MATH 637: Mathematical Techniques in Data Science
Random forest

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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):

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\text{Sample 1} & \text{Sample 2} & \text{Sample 3} \\
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- Each bootstrap sample mimics the statistical properties of the original data.
- Often used to estimate parameter variability (or uncertainty).

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

Simulation:

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

$$P(Y = 1|X_1 \leq 0.5) = 0.2$$
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Example: trees with simulated data (ESL, Example 8.7.1)

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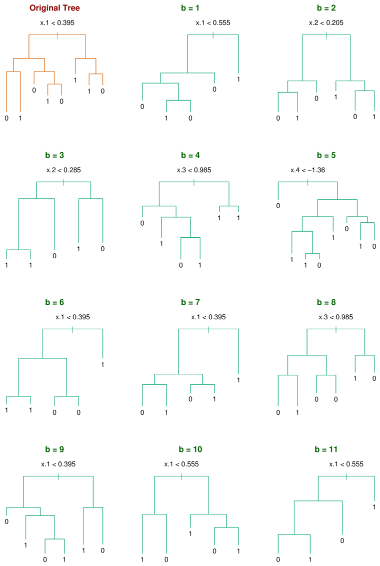
- A test sample of size $2,000$ was also generated using the same model.
- The test error for the original tree and the bagged tree are reported.

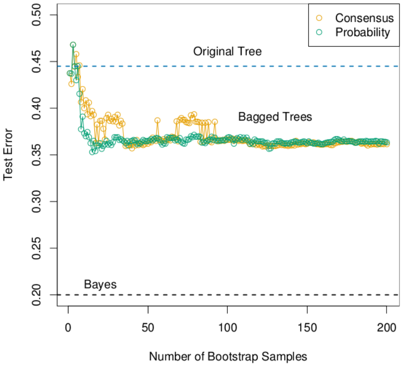
Example (cont.)

Bootstrap trees:



ESL, Figure 8.9.

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.

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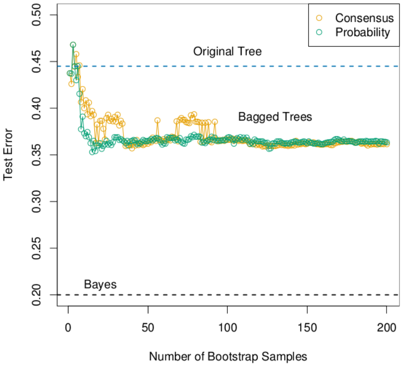

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Out-of-bag error: Mean prediction error on each training sample x_i, using only the trees that did not have x_i in their bootstrap sample.

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.

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

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

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.

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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.
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- 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

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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:
$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \cdot \hat{f}^b(x).$$
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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.

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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.

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- 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:

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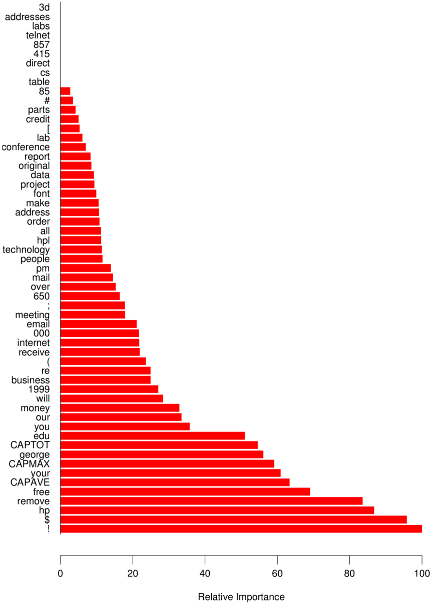
- Taking the square root of the relevance measure, we obtain the *relevance* of X_l.
- Typically, we do not report the actual relevance of a variable. We rather report the percentage of relevance of a given variable with respect to the variable with the largest relevance.

Relative importance of predictor for the spam data



ESL, Figure 10.6.