Boosting

AdaBoost, Gradient Boosting, XGboost

DS 6030 | Fall 2024

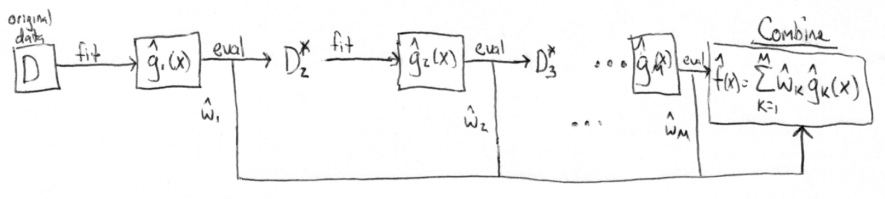
boosting.pdf

Contents

1 Boosting

Boosting is a *sequential* ensemble method.

Boosting Sketch



- A boosting model can be written as a generic ensemble
  - M is the number of base learners
  - $\hat{a}_k$ is the weight for the kth base learner ($\hat{a}_k \geq 0$).
  - $\hat{g}_k(x)$ is the prediction from the kth base learner

the more M's there are, the more complex

$$\hat{f}_M(x) = \sum_{k=1}^{M} \hat{a}_k \, \hat{g}_k(x)$$

- The key distinction of boosting models is that the base learners are **fitted sequentially**, and the best model at stage $m+1$ is dependent on all models fit up to stage m.

$$\hat{f}_{m+1}(x) = \underset{a,\, g(x)}{\arg\min} \sum_{i=1}^{n} L(y_i, \hat{f}_m(x_i) + a\, g(x_i))$$

true outcome label

- Boosting is primarily a *bias* reducer
  - The base models are often simple/weak (low variance, but high bias) models (like shallow trees)

- The complexity of the final model is based on i) the complexity of the base learners, ii) the number of iterations M, and iii) the magnitude of the ensemble weights a_k
  - Boosting models will overfit as the number of iterations increases
    - Early stopping is necessary
    - Less of a problem for hard classification problems with balanced data
  - Can apply *shrinkage* (making a_k smaller), to reduce complexity

- There are two main versions of boosting:
  - *Gradient Boosting*: fits the next model in the sequence $\hat{g}_k(x)$ to the (pseudo) residuals calculated from the predictions on the previous models
  - *AdaBoost*: fits the next model to sequentially *weighted* observations. The weights are proportional to the how poorly the current models predict the observation.

2 AdaBoost

AdaBoost was motivated by the idea that many *weak* leaners can be combined to produce a *strong* aggregate model.

- AdaBoost is for binary classification problems — Categorical outcome
- Trees are a popular base learner
  - *Weak* learners are usually used. For trees, this means shallow depth.
- At each iteration, the current model is evaluated.
  - The *ensemble weight* of model k is based on its performance (on all the training data)
  - The *observation weight* of observation i is increased if it is mis-classified and decreased if it is correctly classified.
  - Thus, at each iteration, those observations that are mis-classified are weighted higher and get extra attention in the next iteration.
- Because Adaboost uses hard-classifiers, it is sensitive to unbalanced data and unequal misclassification costs.
  - Because the thresholds are set at $p > .50$
  - There are, of course, ways to account for unbalance and unequal costs in the algorithm
  - An improvement to AdaBoost, *LogitBoost* explicitly attempts to estimate the class probability during each iteration which will allow easier post-fitting adjustments for unequal costs

Weighted Loss Functions (with observations weights)

Let $w_i \geq 0$ be a *weight* associated with observation i. The weighted loss for predictions $\hat{\mathbf{y}} = \hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n$ is

$$L(\mathbf{y}, \hat{\mathbf{y}}, \mathbf{w}) = \sum_{i=1}^{n} w_i L(y_i, \hat{y}_i)$$

2.1 Adaboost Algorithm

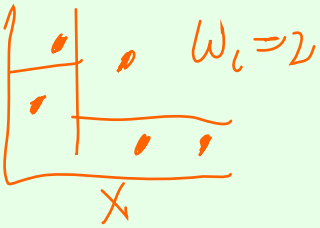
Algorithm: AdaBoost (Discrete)

Inputs:

- $D = \{(x_i, y_i\}_{i=1}^n$, where $y_i \in \{-1, 1\}$
- Tuning parameters for base model $\hat{g}$
- Maximum number of iterations, M or other stopping criteria

Algorithm:

1. Initialize *observation weights* $w_i = 1/n$ for all i



2. For $k = 1$ to M:
   a. Fit a *classifier* $\hat{g}_k(x)$ that maps (x_i, w_i) to $\{-1, 1\}$. In other words, the classifier must make a hard classification using weighted observations.
   b. Compute the weighted mis-classification rate

$$e_k = \frac{\sum_{i=1}^n w_i \mathbb{1}(y_i \neq \hat{g}_k(x_i))}{\sum_{i=1}^n w_i}$$

   Note: $0 \leq e_k \leq .5$ since model fit and evaluated on same training data.
   c. Calculate the *coefficient* for model k (*ensemble weight*)

$$\hat{a}_k = \log\left(\frac{1 - e_k}{e_k}\right)$$

   Note: $0 \leq a_k < \infty$.
   d. Update the *observations weights*. Increase weights for observations that are mis-classified by model $\hat{g}_k$ and decrease weights for the correctly classified observations.

$$\tilde{w}_i = w_i \cdot \exp\left(\hat{a}_k \cdot \mathbb{1}(y_i \neq \hat{g}_k(x_i))\right)$$

$$\tilde{w}_i = \begin{cases} w_i \left(\frac{1-e_k}{e_k}\right) & \text{if obs } i \text{ is misclassified} \\ w_i & \text{if obs } i \text{ is correctly classified} \end{cases}$$

$$w_i = \frac{\tilde{w}_i}{\sum_{j=1}^n \tilde{w}_j} \quad \text{(re-normalize weights)}$$

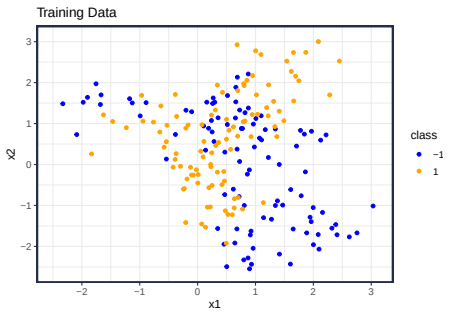
3. Output final ensemble $\hat{f}_M(x)$

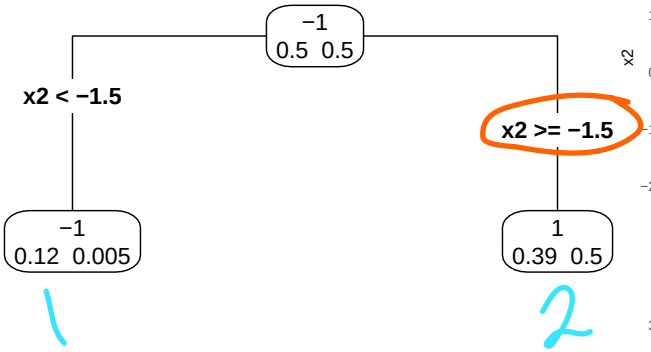
$$\hat{f}_M(x) = \sum_{k=1}^{M} \hat{a}_k \, \hat{g}_k(x)$$

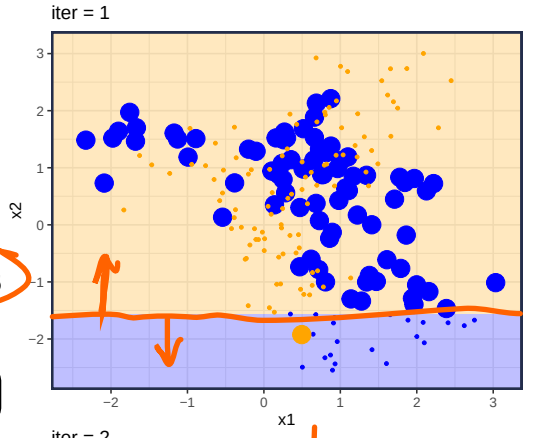
- Where $\hat{f}_k(x) = \hat{a}_k \, \hat{g}_k(x)$
- Hard classification: $\hat{f}_M(x) > 0$
- Or remap to a probability $\hat{p}(x) = \frac{e^{2\hat{f}(x)}}{1+e^{2\hat{f}(x)}}$ for thresholding

2.1.1 Illustration with Stumps (depth = 1, n.nodes=2)

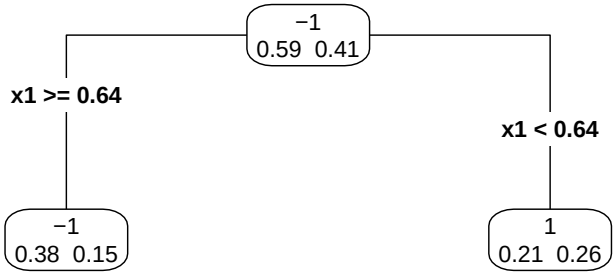
Stumps: all trees have single root w/ 2 nodes

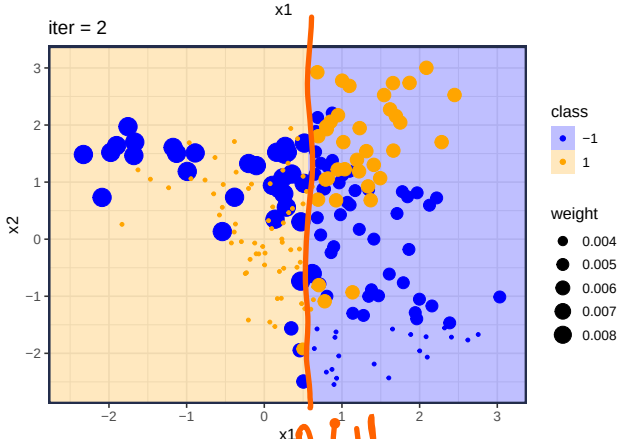




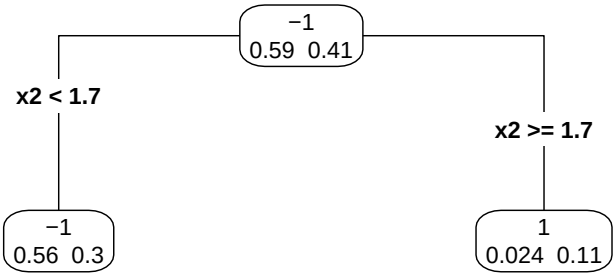


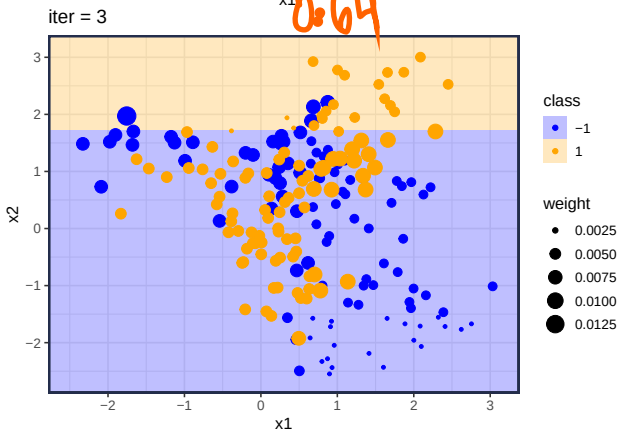
Big dots are mis-classified.

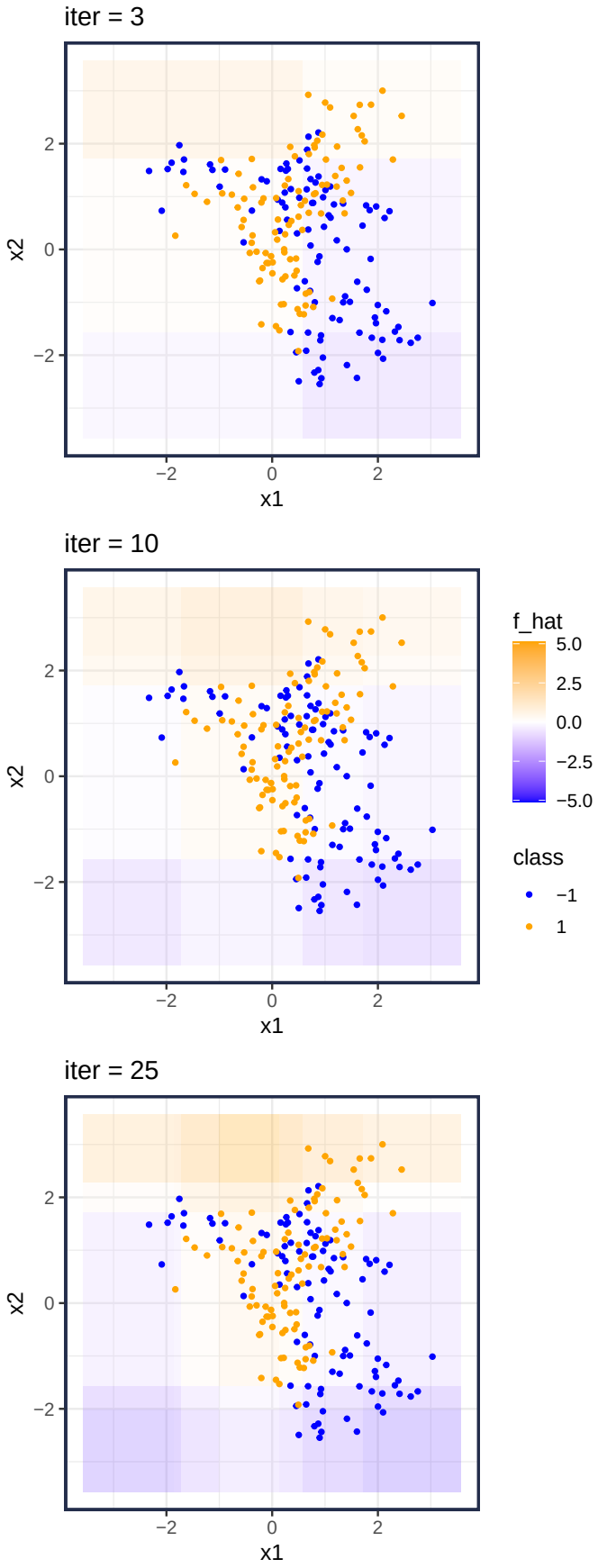




0.64



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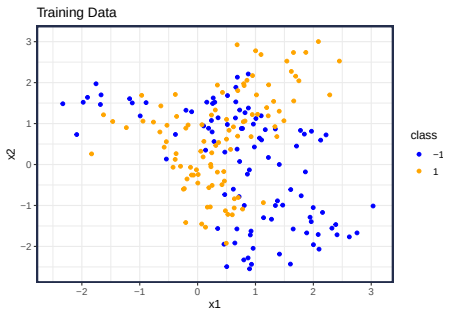
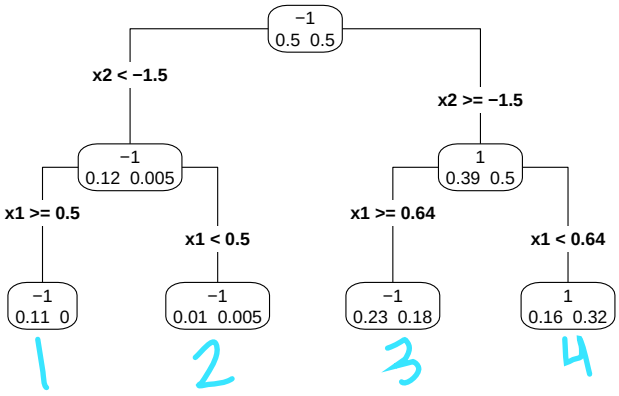
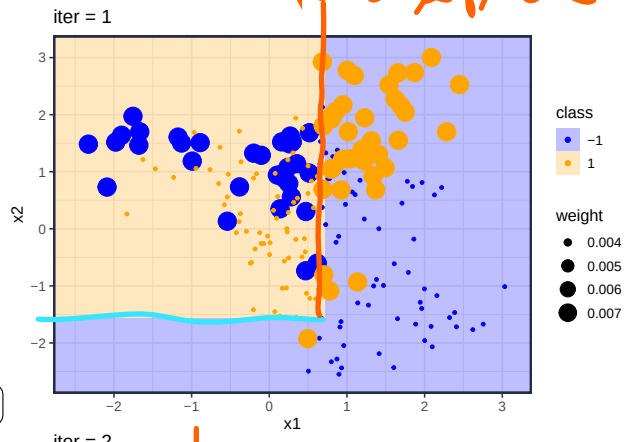
iter = 10
iter = 25
x1
x2
−2
0
2
f_hat
5.0
2.5
0.0
−2.5
−5.0
class
−1
1

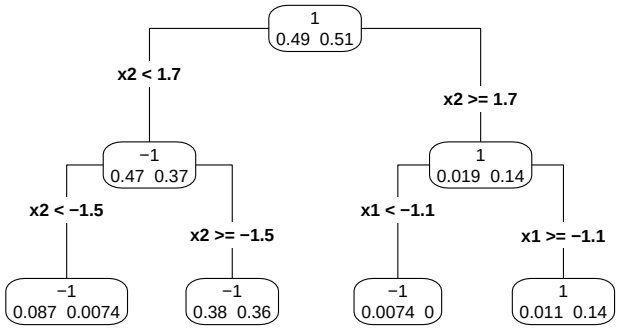
2.1.2 Illustration with depth = 2, n.nodes=4

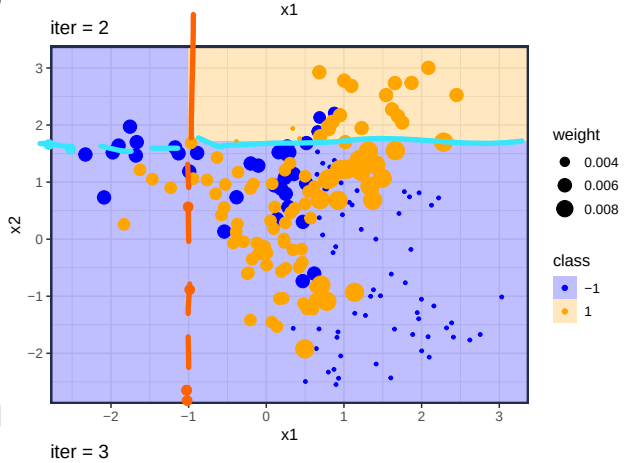


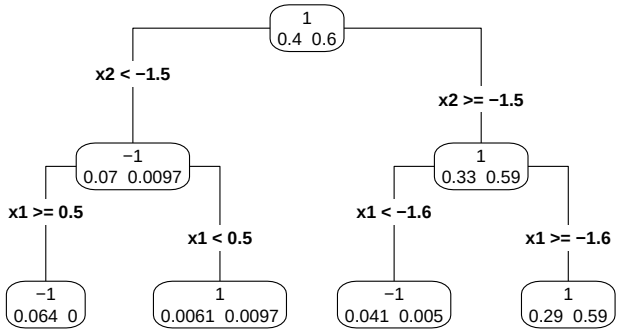
two splits

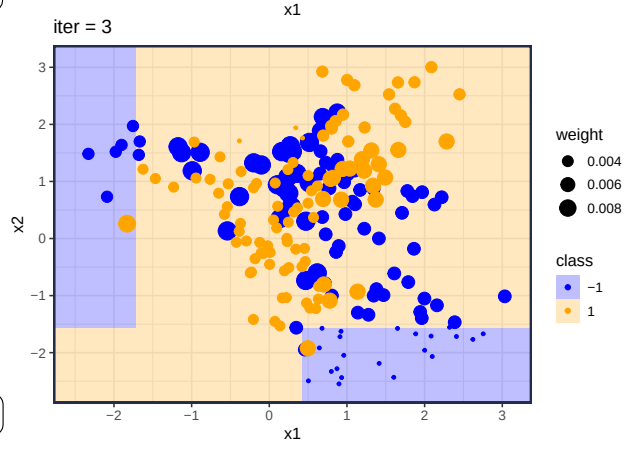


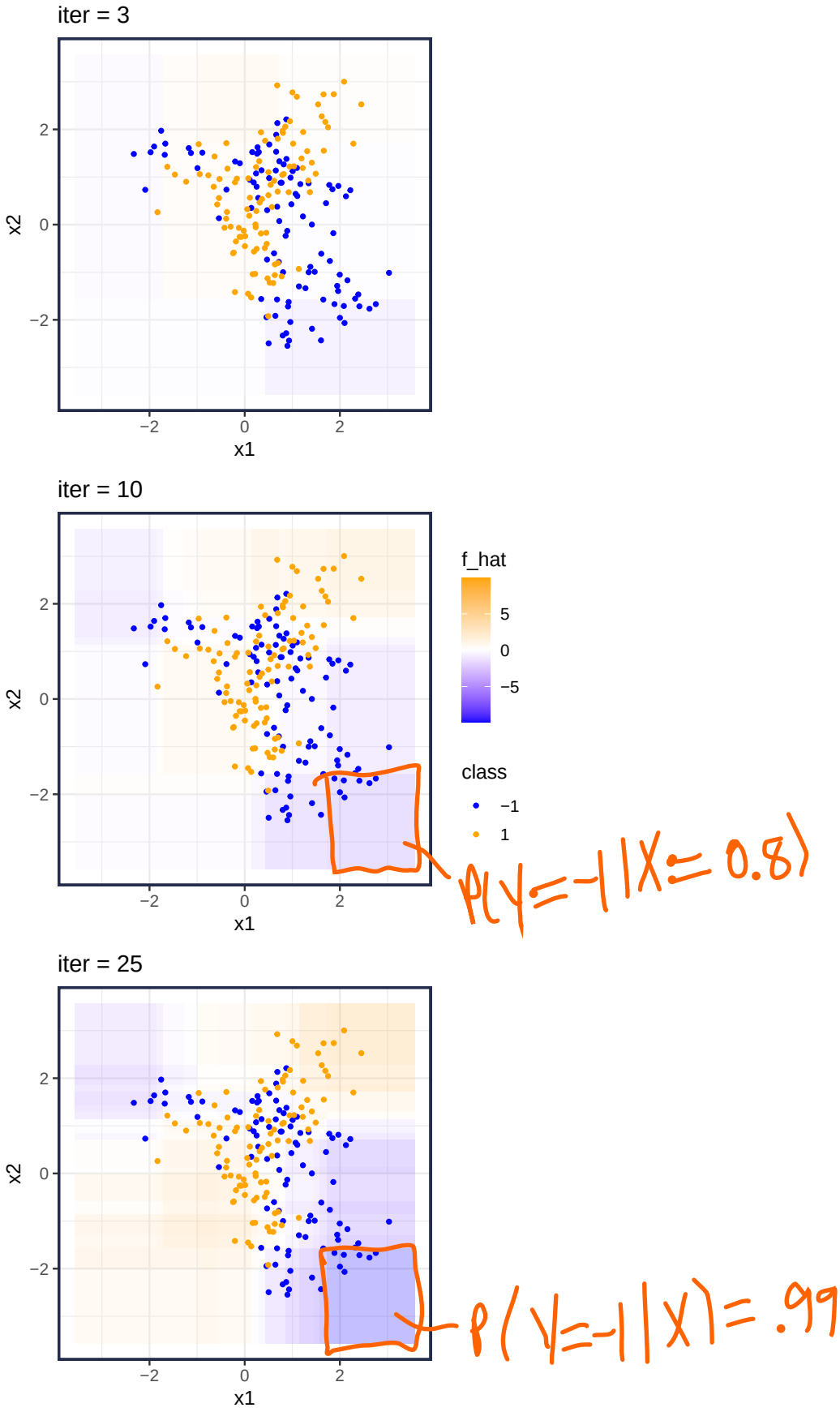


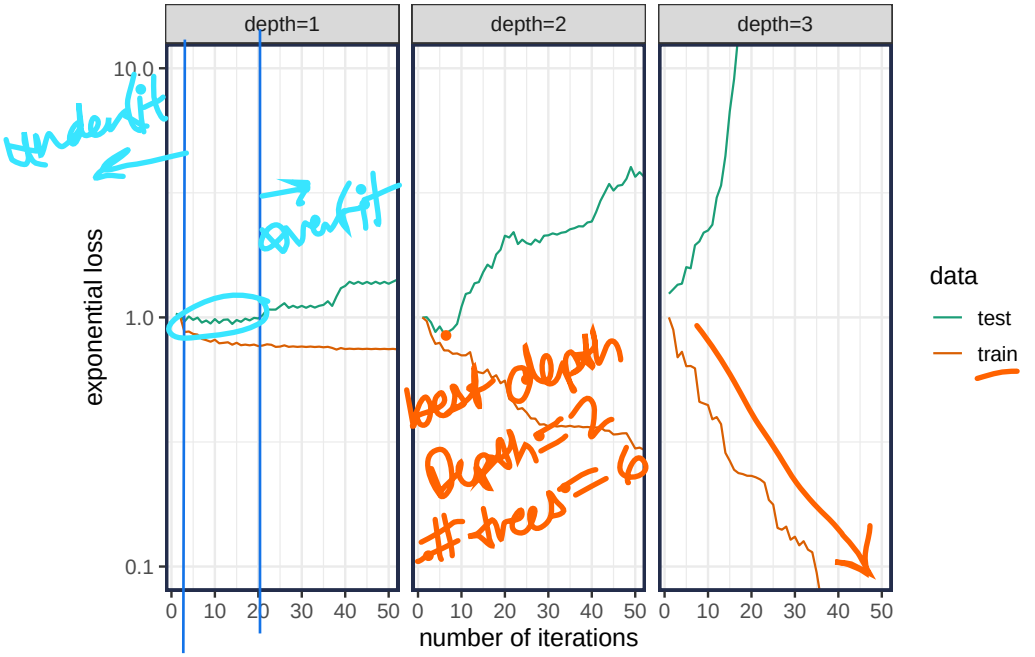


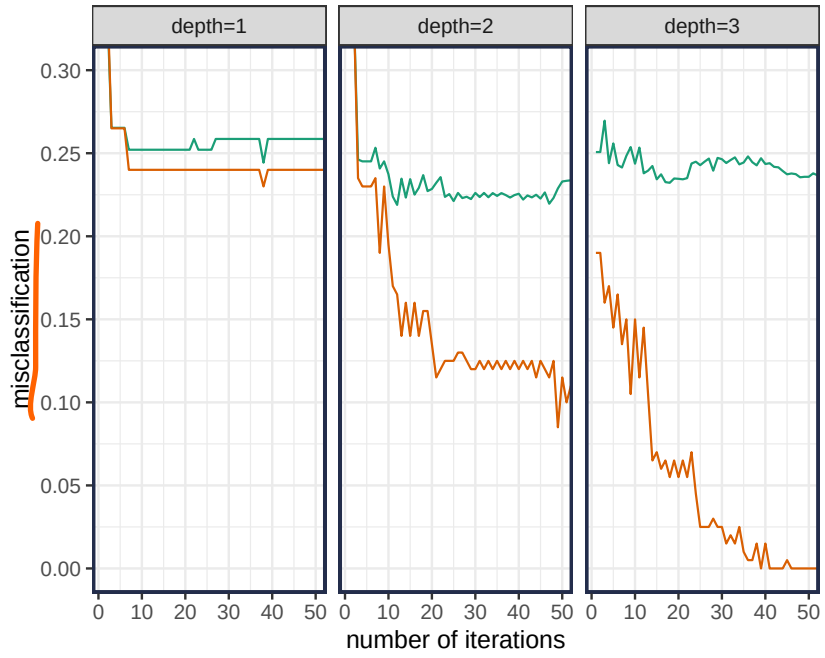







iter = 3
iter = 10
iter = 25
x1
x2
f_hat
5
0
−5
class
−1
1
P(Y=-1|X=0.8)
P(Y=-1|X)=.99





b/c of the loss function here, adaboost doesn't overfit

2.2 AdaBoost Details

- Adaboost uses an outcome variable of $y \in \{-1, 1\}$
- AdaBoost implicitly uses the loss function:

$$L(y, f) = e^{-yf}$$
$$= \begin{cases} e^{-f} & y = +1 \\ e^{f} & y = -1 \end{cases}$$

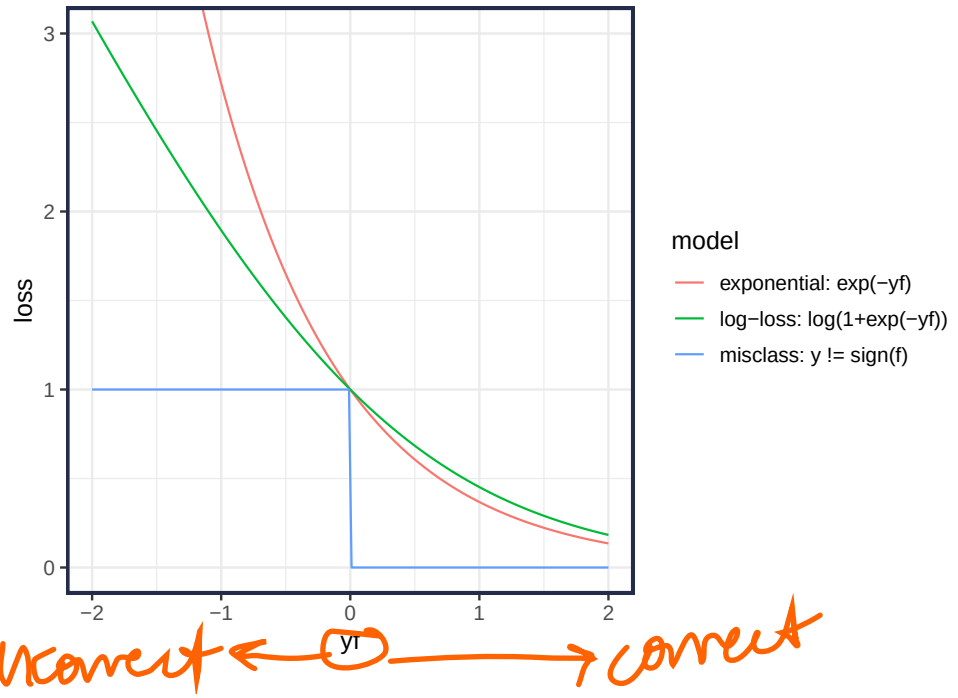
- Adaboost estimates the probability that $Y = +1$ as

$$\hat{p}(x) = \frac{e^{\hat{f}_M(x)}}{e^{-\hat{f}_M(x)} + e^{\hat{f}_M(x)}}$$
$$= \frac{e^{2\hat{f}_M(x)}}{1 + e^{2\hat{f}_M(x)}}$$

where $p(x) = \Pr(Y = +1 \mid X = x)$

- And $\hat{f}(x)$ is an estimate of

$$\hat{f}_M(x) = \frac{1}{2} \log \frac{\hat{p}(x)}{1 - \hat{p}(x)}$$
$$= \frac{1}{2} \text{logit } \hat{p}(x)$$

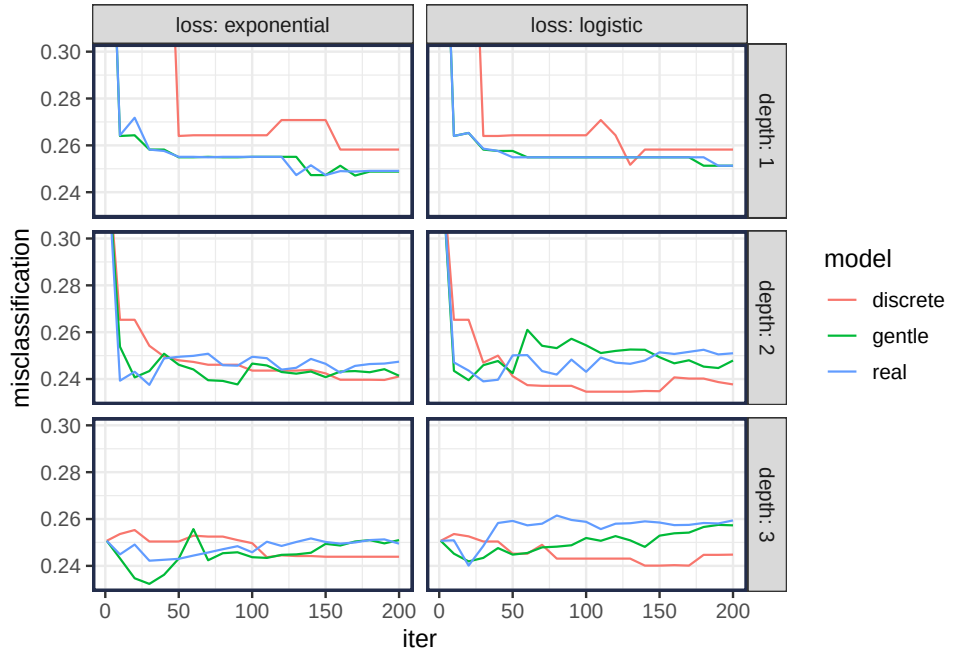


- Comparison with logistic regression (using log-loss / negative binomial log-likelihood)
  - $\hat{f}(x) = \text{logit } \hat{p}(x)$
  - $\hat{p}(x) = \frac{e^{\hat{f}_M(x)}}{1+e^{\hat{f}_M(x)}}$
  - Log-loss: $\log(1 + e^{-yf})$ (using $y \in \{-1, +1\}$)

2.3 R package `ada`

The R package `ada` provides an implementation of AdaBoost (and related methods).

- See Friedman, J., Hastie, T., and Tibshirani, R. (2000). Additive Logistic Regression: A statistical view of boosting. Annals of Statistics, 28(2), 337-374. for the details of model variations
  - {Discrete, Real, Gentle} AdaBoost
  - Logitboost



Algorithm: Real AdaBoost

Inputs:

- $D = \{(x_i, y_i\}_{i=1}^n$, where $y_i \in \{-1, 1\}$
- Tuning parameters for base model $\hat{g}$
- Maximum number of iterations, M

Algorithm:

1. Initialize *observation weights* $w_i = 1/n$ for all i

2. For $k = 1$ to M:

   a. Fit a model $\hat{q}_k(x)$ that uses weighted inputs (x_i, w_i) to estimate a probability $\hat{p}_k(x) = \widehat{\Pr}(Y = 1 \mid X = x)$. In other words, the classifier must make a soft classification using weighted observations.

b. Set $f_m(x) = \frac{1}{2}\text{logit}\,\hat{p}_k(x)$

c. Update the *observations weights*. Increase weights for observations that are mis-classified by model $\hat{g}_k$ and decrease weights for the correctly classified observations.

$$\tilde{w}_i = w_i \cdot \exp\left(-y_i \hat{f}_m(x_i)\right)$$
$$w_i = \frac{\tilde{w}_i}{\sum_{j=1}^n \tilde{w}_j} \qquad \textit{(re-normalize weights)}$$

3. Output final ensemble $\hat{f}_M(x)$

$$\hat{f}_M(x) = \sum_{k=1}^{M} \hat{f}_k(x)$$

- Hard classification: $\hat{f}_M(x) > 0$
- Or remap to a probability $\hat{p}(x) = \frac{e^{2f}}{1+e^{2f}}$ for thresholding

Algorithm: Gentle AdaBoost

Inputs:

- $D = \{(x_i, y_i\}_{i=1}^n$, where $y_i \in \{-1, 1\}$
- Tuning parameters for base model $\hat{g}$
- Maximum number of iterations, M

Algorithm:

1. Initialize *observation weights* $w_i = 1/n$ for all i and $f_0(x) = 0$

2. For $k = 1$ to M:

a. Fit a model $\hat{g}_k(x)$ with weighted least squares that estimates y_i using features x_i and weights w_i.

b. Update the *observations weights*. Increase weights for observations that are mis-classified by model $\hat{g}_k$ and decrease weights for the correctly classified observations.

$$\tilde{w}_i = w_i \cdot \exp\left(-y_i \hat{g}_m(x_i)\right)$$
$$w_i = \frac{\tilde{w}_i}{\sum_{j=1}^n \tilde{w}_j} \qquad \textit{(re-normalize weights)}$$

3. Output final ensemble $\hat{f}_M(x)$

$$\hat{f}_M(x) = \sum_{k=1}^{M} \hat{g}_k(x)$$

- Hard classification: $\hat{f}_M(x) > 0$

Algorithm: LogitBoost

Inputs:

- $D = \{(x_i, y_i\}_{i=1}^n$, where $y_i \in \{-1, 1\}$
- Tuning parameters for base model $\hat{g}$
- Maximum number of iterations, M
- Let $y_i^* = (y + 1)/2 \in \{0, 1\}$

Algorithm:

1. Initialize *observation weights* $w_i = 1/n$ for all i and $f_0(x) = 0$

2. For $k = 1$ to M:

   a. Like in newton-raphson for logistic regression, calculate the working response and weights for all observations

   $$z_i = \frac{y_i^* - p_i}{p_i(1 - p_i)}$$
   $$w_i = p_i(1 - p_i)$$

   b. Fit a model $\hat{g}_k(x)$ with weighted least squares that estimates z_i using features x_i and weights w_i.

   c. Update $\hat{f}_k(x) = \hat{f}_{k-1}(x) + \hat{g}_k(x)/2$ and $p_i = e^{\hat{f}_k(x)}/(e^{\hat{f}_k(x)} + e^{-\hat{f}_k(x)})$

3. Output final ensemble $\hat{f}_M(x) \in \mathbb{R}$

$$\hat{f}_M(x) = \sum_{k=1}^{M} \frac{1}{2} \hat{g}_k(x)$$

- Where $\hat{f}_k(x) = \frac{1}{2} \hat{g}_k(x)$.
- Hard classification: $\hat{f}_M(x) > 0$
- Or remap to a probability $\hat{p}(x) = \frac{e^{2f}}{1+e^{2f}}$ for thresholding

3 Gradient Boosting

a sequential observation technique

The boosting model:

$$\hat{f}_M(x) = \sum_{k=1}^{M} \hat{a}_k \, \hat{g}_k(x)$$

Sequential Fitting:

$$\hat{f}_{k+1}(x) = \underset{a,\, g(x)}{\arg\min} \sum_{i=1}^{n} L(y_i, \hat{f}_k(x_i) + a\, g(x_i))$$

The concept of gradient boosting is to sequentially re-fit to the negative (functional) gradients of the loss function (think of the negative gradients as a type of residual; *pseudo residual*).

- The same structure can be used for many different loss functions
  - it works the same for regression and classification
  - survival analysis, ranking, etc.

3.1 Gradient Descent

- Our objective is to find the model (or model parameters) that minimize the loss function
- From any starting point, we can move toward the optimum using *gradient descent*:

$$f_{k+1} = f_k - \nu_k L'(f_k)$$

  - $\nu_k > 0$ is the step-size
  - $L'(f_k)$ is the functional derivative of the loss with respect to the model f_k

step size

derivative of loss "gradient"

- Boosting fits models sequentially:

$$\hat{f}_{k+1}(x) = \hat{f}_k(x) + \hat{a}_k \, \hat{g}_k(x)$$

- So we see a parallel; each boosting model $\hat{g}_k(x)$ can be viewed as estimating the *negative derivative* of the loss function.

3.2 L_2 Boosting

L_2 boosting is based on the the squared error loss function

$$L(y_i, \hat{f}(x_i)) = \frac{1}{2}(y_i - \hat{f}(x_i))^2$$

- The *negative gradients* are

$$\begin{aligned} r_i &= \left[-\frac{\partial L(y_i, f_i)}{\partial f_i} \right]_{f_i = \hat{f}(x_i)} \\ &= y_i - \hat{f}(x_i) \end{aligned}$$

- L2 Boosting is simply re-fitting to the residuals.

Algorithm: L_2 Boosting

1. Initialize $\hat{f}_0(x) = \bar{y}$

2. For $k = 1$ to M:

   a. Calculate residuals $r_i = y_i - \hat{f}_{k-1}(x_i)$ for all i

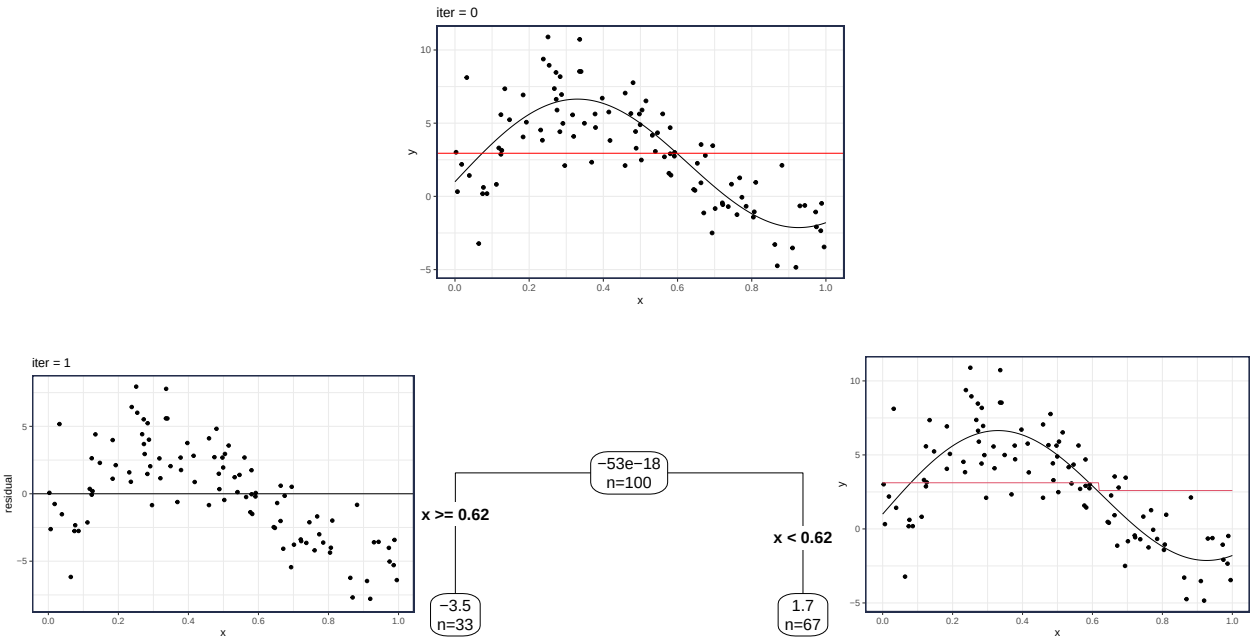
   b. Fit a base learner (e.g., regression trees) to the residuals $\{(x_i, r_i)\}_{i=1}^n$ to get the model $\hat{g}_k(x)$

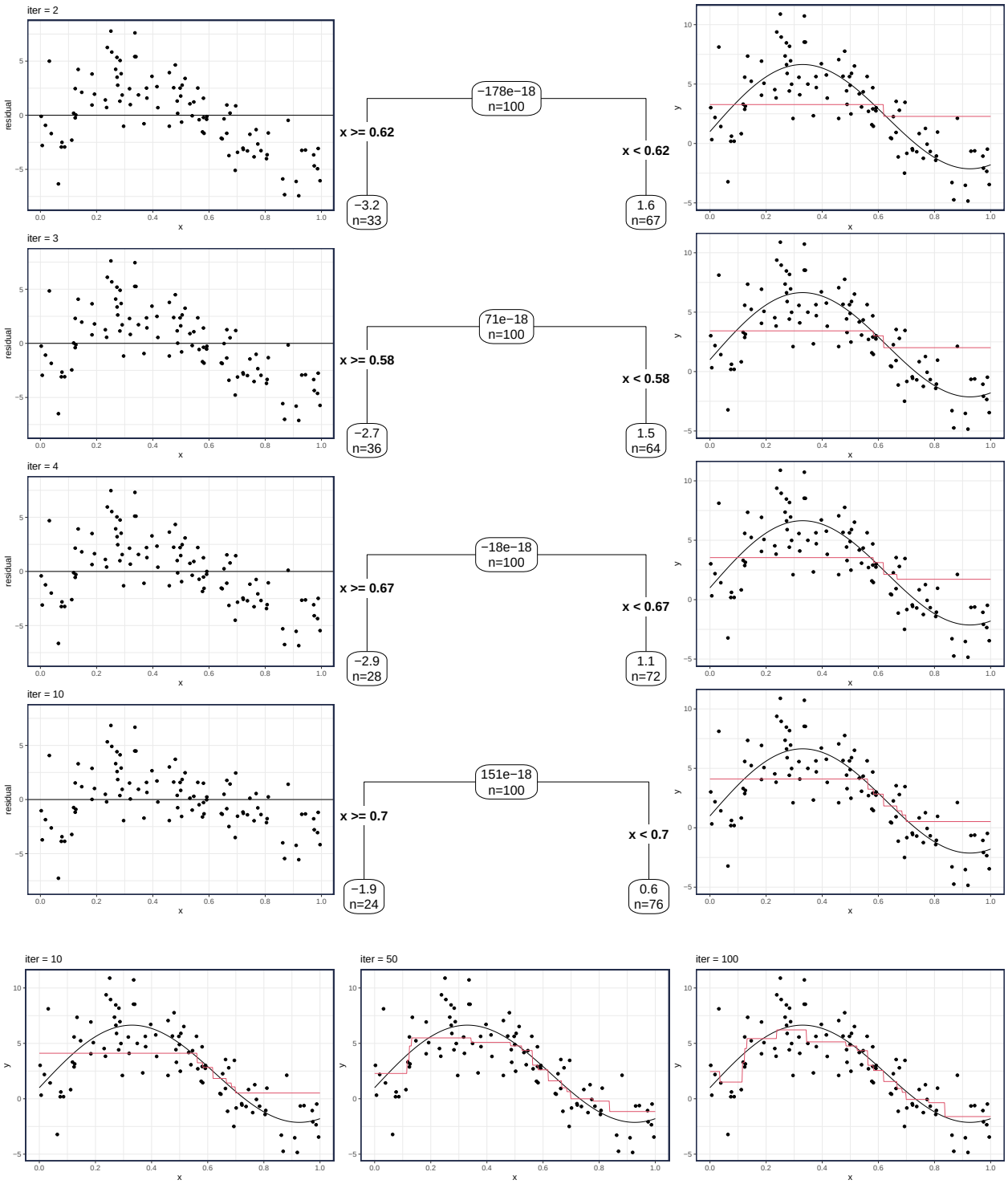
   c. Update the overall model $\hat{f}_k(x) = f_{k-1}(x) + \nu \hat{g}_k(x)$
      - $0 \leq \nu \leq 1$ is the step-size (*shrinkage*)

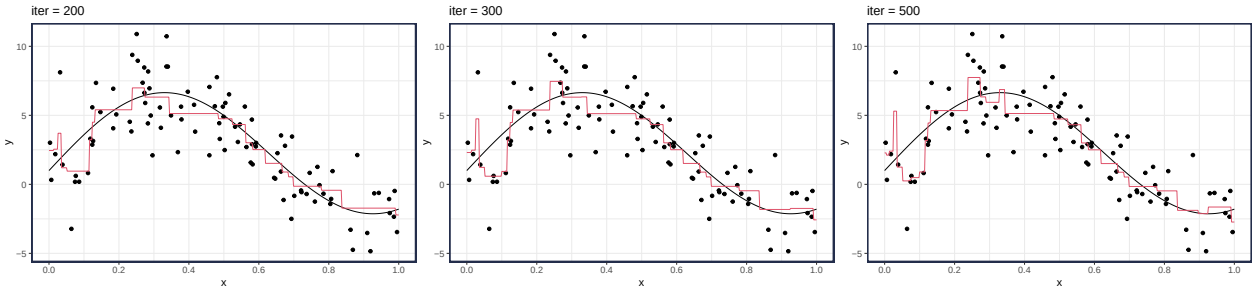
3. Final model is $\hat{f}_M(x) = \bar{y} + \sum_{k=1}^M \nu \hat{g}_k(x)$

- Like AdaBoost, emphasis is given to observations that are predicted poorly (large residuals)

3.2.1 Illustration using stumps (depth=1, n.nodes=2, $\nu = .1$)




iter = 2
residual
x
−178e−18
n=100
x >= 0.62
x < 0.62
−3.2
n=33
1.6
n=67
y
iter = 3
residual
x
71e−18
n=100
x >= 0.58
x < 0.58
−2.7
n=36
1.5
n=64
y
iter = 4
residual
x
−18e−18
n=100
x >= 0.67
x < 0.67
−2.9
n=28
1.1
n=72
y
iter = 10
residual
x
151e−18
n=100
x >= 0.7
x < 0.7
−1.9
n=24
0.6
n=76
y
iter = 10
iter = 50
iter = 100
y
x


iter = 200
iter = 300
iter = 500
y
x
10
5
0
−5
0.0
0.2
0.4
0.6
0.8
1.0

3.3 GBM (Gradient Boosting Machine)

- R package `gbm`
- GBM Documentation
- GBM is a first order approach. It does not consider Hessian.

3.3.1 Model/Tree Tuning Parameters

- Tree depth (`interaction.depth`)
  - Grows trees to a depth specified by `interaction.depth` (unless there are not enough observations in the terminal nodes)
- Minimum number of observations allowed in the terminal nodes (`n.minobsinnode`)
- Sub-sampling (`bag.fraction`)
  - *Stochastic Gradient Boosting*
  - Sample (without replacement) at each iteration
- Loss Function (`distribution`)
  - The loss function is determined by the `distribution` argument
  - Use `distribution="gaussian"` for squared error
  - Other options are: `bernoulli` (for logistic regression), `poisson` (for Poisson regression), `pairwise` (for ranking/LambdaMart), `adaboost` (for the adaboost exponential loss), etc.

3.3.2 Boosting Tuning Parameters

- Number of iterations/trees (`n.trees`)
  - Need to tune
- Shrinkage parameter (`shrinkage`)
  - Set small, but the smaller the `shrinkage`, the more iterations/trees need to be used
  - "Ranges from 0.001 to 0.100 usually work"
- Cross-validation (`cv.folds`)
  - `gbm` has a built in cross-validation
  - no way to manually set the folds

3.3.3 Computational Settings

- Number of Cores (`n.cores`)
  - Only used when cross-validation is implemented

3.4 xgboost (Extreme Gradient Boosting)

- R package `xgboost`
- xgboost Documentation
- xgboost Model
- xbgoost Paper

3.4.1 Model/Tree Tuning Parameters

- Different base leaners (`booster`)
  - `gbtree` is a tree
  - `gblinear` creates a (generalized) liner model (forward stagewise linear model)
- Tree building (`tree_method`)
  - To speed up the fitting, only consider making splits at certain quantiles of the input vector (rather than considering every unique value)
- Sub-sampling (`subsample`)
  - *Stochastic Gradient Boosting*
  - Sample (without replacement) at each iteration
- Feature sampling (`colsample_bytree`, `colsample_bylevel`, `colsample_bynode`)
  - Like used in Random Forest, the features/columns are subsampled
  - Can use a subsample of features for each tree, level, or node

Model Complexity Parameters

- Tree depth (`max_depth`)
  - Grows trees to a depth specified by `max_depth` (unless there are not enough observations in the terminal nodes)
  - Trees may not reach `max_depth` if the `gamma` or `min_child_weight` arguments are set.
- Minimum number of observations (or sum of weights) allowed in the terminal nodes (`min_child_weight`)
- Pruning (`gamma` or `min_split_loss`)
  - Minimum loss reduction required to make a further partition on a leaf node of the tree
  - The larger gamma is, the more conservative the algorithm will be
- ElasticNet type penalty (`lambda` and `alpha`)
  - `lambda` is an L_2 penalty
  - `alpha` is an L_1 penalty

Note

- Recall that trees model the outcome as a *constant* in each region

$$\hat{f}_T(x) = \sum_{m=1}^{M} \hat{c}_m \, \mathbb{1}(x \in \hat{R}_m)$$

- Cost-complexity pruning found the optimal tree as the one that minimized the penalized loss objective function:

$$C_\gamma(T) = \sum_{m=1}^{|T|} \text{Loss}(T) + \gamma |T|$$

- XGBoost selects a tree at each iteration using the following penalized loss:

$$C_{\gamma,\lambda,\alpha}(T) = \sum_{m=1}^{|T|} \text{Loss}(T) + \gamma |T| + \frac{\lambda}{2} \sum_{m=1}^{|T|} \hat{c}_m^2 + \alpha \sum_{m=1}^{|T|} |\hat{c}_m|$$

- Loss Function (`objective`)
  - The loss function is determined by the `objective` argument
  - Use `reg:squarederror` for squared error
  - Other options are: `reg:logistic` or `binary:logistic` (for logistic regression), `count:poisson` (for Poisson regression), `rank:pairwise` (for ranking/LambdaMart), etc.

3.4.2 Boosting Tuning Parameters

- Shrinkage parameter (`eta` or `learning_rate`)
  - Set small, but the smaller the `eta`, the more iterations/trees need to be used
- Number of iterations/trees (`num_rounds`)
- Cross-validation (`xgb.cv`)
  - `xgboost` has a built in cross-validation
  - It is possible to manually set the folds

3.4.3 Computational Settings

- Number of Threads (`nthread`)
- GPU Support (https://xgboost.readthedocs.io/en/latest/gpu/index.html)
  - Used for finding tree split points and evaluating/calculating the loss function

3.5 CatBoost

- R package: (https://github.com/catboost/catboost/tree/master/catboost/R-package)
- CatBoost Documentation
- Model/Tree Tuning Parameters:

- Boosting Tuning Parameters:

3.6 LightGBM

- R Package: https://github.com/microsoft/LightGBM/tree/master/R-package
- LightGBM Documentation
- Model/Tree Tuning Parameters:

- Boosting Tuning Parameters:

4 Appendix: L2 Tree Boosting R Code

```
#: L2 Boost Algorithm
library(rpart)

# L2boost()
#---------------------------------------------------------------------------#
# L2 boosted trees (boosted regression trees)
# Inputs:
#  x,y: training data. x should be data frame or matrix, y a vector
#  xtest optional test data (data frame or matrix)
#  M: number of iterations
#  depth: tree depth. depth = 2 gives 4 leaf nodes.
#  nu: shrinkage parameter
# Outputs:
#  YHAT: matrix of in-sample predictions (predicting x)
#  R: matrix of residuals
#  YHAT.test: matrix of predictions for xtest
#  TREE: list of rpart trees
#---------------------------------------------------------------------------#

L2boost <- function(x, y, xtest=NULL, M=100, depth=2, nu=.1){
```

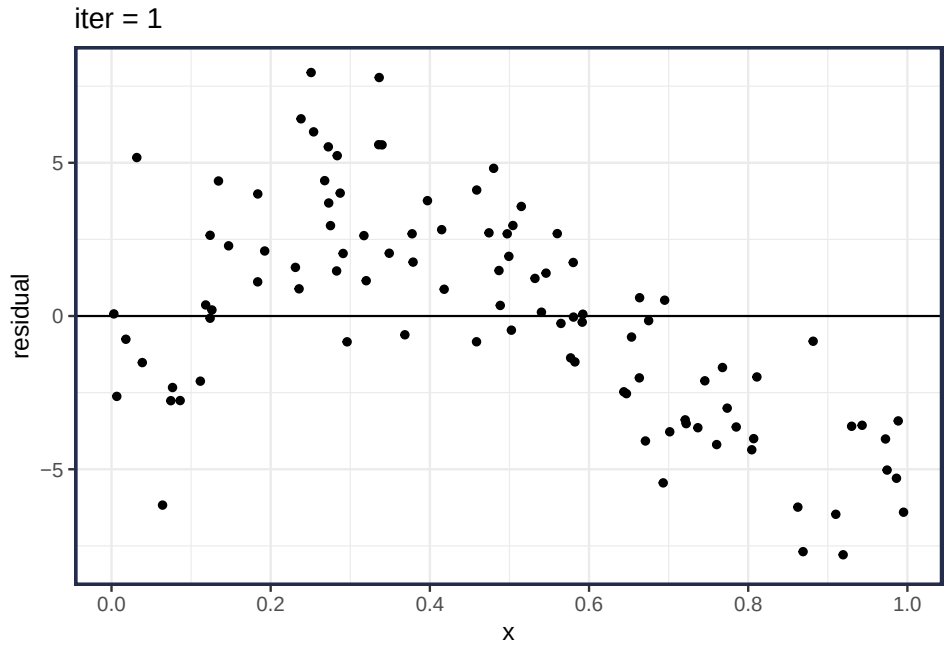
```
  #- use training data if test data is not specified
  if(is.null(xtest)) {
    xtest = x
  }

  #- storage
  n = length(y)
  R = YHAT =  matrix(NA_real_, n, M)
  YHAT_test = matrix(NA_real_, nrow(xtest), M)
  colnames(YHAT) = colnames(YHAT_test) = colnames(R) = paste0("iter = ", 1:M)
  TREE = vector("list", M)
  names(TREE) = paste0("iter = ", 1:M)

  #-- 1) initialize model with mean
  mu = mean(y)
  yhat = rep(mu, nrow(x))
  yhat_test = rep(mu, nrow(xtest))

  for(m in 1:M){

    #-- 2a) Calculate Residuals
    r = y - yhat
    R[,m] = r

    #-- 2b) Fit regression tree
    tree = rpart(r ~ ., data = x,
                 maxdepth = depth,   # control tree depth
                 cp = -1,            # no pruning
                 minsplit = 0,       # allow all splits
                 minbucket = 1,      # no minimum on leaf size
                 method = "anova",   # least-squares loss function
                 xval = 0)           # no cross-validation

    TREE[[m]] = tree

    #-- 2c) Update model
    yhat = yhat + nu*predict(tree, x)
    YHAT[, m] = yhat

    yhat_test = yhat_test + nu*predict(tree, xtest)
    YHAT_test[, m] = yhat_test

  }

  #-- 3) Output
  return(list(YHAT=YHAT, R=R, YHAT.test=YHAT_test, TREE=TREE))
}
```

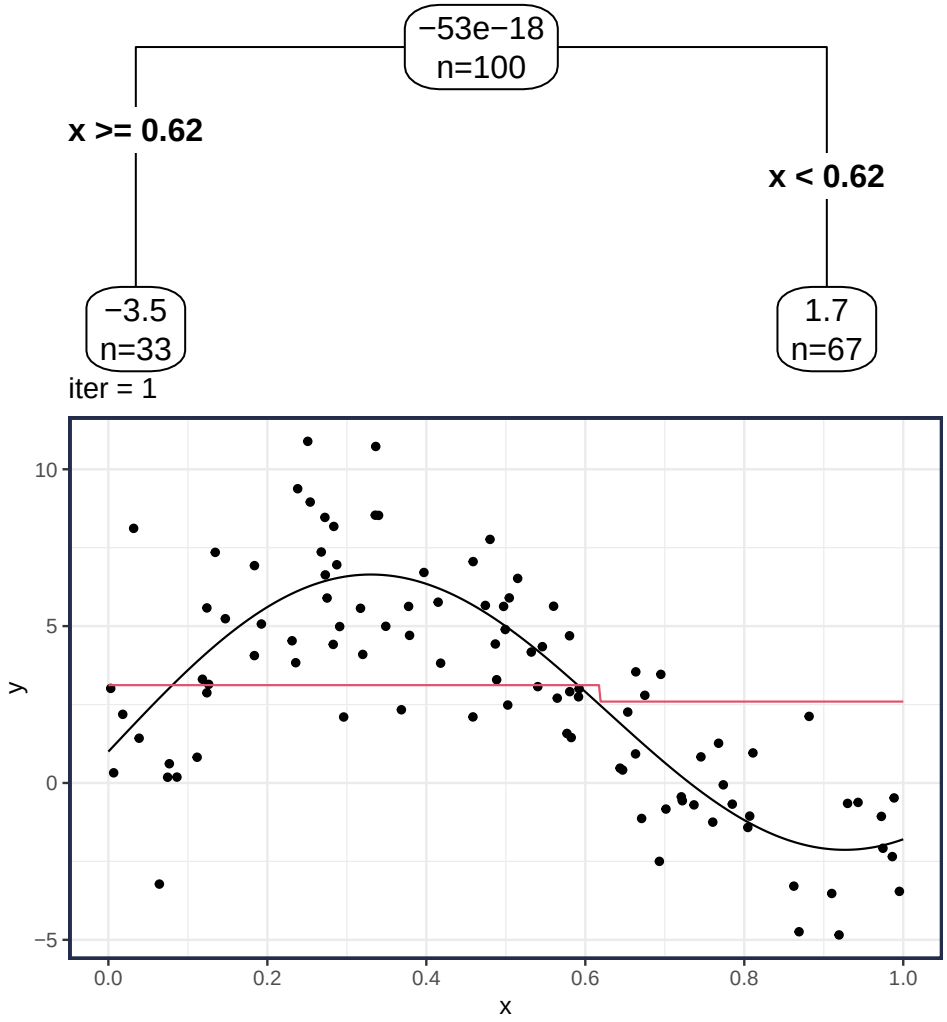
```
#: Data Generation
n = 100                                 # number of observations
generate_x <- function(n) runif(n)      # U[0,1]
f <- function(x) 1 + 2*x + 5*sin(5*x)   # true mean function
sd = 2                                  # stdev for error

set.seed(825)                           # set seed for reproducibility
x = generate_x(n)                       # get x values
y = f(x) + rnorm(n, sd=sd)              # get y values
data_train = data.frame(x, y)           # training data
```

```r
x_eval = seq(0, 1, length=500)           # evaluation points
```

```r
#: Implement L2 boosting
L2 = L2boost(data.frame(x), y, xtest=data.frame(x=x_eval),  # data
             depth = 1, M = 100, nu = .1)              # tuning parameters
```

```r
#: Plotting
library(tidyverse)    # for ggplot2 package
library(rpart.plot)   # for prp()

# set iteration
i = 1

# Residual Plot
ggplot(data_train, aes(x)) +
  geom_point(aes(y = L2$R[,i]), col="black") +
  geom_hline(yintercept=0, col="black")  +
  scale_x_continuous(breaks=seq(0, 1, by=.20)) +
  coord_cartesian(ylim=c(-8, 8)) +
  labs(y="residual", title=colnames(L2$R)[i])

# Tree
prp(L2$TREE[[i]], type=4, extra=1, branch=1, clip.right.labs = FALSE, roundint=FALSE)

# Model prediction
ggplot(data_train, aes(x, y)) +
  geom_point() +
  annotate("line", x=x_eval, y=f(x_eval), color = "black") +
  geom_line(data=tibble(x=x_eval, y=L2$YHAT.test[,i]), col=2) +
  scale_x_continuous(breaks=seq(0, 1, by=.20)) +
  labs(title=colnames(L2$R)[i])
```





5 Appendix: xgboost and lightgbm

```
#: Load required packages
library(tidyverse)
library(palmerpenguins) # data
library(xgboost)
library(lightgbm)
```

We will use the palmer penguins data:

```
palmerpenguins::penguins
#> # A tibble: 344 x 8
#>   species island    bill_length_mm bill_depth_mm flipper_length_mm body_mass_g
#>   <fct>   <fct>              <dbl>         <dbl>             <int>       <int>
#> 1 Adelie  Torgersen           39.1          18.7               181        3750
#> 2 Adelie  Torgersen           39.5          17.4               186        3800
#> 3 Adelie  Torgersen           40.3          18                 195        3250
#> 4 Adelie  Torgersen           NA            NA                  NA          NA
#> 5 Adelie  Torgersen           36.7          19.3               193        3450
```

```
#> 6 Adelie  Torgersen           39.3          20.6               190        3650
#> # i 338 more rows
#> # i 2 more variables: sex <fct>, year <int>
```

with a goal of predicting the `species` from the other variables. This is a three-class probability estimation problem. Most tree-based models can handle multiple classes naturally.

Note that the `sex` and `island` predictors are categorical.

5.1 xgboost

Requires a numeric matrix as input, and suggests using a special xgb formatted matrix for efficiency. The approach here is to create a *recipe* that does some pre-processing to handle missing values and categorical predictors and then create the special matrix.

Notes:

- The recipe removes observations with missing outcomes. It also sets unknown categorical/nominal values to an explicit level. Any missing values in the resulting data are handled internally by xgboost.
- the categorical (or nominal) predictors are dummy encoded.
- the three level outcome variables *species* is recoded to be $\{0, 1, 2\}$. All xgboost data must be numeric, even if it represents a nominal variable.

```
library(recipes) # part of tidymodels
library(xgboost)

#: pre-processing specs
rec_xgb = recipe(species ~ ., data = palmerpenguins::penguins) %>%
  # Handle missing data
  step_naomit(species) %>%  # remove cases with missing outcome label
  step_unknown(all_nominal_predictors()) %>% # add "unknown" level if missing
  # replace categorical/factors with numeric
  step_dummy(all_nominal_predictors(), one_hot = FALSE) %>%
  step_integer(species, zero_based = TRUE) %>%
  # train or prepare the pre-process step using the data provided in recipe()
  prep()

#: xgboost data object
xgb_data =
  xgb.DMatrix(
    data = bake(rec_xgb, new_data = NULL, composition = "matrix",
                all_predictors()),
    label = bake(rec_xgb, new_data = NULL, all_outcomes()) %>% pull()
  )

#: tuning parameters
xgb_tuning = list(
  learning_rate = .1,
  gamma = 1,
  max_depth = 2,
  subsample = .80
)
# Note, the number of iterations, nrounds, is not part of the params.
```

```r
#: fit model
set.seed(1234) # xgboost can use stochastic resampling
xgb = xgboost(data = xgb_data,
              params = xgb_tuning, nrounds = 100, # tuning parameters
              num_class = 3,  # this is required for multi-class problems
              objective = "multi:softprob", # multi-class loss function
              verbose = 0) # don't print output during training

#: make predictions
predict(xgb, xgb_data, reshape = TRUE) %>% head()
#>         [,1]     [,2]     [,3]
#> [1,] 0.9941 0.003113 0.002755
#> [2,] 0.9938 0.003303 0.002924
#> [3,] 0.9938 0.003303 0.002924
#> [4,] 0.5404 0.025182 0.434446
#> [5,] 0.9941 0.003113 0.002755
#> [6,] 0.9941 0.003113 0.002755
```

5.2 lightgbm

Following a similar process to what is required for xgboost. LightGBM requires a matrix as input, and suggests using a special formatted matrix. The approach here follows the recipe that is used for xgboost with the exception that lightgbm can internally handle categorical predictors.

Notes:

- The recipe removes observations with missing outcomes. It also sets unknown categorical/nominal values to an explicit level. Any missing values in the resulting data are handled internally by lightgbm.
- the categorical (or nominal) predictors are integer encoded $\{0, 1, ...\}$ so they are numeric, and then handled internally by lightGBM. The `categorical_features` argument in the `lgb.Dataset()` function is used to specify which predictors should be treated as categorical.
- the three level outcome variables *species* is recoded to be $\{0, 1, 2\}$. All lightgbm data must be numeric, even if it represents a nominal variable.

```r
library(recipes) # part of tidymodels
library(lightgbm)

#: pre-processing specs
rec_lgbm = recipe(species ~ ., data = palmerpenguins::penguins) %>%
  # Handle missing data
  step_naomit(species) %>%  # remove cases with missing outcome label
  step_unknown(all_nominal_predictors()) %>%        # add "unknown" level if missing
  # replace categorical/factors with numeric
  step_integer(all_nominal_predictors(), zero_based = TRUE) %>%
  step_integer(species, zero_based = TRUE) %>%
  # train or prepare the pre-process step using the data provided in recipe()
  prep()

#: lgb data object
X = bake(rec_lgbm, new_data = NULL, composition = "matrix", all_predictors())
lgbm_data =
  lgb.Dataset(
    data = X,
```

```
    colnames = colnames(X),
    categorical_feature = c("island", "sex"),
    label = bake(rec_lgbm, new_data = NULL, all_outcomes()) %>% pull()
  )

#: tuning parameters
lgbm_tuning = list(
  # settings
  objective = "multiclass",
  num_class = 3,
  # tuning parameters
  nrounds = 100,
  min_gain_to_split = 1,
  learning_rate = 0.1,
  max_depth = 2,
  bagging_freq = 1,        # enable subsampling
  bagging_fraction = 0.8, # subsample size
  bagging_seed = 123 # controls the internal sampling
)

#: fit model
lgbm = lightgbm(data = lgbm_data, params = lgbm_tuning, verbose = -1)

#: make predictions
predict(lgbm, X) %>% head()
#>         [,1]     [,2]     [,3]
#> [1,] 0.9979 0.001190 0.000868
#> [2,] 0.9973 0.001540 0.001123
#> [3,] 0.9972 0.001700 0.001123
#> [4,] 0.8176 0.015829 0.166561
#> [5,] 0.9976 0.001413 0.001031
#> [6,] 0.9979 0.001190 0.000868
```

5.3 Tidymodels

The `bonsai` and `xgboost` packages are necessary to use lightgbm and xgboost in `parsnip`.

```
library(tidymodels)
library(bonsai)  # for lightgbm
library(xgboost) # for xgboost
```

This defines the `parsnip` model specification for xgboost, modifies the recipe to leave the outcome as a factor, and adds it to a *workflow*.

```
#: pre-processing specs
rec_xgb = recipe(species ~ ., data = palmerpenguins::penguins) %>%
  # Handle missing data
  step_naomit(species) %>%  # remove cases with missing outcome label
  step_unknown(all_nominal_predictors()) %>% # add "unknown" level if missing
  # replace categorical/factors with numeric
  step_dummy(all_nominal_predictors(), one_hot = FALSE)

# Define the XGBoost model specification
xgb_spec = boost_tree(
  trees = 100,                    # nrounds
  tree_depth = 2,                 # Max depth of the trees
```

```
  learn_rate = 0.1,                # Learning rate
  loss_reduction = 1,              # Gamma (min_split_loss)
  sample_size = 0.8,               # Subsample ratio
  mode = "classification"          # For multi-class classification
) %>%
  set_engine("xgboost", objective = "multi:softprob", num_class = 3)

#: Create XGBoost workflow (combine recipe with model specification)
xgb_wf = workflow(preprocessor = rec_xgb, spec = xgb_spec)


# Fit the model
set.seed(1234)
xgb_fit = fit(xgb_wf, data = palmerpenguins::penguins)
#> Warning: ! The argument `num_class` is guarded by parsnip and will not be passed to
#>   `xgb.train()`.

# Make predictions on the training data
predict(xgb_fit, palmerpenguins::penguins, type = "prob") %>% head()
#> # A tibble: 6 x 3
#>   .pred_Adelie .pred_Chinstrap .pred_Gentoo
#>          <dbl>           <dbl>        <dbl>
#> 1        0.994         0.00311      0.00275
#> 2        0.994         0.00330      0.00292
#> 3        0.994         0.00330      0.00292
#> 4        0.540         0.0252       0.434
#> 5        0.994         0.00311      0.00275
#> 6        0.994         0.00311      0.00275
```

```
#: pre-processing specs
rec_lgbm = recipe(species ~ ., data = palmerpenguins::penguins) %>%
  # Handle missing data
  step_naomit(species) %>%  # remove cases with missing outcome label
  step_unknown(all_nominal_predictors()) # add "unknown" level if missing


# Define the lightgbm model specification
lgbm_spec = boost_tree(
  trees = 100,                     # nrounds
  tree_depth = 2,                  # Max depth of the trees
  learn_rate = 0.1,                # Learning rate
  loss_reduction = 1,              # min_gain_to_split
  sample_size = 0.8,               # Subsample ratio
  mode = "classification"          # For multi-class classification
) %>%
  set_engine("lightgbm", objective = "multiclass", num_class = 3, num_threads = 6) %>%
  set_args(
    bagging_seed = 123, # controls the internal sampling
  )

#: Create XGBoost workflow (combine recipe with model specification)
lgbm_wf = workflow(preprocessor = rec_lgbm, spec = lgbm_spec)


# Fit the model
lgbm_fit = fit(lgbm_wf, data = palmerpenguins::penguins)

# Make predictions on the training data
```

```
predict(lgbm_fit, palmerpenguins::penguins, type = "prob") %>% head()
#> # A tibble: 6 x 3
#>   .pred_Adelie .pred_Chinstrap .pred_Gentoo
#>          <dbl>           <dbl>        <dbl>
#> 1        0.998         0.00119     0.000868
#> 2        0.997         0.00154     0.00112
#> 3        0.997         0.00170     0.00112
#> 4        0.818         0.0158      0.167
#> 5        0.998         0.00141     0.00103
#> 6        0.998         0.00119     0.000868
```