Model Assessment and Selection

Steve Avsec

Illinois Institute of Technology

February 26, 2024

Overview

Additive Models

2 Trees

3 Boosting and Bagging

General Linear Models:

$$g(E[Y|\mathbf{X}]) = c_0 + \sum_{j=1^N} c_j X_j$$

where *g* is a link function (identity, logit, log, etc.)

General Linear Models:

$$g(E[Y|\mathbf{X}]) = c_0 + \sum_{j=1^N} c_j X_j$$

where g is a link function (identity, logit, log, etc.)

General Additive Models:

$$g(E[Y|\mathbf{X}]) = c_0 + \sum_{j=1}^{N} f_j(X_j)$$

Many possibilities:

Linear terms

$$g(E[Y|X]) = c_0 + \sum_{j=1^K} c_j X_j + \sum_{j=K+1}^N f_j(X_j)$$

Many possibilities:

Linear terms

$$g(E[Y|X]) = c_0 + \sum_{j=1^K} c_j X_j + \sum_{j=K+1}^N f_j(X_j)$$

Splines

Many possibilities:

Linear terms

$$g(E[Y|X]) = c_0 + \sum_{j=1^K} c_j X_j + \sum_{j=K+1}^N f_j(X_j)$$

- Splines
- Basis functions (e.g. polynomials, trig polynomials, etc., just least squares).

Many possibilities:

Linear terms

$$g(E[Y|X]) = c_0 + \sum_{j=1^K} c_j X_j + \sum_{j=K+1}^N f_j(X_j)$$

- Splines
- Basis functions (e.g. polynomials, trig polynomials, etc., just least squares).
- Nonparametric functions (Kernel estimation).



Backfitting

1 Let
$$\alpha = \frac{1}{N} \sum_{j=1}^{N} y_j$$
, $f_j := 0$.

Backfitting

- **1** Let $\alpha = \frac{1}{N} \sum_{j=1}^{N} y_j$, $f_j := 0$.
- 2 Iterate $j = 1, \ldots, d$ and do

$$f_j = S_j \left(y_i - \alpha - \sum_{k \neq j} f_k(x_{i,k}) \right)$$

where S_i is some smoothing operation.

3 Stop when differences between iterations become small.

Backfitting

- **1** Let $\alpha = \frac{1}{N} \sum_{j=1}^{N} y_j$, $f_j := 0$.
- 2 Iterate $j = 1, \ldots, d$ and do

$$f_j = S_j \left(y_i - \alpha - \sum_{k \neq j} f_k(x_{i,k}) \right)$$

where S_i is some smoothing operation.

3 Stop when differences between iterations become small.

Smoothing can be taken to be 1-dimensional on pairs $(x_{i,j}, y_i - \alpha - \sum_{k \neq i} f_k(x_{i,k}))$.



Estimate the outcome using

$$f(\mathbf{X}) = \sum_{k=1}^{K} c_k I(\mathbf{X} \in R_k)$$

where R_k are regions (usually rectangles).

Estimate the outcome using

$$f(\mathbf{X}) = \sum_{k=1}^K c_k I(\mathbf{X} \in R_k)$$

where R_k are regions (usually rectangles).

Why is this a "tree"? List of conditions:

$$(root, X_1 \le t_1), (L, X_2 \le t_2), (R, X_1 \le t_3)...$$

Estimate the outcome using

$$f(\mathbf{X}) = \sum_{k=1}^K c_k I(\mathbf{X} \in R_k)$$

where R_k are regions (usually rectangles).

Why is this a "tree"? List of conditions:

$$(\text{root}, X_1 \leq t_1), (L, X_2 \leq t_2), (R, X_1 \leq t_3) \dots$$

Each region defined by and-ing conditions from root to leaf.

Fitting (regression)

For a given region, the best estimator $\tilde{c}_k = \text{mean}(y_i | \mathbf{x}_i \in R_k)$.

Fitting (regression)

For a given region, the best estimator $\tilde{c}_k = \text{mean}(y_i | \mathbf{x}_i \in R_k)$.

For a fixed j, let $R_1(j,s) = \{\mathbf{X}|X_j \leq s\}$ and $R_2 = \{\mathbf{X}|X_j > s\}$. Then consider

$$m_{j,s} = \min_{j,s} \sum_{\mathbf{x}_i \in R_1(j,s)} (y_i - \tilde{c}_1)^2 + \sum_{\mathbf{x}_j \in R_2(j,s)} (y_i - \tilde{c}_2)^2$$

Fitting (regression)

For a given region, the best estimator $\tilde{c}_k = \text{mean}(y_i | \mathbf{x}_i \in R_k)$.

For a fixed j, let $R_1(j,s) = \{\mathbf{X}|X_j \leq s\}$ and $R_2 = \{\mathbf{X}|X_j > s\}$. Then consider

$$m_{j,s} = \min_{j,s} \sum_{\mathbf{x}_i \in R_1(j,s)} (y_i - \tilde{c}_1)^2 + \sum_{\mathbf{x}_j \in R_2(j,s)} (y_i - \tilde{c}_2)^2$$

Optimal s is computationally tractable for each j, so choose optimal j, s pair at each iteration.

We need a stopping condition! Let:

1
$$N_m = |\{\mathbf{x}_i \in R_m\}|.$$

2
$$Q_m(T) = \frac{1}{N_m} \sum_{\mathbf{x}_i \in R_m} (y_i - \tilde{c}_m)^2$$

We need a stopping condition! Let:

1
$$N_m = |\{\mathbf{x}_i \in R_m\}|.$$

2
$$Q_m(T) = \frac{1}{N_m} \sum_{\mathbf{x}_i \in R_m} (y_i - \tilde{c}_m)^2$$

Define

$$C_{\alpha}(T) = \sum_{m=1}^{T} N_{m}Q_{m}(T) + \alpha |T|.$$

We need a stopping condition! Let:

1
$$N_m = |\{\mathbf{x}_i \in R_m\}|.$$

2
$$Q_m(T) = \frac{1}{N_m} \sum_{\mathbf{x}_i \in R_m} (y_i - \tilde{c}_m)^2$$

Define

$$C_{\alpha}(T) = \sum_{m=1}^{T} N_m Q_m(T) + \alpha |T|.$$

Start with a grand tree T_0 found by stopping when a node reaches a fixed number of points (commonly 5). There is a unique smallest subtree T_{α} for each α .

We need a stopping condition! Let:

1
$$N_m = |\{\mathbf{x}_i \in R_m\}|.$$

2
$$Q_m(T) = \frac{1}{N_m} \sum_{\mathbf{x}_i \in R_m} (y_i - \tilde{c}_m)^2$$

Define

$$C_{\alpha}(T) = \sum_{m=1}^{T} N_m Q_m(T) + \alpha |T|.$$

Start with a grand tree T_0 found by stopping when a node reaches a fixed number of points (commonly 5). There is a unique smallest subtree T_{α} for each α .

Tune α using k-fold cross validation, bootstrapping, etc.



• Missing values: Imputing the mean of the non-missing values is a bad idea.

- Missing values: Imputing the mean of the non-missing values is a bad idea.
- Instability: Small perturbations to the training data can lead to wild changes in splits.

- Missing values: Imputing the mean of the non-missing values is a bad idea.
- Instability: Small perturbations to the training data can lead to wild changes in splits.
- Interpretability: Very high interpretability since it is easy to see which training samples influence a prediction.

- Missing values: Imputing the mean of the non-missing values is a bad idea.
- Instability: Small perturbations to the training data can lead to wild changes in splits.
- Interpretability: Very high interpretability since it is easy to see which training samples influence a prediction.
- Non-continuity: Indicators are not continuous/differentiable which can be a negative in some contexts. (MARS and HME)



Consider a classification where $Y \in \{\pm 1\}$.

Consider a classification where $Y \in \{\pm 1\}$. Usual error function

$$\overline{\operatorname{err}} = \frac{1}{N} \sum_{i=1}^{N} I(y_i \neq G(\mathbf{x}_i)).$$

(in sample error).

Consider a classification where $Y \in \{\pm 1\}$. Usual error function

$$\overline{\operatorname{err}} = \frac{1}{N} \sum_{i=1}^{N} I(y_i \neq G(\mathbf{x}_i)).$$

(in sample error).

Let G_1, \ldots, G_M be "weak" learners (ones that are slightly better than random).

Consider a classification where $Y \in \{\pm 1\}$. Usual error function

$$\overline{\operatorname{err}} = \frac{1}{N} \sum_{i=1}^{N} I(y_i \neq G(\mathbf{x}_i)).$$

(in sample error).

Let G_1, \ldots, G_M be "weak" learners (ones that are slightly better than random).

Final model:

$$G(\mathbf{x}) = \operatorname{sign}\left(\sum_{m=1}^{M} \alpha_m G_m(\mathbf{x})\right)$$

1 Let
$$w_i = \frac{1}{N}$$
 for $i = 1, ..., N$.

- **1** Let $w_i = \frac{1}{N}$ for i = 1, ..., N.
- 2 Fit a classifier G_m to the (weighted) training data using current weights.

- **1** Let $w_i = \frac{1}{N}$ for i = 1, ..., N.
- 2 Fit a classifier G_m to the (weighted) training data using current weights.
- 3 Compute

$$\operatorname{err}_{m} = \frac{\sum_{i=1}^{N} w_{i} I(y_{i} \neq G_{m}(\mathbf{x}_{i}))}{\sum_{i=1}^{N} w_{i}}$$

- **1** Let $w_i = \frac{1}{N}$ for i = 1, ..., N.
- 2 Fit a classifier G_m to the (weighted) training data using current weights.
- 3 Compute

$$\mathsf{err}_m = \frac{\sum_{i=1}^N w_i I(y_i \neq G_m(\mathbf{x}_i))}{\sum_{i=1}^N w_i}$$

4 Set

$$\alpha_m = \log(\frac{1 - \operatorname{err}_m}{\operatorname{err}_m})$$

- **1** Let $w_i = \frac{1}{N}$ for i = 1, ..., N.
- 2 Fit a classifier G_m to the (weighted) training data using current weights.
- 3 Compute

$$\operatorname{err}_{m} = \frac{\sum_{i=1}^{N} w_{i} I(y_{i} \neq G_{m}(\mathbf{x}_{i}))}{\sum_{i=1}^{N} w_{i}}$$

4 Set

$$\alpha_m = \log(\frac{1 - \operatorname{err}_m}{\operatorname{err}_m})$$

6 Update:

$$\mathbf{w}_i = \mathbf{w}_i \mathbf{e}^{\alpha_m I(\mathbf{y}_i \neq G_m(\mathbf{x}_i))}$$



Back to Additive Models

Suppose we want to fit

$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m b(\mathbf{x}, \gamma_m)$$

Back to Additive Models

Suppose we want to fit

$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m b(\mathbf{x}, \gamma_m)$$

1 Initialize $f_0 := 0$

Back to Additive Models

Suppose we want to fit

$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m b(\mathbf{x}, \gamma_m)$$

- 1 Initialize $f_0 := 0$
- 2 Compute

$$(c_m, \gamma_m) = \arg\min_{c, \gamma} L(Y, f_{m-1}(\mathbf{X}) + cb(\mathbf{X}, \gamma))$$

Back to Additive Models

Suppose we want to fit

$$f(\mathbf{x}) = \sum_{m=1}^{M} c_m b(\mathbf{x}, \gamma_m)$$

- 1 Initialize $f_0 := 0$
- 2 Compute

$$(c_m, \gamma_m) = \arg\min_{c, \gamma} L(Y, f_{m-1}(\mathbf{X}) + cb(\mathbf{X}, \gamma))$$

Opdate

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + c_m b(\mathbf{x}, \gamma_m)$$



 Previous example can be intractable depending on the Loss function and basis function involved.

- Previous example can be intractable depending on the Loss function and basis function involved.
- However, this can often be reduced to just finding

$$arg \min_{c,\gamma} L(Y, cb(\mathbf{X}, \gamma))$$

- Previous example can be intractable depending on the Loss function and basis function involved.
- However, this can often be reduced to just finding

$$\arg\min_{\boldsymbol{c},\gamma} L(Y, \boldsymbol{cb}(\mathbf{X}, \gamma))$$

For instance,

$$L(Y, f(\mathbf{X})) = \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i))^2$$

reduces to

$$(y_i - f_{m-1}(\mathbf{x}_i) - cb(\mathbf{x}, \gamma))$$



- Previous example can be intractable depending on the Loss function and basis function involved.
- However, this can often be reduced to just finding

$$\arg\min_{\boldsymbol{c},\gamma} L(\boldsymbol{Y}, \boldsymbol{cb}(\mathbf{X}, \gamma))$$

For instance,

$$L(Y, f(\mathbf{X})) = \sum_{i=1}^{N} (y_i - f(\mathbf{x}_i))^2$$

reduces to

$$(y_i - f_{m-1}(\mathbf{x}_i) - cb(\mathbf{x}, \gamma))$$

• So in effect just best fit of current residual.



Suppose the loss function L is differentiable and define

$$L(f) = L(Y, f(\mathbf{X}))$$

Suppose the loss function L is differentiable and define

$$L(f) = L(Y, f(\mathbf{X}))$$

Let

$$\mathbf{f} = (f(\mathbf{x_i}))$$

then

$$\hat{f}(f) = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

Suppose the loss function *L* is differentiable and define

$$L(f) = L(Y, f(\mathbf{X}))$$

Let

$$\mathbf{f} = (f(\mathbf{x_i}))$$

then

$$\hat{f}(f) = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

Start with an initial guess. At each step, compute

$$g_{i,m} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f}\right]_{f = f_m}$$

Suppose the loss function *L* is differentiable and define

$$L(f) = L(Y, f(X))$$

Let

$$\mathbf{f} = (f(\mathbf{x_i}))$$

then

$$\hat{f}(f) = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

Start with an initial guess. At each step, compute

$$g_{i,m} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f}\right]_{f = f_m}$$

Update

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \rho_m g_{i,m}$$

1 Initialize $f_0(\mathbf{x}) = \arg\min_{\gamma} L(Y, \gamma)$.

- 1 Initialize $f_0(\mathbf{x}) = \arg\min_{\gamma} L(Y, \gamma)$.
- 2 Compute

$$r_{i,m} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f}\right]_{f=f_{m-1}}$$

- 1 Initialize $f_0(\mathbf{x}) = \arg\min_{\gamma} L(Y, \gamma)$.
- 2 Compute

$$r_{i,m} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f}\right]_{f=f_{m-1}}$$

3 Fit a regression tree using \mathbf{r}_m as targets.

- 1 Initialize $f_0(\mathbf{x}) = \arg\min_{\gamma} L(Y, \gamma)$.
- 2 Compute

$$r_{i,m} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f}\right]_{f=f_{m-1}}$$

- **3** Fit a regression tree using \mathbf{r}_m as targets.
- 4 Compute

$$\gamma_{j,m} = \arg\min_{\gamma} \sum_{\mathbf{x}_i \in R_{j,m}} L(y, f_{m-1}(\mathbf{x}) + \gamma)$$

- 1 Initialize $f_0(\mathbf{x}) = \arg\min_{\gamma} L(Y, \gamma)$.
- 2 Compute

$$r_{i,m} = \left[\frac{\partial L(y_i, f(\mathbf{x}_i))}{\partial f}\right]_{f=f_{m-1}}$$

- 3 Fit a regression tree using \mathbf{r}_m as targets.
- 4 Compute

$$\gamma_{j,m} = \arg\min_{\gamma} \sum_{\mathbf{x}_i \in R_{i,m}} L(y, f_{m-1}(\mathbf{x}) + \gamma)$$

G Update

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \sum_{j=1}^{J_m} \gamma_{j,m} I(\mathbf{x} \in R_{j,m})$$

