HiOA Big Data Course

Session 6 - Trees

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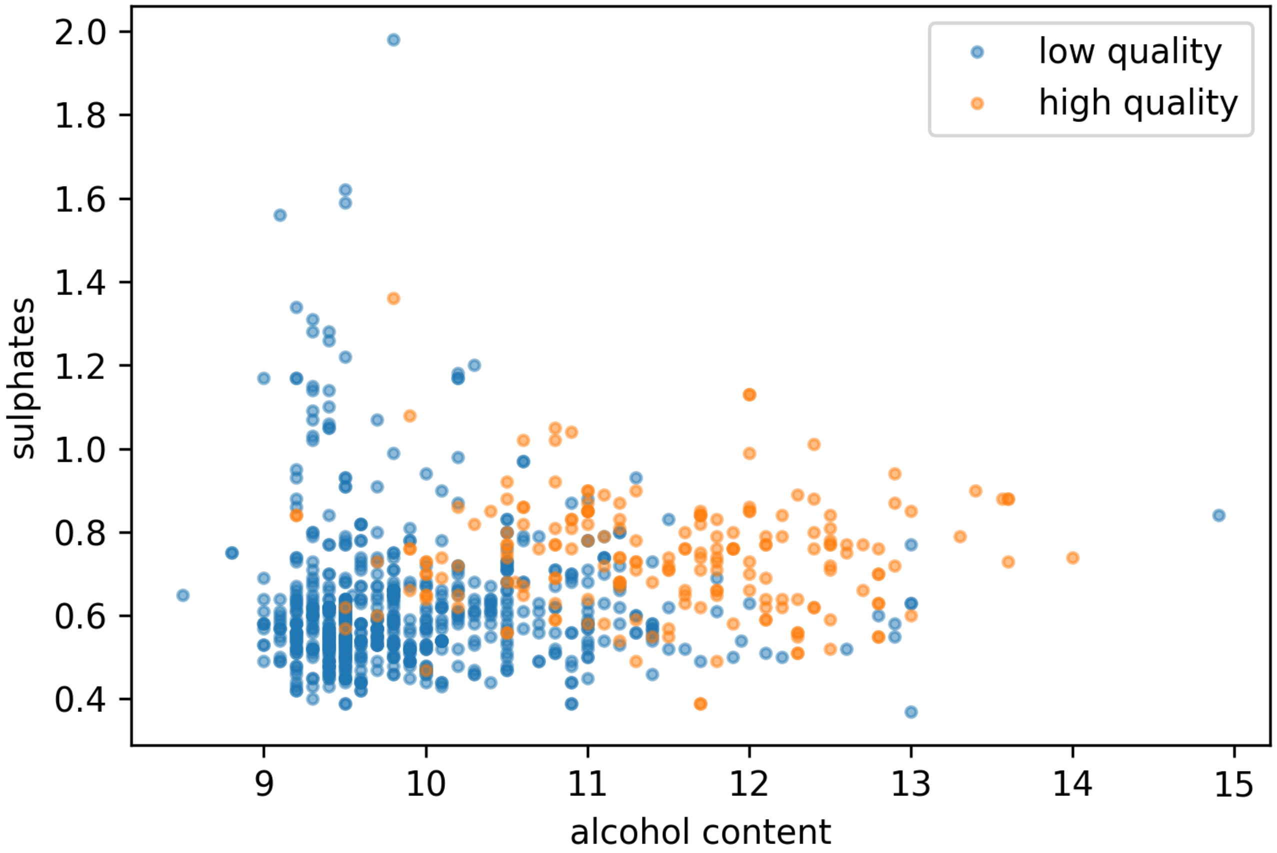
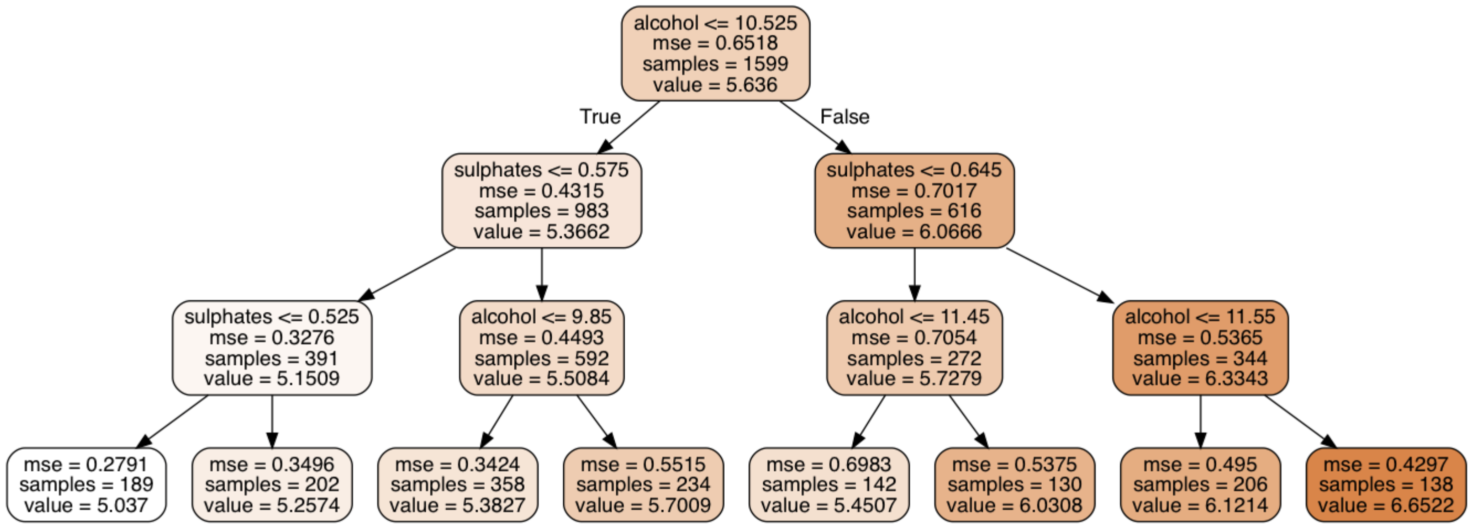
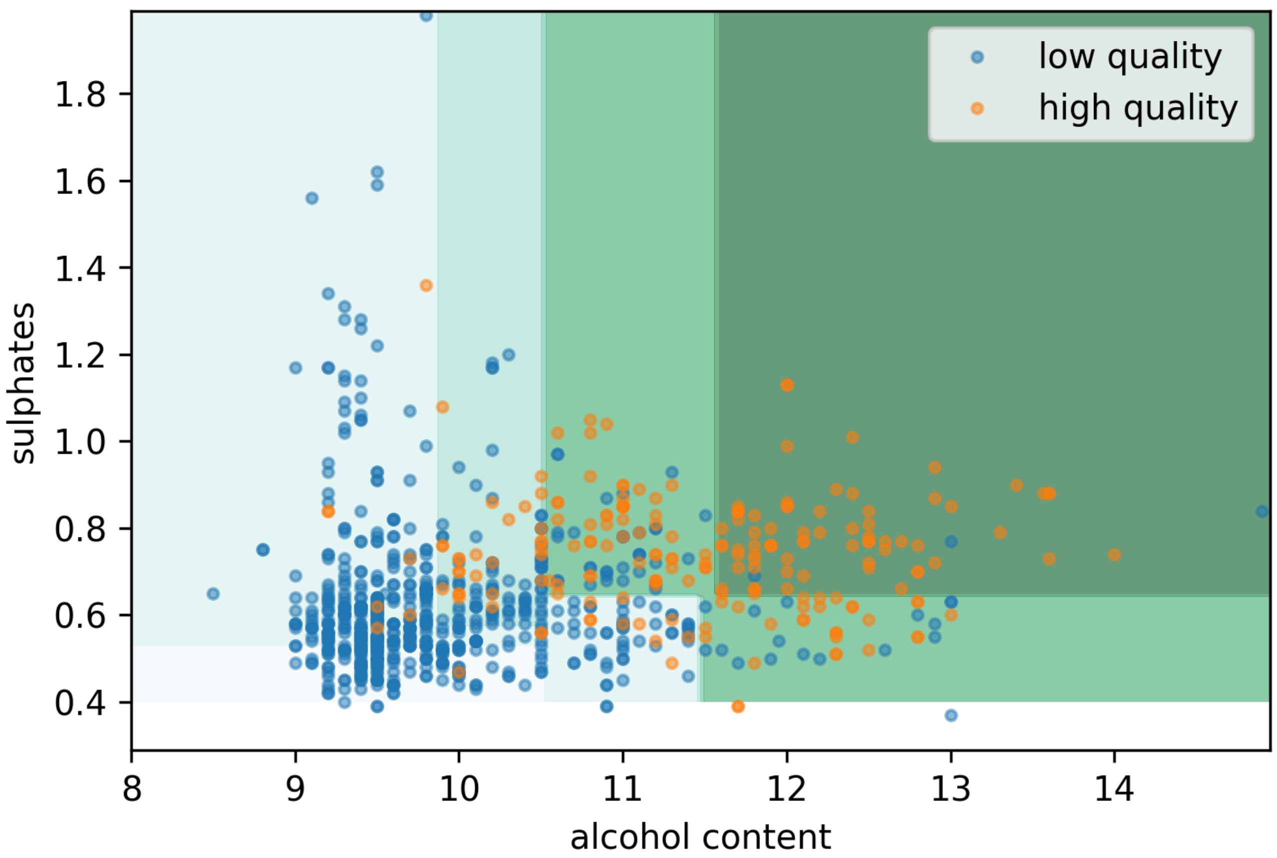
Wine Quality



Wine Quality Tree



Wine Quality Regression Tree



Why trees?

- Simple.
- Easy to explain.
    - Especially to non-experts.
- Powerful.

Calculating Trees

- Divide your data $R_L(j,s) = \{X | X^{(j)} \leq s\}$, $R_R(j,s) = \{X | X^{(j)} > s\}$.
- Find the best a_R, a_L, j, s to minimize

$$\sum_{i, x_i \in R_L(j,s)} (a_L - y_i)^2 + \sum_{i, x_i \in R_R(j,s)} (a_R - y_i)^2$$

- For given j, s, we find that $a_{R,L} = \underset{i, x_i \in R_{R,L}}{\operatorname{avg}} y_i$.
- Repeat on the sub-sets.
  - Until a maximum depth is reached.
  - Until a minimum number of samples is reached.

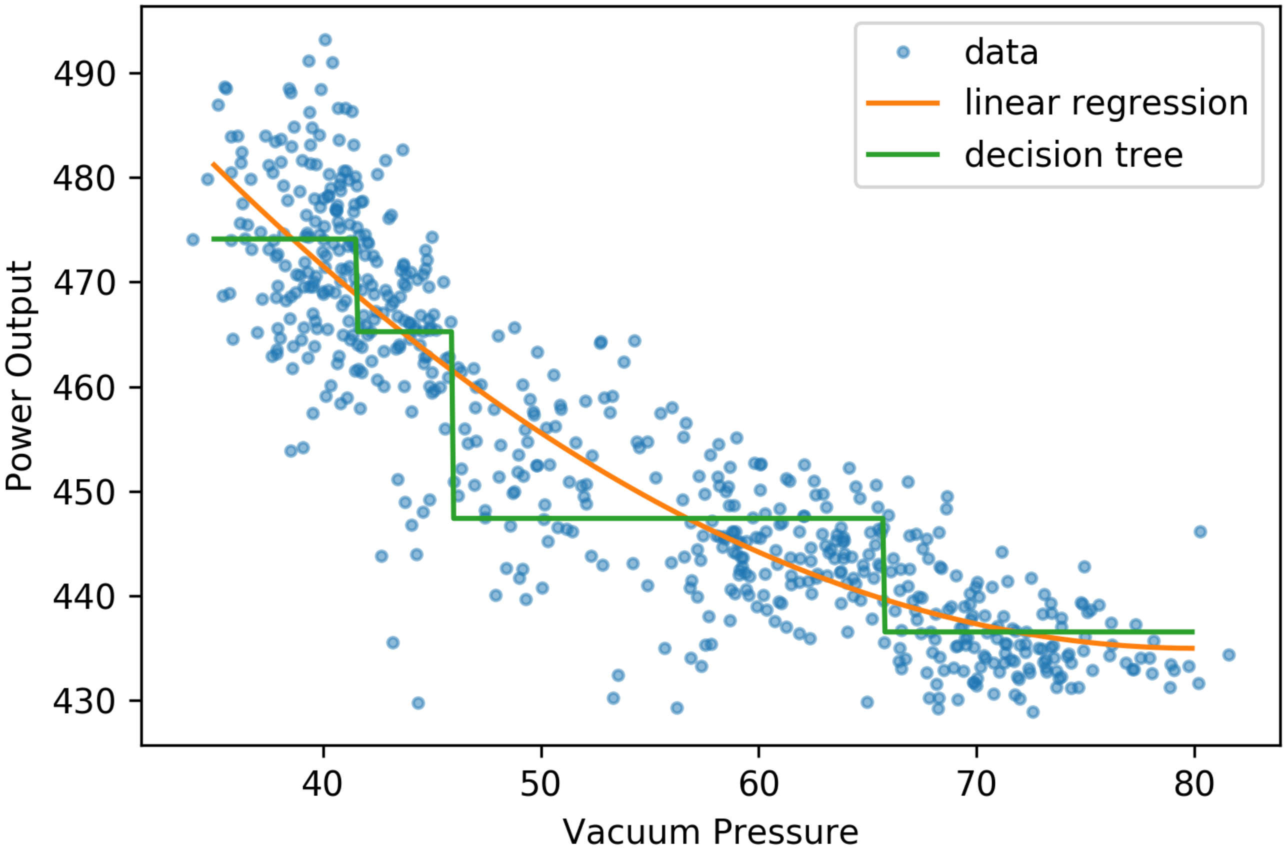
Regression Tree

Our resulting model reads

$$\hat{f}(X) = \sum_m c_m I\{X \in R_m\}.$$

Hence trees are an example of a general class of *additive models*.

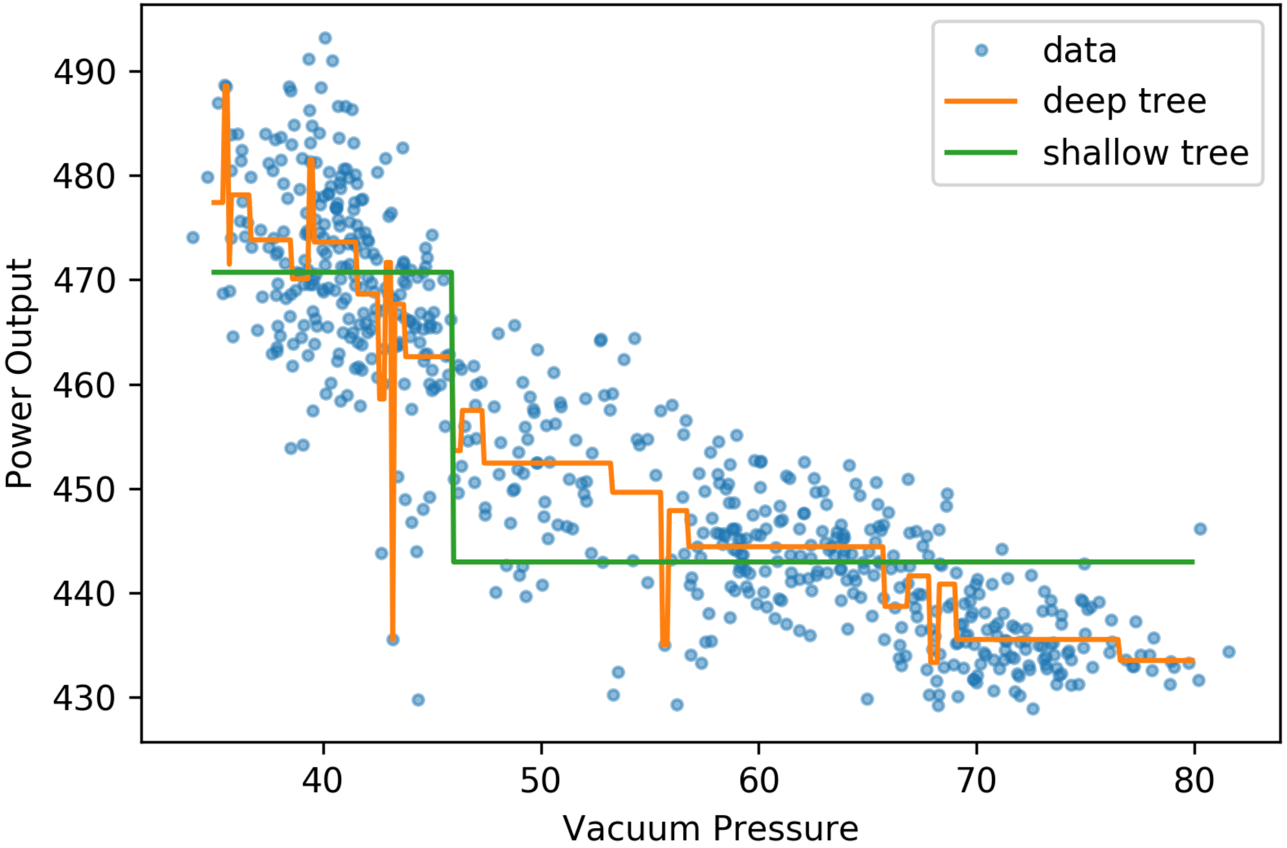
Tree Vs Linear Regression



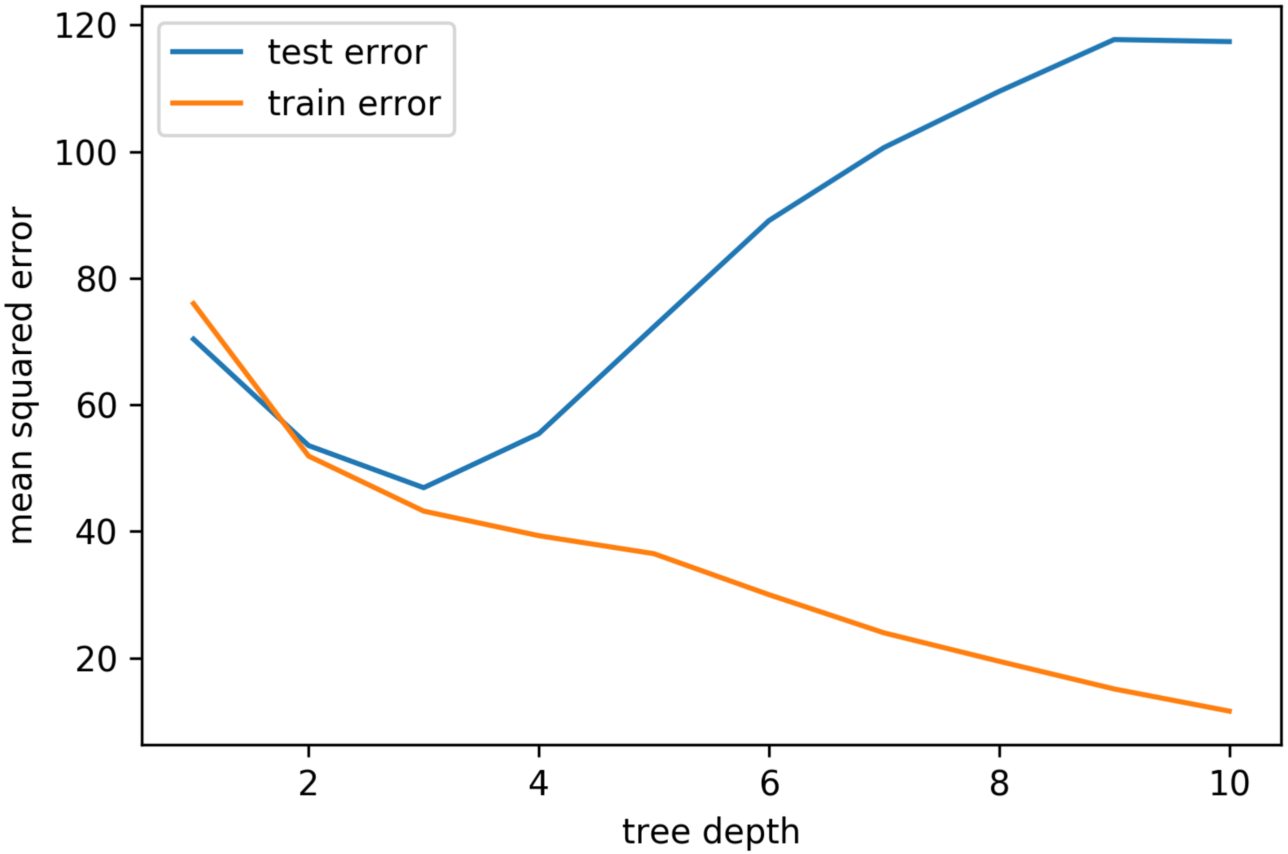
How Deep Should You Go?

- Deep trees have many degrees of freedom and hence high **variance**.
- Too shallow trees can't capture the *shape* of the data.
    - Hence have high **bias**.

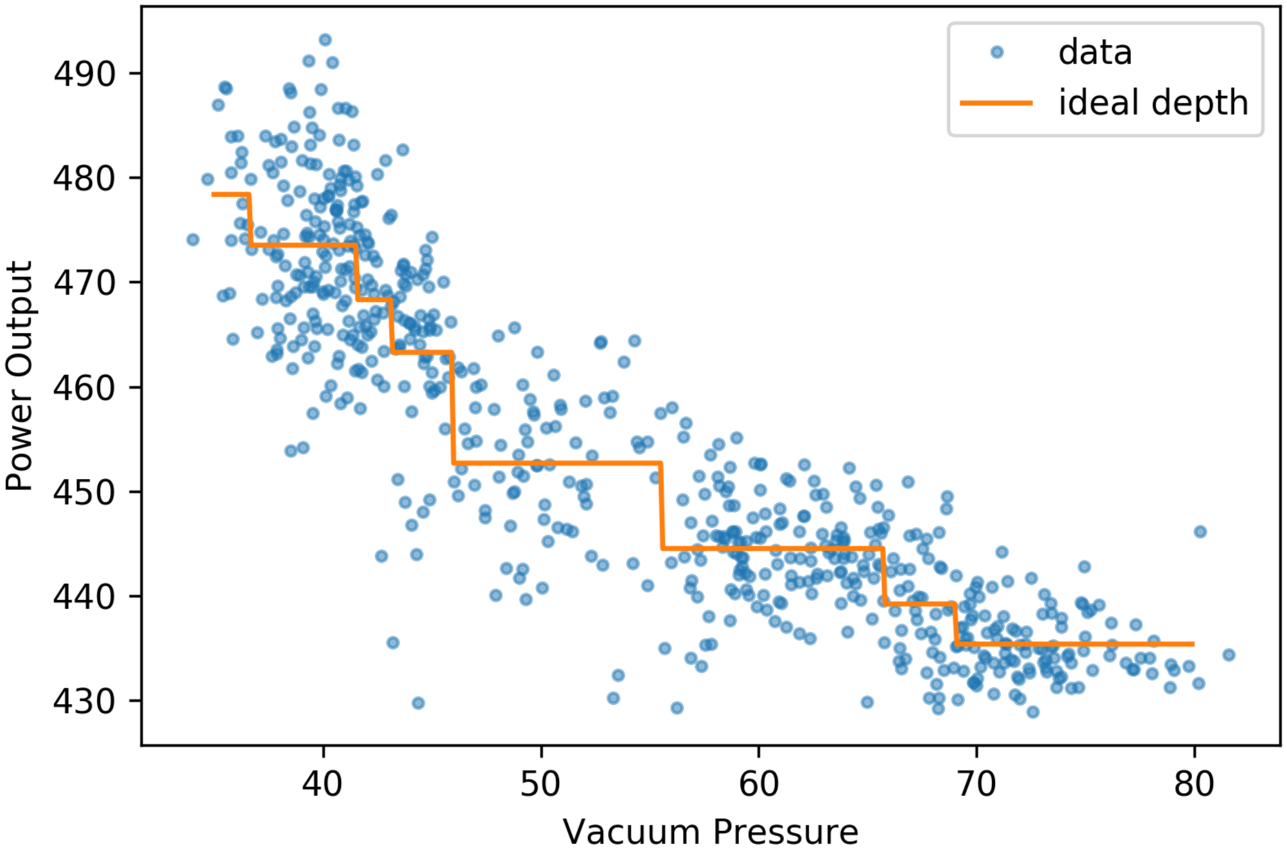
Bias-Variance Trade-off for Trees



Training and Test Error



The Best Tree



Trees for Classification

Just *modifying* our tree formulas to use the **mode**

$$a_{R,L} = \underset{i, x_i \in R_{R,L}}{\text{mode}}\ y_i$$

yields a classification algorithm.

How Find the Splits for Classification?

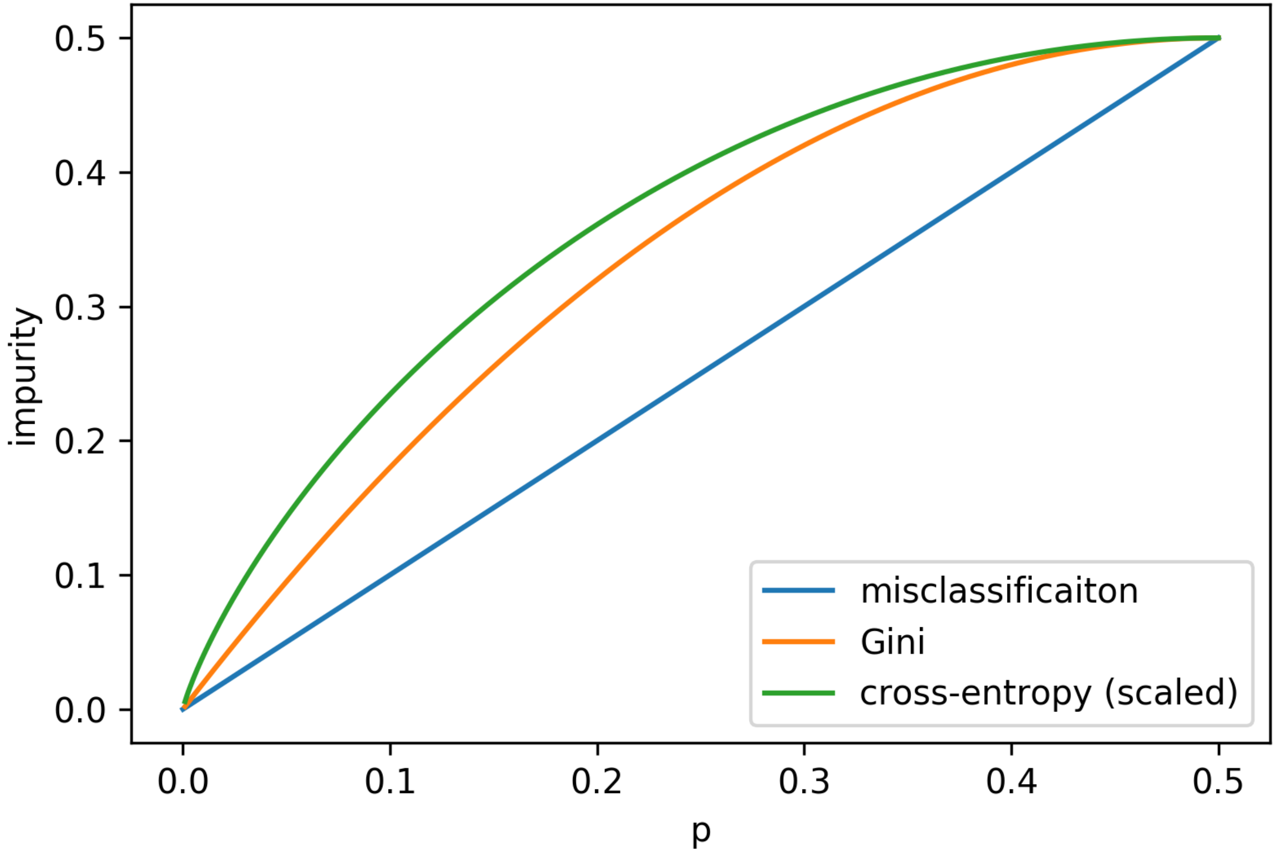
Define

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{i; x_i \in R_m} I(y_i = k),$$

such that $k(m) = \mathrm{argmax}_k \, \hat{p}_{mk}$

- Misclassification: $1 - \hat{p}_{mk(m)}$.
- Gini index: $\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$.
- Cross-entropy: $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$.

Two-Class impurity Measures



Tree pruning

- Stopping criteria:
  - Depth d.
  - Terminal node size.
  - Maximum split size.
  - Minimum impurity.
- Stopping at given d or impurity threshold might miss good splits later on.
- Often better to stop at e.g. minimal node size 10.
- Prune resulting tree.

Pruning by complexity

- Fitted tree T_0, let T be subtree with $|T|$ terminal nodes R_m.

$$N_m = |\{x_i \in R_m\}|$$
$$\hat{c}_M = \frac{1}{N_m} \sum_{x_i \in R_m} y_i$$
$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$
$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|$$

- For each α, $\exists$ unique smallest subtree minimizing C_α.

Practical considerations.

- Categorical inputs.
  - *Many* possible splits.
  - Easy for binary targets.
- Loss matrix.
  - L_{kl} loss for classifying k as l.
  - Classify $k(m) = \mathrm{argmin}_k \sum_l L_{lk}\hat{p}_{ml}$.
- Missing values.
- Multiple child nodes.
- Smoothness.
- Variance.

Ensemble Methods

- Reduce over-fitting and increase accuracy by using *multiple* models.
  - Reduce variance.
  - Possibly increase bias.
- Most commonly used:
  - Boosting.
  - Bagging.

Boosting

Additive Models

Instead of using one complex predictor, use many instances of a very basic one b (e.g. a tree with one split).

$$f(x) = \sum_{m=1}^{M} \beta_m b(x; \gamma_m)$$

The parameters are given by

$$\min_{\beta,\gamma} \sum_{i=1}^{N} L\left(y_i, \sum_{m=1}^{M} \beta_m b(x; \gamma_m)\right).$$

Forward stepwise additive modeling

1. Set $f_0 \equiv 0$.
2. For $m = 1m \ldots, M$
    - Set

$$(\beta_m, \gamma_m) = \operatorname*{argmin}_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma).$$

    - Set

$$f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m).$$

3. Return f_m.

FSAM and Square Error loss

For square error loss, we fit in each step to the residuals of the previous step.

$$
\begin{aligned}
L\left(y_i, f_{m-1}(x_i) + \beta b(x_i;\gamma)\right) &= \left[y_i - f_{m-1}(x_i) - \beta b(x_i,\gamma)\right]^2 \\
&= \left[r_{im} - \beta b(x_i,\gamma)\right]^2
\end{aligned}
$$

ADABOOST

Using

$$L(y, f(x)) = \exp(-yf(x))$$

for targets $y \in \{-1, 1\}$, gives raise to the AdaBoost algorithm.

AdaBoost

1. Initialize $w_i = 1/N,\ i = 1, \ldots, N$.
2. For $m = 1, \ldots, M$
   - Fit classifier $b_m(x)$ to data with weights w_i.
   - Set

$$e_m = \frac{\sum_i w_i I(y_i \neq b_m(x_i))}{\sum_i w_i}.$$

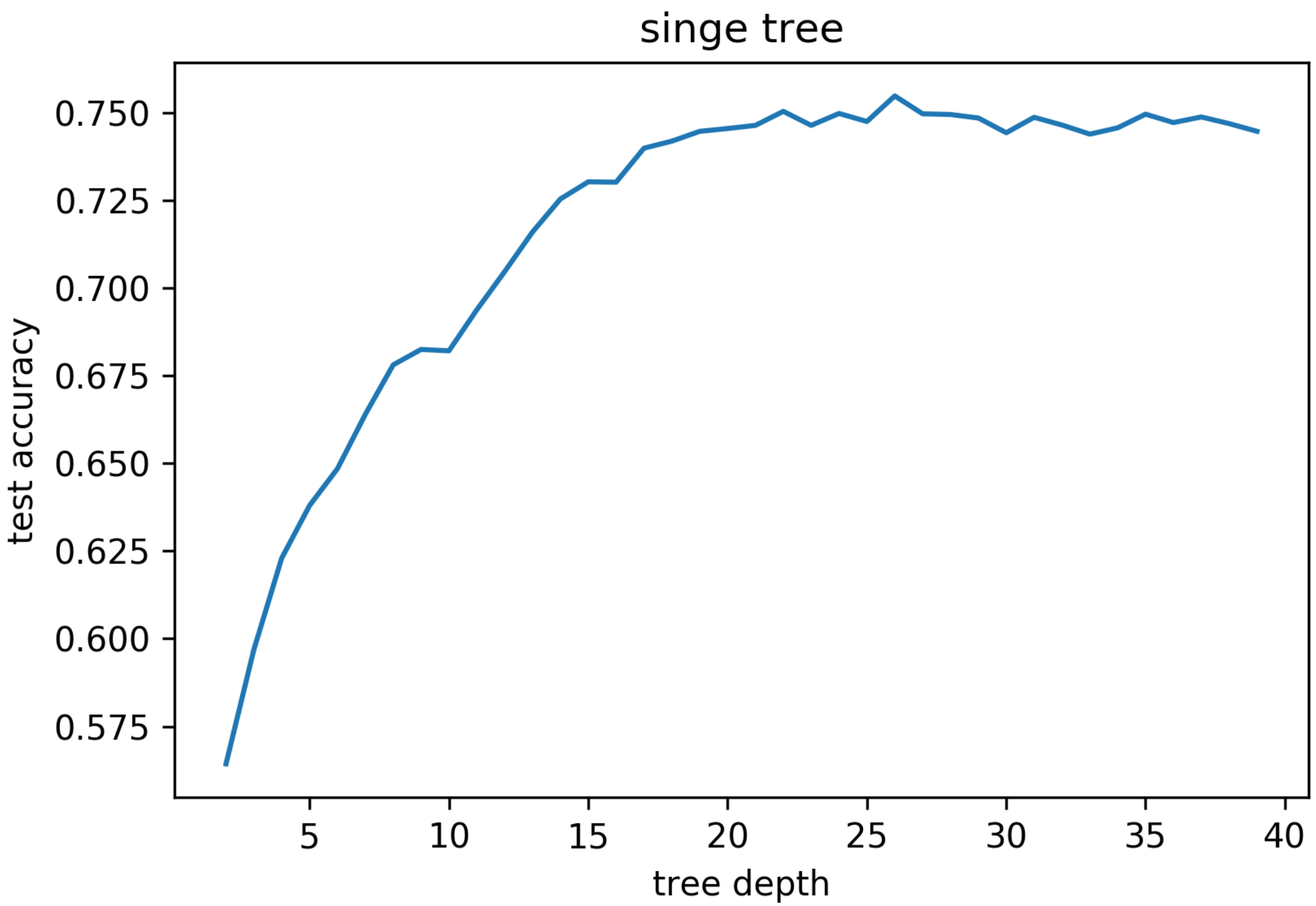
   - Set $\alpha_m = \log((1 - e_m)/e_m)$.
   - Set $w_i \leftarrow w_i \exp[\alpha_m I(y_i \neq b_m(x_i))]$.
3. Return $f(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m b_m(x)\right]$.

This can be adapted to *regression* as well.

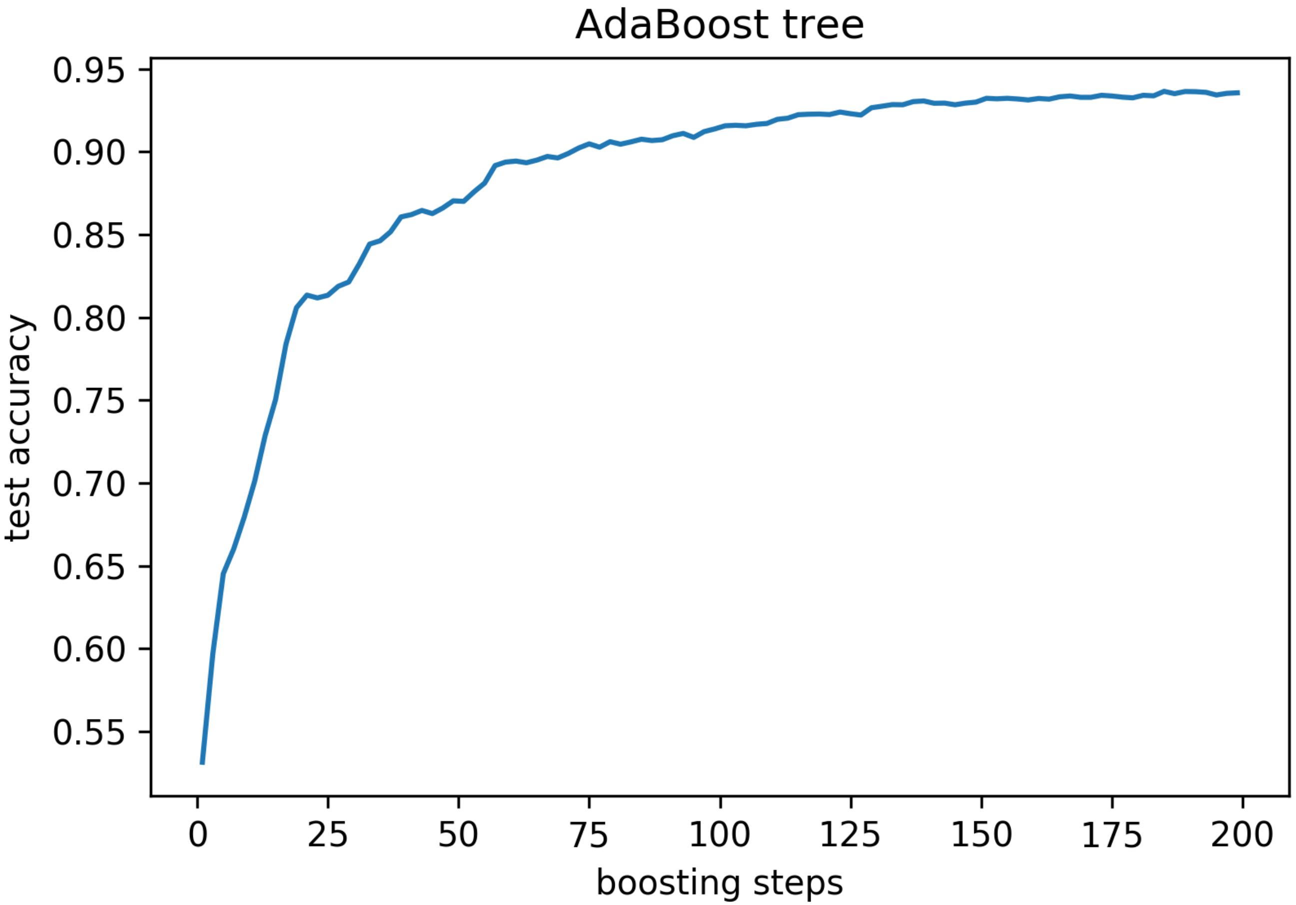
Generated Data

- Taken from Elements of Statistical Learning.
- $X_1, \ldots, X_{10}$ standard Gaussians.
- $Y = \begin{cases} 1 & \text{if } \sum_j X_j^2 > 9.34 = \chi^2_{10}(0.5) \\ 1 & \text{else} \end{cases}$
- 2k training cases, 10k test cases.

Single Tree on Generated Data



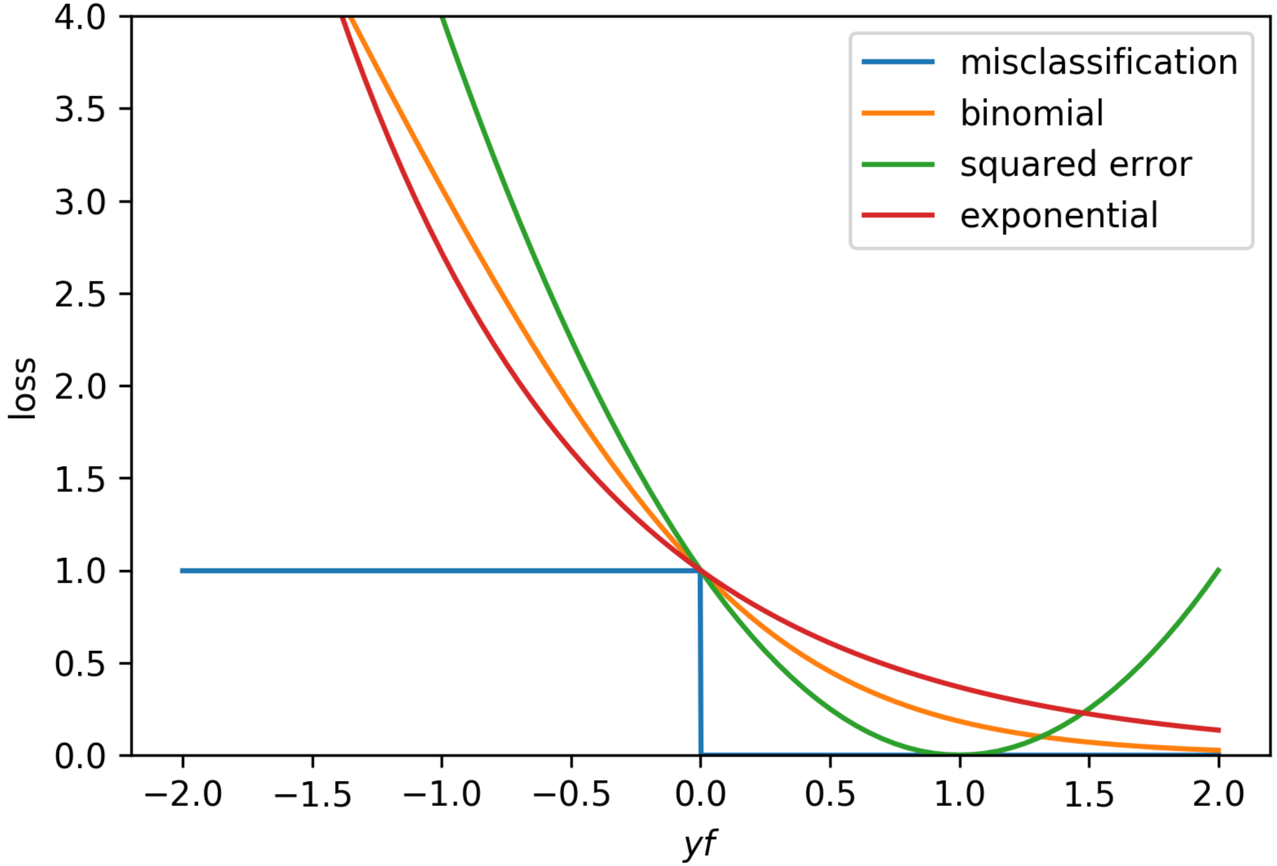
AdaBoost on Generated Data



More on Loss Functions

- Let's compare some loss functions for **classification**.
- We'll classify to $\mathrm{sign}(f)$.
- Misclassification: $I(\mathrm{sign}(f) \neq y)$.
- Exponential: $\exp(-yf)$.
- Binomial: $\log(1 + \exp(-2fy))$.
- Squared error: $(y - f)^2$.

Loss functions for classification



Conclusion

AdaBoost works great, but we'd like to plug in arbitrary loss functions. This seems like a hard task looking at

$$\min_{\beta,\gamma} \sum_{i=1}^{N} L\left(y_i, \sum_{m=1}^{M} \beta_m b(x;\gamma_m)\right).$$

The way out: **Gradient boosting**.

Questions?

Regression Algorithms

for Anomaly Detection

in Time Series Data

Time series data

- Given $x_i = x(t_i), i = 1, \ldots, n$.
  - Quantities measured at a given *time*.
    - E.g. number of users.
    - Bike trips taken.
- Want to predict an $x(t_i)$ in the future.
- Assume that t_i are periodic and equidistant.

Auto-regressive models

- Fit

  $$x(t) \approx \hat{f}\,(x(t)) = \hat{f}\,(x(t-\Delta_1), \ldots, x(t-\Delta_p))$$

  for chosen shifts Δ_k.
- Need to take into account periodicity in data.
  - E.g. $\Delta_1 = 1 \text{ day}$, $\Delta_2 = 1 \text{ week}$.

Detecting Anomalies

- Predict values using $\hat{f}$, compare to actuals.
- Let $\delta_i = \hat{f}(x(t_i)) - x(t_i)$.
- Let $\sigma = \sqrt{\frac{1}{N_t} \sum_i (\delta_i - \hat{\delta})^2}$.
- Let $z_i = \delta_i / \sigma$.
- Flag data points as anomalous if $z_i > z_{\mathrm{max}}$.