

The assumption of **Linear Discriminant Analysis** (LDA) is not that the joint density function  $f(\mathbf{x})$  is linear in  $\mathbf{x}$ . Rather, LDA assumes that the conditional probability distribution of the independent variables  $\mathbf{X}$  given the category  $Y=k$  is multivariate normal, with a class-specific mean vector and a covariance matrix that is common to all  $K$  classes. The discriminant functions, which are derived from these densities, are linear in  $\mathbf{x}$ . This is where the "linear" in Linear Discriminant Analysis comes from. The discriminant function, not the density function, is linear in  $\mathbf{x}$ .

**Bootstrap dataset (size n)** is drawing from the original dataset  $n$  time with replacement.

**P-value Logistic Regression:** each coefficient represents the change in the log-odds of the dependent variable for a one-unit change in the predictor variable. The p-value for each coefficient tests the null hypothesis that the coefficient is equal to zero (no effect). A low p-value ( $< 0.05$ ) indicates that you can reject the null hypothesis. In the context given:

**LINEAR REGRESSION: Adding a variable transformation: AgeSquared = (Age)<sup>2</sup>**

It is possible for this new variable to improve the result. By default linear regression assumes a functional form that provides a linear mapping of independent variables to the dependent variable. If one suspects that the relationship between the independent variables and the dependent variable is more complex than a linear relationship, one can add new features which are a non-linear transformation of one or multiple of the existing features. Since these non-linear relations were not considered before with the original set of features, these new variables can improve the model.

\*Response variable  $Y$  is continuous      \* $R^2$  is for train, OSR2 is for test.

Categorical Variables in linear regression: **can only use dummy variable**. NO one-hot encoding

CART can use either dummy or on-hot encoding.

**A CART model** is more easily interpretable than a linear regression or logistic regression model

- \* Simple rules to determine a prediction
- \* Provides transparency to decision process
- \* Graphical display
- CART selects the significant variables for us.**

**CART can deliver nonlinear predictions**

- \* Difficult to capture "high but not too high" with linear regression (or logistic regression)
- \* CART creates its "partitions" based on simple rules (e.g. high GPA and moderate experience)

**\* How can we handle categorical features?:** \* Splitting requires considering all possible partitions of  $k$  categories into two groups \* The amount of computation is naively exponential in  $k$  but there are a few non-trivial tricks to improve this \* Implemented in part, but not in sklearn      \* sklearn requires manually creating dummy variables

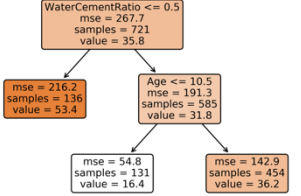
**\*What if our data has some missing values?:** \* This is a general problem in all of statistical learning \* It turns out that CART handles this problem relatively gracefully via the more advanced concept of surrogate splits

**LOSS: Loss = L<sub>FP</sub> + # False Positive + L<sub>FN</sub> + # False Negative**

In CART, if we want to modify the loss table then we need to **re-run the model**.

In **logistic regression**, we can tradeoff between false positive and false negative errors by changing the threshold but still **using the same model**.

**Setting the "Technical Parameters":** \* In linear and logistic regression, the model coefficients are computed to best fit the training data; \* **We could take the same approach with CART;** \* **Set the min\_samples\_leaf parameter to 1:** split data all the way down to a single observation in a bucket – ensures that each bucket would have no impurity; \* **Set the cp parameter to 0.0:** retain any split as long as it helps improve predictions; \* **This approach will overfit the training data;** \* **Instead**, try to optimize for the prediction error, using k-fold cross validation to estimate the prediction error with the training set



**IMPURITY Ccp\_alpha** is the pruning parameter. We prune the CART tree by removing splits that do not sufficiently improve the model fit. For regression trees, a split must reduce the total impurity by at least **ccp\_alpha** to remain. If we would like to produce a **tree with more splits, we would want to prune less**. To produce a tree with more splits we must set **lower ccp\_alpha** value.

**BASELINE/NULL**

**IMPURITY COST VALUE OF THE CURRENT TREE:**

**Solution:** We calculate the impurity of bucket  $m$  for CART regression trees using:  $Q_m(T) = \frac{1}{N_m} \sum_{i: x_i \in R_m} (y_i - \bar{y}_m)^2$ . We compute the total impurity cost of the tree by:  $C_{imp}(T) = \sum_{m=1}^{|T|} N_m Q_m(T)$ . Using these equations and the values from the CART tree we get:  $C_{imp}(T) = \sum_{m=1}^{|T|} N_m MSE_m = 136 * 216.2 + 131 * 54.8 + 454 * 142.9 = 101,458.6$

**Solution:** We will use our answers from the previous two parts:  
 $R^2 = 1 - \frac{SSE}{TSS} = 1 - \frac{C_{imp}(T)}{C_{imp}(T_{baseline})} = 1 - \frac{101,458.6}{193,011.7} = 0.474$

**CART: Adding a variable transformation: AgeSquared = (Age)<sup>2</sup>**

Unlike the case in the linear regression model, **this feature would NOT improve the CART regression tree model**. As Age is always a positive integer variable and  $f(x)=x^2$  is an increasing function in positive domain, **AgeSquared** would have the same split as Age. For example, a split Age  $\leq 10$  is equivalent to **AgeSquared  $\leq 100$** . So, the performance of our model remains same.

**Linear Regression: (multiple)** \* Predicts a continuous response variable – the dependent variable

\* Prediction is based on a set of independent variables

- \* The (true) regression coefficients  $\beta = (\beta_0, \beta_1, \dots, \beta_p)$  are unknown to us
- \* Recall the 2-norm of an  $n$ -vector  $\mathbf{z}$  is defined by:  
 $\|\mathbf{z}\|_2 = \sqrt{z_1^2 + z_2^2 + \dots + z_n^2}$

- \* How do we estimate the regression coefficients?
- \* Minimize prediction error, as measured by the residual sum of squares (RSS):

$$RSS(\beta) := \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \dots - \beta_p x_{ip})^2$$

**R SQUARED:  $R^2$**  is the coefficient of determination.  $R^2$  is a measure of the overall quality of the regression model  $R^2$  is a number between 0.0 and 1.0. A higher  $R^2$  means the regression model is a better fit to the (training) data.

- \* Using the representation  $RSS(\beta) = \|\mathbf{y} - \mathbf{X}\beta\|_2^2$  and assuming that  $\text{rank}(\mathbf{X}) = p + 1 < n$ , then one may use calculus/linear algebra to show that the solution of  $\min_{\beta} RSS(\beta)$  is given by:

$$\begin{aligned} \nabla RSS(\hat{\beta}) &= 0 \Leftrightarrow \\ -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\hat{\beta}) &= 0 \Leftrightarrow \\ 2\mathbf{X}^T\mathbf{X}\hat{\beta} &= 2\mathbf{X}^T\mathbf{y} \Leftrightarrow \\ \hat{\beta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \end{aligned}$$

**$R^2$  compares two models:**

\* 1) the regression model (the one determined by minimizing the RSS (residual sum of squares error), and 2) the "baseline" model. Think of the baseline model as a model you might have built using this data but without any real mathematical thinking.

\* Baseline model predicts simplistically using only the mean/average of the sample outcomes

$$R^2 = 1 - \frac{\text{Sum of squared residuals of regression model}}{\text{Sum of squared residuals of baseline model}}$$

$$= 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

$$= 1 - \frac{SSE}{SST}$$

$$SST = \sum_{i=1}^n (y_i - \bar{y})^2$$

\* We will see how to address this issue throughout the course, including today's lecture

\* Overfitting is related to the "bias-variance tradeoff"

\* Adjusted  $R^2$  is a simplistic way to account for the risk of overfitting for a linear reg. model

\* It is an adjustment to the training set  $R^2$  to account for "degrees of freedom".

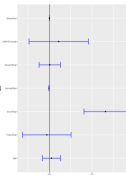
$$\begin{aligned} \text{Adjusted } R^2 &= 1 - \frac{\frac{1}{n-p-1} \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} \\ &= 1 - \frac{SSE}{SST} \cdot \frac{n-1}{n-p-1} \end{aligned}$$

estimated function changes when you slightly change the dataset \* More flexibility usually comes at the cost of higher variance \* The bias-variance tradeoff is a common theme in this course that we will continue discussing

### Testing the Significance of Regression Coefficients

$H_0: \beta_j = 0$  vs.  $H_a: \beta_j \neq 0$

- \* Hypothesis test is equivalent to looking at confidence intervals
- \* Reject null hypothesis as significance level  $\alpha$  if and only if  $(1-\alpha)\%$  confidence interval does not contain 0



- \* Under the previous set of assumptions, it is possible to prove mathematically that:

1.)  $\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$  is an unbiased estimator of the true vector of coefficients  $\beta$ :

$$\mathbb{E}[\hat{\beta} | \mathbf{X}] = \beta$$

2.) The covariance matrix of  $\hat{\beta}$  given  $\mathbf{X}$  is:

$$\text{cov}(\hat{\beta} | \mathbf{X}) = \sigma^2 (\mathbf{X}^T\mathbf{X})^{-1}$$

3.)  $\hat{\beta}$  is a normally distributed random vector given  $\mathbf{X}$

\* Question: What's the problem?

\* Answer: we usually don't know  $\sigma^2$  and must estimate that from the data in order to construct the matrix  $\text{cov}(\hat{\beta} | \mathbf{X}) = \sigma^2 (\mathbf{X}^T\mathbf{X})^{-1}$

\* Letting  $\mathbf{e} = \mathbf{y} - \mathbf{X}\hat{\beta}$  denote the vector of training set residuals, then use the estimate:

$$\hat{\sigma}^2 = \frac{\|\mathbf{e}\|_2^2}{n-p-1} = \frac{1}{n-p-1} \sum_{i=1}^n e_i^2$$

- \* Makes the estimated coefficients very sensitive to noise in the training data
- \* can produce very inaccurate estimates hurting interpretability and predictive performance
- \* **Tell-tale signs:** \* Some of the estimated coefficients have the "wrong" sign.
- \* Some of the coefficients are not significantly different from zero.
- \* **Multicollinearity** can usually be fixed by deleting one or more independent variable

Multicollinearity can exist without evidence of large correlations in the correlation table.  
\* **Rule of thumb:** \*  $VIF > 10$ : definitely a problem  
\*  $VIF > 5$ : could be a problem  
\*  $VIF \leq 5$ : probably okay \* **VIF: Greater than 10**, remove. It is a sign of multicollinearity.

**Regression vs. Classification**

\* Two important classes of supervised learning problem \* Regression involves predicting a continuous response variable \* The value of a household \* The logarithm of the auction price of a vintage wine \* Classification involves predicting a binary yes/no outcome \* Did the user click on the ad or not? \* Overarching themes but different methods for each

**Prediction for the  $i^{\text{th}}$  observation:**

$$\hat{y}_i := \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \dots + \hat{\beta}_p x_{ip}$$

**Residuals:**  $e_i = y_i - \hat{y}_i$

**RSS with respect to the estimated coefficients:**

$$RSS = SSE = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

\* SSE is the sum of squared errors (both conventions often used)

**OSR2 is an assessment of the real-world**

performance of the model we have built  
\* It should only be computed once, at the end of your analysis, as a final metric  
\* If OSR2 is significantly smaller than  $R^2$  (on the training data), this is an indicator of potential overfitting  
**Overfitting is more likely when:**  
\* The number of parameters to be estimated is large \* Data is limited \* Care must be taken to make sure that the model we estimate does not suffer from overfitting

**Bias and Variance of Learning Methods**

\* Bias refers to the error that is introduced by modeling a complicated relationship with a simple one \* Less flexible methods have more bias. \* Variance refers to the amount that our

1.) The observed data  $(x_i, y_i) \quad i = 1, \dots, n$  satisfies  
 $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} + \epsilon_i$

where  $\beta = (\beta_0, \beta_1, \dots, \beta_p)$  are the true but unknown regression coefficients and the  $\epsilon_i$  are noise terms

- 2.)  $\epsilon_1, \epsilon_2, \dots, \epsilon_n$  are independent and identically distributed **normal** random variables with mean 0 and variance  $\sigma^2$
- 3.) If the features  $x_1, x_2, \dots, x_n$  are also regarded as random variables, then they are independent of  $\epsilon_1, \epsilon_2, \dots, \epsilon_n$

\* Given the formula  $\text{cov}(\hat{\beta} | \mathbf{X}) = \sigma^2 (\mathbf{X}^T\mathbf{X})^{-1}$ , we can read off the diagonal entries of this matrix to get the standard errors for each coefficient

\* Given that  $\hat{\beta}$  is normally distributed, we can now easily construct confidence intervals in the usual way, i.e., for some z-score (such as  $z^* = 1.96$ ):

$$\hat{\beta}_j \pm z^* \sqrt{\text{cov}(\hat{\beta} | \mathbf{X})_{jj}}$$

**OUT-OF-SAMPLE**

It is important to understand the assumptions that lead to the results of your analysis (e.g., which variables you retain in your model)  
\* Ultimately though – regardless of whether you believe or doubt that the assumptions hold for your dataset – it is critical to validate your final model on an out of sample testing set  
**Multicollinearity** \* Occurs when two or more predictors are highly correlated

### What is VIF?

\* Consider regressing each predictor variable  $X_j$  on all of the others:

$$X_j = \alpha_0 + \alpha_1 X_1 + \dots + \alpha_{j-1} X_{j-1} + \alpha_{j+1} X_{j+1} + \dots + \alpha_p X_p$$

\* If the  $R^2$  for the above (call it  $R_j^2$ ) is equal to 1, then there exists a perfect linear relationship between  $X_j$  and all other independent variables (at least according to the training data)

\* So, define:  $VIF_j = \frac{1}{1 - R_j^2}$

### Interpreting the Coefficients Using Odds, cont.

$$\text{Odds}(Y = 1) = \frac{\Pr(Y = 1)}{1 - \Pr(Y = 1)}$$

\* The logistic regression model is naturally expressed using odds:

$$\log(\text{Odds}(Y = 1|X)) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$

Logistic Regression

- \* Logistic Regression is a classification method
  - \* The dependent variable is modeled as a Bernoulli random variable (think success or failure):  $Y = 0$  or  $Y = 1$  \*  $Y = 1$  if "success" – default on loan \*  $Y = 0$  if "failure" – not default on loan
  - \* We seek to predict the probability of a success outcome of the dependent variable  $Y$ :
  - \* Predict probability that the loan defaults, namely  $\Pr(Y=1)$
  - \* Probability of success is a particular function of the independent variables  $X_1, X_2, \dots, X_p$ .
- \* logistic regression model gives us predicted probability values that don't always represent the true probability of the corresponding event.

Interpreting Positive Coefficients

- \*Inquiries in last 6 months has positive coefficient (Beta=0.1171)
- \* Higher value of the variable will result in a higher value of the probability
- \* Lower value of the variable will result in a lower value of the probability
- \* Consider the probability of default for applicants with different number of inquiries

Interpreting Negative Coefficients

- \* log(Annual Income) has negative coefficient (Beta = -0.8537)
- \* Higher variable values yield lower probability estimates
- \* Lower variable values yield higher probability estimates
- \* Consider estimated default risk for applicants with different annual incomes but all other variables as in the earlier slide

Change in Outputted Probability is NOT Linear

- \* A change in a variable does not yield a linear change in the probability outputted by the model.
- \* This makes it challenging to communicate the precise meaning of a model coefficient (unlike the situation in linear regression).

Bayes Optimal Classifier

Given the classifier  $\hat{h}$  trained on the data, we would naturally like to know its error rate:  $R(\hat{h}) = \Pr(Y \neq \hat{h}(X))$

- \* In practice, we estimate the error rate using test data
- \* In theory, note that the Bayes optimal classifier gives us a lower bound:  $R(\hat{h}) \geq R(h^*)$
- \* the error rate of the Bayes optimal classifier is the irreducible error that can never do better
- \* the difference  $R(\hat{h}) - R(h^*)$  is the reducible error in a classification problem.

**Two sources of reducible error:**

- \* Approximation error (a.k.a. bias), which relates to how well the learning method approximates the Bayes optimal classifier  $h^*$
- \* Estimation error (a.k.a. variance), which relates to the error due to the fact that the training data only provides partial information about the distribution  $P_{X,Y}$

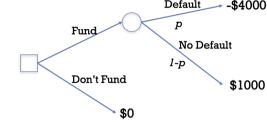
Consider a binary classification problem where  $L_{FP} > 0$  and  $L_{FN} > 0$   $L_{TP} = L_{TN} = 0$

- Given  $p = \Pr(Y = 1 | X = x)$ , derive a threshold  $q$  so that it is optimal to predict that  $Y = 1$  if and only if  $p \geq q$

$$\begin{aligned} EL[\hat{Y} = 1|X] &= L_{FP} * p_{Y=1} \\ EL[\hat{Y} = 0|X] &= L_{FN} * p_{Y=0} = L_{FN} * (1 - p) \\ L_{FP} * p_{Y=1} &= L_{FN} * (1 - p) \Rightarrow p = \frac{L_{FP}}{L_{FP} + L_{FN}} \end{aligned}$$

Recall the Simple Lending Decision Tree

- If borrower defaults (probability  $p$ ), the lender loses \$4000
- If borrower does not default (probability  $1-p$ ), the lender makes \$1000



Predictions with a Loss Table

Model		
	Predict Y = 0	Predict Y = 1
Reality Y = 0	$L_{TN}$	$L_{FN}$
Reality Y = 1	$L_{FP}$	$L_{TP}$

- Answer: make a prediction by comparing the expected loss of each option
- Expected Loss (EL) of Predicting  $Y = 0$  is:

$$\begin{aligned} EL(0|x) &= L_{TN} \cdot \Pr(Y = 0|x) + L_{FN} \cdot \Pr(Y = 1|x) \\ &= L_{TN} \cdot (1 - f(x)) + L_{FN} \cdot f(x) \end{aligned} \quad \begin{aligned} EL(1|x) &= L_{FP} \cdot \Pr(Y = 0|x) + L_{TP} \cdot \Pr(Y = 1|x) \\ &= L_{FP} \cdot (1 - f(x)) + L_{TP} \cdot f(x) \end{aligned}$$

Predictions with a Loss Table, cont.

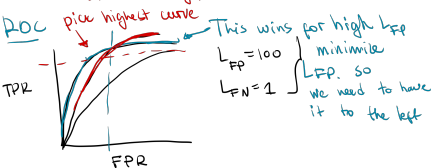
Model		
	Predict Y = 0	Predict Y = 1
Reality Y = 0	$L_{TN}$	$L_{FN}$
Reality Y = 1	$L_{FP}$	$L_{TP}$

- Given perfect knowledge of  $f(x) = \Pr(Y = 1|X = x)$  the optimal strategy is to choose the option with smaller expected loss (ties broken arbitrarily)

$$h^*(x) = \begin{cases} 1 & \text{if } EL(1|x) \leq EL(0|x) \\ 0 & \text{if } EL(1|x) > EL(0|x) \end{cases}$$

- $h^*$  defined above is called the "Bayes decision rule"

to minimize  $L_{FN}$ , we maximize TPR in the case  $L_{FN} = 100$  (high)  $L_{FP} = 1$



Accuracy

- **Accuracy:** the proportion of loans that we correctly classified
- Loans that did not default classified as Good Risk
- Loans that did default classified as Bad Risk

$$Accuracy = \frac{Number\ Correct}{Number\ Total} = \frac{1865 + 178}{1865 + 178 + 534 + 278} = 0.716$$

Model		
	Good Risk $\Pr(Y = 1) < 0.2$	Bad Risk $\Pr(Y = 1) > 0.2$
Reality No Default (Y = 0)	1865	534
Default (Y = 1)	278	178

False Positive Rate (FPR)

- **False Positive Rate (FPR):** the proportion of non-defaulting loans ( $Y_i = 0$ ) incorrectly identified as bad risks ( $\Pr(Y_i = 1) > 0.2$ )
- Synonyms you may hear: 1-specificity or fall-out

$$False\ Positive\ Rate\ (FPR) = \frac{False\ Positives}{All\ Negatives} = \frac{534}{534 + 1865} = 0.223$$

Model		
	Good Risk $\Pr(Y = 1) < 0.2$	Bad Risk $\Pr(Y = 1) > 0.2$
Reality No Default (Y = 0)	1865	534
Default (Y = 1)	278	178

Interpreting the AUC

- \* Interpretation: given a randomly selected positive observation (customer who churned) and a randomly selected negative observation (customer who did not churn), AUC is the likelihood that the model would correctly differentiate which is which.
- \* That is, it is the likelihood that the model would assign a higher churn probability to the customer who churned
- \* AUC measures the model's discriminative ability
- \* LDA is popular for multiclass classification – when there are more than 2 response categories
- \* LDA is more "stable" in certain situations

**Validation Set Approach:**

- Step 1:** Split into 3 sets – training, validation, and test;
- Step 2:** Build a sequence of models using the training data (for example, using different  $c_p$  values in CART);
- Step 3:** Evaluate each model's performance (e.g. R2, accuracy, TPR, FPR, ...) on the validation set;
- Step 4:** Pick the best model and use the test set to estimate future real-world performance of the model;

**k-fold Cross-Validation method:**

- For  $max\_features = 1, 2, \dots, 18$ :
- Do cross-validation with the current value of  $max\_features$
- Record the averaged cross-validated R2 (over the 5 folds) using the current  $max\_features$  value
- Then set the  $max\_features$  value to be that value that yielded the highest R2 value
- \* Looking at R2 is equivalent to looking at RMSE

**Interpreting Random Forest Models:**

- \* Random forests consist of hundreds of large CART trees, so interpreting models is much more difficult than for the models
- \* Some interpretability of the relative importance of variables is possible through variable importance measures
- \* For numeric/regression outcomes, we look at the improvement in the sum of squared errors from splitting with the variable, averaged across all trees
- \* Provides an ordering of variables by importance (even though the actual values cannot be readily interpreted)

**BOOSTING:** The key idea of boosting is to intelligently combine a bunch of "weak" models

- \* Each model is a very shallow tree (for example, 1, 2, or 3 splits only)
- \* But the models are combined adaptively – each model is designed to perform well on parts of the data that the previous models do not perform as well on

- Boosting produces trees  $f_1, f_2, \dots, f_B$  sequentially
- Tree  $\hat{f}_k$  is designed in such a way that it performs well on the parts of the data that trees  $f_1, f_2, \dots, f_{k-1}$  perform weakest on
- The final model is a rescaled average of the trees:
  - $\lambda$  is called the shrinkage parameter

How do we take this analysis and "back out" a prediction for our original dependent variable  $Y$ ?

$$\begin{aligned} R_1 &= Y - \hat{f}_1(X) \\ R_2 &= R_1 - \hat{f}_2(X) \\ R_3 &= R_2 - \hat{f}_3(X) \\ R_4 &= R_3 - \hat{f}_4(X) \end{aligned}$$

Hence, a prediction for  $Y$  is given by:

$$\hat{Y} = \sum_{i=1}^4 \hat{f}_i(X)$$

AdaBoost \*It is not clear

how to extend the concept of "residuals" for classification problems

- \* Again, trees are added to the model in a sequential way whereby the next tree performs well on parts of the data that are poorly explained by the current model
- \* AdaBoost uses reweighted versions of the training data to achieve this.

**Boosting vs. Random Forests**

- \* How does boosting compare to random forests?
- \* Contrast the adaptive design of trees in boosting with random forests' completely independent construction of trees
- \* forests' trees are strong (i.e., deep), so each tree fits the data well and they are averaged to reduce variance
- \* Boosting's trees are weak (i.e., shallow), so each tree has low variance, but they are added together in such a way that the overall model fits the data progressively better

Comparison of Models Seen so Far

	Linear Regression	Logistic Regression	LDA	CART	Random Forests	Boosting
Captures non-linear structure				✓	✓	✓
Simple and interpretable	✓	✓	✓	✓		
Best out-of-sample prediction quality				✓	✓	✓
Can be used for binary classification problems		✓	✓	✓	✓	✓
Can be used for multiclass classification problems			✓	✓	✓	✓
Can be used to predict continuous outcomes	✓			✓	✓	✓