Statistical Machine Learning (BE4M33SSU)
Lecture 12: Ensembling

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Overview

Topics covered in the lecture:

- Ensemble Methods
- Bias-Variance Decomposition
- Bagging
- Random Forests
- Boosting and Gradient Boosting
- Gradient Boosted Trees

Ensemble Methods

- Inspired in *Wisdom of the crowd*
  - (weighted) averaging or taking majority vote
  - cancelling effect of noise of individual opinions,
  - examples: politics, trial by jury (vs. trial by judge), sports (figure skating, gymnastics), Wikipedia, Quora, Stack Overflow, . . .
- Learning and aggregating multiple predictors
- Ensemble may be built using single or different types of predictors

Wikimedia Commons

Prediction Problem: Expected Risk and Error Decomposition

Expected risk for data generated by $p(x, y)$:

$$R(h) = \mathbb{E}_{(x,y)\sim p}\Big(\ell(y, h(x))\Big)$$

- The best attainable (Bayes) risk is $R^* = \inf_{h\in\mathcal{Y}^{\mathcal{X}}} R(h)$
- The best predictor in $\mathcal{H}$ is $h_{\mathcal{H}} \in \operatorname{Argmin}_{h\in\mathcal{H}} R(h)$
- The predictor $h_m = A(\mathcal{T}^m)$ learned from $\mathcal{T}^m$ has risk $R(h_m)$

Excess error measures deviation of the learned predictor from the best one:

$$\underbrace{\Big(R(h_m) - R^*\Big)}_{\text{excess error}} = \underbrace{\Big(R(h_m) - R(h_{\mathcal{H}})\Big)}_{\text{estimation error}} + \underbrace{\Big(R(h_{\mathcal{H}}) - R^*\Big)}_{\text{approximation error}}$$

Risk Averaged over Datasets

- How will our predictor behave when sampling different training sets?
- We can define the errors considering average over all possible datasets $\mathcal{T}^m$, i.e., $\mathbb{E}_{\mathcal{T}^m}\Big(R(h_m)\Big)$
- The errors can be redefined as:

$$\underbrace{\Big(\mathbb{E}_{\mathcal{T}^m}(R(h_m)) - R^*\Big)}_{\text{excess error}} = \underbrace{\Big(\mathbb{E}_{\mathcal{T}^m}(R(h_m)) - R(h_{\mathcal{H}})\Big)}_{\text{estimation error}} + \underbrace{\Big(R(h_{\mathcal{H}}) - R^*\Big)}_{\text{approximation error}}$$

Predictors Averaged over Datasets

- Let us also define a model averaged over all possible datasets:

$$g_m(x) = \mathbb{E}_{\mathcal{T}^m}\Big(h_m(x)\Big)$$

- Unlike individual h_m models, g_m has an access to the whole $p(x, y)$
- Note: g_m can't be actually evaluated for infinite number of $\mathcal{T}^m$ datasets

Bias-Variance Decomposition for Regression

- Consider a regression problem with data generated as follows:

$$y = h^*(x) + \epsilon$$

where ϵ is noise: $\mathbb{E}(\epsilon) = 0$ and $\mathrm{Var}(\epsilon) = \sigma^2$, e.g., $\epsilon \sim \mathcal{N}(0, \sigma^2)$

- Use squared loss:

$$\ell(y, h(x)) = \Big(h(x) - y\Big)^2$$

- The optimal predictor $h^*(x)$ has a nonzero risk (for $\sigma^2 > 0$):

$$R^* = \mathbb{E}_{x,y}\bigg(\Big(h^*(x) - y\Big)^2\bigg) = \mathbb{E}_{\epsilon}\Big(\epsilon^2\Big) = \mathrm{Var}(\epsilon) = \sigma^2$$

Bias-Variance Decomposition for Regression 2

- The expected risk for h_m can be decomposed:

$$\begin{aligned}
\mathbb{E}_{\mathcal{T}^m}\Big(R(h_m)\Big) &= \mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x) - y\Big)^2\Big) \\
&= \cdots \\
&= \underbrace{\mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x) - g_m(x)\Big)^2\Big)}_{\text{variance}} + \\
&+ \underbrace{\mathbb{E}_{x,y}\Big(\Big(g_m(x) - h^*(x)\Big)^2\Big)}_{\text{bias}^2} + \underbrace{\sigma^2}_{\text{noise}}
\end{aligned}$$

- The error splits into three terms
  - **variance**: difference of h_m from the averaged predictor g_m,
  - **bias**^{2}: difference of the averaged predictor g_m from the optimal one,
  - **noise**: irreducible determined by data

Excess Error vs. Bias and Variance

- The excess error is defined as:

$$\mathbb{E}_{\mathcal{T}^m}(R(h_m)) - R^*$$

- As $R^* = \sigma^2$ we get:

$$\mathbb{E}_{\mathcal{T}^m}(R(h_m)) - R^* = \underbrace{\mathbb{E}_{x,y}\left(\left(g_m(x) - h^*(x)\right)^2\right)}_{\text{bias}^2} + \underbrace{\mathbb{E}_{x,y,\mathcal{T}^m}\left(\left(h_m(x) - g_m(x)\right)^2\right)}_{\text{variance}}$$

- We have
  - **bias**^{2} $\approx$ approximation error,
  - **variance** $\approx$ estimation error

Derivation of the Bias-Variance Decomposition

$$
\begin{aligned}
\mathbb{E}_{\mathcal{T}^m}\Big(R(h_m)\Big) &= \mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x)-y\Big)^2\Big) \\
&= \mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x)-g_m(x)+g_m(x)-y\Big)^2\Big) \\
&= \mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x)-g_m(x)\Big)^2+\Big(g_m(x)-y\Big)^2 \\
&\quad +2\Big(h_m(x)-g_m(x)\Big)\Big(g_m(x)-y\Big)\Big) \\
&= \mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x)-g_m(x)\Big)^2\Big)+\mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(g_m(x)-y\Big)^2\Big) \\
&\quad \underbrace{+\mathbb{E}_{x,y}\Big(2\Big(\underbrace{\mathbb{E}_{\mathcal{T}^m}\Big(h_m(x)\Big)}_{g_m(x)}-g_m(x)\Big)\Big(g_m(x)-y\Big)\Big)}_{=0}
\end{aligned}
$$

Derivation of the Bias-Variance Decomposition 2

We get:

$$\mathbb{E}_{\mathcal{T}^m}\Big(R(h_m)\Big) = \underbrace{\mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(h_m(x) - g_m(x)\Big)^2\Big)}_{\text{variance}} + \mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(g_m(x) - y\Big)^2\Big)$$

Note that the second term does not depend on $\mathcal{T}^m$:

$$\mathbb{E}_{x,y,\mathcal{T}^m}\Big(\Big(g_m(x) - y\Big)^2\Big) = \mathbb{E}_{x,y}\Big(\Big(g_m(x) - y\Big)^2\Big)$$

Derivation of the Bias-Variance Decomposition 3

Let us continue with the second term:

$$\begin{aligned}
\mathbb{E}_{x,y}\Big(\big(g_m(x)-y\big)^2\Big) &= \mathbb{E}_{x,\epsilon}\Big(\big(g_m(x)-h^*(x)-\epsilon\big)^2\Big) \\
&= \mathbb{E}_{x,\epsilon}\Big(\big(g_m(x)-h^*(x)\big)^2+\epsilon^2-2\epsilon\big(g_m(x)-h^*(x)\big)\Big) \\
&= \mathbb{E}_x\Big(\big(g_m(x)-h^*(x)\big)^2\Big)+\mathbb{E}_\epsilon\big(\epsilon^2\big) \\
&\quad \underbrace{-2\mathbb{E}_{x,\epsilon}\Big(\epsilon\big(g_m(x)-h^*(x)\big)\Big)}_{=0} \\
&= \underbrace{\mathbb{E}_x\Big(\big(g_m(x)-h^*(x)\big)^2\Big)}_{\text{bias}^2}+\underbrace{\sigma^2}_{\text{noise}}
\end{aligned}$$

Pointwise Bias-Variance

We can express the bias and variance as function of x by not integrating over in expected values

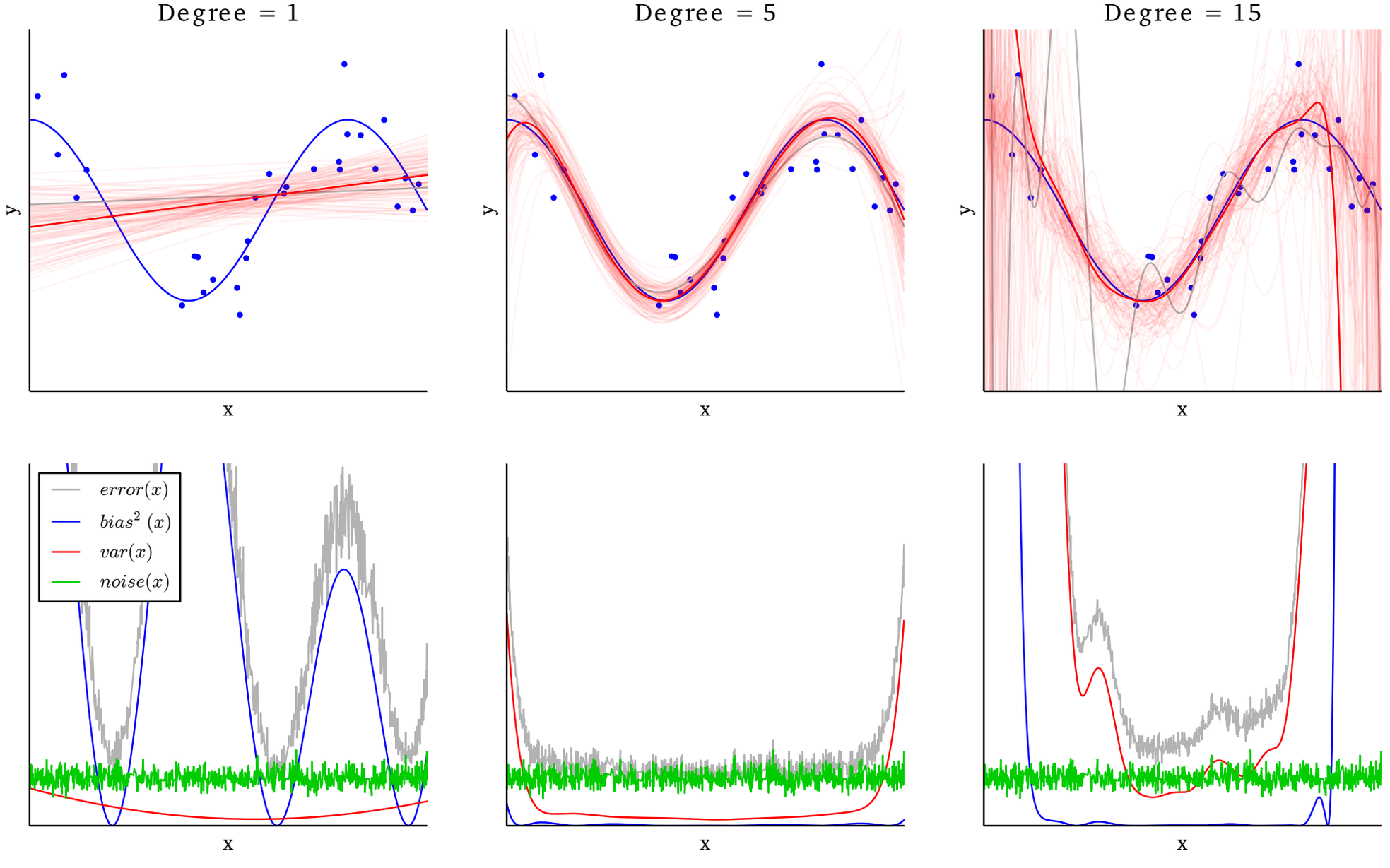
$$\mathbb{E}_{y|x,\mathcal{T}^m}\Big(\ell(y, h_m(x))\Big) = \mathbb{E}_{y|x,\mathcal{T}^m}\Big(\Big(h_m(x) - y\Big)^2\Big)$$

$$= \underbrace{\mathrm{Var}_{y|x,\mathcal{T}^m}\Big(h_m(x)\Big)}_{\text{variance(x)}} +$$

$$+ \underbrace{\mathbb{E}_{y|x}\Big(\Big(g_m(x) - h^*(x)\Big)^2\Big)}_{\text{bias(x)}^2} + \underbrace{\sigma^2}_{\text{noise}}$$

Bias-Variance: Example

- Polynomial regression with a varying degree of polynomial



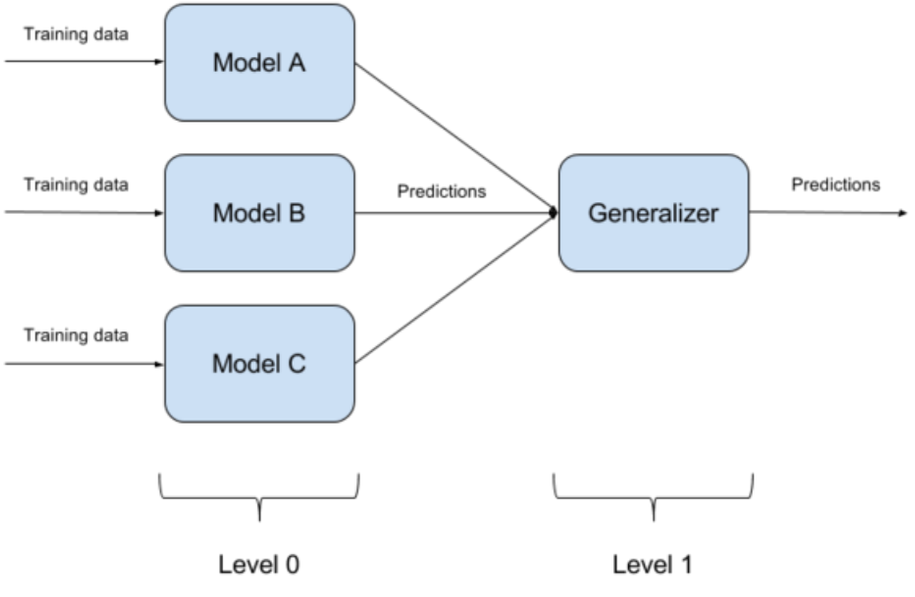
Gilles Louppe: *Understanding Random Forests: From Theory to Practice*, 2014

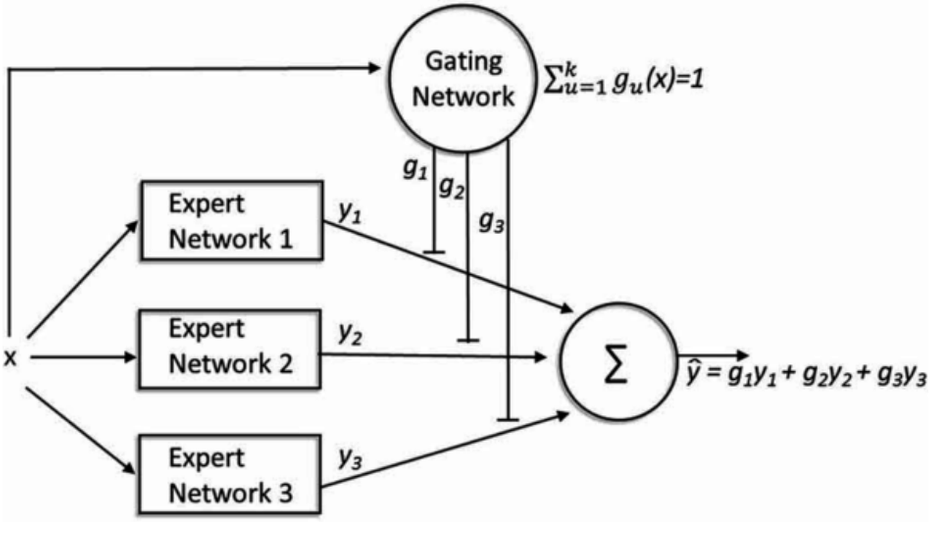
Ensembling Approaches

- Bagging (Bootstrap AGGregatING):
  - sample different training sets from the original training set
  - train *high variance low bias* predictors based on these sets and average them
  - exploits independence between predictors
- Boosting:
  - sequentially train *low variance high bias* predictors
  - subsequent predictors learn to fix the mistakes of the previous ones
  - exploits dependence between learners

Stacking and Mixture of Experts

- Combine *base-learners* with *meta-learner*

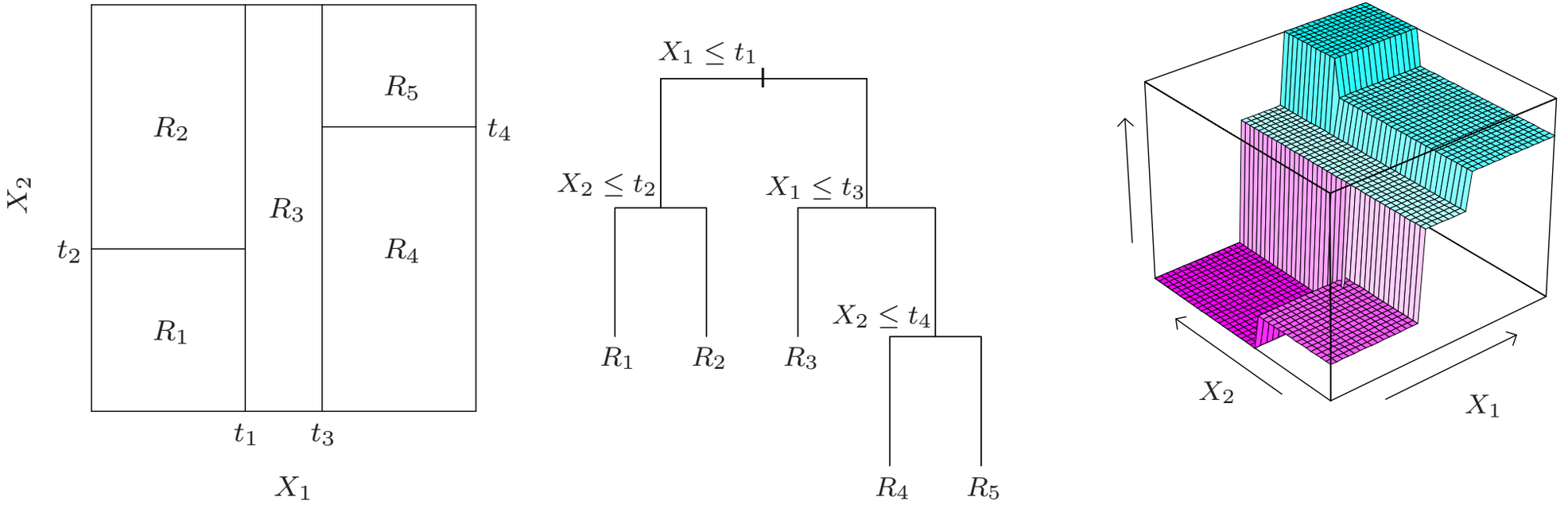




https://www.commonlounge.com/discussion/9331c0d004704e89bd4d1da08fd7c7bc

Decision/Regression Trees

- Nodes correspond to mutually exclusive subsets of the original training data as well as mutually exclusive subsets of the input space $\mathcal{X}$
- Inner node further splits its subset



Hastie et al.: *The Elements of Statistical Learning*, 2009

Decision/Regression Trees (contd.)

- Training set: $\mathcal{T}^m = \{(\boldsymbol{x}_i, y_i) \mid i = 1, \ldots, m\}$, $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$
- Input space split into regions defined in leaves: $R_r,\ r \in \{1, \ldots, M\}$
- We can model *region responses* by constants $c_r,\ r \in \{1, \ldots, M\}$ but other possibilities, e.g., linear regression are possible
- Prediction:

$$h(\boldsymbol{x}) = \sum_{r=1}^{M} c_r [\![\boldsymbol{x} \in R_r]\!]$$

- For sum of squares *loss function* $\sum_{i=1}^{m} (y_i - h(\boldsymbol{x}_i))^2$ we set the responses to be the averages over regions:

$$\hat{c}_r = \frac{1}{|S_r|} \sum_{\boldsymbol{x}_i \in R_r} y_i \qquad \text{(see seminar)}$$

where we define samples per region sets :
$S_r = \{(\boldsymbol{x}_i, y_i) : (\boldsymbol{x}_i, y_i) \in \mathcal{T}^m \wedge \boldsymbol{x}_i \in R_r\}$

Greedy Learning of Decision/Regression Trees

- How many distinct decision trees with n Boolean attributes for binary classification?
  - at least as many as boolean functions of p attributes
  - $=$ number of distinct truth tables with 2^p rows: 2^{2^p}
  - For 6 Boolean attributes at least 18,446,744,073,709,551,616 trees!
- Learning is NP-complete: [Hyafil and Rivest 1976]
- We need heuristics $\Rightarrow$ **greedy approach**
- Recursively choose the "most important" attribute to find a small tree consistent with the training data
- Split points:
  - **nominal attribute**: try all possibilities
  - **ordinal/continuous attribute**: try attribute values based on all training data samples or their subset

Regression Trees: Which Attribute to Split?

- The "most important" attribute for regression trees would be the one, for which the split reduces the loss (sum of squared errors) by the greatest amount
- We have:

$$h(\boldsymbol{x}) = \sum_{r=1}^{M} c_r [\boldsymbol{x} \in R_r]$$

- Consider splitting attribute j and split point s, we split an original region R into a pair of half-planes for an ordinal (e.g., continuous) attribute:

$$R_L(j,s) = \{\boldsymbol{x} | \boldsymbol{x} \in R \wedge x_j \leq s\} \text{ and } R_R(j,s) = \{\boldsymbol{x} | \boldsymbol{x} \in R \wedge x_j > s\}$$

similarly for a nominal attribute:

$$R_L(j,s) = \{\boldsymbol{x} | \boldsymbol{x} \in R \wedge x_j = s\} \text{ and } R_R(j,s) = \{\boldsymbol{x} | \boldsymbol{x} \in R \wedge x_j \neq s\}$$

Regression Trees: Which Attribute to Split? (contd.)

- We seek for an attribute j and a split point s which minimize:

$$\min_{c_L} \sum_{\boldsymbol{x}_i \in R_L(j,s)} (y_i - c_L)^2 + \min_{c_R} \sum_{\boldsymbol{x}_i \in R_R(j,s)} (y_i - c_R)^2$$

for $(\boldsymbol{x}_i, y_i) \in S \subseteq \mathcal{T}^m$ ($S = \mathcal{T}^m$ for the root node) and $R = R_L \cup R_R$

- Inner minimizations (region response values) are solved by averaging tree outputs per region:

$$\hat{c}_L = \frac{1}{|S_L(j,s)|} \sum_{\boldsymbol{x}_i \in R_L(j,s)} y_i \qquad \text{and} \qquad \hat{c}_R = \frac{1}{|S_R(j,s)|} \sum_{\boldsymbol{x}_i \in R_R(j,s)} y_i$$

where $S_k(j,s) = \{(\boldsymbol{x}_i, y_i) \mid (\boldsymbol{x}_i, y_i) \in \mathcal{T} \wedge \boldsymbol{x}_i \in R_k(j,s)\}$

Tree Learning Algorithm

BUILD-TREE(S)

```
 1  i = IMPURITY(S)                                   // e.g., the squared loss
 2  î, ĵ, ŝ, Ŝ_L, Ŝ_R = 0, 0, 0, ∅, ∅                 // current best kept in these
 3  for j ∈ {1, ..., p}                               // iterate over attributes
 4      for s ∈ SPLIT-POINTS(S, j)                    // iterate over all split points
 5          S_L, S_R = SPLIT(S, j, s)
 6          i_L = IMPURITY(S_L)
 7          i_R = IMPURITY(S_R)
 8          if i_L + i_R < î  and  |S_L| > 0  and  |S_R| > 0
 9              î, ĵ, ŝ, Ŝ_L, Ŝ_R = (i_L + i_R), j, s, S_L, S_R
10  if î > i
11      N_L = BUILD-TREE(Ŝ_L)
12      N_R = BUILD-TREE(Ŝ_R)
13      return DECISION-NODE(ĵ, ŝ, N_L, N_R)
14  else return LEAF-NODE(S)
```

Bias and Variance of Decision Trees

- Small changes of training data lead to big differences in final trees
- Decision trees grown deep enough have typically:
  - low bias
  - high variance

  $\Rightarrow$ **overfitting**
- Idea: *average multiple models* to reduce variance while (happily) not increasing bias much

Averaging Models

- Define regression model b as an average of K models:

$$b(x) = \frac{1}{K} \sum_{i=1}^{K} h_m^{(i)}(x)$$

  trained using a set of i.i.d. datasets of size m: $\mathcal{D}^m = \{\mathcal{T}_1^m, \ldots, \mathcal{T}_K^m\}$

- Note that $b(x)$ approximates the averaging model

$$g_m(x) = \mathbb{E}_{\mathcal{T}^m}\Big(h_m(x)\Big)$$

- The need for K different training sets $\mathcal{T}_i^m$ is still impractical – why not to train a single model using $\mathcal{T}_1^m \cup \mathcal{T}_2^m \cup \ldots \mathcal{T}_K^m$ instead of $b(x)$?

Averaging Models: Bias

- Bias remains unchanged when compared to a single model:

$$
\begin{aligned}
\text{bias(x)}^2 &= \mathbb{E}_{y|x}\left(\left(g_m(x) - h^*(x)\right)^2\right) \\
&= \mathbb{E}_{y|x}\left(\left(\mathbb{E}_{\mathcal{D}^m}\left(b(x)\right) - h^*(x)\right)^2\right) \\
&= \mathbb{E}_{y|x}\left(\left(\mathbb{E}_{\mathcal{D}^m}\left(\frac{1}{K}\sum_{i=1}^{K} h_m^{(i)}(x)\right) - h^*(x)\right)^2\right) \\
&= \mathbb{E}_{y|x}\left(\left(\frac{1}{K}\sum_{i=1}^{K} \mathbb{E}_{\mathcal{T}_i^m}\left(h_m^{(i)}(x)\right) - h^*(x)\right)^2\right) \\
&= \mathbb{E}_{y|x}\left(\left(\mathbb{E}_{\mathcal{T}^m}\left(h_m(x)\right) - h^*(x)\right)^2\right)
\end{aligned}
$$

where $\mathbb{E}_{\mathcal{T}^m}\left(h_m(x)\right)$ was the $g_m(x)$ defined for a single model $h_m(x)$

Averaging Models: Variance

- For uncorrelated component models $h_m^{(i)}(x)$:

$$\mathrm{Var}_{\mathcal{D}^m}\left(b(x)\right) = \mathrm{Var}_{\mathcal{D}^m}\left(\frac{1}{K}\sum_{i=1}^{K} h_m^{(i)}(x)\right)$$

$$= \frac{1}{K^2}\sum_{i=1}^{K}\mathrm{Var}_{\mathcal{T}_i^m}\left(h_m^{(i)}(x)\right) = \frac{1}{K}\mathrm{Var}_{\mathcal{T}^m}\left(h_m(x)\right)$$

  which is a great improvement based on the **strong** assumption

- There is no improvement for maximum correlation, i.e., all component models equal: $h_m^{(i)}(x) = h_m(x)$ for $i = 1, \ldots, K$, we get:

$$\mathrm{Var}_{\mathcal{D}^m}\left(b(x)\right) = \mathrm{Var}_{\mathcal{D}^m}\left(\frac{1}{K}\sum_{i=1}^{K} h_m^{(i)}(x)\right) = \mathrm{Var}_{\mathcal{T}^m}(h_m(x))$$

  $\Rightarrow$ we need to train **uncorrelated** (diverse) component models while **keeping their bias reasonably low**

Bootstrapping

- In practice we have only a single training dataset $\mathcal{T}^m$
- Bootstrapping is a method producing datasets $\mathcal{T}_i^m$ for $i = 1, \dots K$ by sampling $\mathcal{T}^m$ uniformly with *replacement*
- Bootstrap datasets have the same size as the original dataset $|\mathcal{T}_i^m| = |\mathcal{T}^m|$
- $\mathcal{T}_i^m$ is expected to have the fraction $1 - \frac{1}{e} \approx 63.2\%$ of unique samples from $\mathcal{T}^m$, others are duplicates (see seminar)

Bagging

- Bagging = Bootstrap AGGregating [Breiman 1994]:
  1. Use bootstrapping to generate K datasets
  2. Train a model $h_m^{(i)}$ on each dataset $\mathcal{T}_i^m$
  3. Average the models
- When decision trees are used as the models $\Rightarrow$ **random forests**
- Low bias is achieved by growing the trees to maximal depth
- Trees are decorrelated by:
  - training each tree on a different bootstrap dataset
  - randomization of split attribute selection

Random Forest Algorithm

1. For $i = 1 \ldots K$:
   (a) draw a bootstrap dataset $\mathcal{T}_i^m$ from $\mathcal{T}^m$, $|\mathcal{T}_i^m| = |\mathcal{T}^m| = m$
   (b) grow a tree $h_m^{(i)}$ using $\mathcal{T}_i^m$ by recursively repeating the following, until the minimum node size n_{min} is reached:
      i. select k attributes at random from the p attributes
      ii. pick the best attribute and split-point among the k
      iii. split the node into two daughter nodes

2. Output ensemble of trees $b(x)$ averaging $h_m^{(i)}$ (regression) or selecting a majority vote (classification)

- Node size n_{min} is the number of dataset samples associated with the node, limits tree depth

Out-of-Bag (OOB) Error

- Cheap way of generalization error assessment for bagging
- Bagging produces bootstrapped sets $\mathcal{T}_1^m, \mathcal{T}_2^m, \ldots \mathcal{T}_K^m$
- For each $(\boldsymbol{x}_i, y_i) \in \mathcal{T}^m$ select only trees which were not trained on this sample: $H_i = \{h_m^{(j)} \mid (\boldsymbol{x}_i, y_i) \notin \mathcal{T}_j^m\}$
- Average only the OOB trees in H_i when evaluating error for $(\boldsymbol{x}_i, y_i)$
- Replacement for K-fold cross-validation

Feature Importance

- Random forests allow easy evaluation of feature importances
- Mean Decrease Impurity (MDI):
  - set $f_j = 0$ for all attributes $j = 1, \ldots, p$
  - traverse all trees processing all internal nodes
  - for each node having a split attribute j add its *impurity decrease* multiplied by the proportion of the *node size* to f_j
- Mean Decrease Accuracy (MDA), permutaion importance:
  - evaluate the forest using OOB
  - do the same with permuted values of an attribute j
  - watch decrease in accuracy: low decrease means unimportant feature

Boosting

- Sequentially train weak learners/predictors *low variance high bias*
- Subsequent predictors fix the mistakes of the previous ones reducing bias
- Methods discussed here:
  - AdaBoost
  - Forward Stagewise Additive Modeling
  - Gradient Boosting Machine
  - Gradient Boosted Trees

Forward Stagewise Additive Modeling (FSAM)

1. Initialize $f_0(x) = 0$

2. For $k = 1$ to K:

   (a) Find

$$(\beta_k, \theta_k) = \underset{\beta,\theta}{\operatorname{argmin}} \sum_{i=1}^{m} \ell\Big(y_i, f_{k-1}(x_i) + \beta b(x_i; \theta)\Big)$$

   where $b(x_i; \theta_k)$ is the *basis function* and β_k the corresponding coefficient

   (b) Set $f_k(x) = f_{k-1}(x) + \beta_k b(x; \theta_k)$

3. Return $h_m(x) = f_K(x)$

AdaBoost M1

Binary classifier: $\mathcal{Y} = \{-1, 1\}$

1. Initialize the weights $w_i = 1/m$ for $i = 1, 2, \ldots m$

2. For $k = 1$ to K:

   (a) Fit a classifier $f_k(x; \theta_k)$ to the training data using loss weighted by w_i:

$$\theta_k = \underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{m} w_i [\![y_i \neq f_k(x_i; \theta)]\!]$$

   (b) Compute the weighted error rate

$$\epsilon_k = \frac{\sum_{i=1}^{m} w_i [\![y_i \neq f_k(x_i; \theta_k)]\!]}{\sum_{i=1}^{m} w_i}$$

   (c) Compute the weight $\alpha_k = \log((1 - \epsilon_k)/\epsilon_k)$
   (d) Set $w_i \leftarrow w_i \cdot \exp(\alpha_k \cdot [\![y_i \neq f_k(x_i; \theta_k)]\!])$ for $i = 1, 2, \ldots m$

3. Return $h_m(x) = \operatorname{sign}\left[\sum_{k=1}^{K} \alpha_k f_k(x; \theta_k)\right]$

AdaBoost is FSAM

- Claim: AdaBoost is FSAM using the exponential loss

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

- We get:

$$\begin{aligned}
(\beta_k, \theta_k) &= \operatorname*{argmin}_{\beta,\theta} \sum_{i=1}^{m} \ell\Big(y_i, f_{k-1}(x_i) + \beta b(x_i;\theta)\Big) \\
&= \operatorname*{argmin}_{\beta,\theta} \sum_{i=1}^{m} \exp\Big(-y_i\Big(f_{k-1}(x_i) + \beta b(x_i;\theta)\Big)\Big) \\
&= \operatorname*{argmin}_{\beta,\theta} \sum_{i=1}^{m} w_i^{(k)} \exp\Big(-y_i \beta b(x_i;\theta)\Big),
\end{aligned}$$

where $w_i^{(k)} = \exp(-y_i f_{k-1}(x_i))$

AdaBoost is FSAM II

- We can rearrange further:

$$
\begin{aligned}
(\beta_k, \theta_k) &= \operatorname*{argmin}_{\beta,\theta} \sum_{i=1}^{m} w_i^{(k)} \exp\Big(- y_i \beta b(x_i;\theta) \Big) \\
&= \operatorname*{argmin}_{\beta,\theta} \left[e^{-\beta} \sum_{y_i = b(x_i;\theta)} w_i^{(k)} + e^{\beta} \sum_{y_i \neq b(x_i;\theta)} w_i^{(k)} \right] \\
&= \operatorname*{argmin}_{\beta,\theta} \left[\underbrace{(e^{\beta} - e^{-\beta})}_{>0 \text{ for } \beta>0} \sum_{i=1}^{m} w_i^{(k)} [\![y_i \neq b(x_i;\theta)]\!] + e^{-\beta} \sum_{i=1}^{m} w_i^{(k)} \right]
\end{aligned}
$$

- For any $\beta > 0$ we can minimize θ separately:

$$
\theta_k = \operatorname*{argmin}_{\theta} \sum_{i=1}^{m} w_i^{(k)} [\![y_i \neq b(x_i;\theta)]\!] \quad \text{(same as } \textit{AdaBoost 2(a)}\text{)}
$$

AdaBoost is FSAM III

- Let's minimize

$$(e^{\beta} - e^{-\beta}) \sum_{i=1}^{m} w_i^{(k)} [\![y_i \neq b(x_i; \theta_k)]\!] + e^{-\beta} \sum_{i=1}^{m} w_i^{(k)}$$

with respect to β

$$(e^{\beta_k} + e^{-\beta_k}) \sum_{i=1}^{m} w_i^{(k)} [\![y_i \neq b(x_i; \theta_k)]\!] - e^{-\beta_k} \sum_{i=1}^{m} w_i^{(k)} = 0$$

$$(e^{\beta_k} + e^{-\beta_k}) \epsilon_k - e^{-\beta_k} = 0$$

where $\epsilon_k = \frac{\sum_{i=1}^{m} w_i [\![y_i \neq b(x_i; \theta_k)]\!]}{\sum_{i=1}^{m} w_i}$ as in *AdaBoost 2(b)*

- Solving for β_k:

$$\beta_k = \frac{1}{2} \log \frac{1 - \epsilon_k}{\epsilon_k}$$

- Define $\alpha_k \triangleq 2\beta_k$ and compare to *AdaBoost 2(c)*

AdaBoost is FSAM IV

- We have $w_i^{(k)} = e^{-y_i f_{k-1}(x_i)}$ and $f_k(x) = f_{k-1}(x) + \beta_k b(x; \theta_k)$ so:

$$w_i^{(k+1)} = e^{-y_i\left(f_{k-1}(x_i)+\beta_k b(x_i;\theta_k)\right)} = w_i^{(k)} \cdot e^{-y_i \beta_k b(x_i;\theta_k)}$$

- Finally $-y_i b(x_i; \theta_k) = 2 \cdot [\![y_i \neq b(x_i; \theta_k)]\!] - 1$ gives the weight update:

$$w_i^{(k+1)} = w_i^{(k)} \cdot e^{\alpha_k [\![y_i \neq b(x_i;\theta_k)]\!]} \cdot e^{-\beta_k}$$

corresponding to *AdaBoost 2(d)* up to the factor $e^{-\beta_k}$ which is same for all weights and hence has no effect

FSAM and Gradient Descent

- FSAM update looks very similar to the gradient descent one:

$$f_k(x) = f_{k-1}(x) + \beta_k b(x; \theta_k)$$

- Just think of
  - $\beta_k \approx$ step size (learning rate)
  - $b(x_i; \theta_k) \approx$ the negative of gradient

FSAM for Squared Loss

- Again consider regression with the squared loss:

$$\ell(y, f(x)) = (y - f(x))^2$$

- For FSAM we get:

$$\begin{aligned}\ell(y_i, f_k(x_i)) &= \ell(y_i, f_{k-1}(x_i) + \beta_k b(x_i; \theta_k)) \\ &= (y_i - f_{k-1}(x_i) - \beta_k b(x_i; \theta_k))^2 \\ &= (r_{ik} - \beta_k b(x_i; \theta_k))^2\end{aligned}$$

  where $r_{ik} = y_i - f_{k-1}(x_i)$ is the *residual* of the current model for the i-th sample

- The task of FSAM is to fit the model $\beta_k b(x_i; \theta_k)$ to match the residuals
- The method is sometimes called the *least-squares boosting*

Gradient Boosting for Regression

- In case of regression with squared loss we minimize:

$$\mathcal{L} = \sum_{i=1}^{m} \ell(y_i, f(x_i)) = \sum_{i=1}^{m} \frac{1}{2}(y_i - f(x_i))^2,$$

  which is same as minimization of the empirical risk

- We can treat $f(x_1), f(x_2), \ldots, f(x_m)$ as parameters and take derivatives:

$$\frac{\partial \mathcal{L}}{\partial f(x_i)} = \frac{\partial \left(\sum_{j=1}^{m} \ell(y_j, f(x_j)) \right)}{\partial f(x_i)} = \frac{\partial \ell(y_i, f(x_i))}{\partial f(x_i)}$$
$$= f(x_i) - y_i = -r_i$$

- The *least-squares boosting* hence takes steps in the negative gradient direction where $r_i = -\frac{\partial \mathcal{L}}{\partial f(x_i)}$
- This approach can be generalized for any differentiable loss function!

Gradient Boosting Machine

1. Initialize $f_0(x) = 0$ or $f_0(x) = \operatorname{argmin}_\gamma \sum_{i=1}^m \ell(y_i, \gamma)$

2. For $k = 1$ to K:

   (a) Compute:

$$\boldsymbol{g}_k = \left[\frac{\partial \ell(y_i, f_{k-1}(x_i))}{\partial f_{k-1}(x_i)}\right]_{i=1}^m$$

   (b) Fit a regression model $b(\cdot;\theta)$ to $-\boldsymbol{g}_k$ using squared loss:

$$\theta_k = \operatorname*{argmin}_\theta \sum_{i=1}^m \left[(-\boldsymbol{g}_k)_i - b(x_i;\theta)\right]^2$$

   (c) Choose a fixed step size $\beta_k = \beta > 0$ or use line search:

$$\beta_k = \operatorname*{argmin}_{\beta>0} \sum_{i=1}^m \ell\Big(y_i, f_{k-1}(x_i) + \beta b(x_i;\theta_k)\Big)$$

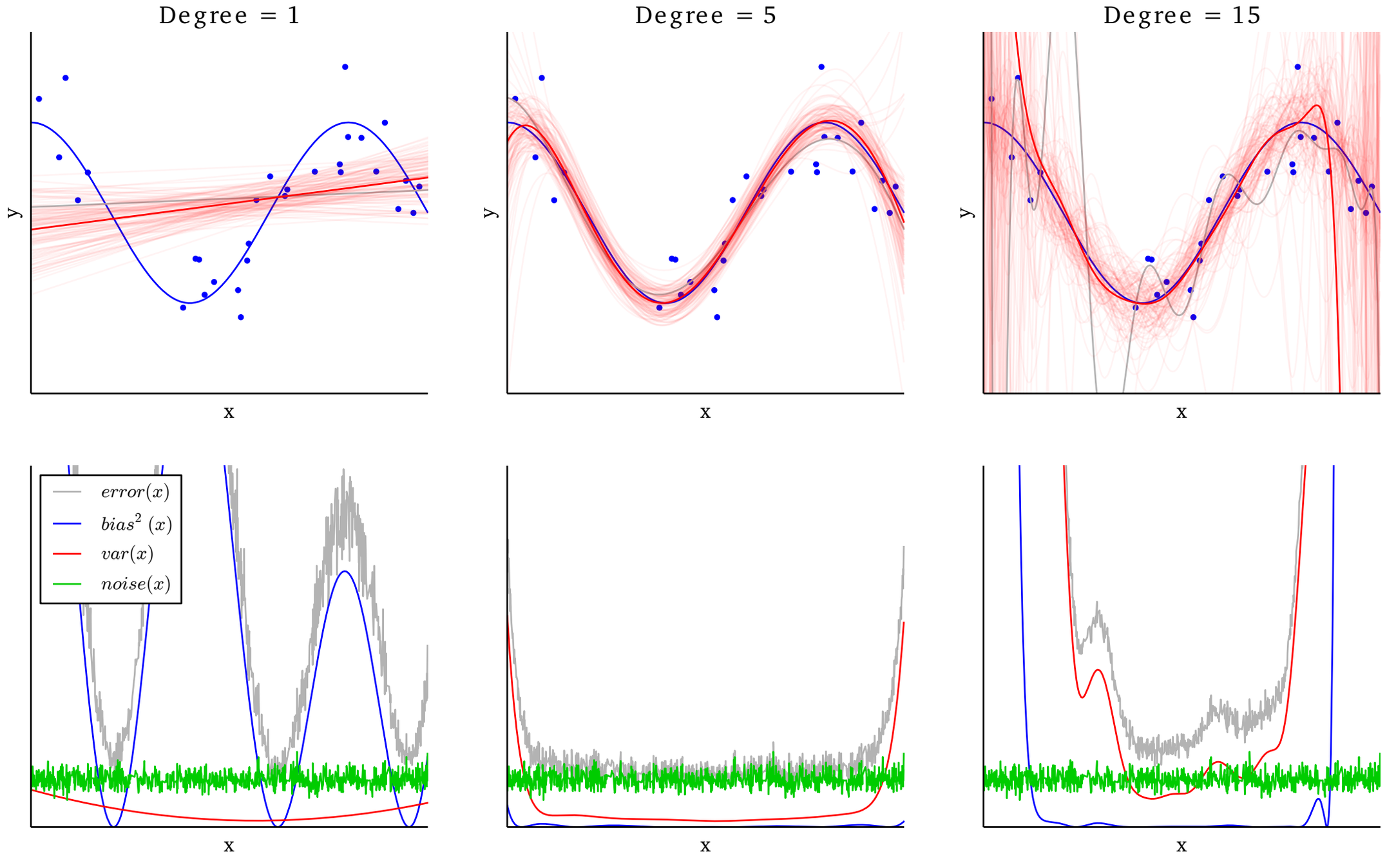
   (d) Set $f_k(x) = f_{k-1}(x) + \beta_k b(x;\theta_k)$

3. Return $h_m(x) = f_K(x)$

Gradient Boosted Trees

- Gradient Boosting Tree is GBM where all weak learners f_k are decision or regression trees
- Use limit on depth/number of leaves/node size for the weak learners $\Rightarrow$ high bias
- Meta-parameters such as K (number of trees) and β (learning rate) have to be found using cross validation
- Model is built sequentially (unlike random forests)
- Highly optimized algorithms based on Gradient Boosting Trees:
  - XGBoost, LightGBM
  - parallelization, scalability, regularization


3
3
5
3
5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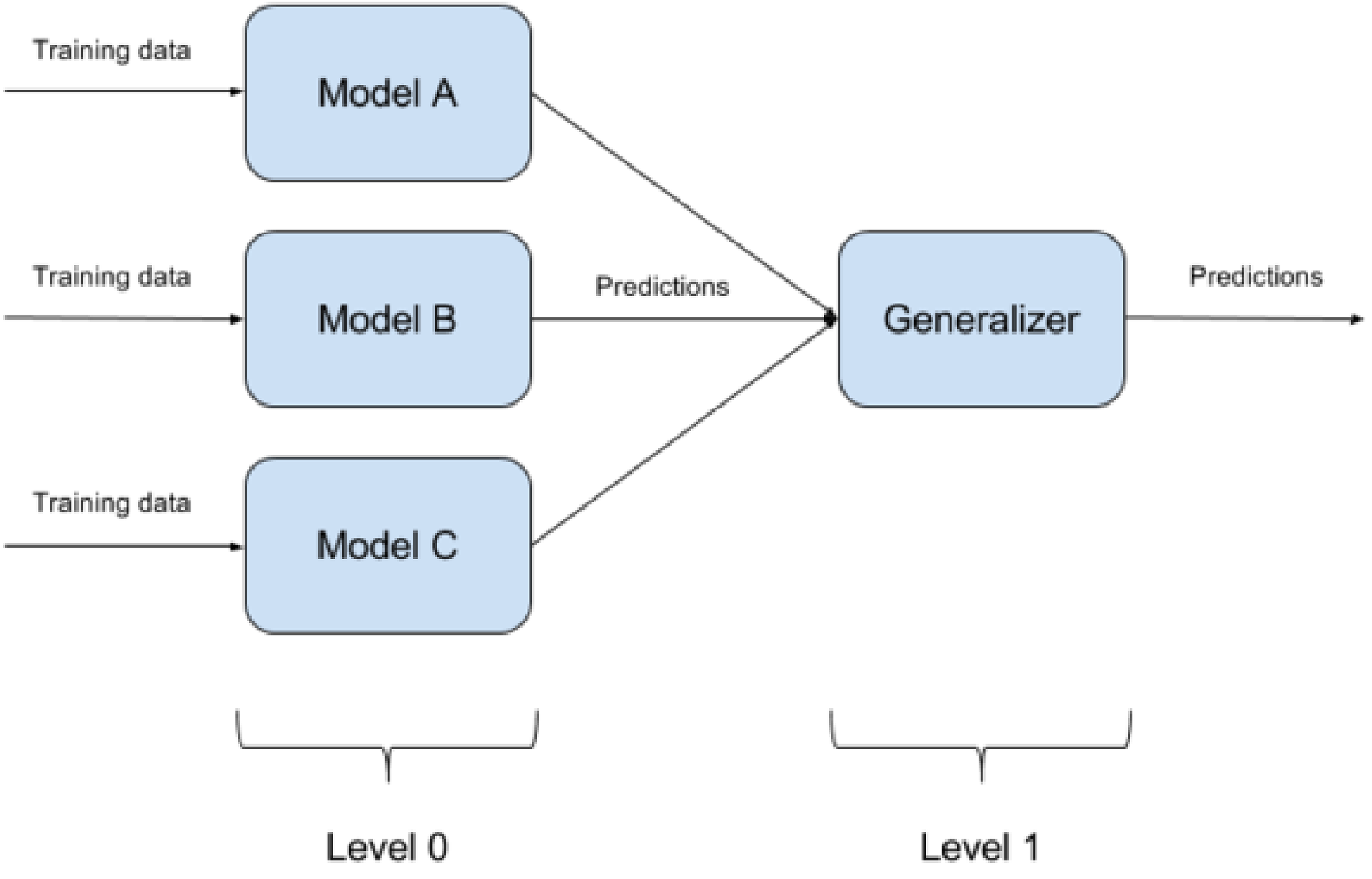
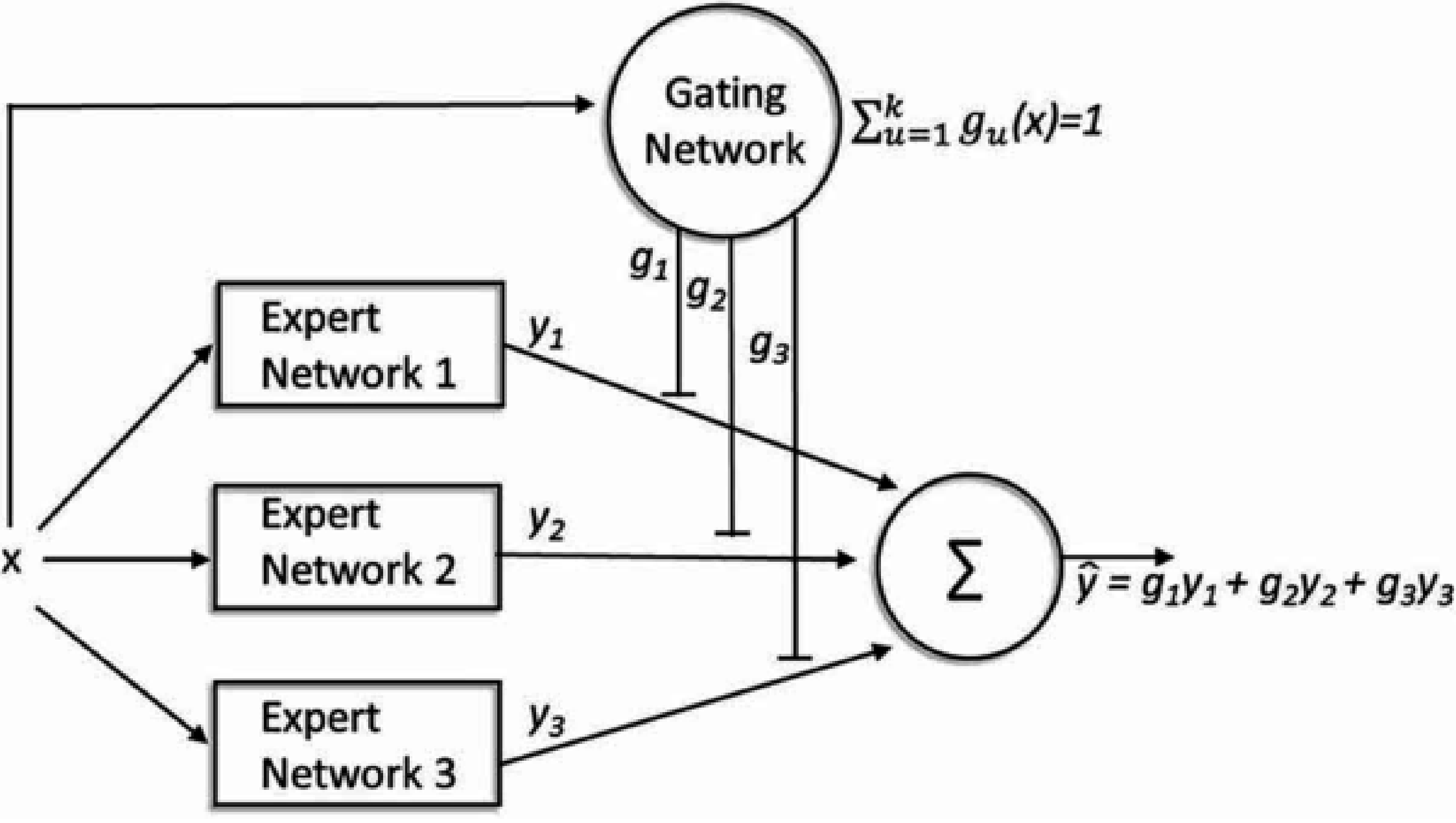
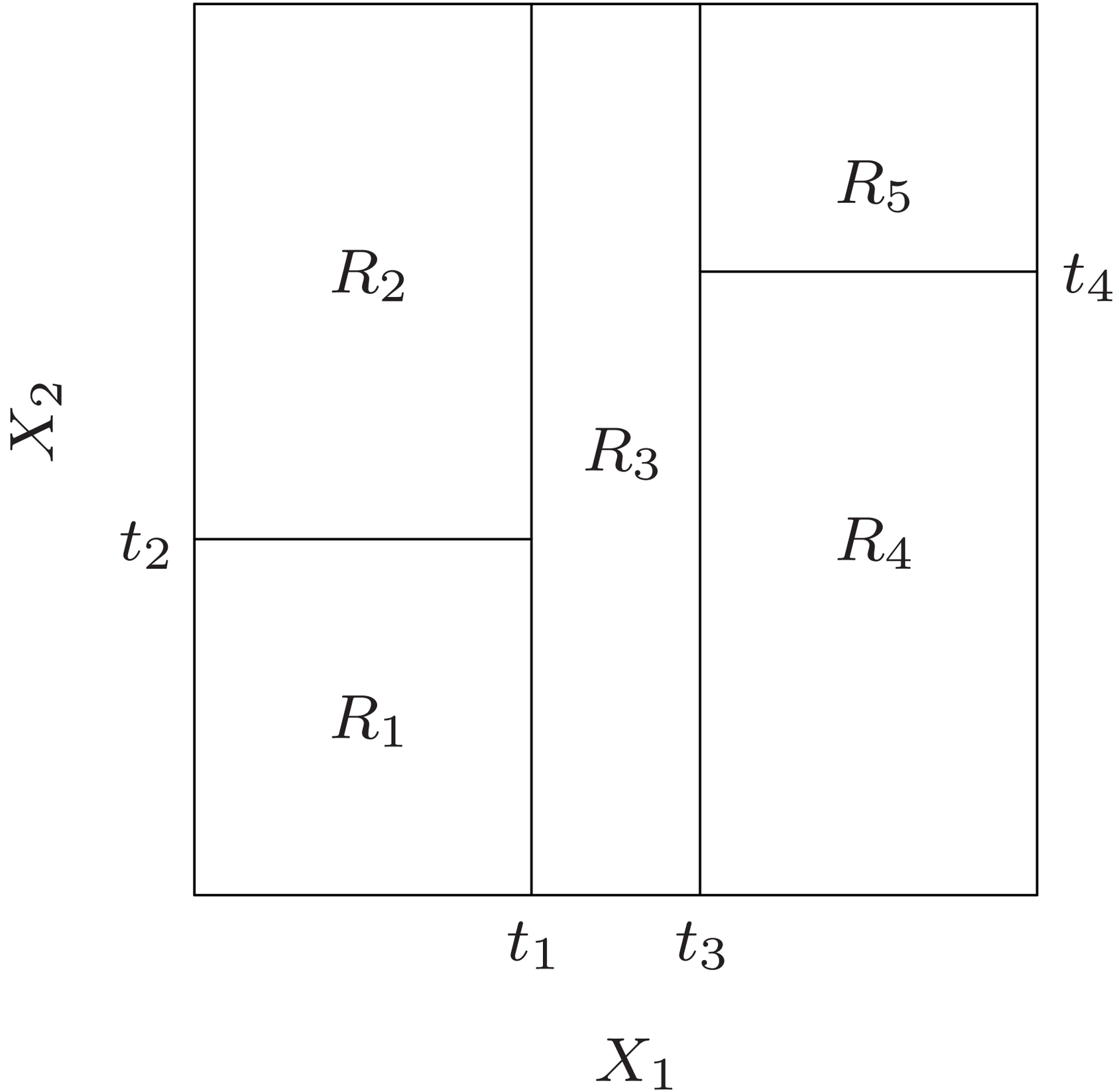
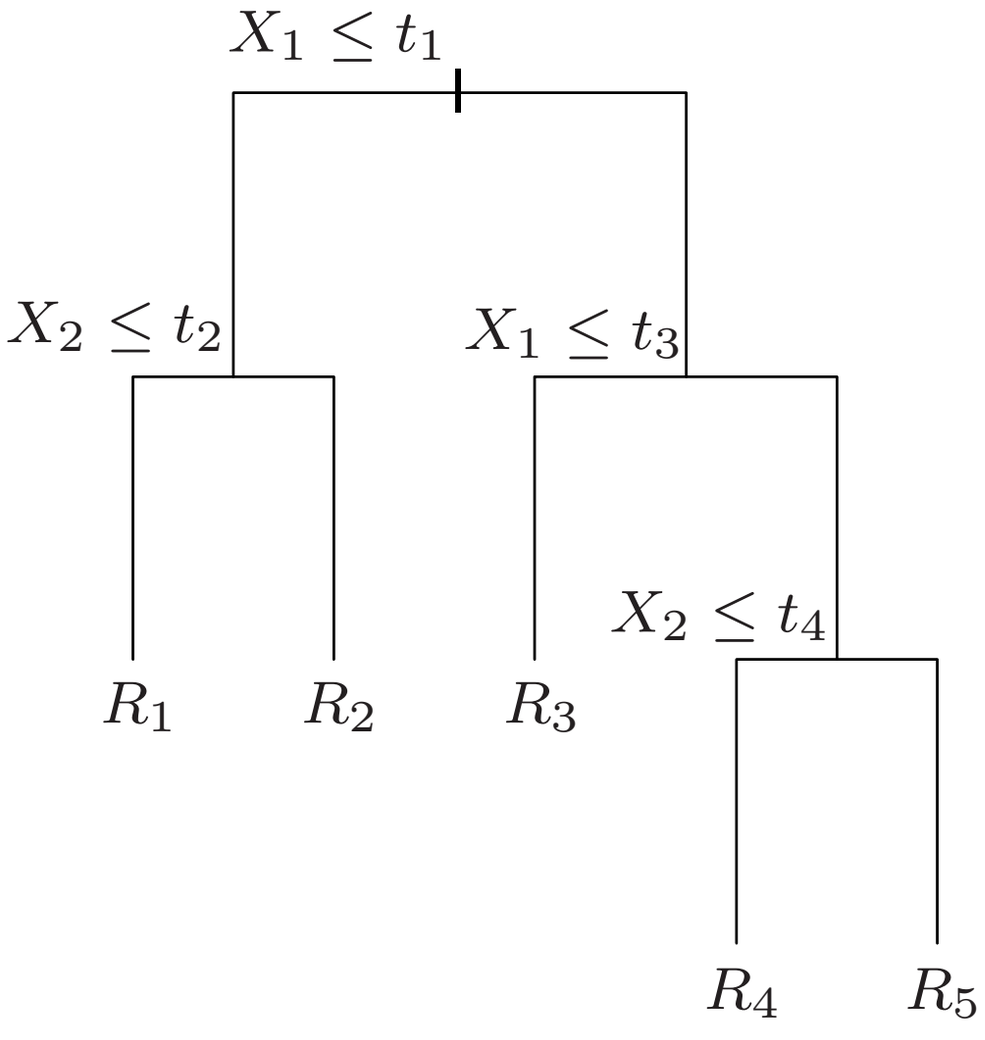
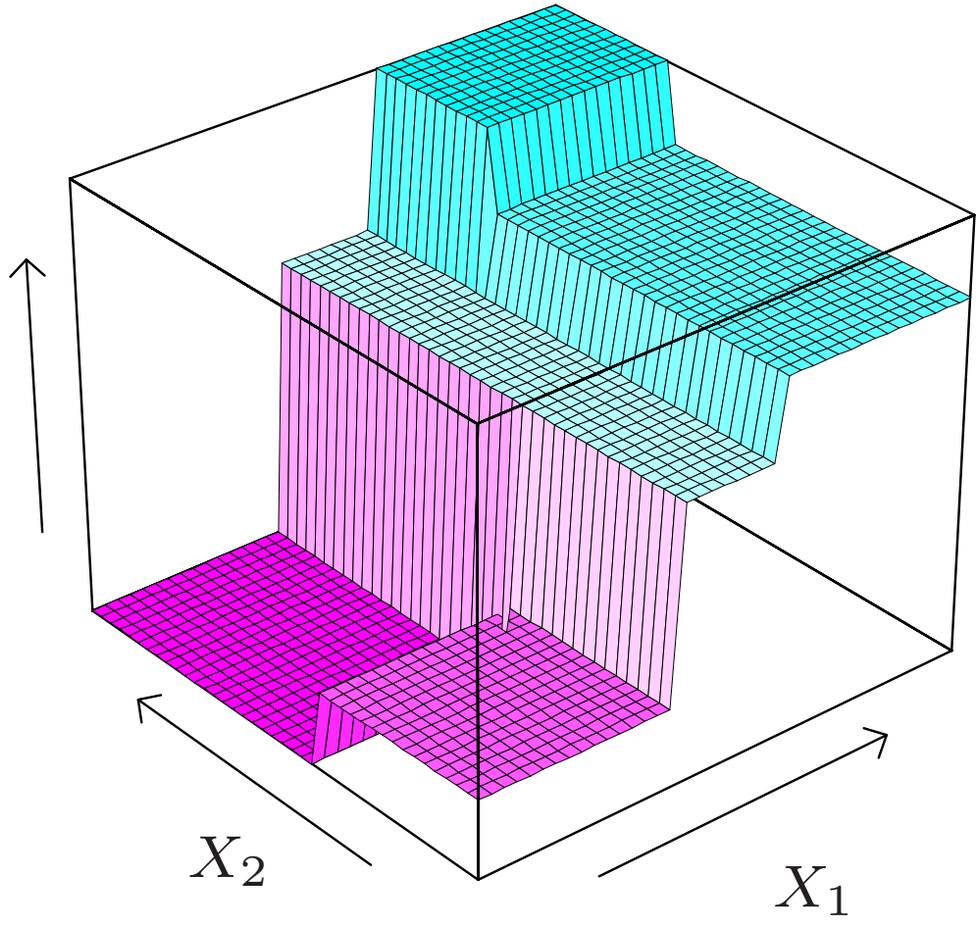
Degree = 5
Degree = 15
y
x
error(x)
bias² (x)
var(x)
noise(x)


Training data
Model A
Training data
Model B
Predictions
Generalizer
Predictions
Training data
Model C
Level 0
Level 1


Gating Network
$\sum_{u=1}^{k} g_u(x)=1$
g_1
g_2
g_3
Expert Network 1
y_1
Expert Network 2
y_2
Expert Network 3
y_3
x
$\sum$
$\hat{y} = g_1y_1 + g_2y_2 + g_3y_3$


R_5
R_2
t_4
X_2
R_3
t_2
R_4
R_1
t_1
t_3
X_1


$X_1 \leq t_1$
$X_2 \leq t_2$
$X_1 \leq t_3$
$X_2 \leq t_4$
R_1
R_2
R_3
R_4
R_5


X_2
X_1