MATH 567: Mathematical Techniques in Data Science
Random forest

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

April 24, 2017

The bootstrap

- We saw before that decision trees often overfit the data.
- We will now discuss techniques that can be used to mitigate that problem.

Bootstrapping: General statistical method that relies on resampling data with replacement.

Idea: Given data (y_i, x_i), $i = 1, \dots, n$, construct *bootstrap samples* by sampling n of the observations **with replacement** (i.e., allow repetitions):

Sample 1	Sample 2	Sample 3
(y_{i_1}, x_{i_1})	(y_{j_1}, x_{j_1})	(y_{k_1}, x_{k_1})
(y_{i_2}, x_{i_2})	(y_{j_2}, x_{j_2})	(y_{k_2}, x_{k_2})
$\vdots$	$\vdots$	$\vdots$
(y_{i_n}, x_{i_n})	(y_{j_n}, x_{j_n})	(y_{k_n}, x_{k_n})

- Each bootstrap sample mimics the statistical properties of the original data.
- Often used to estimate parameter variability (or uncertainty).

Bagging

Bagging:(bootstrap aggregation) Suppose we have a model $y \approx \hat{f}(x)$ for data $(y_i, x_i) \in \mathbb{R}^{p+1}$.

1. Construct $B \in \mathbb{N}$ bootstrap samples.
2. Train the method on the b-th bootstrap sample to get $\hat{f}^{*b}(x)$.
3. Compute the average of the estimators:

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B} \sum_{i=1}^{B} \hat{f}^{*b}(x).$$

- Bagging is often used with regression trees.
- Can improve estimators significantly.

Note: Each bootstrap tree will typically involve different features than the original, and might have a different number of terminal nodes.

The bagged estimate is the average prediction at x from these B trees.

For classification: Use a majority vote from the B trees.

Example: trees with simulated data (ESL, Example 8.7.1)

Simulation:

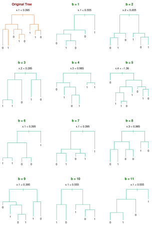
- $N = 30$ samples with $p = 5$ features.
- Features from a standard Gaussian distribution with pairwise correlation 0.95.
- Y generated according to

$$P(Y = 1 | X_1 \leq 0.5) = 0.2$$
$$P(Y = 1 | X_1 > 0.5) = 0.8.$$

- A test sample of size $2,000$ was also generated using the same model.
- The test error for the original tree and the bagged tree are reported.

Example (cont.)

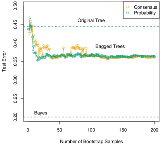
Bootstrap trees:



ESL, Figure 8.9.

Example (cont.)

Test error:



Errors for the bagging example. (ESL, Figure 8.10.)

The orange points correspond to the consensus vote, while the green points average the probabilities.

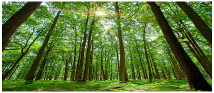
Out-of-bag error: Mean prediction error on each training sample x_i, using only the trees that did not have x_i in their bootstrap sample.

Can be used to approximate the prediction error.

Random forests

- Idea of bagging: average many noisy but approximately unbiased models, and hence reduce the variance.
- However, the bootstrap trees are generally correlated.
- Random forests improve the variance reduction of bagging by reducing the correlation between the trees.
- Achieved in the tree-growing process through random selection of the input variables.
- Popular method.

Random forests (cont.)



Random forests: Each time a split in a tree is considered, a random selection of m predictors is chosen as split candidates from the full set of p predictors.

- Typical value for m is $\sqrt{p}$.
- We construct $T_1, \dots, T_B$ trees using that method on bootstrap samples. The **random forest (regression) predictor** is

$$\hat{f}^B_{\text{rf}}(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x).$$

For classification: use majority vote.

Example (Izenman, 2013)

Diagnostic classification of four childhood tumors (Khan et al., 2001):

- Small, round, blue-cell tumors (SRBCTs) of childhood.
- Four types of SRBCTs (EWS, BL, NB, RMS).
- Tumors have a similar appearance.
- Getting the diagnosis correct impacts directly upon the type of treatment, therapy, and prognosis the patient receives.
- Currently, no single clinical test that can discriminate between these cancers.

Data:

- 83 cases (29 EWS, 11 BL, 18 NB, 25 RMS).
- Gene expression data for $6,567$ genes, reduced to $2,308$ by requiring a minimum intensity.
- `research.nhgri.nih.gov/microarray/Supplement`.

- A random forest was applied to these data using 500 fully grown trees with $m = 25$ variables at each split.
- Able to get a 0% Out-of-bag misclassification rate.

Boosting

Like bagging, boosting is a general approach that can be applied to many models. *Combines weak learners into a single strong learner.*

Boosting: Recursively fit trees to residuals. (Compensate the shortcoming of previous model.)

Input: $(y_i, x_i) \in \mathbb{R}^{p+1}$, $i = 1, \dots, n$. Initialize $\hat{f}(x) = 0$, $r_i = y_i$.

For $b = 1, \dots, B$:

1. Fit a tree estimator $\hat{f}^b$ with d splits to the training data.
2. Update the estimator using:
$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \cdot \hat{f}^b(x).$$
3. Update the residuals:
$$r_i \leftarrow r_i - \lambda \cdot \hat{f}^b(x_i).$$

Output: Boosted tree:

$$\hat{f}(x) = \sum_{i=1}^{B} \lambda \hat{f}^b(x).$$

Note: $\lambda > 0$ is a *learning rate*.

Boosting (cont.)

Can use many small trees (by choosing d small) and learn slowly (λ small) to avoid overfitting.

Choosing the parameters:

1. Number of trees B: choose by cross-validation.
2. Number of splits: can use a small value (e.g. $d = 1$).
3. Learning rate: can use 0.01, 0.001. Note: A small λ will generally require a larger B...

Gradient boosting: More generally, one can work with a general loss function (instead of sum of squares) and replace the residuals with the (negative) of the gradient of the loss function.

Relative importance of predictor variables

- The previous methodologies can improve decision trees considerably.
- However, we lose the nice interpretability of decision trees.

A *relative importance* of each predictor can be computed to help understand a model with multiple trees.

- Let T be a (binary) decision tree with $J - 1$ internal nodes.
- At each internal node t, a variable $X_{v(t)}$ is split, resulting in an improvement $\hat{\imath}_t^2$ in squared error.
- We define a *measure of relevance* of X_l by
$$\mathcal{I}_l^2(T) := \sum_{t=1}^{J-1} \hat{\imath}_t^2 \cdot I(v(t) = l).$$
In other words, we add-up the improvements at the nodes where X_l is split.

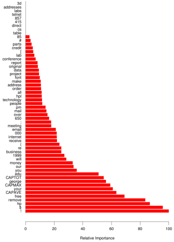
Relative importance of predictor variables (cont.)

- Similarly, in a model obtained from M trees (e.g. bagging, random forest), we use:

$$\mathcal{I}_l^2 = \frac{1}{M}\sum_{m=1}^{M}\mathcal{I}_l^2(T_m).$$

- Taking the square root of the relevance measure, we obtain the *relevance* of X_l.
- Typically, we do not report the actual relevance of a variable. We rather report the percentage of relevance of a given variable with respect to the variable with the largest relevance.

Relative importance of predictor for the spam data



ESL, Figure 10.6.