Machine Learning – Lecture 10

AdaBoost

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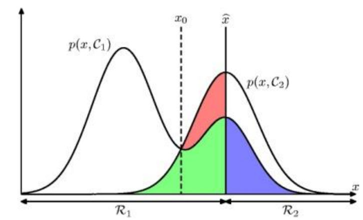
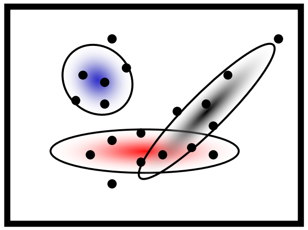
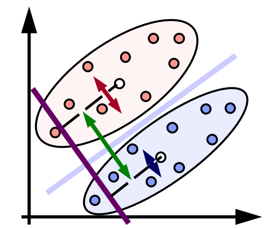
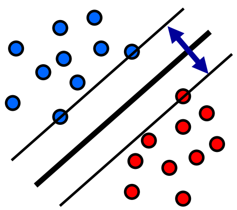
Course Outline

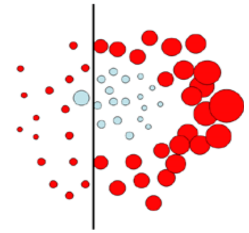
- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Random Forests
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks

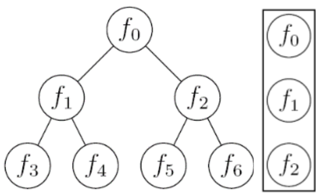


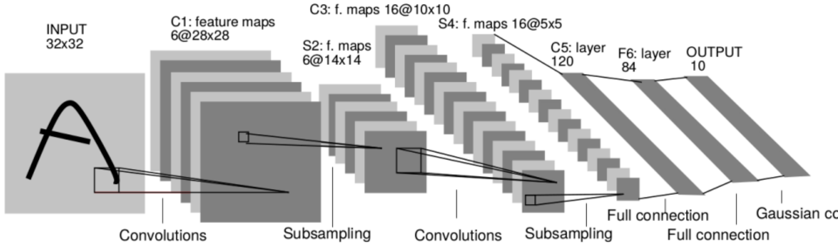












Recap: SVM – Analysis

- Traditional soft-margin formulation

$$\min_{\mathbf{w}\in\mathbb{R}^D,\, \xi_n\in\mathbb{R}^+} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

“Maximize the margin”

subject to the constraints

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

“Most points should be on the correct side of the margin”

- Different way of looking at it
  - We can reformulate the constraints into the objective function.

$$\min_{\mathbf{w}\in\mathbb{R}^D} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2}_{L_2\text{ regularizer}} + \underbrace{C\sum_{n=1}^{N}[1 - t_n y(\mathbf{x}_n)]_+}_{\text{“Hinge loss”}}$$

where $[x]_+ := \max\{0,x\}$.

Recap: Bayesian Model Averaging

- Model Averaging
  - Suppose we have H different models $h = 1,\ldots,H$ with prior probabilities $p(h)$.
  - Construct the marginal distribution over the data set

$$p(\mathbf{X}) = \sum_{h=1}^{H} p(\mathbf{X}|h)p(h)$$

- Average error of committee

$$\mathbb{E}_{COM} = \frac{1}{M}\mathbb{E}_{AV}$$

  - This suggests that the average error of a model can be reduced by a factor of M simply by averaging M versions of the model!
  - Unfortunately, this assumes that the errors are all uncorrelated. In practice, they will typically be highly correlated.

Topics of This Lecture

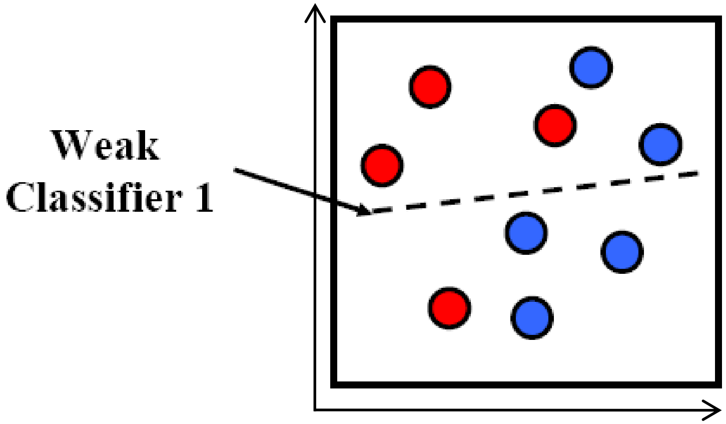
- AdaBoost
  - Algorithm
  - Analysis
  - Extensions
- Analysis
  - Comparing Error Functions
- Applications
  - AdaBoost for face detection
- Decision Trees
  - CART
  - Impurity measures, Stopping criterion, Pruning
  - Extensions, Issues
  - Historical development: ID3, C4.5

AdaBoost – "Adaptive Boosting"

- Main idea [Freund & Schapire, 1996]
  - Iteratively select an ensemble of component classifiers
  - After each iteration, reweight misclassified training examples.
    - Increase the chance of being selected in a sampled training set.
    - Or increase the misclassification cost when training on the full set.
- Components
  - $h_m(\mathbf{x})$: "weak" or base classifier
    - Condition: <50% training error over any distribution
  - $H(\mathbf{x})$: "strong" or final classifier
- AdaBoost:
  - Construct a strong classifier as a thresholded linear combination of the weighted weak classifiers:

$$H(\mathbf{x}) = sign\left(\sum_{m=1}^{M} \alpha_m h_m(\mathbf{x})\right)$$

AdaBoost: Intuition



Consider a 2D feature space with positive and negative examples.

Each weak classifier splits the training examples with at least 50% accuracy.

Examples misclassified by a previous weak learner are given more emphasis at future rounds.

Slide credit: Kristen Grauman

Figure adapted from Freund & Schapire

AdaBoost: Intuition

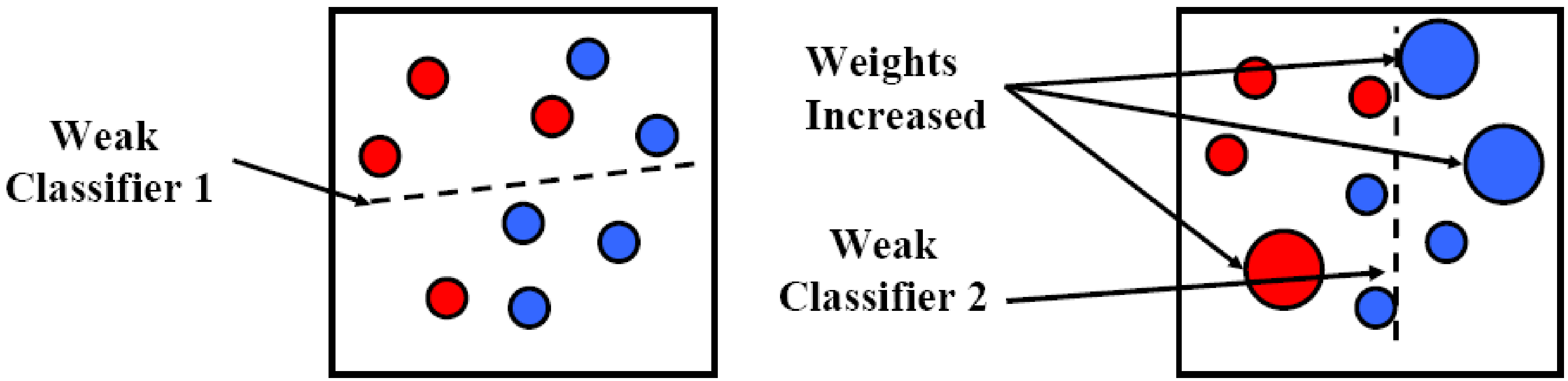
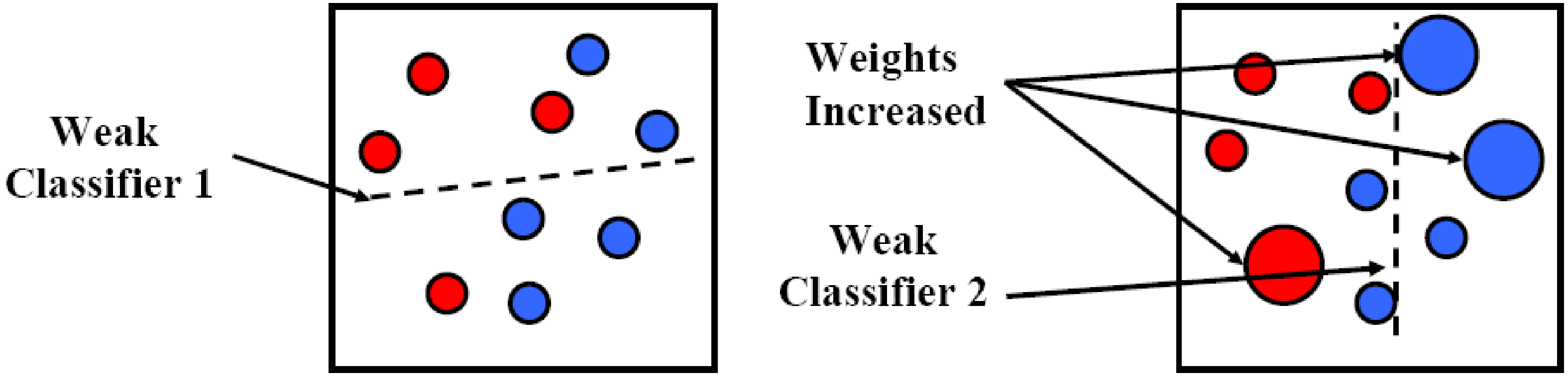
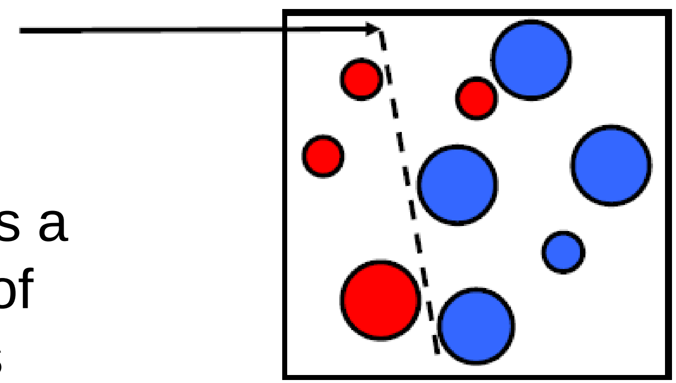


Figure adapted from Freund & Schapire

AdaBoost: Intuition





The final classifier is a linear combination of the weak classifiers

AdaBoost – Formalization

- 2-class classification problem
  - Given: training set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ with target values $\mathbf{T} = \{t_1, \ldots, t_N\}$, $t_n \in \{-1,1\}$.
  - Associated weights $\mathbf{W}=\{w_1, \ldots, w_N\}$ for each training point.
- Basic steps
  - In each iteration, AdaBoost trains a new weak classifier $h_m(\mathbf{x})$ based on the current weighting coefficients $\mathbf{W}^{(m)}$.
  - We then adapt the weighting coefficients for each point
    - Increase w_n if $\mathbf{x}_n$ was misclassified by $h_m(\mathbf{x})$.
    - Decrease w_n if $\mathbf{x}_n$ was classified correctly by $h_m(\mathbf{x})$.
  - Make predictions using the final combined model

$$H(\mathbf{x}) = sign\left(\sum_{m=1}^{M} \alpha_m h_m(\mathbf{x})\right)$$

AdaBoost – Algorithm

1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ for $n = 1,\ldots,N$.
2. For $m = 1,\ldots,M$ iterations
   a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function

$$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$

$$I(A) = \begin{cases} 1, & \text{if } A \text{ is true} \\ 0, & \text{else} \end{cases}$$

   b) Estimate the weighted error of this classifier on $\mathbf{X}$:

$$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}}$$

   c) Calculate a weighting coefficient for $h_m(\mathbf{x})$:

$$\alpha_m = \ ?$$

   d) Update the weighting coefficients:

$$w_n^{(m+1)} = \ ?$$

How should we do this exactly?

AdaBoost – Historical Development

- Originally motivated by Statistical Learning Theory
  - AdaBoost was introduced in 1996 by Freund & Schapire.
  - It was empirically observed that AdaBoost often tends not to overfit. (Breiman 96, Cortes & Drucker 97, etc.)
  - As a result, the margin theory (Schapire et al. 98) developed, which is based on loose generalization bounds.
    - Note: margin for boosting is *not* the same as margin for SVM.
    - A bit like retrofitting the theory…
  - However, those bounds are too loose to be of practical value.

- Different explanation [Friedman, Hastie, Tibshirani, 2000]
  - Interpretation as sequential minimization of an exponential error function ("Forward Stagewise Additive Modeling").
  - Explains why boosting works well.
  - Improvements possible by altering the error function.

AdaBoost – Minimizing Exponential Error

- Exponential error function

$$E = \sum_{n=1}^{N} \exp\{-t_n f_m(\mathbf{x}_n)\}$$

  - where $f_m(\mathbf{x})$ is a classifier defined as a linear combination of base classifiers $h_l(\mathbf{x})$:

$$f_m(\mathbf{x}) = \frac{1}{2}\sum_{l=1}^{m} \alpha_l h_l(\mathbf{x})$$

- Goal
  - Minimize E with respect to both the weighting coefficients α_l and the parameters of the base classifiers $h_l(\mathbf{x})$.

AdaBoost – Minimizing Exponential Error

- Sequential Minimization
  - Suppose that the base classifiers $h_1(\mathbf{x}),\ldots, h_{m-1}(\mathbf{x})$ and their coefficients $\alpha_1,\ldots,\alpha_{m-1}$ are fixed.

$\Rightarrow$ Only minimize with respect to α_m and $h_m(\mathbf{x})$.

$$E = \sum_{n=1}^{N} \exp\left\{-t_n f_m(\mathbf{x}_n)\right\} \quad \text{with} \quad f_m(\mathbf{x}) = \frac{1}{2}\sum_{l=1}^{m} \alpha_l h_l(\mathbf{x})$$

$$= \sum_{n=1}^{N} \exp\left\{\underbrace{-t_n f_{m-1}(\mathbf{x}_n)}_{= \textit{const.}} - \frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\}$$

$$= \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\}$$

AdaBoost – Minimizing Exponential Error

$$E = \sum_{n=1}^{N} w_n^{(m)} \exp\left\{ -\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n) \right\}$$

- Observation:
  - Correctly classified points: $t_n h_m(\mathbf{x}_n) = +1$ $\Rightarrow$ collect in $\mathcal{T}_m$
  - Misclassified points: $t_n h_m(\mathbf{x}_n) = -1$ $\Rightarrow$ collect in $\mathcal{F}_m$
- Rewrite the error function as

$$E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in \mathcal{F}_m} w_n^{(m)}$$

$$= \left(e^{\alpha_m/2} \qquad\qquad \right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n)$$

AdaBoost – Minimizing Exponential Error

$$E = \sum_{n=1}^{N} w_n^{(m)} \exp\left\{-\frac{1}{2}t_n \alpha_m h_m(\mathbf{x}_n)\right\}$$

- Observation:
  - Correctly classified points: $t_n h_m(\mathbf{x}_n) = +1$ $\Rightarrow$ collect in $\mathcal{T}_m$
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- Rewrite the error function as

$$E = e^{-\alpha_m/2} \sum_{n \in \mathcal{T}_m} w_n^{(m)} + e^{\alpha_m/2} \sum_{n \in \mathcal{F}_m} w_n^{(m)}$$

$$= \left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$$

AdaBoost – Minimizing Exponential Error

- Minimize with respect to $h_m(\mathbf{x})$: $\quad \frac{\partial E}{\partial h_m(\mathbf{x}_n)} \stackrel{!}{=} 0$

$$E = \underbrace{\left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right)}_{=\ const.} \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + \underbrace{e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}}_{=\ const.}$$

$\Rightarrow$ This is equivalent to minimizing

$$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$

(our weighted error function from step 2a) of the algorithm)

$\Rightarrow$ *We're on the right track. Let's continue…*

AdaBoost – Minimizing Exponential Error

- Minimize with respect to α_m: $\frac{\partial E}{\partial \alpha_m} \stackrel{!}{=} 0$

$$E = \left(e^{\alpha_m/2} - e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) + e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$$

$$\left(\cancel{\tfrac{1}{2}} e^{\alpha_m/2} + \cancel{\tfrac{1}{2}} e^{-\alpha_m/2}\right) \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n) \stackrel{!}{=} \cancel{\tfrac{1}{2}} e^{-\alpha_m/2} \sum_{n=1}^{N} w_n^{(m)}$$

weighted error

$$\epsilon_m := \frac{\sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}_n) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}} = \frac{e^{-\alpha_m/2}}{e^{\alpha_m/2} + e^{-\alpha_m/2}}$$

$$\epsilon_m = \frac{1}{e^{\alpha_m} + 1}$$

$\Rightarrow$ *Update for the α coefficients:* $$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$

AdaBoost – Minimizing Exponential Error

- Remaining step: update the weights
  - Recall that

$$E = \sum_{n=1}^{N} \underbrace{w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\}}_{\text{This becomes } w_n^{(m+1)} \text{ in the next iteration.}}$$

  - Therefore

$$\begin{aligned} w_n^{(m+1)} &= w_n^{(m)} \exp\left\{-\frac{1}{2} t_n \alpha_m h_m(\mathbf{x}_n)\right\} \\ &= \ldots \\ &= w_n^{(m)} \exp\left\{\alpha_m I(h_m(\mathbf{x}_n) \neq t_n)\right\} \end{aligned}$$

$\Rightarrow$ *Update for the weight coefficients.*

AdaBoost – Final Algorithm

1. Initialization: Set $w_n^{(1)} = \frac{1}{N}$ for $n = 1,\dots,N$.
2. For $m = 1,\dots,M$ iterations
   a) Train a new weak classifier $h_m(\mathbf{x})$ using the current weighting coefficients $\mathbf{W}^{(m)}$ by minimizing the weighted error function
   $$J_m = \sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)$$
   b) Estimate the weighted error of this classifier on $\mathbf{X}$:
   $$\epsilon_m = \frac{\sum_{n=1}^{N} w_n^{(m)} I(h_m(\mathbf{x}) \neq t_n)}{\sum_{n=1}^{N} w_n^{(m)}}$$
   c) Calculate a weighting coefficient for $h_m(\mathbf{x})$:
   $$\alpha_m = \ln\left\{\frac{1-\epsilon_m}{\epsilon_m}\right\}$$
   d) Update the weighting coefficients:
   $$w_n^{(m+1)} = w_n^{(m)} \exp\left\{\alpha_m I(h_m(\mathbf{x}_n) \neq t_n)\right\}$$

AdaBoost – Analysis

- Result of this derivation
  - We now know that AdaBoost minimizes an exponential error function in a sequential fashion.
  - This allows us to analyze AdaBoost's behavior in more detail.
  - In particular, we can see how robust it is to outlier data points.

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  - Extensions
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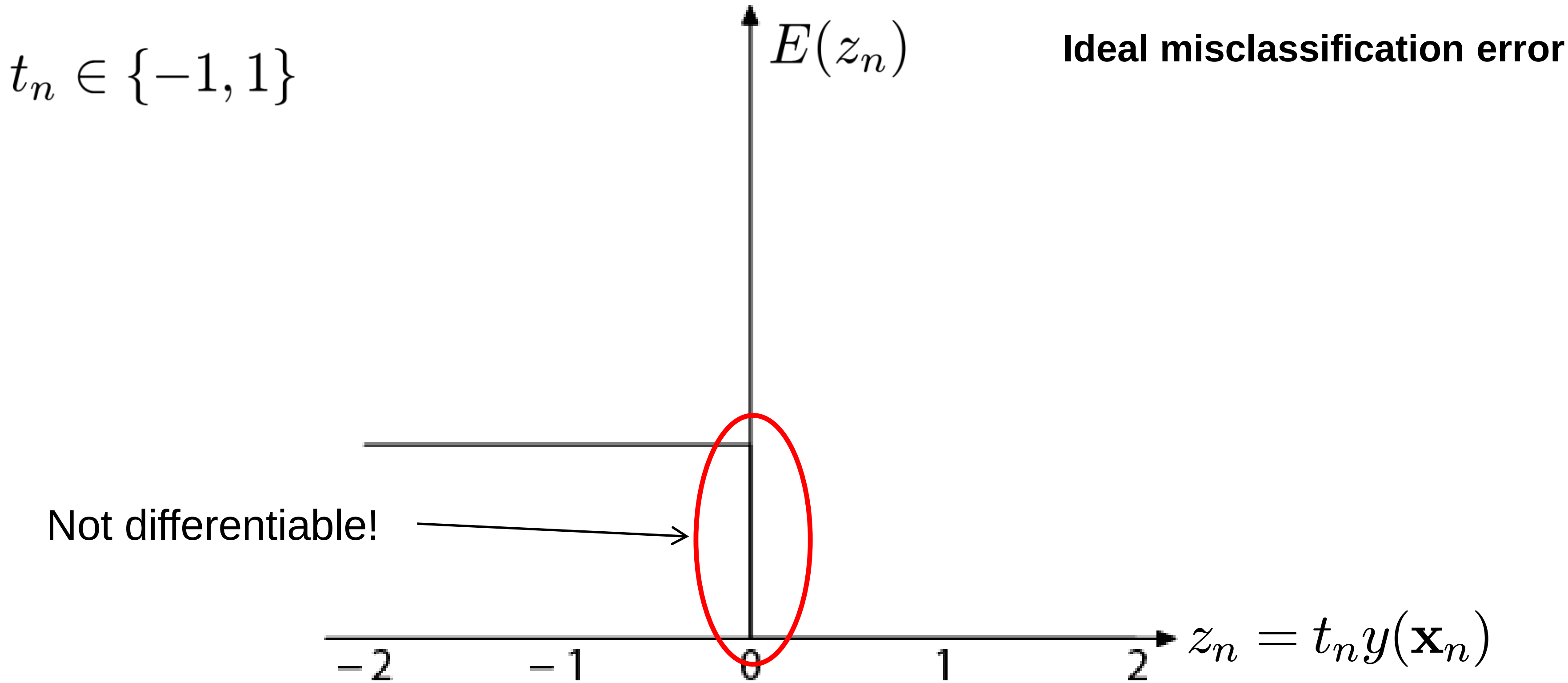
  - Comparing Error Functions
- Applications
  - AdaBoost for face detection
- Decision Trees
  - CART
  - Impurity measures, Stopping criterion, Pruning
  - Extensions, Issues
  - Historical development: ID3, C4.5

Recap: Error Functions

$t_n \in \{-1, 1\}$



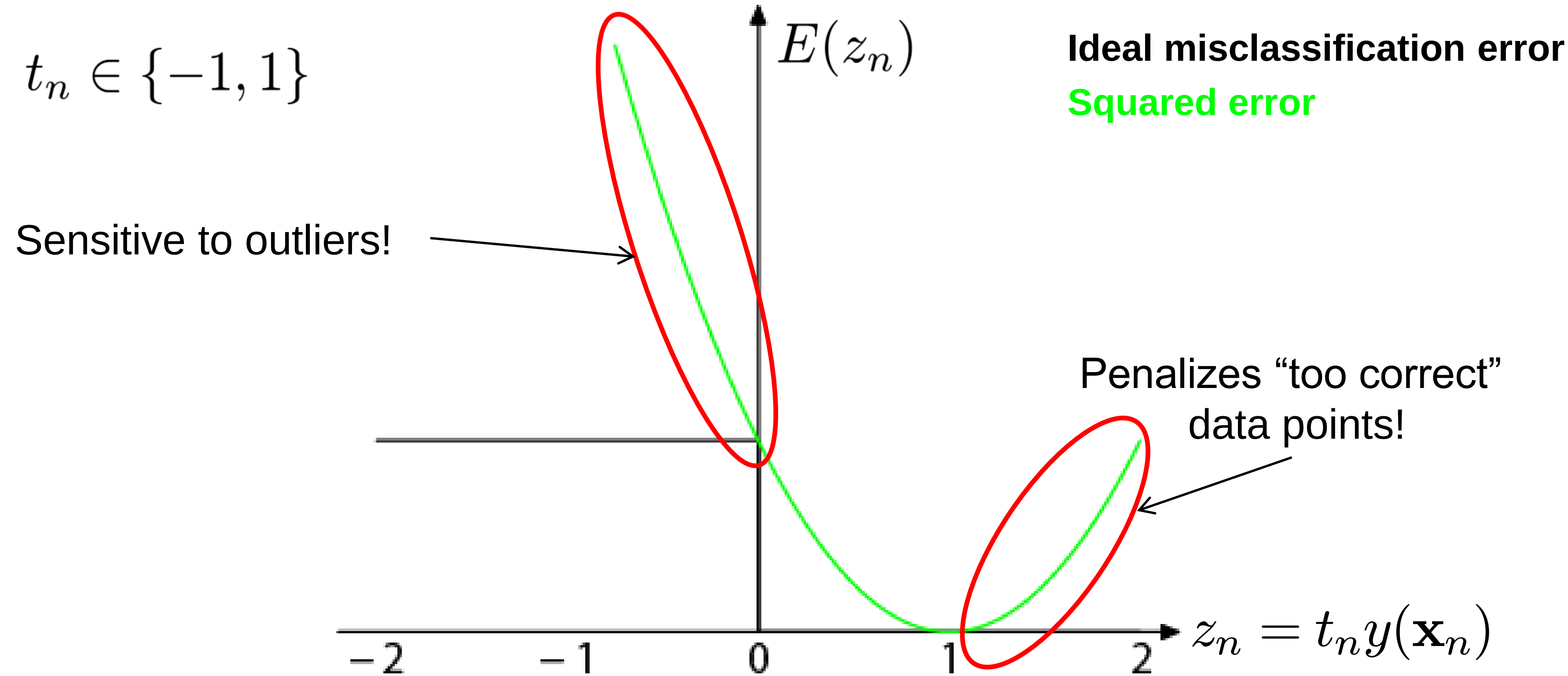
- Ideal misclassification error function (black)
  - This is what we want to approximate,
  - Unfortunately, it is not differentiable.
  - The gradient is zero for misclassified points.

  $\Rightarrow$ We cannot minimize it by gradient descent.

Image source: Bishop, 2006

Recap: Error Functions

$t_n \in \{-1, 1\}$

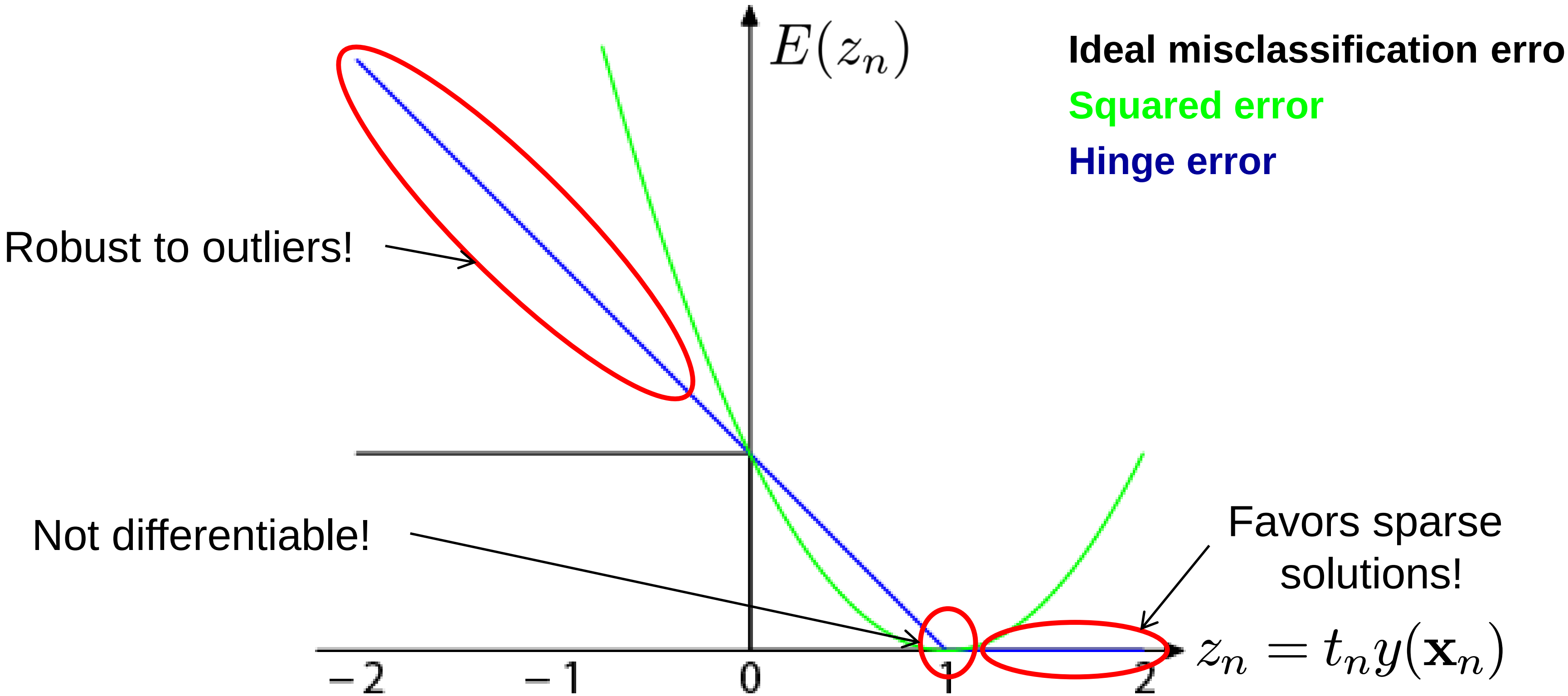


- Squared error used in Least-Squares Classification
  - Very popular, leads to closed-form solutions.
  - However, sensitive to outliers due to squared penalty.
  - Penalizes "too correct" data points

$\Rightarrow$ Generally does not lead to good classifiers.

Image source: Bishop, 2006

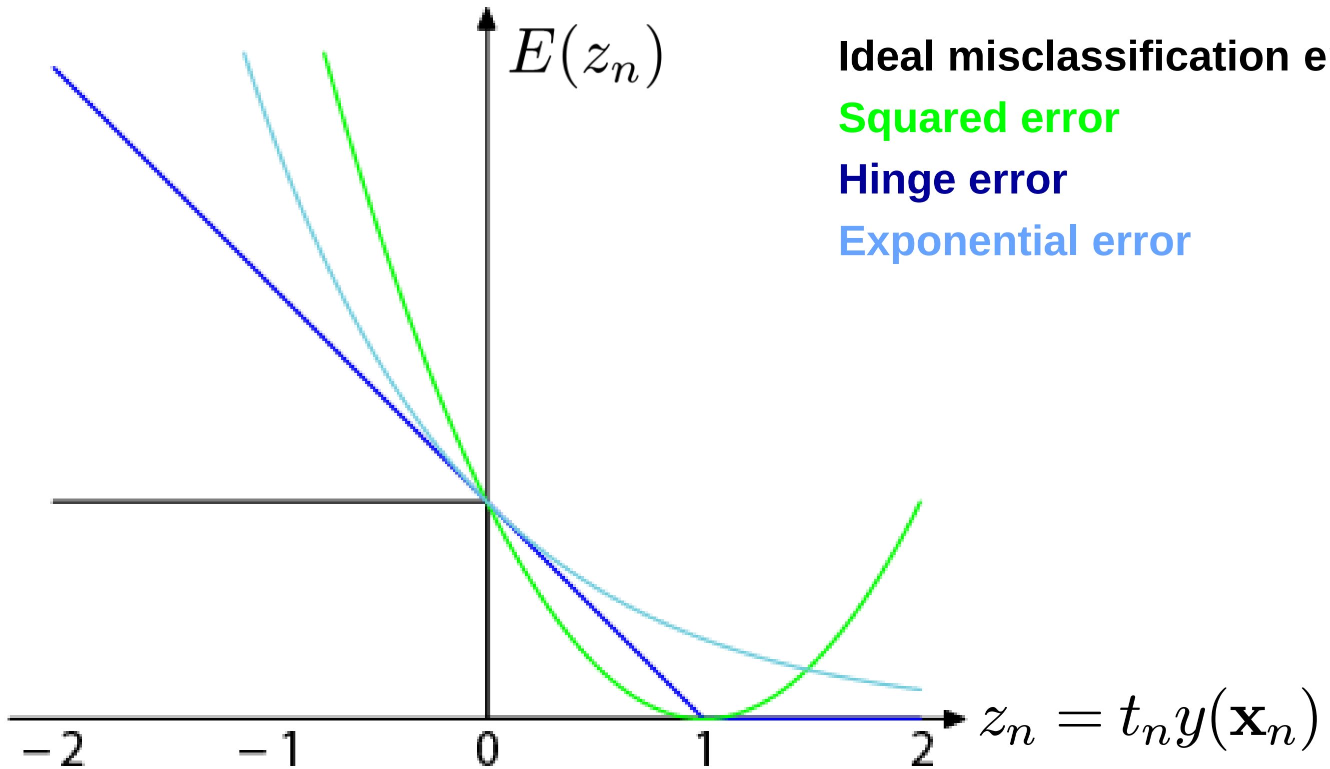
Recap: Error Functions



- "Hinge error" used in SVMs
  - Zero error for points outside the margin ($z_n > 1$) $\Rightarrow$ sparsity
  - Linear penalty for misclassified points ($z_n < 1$) $\Rightarrow$ robustness
  - Not differentiable around $z_n = 1$ $\Rightarrow$ Cannot be optimized directly.

Image source: Bishop, 2006

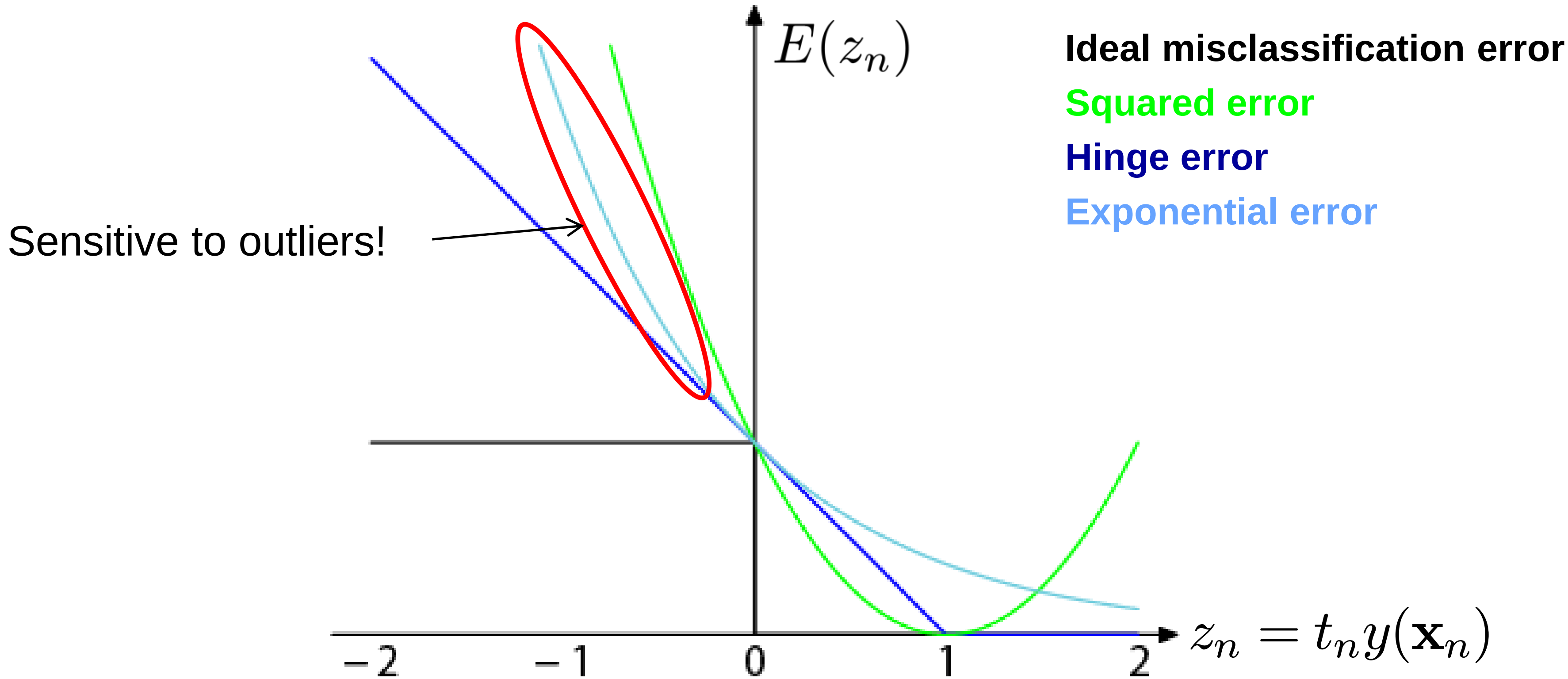
Discussion: AdaBoost Error Function



- Exponential error used in AdaBoost
  - Continuous approximation to ideal misclassification function.
  - Sequential minimization leads to simple AdaBoost scheme.
  - Properties?

Image source: Bishop, 2006

Discussion: AdaBoost Error Function

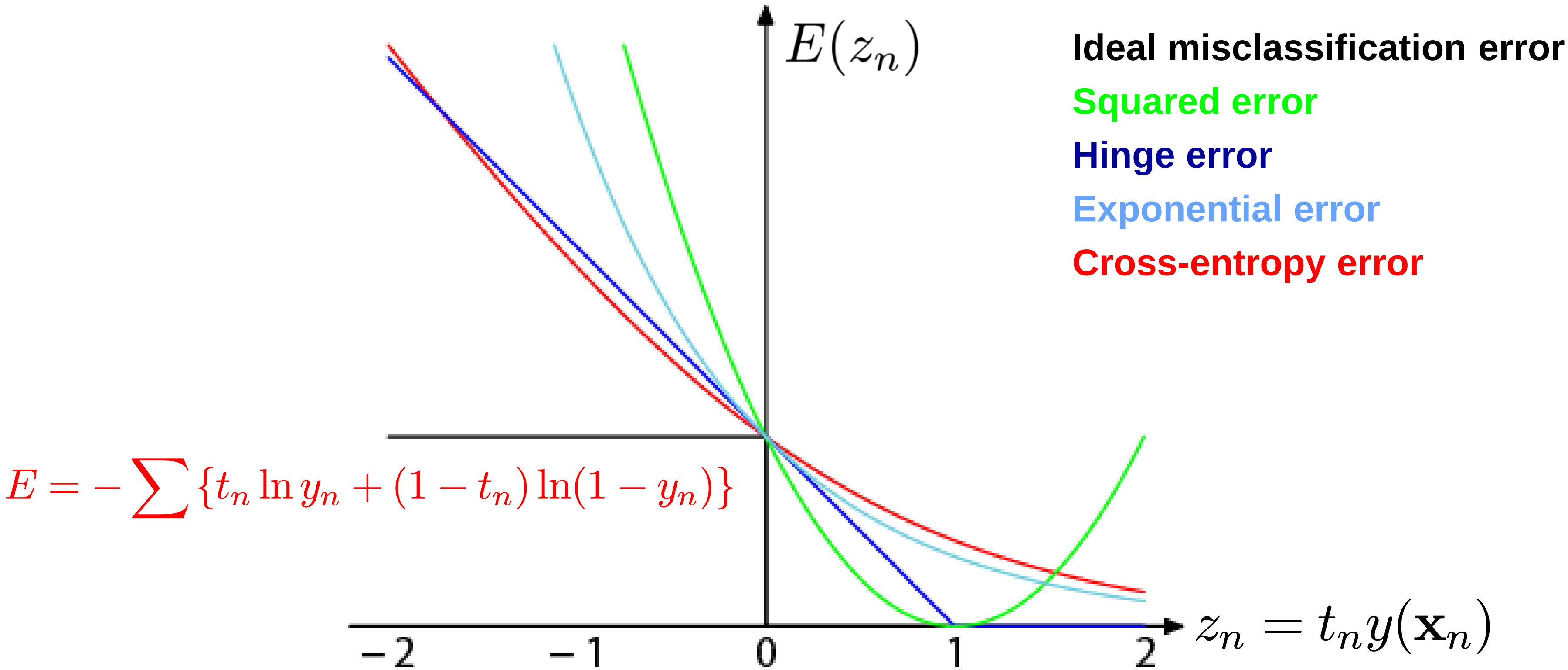


- Exponential error used in AdaBoost
  - No penalty for too correct data points, fast convergence.
  - Disadvantage: exponential penalty for large negative values!

  $\Rightarrow$ Less robust to outliers or misclassified data points!

Image source: Bishop, 2006

Discussion: Other Possible Error Functions



- "Cross-entropy error" used in Logistic Regression
  - Similar to exponential error for $z>0$.
  - Only grows linearly with large negative values of z.

  $\Rightarrow$ Make AdaBoost more robust by switching to this error function.

  $\Rightarrow$ "GentleBoost"

Image source: Bishop, 2006

Summary: AdaBoost

- Properties
  - Simple combination of multiple classifiers.
  - Easy to implement.
  - Can be used with many different types of classifiers.
    - None of them needs to be too good on its own.
    - In fact, they only have to be slightly better than chance.
  - Commonly used in many areas.
  - Empirically good generalization capabilities.

- Limitations
  - Original AdaBoost sensitive to mislabeled training data points.
    - Because of exponential error function.
    - Improvement by GentleBoost
  - Single-class classifier
    - Multiclass extensions available

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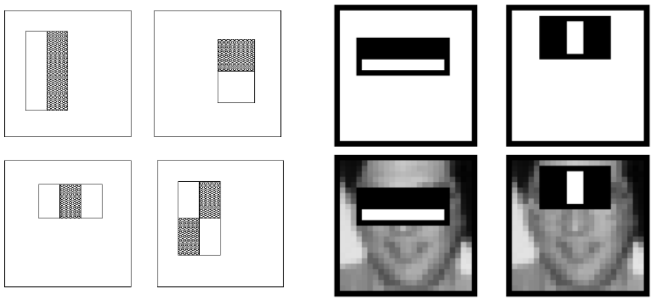
Example Application: Face Detection

- Frontal faces are a good example of a class where global appearance models + a sliding window detection approach fit well:
  - Regular 2D structure
  - Center of face almost shaped like a “patch”/window

- Now we’ll take AdaBoost and see how the Viola-Jones face detector works

Feature extraction

"Rectangular" filters

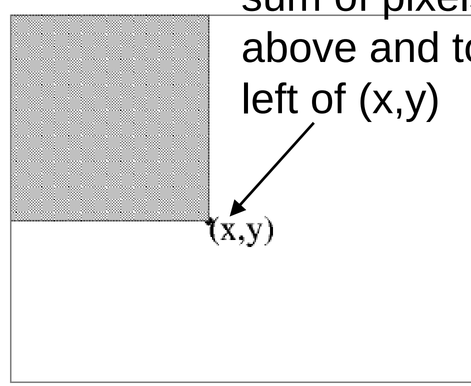


Feature output is difference between adjacent regions

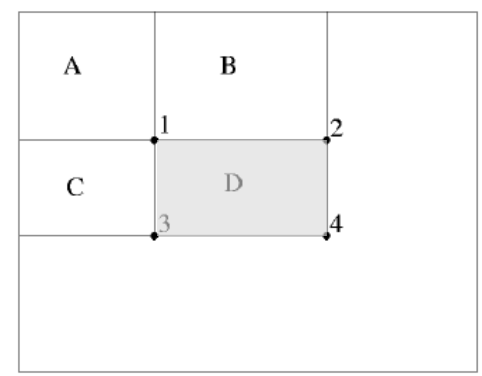
Efficiently computable with integral image: any sum can be computed in constant time

Avoid scaling images → scale features directly for same cost

Value at (x,y) is sum of pixels above and to the left of (x,y)



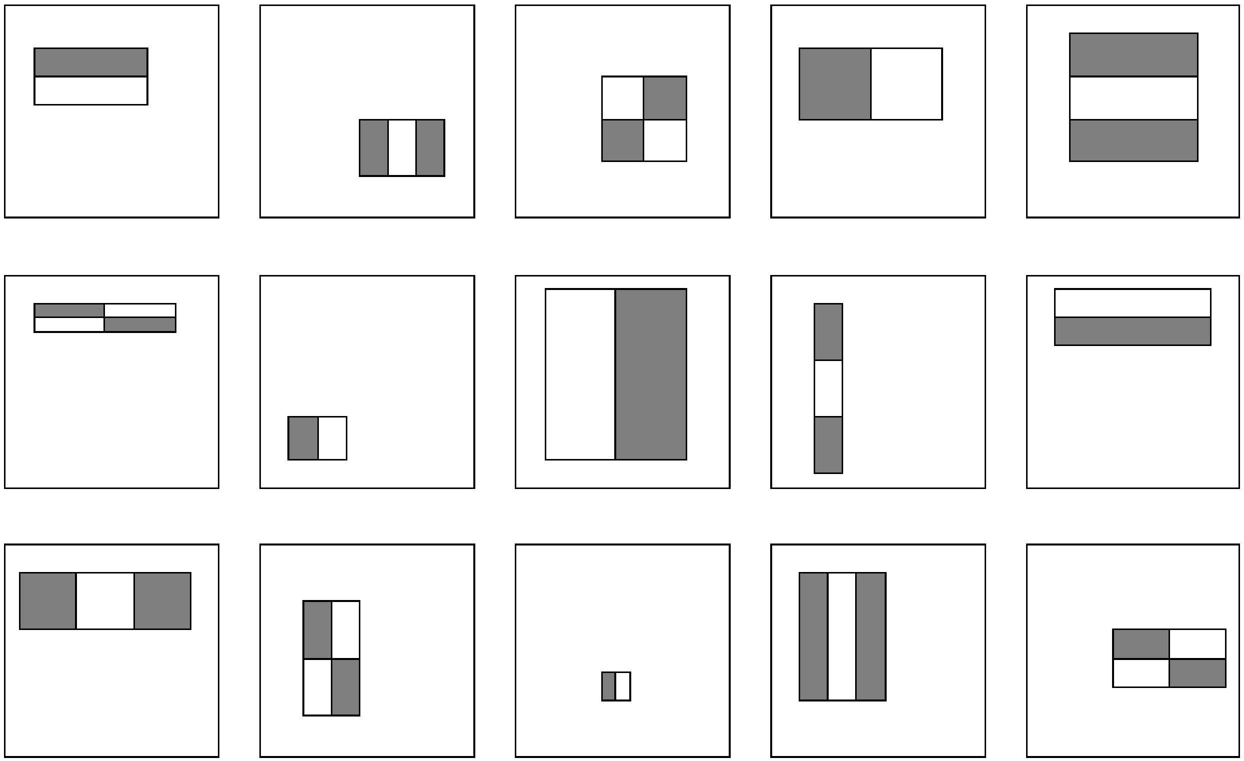
Integral image



$$D = I(1) + I(4) - (I(2) + I(3))$$

[Viola & Jones, CVPR 2001]

Large Library of Filters



Considering all possible filter parameters: position, scale, and type:

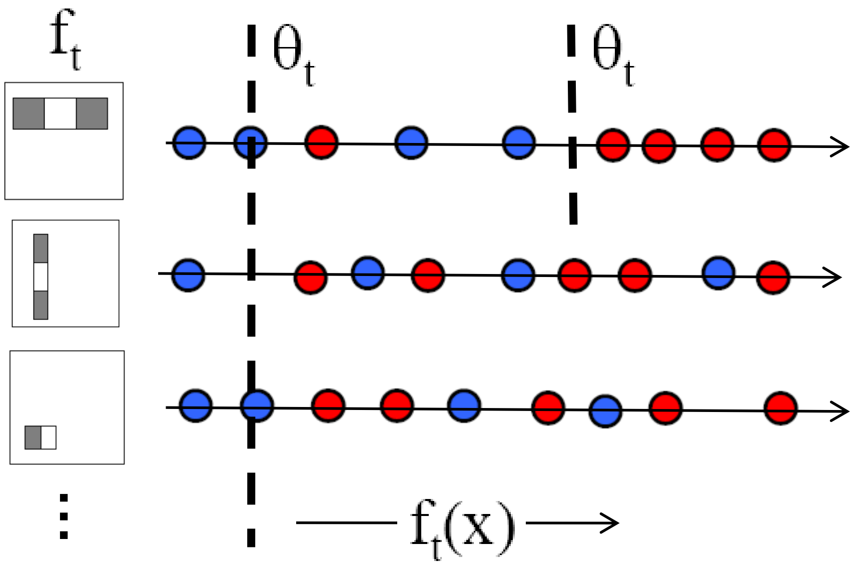
180,000+ possible features associated with each 24 x 24 window

Use AdaBoost both to select the informative features and to form the classifier

[Viola & Jones, CVPR 2001]

AdaBoost for Feature+Classifier Selection

- Want to select the single rectangle feature and threshold that best separates positive (faces) and negative (non-faces) training examples, in terms of *weighted* error.



Outputs of a possible rectangle feature on faces and non-faces.

Resulting weak classifier:

$$h_t(x) = \begin{cases} +1 & \text{if } f_t(x) > \theta_t \\ -1 & \text{otherwise} \end{cases}$$

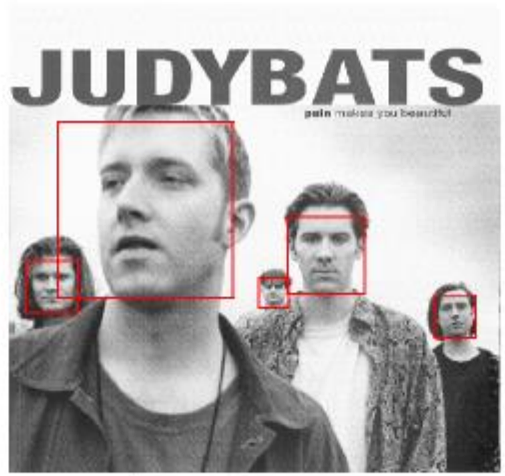
For next round, reweight the examples according to errors, choose another filter/threshold combo.

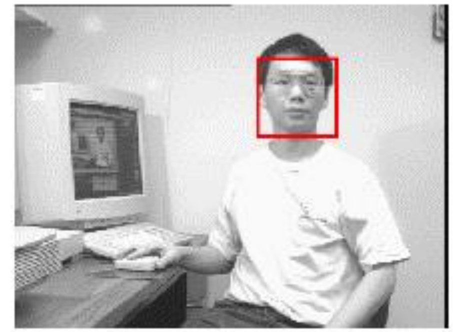
AdaBoost for Efficient Feature Selection

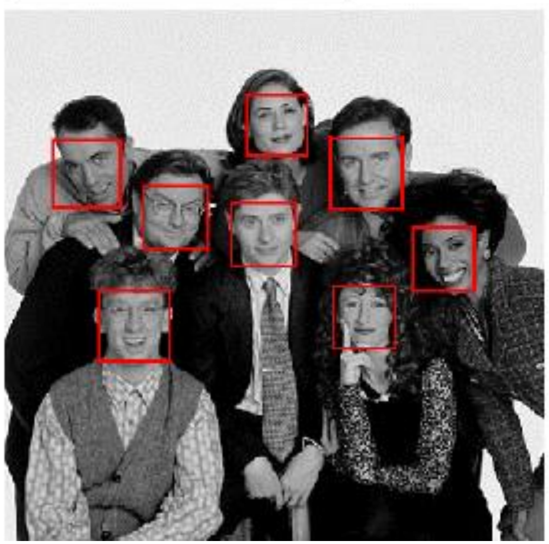
- Image features = weak classifiers
- For each round of boosting:
  - Evaluate each rectangle filter on each example
  - Sort examples by filter values
  - Select best threshold for each filter (min error)
    - Sorted list can be quickly scanned for the optimal threshold
  - Select best filter/threshold combination
  - Weight on this features is a simple function of error rate
  - Reweight examples

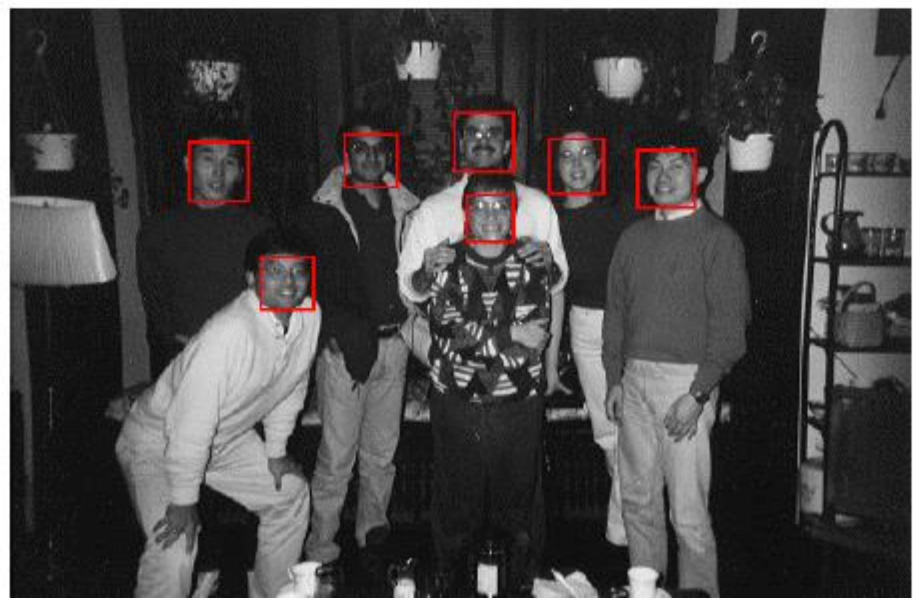
P. Viola, M. Jones, Robust Real-Time Face Detection, IJCV, Vol. 57(2), 2004.
(first version appeared at CVPR 2001)

Viola-Jones Face Detector: Results

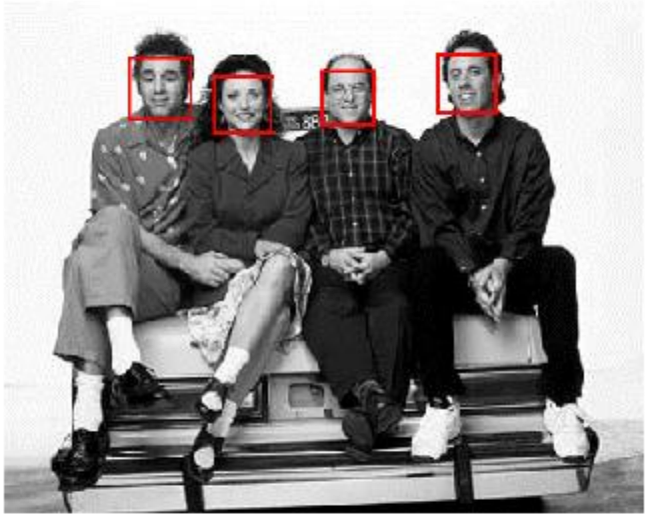


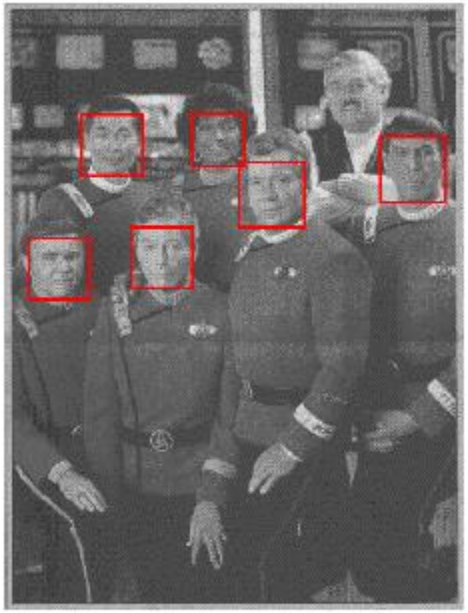


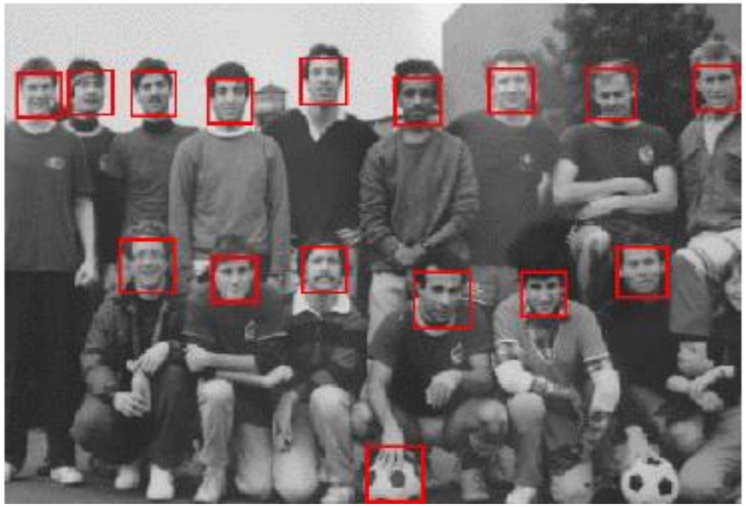


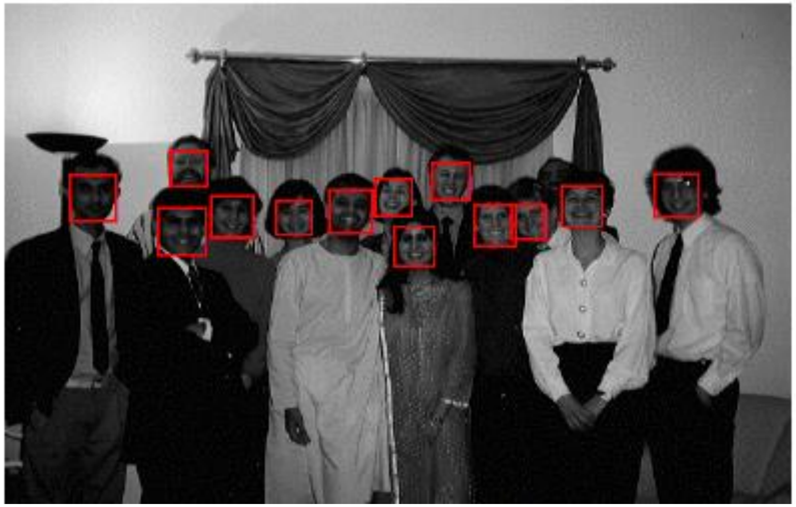


Viola-Jones Face Detector: Results







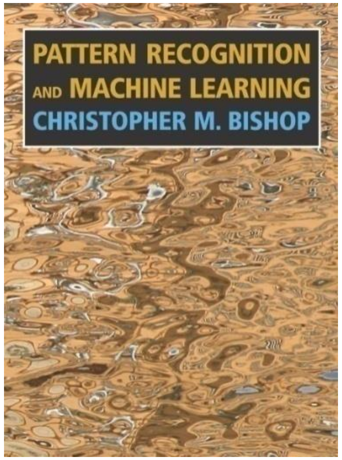


Slide credit: Kristen Grauman

References and Further Reading

- More information on Classifier Combination and Boosting can be found in Chapters 14.1-14.3 of Bishop’s book.

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006



- A more in-depth discussion of the statistical interpretation of AdaBoost is available in the following paper:
  - J. Friedman, T. Hastie, R. Tibshirani, Additive Logistic Regression: a Statistical View of Boosting, *The Annals of Statistics*, Vol. 38(2), pages 337-374, 2000.

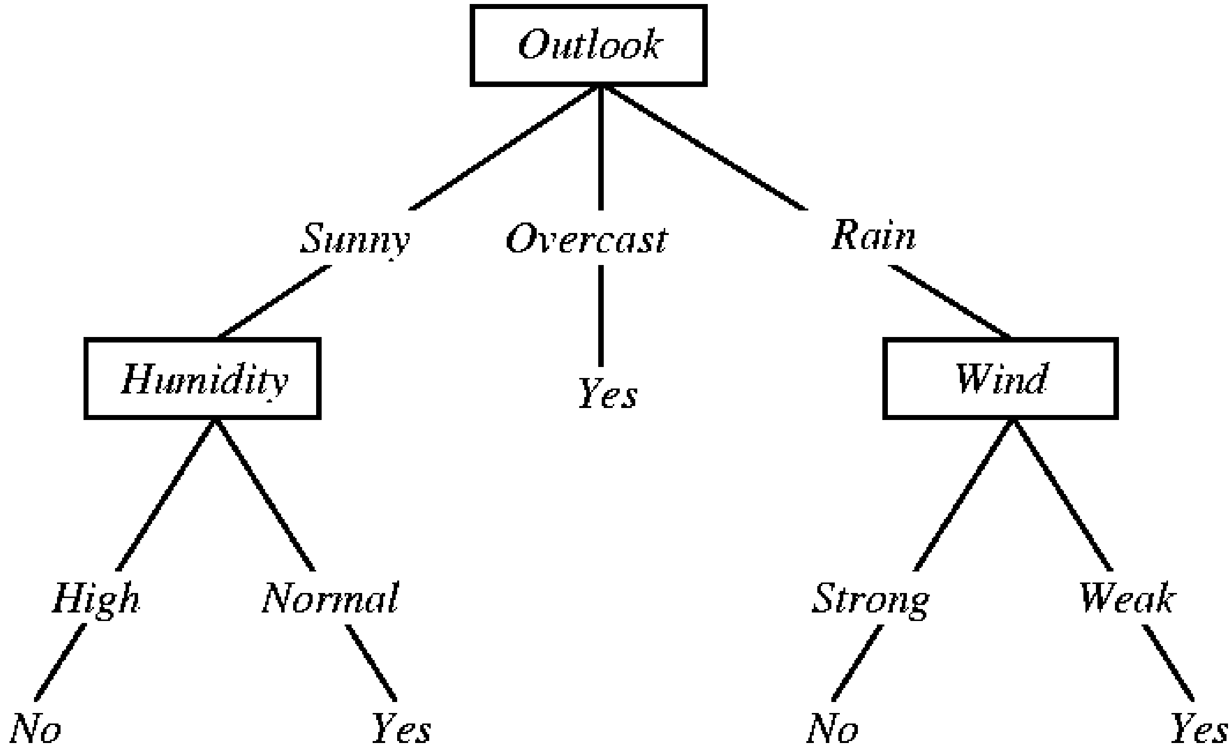
Topics of This Lecture

- AdaBoost
  - Algorithm
  - Analysis
  - Extensions
- Analysis
  - Comparing Error Functions
- Applications
  - AdaBoost for face detection
- Decision Trees
  - CART
  - Impurity measures, Stopping criterion, Pruning
  - Extensions, Issues
  - Historical development: ID3, C4.5

Decision Trees

- Very old technique
  - Origin in the 60s, might seem outdated.
- But…
  - Can be used for problems with nominal data
    - E.g. attributes color $\in$ {red, green, blue} or weather $\in$ {sunny, rainy}.
    - Discrete values, no notion of similarity or even ordering.
  - Interpretable results
    - Learned trees can be written as sets of if-then rules.
  - Methods developed for handling missing feature values.
  - Successfully applied to broad range of tasks
    - E.g. Medical diagnosis
    - E.g. Credit risk assessment of loan applicants
  - Some interesting novel developments building on top of them…

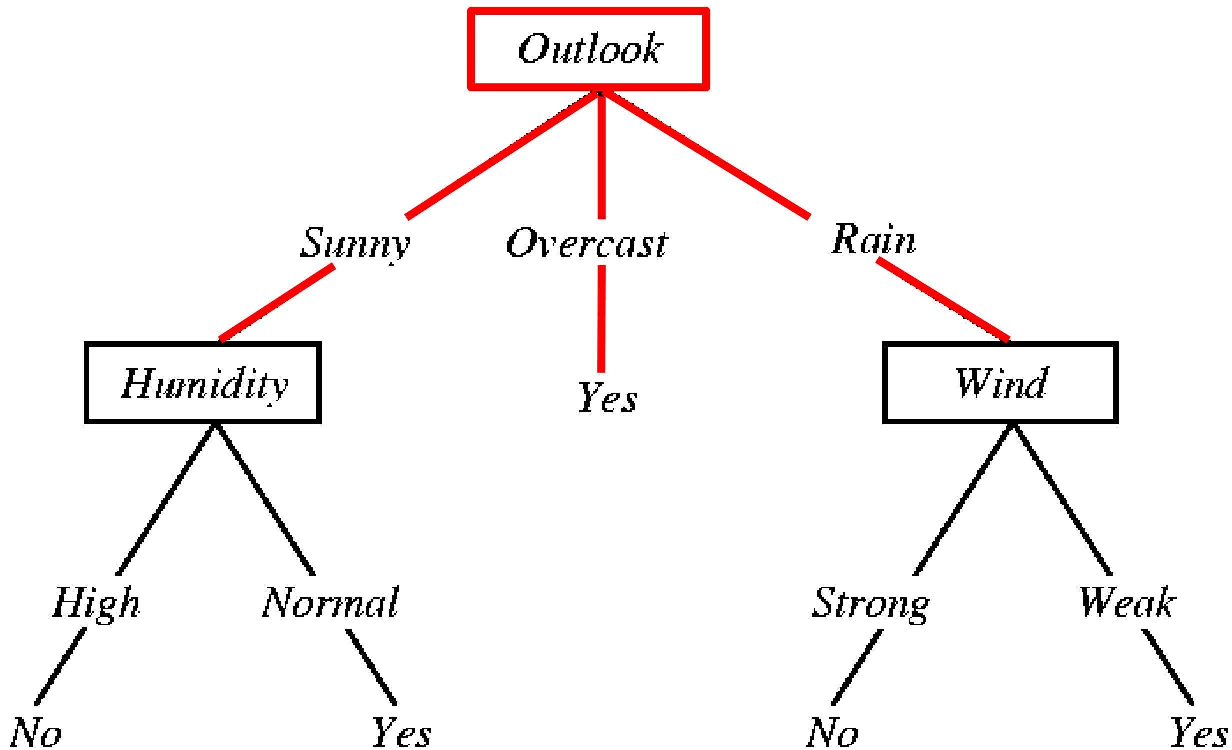
Decision Trees



- Example:
  - "Classify Saturday mornings according to whether they're suitable for playing tennis."

Image source: T. Mitchell, 1997

Decision Trees

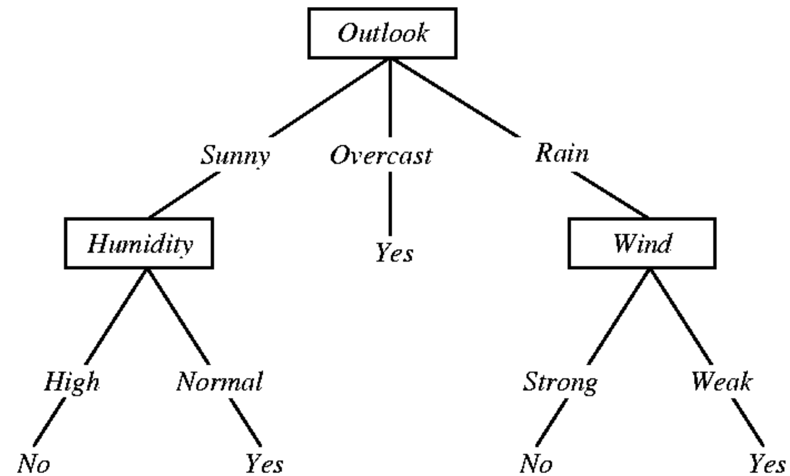


- Elements
  - Each node specifies a test for some attribute.
  - Each branch corresponds to a possible value of the attribute.

Image source: T. Mitchell, 1997

Decision Trees

- Assumption
  - Links must be mutually distinct and exhaustive
  - I.e. one and only one link will be followed at each step.



- Interpretability
  - Information in a tree can then be rendered as logical expressions.
  - In our example:

$$\begin{aligned} &(Outlook = Sunny \wedge Humidity = Normal) \\ \vee\ &(Outlook = Overcast) \\ \vee\ &(Outlook = Rain \wedge Wind = Weak) \end{aligned}$$

Image source: T. Mitchell, 1997

Training Decision Trees

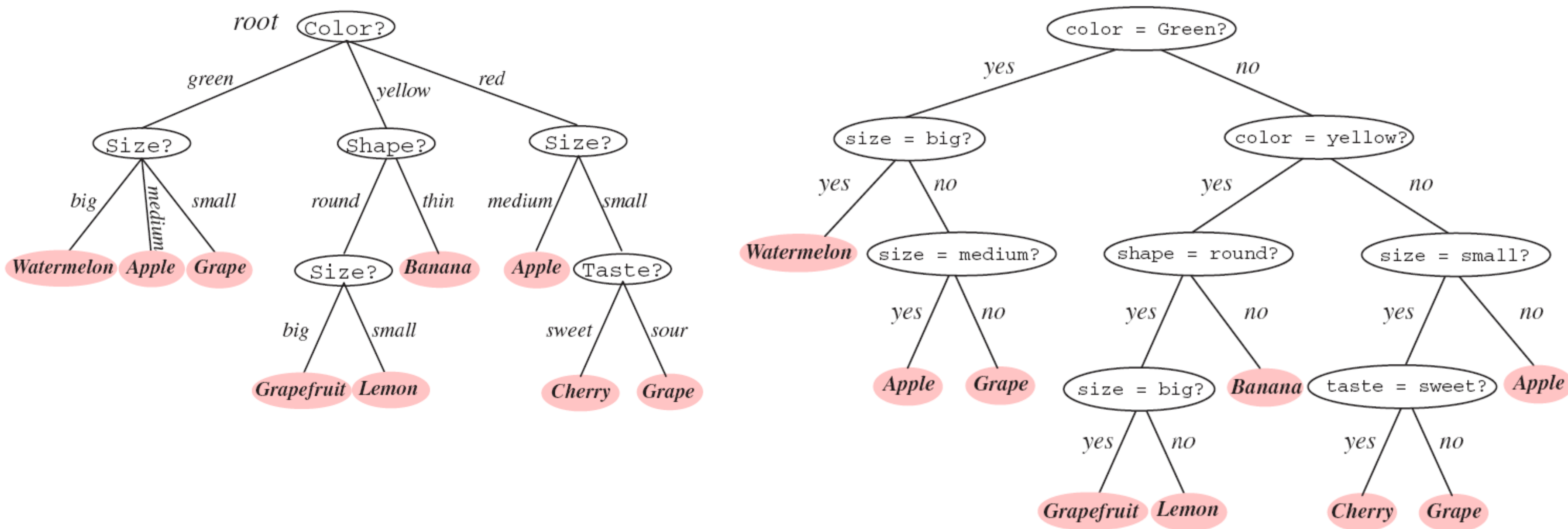
- Finding the optimal decision tree is NP-hard…
- Common procedure: Greedy top-down growing
  - Start at the root node.
  - Progressively split the training data into smaller and smaller subsets.
  - In each step, pick the *best attribute* to split the data.
  - If the resulting subsets are pure (only one label) or if no further attribute can be found that splits them, terminate the tree.
  - Else, recursively apply the procedure to the subsets.
- CART framework
  - Classification And Regression Trees (Breiman et al. 1993)
  - Formalization of the different design choices.

CART Framework

- Six general questions
  1. Binary or multi-valued problem?
     – I.e. how many splits should there be at each node?
  2. Which property should be tested at a node?
     – I.e. how to select the query attribute?
  3. When should a node be declared a leaf?
     – I.e. when to stop growing the tree?
  4. How can a grown tree be simplified or pruned?
     – Goal: reduce overfitting.
  5. How to deal with impure nodes?
     – I.e. when the data itself is ambiguous.
  6. How should missing attributes be handled?

CART – 1. Number of Splits

- Each multi-valued tree can be converted into an equivalent binary tree:



⇒ Only consider binary trees here…

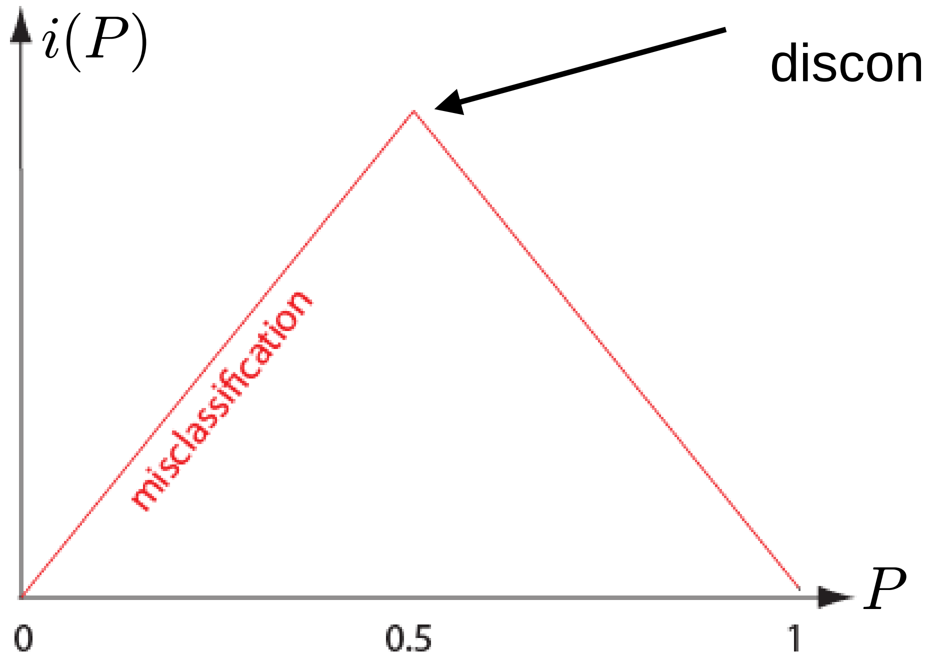
Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – 2. Picking a Good Splitting Feature

- Goal
  - Want a tree that is as simple/small as possible (Occam's razor).
  - But: Finding a minimal tree is an NP-hard optimization problem.

- Greedy top-down search
  - Efficient, but not guaranteed to find the smallest tree.
  - Seek a property T at each node s_j that makes the data in the child nodes as pure as possible.
  - For formal reasons more convenient to define impurity $i(s_j)$.
  - Several possible definitions explored.

CART – Impurity Measures



Problem:
discontinuous derivative!

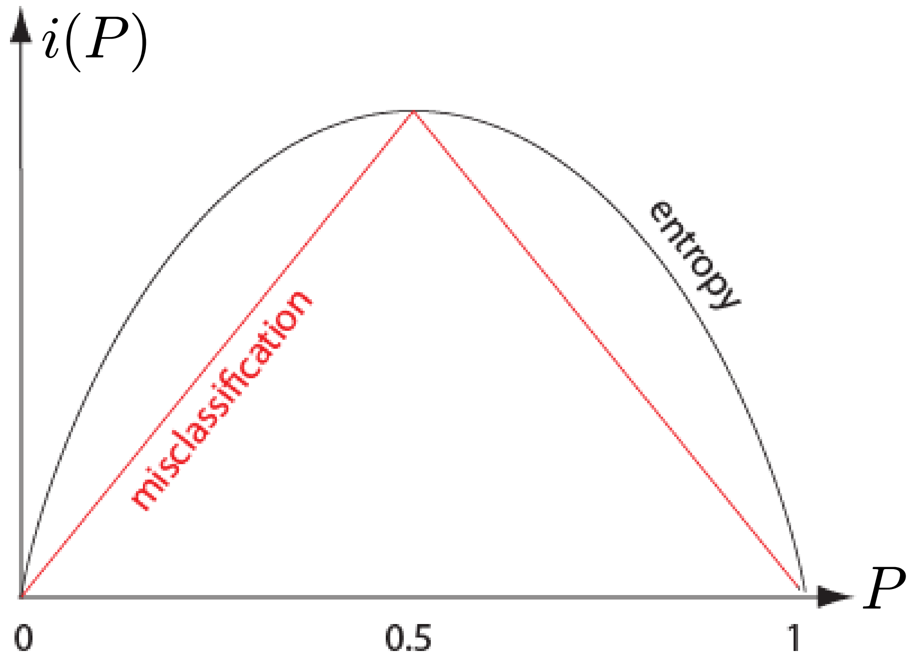
- Misclassification impurity

$$i(s_j) = 1 - \max_k \boxed{p(C_k|s_j)}$$

"Fraction of the training patterns in category $\mathcal{C}_k$ that end up in node s_j."

Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – Impurity Measures



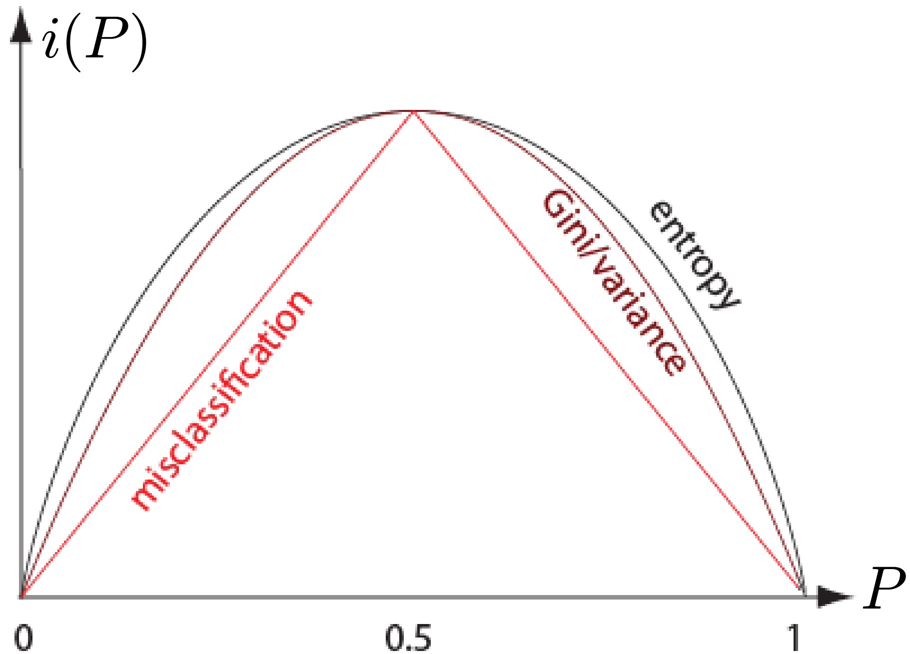
- Entropy impurity

$$i(s_j) = -\sum_k p(C_k|s_j)\log_2 p(C_k|s_j)$$

"Reduction in entropy = gain in information."

Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – Impurity Measures



- Gini impurity (variance impurity)

$$i(s_j) = \sum_{k \neq l} p(C_k|s_j)\, p(C_l|s_j)$$

$$= \frac{1}{2}\left[1 - \sum_k p^2(C_k|s_j)\right]$$

"Expected error rate at node s_j if the category label is selected randomly."

Image source: R.O. Duda, P.E. Hart, D.G. Stork, 2001

CART – Impurity Measures

- Which impurity measure should we choose?
  - Some problems with misclassification impurity.
    - Discontinuous derivative.

      $\Rightarrow$ Problems when searching over continuous parameter space.
    - Sometimes misclassification impurity does not decrease when Gini impurity would.
  - Both entropy impurity and Gini impurity perform well.
    - No big difference in terms of classifier performance.
    - In practice, stopping criterion and pruning method are often more important.

CART – 2. Picking a Good Splitting Feature

- Application
  - Select the query that decreases impurity the most

$$\Delta i(s_j) = i(s_j) - P_L i(s_{j,L}) - (1 - P_L) i(s_{j,R})$$

$P_L =$ fraction of points at left child node $s_{j,L}$

- Multiway generalization (gain ratio impurity):
  - Maximize

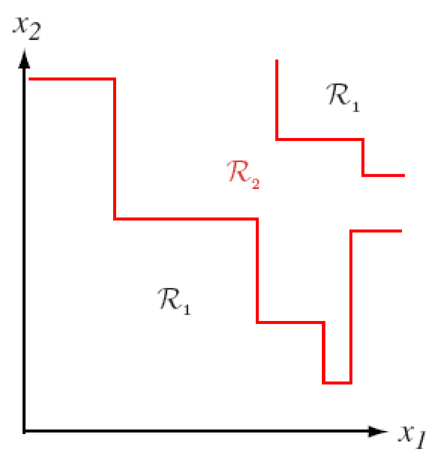
$$\Delta i(s_j) = \frac{1}{Z}\left(i(s_j) - \sum_{m=1}^{M} P_m i(s_{j,m}) \right)$$

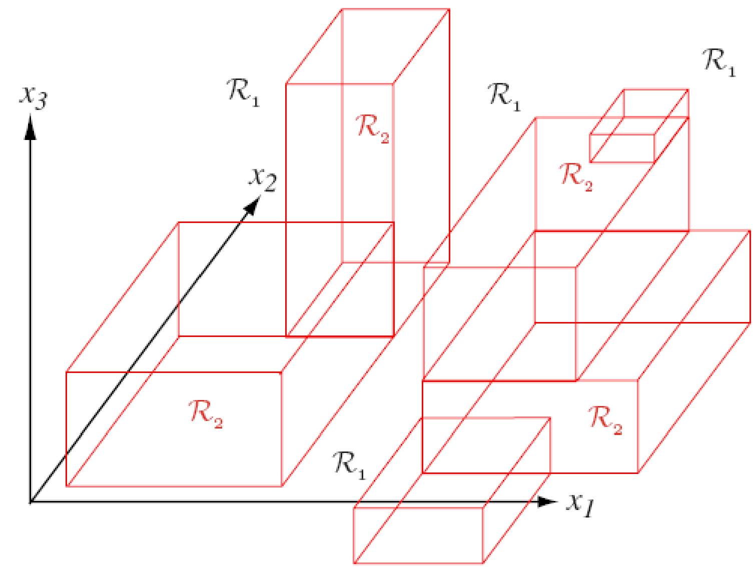
  - where the normalization factor ensures that large K are not inherently favored:

$$Z = -\sum_{m=1}^{M} P_m \log_2 P_m$$

CART – Picking a Good Splitting Feature

- For efficiency, splits are often based on a single feature
  - "Monothetic decision trees"



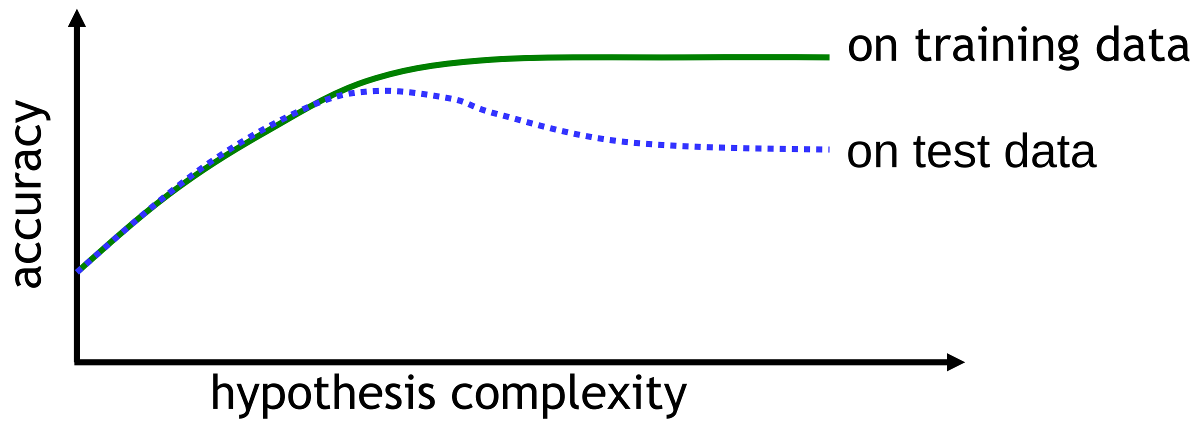


- Evaluating candidate splits
  - Nominal attributes: exhaustive search over all possibilities.
  - Real-valued attributes: only need to consider changes in label.
    - Order all data points based on attribute x_i.
    - Only need to test candidate splits where *label*(x_i) ≠ *label*(x_{i+1}).

CART – 3. When to Stop Splitting

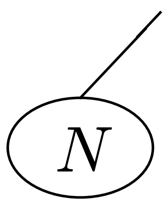
- Problem: Overfitting
  - Learning a tree that classifies the training data perfectly may not lead to the tree with the best generalization to unseen data.
  - Reasons
    - Noise or errors in the training data.
    - Poor decisions towards the leaves of the tree that are based on very little data.

- Typical behavior

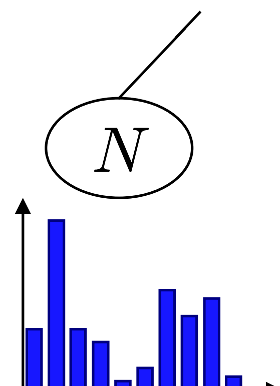


CART – Overfitting Prevention (Pruning)

- Two basic approaches for decision trees
  - Prepruning: Stop growing tree as some point during top-down construction when there is no longer sufficient data to make reliable decisions.
  - Postpruning: Grow the full tree, then remove subtrees that do not have sufficient evidence.
- Label leaf resulting from pruning with the majority class of the remaining data, or a class probability distribution.



$$\mathcal{C}_N = \arg\max_k p(\mathcal{C}_k|N)$$



$p(\mathcal{C}_k|N)$

Decision Trees – Computational Complexity

- Given
  - Data points $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
  - Dimensionality D
- Complexity
  - Storage: $O(N)$
  - Test runtime: $O(\log N)$
  - Training runtime: $O(DN^2 \log N)$
    - Most expensive part.
    - Critical step: selecting the optimal splitting point.
    - Need to check D dimensions, for each need to sort N data points.

$$O(DN \log N)$$

Summary: Decision Trees

- Properties
  - Simple learning procedure, fast evaluation.
  - Can be applied to metric, nominal, or mixed data.
  - Often yield interpretable results.

Summary: Decision Trees

- Limitations
  - Often produce noisy (bushy) or weak (stunted) classifiers.
  - Do not generalize too well.
  - Training data fragmentation:
    - As tree progresses, splits are selected based on less and less data.
  - Overtraining and undertraining:
    - Deep trees: fit the training data well, will not generalize well to new test data.
    - Shallow trees: not sufficiently refined.
  - Stability
    - Trees can be very sensitive to details of the training points.
    - If a single data point is only slightly shifted, a radically different tree may come out!

    $\Rightarrow$ Result of discrete and greedy learning procedure.
  - Expensive learning step
    - Mostly due to costly selection of optimal split.

References and Further Reading

- More information on Decision Trees can be found in Chapters 8.2-8.4 of Duda & Hart.

R.O. Duda, P.E. Hart, D.G. Stork
Pattern Classification
2nd Ed., Wiley-Interscience, 2000