Introduction to Machine Learning

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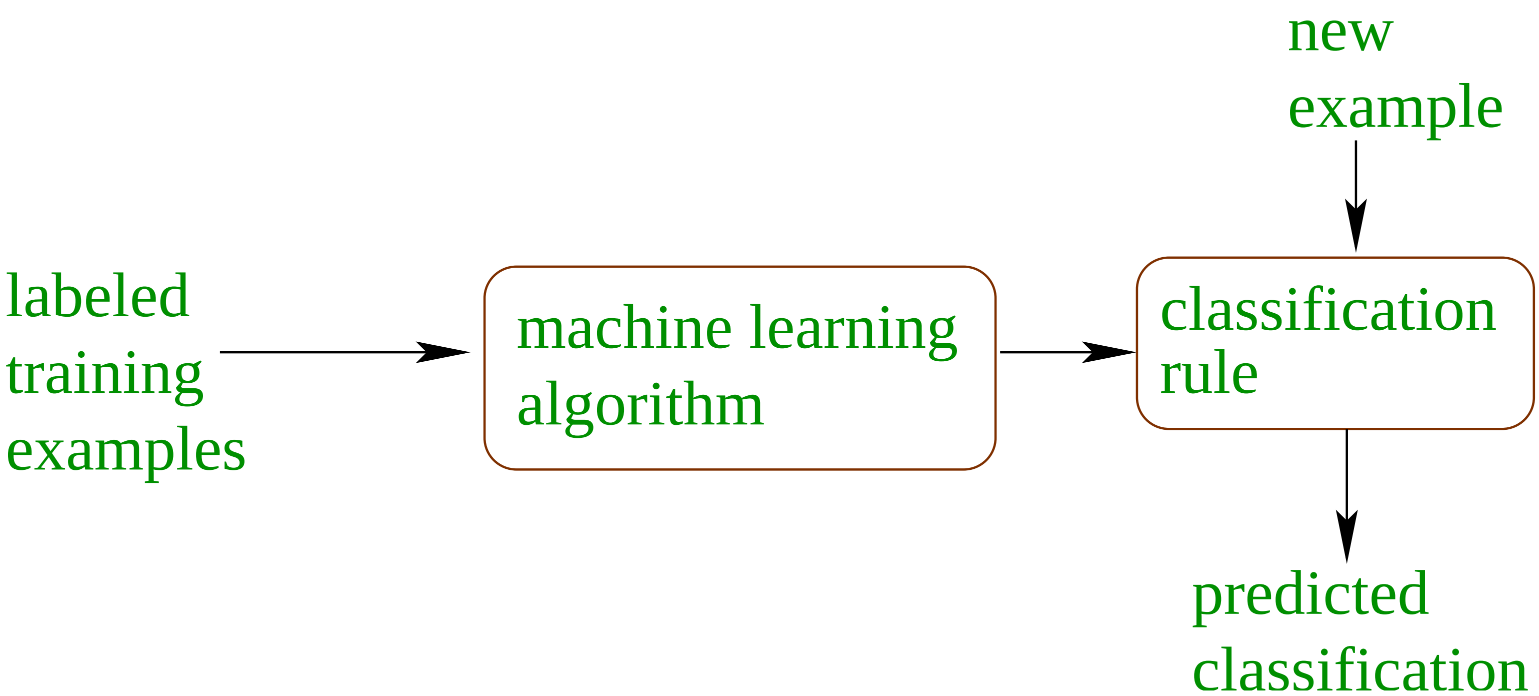
Machine Learning

- studies how to automatically learn to make accurate predictions based on past observations
- classification problems:
  - classify examples into given set of categories



Examples of Classification Problems

- bioinformatics
  - classify proteins according to their function
  - predict if patient will respond to particular drug/therapy based on microarray profiles
  - predict if molecular structure is a small-molecule binding site
- text categorization (e.g., spam filtering)
- fraud detection
- optical character recognition
- machine vision (e.g., face detection)
- natural-language processing (e.g., spoken language understanding)
- market segmentation (e.g.: predict if customer will respond to promotion)

Characteristics of Modern Machine Learning

- primary goal: highly accurate predictions on test data
  - goal is not to uncover underlying “truth”
- methods should be general purpose, fully automatic and “off-the-shelf”
  - however, in practice, incorporation of prior, human knowledge is crucial
- rich interplay between theory and practice
- emphasis on methods that can handle large datasets

Why Use Machine Learning?

- advantages:
  - often much more accurate than human-crafted rules (since data driven)
  - humans often incapable of expressing what they know (e.g., rules of English, or how to recognize letters), but can easily classify examples
  - automatic method to search for hypotheses explaining data
  - cheap and flexible — can apply to any learning task
- disadvantages
  - need a lot of labeled data
  - error prone — usually impossible to get perfect accuracy
  - often difficult to discern what was learned

This Talk

- conditions for accurate learning
- two state-of-the-art algorithms:
  - boosting
  - support-vector machines

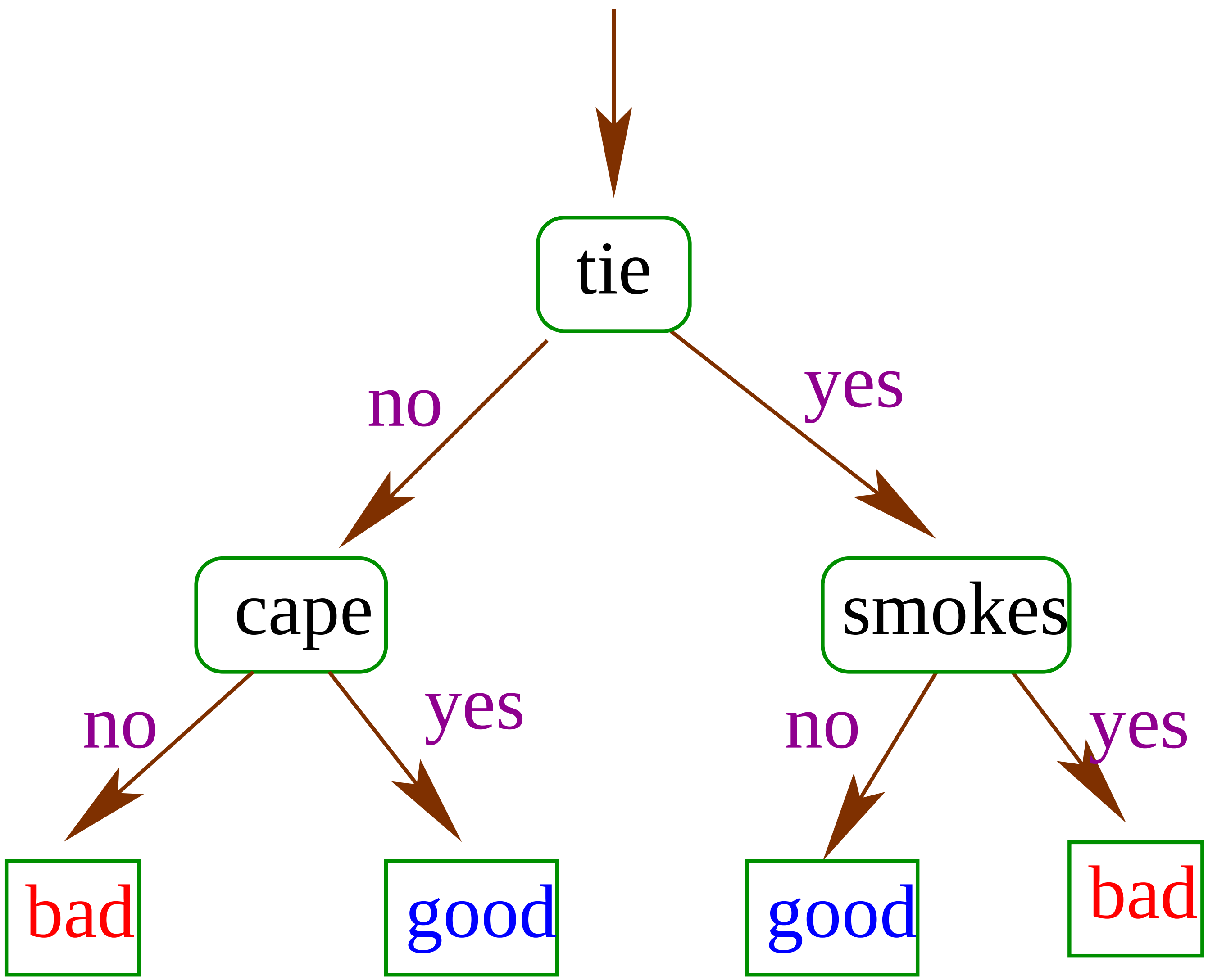
Conditions for Accurate Learning

Example: Good versus Evil

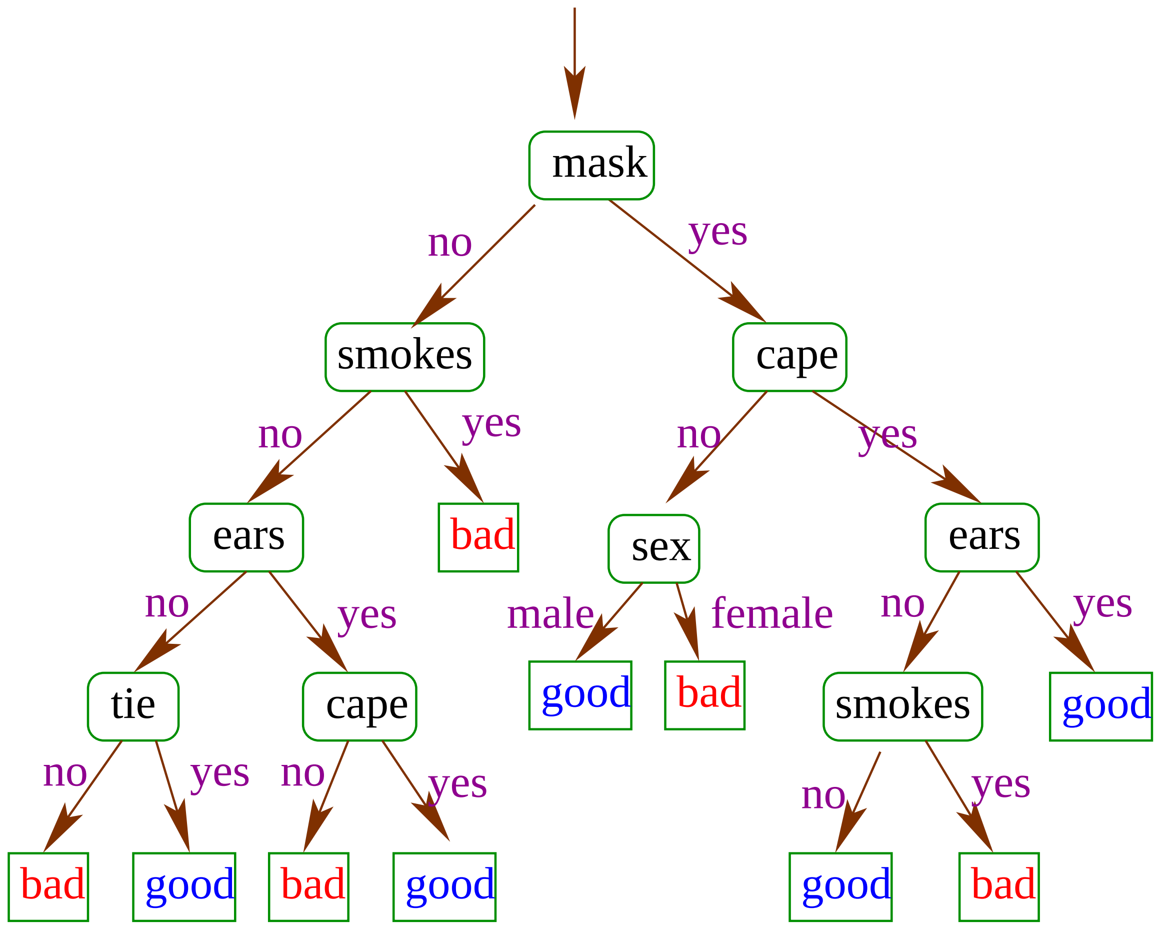
- problem: identify people as good or bad from their appearance

	sex	mask	cape	tie	ears	smokes	class
				training data			
batman	male	yes	yes	no	yes	no	Good
robin	male	yes	yes	no	no	no	Good
alfred	male	no	no	yes	no	no	Good
penguin	male	no	no	yes	no	yes	Bad
catwoman	female	yes	no	no	yes	no	Bad
joker	male	no	no	no	no	no	Bad
				test data			
batgirl	female	yes	yes	no	yes	no	??
riddler	male	yes	no	no	no	no	??

An Example Classifier

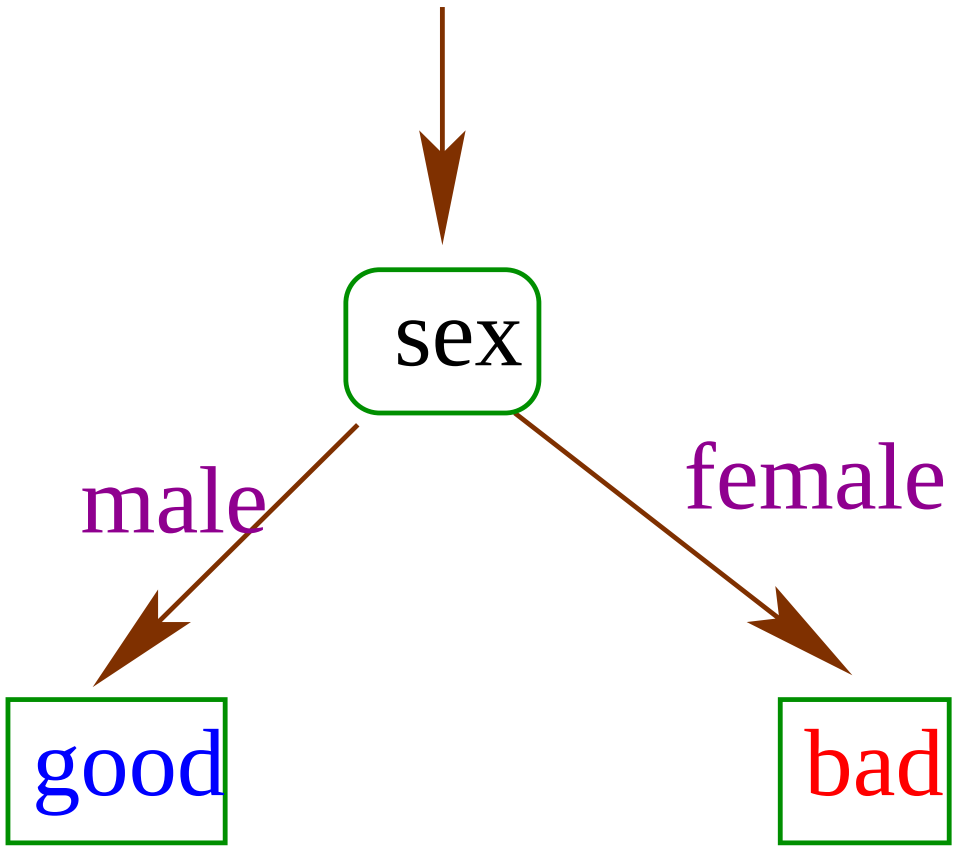


Another Possible Classifier



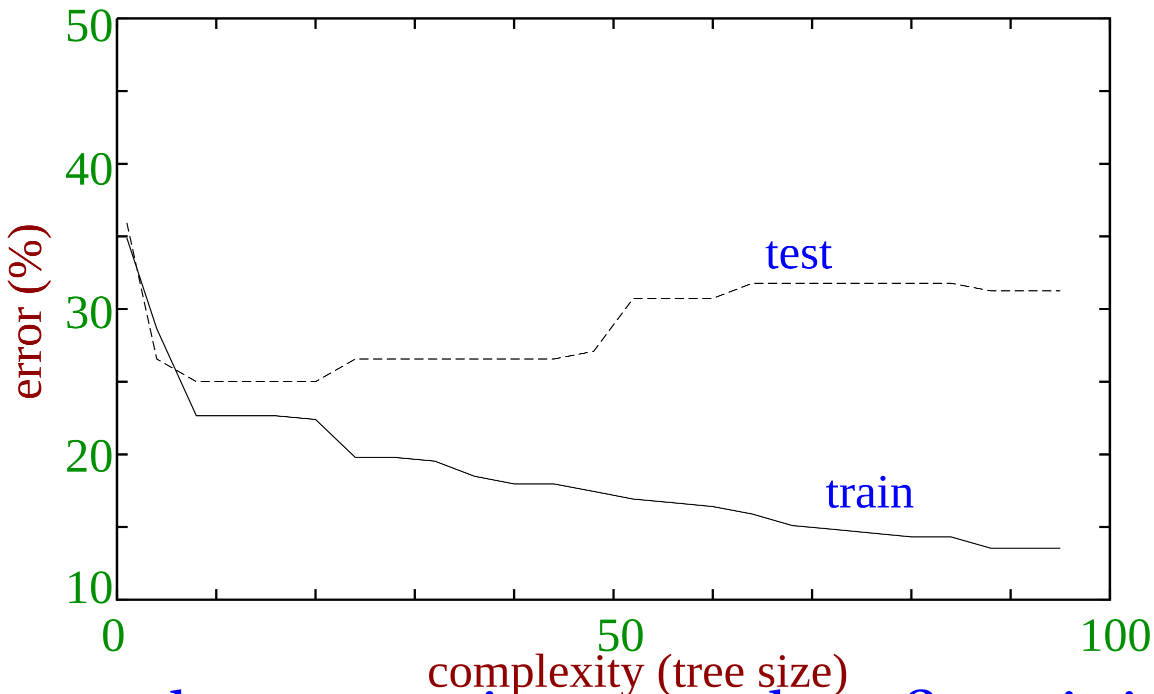
- perfectly classifies training data
- BUT: intuitively, overly complex

Yet Another Possible Classifier



- overly simple
- doesn't even fit available data

Complexity versus Accuracy on An Actual Dataset



- classifiers must be expressive enough to fit training data (so that "true" patterns are fully captured)
- BUT: classifiers that are too complex may overfit (capture noise or spurious patterns in the data)
- problem: can't tell best classifier complexity from training error
- controlling overfitting is the central problem of machine learning

Building an Accurate Classifier

- for good test peformance, need:
  - enough training examples
  - good performance on training set
  - classifier that is not too "complex" ("Occam's razor")
    - measure "complexity" by:
      - number bits needed to write down
      - number of parameters
      - VC-dimension
- classifiers should be "as simple as possible, but no simpler"
- "simplicity" closely related to prior expectations

Theory

- can prove:

$$(\text{generalization error}) \leq (\text{training error}) + \tilde{O}\left(\sqrt{\frac{d}{m}}\right)$$

  with high probability

  - $d =$ VC-dimension
  - $m =$ number training examples

Boosting

Example: Spam Filtering

- problem: filter out spam (junk email)
- gather large collection of examples of spam and non-spam:

From: yoav@att.com	Rob, can you review a paper...	non-spam
From: xa412@hotmail.com	Earn money without working!!!! ...	spam
⋮	⋮	⋮

- main observation:
  - easy to find "rules of thumb" that are "often" correct
    - *If* 'buy now' *occurs in message, then predict* 'spam'
  - hard to find single rule that is very highly accurate

The Boosting Approach

- devise computer program for deriving rough rules of thumb
- apply procedure to subset of emails
- obtain rule of thumb
- apply to 2nd subset of emails
- obtain 2nd rule of thumb
- repeat T times

Details

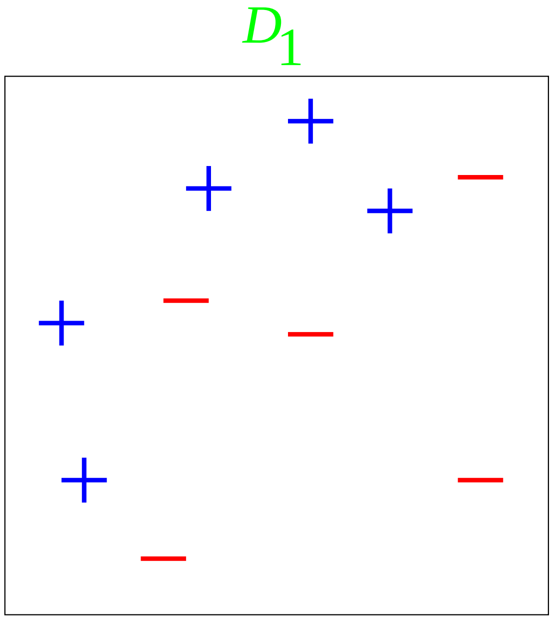
- how to choose examples on each round?
  - concentrate on "hardest" examples
    (those most often misclassified by previous rules of thumb)
- how to combine rules of thumb into single prediction rule?
  - take (weighted) majority vote of rules of thumb

- can prove: if can always find weak rules of thumb slightly better than random guessing (51% accuracy), then can learn almost perfectly (99% accuracy) using boosting

AdaBoost

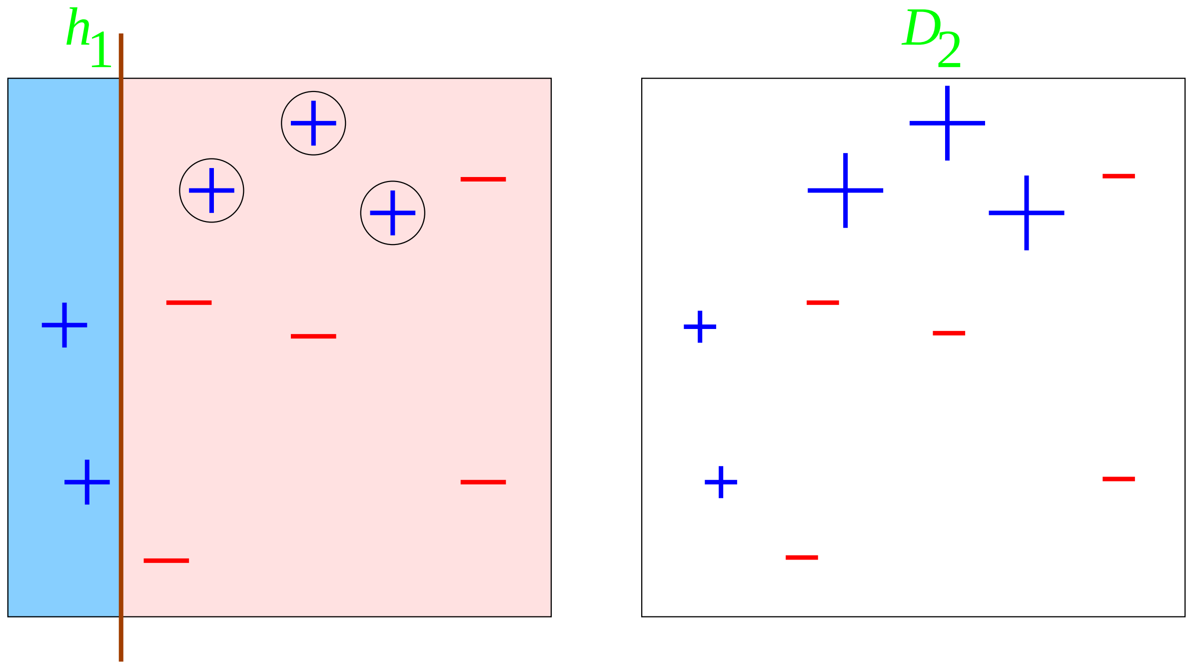
- given training examples
- initialize weights D_1 to be uniform across training examples
- for $t = 1, \ldots, T$:
  - train weak classifier ("rule of thumb") h_t on D_t
  - compute new weights D_{t+1}:
    - decrease weight of examples correctly classified by h_t
    - increase weight of examples incorrectly classified by h_t
- output final classifier
  - $H_{\text{final}} =$ weighted majority vote of $h_1, \cdots, h_T$

Toy Example



weak classifiers = vertical or horizontal half-planes

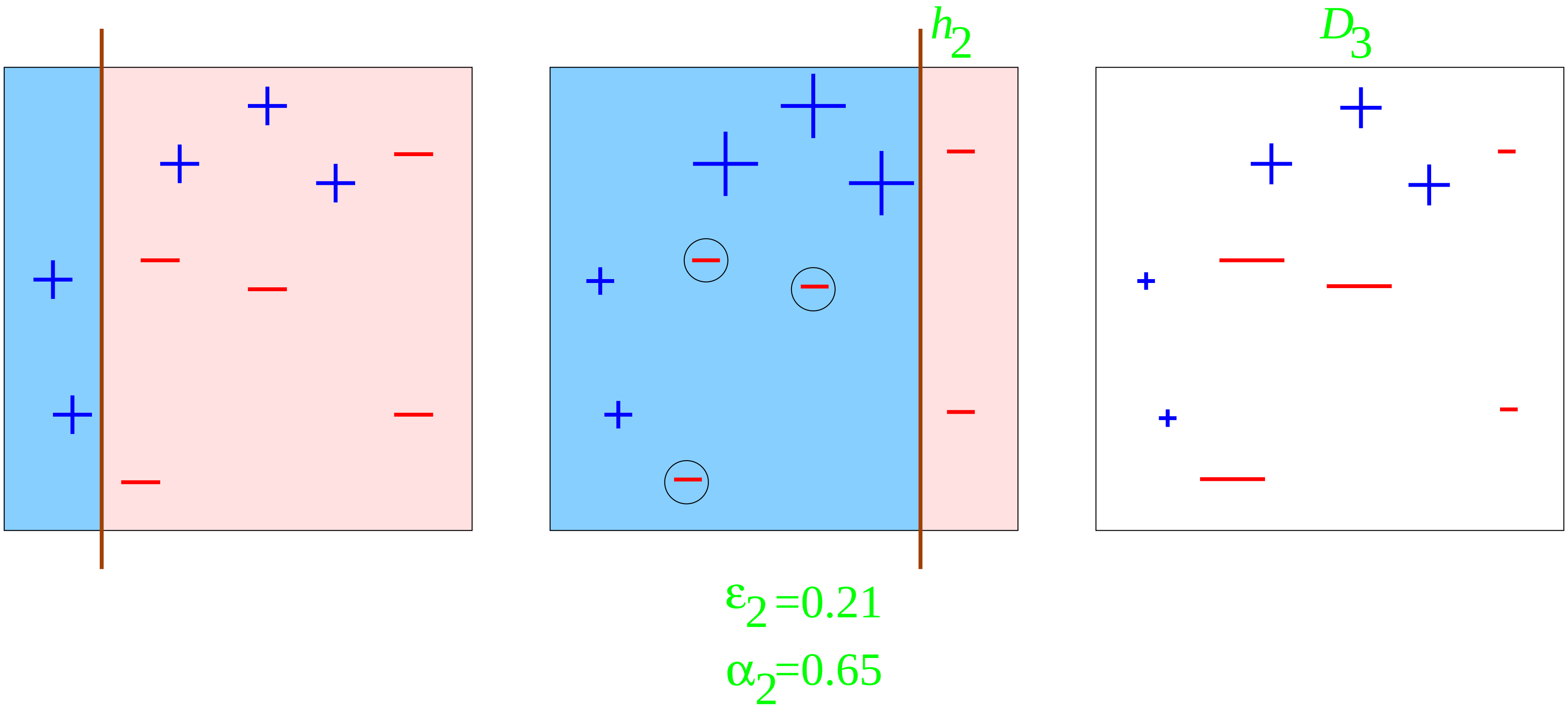
Round 1



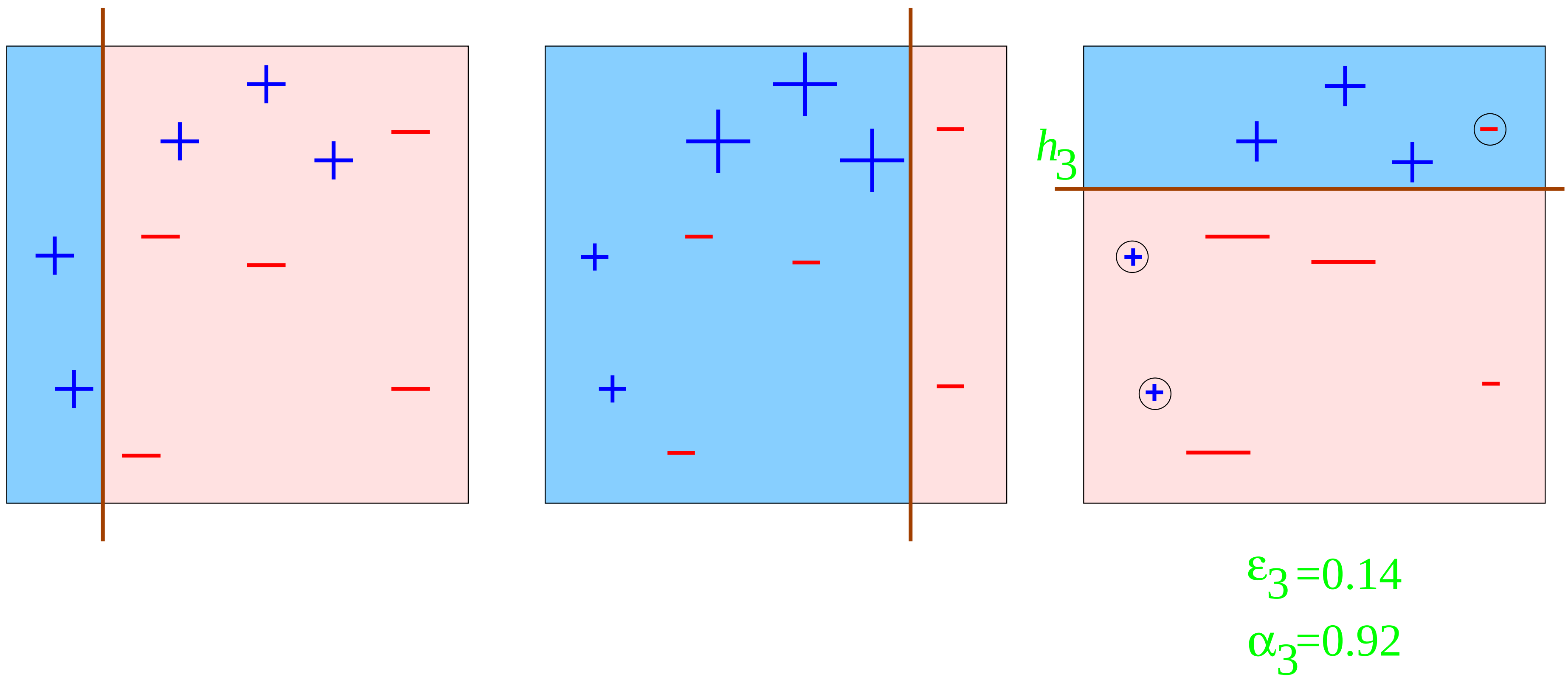
$\varepsilon_1 = 0.30$

$\alpha_1 = 0.42$

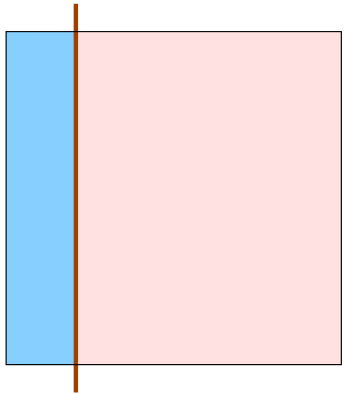
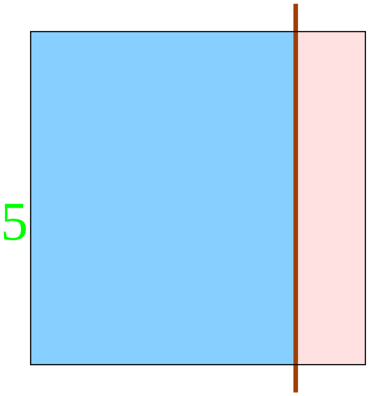
Round 2

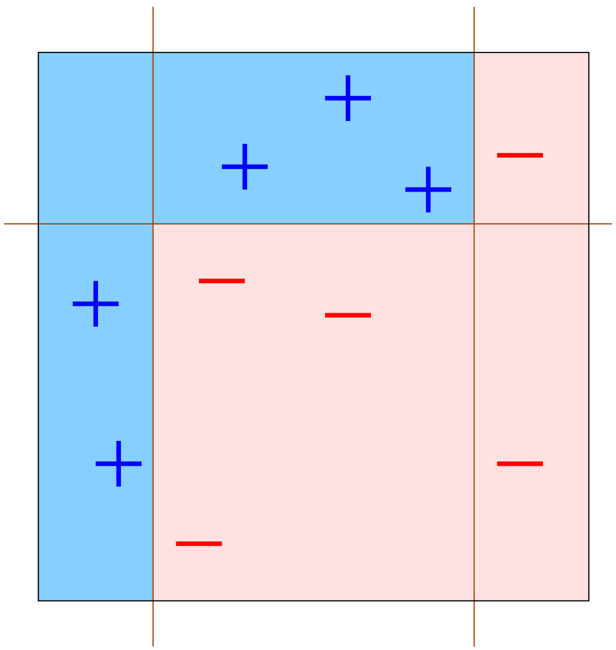


Round 3



Final Classifier

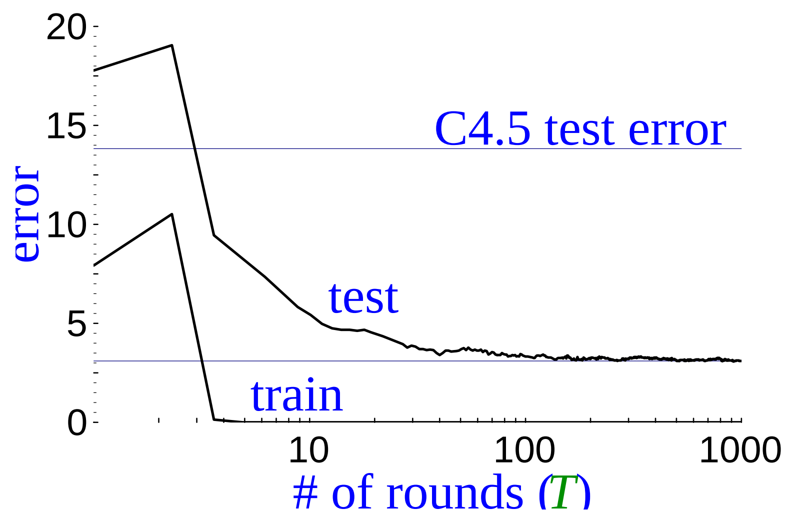
H_{final} = sign (0.42  + 0.65  + 0.92 )

= 

Theory of Boosting

- assume each weak classifier slightly better than random
- can prove training error drops to zero exponentially fast
- even so, naively expect significant overfitting, since a large number of rounds implies a large final classifier
- surprisingly, usually does not overfit

Theory of Boosting (cont.)

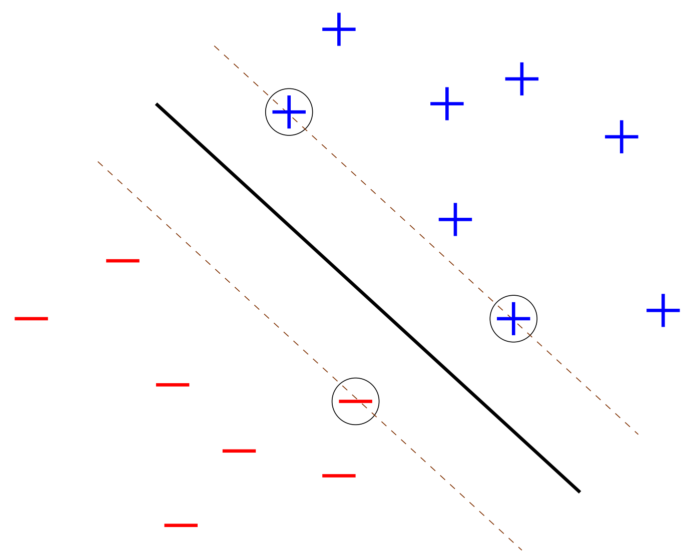


(boosting C4.5 on "letter" dataset)

- test error does not increase, even after 1000 rounds
- test error continues to drop even after training error is zero!
- explanation:
  - with more rounds of boosting, final classifier becomes more confident in its predictions
  - increase in confidence implies better test error (regardless of number of rounds)

Support-Vector Machines

Geometry of SVM's



- given linearly separable data
- margin = distance to separating hyperplane
- choose hyperplane that maximizes minimum margin
- intuitively:
  - want to separate $+$'s from $-$'s as much as possible
  - margin = measure of confidence
- support vectors = examples closest to hyperplane

Theoretical Justification

- let $\gamma =$ minimum margin
  $R =$ radius of enclosing sphere
- then

$$\text{VC-dim} \leq \left(\frac{R}{\gamma}\right)^2$$

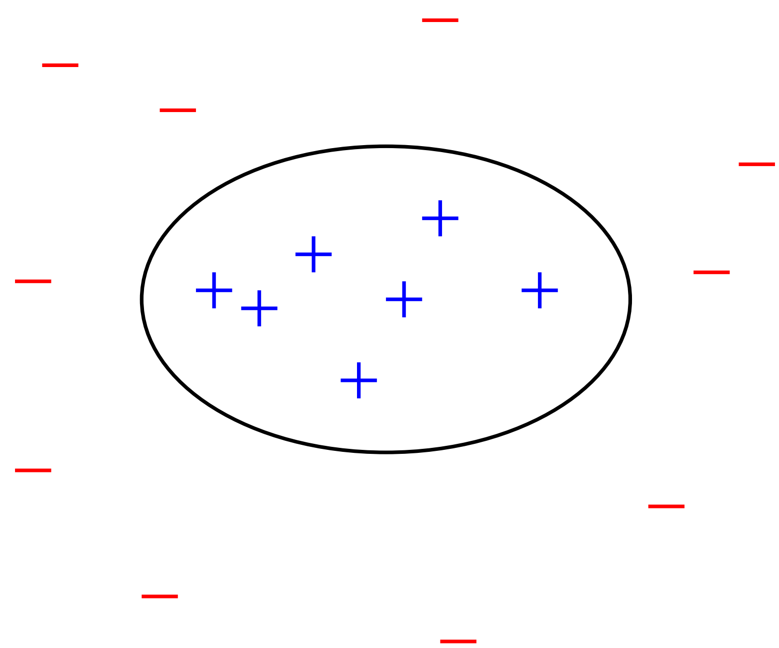
  - so larger margins $\Rightarrow$ lower "complexity"
  - independent of number of dimensions
- in contrast, unconstrained hyperplanes in $\mathbb{R}^n$ have

$$\text{VC-dim} = (\text{\# parameters}) = n + 1$$

What If Not Linearly Separable?

- answer #1: penalize each point by distance must be moved to obtain large margin
- answer #2: map into higher dimensional space in which data becomes linearly separable

<u>Example</u>



- <u>not</u> linearly separable
- map $\mathbf{x} = (x_1, x_2) \mapsto \Phi(\mathbf{x}) = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$
- hyperplane in mapped space has form

$$a + bx_1 + cx_2 + dx_1x_2 + ex_1^2 + fx_2^2 = 0$$

$=$ conic in original space

- linearly separable in mapped space

Higher Dimensions Don't (Necessarily) Hurt

- may project to very high dimensional space
- statistically, may not hurt since VC-dimension independent of number of dimensions ($(R/\gamma)^2$)
- computationally, only need to be able to compute inner products

$$\Phi(\mathbf{x}) \cdot \Phi(\mathbf{z})$$

  - sometimes can do very efficiently using kernels

Example (cont.)

- modify Φ slightly:

$$\Phi(\mathbf{x}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2)$$

- then

$$\begin{aligned} \Phi(\mathbf{x}) \cdot \Phi(\mathbf{z}) &= 1 + 2x_1z_1 + 2x_2z_2 + 2x_1x_2z_1z_2 + x_1^2z_1^2 + x_2^2 + z_2^2 \\ &= (1 + x_1z_1 + x_2z_2)^2 \\ &= (1 + \mathbf{x} \cdot \mathbf{z})^2 \end{aligned}$$

- in general, for polynomial of degree d, use $(1 + \mathbf{x} \cdot \mathbf{z})^d$
- very efficient, even though finding hyperplane in $O(n^d)$ dimensions

Kernels

- kernel = function K for computing

$$K(\mathbf{x}, \mathbf{z}) = \Phi(\mathbf{x}) \cdot \Phi(\mathbf{z})$$

- permits efficient computation of SVM's in very high dimensions
- many kernels have been proposed and studied
  - provides power, versatility and opportunity for incorporation of prior knowledge

Significance of SVM's and Boosting

- grounded in rich theory with provable guarantees
- flexible and general purpose
- off-the-shelf and fully automatic
- fast and easy to use
- able to work effectively in very high dimensional spaces
- performs well empirically in many experiments and in many applications

Summary

- central issues in machine learning:
  - avoidance of overfitting
  - balance between simplicity and fit to data
- quick look at two learning algorithms: boosting and SVM's
- many other algorithms not covered:
  - decision trees
  - neural networks
  - nearest neighbor algorithms
  - Naive Bayes
  - bagging

  ⋮
- also, classification just one of many problems studied in machine learning

Other Machine Learning Problem Areas

- supervised learning
  - classification
  - regression – predict real-valued labels
  - rare class / cost-sensitive learning
- unsupervised – no labels
  - clustering
  - density estimation
- semi-supervised
  - in practice, unlabeled examples much cheaper than labeled examples
  - how to take advantage of both labeled and unlabeled examples
  - active learning – how to carefully select which unlabeled examples to have labeled

Further reading on machine learning in general:

Ethem Alpaydin. *Introduction to machine learning*. MIT Press, 2004.

Luc Devroye, Lázló Györfi and Gábor Lugosi. *A Probabilistic Theory of Pattern Recognition*. Springer, 1996.

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Trevor Hastie, Robert Tibshirani and Jerome Friedman. *The Elements of Statistical Learning : Data Mining, Inference, and Prediction*. Springer, 2001.

Michael J. Kearns and Umesh V. Vazirani. *An Introduction to Computational Learning Theory*. MIT Press, 1994.

Tom M. Mitchell. *Machine Learning*. McGraw Hill, 1997.

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Boosting:

Ron Meir and Gunnar Rätsch. An Introduction to Boosting and Leveraging. In *Advanced Lectures on Machine Learning (LNAI2600)*, 2003. http://www.boosting.org/papers/MeiRae03.pdf

Robert E. Schapire. The boosting approach to machine learning: An overview. In *MSRI Workshop on Nonlinear Estimation and Classification*, 2002. http://www.cs.princeton.edu/∼schapire/boost.html

Many more papers, tutorials, etc. available at www.boosting.org.

Support-vector machines:

Nello Cristianni and John Shawe-Taylor. *An Introduction to Support Vector Machines and Other Kernel-based Learning Methods*. Cambridge University Press, 2000. See www.support-vector.net.

Many more papers, tutorials, etc. available at www.kernel-machines.org.