

# GBUS 738 Data Mining

## Logistic Regression

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# Multiple Linear Regression

## Advertising Data Analysis – Putting It All Together

Is there a relationship between sales revenue and advertising budget?

We can answer this question by fitting a multiple linear regression of **Sales** using TV, Radio, and Newspaper as predictor variables and testing the following hypothesis:

$$H_0: \beta_1 = \beta_2 = \beta_3 = 0 \text{ vs } H_a: \text{At least one } \beta_j \text{ is non-zero}$$

From the output on the right, we have an F statistic of **570.3** with a highly significant p-value.

This provides strong evidence **against** the null hypothesis, and we conclude that Sales revenue is associated with **at least one advertising type**.

$$\text{Sales} = \beta_0 + \beta_1 \text{TV} + \beta_2 \text{Radio} + \beta_3 \text{Newspaper}$$

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	2.938889	0.311908	9.422	<2e-16	***
TV	0.045765	0.001395	32.809	<2e-16	***
Radio	0.188530	0.008611	21.893	<2e-16	***
Newspaper	-0.001037	0.005871	-0.177	0.86	

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Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.686 on 196 degrees of freedom  
Multiple R-squared: 0.8972, Adjusted R-squared: 0.8956  
F-statistic: 570.3 on 3 and 196 DF, p-value: < 2.2e-16

# Multiple Linear Regression

## Advertising Data Analysis – Putting It All Together

Which advertising media contribute to sales revenue?

To answer this question, we must examine the **partial F-test results** in the summary output. We find that the coefficient of Newspaper is not statistically significant. This corresponds to the following hypothesis:

$$H_0: \beta_3 = 0 \text{ vs } H_a: \beta_3 \neq 0$$

**Interpretation:** given that I am using TV and Radio as predictors, Newspaper does not provide increased accuracy to the multiple linear regression model. This suggests that TV and Radio are the primary drivers of Sales revenue

$$\text{Sales} = \beta_0 + \beta_1 \text{TV} + \beta_2 \text{Radio} + \beta_3 \text{Newspaper}$$

Coefficients:

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# Multiple Linear Regression

## Advertising Data Analysis – Putting It All Together

### How large is the effect of each advertising type on Sales revenue?

The estimated coefficients associated with TV and Radio advertising budgets are:

0.045 and 0.19 [remember that all units in the Advertising data set are in **thousands**]

**Interpretation:** For a \$1,000 increase in TV advertising budget, we estimate that the increase in **average** Sales revenue will be **\$45 for a fixed budget of Radio**

For a \$1,000 increase in Radio advertising budget, we estimate that the increase in **average** Sales revenue will be **\$190, for a fixed budget of TV**

Overall, the effect of Radio advertising on average Sales is nearly **5 times greater** than that of TV advertising

$$\text{Sales} = \beta_0 + \beta_1 \text{TV} + \beta_2 \text{Radio}$$

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	2.92110	0.29449	9.919	<2e-16	***
TV	0.04575	0.00139	32.909	<2e-16	***
Radio	0.18799	0.00804	23.382	<2e-16	***

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Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.681 on 197 degrees of freedom  
Multiple R-squared: 0.8972, Adjusted R-squared: 0.8962

# Multiple Linear Regression

## Advertising Data Analysis – Putting It All Together

*How strong is the relationship between sales revenue and advertising budgets for TV and Radio?*

$$Sales = \beta_0 + \beta_1 TV + \beta_2 Radio$$

The  $R^2$  of the multiple linear regression on the right is **0.90** when rounded to 2 decimal places

**Interpretation:** TV and Radio advertising budgets explain approximately 90% of the total variance in Sales revenue, indicating a strong relationship between Sales revenue and advertising budgets

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )	
(Intercept)	2.92110	0.29449	9.919	<2e-16	***
TV	0.04575	0.00139	32.909	<2e-16	***
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# Multiple Linear Regression

## Advertising Data Analysis – Putting It All Together

$$\text{Sales} = \beta_0 + \beta_1 \text{TV} + \beta_2 \text{Radio}$$

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Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

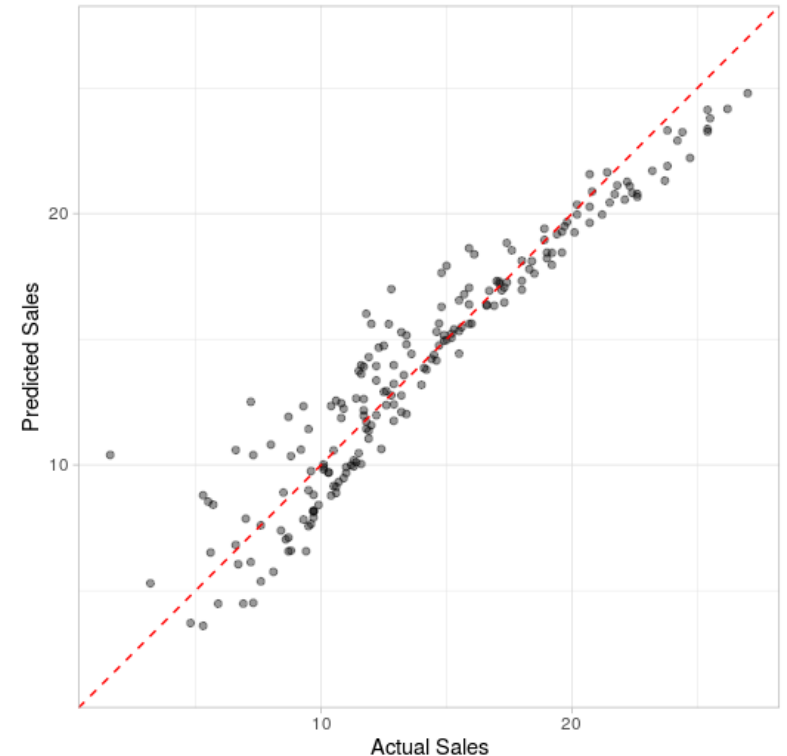
Residual standard error: 1.681 on 197 degrees of freedom  
Multiple R-squared: 0.8972, Adjusted R-squared: 0.8962

### How accurately can we predict future Sales revenue?

The residual standard error (RSE) for this model is 1.681. As a proportion of the average Sales revenue in the data (14.02), the RSE represents approximately 12%.

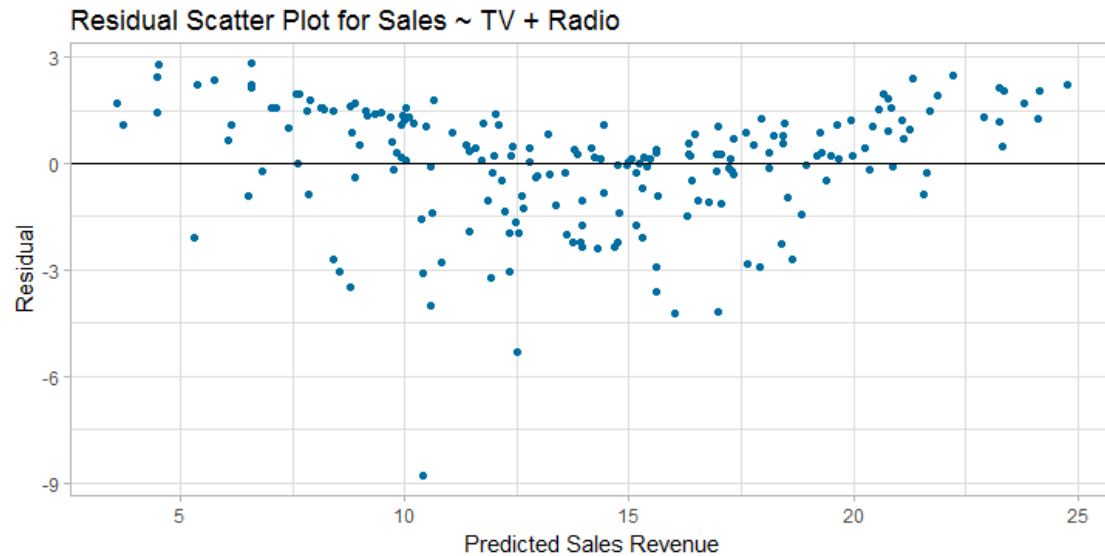
**Interpretation:** Roughly speaking, we can expect 12% prediction error, on average. We also note from the visualization of  $R^2$  that the highest prediction accuracy occurs for Sales values between approximately \$14,000 and \$22,000

Actual Sales vs Predicted



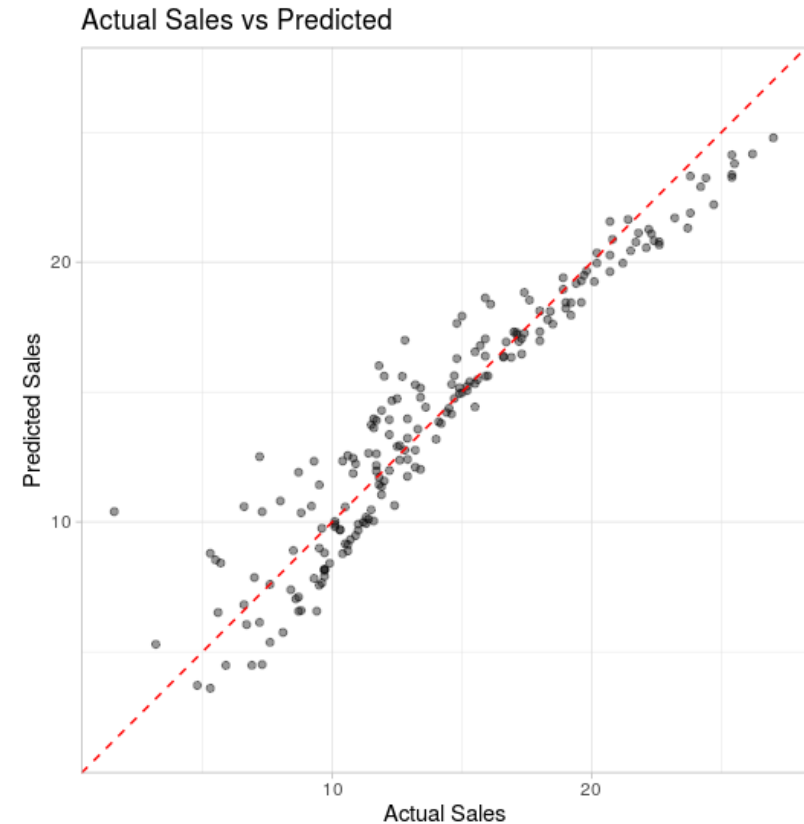
# Multiple Linear Regression

## Advertising Data Analysis – Putting It All Together



*Is the relationship between average Sales revenue and advertising budgets linear?*

We see a slight *non-linear* relationship in both the residual plot and the  $R^2$  visualization of predicted Sales versus actual Sales. The non-linearity mainly occurs at the lower and upper bounds of Sales revenue. However, the model provides a reasonable approximation that is easy to interpret



# Machine Learning Methods

## Supervised Learning - Classification

### Classification

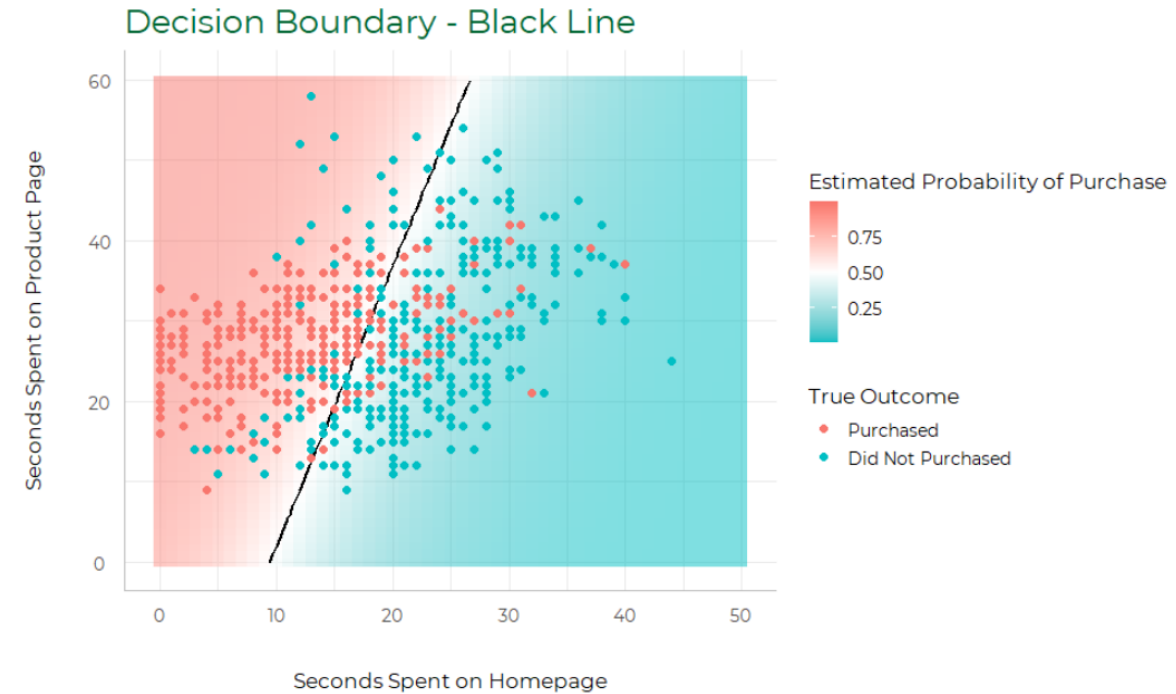
Supervised learning methods used to predict **categorical** response variables

#### Example

- Predict whether a customer will purchase a product based on the seconds they have spent browsing a company's homepage and product page

Outcome	Predictors	
Outcome	Seconds Homepage	Seconds Product Page
Did Not Purchase	4	30
Purchased	32	43
Did Not Purchase	2	22
Purchased	24	36

Segmenting the predictor values into distinct, non-overlapping regions to predict a category





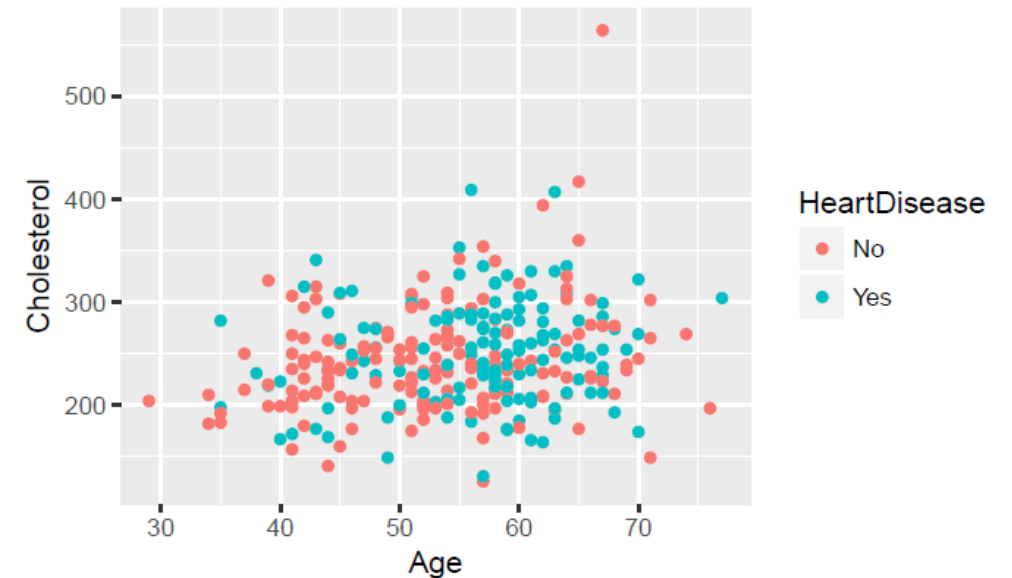
# Classification

## Predicting Categorical Outcomes

An example of classification would include predicting whether a patient will develop heart disease (Yes/No) using the Heart Disease data set on the right

- There are many classification techniques, or *classifiers*, that can be used to predict categorical outcome variables
- This lecture will focus on *logistic regression*
  - Logistic regression is used to predict **dichotomous** outcome variables – these are categorical variables with two levels
  - The *heart\_disease* variable on the right is dichotomous

heart_disease	age	chest_pain	resting_bp	cholesterol
No	63	typical	145	233
Yes	67	asymptomatic	160	286
Yes	67	asymptomatic	120	229
No	37	nonanginal	130	250
No	41	nontypical	130	204



# Logistic Regression

## The Bernoulli Distribution

A Bernoulli random variable can be used to model the probabilistic behavior of dichotomous outcomes

- A common example would be tossing a fair coin

### Positive class

- Event of interest to predict
- “Yes” in *heart\_disease* outcome

### Negative class

- Remaining class
- “No”

The Bernoulli distribution is indexed by a parameter  $p$ , which represents the probability that the outcome variable will be the **positive class**

# Logistic Regression

## The Logistic Regression Setting

In *logistic regression*, we are predicting a **dichotomous outcome variable Y**

- We map the event of interest to the **Positive** class
- “Yes” in the *heart\_disease* variable

We assume that each individual observation of Y follows a **Bernoulli distribution**

Given predictor variables  $X_1, X_2, \dots, X_p$ , we assume that

$$E(Y_i | X_1 = x_1, \dots, X_p = x_p) = p_i$$

heart_disease	age	chest_pain	resting_bp	cholesterol
No	63	typical	145	233
Yes	67	asymptomatic	160	286
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# Logistic Regression

## The Logistic Regression Setting

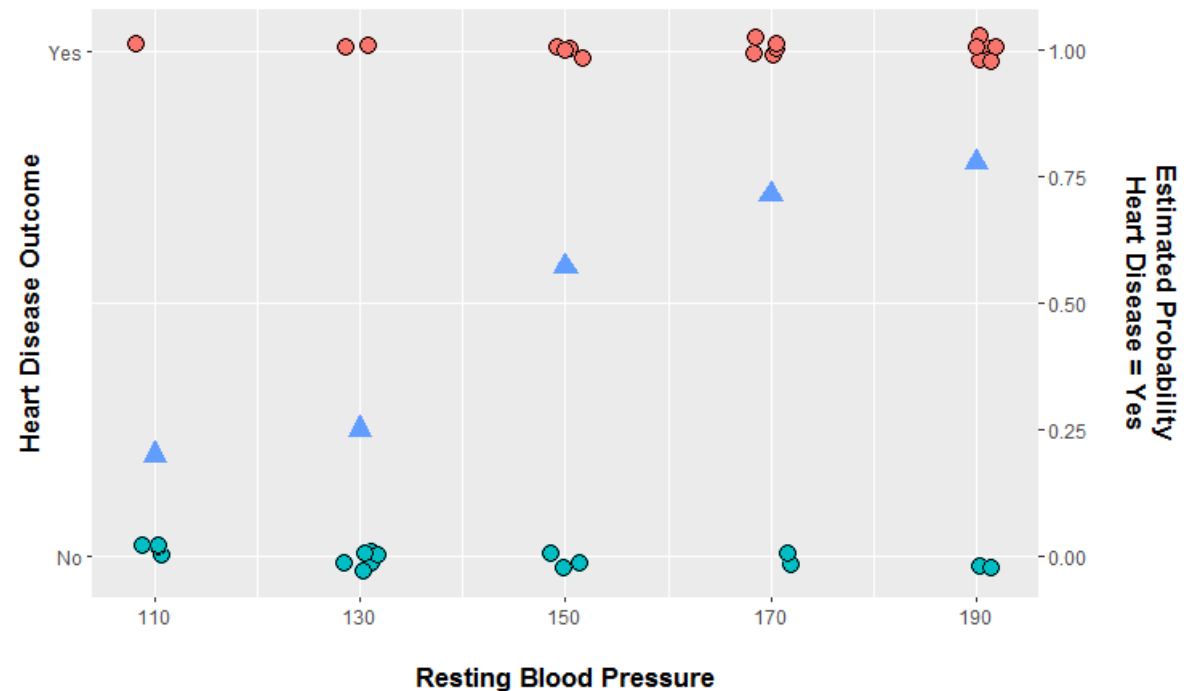
$$E(Y_i | X_1 = x_1, \dots, X_p = x_p) = p_i$$

In most textbooks, the above is denoted as  $p(x)$  and represents the probability of the positive class given the values of the predictor variable(s)

In *logistic regression*, we are modeling the relationship between  $p(x)$  and the predictor variable values

*We are interested in estimating  $p(x)$  as a continuous function of the predictor variable values*

Resting Blood Pressure	Heart Disease Yes	Heart Disease No	Estimated Probability of (Heart Disease = Yes)
110	1	4	0.20
130	2	6	0.25
150	4	3	0.57
170	5	2	0.71
190	7	2	0.78



# Logistic Regression

## Why not linear regression?

How should we estimate  $p(x)$ ?

For the case of one predictor variable  $X$ , why not use linear regression? This would be represented by the following model

$$E(Y|X = x) = p(x) = \beta_0 + \beta_1 x + \varepsilon$$

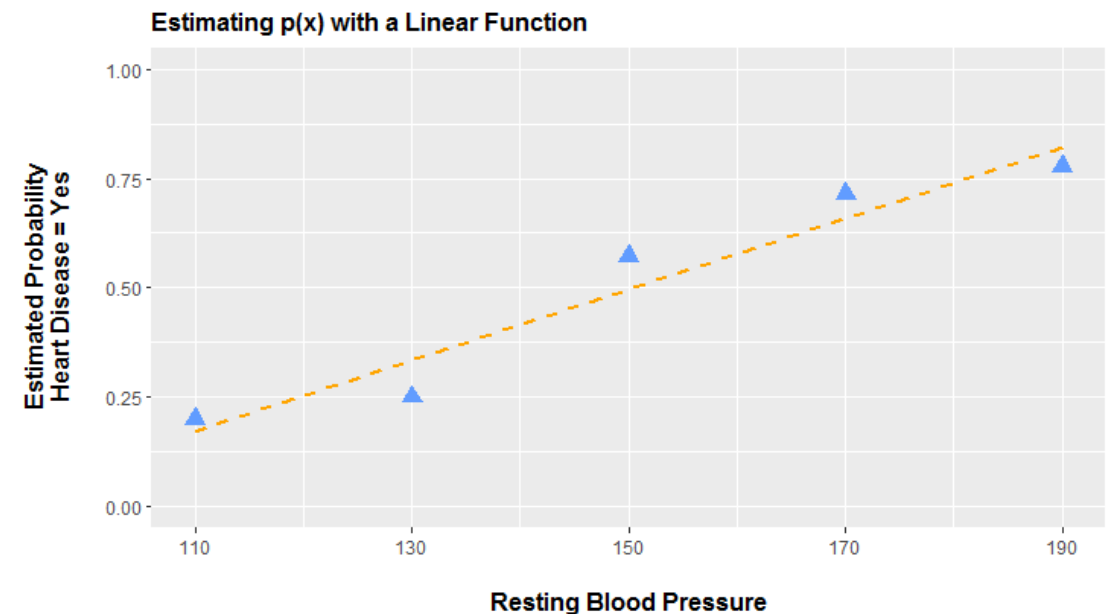
For our example on the right, this gives us an estimated regression line of

$$p(x) = -0.71 + 0.008(\text{Resting Blood Pressure})$$

### Problems with this model

- For resting blood pressure of 70, the estimated probability that a patient will develop heart disease is **-0.15**
- In linear regression the  $\varepsilon$  are assumed to have the same common variance, but by the properties of the Bernoulli distribution make this impossible

Resting Blood Pressure	Heart Disease Yes	Heart Disease No	Estimated Probability of (Heart Disease = Yes)
110	1	4	0.20
130	2	6	0.25
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190	7	2	0.78



# Logistic Regression

## The logistic function

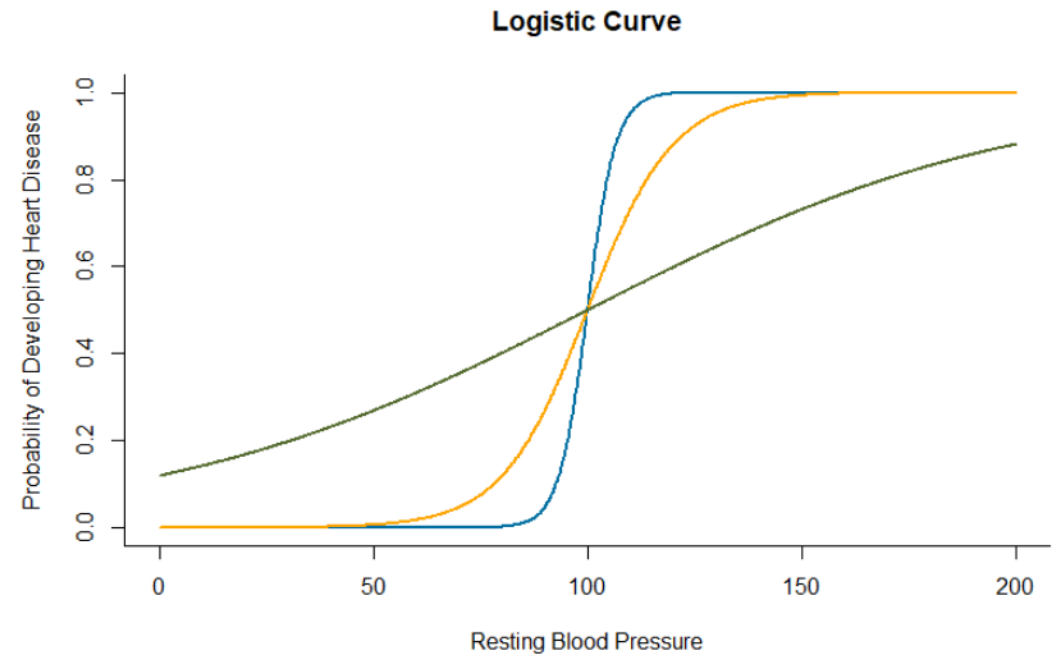
To avoid the problems we encountered on the previous slide, we must model  $p(x)$  using a function that gives outputs between 0 and 1

In logistic regression, we use the **logistic function**. For the case of one predictor variable  $X$ , the logistic function takes the form below

$$p(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

Three logistic curves are plotted to the right, using various values of  $\beta_0$  and  $\beta_1$

Estimating  $p(x) = P(Y = \textit{positive class} | X = x)$  with the logistic function is a good choice since the logistic curve can take various shapes, from almost linear to extremely “S” shaped



# Logistic Regression

## The *logit* Transformation

$p(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$  is not a linear function of the predictor variable  $X$

However, using a **logit transformation**, we can transform both sides of the equation to get a linear function of the predictor variable  $X$

$$\begin{aligned} \text{logit}(p(x)) &= \log\left(\frac{p(x)}{1 - p(x)}\right) = \log\left(\frac{\frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}}{1 - \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}}\right) = \log\left(\frac{\frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}}{\frac{1 + e^{-(\beta_0 + \beta_1 x)} - 1}{1 + e^{-(\beta_0 + \beta_1 x)}}}\right) \\ &= \log\left(\frac{\frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}}{\frac{e^{-(\beta_0 + \beta_1 x)}}{1 + e^{-(\beta_0 + \beta_1 x)}}}\right) = \log\left(\frac{1}{e^{-(\beta_0 + \beta_1 x)}}\right) = \log(e^{(\beta_0 + \beta_1 x)}) = \beta_0 + \beta_1 x \end{aligned}$$

# Logistic Regression

## The *logit* Transformation

Once we have our estimated coefficients, we can obtain an estimated probability for the **positive** class for any predictor value,  $\mathbf{x}$ , with:

$$p(\mathbf{x}) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 \mathbf{x})}}$$

How do we predict the outcome categories?

- If our estimated probability for a given  $\mathbf{x}$  is **greater than or equal to 0.5**
  - We predict the **positive** class
  - Negative class otherwise



# Logistic Regression

## Modeling Process

heart_disease	resting_bp
No	127
Yes	145
Yes	135
No	130
No	135
No	90
Yes	130

Estimated  
Parameters



$$\beta_0 = -33.94$$

$$\beta_1 = 0.25$$

Logit (resting_bp)
-2.19
2.31
-0.19
-1.44
-0.19
-11.44
-1.44

Logistic Function



$$\frac{1}{1 + e^{-(-33.94 + 0.25x)}}$$

Probability of Positive Class "Yes"
0.10
0.91
0.45
0.19
0.45
0.0
0.19

Threshold



0.5

Predicted Heart Disease
No
Yes
No
No
No
No
No

# Logistic Regression

## Multiple Logistic Regression

The logistic regression model can easily be extended to incorporate multiple predictor variables

Just like in the multiple regression setting, predictors can be quantitative or categorical

In this case

$$p(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p)}}$$

and

$$\text{logit}(p(x)) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$

# Confusion Matrix

## Evaluating Prediction Accuracy

A **confusion matrix** can be created for any classifier that is used to predict a dichotomous outcome variable

The positive class is associated with the level of the outcome variable representing our event of interest

In the heart disease data set, a positive (+) is associated with the “Yes” outcome for the *heart\_disease* variable

		Truth		Row Total
		+	-	
Predicted	+	TP	FP	P*
	-	FN	TN	N*
Column Total		P	N	

### Key Performance Measures:

Metric	Meaning
True Positive (TP)	Predicted Positive – Truth is Positive
True Negative (TN)	Predicted Negative – Truth is Negative
False Positive (FP)	Predicted Positive – Truth is Negative
False Negative (FN)	Predicted Negative – Truth is Positive

# Confusion Matrix

## An Example Using the Heart Disease Data Set

```
conf_mat(test_results, truth = heart_disease, estimate = .pred_class)
```

```
      Truth
Prediction yes no
yes      26  9
no       8 32
```

### Interpretation

Overall, 58 patients (77%) were correctly classified. We predicted that 8 patients would not develop heart disease when in fact they did develop heart disease (*false negative*).

		Truth		Row Total
		+	-	
Predicted	+	26	9	35
	-	8	32	40
Column Total		34	41	

# Performance Metrics

## Sensitivity (Recall)

### Sensitivity

- Proportion of actual positive cases that were correctly classified
- Also called **recall**
- Values near 1 are optimal

Of patients who **did** develop heart disease, what proportion did our model predict correctly?

		Truth	
		Positive (+)	Negative (-)
Predicted	Positive (+)	TP	FP
	Negative (-)	FN	TN

$$\frac{TP}{TP + FN}$$

# Performance Metrics

## Specificity

### Specificity

- Proportion of actual negative cases that were correctly classified
- Values near 1 are optimal

Of patients who **did not** develop heart disease, what proportion did our model predict correctly?

### 1 – Specificity

- False positive rate (FPR)
- Proportion of false positives among true negatives

		Truth	
		Positive (+)	Negative (-)
Predicted	Positive (+)	TP	FP
	Negative (-)	FN	TN

$$\frac{TN}{TN + FP}$$

# Performance Metrics

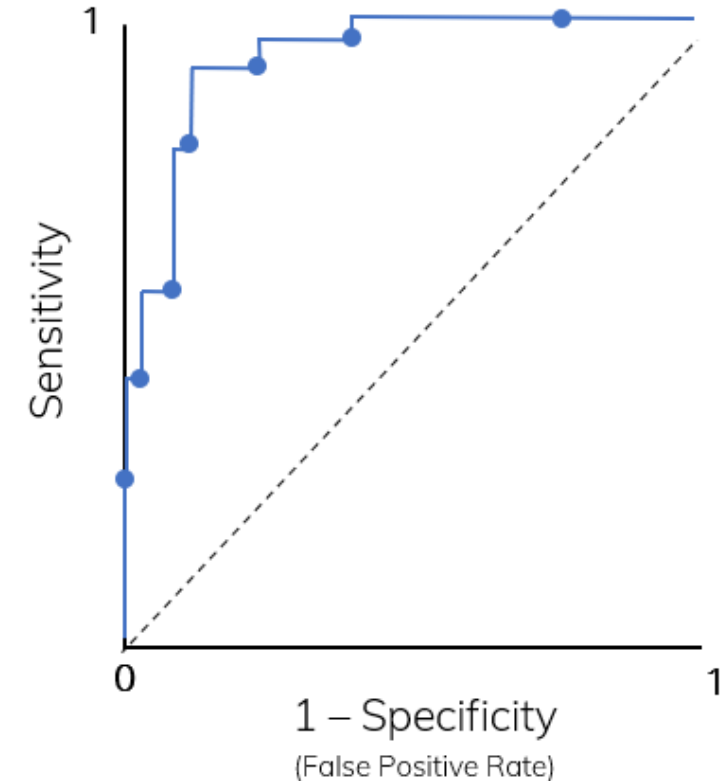
## ROC Curves and Area Under the ROC Curve

ROC curve plots the **sensitivity** vs (**1 – specificity**) for all possible probability cut-off values.

- The default probability cut-off value used by classification models is 0.5
  - Changing this can guard against either false positives or false negatives. The ROC curve plots all this information in one plot

### What to look for

- The best ROC curve is as close as possible to the point (0, 1) that is at the top left corner of the plot. The closer the ROC curve is to that point throughout the entire range, the better the classification model



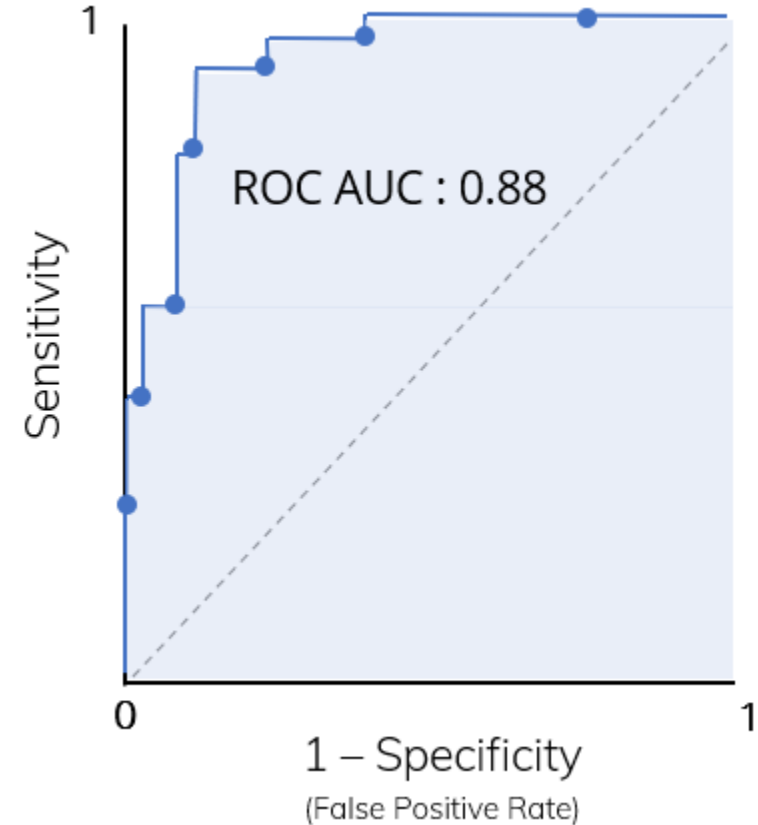
# Performance Metrics

## ROC Curves and Area Under the ROC Curve

### Area Under the ROC Curve (AUC)

Another common performance metric. Can be interpreted as a letter grade for model performance:

- $0.9 - 1 = A$
- $0.8 - 0.89 = B$
- $0.7 - 0.79 = C$
- $0.6 - 0.69 = D$
- Below  $0.6 = F$





# Performance Metrics

## Precision

### Precision

- Proportion of **predicted** positive cases that were correctly classified
- Values near 1 are optimal

Of patients who **were predicted to develop heart disease**, what proportion did our model predict correctly?

		Truth	
		Positive (+)	Negative (-)
Predicted	Positive (+)	TP	FP
	Negative (-)	FN	TN

$$\frac{TP}{TP + FP}$$

# Performance Metrics

F1 Score – a single measure of performance

Instead of having to look at both false positive and false negative rates, the  $F_1$  score combines both metrics into one overall score

- The  $F_1$  score gives **equal weight** to precision and recall
  - Precision – function of false positives
  - Recall (Sensitivity) – function of false negatives
- The  $F_1$  score ranges from 0 (worst) to 1 (best)

## Precision

$$\frac{TP}{TP + FP} = \frac{26}{26+9} = 0.74$$

## Recall

$$\frac{TP}{TP + FN} = \frac{26}{26+8} = 0.76$$

## $F_1$ Score

$$2 \left( \frac{PR}{P+R} \right) = 2 * \frac{(0.74)(0.76)}{0.74 + 0.76} = 0.75$$

		Truth		Row Total
		+	-	
Predicted	+	26	9	35
	-	8	32	40
Column Total		34	41	