Committee Machines

CS6140

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Fall 2024

Motivation

Given: a set of observations $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$, $x_i \in \mathcal{X}, y_i \in \mathcal{Y}$

Objective: learn the posterior $p(y|x, \mathcal{D})$

Optimal Bayes Model:

$$p(y|x, \mathcal{D}) = \sum_{f \in \mathcal{F}} p(y|x, \mathcal{D}, f)p(f|x, \mathcal{D}) \qquad \text{Finite } \mathcal{F}$$

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Idea:

Don't just train a single model, train multiple models.

Average the outputs in some way.

Motivation

Given: a set of observations $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$, $x_i \in \mathcal{X}, y_i \in \mathcal{Y}$

Objective: learn $s(x|\mathcal{D})$ to approximate the posterior $p(y|x, \mathcal{D})$

The problem of local optima with rich hypothesis spaces:

- every time we train, we find a different local optimium; i.e. $s'(x|\mathcal{D})$

$$s(x) = \sum_{s' \in \mathcal{S}_{\text{strong}}} w_{(s',x)} s'(x|\mathcal{D}) \qquad \text{Finite } \mathcal{S}_{\text{strong}}$$

The problem of weak hypothesis space $\mathcal{S}_{\text{weak}}$:

- we can only find a weak learner $s'(x)$

$$s(x) = \sum_{s' \in \mathcal{S}_{\text{weak}}} w_{(s',x)} s'(x|\mathcal{D}) \qquad \text{Finite } \mathcal{S}_{\text{weak}}$$

Two Ways of Averaging

Static structures:

pre-trained models, applied independently of x

examples: bagging, boosting, random forests

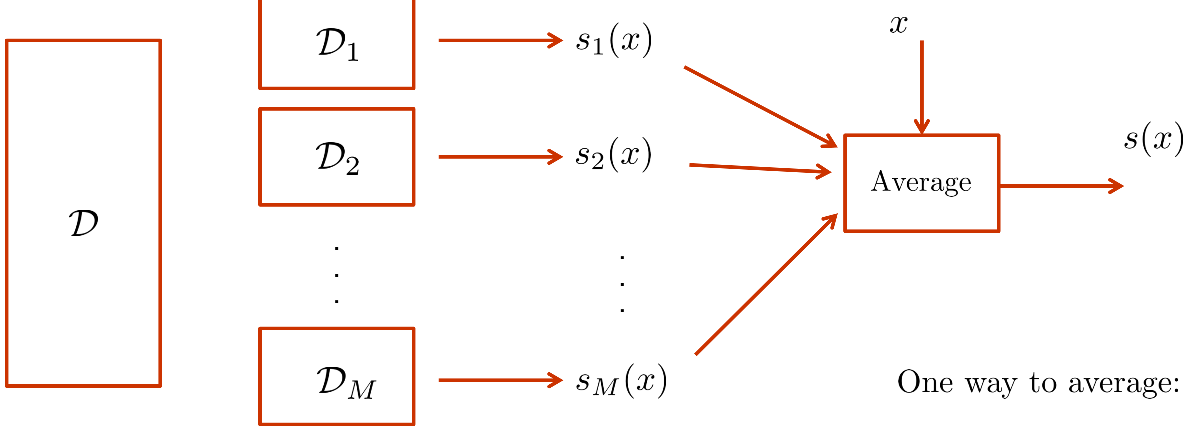
Dynamic structures:

pre-trained models, applied depending on x

examples: mixtures of experts

Haykin. Neural networks, 1999.

Static Structure



One way to average:

$$s(x) = \frac{1}{M} \sum_{i=1}^{M} s_i(x)$$

Why Should it Work?

Given: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}\ ,\ x_i \in \mathcal{X}, y_i \in \mathcal{Y}$

Idea:

Let $f_A(x) = \mathbb{E}[f(x|D)]$ be an "averaged" model. Then, for a fixed x

$$\mathbb{E}[(y - f(x|D))^2] = y^2 - 2y\mathbb{E}[f(x|D)] + \mathbb{E}[f^2(x|D)]$$

$$\mathbb{E}[(y - f(x|D))^2] \geq (y - f_A(x))^2$$

Jensen's inequality

$$\mathbb{E}[Z^2] \geq \mathbb{E}^2[Z]$$

Bagging

Bagging: Bootstrap aggregating

Approach:

- create B bootstrap samples $\mathcal{D}_b$, where $b = 1, 2, ..., B$
- train a model $f_b(x)$ for each $\mathcal{D}_b$
- let the final decision $f(x)$ be a majority vote by $\{f_1(x), \ldots, f_B(x)\}$; technically, $f(x) = \arg\max_{y \in \mathcal{Y}} \sum_{b=1}^{B} I(f_b(x) = y)$

Averaging scenarios:

- use majority vote (original idea by Leo Breiman)
- average soft predictions, then threshold the model
- create soft predictions by averaging thresholded models $f_b(x)$

Breiman. Bagging predictors. *Mach Learn*, 1996.

Random Forests

Idea. Construct an ensemble of trees, 100 to 1000.

In practice:

Randomize dataset

- bootstrap the dataset

Randomize features upon which we split

- at each node, keep e.g. $F = \log_2 d + 1$ features, then split

Breiman. Random forests. *Mach Learn*, 2001.

Boosting

Idea: Combine "weak" models to create "strong" models.

Methodologies that answer theoretical questions (PAC learning).

Models trained sequentially on different distributions or problems.

Three approaches:

Boosting by filtering

Boosting by subsampling or reweighting

Functional gradient boosting

Boosting by Filtering

Idea: Construct a committee of 3 experts.

1) Expert f_1 is trained on n_1 examples picked randomly

2) Expert f_2 is trained as follows

2.1. Flip a coin

Heads $\rightarrow$ pass examples through f_1 until one is misclassified

include that example in training set for f_2

Tails $\rightarrow$ pass examples through f_1 until one is correctly classified

include that example in training set for f_2

2.2. Continue until n_1 examples are collected, then train f_2

BOOSTING BY FILTERING

Idea: Construct a committee of 3 experts.

3) Expert f_3 is trained as follows

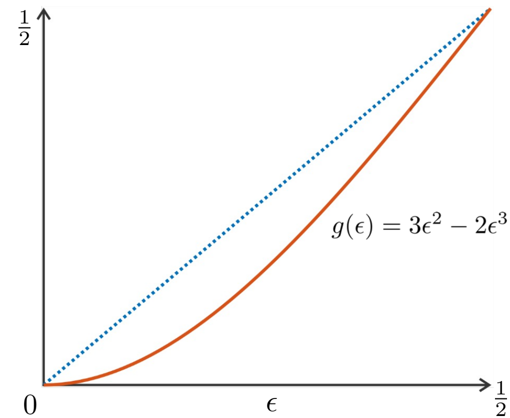
3.1. Select n_1 examples by keeping those where f_1 and f_2 disagree

Data distributions are different for training f_1, f_2, and f_3

The final prediction obtained by majority voting.

It can be proved that if f_1, f_2, f_3 all have error rate of $\epsilon < \frac{1}{2}$

then the committee machine has error $g(\epsilon) = 3\epsilon^2 - 2\epsilon^3$



Idea: Repeat the process recursively.

Algorithm 1 AdaBoost algorithm. Typically, $T = 100$.

Input:

$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$, where $x_i \in \mathcal{X}$ and $y_i \in \mathcal{Y}$.
Weak learning algorithm a that maps a data set to $\mathcal{F}$
Positive integer T

Initialization:

Initialize sampling distribution $p^{(1)}(i) = \frac{1}{n}$ for $\forall i \in \{1, 2, \ldots, n\}$

Loop:

for $t = 1$ to T
Sample data set $\mathcal{D}^{(t)}$ from $\mathcal{D}$ according to $p^{(t)}(i)$
Learn model $f_t(x)$ from $\mathcal{D}^{(t)}$
Calculate error ϵ_t on training data $\mathcal{D}$ as $\epsilon_t = \sum_{i: f_t(x_i) \neq y_i} p^{(t)}(i)$
Set $\beta_t = \frac{\epsilon_t}{1 - \epsilon_t}$
Set $w_t = \ln \frac{1}{\beta_t}$
Set $p^{(t+1)}(i) = \frac{p^{(t)}(i)}{Z} \cdot \begin{cases} \beta_t & \text{if } f_t(x_i) = y_i \\ 1 & \text{otherwise} \end{cases}$, where Z is a normalizer
end

Output:

$f(x) = \arg\max_{y \in \mathcal{Y}} \left(\sum_{t=1}^{T} w_t \cdot I(f_t(x) = y) \right)$

AdaBoost

Theorem. Assume $\epsilon_t < \frac{1}{2}$ and let $\gamma_t = \frac{1}{2} - \epsilon_t$. Then the following bound holds

$$\frac{1}{n}\left|\{i : f(x_i) \neq y_i\}\right| \leq \prod_{t=1}^{T} \sqrt{1 - 4\gamma_t^2} \leq e^{-2\sum_{t=1}^{T} \gamma_t^2}$$

In practice:

Training error $\to 0$, but the test error continues to decrease

AdaBoost theory shows relationship to SVMs

Minimizing ϵ_t is equivalent to minimizing $E = \sum_{i=1}^{n} e^{-y_i f(x_i)}$

Gradient Boosting: Intuition

Objective: $L = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$ $\longleftarrow$ minimize mean squared error

Idea:

- prediction $f(x_i)$ is imperfect
- can we improve it by learning $g(x_i) = y_i - f(x_i)$
- we want to predict the residual $y_i - f(x_i)$

Incorporate into boosting:

$$f^{(0)}(x) = \arg\min_{c\in\mathbb{R}} \sum_{i=1}^{n}(y_i - c)^2$$

$t = 1 \ldots T$

$$f^{(t)}(x) = f^{(t-1)}(x) + \gamma^{(t)} g^{(t)}(x) \qquad \text{where} \qquad g^{(t)}(x) = \arg\min_{h\in\mathcal{F}} \sum_{i=1}^{n}(y_i - f^{(t-1)}(x_i) - h(x_i))^2$$

$$\gamma^{(t)} = \arg\min_{\gamma\in\mathbb{R}} \sum_{i=1}^{n}(y_i - f^{(t-1)}(x_i) - \gamma g^{(t)}(x_i))^2$$

$\uparrow$ needed for more complex loss functions

Output: $f^{(T)}(x)$

Why is it Gradient Boosting

Objective: $L = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$

Differentiate:

$$-\frac{\partial L}{\partial f(x_i)} = \frac{2}{n}(y_i - f(x_i))$$
$$= \frac{2}{n}g(x_i) \qquad \longleftarrow \qquad \text{residual}$$

Generalize:

- L can be any differentiable loss function, ideally convex
- we can find the gradient ∇L to optimize the "generalized residual"
- we can also find Hessian of L to improve optimization
- good idea to regularize

Gradient Boosting: XGBoost

Convex loss: $L^{(t)} = \sum_{i=1}^{n} \left(\ell(y_i, f^{(t-1)}(x_i) + g^{(t)}(x_i))\right) + \text{regularizer}(g^{(t)}(x))$

Second order approximation:

$$L^{(t)} \approx \sum_{i=1}^{n} [\ell(y_i, f^{(t-1)}(x_i)) + \text{gradient} \cdot g^{(t)}(x_i) + \frac{1}{2} \cdot \text{Hessian} \cdot g^{(t)2}(x_i)] + \text{regularizer}$$

Details:

- boost trees
- improved splitting function
- many speedups
- added shrinkage for regularization

Chen & Guestrin. XGBoost: a scalable tree boosting system. *KDD*, 2016.

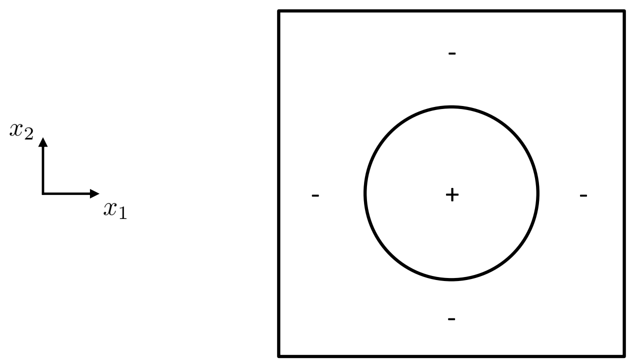
Experiment: Bagging

Data set:

- binary classification
- a unit-radius circle within a 4×4 square
- 200 examples, added a small amount of noise

Models:

- neural networks
- regression trees
- w/ and w/o bagging



$$\mathcal{X} = [-2, 2] \times [-2, 2]$$

$$\mathcal{Y} = \{-, +\}$$

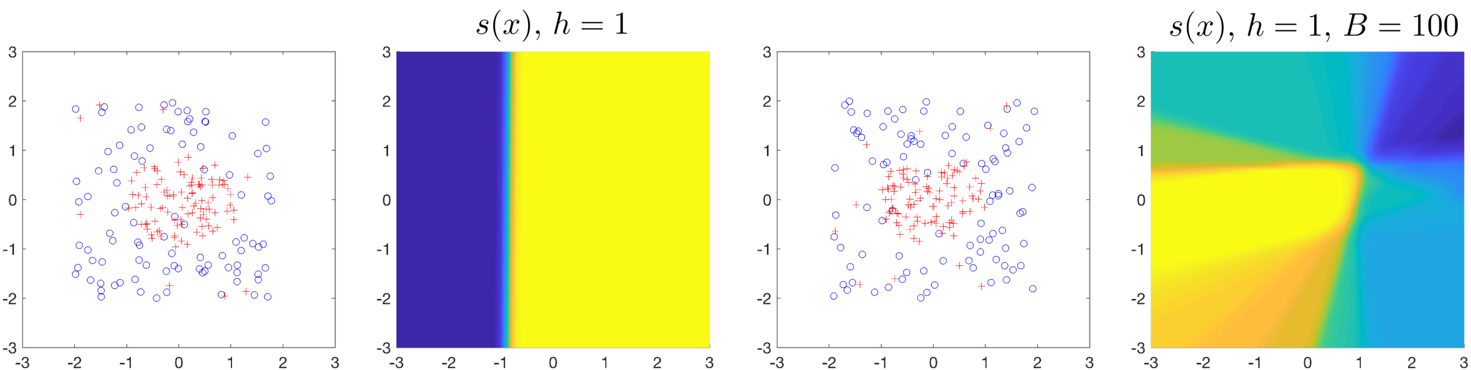
Experiment: Bagging

Data set:

- a unit-radius circle within a 4×4 square
- $n_+ = 100$, $n_- = 100$
- 5% error in positives, 10% error in negatvies

Models:

- single-output two-layer neural networks
- h hidden neurons, $\tanh(x)$ activation
- RPROP optimization



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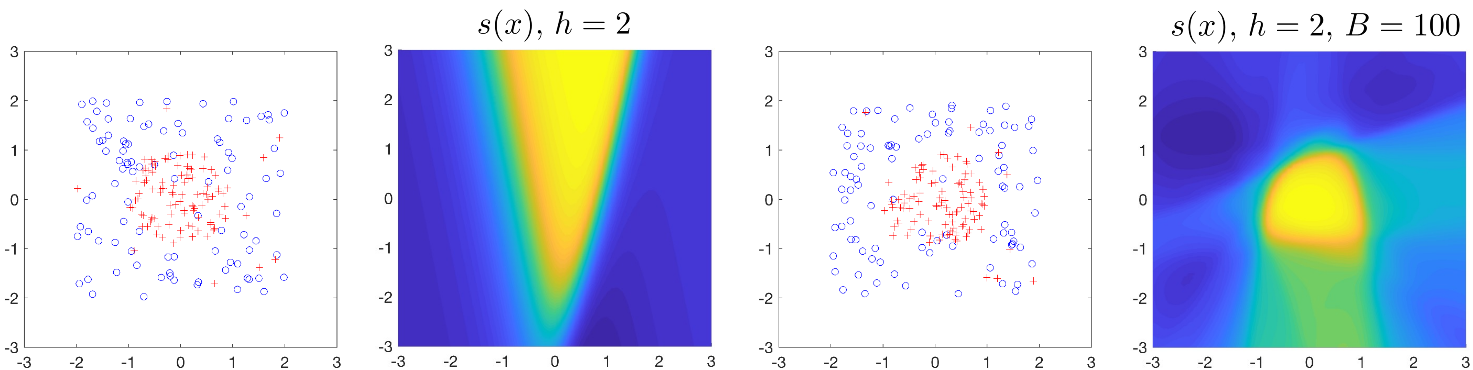

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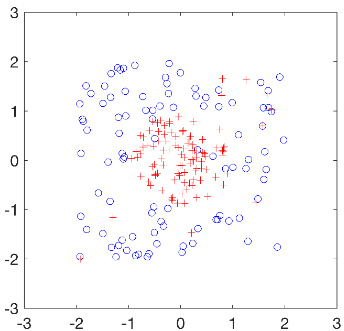
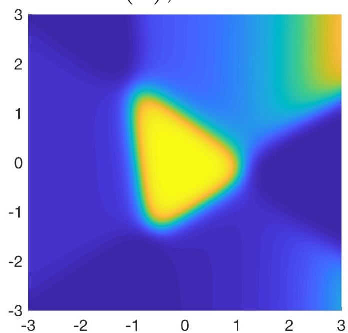
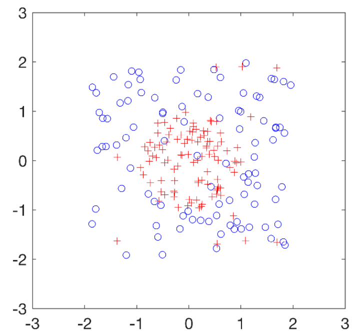
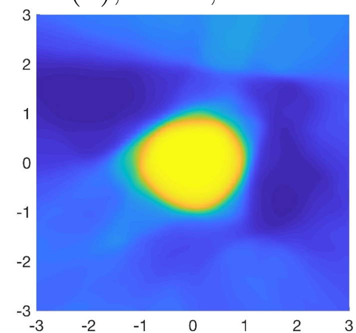


$s(x)$, $h = 4$





$s(x)$, $h = 4$, $B = 100$



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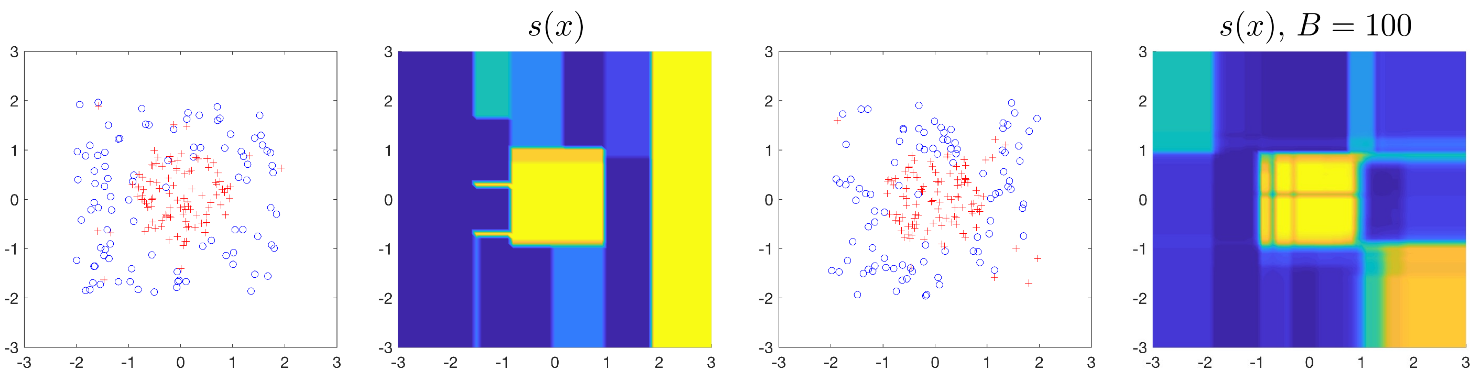


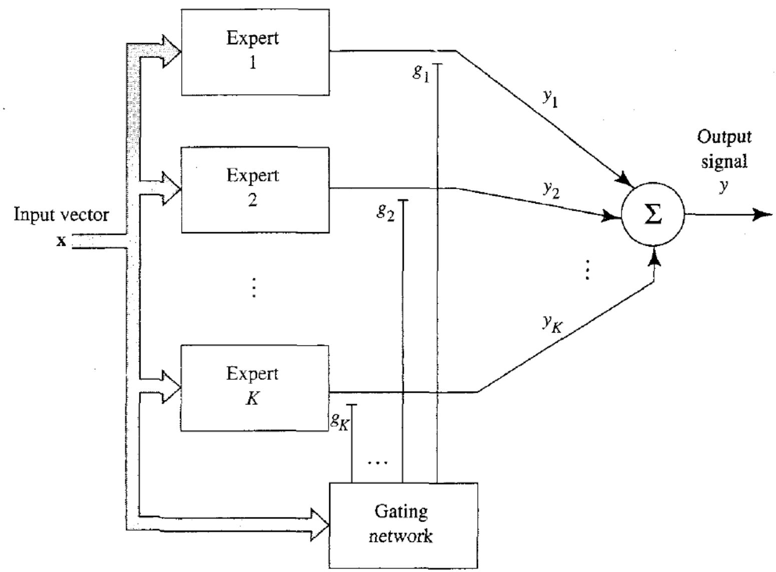
Probabilistic Generative Mixture Models

Model:

- x drawn according to $p(x)$
- pick model k to generate a target according to $p(k|x)$
- generate target using a linear model with additive zero-mean error
  e.g., $Y = \sum w_{kj} X_j + \epsilon_k$, where $\epsilon_k \sim \mathcal{N}(0, \sigma_k^2)$

$$p(y|x, \theta) = \sum_{k=1}^{K} p(y|x, w_k) p(k|x)$$

Mixture of Experts



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