Day 8: Ensemble methods, boosting

Introduction to Machine Learning Summer School
June 18, 2018 - June 29, 2018, Chicago

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TOYOTA TECHNOLOGICAL INSTITUTE AT CHICAGO
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Topics so far

- Linear regression
- Classification
  - Logistic regression
  - Maximum margin classifiers, kernel trick
  - Generative models
  - Neural networks, backpropagation, NN training – optimization and regularization, special architectures – CNNs, RNNs, encoder-decoder
- Remaining Topics
  - Ensemble methods, boosting
  - Unsupervised learning – clustering, dimensionality reduction
  - Review and topics not covered!

Ensemble learning

- Ensemble learning
  - Create a population of base learning $f_1, f_2, \ldots f_M \colon \mathcal{X} \to \mathcal{Y}$
  - Combine the predictors to form a composite predictor
- Example in classification with $\mathcal{Y} = \{-1,1\}$ → assign "votes" α_m to each classifier f_m and take weighted-majority vote

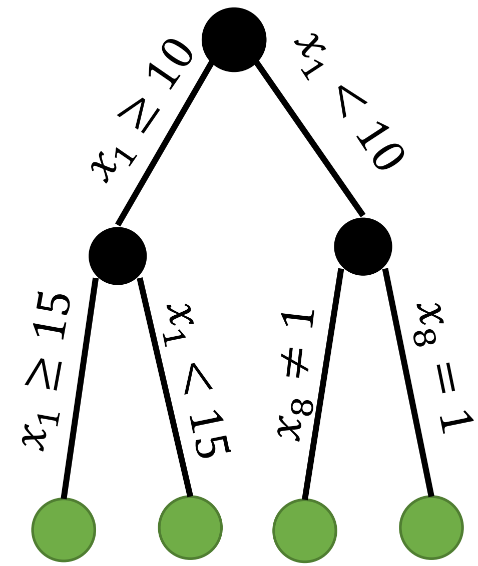
$$F(x) = \operatorname{sign}\left(\sum_{m=1}^{M} \alpha_m f_m(x)\right)$$

  - Individual classifiers can be very simple, e.g., $x_1 \geq 10$, $x_5 \leq 5$
- Why?
  - more powerful models → reduce bias
    - e.g., majority vote of linear classifiers can give decision boundaries that are intersections of halfspaces
  - reduce variance
    - averaging classifiers $f_1, f_2, \ldots f_M$ trained independently on different iid datasets $S_1, S_2, \ldots, S_M$ can reduce variance of composite classifier

Reducing bias using ensembles

Decision trees

- Each non-leaf node tests a binary condition on some feature x_k
  - if condition satisfies then go left, else go right
  - leaf nodes have label (typically the label of majority class of training examples at that node
- Classifying a point by decision tree can be seen as a sequence of classifiers refined as we follow the path to a leaf.



Combining "simple" models

- Smooth-ish tradeoff between bias-complexity
  - start with simple models with large bias and low variance
  - learn more complex classes by composign simple models
- For example consider classifiers $f_1, f_2, \ldots, f_M$ based on only one feature (decision stumps), i.e., each

$$f_m(x; \theta_m) = 1\left(x_{k_m} \geq \tau_m\right) \text{ where } \theta_m = (k_m, \tau_m)$$

- $\mathcal{H} = \{x \rightarrow majority(\alpha_1 f_1(x; \theta_1), \alpha_2 f_2(x; \theta_2), \ldots, \alpha_M f_M(x; \theta_M))\}$ contains very complex boundaries
- demo (by Nati Srebro)
- So clearly combining simple classifiers can reduce bias. How do we combine classifiers?

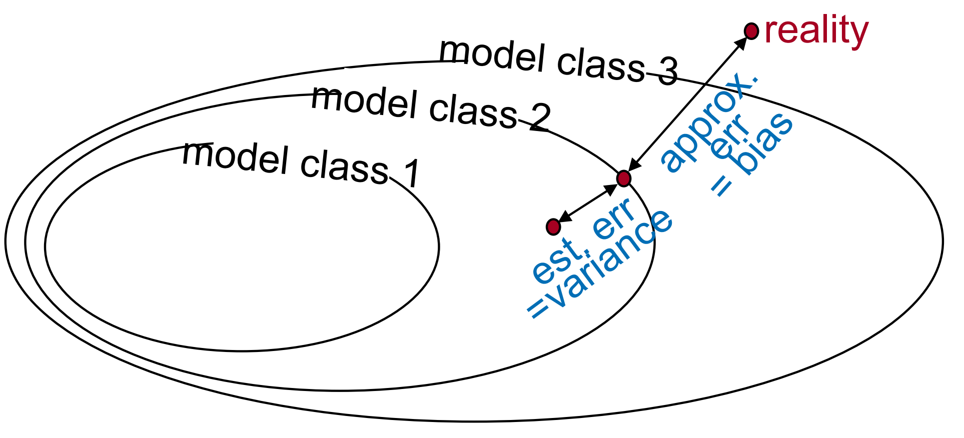


Figure credit: Nati Srebro

Combining "simple" models

- Given a family of models $f_1, f_2, \ldots : \mathcal{X} \to \mathcal{Y}$, we want to combine?
- Weighted averaging of models:
  - parameterize combined classifier using α_m as

$$F_\alpha(x) = \sum_{m=1}^{M} \alpha_m f_m(x)$$

  - minimize loss over combined model

$$\min_{\alpha} \sum_{i=1}^{N} \ell\left(F_\alpha\left(x^{(i)}\right), y^{(i)}\right)$$

- Alternative algorithm: greedy approach
  - $F_0(x) = 0$
  - for each round $t = 1,2, \ldots, T$
    - find the best model to minimize the incremental change from F_{t-1}

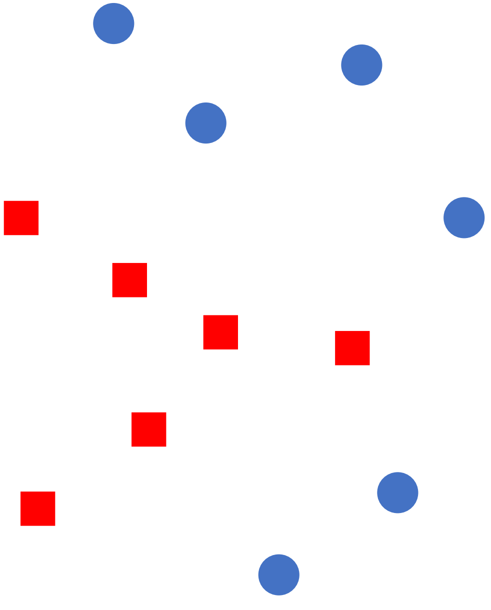
$$\min_{\alpha_t, f^{(t)}} \sum_{i=1}^{N} \ell\left(F_{t-1}\left(x^{(i)}\right) + \alpha_t f^{(t)}\left(x^{(i)}\right), y^{(i)}\right)$$

  - Output classifier $F_T(x) = \sum_{t=1}^{T} \alpha_t f^{(t)}(x)$

Adaboost

Training data $S = \{(x^{(i)}, y^{(i)}) : i = 1,2, \dots, N\}$

- Maintain weights $W_i^{(t)}$ for each example $(x^{(i)}, y^{(i)})$, initially all $W_i^{(1)} = \frac{1}{N}$



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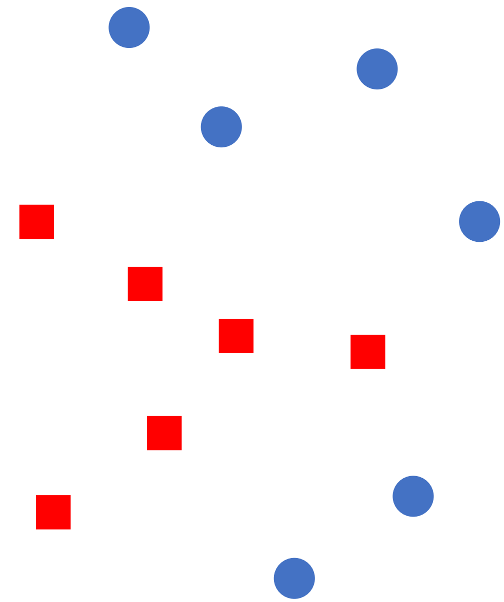

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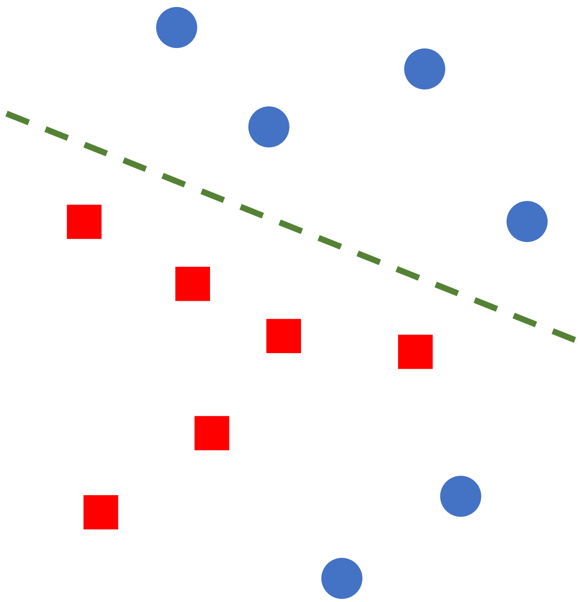

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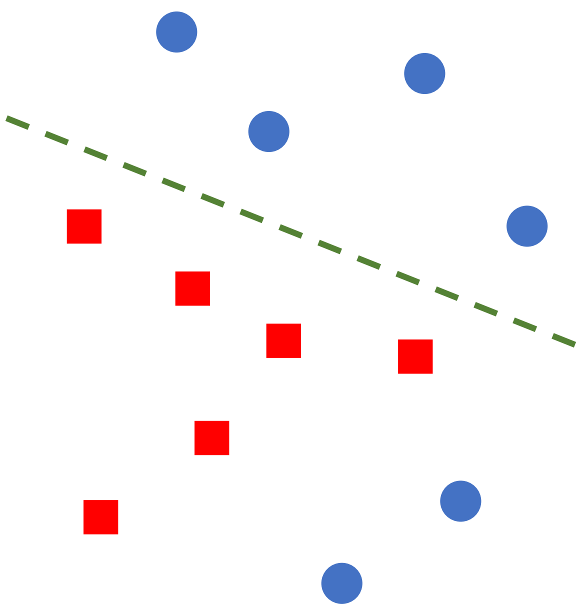

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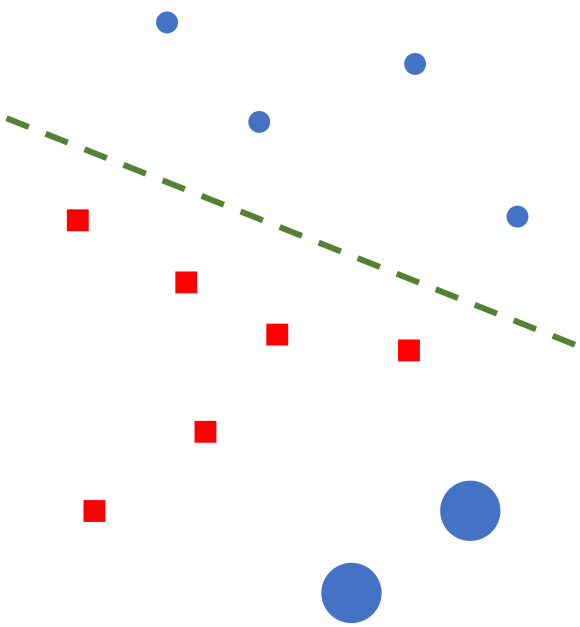

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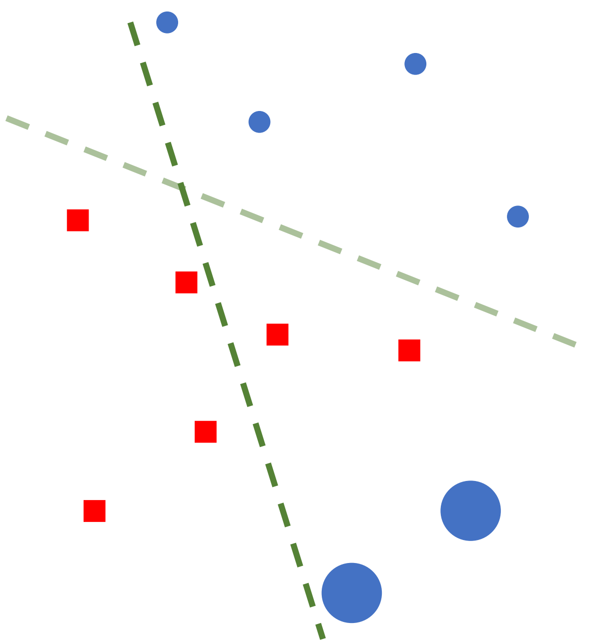

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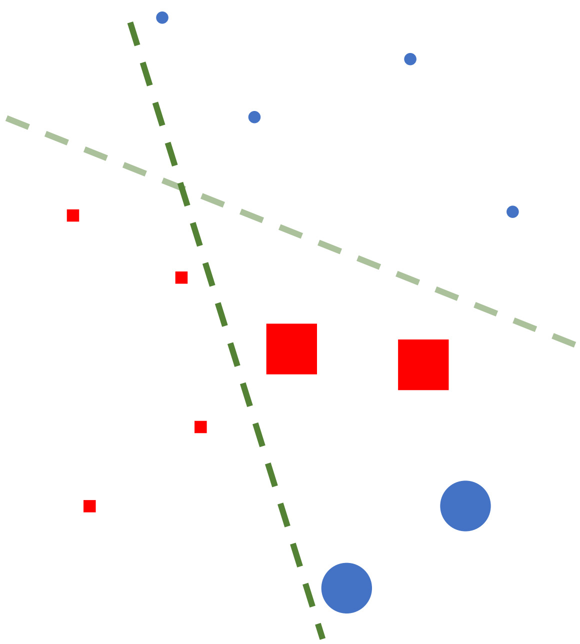

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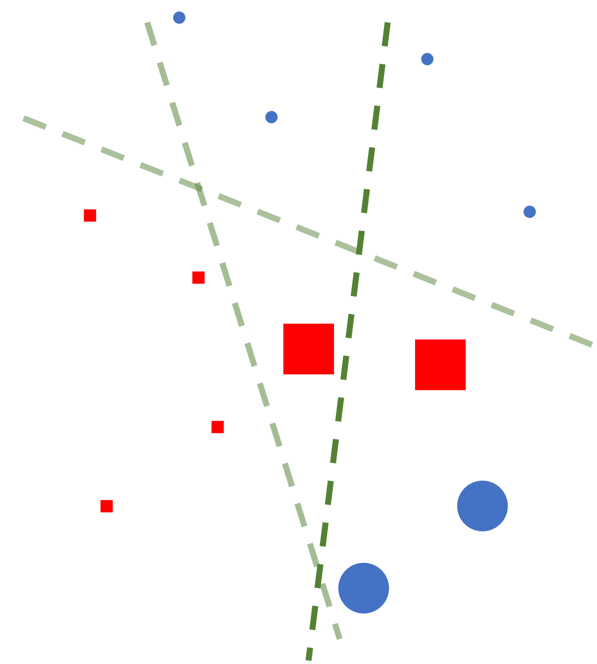

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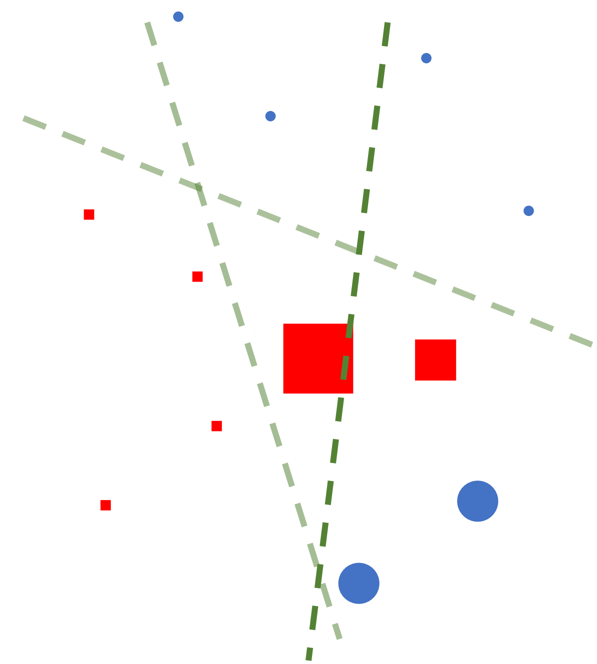

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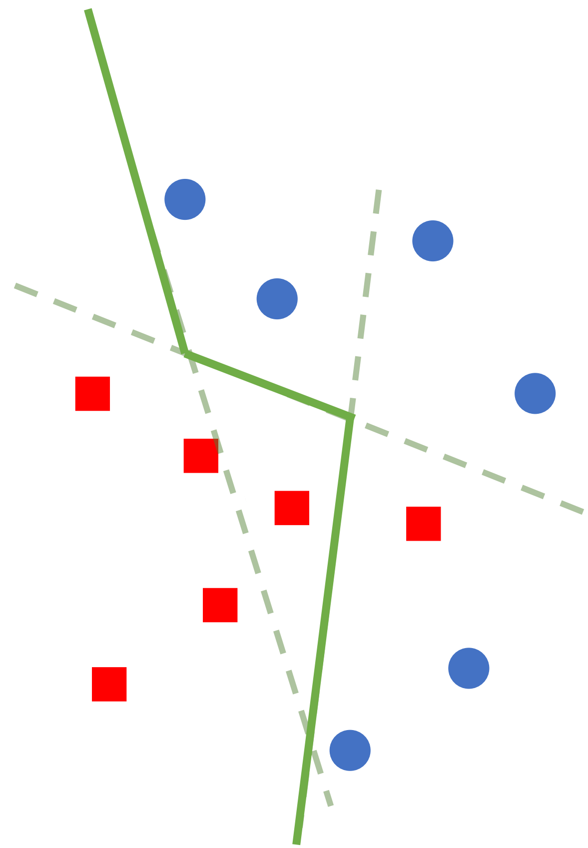

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  - Update weights $W_i^{(t+1)} = W_i^{(t)} \exp\left(-\alpha_t y^{(i)} f_t\left(x^{(i)}\right)\right)$
- Output strong classifier $F_T(x) = \mathrm{sign}(\sum_t \alpha_t f_t(x))$

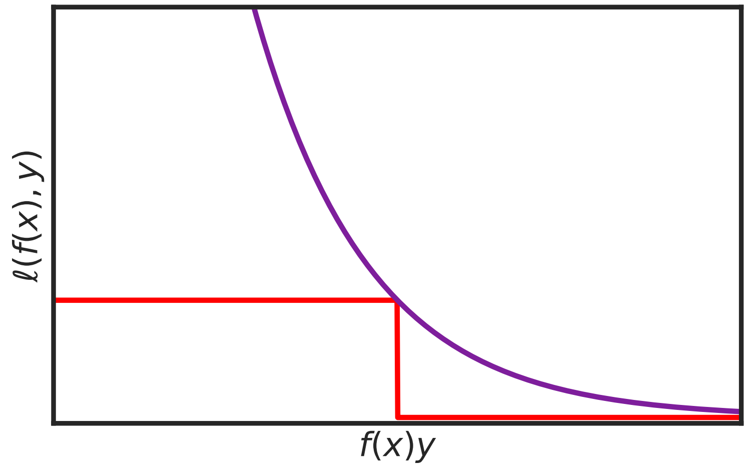
Example credit: Greg Shaknarovich

Adaboost

- Demo again (code by Nati Srebro)
- What are we doing in Adaboost?
    - Some algorithm to do ensembles
    - Learning ***sparse*** linear predictors with large (infinite?) dimensional features
        - Sparsity controls complexity
        - Number of iterations controls sparsity
          ➔ early stopping as regularization
    - Coordinate descent on exponential loss (briefly next)
- Variants of AdaBoost
    - FloatBoost: After each round, see if removal of a previously added classier is helpful.
    - Totally corrective AdaBoost: update the α's for all weak classifiers selected so far by minimizing loss

Exponential loss

- Exponential loss $\ell(f(x), y) = \exp(-f(x)y)$ another surrogate loss
- Ensemble classifier
  $F_\alpha(x) = \text{sign}(\sum_t \alpha_t f_t(x))$



- We will not derive, but can show that adaboost updates correspond to coordinate descent on ERM with exp loss

$$\min_\alpha \sum_{i=1}^{N} \exp\left(-\sum_t \alpha_t f_t(x^{(i)}) y^{(i)}\right)$$

Example: Viola-Jones Face Detector

- Classify each square in an image as “face” or “no-face”

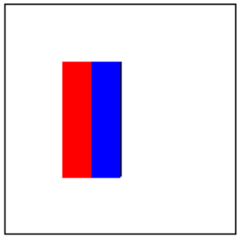
- $\mathcal{X}$ = patches of 24x24 pixels, say

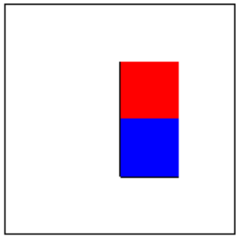
Slide credit: Nati Srebro

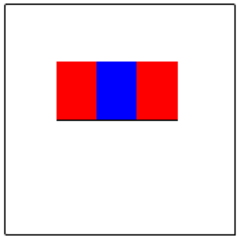
Viola-Jones "Weak Predictors"/Features

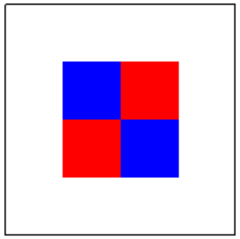
$$\mathcal{B} = \left\{ 1\big(g_{r,t}(x) < \theta\big) \mid \theta \in \mathbb{R}, \text{rect } r \text{ in image}, t \in \{A, B, C, D, \bar{A}, \bar{B}, \bar{C}, \bar{D}\} \right\}$$

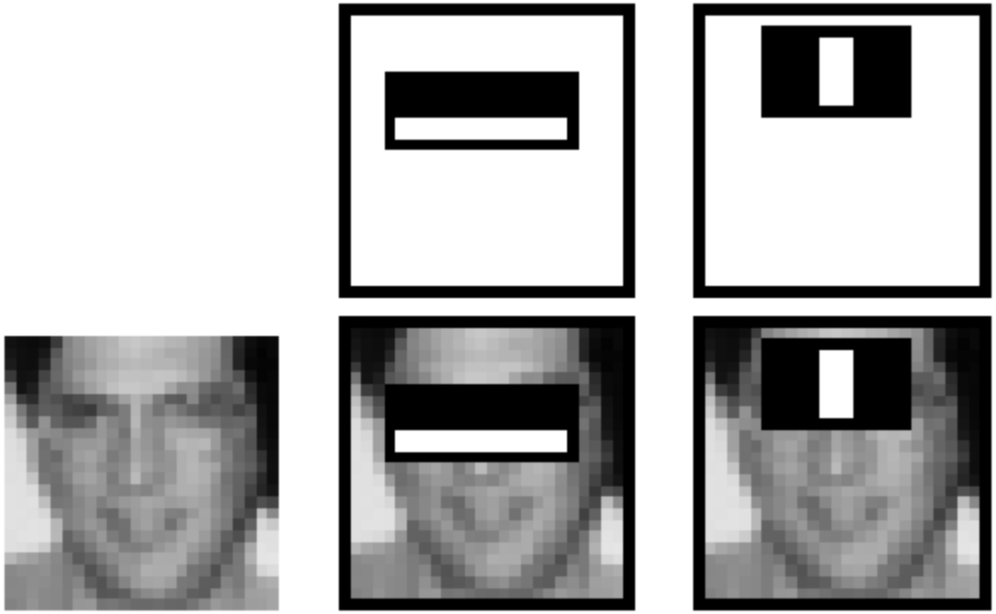
where $g_{r,t}(x)$ =sum of "blue" pixels – sum of "red" pixels

A: 

B: 

C: 

D: 



Slide credit: Nati Srebro

Viola-Jones Face Detector

- Simple implementation of boosting using generic (non-face specific) “weak learners”/features
  - Can be used also for detecting other objects
- Efficient method using dynamic programing and caching to find good weak predictor
- About 1 million possible $g_{r,t}$, but only very few used in returned predictor
- Sparsity:
  - ➔ Generalization
  - ➔ Prediction speed! (and small memory footprint)
- To run in real-time (on 2001 laptop), use sequential evaluation
  - First evaluate first few h_t to get rough prediction
  - Only evaluate additional h_t on patches where the leading ones are promising

Slide credit: Nati Srebro

Ensembling to reduce variance

Averaging predictors

- Averaging reduces variance: if $Z_1, Z_2, \ldots, Z_M$ are independent random variables each with mean μ and variance of σ^2

$$var\left(\frac{1}{M}\sum_{m=1}^{M} Z_m\right) = \frac{\sigma^2}{M}$$

- What happens to mean?

$$\mathbb{E}\left(\frac{1}{M}\sum_{m=1}^{M} Z_m\right) = \mu$$

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- If we had M models $f_1, f_2, \dots f_M$ trained independently on different iid datasets $S_1, S_2, \dots, S_M$, then averaging the results of the models will
  - reduce variance: it will be less sensitive to specific training data
  - without increasing the bias: on average all classifiers will do as well
- But we have only one dataset! How do we get multiple models
  - Remember the models have to be independent!

Bagging: Bootstrap aggregation

Averaging independent models reduces variance without increasing bias.

- But we don't have independent datasets!
  - Instead take repeated bootstrap samples from training set S
- Bootstrap sampling: Given dataset $S = \{(x^{(i)}, y^{(i)}): i = 1,2, \dots, N\}$, create S' by drawing N examples at random **with replacement** from S
- Bagging:
  - Create M bootstrap datasets $S_1, S_2, \dots, S_M$
  - Train distinct models $f_m: \mathcal{X} \to \mathcal{Y}$ by training only on S_m
  - Output final predictor $F(x) = \frac{1}{M}\sum_{m=1}^{M} f_m(x)$ (for regression) or $F(x) = \text{majority}(f_m(x))$ (for classification)

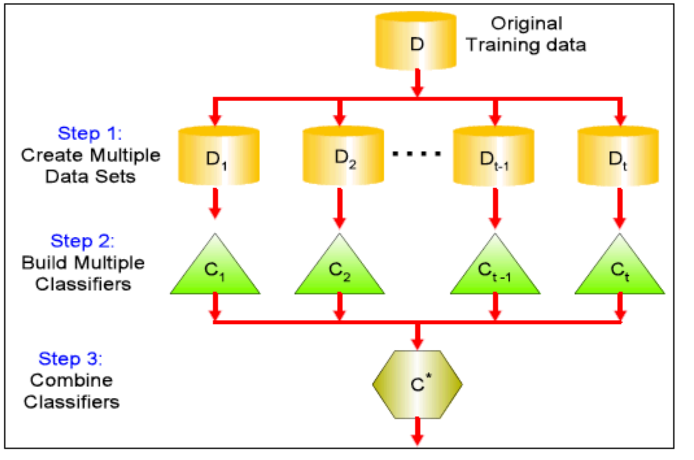


Figure credit: David Sontag

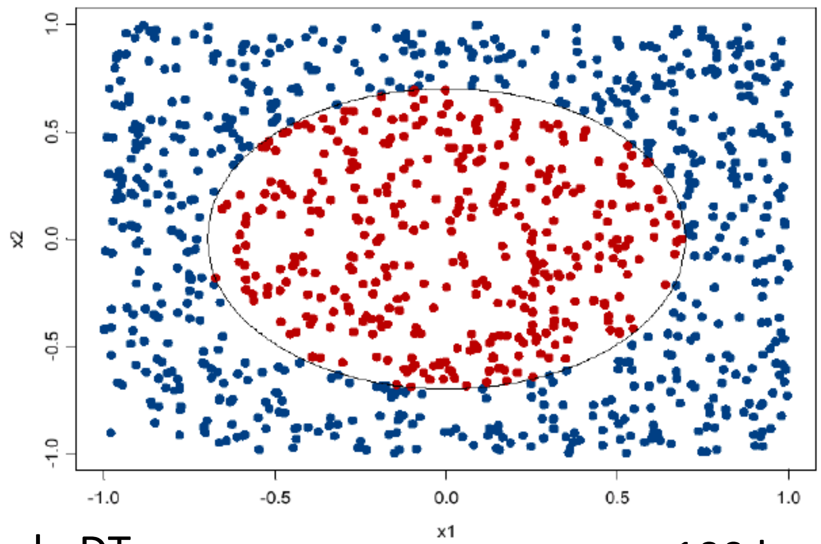
Bagging

- Most effective while combining high variance, low bias predictors
  - unstable non-linear predictors like decision trees
  - "overfitting quirks" of different trees canceling out

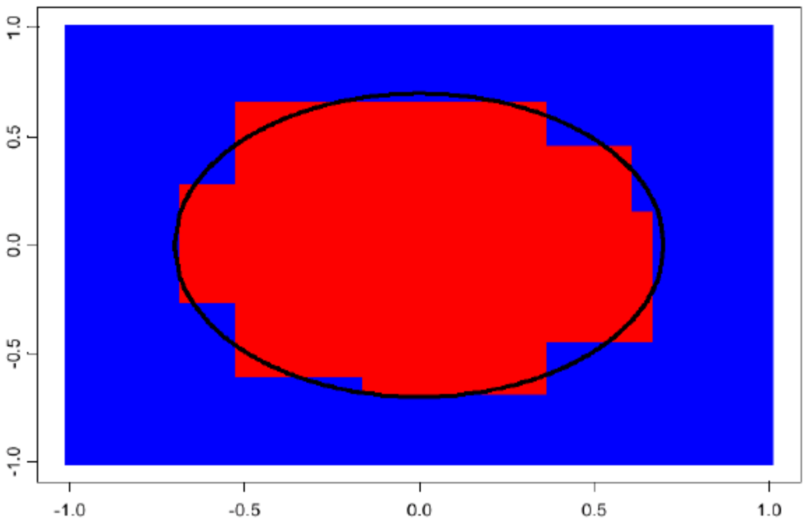
- Not very useful with linear predictors

- Useful property of bagging: "out of bag" (OOB) data
  - in each "bag", treat the examples that didn't make it to the bag as a kind of validation set
  - while learning predictors, keep track of OOB accuracy

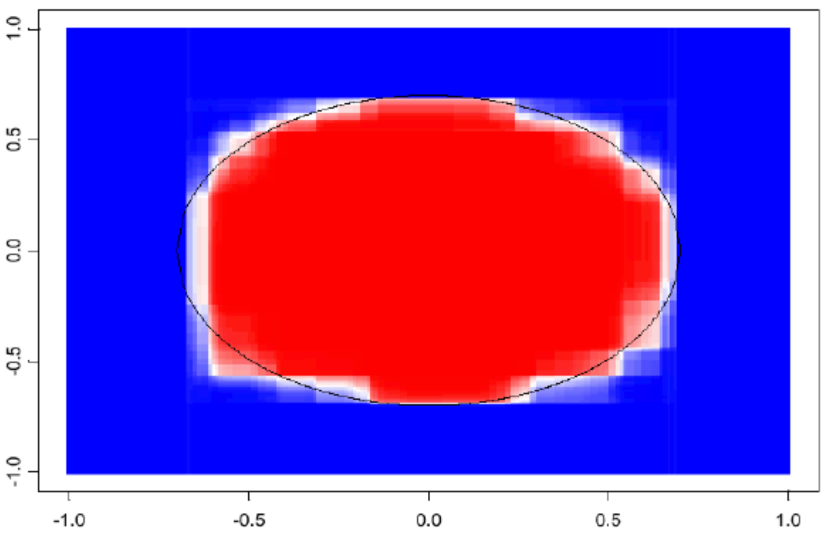
Bagging example



Output of single DT



100 bagged trees



Slide/example credit: David Sontag

Random forests

- Ensemble method specifically built for decision trees
- Two sources of randomness
  - Sample bagging: Each tree grown with a bootstrapped training data
  - Feature bagging: at each node, best split decided over only a subset of random features → increases diversity among trees
- Algorithm
  - Create bootsrapped datasets $S_1, S_2, \ldots, S_M$
  - For each m, grow a decision tree T_m by repeating the following at each node until some stopping condition
    - select K features at random from d features of x
    - pick best variable/split threshold among the K selected features
    - split the node into two child nodes based on above condition
  - Output majority vote of $\{T_m\}_{m=1}^{M}$

Ensembles summary

- Reduce bias:
  - build ensemble of low-variance, high-bias predictors sequentially to reduce bias
  - AdaBoost: binary classication, exponential surrogate loss
- Reduce variance:
  - build ensemble of high-variance, low-bias predictors in parallel and use randomness and averaging to reduce variance
  - random forests, bagging
- Problems
  - Computationally expensive (train and test time)
  - Often loose interpretability