Ensemble Methods

COMP9417, 23T1

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Section 1

Ensemble Methods

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Why?

Section 2

Quick Recap: Bias and Variance of Estimators

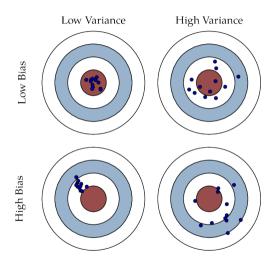
Quick Recap: Bias and Variance of Estimators

Recall the bias of an estimator $\hat{\theta}$ is defined as:

$$\mathsf{bias}(\hat{ heta}) = \mathbb{E}(\hat{ heta}) - heta$$

And its variance is defined as:

$$\mathsf{var}(\hat{ heta}) = \mathbb{E}\left[(heta - \mathbb{E}[\hat{ heta}])^2
ight]$$



Section 3

Bias-Variance Tradeoff

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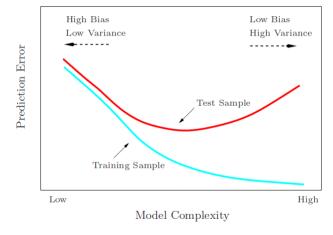
Recall the bias-variance decomposition of the MSE for an estimator $\hat{\theta}$:

$$\mathsf{MSE}(\hat{\theta}) = \mathsf{var}(\hat{\theta}) + \mathsf{bias}(\hat{\theta})^2$$

obviously for the best estimator we need to minimise the variance and minimise the bias.

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Section 4

Bagging

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For example, if we have a dataset $D=(x_i,y_i)$ for $i\in[1,n]$, we might train 4 decision trees on m points (where m=n/4) randomly picked from our dataset. We then have a committee of four trees with distinct knowledge on the dataset, which we can then average for our final prediction.

Ensemble Methods

Bagging

Generally, if we take ${\cal B}$ separate training sets from data ${\cal D}$, our bootstrapped models will be:

$$\hat{f}^1(D_1), \hat{f}^2(D_2), \dots, \hat{f}^B(D_B)$$

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and the final prediction for a point x is

$$\hat{f}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^b(x)$$

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$$\operatorname{var}\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}\right) = \frac{1}{n^{2}}\operatorname{var}\left(\sum_{i=1}^{n}X_{i}\right)$$

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Random Forests

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In bootstrap aggregation, the trees we generate may be *correlated*. To combat this we introduce *random forests* where:

- Randomly pick bootstrap samples
- At every step of tree learning, randomise what features the tree splits on
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Rationale: if we have strong predictors/features in our dataset, bagged trees will all typically pick the same features, leading to highly correlated predictions within the committee. This methods reduces this correlation and therefore the variance.

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$$C_m(X) = \alpha_1 h_1(X) + \alpha_2 h_2(X) + \ldots + \alpha_m h_m(X)$$

where α_i signifies the influence/weighting we give a model h_i for the final decision.

Boosting

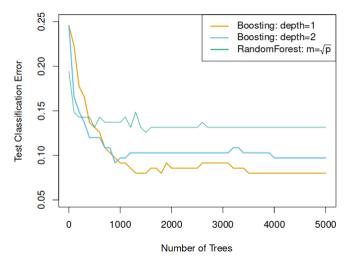
In boosting, we use a weak learner and improve it incrementally by adding more weak learners to make up for its mistakes. So we'll have a final model in the form,

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where α_i signifies the influence/weighting we give a model h_i for the final decision.

We also define a w_i for each iteration, signifying the weighting of each point. As each subsequent model needs to be an improvement on the last, we use these weights to signify which point the previous model misclassified.

Ensemble Methods



Let's take a look at the **Ada**ptive **Boost**ing algorithm.

Adaboost

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For a binary classification problem, we'll define the exponential loss as:

$$L(h(x_i), y_i) = e^{-y_i h(x_i)}$$

this loss typically isn't used in practice, but gives us a way of *weighting* how good a model performs on a dataset.

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Bias-Variance Tradeoff

Recall, our boosted model takes the form:

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$$L(C_m(X), Y) = \sum_{i=1}^{n} e^{-y_i C_m(x_i)}$$
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So, our problem is essentially,

$$\underset{\alpha,h}{\operatorname{arg\,min}} \left(\sum_{y_i = h_m(x_i)} w_i^m e^{-\alpha_m} + \sum_{y_i \neq h_m(x_i)} w_i^m e^{\alpha_m} \right)$$

$$\frac{\partial L}{\partial \alpha} = -e^{-\alpha_m} \sum_{y_i = h_m(x_i)} w_i^m + e^{\alpha_m} \sum_{y_i \neq h_m(x_i)} w_i^m$$

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At the minimum:

$$-e^{-\alpha_m} \sum_{y_i = h_m(x_i)} w_i^m + e^{\alpha_m} \sum_{y_i \neq h_m(x_i)} w_i^m = 0$$

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$$e^{2\alpha_m} = \frac{\sum_{y_i = h_m(x_i)} w_i^m}{\sum_{y_i \neq h_m(x_i)} w_i^m}$$

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$$\alpha_m = \frac{1}{2} \log \left(\frac{\sum_{y_i = h_m(x_i)} w_i^m}{\sum_{y_i \neq h_m(x_i)} w_i^m} \right)$$

If we let

$$\epsilon_m = \frac{\sum_{y_i \neq h_m(x_i)} w_i^m}{\sum_{i=1}^n w_i^m}$$

We can redefine α_m as:

$$\alpha_m = \frac{1}{2} \log \left(\frac{1 - \epsilon_m}{\epsilon_m} \right)$$

To actually get a form for $w_i^{(m)}$, we can apply the same trick of recursion,

$$w_i^{(m)} = e^{-y_i C_{m-1}(x_i)}$$

$$= e^{-y_i (C_{m-2}(x_i) + \alpha_{m-1} h_{m-1}(x_i))}$$

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So, when $y_i = h_{m-1}(x_i)$:

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When $y_i \neq h_{m-1}(x_i)$:

$$w_i^{(m)} = w_i^{(m-1)} e^{\alpha_{m-1}}$$

Now we have our definitions, we can define the Adaboost algorithm.

If we have a dataset D=(X,y) where $X\in\mathbb{R}^{n\times p}$ and $y\in\mathbb{R}^n$. Where T is our ensemble size and we have a learning algorithm A.

$$\begin{split} w^{(1)} &\leftarrow \frac{1}{n} \\ \text{for } t = 1, \dots, T \text{ do} \\ &M_t \leftarrow A(X, w^{(t)}) \\ &\alpha_t \leftarrow \frac{1}{2} \log \left(\frac{1 - \epsilon_t}{\epsilon_t} \right) \\ &w_i^{(t+1)} \leftarrow w_j^{(t)} \exp(\alpha_t) \quad j \text{ where } y_j \neq M_t(x_j) \\ &w_j^{(t+1)} \leftarrow w_j^{(t)} \exp(-\alpha_t) \quad j \text{ where } y_j = M_t(x_j) \end{split}$$
 end forreturn $M(X) = \operatorname{sgn} \left(\sum_{t=1}^T \alpha_t M_t(X) \right)$