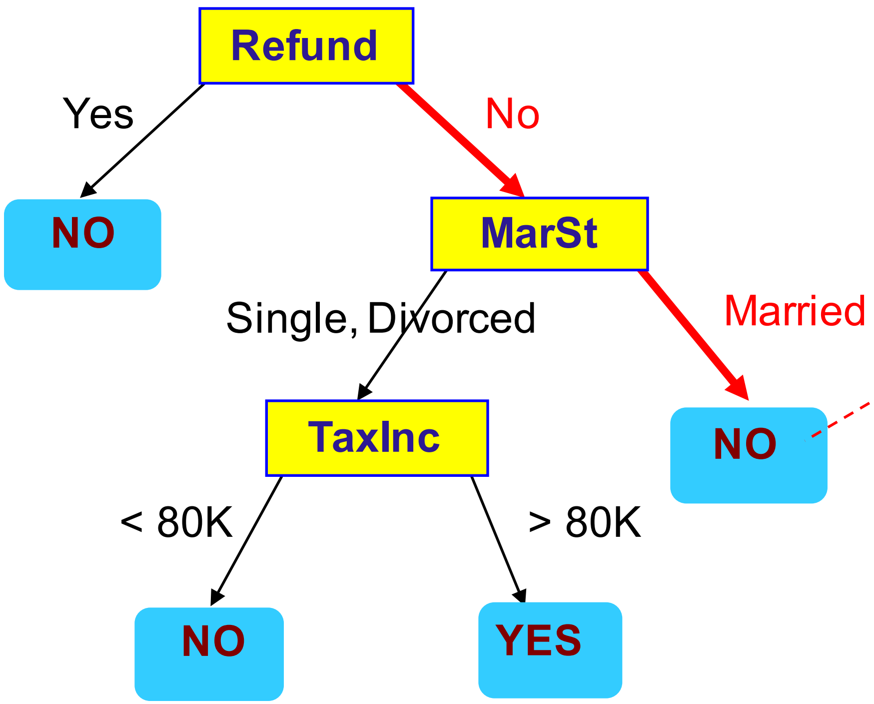
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



Test Data

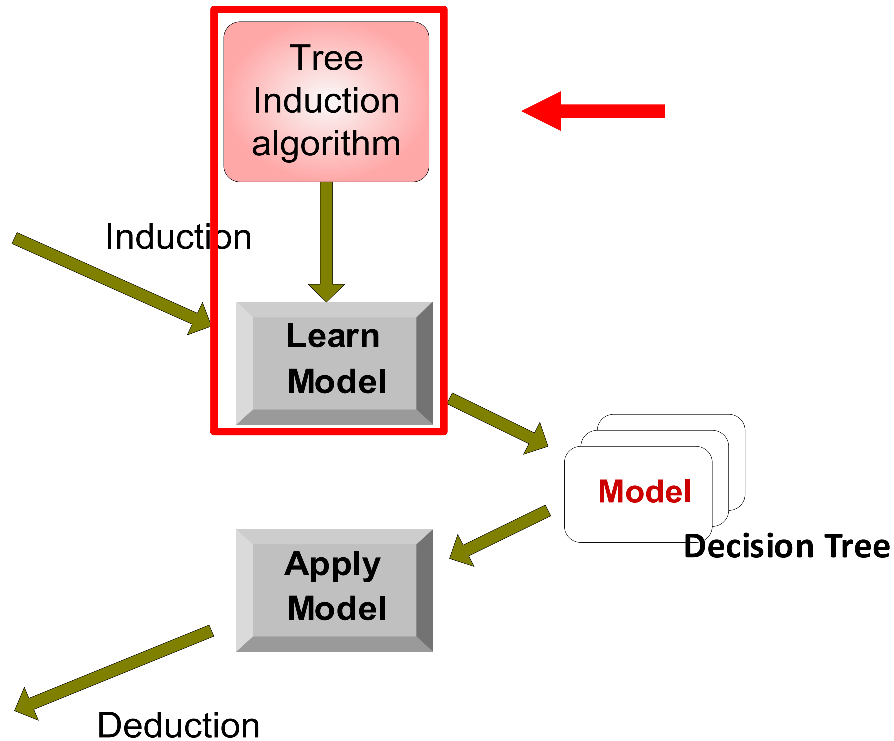
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to “No”

Decision Tree Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set



Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set

Decision Tree Induction

- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - **ID3**, C4.5
  - SLIQ,SPRINT
- The basic idea behind any decision tree algorithm is as follows:
  - Choose the *best* attribute(s) to split the remaining instances and make that attribute a decision node
  - Repeat this process for recursively for each child
  - Stop when:
    - All the instances have the same target attribute value
    - There are no more attributes
    - There are no more instances

Many classifiers to choose from

- SVM
- Neural networks
- Naïve Bayes
- Bayesian network
- Logistic regression
- Randomized Forests
- Boosted Decision Trees
- K-nearest neighbor
- Etc.

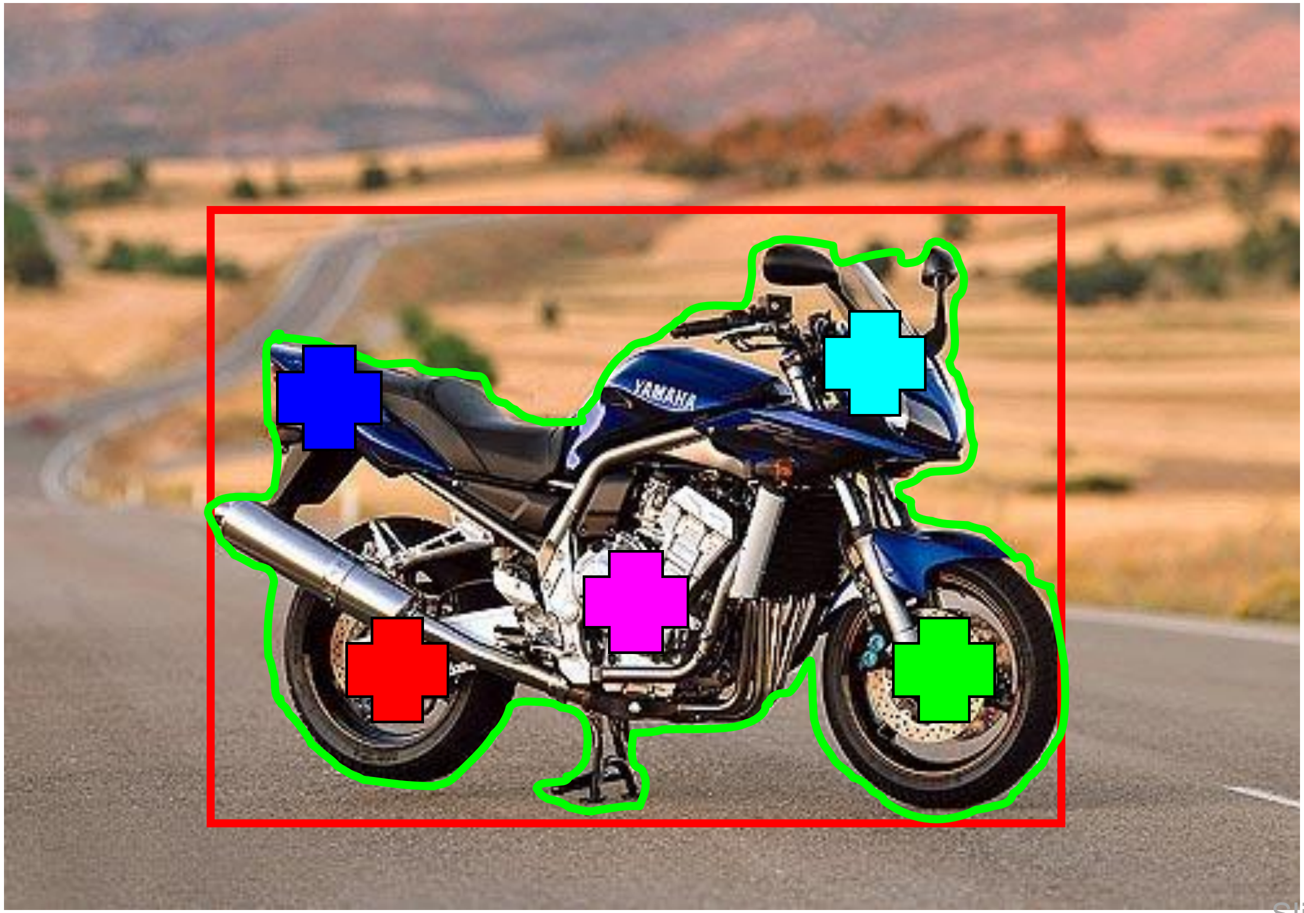
Which is the best one?

Slide credit: D. Hoiem

Recognition task and supervision

- Images in the training set must be annotated with the "correct answer" that the model is expected to produce

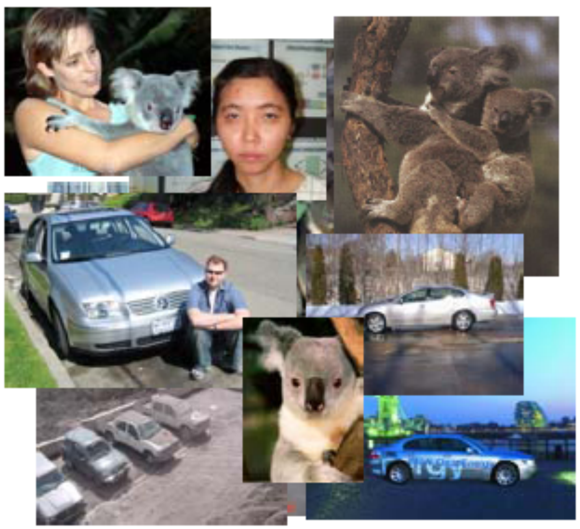
Contains a motorbike



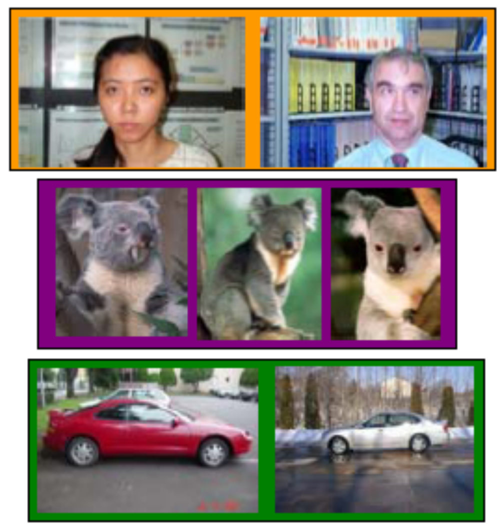
Slide credit: L. Lazebnik

Spectrum of supervision

Less **More**



Unsupervised



“Weakly” supervised

Fully supervised

Definition depends on task

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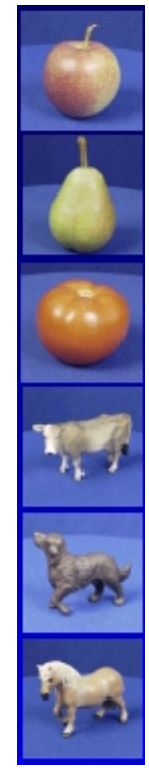
Generalization

Training set (labels known)



Test set (labels unknown)

- How well does a learned model generalize from the data it was trained on to a new test set?

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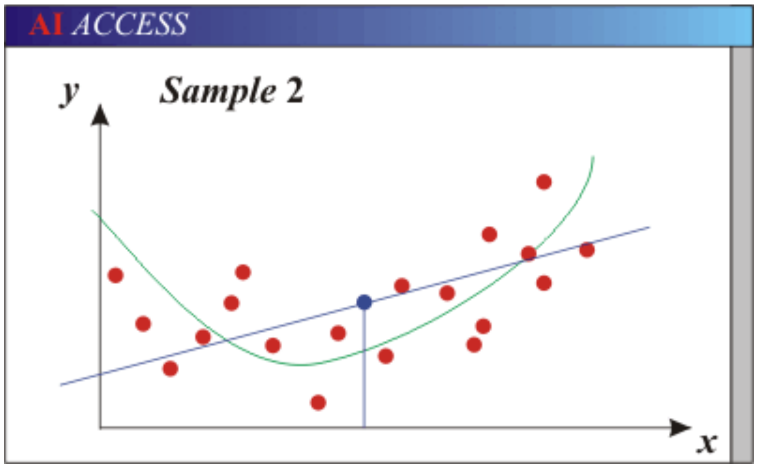
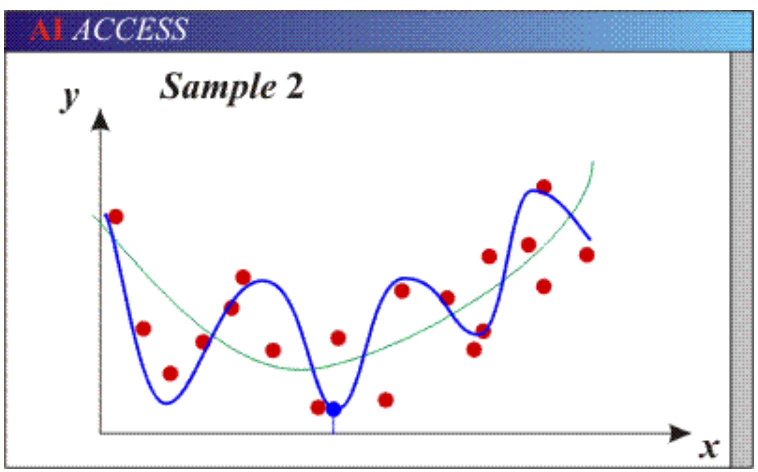
Generalization

- Components of generalization error
  - **Bias:** how much the average model over all training sets differ from the true model?
    - Error due to inaccurate assumptions/simplifications made by the model
  - **Variance:** how much models estimated from different training sets differ from each other
- **Underfitting:** model is too "simple" to represent all the relevant class characteristics
  - High bias and low variance
  - High training error and high test error
- **Overfitting:** model is too "complex" and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - Low training error and high test error

Slide credit: L. Lazebnik

Bias-Variance Trade-off





- Models with too few parameters are inaccurate because of a large bias (not enough flexibility).
- Models with too many parameters are inaccurate because of a large variance (too much sensitivity to the sample).

Bias-Variance Trade-off

$$E(MSE) = noise^2 + bias^2 + variance$$

Unavoidable error

Error due to incorrect assumptions

Error due to variance of training samples

See the following for explanations of bias-variance (also Bishop's "Neural Networks" book):

- http://www.inf.ed.ac.uk/teaching/courses/mlsc/Notes/Lecture4/BiasVariance.pdf

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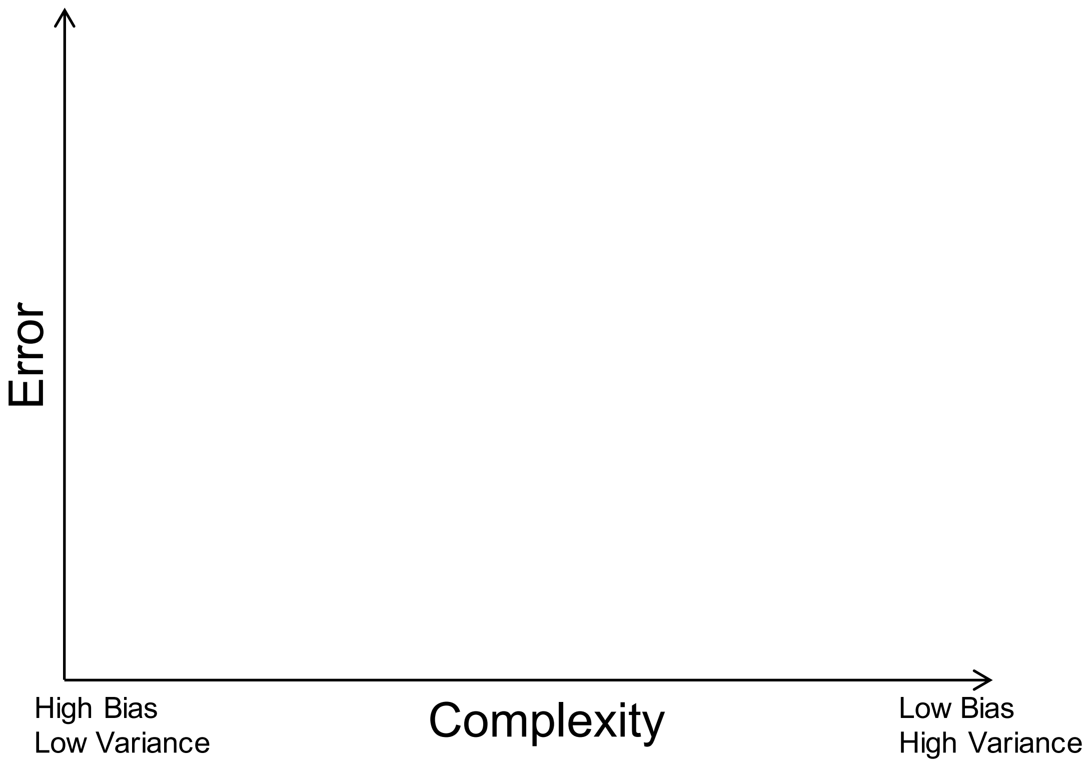
Bias-variance tradeoff

Underfitting **Overfitting**



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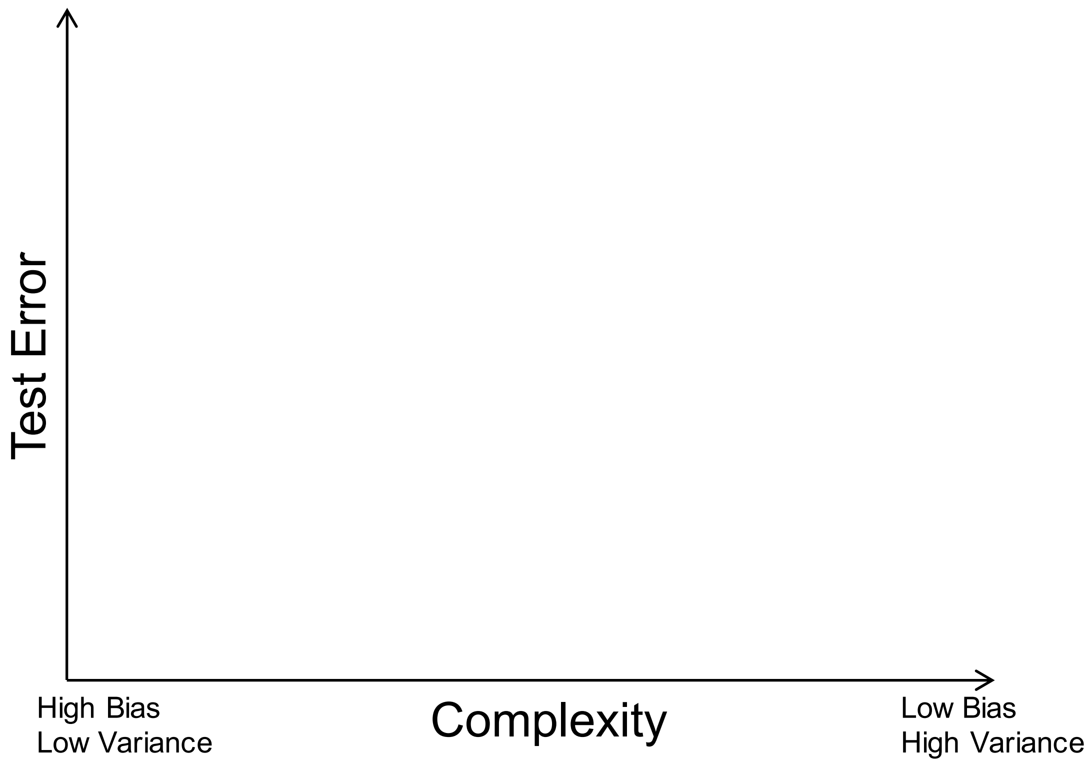
Bias-variance tradeoff



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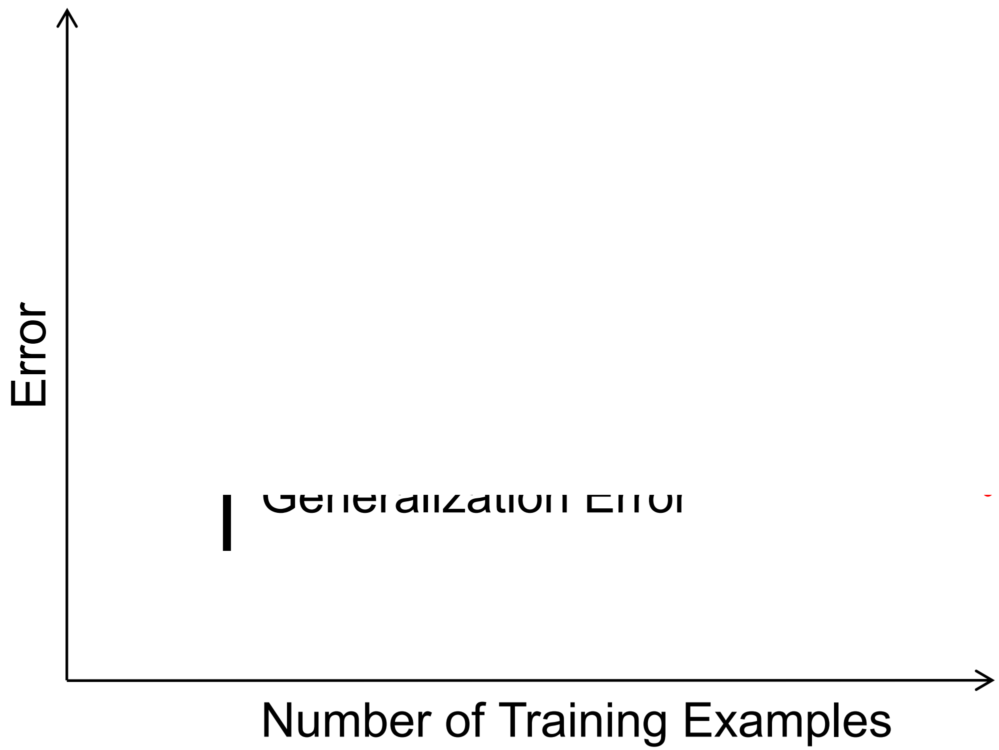
Effect of Training Size

Fixed prediction model



The perfect classification algorithm

- Objective function: encodes the right loss for the problem
- Parameterization: makes assumptions that fit the problem
- Regularization: right level of regularization for amount of training data
- Training algorithm: can find parameters that maximize objective on training set
- Inference algorithm: can solve for objective function in evaluation

Slide credit: D. Hoiem

How to reduce variance?

- Choose a simpler classifier
- Regularize the parameters
- Get more training data

Slide credit: D. Hoiem

Generative vs. Discriminative Classifiers

Generative Models

- Represent both the data and the labels
- Often, makes use of conditional independence and priors
- Examples
  - Naïve Bayes classifier
  - Bayesian network

- Models of data may apply to future prediction problems

Discriminative Models

- Learn to directly predict the labels from the data
- Often, assume a simple boundary (e.g., linear)
- Examples
  - Logistic regression
  - SVM
  - Boosted decision trees

- Often easier to predict a label from the data than to model the data

Slide credit: D. Hoiem

Ideals for a classification algorithm

- Objective function: encodes the right loss for the problem

- Parameterization: takes advantage of the structure of the problem

- Regularization: good priors on the parameters

- Training algorithm: can find parameters that maximize objective on training set

- Inference algorithm: can solve for labels that maximize objective function for a test example

Two ways to think about classifiers

1. What is the objective? What are the parameters? How are the parameters learned? How is the learning regularized? How is inference performed?

2. How is the data modeled? How is similarity defined? What is the shape of the boundary?

Slide credit: D. Hoiem

What to remember about classifiers

- No free lunch: machine learning algorithms are tools, not dogmas

- Try simple classifiers first

- Better to have smart features and simple classifiers than simple features and smart classifiers

- Use increasingly powerful classifiers with more training data (bias-variance tradeoff)

Slide credit: D. Hoiem

- Neural Network and Deep Learning
    - Reinforcement Learning