Classification

Tian-Li Yu

Taiwan Evolutionary Intelligence Laboratory (TEIL)
Department of Electrical Engineering
National Taiwan University
tianliyu@ntu.edu.tw

Readings: AIMA 18.3, 18.4, 18.9, 18.10

Outline

1. Learning Decision Trees
   - Choosing Attributes
   - Generalization and Overfitting
2. Model Evaluation
   - Metrics
   - Cross-Validation
   - Comparison
3. Ensemble Methods
4. Support Vector Machines
   - Kernel Trick

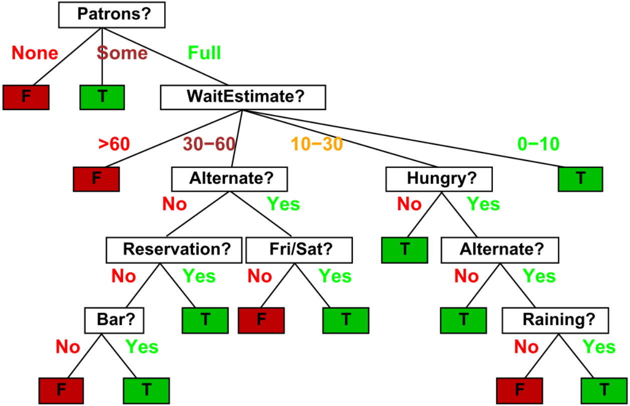
Attribute-based Representations

- Restaurant example.

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	*T*	*F*	*F*	*T*	*Some*	*$$$*	*F*	*T*	*French*	*0–10*	*T*
X_2	*T*	*F*	*F*	*T*	*Full*	*$*	*F*	*F*	*Thai*	*30–60*	*F*
X_3	*F*	*T*	*F*	*F*	*Some*	*$*	*F*	*F*	*Burger*	*0–10*	*T*
X_4	*T*	*F*	*T*	*T*	*Full*	*$*	*F*	*F*	*Thai*	*10–30*	*T*
X_5	*T*	*F*	*T*	*F*	*Full*	*$$$*	*F*	*T*	*French*	*>60*	*F*
X_6	*F*	*T*	*F*	*T*	*Some*	*$$*	*T*	*T*	*Italian*	*0–10*	*T*
X_7	*F*	*T*	*F*	*F*	*None*	*$*	*T*	*F*	*Burger*	*0–10*	*F*
X_8	*F*	*F*	*F*	*T*	*Some*	*$$*	*T*	*T*	*Thai*	*0–10*	*T*
X_9	*F*	*T*	*T*	*F*	*Full*	*$*	*T*	*F*	*Burger*	*>60*	*F*
X_{10}	*T*	*T*	*T*	*T*	*Full*	*$$$*	*F*	*T*	*Italian*	*10–30*	*F*
X_{11}	*F*	*F*	*F*	*F*	*None*	*$*	*F*	*F*	*Thai*	*0–10*	*F*
X_{12}	*T*	*T*	*T*	*T*	*Full*	*$*	*F*	*F*	*Burger*	*30–60*	*T*

Decision Trees

- One possible representation for hypotheses.



Expressiveness of Decision Trees

- $Goal \Leftrightarrow (Path_1 \vee Path_2 \vee \cdots)$.
- $Path_i \Leftrightarrow (Attribute_1 = a_1 \wedge Attribute_2 = a_2 \wedge \cdots)$.
- Decision trees can express any function of the input attributes.
- Trivially, there is a consistent decision tree for any training set with one path to leaf for each example, but it won't generalize to new examples.
- Prefer to find more compact decision trees.

Hypothesis Space

- How many distinct decision trees with n Boolean attributes?
  - Truth table with 2^n rows.
  - Every truth table can be expressed by one decision tree $\Rightarrow$ At least 2^{2^n} decision trees.
  - If different order of attributes counts as $\Rightarrow$ At least $n! \cdot 2^{2^n}$ decision trees.
- More expressive hypothesis space
  - Increase the chance that c can be expressed.
  - May be weak at generalization if we let the decision tree be too expressive.

Learning Decision Trees (ID3 [Quinlan, 1986])

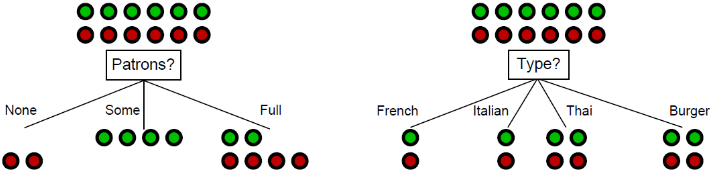
- Aim: Find a small tree consistent with training examples.
- Idea: Recursively choose the best attribute.

DTL(*examples*, *attributes*, *examples*$_{parent}$)

```
if examples is empty then return PLURALITY-VALUE(examples_parent)
elseif all examples have same classification then return the classification
elseif attributes is empty then return PLURALITY-VALUE(examples)
else
    A ← argmax_{a∈attributes} IMPORTACE(a, examples)
    tree ← a new decision tree with root A
    for textbfeach value v_k of A
        exs ← elements of examples with A = v_k
        subtree ← DTL(exs, attributes − A, examples)
        add a branch to tree with label A = v_k and subtree subtree
    return tree
```

Choosing Attributes

- The restaurant example consist of 6 positive and 6 negative examples.
- *Patrons* is a better choice — gives more information about the classification.



Information

- Measure of information: Shannon's entropy.
  - Gives the lower bound of the most compact encoding of a random variable in bits.
- The entropy of a random variable V with values v_k, each with probability $P(v_k)$, is defined as

$$H(V) = -\sum_k P(v_k) \log_2 P(v_k). \geq 0.08 \, ?$$

- For Boolean variables, define

$$B(q) = -q \log_2 q - (1-q) \log_2 (1-q).$$

- The entropy of a fair coin:
  $H = B(0.5) = -(0.5 \log_2 0.5 + 0.5 \log_2 0.5) = 1 bit.$
- The entropy of a unfair coin (99% head):
  $H = B(0.99) = -(0.99 \log_2 0.99 + 0.01 \log_2 0.01) = 0.08 bits.$

Information

- p positive and n negative examples at the root $\Rightarrow B(p/(p+n))$ bits needed to classify a new example.
- Attribute A splits the examples E into subsets E_k, each of which (we hope) needs less information to complete the classification.
- Let E_k have p_k positive and n_k negative examples
  $\Rightarrow B(p_k/(p_k+n_k))$ bits needed to classify a new example
  $\Rightarrow$ expected number of bits per example over all branches is

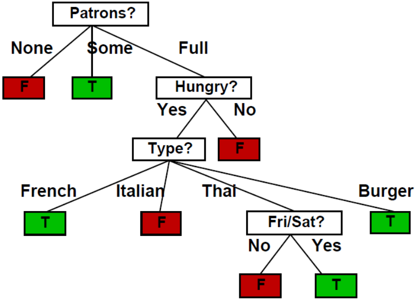
$$Remainder(A) = \sum_k \frac{p_k+n_k}{p+n} B\left(\frac{p_k}{p_k+n_k}\right).$$

- For *Patrons*, this is 0.459 bits; for *Type*, this is (still) 1 bit
  $\Rightarrow$ Choose the attribute that minimizes the remaining information.
  $\Rightarrow$ Choose the attribute with the most information gain:

$$Gain(A) = B\left(\frac{p}{p+n}\right) - Remainder(A)$$

Decision Tree Learned from the Examples

- Decision tree learned from the 12 examples:



- Substantially simpler than a full tree — a more complex hypothesis isn't justified by small amount of data.

Generalization and Overfitting

- If some attributes are irrelevant, DTL still outputs a large tree.
  - The outputs of fair dices with attributes of color, size, and so on.
- To overcome overfitting,
  - we can stop growing the tree before overfitting,
  - or we can allow overfitting, and then post-prune the tree (most common).
- How to decide what to post-prune?
  - Use the testing set.
  - Use statistical tests.
  - Use explicit measures the complexity of the encoding of the tree and training examples (minimum description length principle).

χ^2 Pruning

- Information gain of an irrelevant attribute is expected to be zero, but the sampling noise may still yield some gain.
- Assuming true irrelevant, the expected number of p_k and n_k can be expressed as

$$\hat{p}_k = \frac{p}{p+n} \times (p_k + n_k) \qquad \hat{n}_k = \frac{n}{p+n} \times (p_k + n_k)$$

- Define $\triangle = \sum_k \frac{(p_k - \hat{p}_k)^2}{\hat{p}_k} + \frac{(n_k - \hat{n}_k)^2}{\hat{n}_k}$, $\triangle$ is of χ^2 distribution with $(n + p - 1)$ degree of freedom.
- For example, with 3 degree of freedom, $\triangle \leq 7.82$ encourages the pruning with 5% level of significance.

Rule Post-Pruning

- Used by C4.5rules [Quinlan, 1993].

1. Convert the decision tree into rules (one rule per path).
2. Prune each rule by removing any preconditions that improves its accuracy (by testing set).
3. Sort the the pruned rules by their accuracy, and consider them in this sequence when classifying instances.

- For example,
  $(Patron = Full) \wedge (Hungry = No) \Rightarrow (WillWait = False)$.
- Rule post-pruning considers removing $(Patron = Full)$ and $(Hungry = NO)$ in this example.

Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

Metrics for Performance Evaluation

- Confusion matrix:

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	True Positive	False Negative
	Class=No	False Positive	True Negative

Accuracy

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

- Probably most widely-used metric.
- Can be misleading. Consider class 0 consisting of 9990 instances and class 1 consisting of 10 instances. Classifying everything as class 0 yields 99.9% accuracy.

Other Metrics

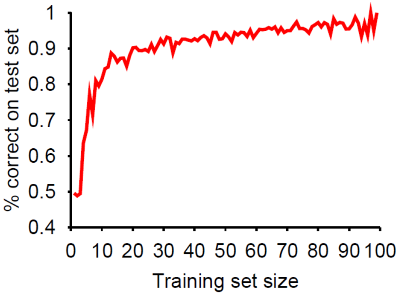
$$Precision(p) = \frac{TP}{TP + FP}$$

$$Recall(r) = \frac{TP}{TP + FN}$$

$$F - measure(F) = \frac{2pr}{p + r} = \frac{2TP}{2TP + FP + FN}$$

Performance Measurement

- How do we know whether $h \approx c$?
  1. Use theorems of computational/statistical learning theory
  2. Try h on a new test set of examples
     (use same distribution over example space as training set)
- Learning curve = % correct on test set as a function of training set size



Cross-Validation

- The idea of having training and testing sets is called cross-validation.
- Holdout cross-validation
  - Randomly split the available data into a training set and a testing set.
  - Simple, fast, but not able to use all available data.
- k-fold cross-validation
  - Randomly split the data into k equal-sized subsets.
  - Perform k rounds of learning using $k-1$ subsets as training and the rest as testing.
  - Popular choice of k is 5 to 10.
  - Accurate statistics, but longer computation.

ROC

- Receiver operating characteristic.
- ROC curve: FPR as x-axis; TPR as y-axis.

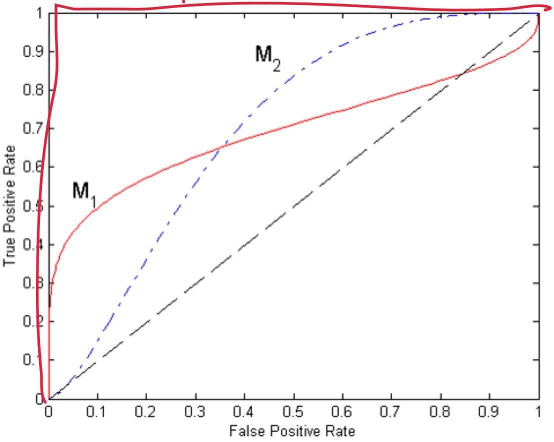
$$FPR(FP\ rate) = \frac{FP}{FP + TN}$$

$$TPR(TP\ rate) = \frac{TP}{TP + FN}$$

- (FPR, TPR):
  - (0,0): Classify everything as negative.
  - (1,1): Classify everything as positive.
  - (0,1): Ideal.

AUC

- Model 1 is better for small FPR.
- Model 2 is better for large FPR.
- Area under the ROC curve (AUC).
  - Ideal: 1.
  - Random guess: 0.5.

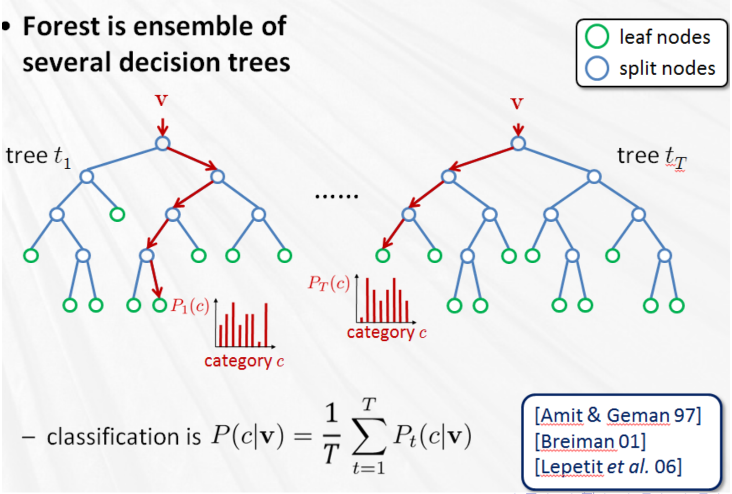


Ensemble

- Use multiple weak classifiers to prevent from overfitting.
- Embedding
- Bagging
- Boosting

Embedding

- Random forest: randomly select *k* attributes to create weak classifiers.



Bagging

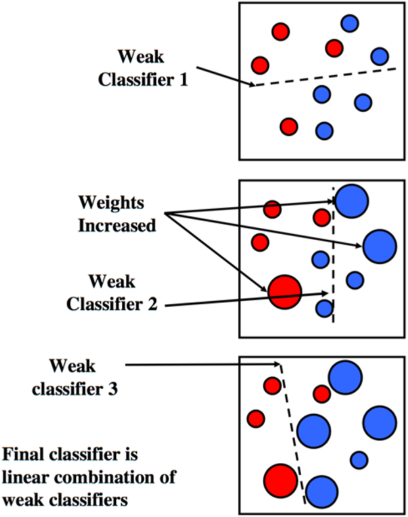
- Sampling with replacement from the dataset to form new datasets.

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Build classifier on each bootstrap sample (supposedly n items).
- Probability $(1-1/n)^n$ of not being selected.
- When n is large, it is about $1/e \simeq 37\%$
- About 37% of noise (if any) not being selected.

Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records.
- Initially, all *n* items are assigned equal weights.
- Unlike bagging, weights vary at the end of boosting round.



AdaBoost

- Weak classifiers: C_i
- Error rates:

$$\epsilon_i = \frac{1}{N}\sum_{j=i}^{N} w_j \cdot \delta[C_i(x_j) \neq y_j]$$

.

- Importance of a classifier:

$$\alpha_i = \frac{1}{2}\ln\frac{1-\epsilon_i}{\epsilon_i}$$

- Weight update (c normalization factor):

$$w_j \leftarrow c \cdot w_j \begin{cases} e^{-\alpha_i} & C_i(x_j) = y_j \\ e^{\alpha_i} & C_i(x_j) \neq y_j \end{cases}$$

AdaBoost

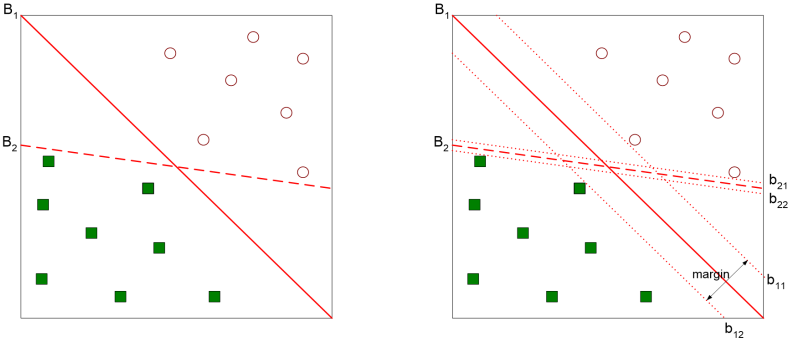
- The equations of the previous slide are such to minimize the total error. We omit the derivations here.

- Initially, $w_j = \frac{1}{N}$.
- Any intermediate round yields error rate higher than 0.5, weights are reverted back to $\frac{1}{N}$.
- Classification:

$$C^*(x) = \underset{y}{\operatorname{argmax}} \sum_j \alpha_j \cdot \delta[C_j(x) = y]$$

Linear Separable Data

- Which separator is better?



- Key: margins

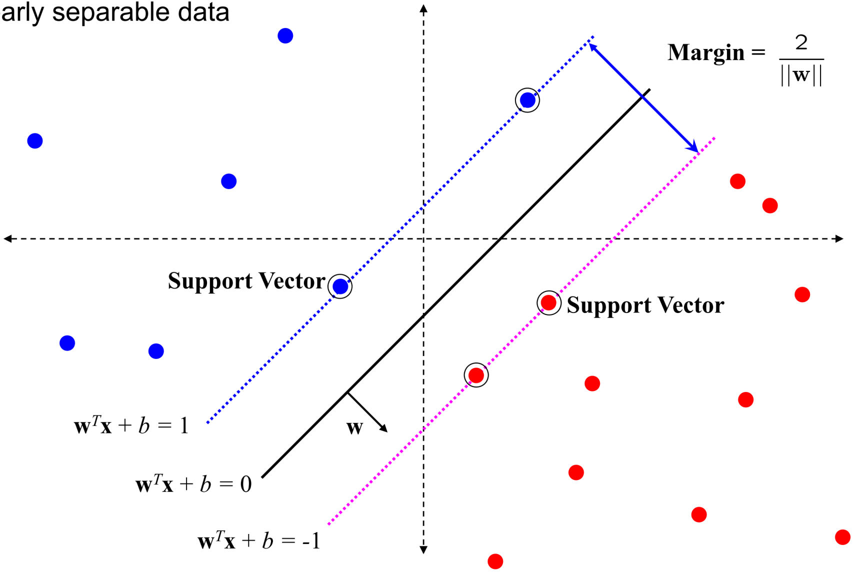
Sketch of Derivations

- Since $\vec{w} \cdot \vec{x} + b = 0$ and $c(\vec{w} \cdot \vec{x} + b) = 0$ defines the same plane, we can choose any normalization factor as desired.
- Choose normalization factor such that $\vec{w} \cdot \vec{x} + b = 1$ positive support vectors and $\vec{w} \cdot \vec{x} + b = -1$ for negative ones.
- The margin is given by

$$\frac{\vec{w} \cdot (\vec{x}_+ - \vec{x}_-)}{|w|} = \frac{2}{|\vec{w}|}$$

Support Vector Machines

linearly separable data



SVM: Optimization

- Can be formulated as an optimization problem:

$$\max_{\vec{w}} \frac{2}{|\vec{w}|}$$

subject to

$$\vec{w} \cdot \vec{x}_i + b \geq 1 \text{ for } y_i = 1$$

$$\vec{w} \cdot \vec{x}_i + b \leq -1 \text{ for } y_i = -1$$

- Or equivalently,

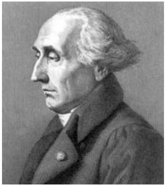
$$\min_{\vec{w}} |\vec{w}|^2$$

subject to

$$y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1$$

- Quadratic problem with linear constraints: quadratic programming.
- Practically, we'll solve the dual problem by finding the Lagrange multipliers.

Lagrange Multiplier for SVM



- Define

$$L(\vec{w}, b, \lambda_i) = \frac{1}{2}|\vec{w}|^2 - \sum_i \lambda_i \left(y_i(\vec{w} \cdot \vec{x}_i + b) - 1\right)$$

- Primal problem:

$$\min_{\vec{w},b} \max_{\lambda_i \geq 0} L(\vec{w}, b, \lambda_i)$$

- Dual problem (convex):

$$\max_{\lambda_i \geq 0} \min_{\vec{w},b} L(\vec{w}, b, \lambda_i)$$

Lagrange Multipliers for SVM

$$\frac{\partial L}{\partial \vec{w}} = 0, \qquad \frac{\partial L}{\partial b} = 0$$

$$\vec{w} - \sum_i \lambda_i y_i \vec{x}_i = 0, \qquad \sum_i \lambda_i y_i = 0$$

$\vec{w}$ =

代入

- Maximizing

$$\max_{\lambda_i} L_D(\lambda_i) = \sum_i \lambda_i - \frac{1}{2} \sum_i \sum_j \lambda_i \lambda_j y_i y_j \vec{x}_i \cdot \vec{x}_j$$

subject to $\sum_i \lambda_i y_i = 0, \lambda_i \geq 0$

Classification

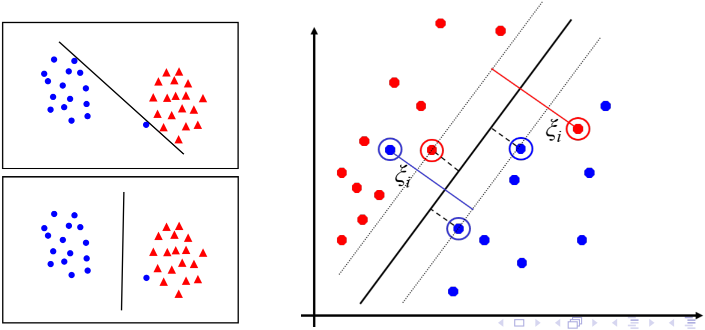
- For $y_i(\vec{w} \cdot \vec{x}_i + b) > 1$, $\lambda_i = 0$
- For $y_i(\vec{w} \cdot \vec{x}_i + b) = 1$, $\lambda_i \geq 0$ (support vector)

$$g(\vec{x}) = sign(\vec{w} \cdot \vec{x} + b),$$

where $\vec{w} = \sum_i \lambda_i y_i \vec{x}_i$ and $b = \frac{1}{2}(\vec{x}_{+1} + \vec{x}_{-1}) \cdot \vec{w}$

Soft Margins

- Small margin vs. slack variables.
- Not purely linear separable (but most are).
- Consider slack variable with margin $\frac{\xi}{|\vec{w}|}$
    - Normally: $\xi = 0$.
    - Within margin, but right side: $0 < \xi \leq 1$.
    - Wrong side: $1 < \xi$.



SVM with Soft Margins

$$\min_{\vec{w},\xi_i} |\vec{w}|^2 + C \sum_i \xi_i$$

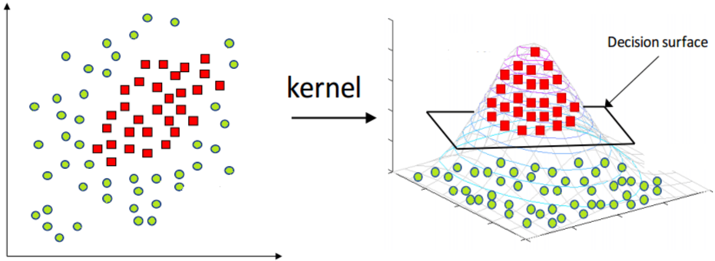
subject to

$$y_i(\vec{w} \cdot \vec{x}_i + b) \geq 1 - \xi_i$$

- C is a regularization parameter (the only parameter):
  - Large C: narrow margin
  - Small C: wide margin
- Every constraint can be satisfied if ξ_i is sufficiently large.
- Still a quadratic optimization with linear constraints.

Kernel Trick

- What if the data is clearly not linear separable?
- We can use kernel function to transfer the input space into feature space such that the data is linear separable.



Kernel Trick

- Recall the dual problem

$$\max_{\lambda_i} L_D(\lambda_i) = \sum_i \lambda_i - \frac{1}{2}\sum_i \sum_j \lambda_i \lambda_j y_i y_j \vec{x}_i \cdot \vec{x}_j$$

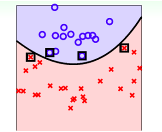
- Suppose we have a mapping function $\vec{x}' = \phi(\vec{x})$.
- All that matters is only the kernel $K(\vec{x}_i, \vec{x}_j) = \phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$
- A necessary and sufficient condition for K to be a kernel is that

$$\sum_i \sum_j \lambda_i \lambda_j K(\vec{x}_i, \vec{x}_j) \geq 0$$

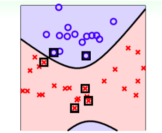
Poly-2 Kernel

$$K(\vec{x}_i, \vec{x}_j) = (\vec{x}_i \cdot \vec{x}_j + c)^2$$

$$\begin{aligned}\phi(\vec{x}) \;=\; & (x_d^2, \ldots, x_1^2, \\ & \sqrt{2}x_d x_{d-1}, \ldots, \sqrt{2}x_d x_1, \ldots, \sqrt{2}x_2 x_1, \\ & \sqrt{2c}x_d, \ldots, \sqrt{2c}x_1)\end{aligned}$$



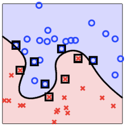
$(1 + 0.001\mathbf{x}^T\mathbf{x}')^2$



$(1 + 1000\mathbf{x}^T\mathbf{x}')^2$

In general, higher-order polynomial kernel

$$K(\vec{x}_i, \vec{x}_j) = (c_1 \vec{x}_i \cdot \vec{x}_j + c_2)^Q$$



10-th order polynomial with margin 0.1

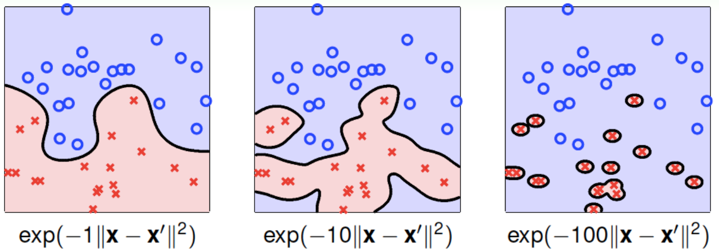
Gaussian Kernel

$$K(\vec{x}_i, \vec{x}_j) = e^{-(\vec{x}_i - \vec{x}_j)^2}$$

$$\phi(\vec{x}) = e^{-\vec{x}^2}\left(1, \sqrt{\frac{2}{1!}}\vec{x}, \sqrt{\frac{2^2}{2!}}\vec{x}^2, \dots\right)$$

More generally,

$$K(\vec{x}_i, \vec{x}_j) = e^{-\gamma(\vec{x}_i - \vec{x}_j)^2}$$



Summary

- Decision tree learning using information gain.
- Learning performance = prediction accuracy measured on test set.
- Cross-validation combats overfitting.
- Different ways to compare the performances of learning models, including F-measure and AUC.
- Ensemble methods: embedding (random forest), bagging, boosting.
- Support vector machine aims to minimize misclassification by maximizing margin.
- Kernel trick for non-linear classification, but be careful of overfitting.