

Bagging and Model Averaging

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Spring 2024

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Introduction

Introduction

Bootstrap aggregating (bagging) and boosting are useful techniques to improve the predictive performance of models.

- ▶ Boosting may also be useful in connection with many other models, e.g. for additive models with high-dimensional predictors
- ▶ bagging is most prominent for improving tree algorithms.

Bagging in Regression problems

Bagging in Regression problems

Let training data be $z = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, from z , obtain the prediction $\hat{f}(x)$ at input x .

Bagging works as follows:

1. Generate a bootstrap sample

$$(X_1^*, Y_1^*), \dots, (X_n^*, Y_n^*)$$

and compute the bootstrapped estimator $\hat{f}^*(\cdot)$.

2. Repeat step B times, yielding

$$\hat{f}^{*(1)}(\cdot), \dots, \hat{f}^{*(B)}(\cdot)$$

3. Aggregate the bootstrap estimates

$$\hat{f}_{bag}(\cdot) = B^{-1} \sum_{b=1}^B \hat{f}^{*(b)}(\cdot)$$

The bagging estimator is essentially (with $B = \infty$)

$$\hat{f}_{bag}(\cdot) \cong E^*(\hat{f}^*(\cdot))$$

here, E^* is with respect to the bootstrap distribution

The bagged estimate will differ from the original estimate $\hat{f}(x)$ **only when** the latter is a nonlinear or adaptive function of the data.

A trivial identity hints at some properties of bagging: with $B = \infty$

$$\begin{aligned}\hat{f}_{bag}(\cdot) &\cong \hat{f}(\cdot) + \left(\mathbb{E}^*(\hat{f}^*(\cdot)) - \hat{f}(\cdot) \right) \\ &\cong \hat{f}(\cdot) + \text{bootstrap bias estimate.}\end{aligned}$$

- ▶ Adding the bootstrap bias estimate
- ▶ What we can hope for is a variance reduction at the price of a higher bias.
 - ▶ True if $\hat{f}(\cdot)$ is a tree-based estimator
- ▶ An **ideal aggregate estimator** ($\mathbb{E}_{\mathbb{P}^* = \mathbb{P}} \hat{f}^*(\cdot)$) never increases MSE.

Bagging in Classification

Hard classification

Hard classification: If $\hat{f}^{*(b)}(x)$ is indicator-vector, with one 1 and $K - 1$ 0's (**hard classification**), equivalently, for some $\hat{h}^{*(b)}(x) \in \{1, \dots, K\}$.

- This is called “Consensus vote” (majority vote): selects the most “votes” from the B classifiers.

$$\hat{f}_{bag,k}(x) = \frac{1}{B} \sum_{b=1}^B 1\{\hat{h}^{*(b)}(x) = k\}$$

so the classifier is

$$\hat{f}_{bag}(x) = \arg \max_k \hat{f}_{bag,k}(x)$$

Soft classification

If $\hat{f}^{*(b)}(x) = \left(\hat{p}_1^{*(b)}, \dots, \hat{p}_K^{*(b)}\right)$, the estimates of class probabilities $\hat{p}_k^{*(b)} := \hat{P}^{(b)}(Y = k \mid X = x), k = 1, \dots, K$.

Consider “averaging probabilities”: the bagged estimates are the average prediction at x from B classifiers

$$\hat{p}_{\text{bag},k}(x) = B^{-1} \sum_{b=1}^B \hat{p}_k^{*(b)}(x), \quad k = 1, \dots, K$$

$$\hat{p}_{\text{bag}}(x) = \arg \max_k \hat{f}_{\text{bag},k}(x)$$

Effects of bagging

In the classification under 0 – 1 loss, bagging a good classifier can make it better, but bagging a bad classifier can make it worse.

The **Wisdom of Crowds** asserts that the collective knowledge of a diverse and independent body of people typically exceeds the knowledge of any single individual and can be harnessed by voting.

The Wisdom of Crowds

Consider an example: optimal decision at x be $h^*(x) = 1$ in a two-class example.

- ▶ Suppose each of the weak learners $h^{*(b)}$ have an error-rate $e_b = e < 0.5$,
- ▶ let $S_1(x) = \sum_{b=1}^B 1(h^{*(b)}(x) = 1)$ be the consensus vote for class 1.
- ▶ the weak learners are assumed to be independent

So

$$S_1(x) \sim \text{Bin}(B, 1 - e),$$

$$\Pr(S_1/B > 1/2) \rightarrow 1,$$

as B gets large.

Note the assumption here is that all weak learners are independent of each other.

Model Averaging

Bayesian model averaging

- ▶ J models, denoted by $M_j, j = 1, 2, \dots, J$.
- ▶ ζ be some quantity of interest, e.g., prediction $f(x)$ at some x .

The posterior distribution of ζ is

$$\Pr(\zeta \mid Z) = \sum_{m=1}^M \Pr(\zeta \mid M_m, Z) \Pr(M_m \mid Z)$$

with posterior mean

$$\mathbb{E}(\zeta \mid Z) = \sum_{m=1}^M \mathbb{E}(\zeta \mid M_m, Z) \Pr(M_m \mid Z)$$

Note:

- ▶ $\Pr(M_m \mid Z)$ are the weights proportional to posterior probability of each model.
- ▶ The **committee method** simply uses a simple unweighted average (equal probability).

$$Pr(M_m|Z)$$

To obtain $Pr(M_m|Z)$, there are two methods

- Use BIC

$$P(M_m | Z) \approx \frac{\exp(-\frac{1}{2}BIC_m)}{\sum_{l=1}^J \exp(-\frac{1}{2}BIC_l)}$$

- carry out a full Bayesian procedure: suppose each model M_m has parameters θ_m

$$\begin{aligned} Pr(M_m|Z) &\propto Pr(M_m)Pr(Z|M_m) \\ &\propto Pr(M_m) \int p(Z|M_k, \theta_k)p(\theta_k|M_k)d\theta_k \end{aligned}$$

Frequentist model averaging

Given predictions $\hat{f}_1(x), \hat{f}_2(x), \dots, \hat{f}_M(x)$, under squared-error loss, we can seek the weights $w = (w_1, w_2, \dots, w_M)$ such that

$$\hat{w} = \operatorname{argmin}_w \mathbb{E} \left(Y - \sum_{m=1}^M w_m \hat{f}_m(x) \right)^2$$

The solution is the population LS of Y on

$$\hat{F}(x)^\top \equiv (\hat{f}_1(x), \hat{f}_2(x), \dots, \hat{f}_M(x)):$$

$$\hat{w} = \mathbb{E} \left(\hat{F}(x) \hat{F}(x)^\top \right)^{-1} \mathbb{E}(\hat{F}(x)Y)$$

It holds that

$$\mathbb{E} \left(Y - \sum_{m=1}^M \hat{w}_m \hat{f}_m(x) \right)^2 \leq \mathbb{E} \left(Y - \hat{f}_m(x) \right)^2, \quad \forall m$$

so combining models never makes things worse, at the population level.

Stacking (ensemble)

- ▶ $\hat{f}_m^{-(i)}(x)$ is the **cross validation prediction** at x , i.e., using the m th model learned from the dataset with the i th training example removed.
- ▶ Then the stacking weights are given by

$$\hat{w}^{\text{st}} = \arg \min_w \sum_{i=1}^n \left(y_i - \sum_{m=1}^M w_m \hat{f}_m^{-(i)}(x_i) \right)^2$$

- ▶ The final prediction at point x is

$$\sum_m \hat{w}_m^{\text{st}} \hat{f}_m(x)$$

- ▶ the weights may be restricted to be sum up to 1.

- ▶ Stacking and model selection with via leave-one-out cross-validation are closely related

$$\text{LOOCV}(\hat{f}) = \frac{1}{n} \sum_{i=1}^n \left(y_i - \hat{f}^{-(i)}(x_i) \right)^2$$

- ▶ If the weight vectors w are restricted so that have one unit weight and the rest zero, this leads to a model choice with smallest leave-one-out cross-validation error.
- ▶ Stacking combines them with estimated optimal weights. This will often lead to better prediction, but less interpretability than the choice of only one of the M models.

Estimate weights

Suppose there are M methods to predict f . We choose $w = (w_1, \dots, w_M) \in \mathcal{W}$ (a grid of weights) by minimizing the K -fold cross validation loss. Suppose the data is divided into K folds, say C_1, \dots, C_k .

1. For $k = 1, \dots, K$:
 - (1) For $m = 1, \dots, M$:
 - (i) Estimate $\hat{f}_m^{(-k)}$ based on the $\{i \in C_k^c\}$
 - (ii) Obtain the out-of-sample estimate $\hat{f}_m^{(-k)}(x_i)$ for all $i \in C_k$
 - (2) For each $\tilde{w} \in \mathcal{W}$: Obtain the out-of-sample loss
$$MSE_k(\tilde{w}) = \sum_{i \in C_k} (Y_i - \sum_{m=1}^M \tilde{w} \hat{f}_m^{(-k)}(x_i))^2$$
2. Obtain the overall out-of-sample loss $MSE(\tilde{w}) = \sum_{k=1}^K MSE_k(\tilde{w})$ for each $\tilde{w} \in \mathcal{W}$.
3. Choose $w^* = \arg \min_{\tilde{w} \in \mathcal{W}} MSE(\tilde{w})$

Bumping

Bumping

Bumping is a technique for finding a better single model: uses bootstrap sampling to move randomly through model space.

- ▶ Draw bootstrap samples $\mathbf{Z}^{*(1)}, \dots, \mathbf{Z}^{*(B)}$, for $b = 1, \dots, B$
 - ▶ By convention, the original training sample is included in the set of bootstrap samples.
- ▶ Fit the model to $\mathbf{Z}^{*(b)}$ giving $\hat{f}^{*(b)}(x)$.
- ▶ Choose the model obtained from bootstrap sample \hat{b} which minimizes training error:

$$\hat{b} = \arg \min_b \frac{1}{n} \sum_{i=1}^n \left(y_i - \hat{f}^{*(b)}(x_i) \right)^2$$

- ▶ The prediction is

$$\hat{f}^{*(\hat{b})}(x)$$

- ▶ Bumping introduces variations in the data to navigate the model fitting process towards more favorable regions within the model space. This method assumes that if certain data points lead to suboptimal solutions, any bootstrap sample that exclude these point should result in improved outcomes.
- ▶ When employing bumping to compare models based on the training data, it's crucial to match the complexity across the models under comparison. For each bootstrap sample, the resulting model may vary but should maintain comparable complexity levels.
 - ▶ Models from the same family may be used as well. For example, in the context of decision trees, this could involve adjusting trees to have the same number of terminal nodes for each bootstrap sample.
- ▶ It's a standard practice to include the original training sample within the pool of bootstrap samples during the bumping process.