Week 2

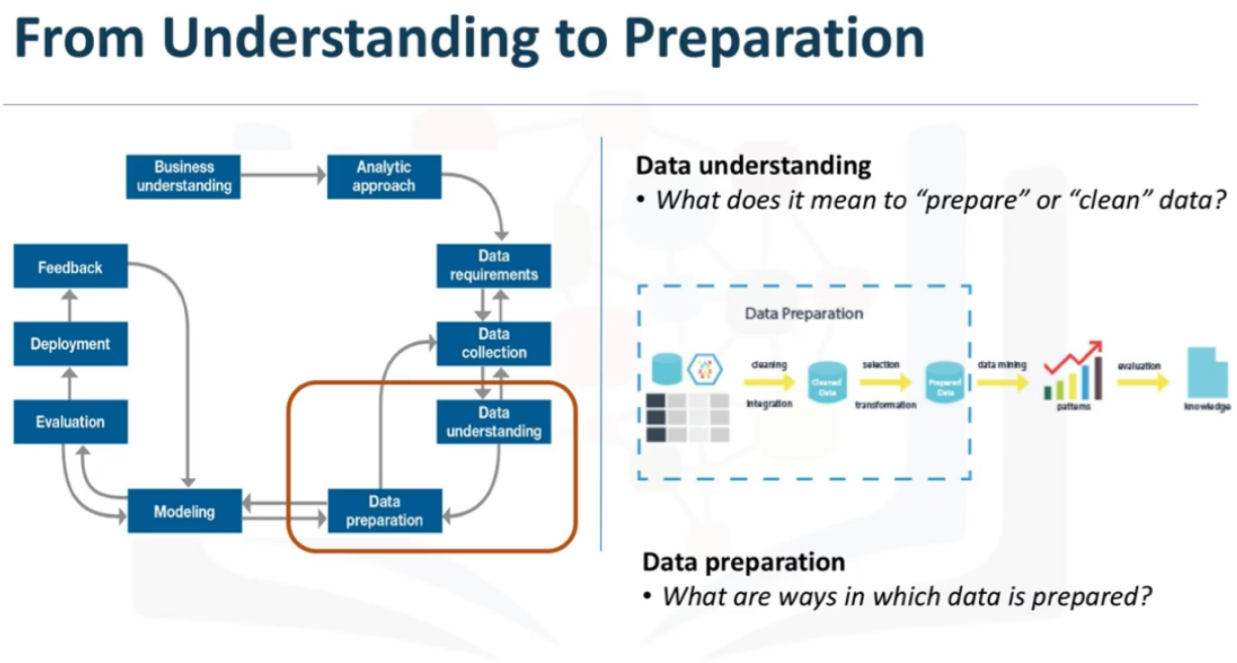
#Data Science/3 - Data Science Methodology#

From Understanding to Preparation

Data Understanding

Data understanding encompasses all activities related to constructing the data set. Essentially, the **data understanding** section of the data science methodology **answers the question**:

- Is the data that you collected representative of the problem to be solved?



Let's apply the data understanding stage of our methodology, to the case study we've been examining. In order **to understand the data** related to congestive heart failure admissions, **descriptive statistics needed** to be run against the data columns that would become variables in the model.

Case Study – Understanding the data

- Descriptive statistics
  - Univariate statistics
  - Pairwise correlations
  - Histogram

$$f(a) + \sum_{k=1}^{n} \frac{1}{k!} \frac{d^k}{dt^k}\Big|_{t=0} f(u(t)) + \int_0^1 \frac{(1-t)^n}{n!} \frac{d^{n+1}}{dt^{n+1}} f(u(t))\, dt.$$

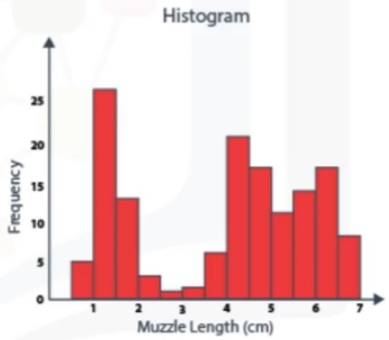
$F_{X,Y}(x, y)$ satisfies

$$F_{X,Y}(x, y) = F_X(x) F_Y(y),$$

or equivalently, their joint density $f_{X,Y}(x, y)$ satisfies

$$f_{X,Y}(x, y) = f_X(x) f_Y(y).$$

Histograms are a good way to understand how values or a variable are distributed, and what sorts of data preparation may be needed to make the variable more useful in a model.



- First, these statistics included Hearst, univariates, and statistics on each variable, such as mean, median, minimum, maximum, and standard deviation.
- Second, pairwise correlations were used, to see how closely certain variables were related, and which ones, if any, were very highly correlated, meaning that they would be essentially redundant, thus making only one relevant for modeling.
- Third, histograms of the variables were examined to understand their distributions.

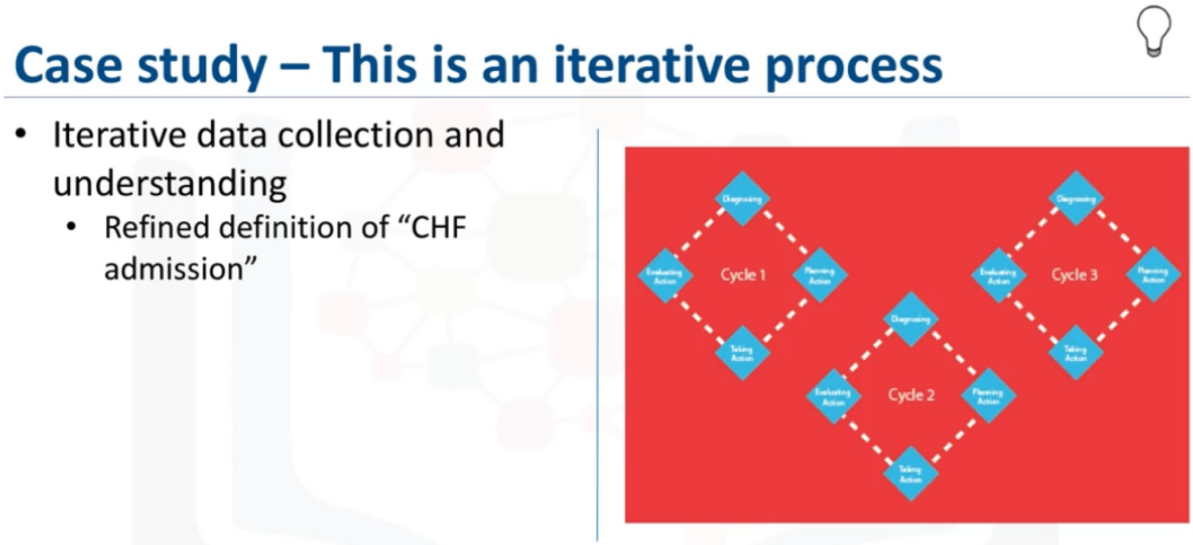
Histograms are a good way to understand how values or a variable are distributed, and which sorts of data preparation may be needed to make the variable more useful in a model. For example, for a categorical variable that has too many distinct values to be informative in a model, the histogram would help them decide how to consolidate those values.

Case study – Looking at data quality

- Data quality
  - Missing values
  - Invalid or misleading values

The univariates, statistics, and histograms are also used to assess data quality. From the information provided, certain values can be re-coded or perhaps even dropped if necessary,

such as when a certain **variable has missing values**.
The question then becomes, **does "missing" mean anything**? Sometimes a missing value might mean "no", or "0" (zero), or at other times it simply means "we don't know". Or, if a variable contains invalid or misleading values, such as a numeric variable called "age" that contains 0 to 100 and also 999, where that "triple-9" actually means "missing", but would be treated as a valid value unless we corrected it.



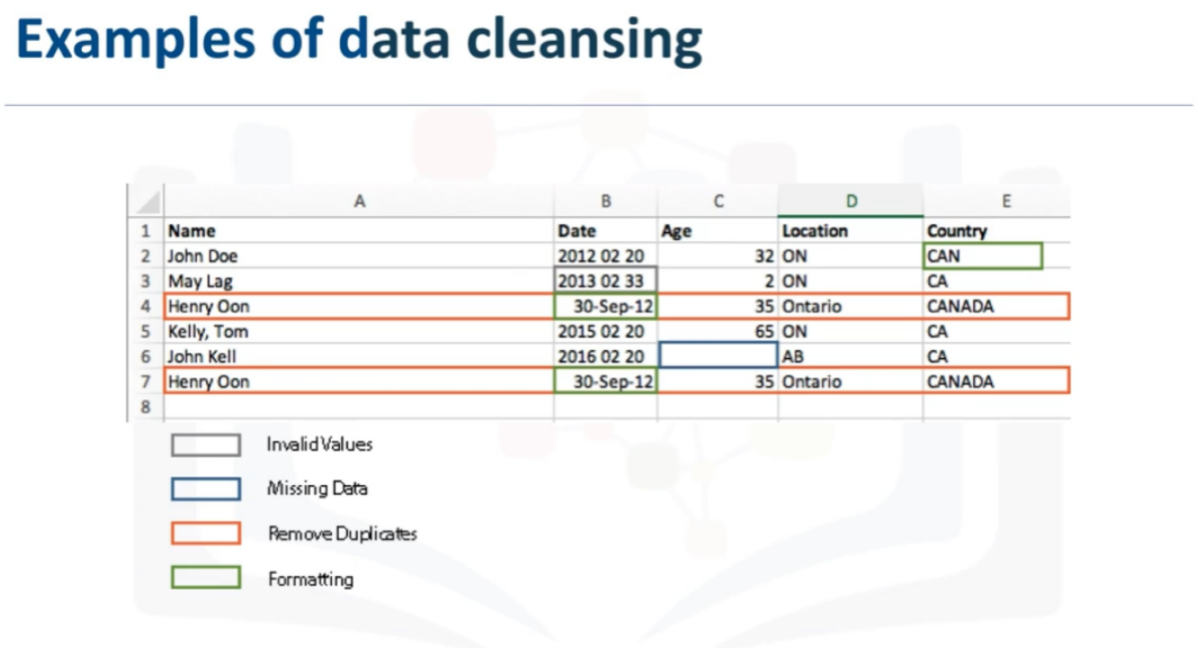
Initially, the meaning of congestive heart failure admission was decided on the basis of a primary diagnosis of congestive heart failure. But working through the data understanding stage revealed that the initial definition was not capturing all of the congestive heart failure admissions that were expected, based on clinical experience. This meant **looping back** to the data collection stage and adding secondary and tertiary diagnoses, and building a more comprehensive definition of congestive heart failure admission.
This is just one example of the interactive processes in the methodology. The more one works with the problem and the data, the more one learns and therefore the more refinement that can be done within the model, ultimately leading to a better solution to the problem.

Data Preparation - Concepts

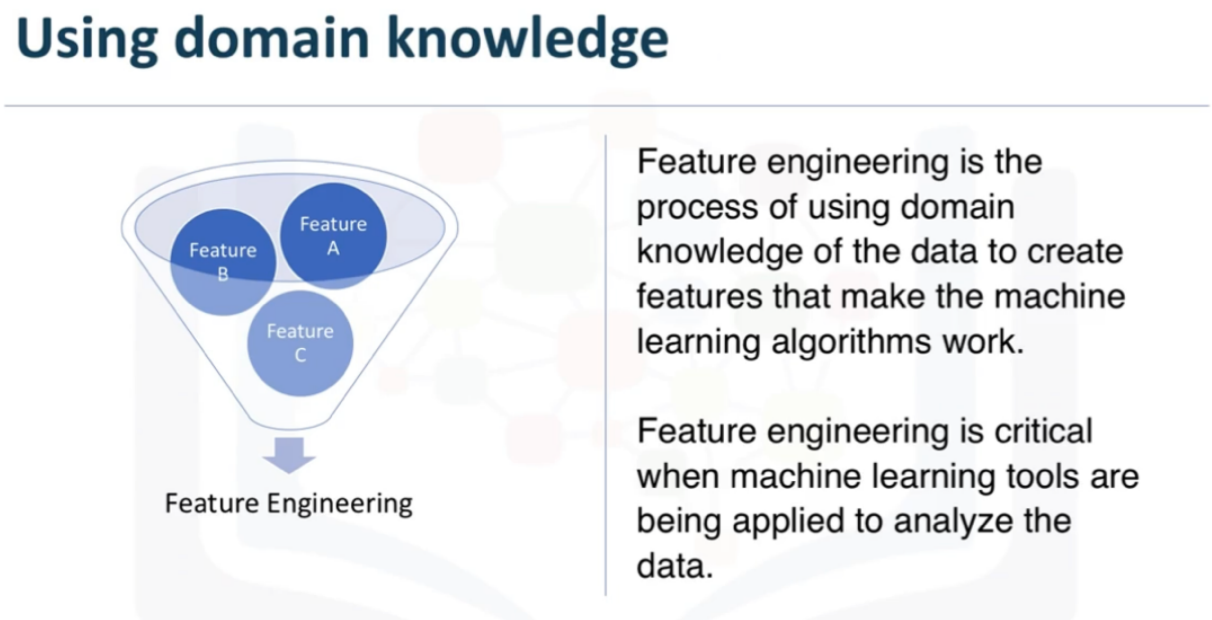
In a sense, data preparation is similar to washing freshly picked vegetables in so far as unwanted elements, such as dirt or imperfections, are removed. Together with data collection and data understanding, **data preparation is the most time-consuming phase of a data science project**, typically taking seventy percent and even up to even ninety percent of the overall project time. Automating some of the data collection and preparation processes in the database, can reduce this time to as little as 50 percent. This time savings translates into increased time for data scientists to focus on creating models.
To continue with our cooking metaphor, we know that the process of chopping onions to a finer state will allow for its flavours to spread through a sauce more easily than that would be the case

if we were to drop the whole onion into the sauce pot. Similarly, transforming data in the **data preparation phase is the process of getting the data into a state where it may be easier to work with**. Specifically, the data preparation stage of the methodology answers the question:

- What are the ways in which data is prepared?

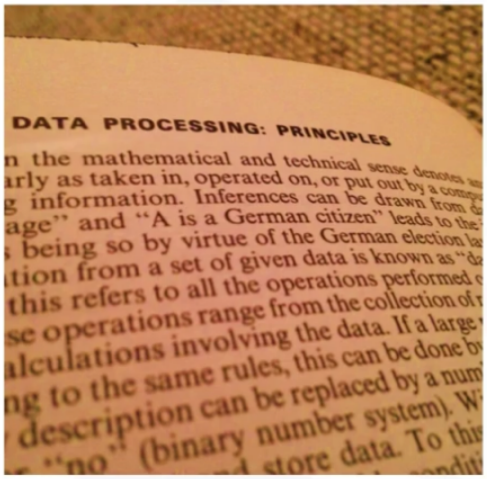


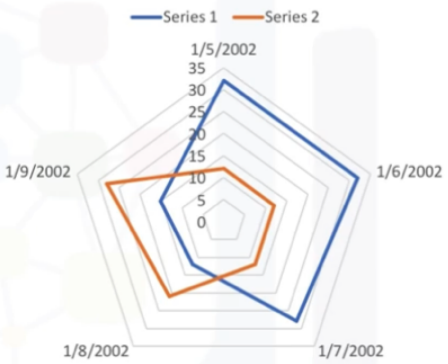
To work effectively with the **data**, it **must be prepared in a way that addresses missing or invalid values and removes duplicates**, toward ensuring that everything is properly formatted.



Feature engineering is also part of data preparation. It is the process of using domain knowledge of the data to create features that make the machine learning algorithms work. A **feature is a characteristic that might help when solving a problem**. Features within the data **are important to predictive models and will influence the results you want to achieve**. Feature engineering is critical when machine learning tools are being applied to analyze the data.

Working with text analysis





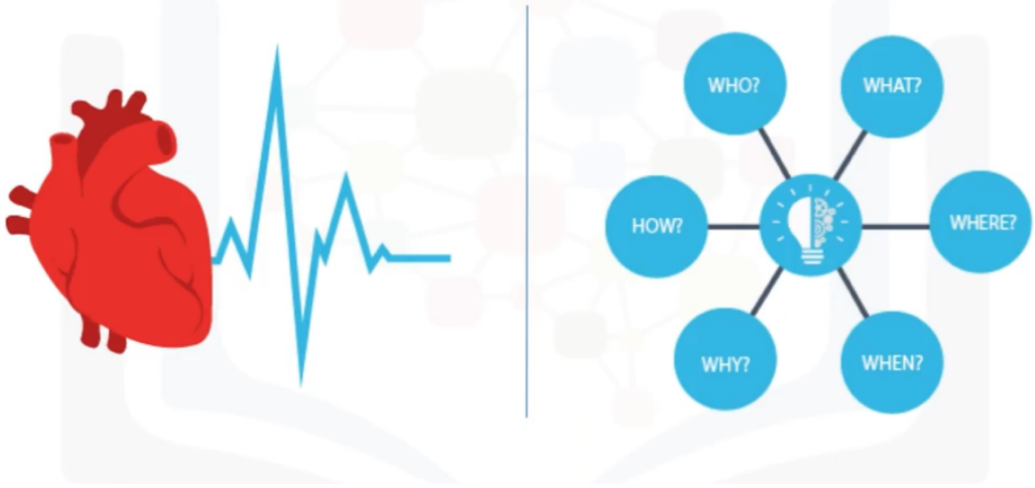
When working with text, text analysis steps for coding the data are required to be able to manipulate the data. The data scientist needs to know what they're looking for within their dataset to address the question. The text analysis is critical to ensure that the proper groupings are set, and that the programming is not overlooking what is hidden within.

The data preparation phase sets the stage for the next steps in addressing the question. While this phase may take a while to do, if done right the results will support the project. If this is skipped over, then the outcome will not be up to par and may have you back at the drawing board. **It is vital to take your time in this area, and use the tools available to automate common steps to accelerate data preparation**. Make sure to pay attention to the detail in this area. After all, it takes just one bad ingredient to ruin a fine meal.

Data Preparation - Case Study

In a sense, data preparation is similar to washing freshly picked vegetables insofar as unwanted elements, such as dirt or imperfections, are removed. So now, let's look at the case study related to applying Data Preparation concepts.

Case Study – Data preparation



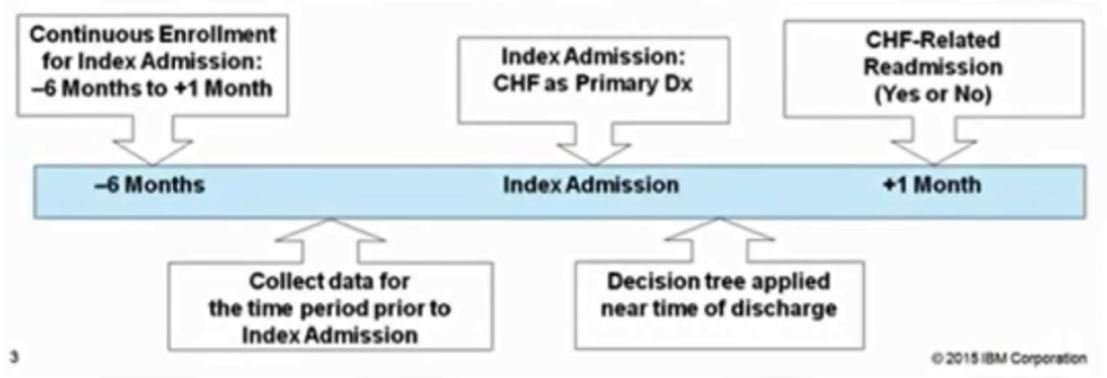
In the case study, an important **first step** in the data preparation stage was to actually **define congestive heart failure**. This sounded easy at first but defining it precisely, was not straightforward. First, the set of diagnosis-related group codes needed to be identified, as congestive heart failure implies certain kinds of fluid buildup. We also needed to consider that congestive heart failure is only one type of heart failure. **Clinical guidance was needed** to get the right codes for congestive heart failure.

Case Study – Defining readmission

The next step involved defining the re-admission criteria for the same condition. The timing of events needed to be evaluated in order to define whether a particular congestive heart failure admission was an initial event, which is called an index admission, or a congestive heart failure-related re-admission. Based on clinical expertise, a time period of 30 days was set as the window for readmission relevant for congestive heart failure patients, following the discharge from the initial admission.

Case Study – Defining CHF admission

Define “CFF admission” and “CHF readmission”



Next, the records that were in transactional format were aggregated, meaning that the data included multiple records for each patient.

Case Study – Aggregating records

Transactional records

- Claims: professional provider, facility, pharmaceutical
- Inpatient & outpatient records: diagnoses, procedures, prescriptions, etc.
- Possibly thousands per patient, depending on clinical history

Transactional records included professional provider facility claims submitted for physician, laboratory, hospital, and clinical services. Also included were records describing all the diagnoses, procedures, prescriptions, and other information about in-patients and out-patients. A given patient could easily have hundreds or even thousands of these records, depending on their clinical history.

Case Study – Aggregating to patient level

Aggregate to patient level

- Roll up to 1 record per patient
- Create new columns representing the transaction
  - Outpatients visits/ Inpatient episodes: frequency, recency, diagnoses/length of stay, procedures, prescriptions
  - Comorbidities with CHF

Then, all the transactional records were aggregated to the patient level, yielding a single record for each patient, as required for the decision-tree classification method that would be used for modeling. As part of the aggregation process, many new columns were created representing the information in the transactions. For example, frequency and most recent visits to doctors, clinics and hospitals with diagnoses, procedures, prescriptions, and so forth. Co-morbidities with congestive heart failure were also considered, such as diabetes, hypertension, and many other diseases and chronic conditions that could impact the risk of re-admission for congestive heart failure.

Case Study – More or less data needed?

Literature review of important factors for CHF readmission

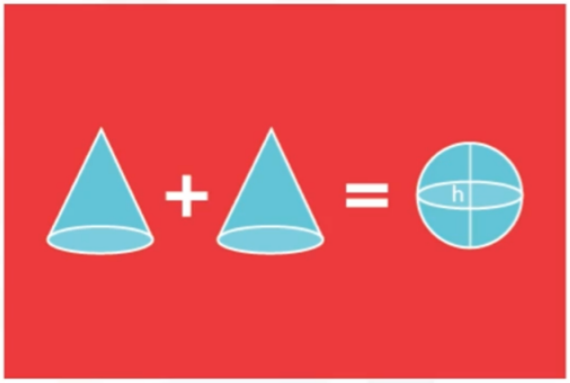
MORE LIKELY TO BE READMITTED

- Medicare / Medicaid insurance holders
- Comorbid conditions including:
  - Ischemic heart disease
  - Idiopathic Cardiomyopathy
  - Prior Cardiac surgery
  - Peripheral vascular disease
  - Diabetes mellitus
  - Anemia

LESS LIKELY TO BE READMITTED

- Patients treated at rural hospitals
- Patients discharged to skilled nursing facilities
- Patients receiving echocardiograms or cardiac catheterization

- Loop back to data collection stage and add additional data, if needed



During discussions around data preparation, a literary review on congestive heart failure was also undertaken to see whether any important data elements were overlooked, such as co-morbidities that had not yet been accounted for. The literary review involved looping back to the data collection stage to add a few more indicators for conditions and procedures.

Case Study – Completing the data set

Merge all data into one table

- One record per patient
- List of variables used in modeling
  - Target: CHF readmission with 30 days (Yes/No), following discharge from CHF hospitalization

Aggregating the transactional data at the patient level, meant merging it with the other patient data, including their demographic information, such as age, gender, type of insurance, and so forth. T**he result was the creation of one table containing a single record per patient, with many columns representing the attributes about the patient in his or her clinical history**. These columns would be used as variables in the predictive modeling.

Case Study – Creating new variables

Merge all data into one table

- One record per patient
- List of variables used in modeling

– Target

CHF readmission with 30 days (Yes/No), following discharge from CHF hospitalization

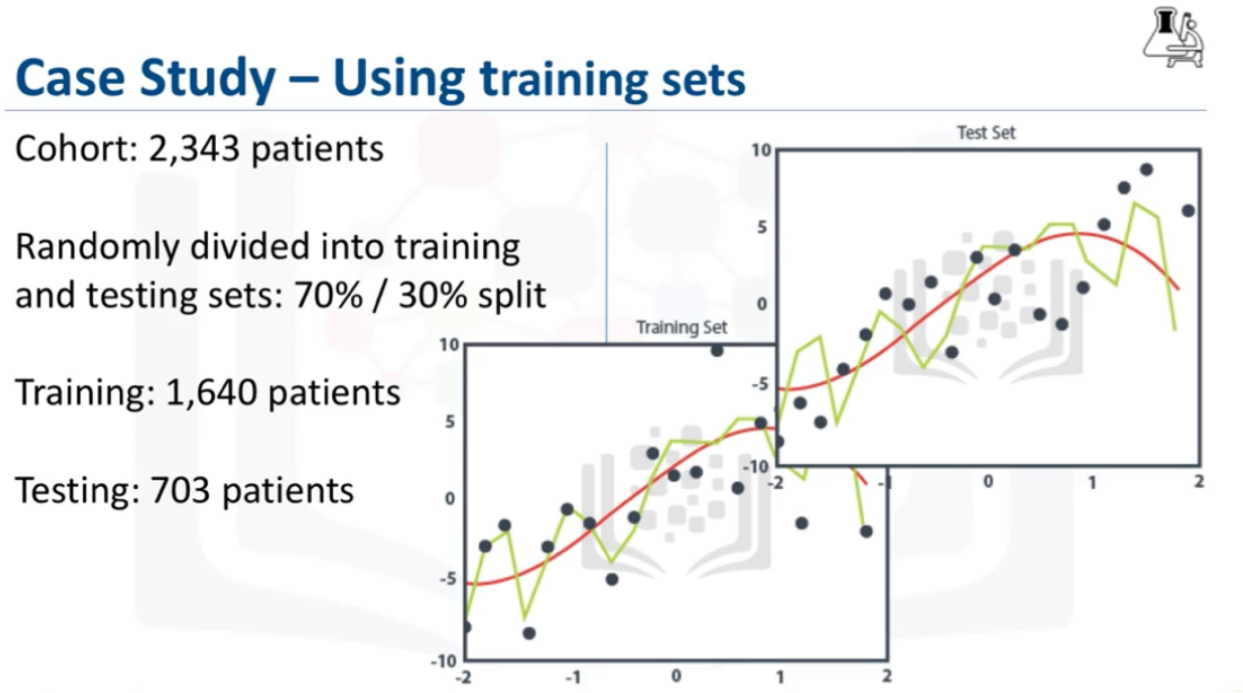
– Measures

Gender	Length of stay	CHF Diagnosis importance
Age	Prior admissions	(primary, secondary, tertiary)
Primary DRG	Line of business	

– Diagnosis flags (Y/N)

CHF	Atrial fibrillation	Pneumonia
Diabetes	Renal failure	Hypertension

Here is a list of the variables that were ultimately used in building the model. The dependent variable, or target, was congestive heart failure readmission within 30 days following discharge from a hospitalization for congestive heart failure, with an outcome of either yes or no.



The data preparation stage resulted in a cohort of 2,343 patients meeting all of the criteria for this case study. The cohort was then split into training and testing sets for building and validating the model, respectively.

From Modeling to Evaluation

Modeling - Concepts

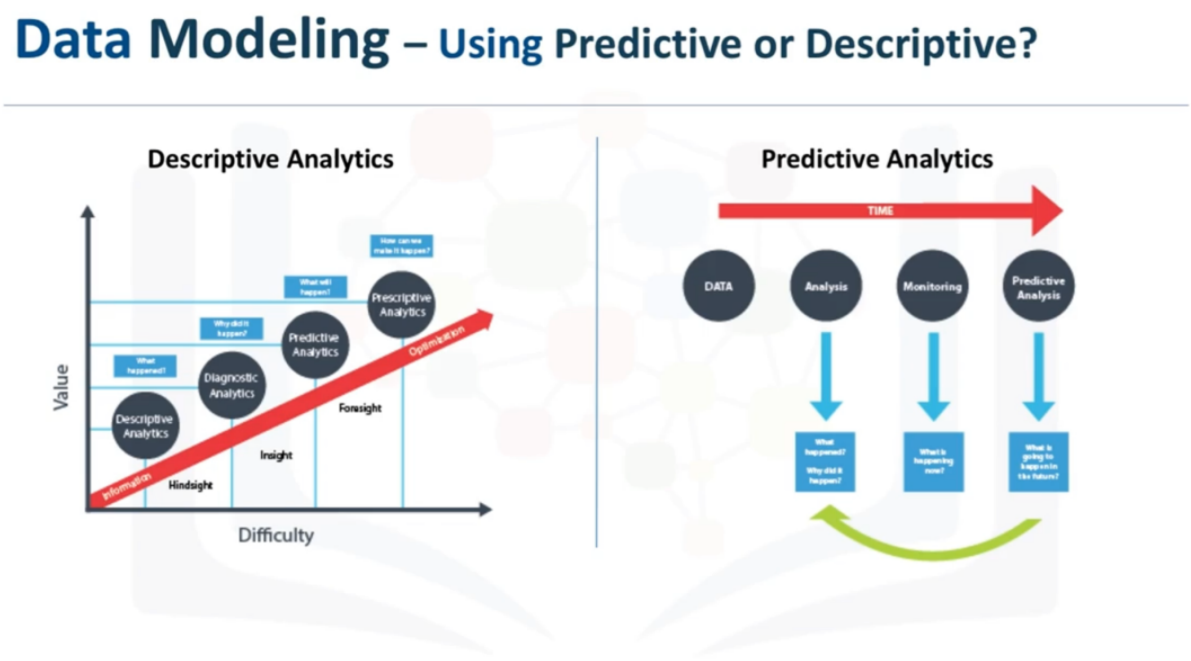
Modelling is the stage in the data science methodology, **where the data scientist has the chance to sample the sauce and determine**, if it's bang on or in need of more seasoning! This portion of the course is geared toward answering two key questions:

- First, what is the purpose of data modeling?
- second, what are some characteristics of this process?

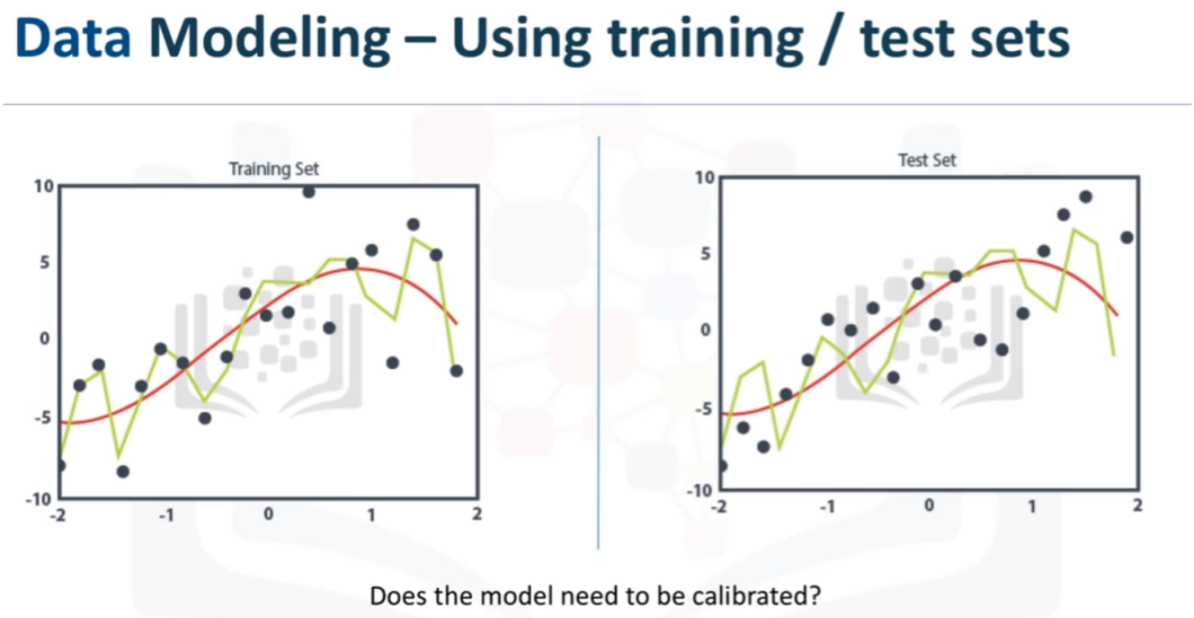
Data Modelling focuses on **developing models that are either descriptive or predictive**. An example of a descriptive model might examine things like:

- if a person did this, then they're likely to prefer that.

A **predictive model** tries to **yield yes/no**, or **stop/go** type outcomes. These models are based on the analytic approach that was taken, either statistically driven or machine learning driven.



The data scientist will use a training set for predictive modelling. A training set is a set of historical data in which the outcomes are already known. The training set acts like a gauge to determine if the model needs to be calibrated.



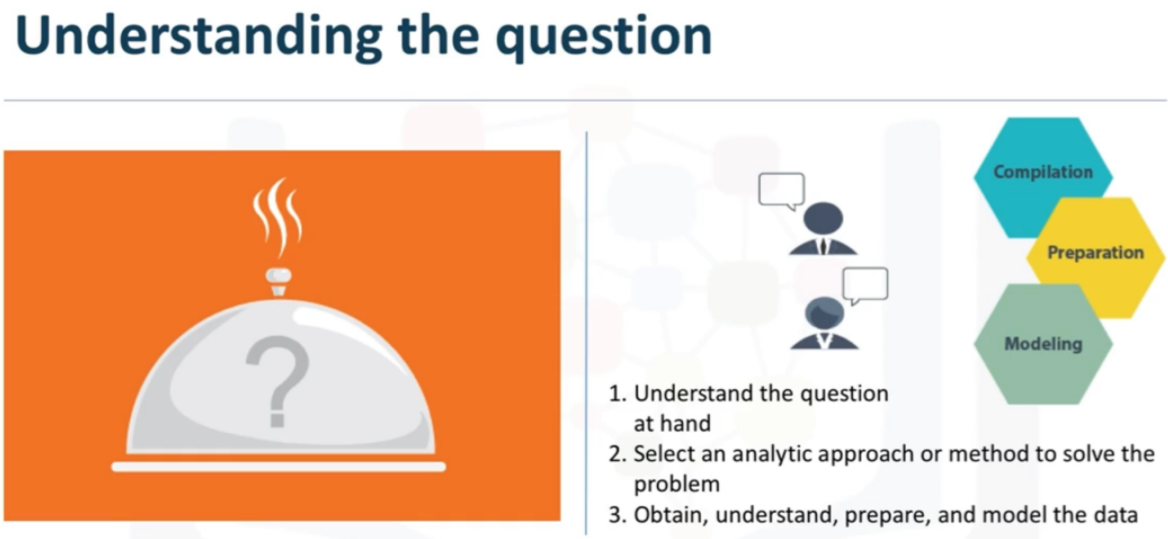
In this stage, the **data scientist will play around with different algorithms** to ensure that the variables in play are actually required. The success of data compilation, preparation and modelling, depends on the understanding of the problem at hand, and the appropriate analytical approach being taken.

The data supports the answering of the question, and like the quality of the ingredients in cooking, sets the stage for the outcome. Constant refinement, adjustments and tweaking are necessary within each step to ensure the outcome is one that is solid.

In John Rollins' descriptive Data Science Methodology, the framework is geared to do 3 things:

- First, understand the question at hand.

- Second, select an analytic approach or method to solve the problem,
- Third, obtain, understand, prepare, and model the data.



The end goal is to move the data scientist to a point where a data model can be built to answer the question. With dinner just about to be served and a hungry guest at the table, the key question is:

- Have I made enough to eat? Well, let's hope so.

In this stage of the methodology, **model evaluation**, **deployment**, and **feedback loops** ensure that the answer is near and relevant. **This relevance is critical** to the data science field overall, as it ís a fairly new field of study, and we are interested in the possibilities it has to offer. The more people that benefit from the outcomes of this practice, the further the field will develop. This ends the Modeling to Evaluation section of this course, in which we reviewed the key concepts related to modeling.

Modeling - Case Study

Modelling is the stage in the data science methodology **where the data scientist has the chance to sample the sauce and determine if it's bang on or in need of more seasoning**! Now, let's apply the case study to the modeling stage within the data science methodology. Here, we'll discuss one of the many aspects of model building, in this case, **parameter tuning to improve the model**. With a prepared training set, the first decision tree classification model for congestive heart failure readmission can be built.

Case Study – Analyzing the 1st model

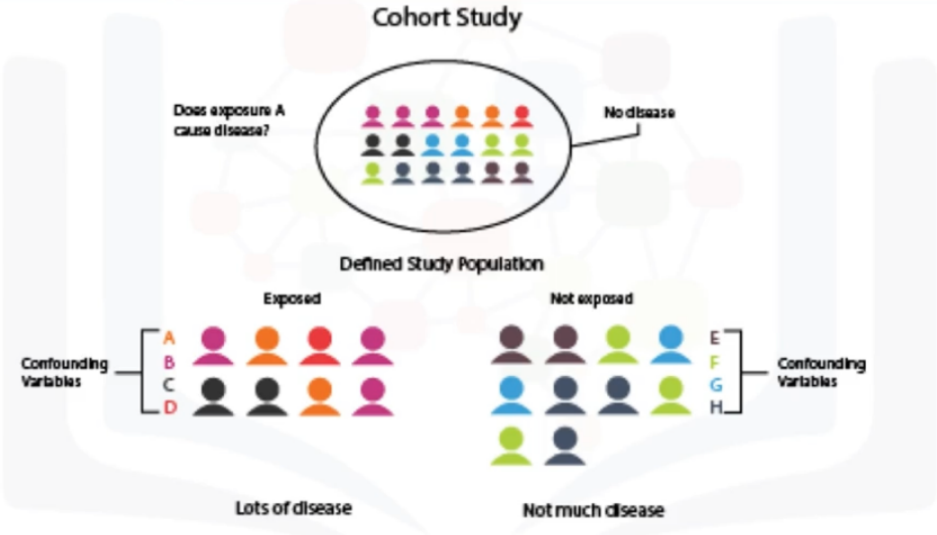
Initial decision tree classification model

- Low accuracy on "Yes" outcome

Model	Relative Cost Y:N	Overall Accuracy (% correct Y & N)	Sensitivity (Y accuracy)	Specificity (N accuracy)
1	1:1	85%	45%	97%
2	9:1	49%	97%	35%
3	4:1	81%	68%	85%

We are looking for patients with high-risk readmission, so the outcome of interest will be congestive heart failure readmission equals "yes". In this first model, overall accuracy in classifying the yes and no outcomes was 85%. This sounds good, but it represents only 45% of the "yes". The actual readmissions are correctly classified, meaning that the model is not very accurate. The question then becomes: How could the accuracy of the model be improved in predicting the yes outcome? For decision tree classification, the best parameter to adjust is the relative cost of misclassified yes and no outcomes.

Case Study – How to improve the model?



Think of it like this: **When** a true, **non-readmission is misclassified**, and action is taken to reduce that patient's risk, **the cost of that error is the wasted intervention**. A statistician calls this a **type I error**, or a false-positive. But **when a true readmission is misclassified**, and **no action is taken** to reduce that risk, then t**he cost of that error is the readmission and all its**

attended costs, plus the trauma to the patient. This is a **type II error**, or a false-negative.
So we can see that the costs of the two different kinds of misclassification errors can be quite different. For this reason, it's reasonable to adjust the relative weights of misclassifying the yes and no outcomes. The default is 1-to-1, but the decision tree algorithm, allows the setting of a higher value for yes.

Case Study – Analyzing the 2nd model

Second model
- High accuracy on "Yes" but poor on "No"

Model	Relative Cost Y:N	Overall Accuracy (% correct Y & N)	Sensitivity (Y accuracy)	Specificity (N accuracy)
1	1:1	85%	45%	97%
2	9:1	49%	97%	35%
3	4:1	81%	68%	85%

For the second model, the relative cost was set at 9-to-1. This is a very high ratio, but gives more insight to the model's behaviour. This time the model correctly classified 97% of the yes, but at the expense of a very low accuracy on the no, with an overall accuracy of only 49%. This was clearly not a good model. The problem with this outcome is the large number of false-positives, which would recommend unnecessary and costly intervention for patients, who would not have been re-admitted anyway.

Case Study – Analyzing the 3rd model

Third model
- Better balance on "Yes" and "No" accuracy

Model	Relative Cost Y:N	Overall Accuracy (% correct Y & N)	Sensitivity (Y accuracy)	Specificity (N accuracy)
1	1:1	85%	45%	97%
2	9:1	49%	97%	35%
3	4:1	81%	68%	85%

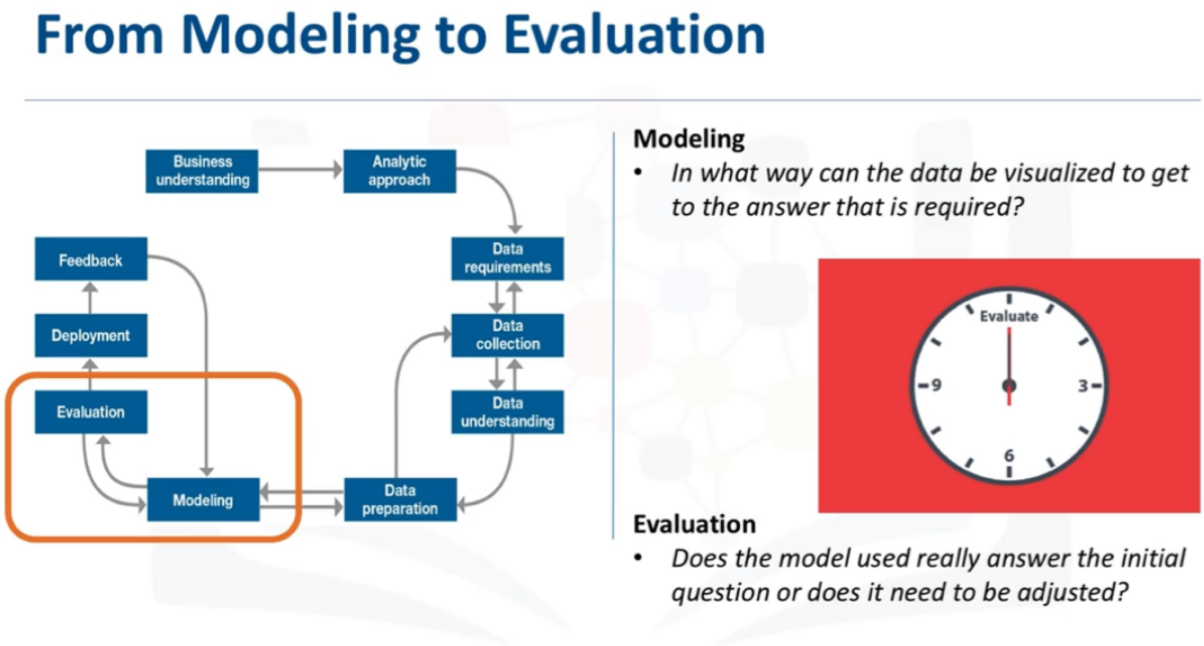
Therefore, the data scientist needs to try again to find a better balance between the yes and no

accuracies. For the third model, the relative cost was set at a more reasonable 4-to-1. This time 68% accuracy was obtained on only yes, called sensitivity by statisticians, and 85% accuracy on the no, called specificity, with an overall accuracy of 81%. This is the best balance that can be obtained with a rather small training set through adjusting the relative cost of misclassified yes and no outcomes parameter.

A lot more work goes into the modeling, of course, including iterating back to the data preparation stage to redefine some of the other variables, so as to better represent the underlying information, and thereby improve the model. This concludes the Modeling section of the course, in which we applied the Case Study to the modeling stage within the data science methodology.

Evaluation

A model evaluation goes hand-in-hand with model building as such, the modeling and evaluation stages are done iteratively.

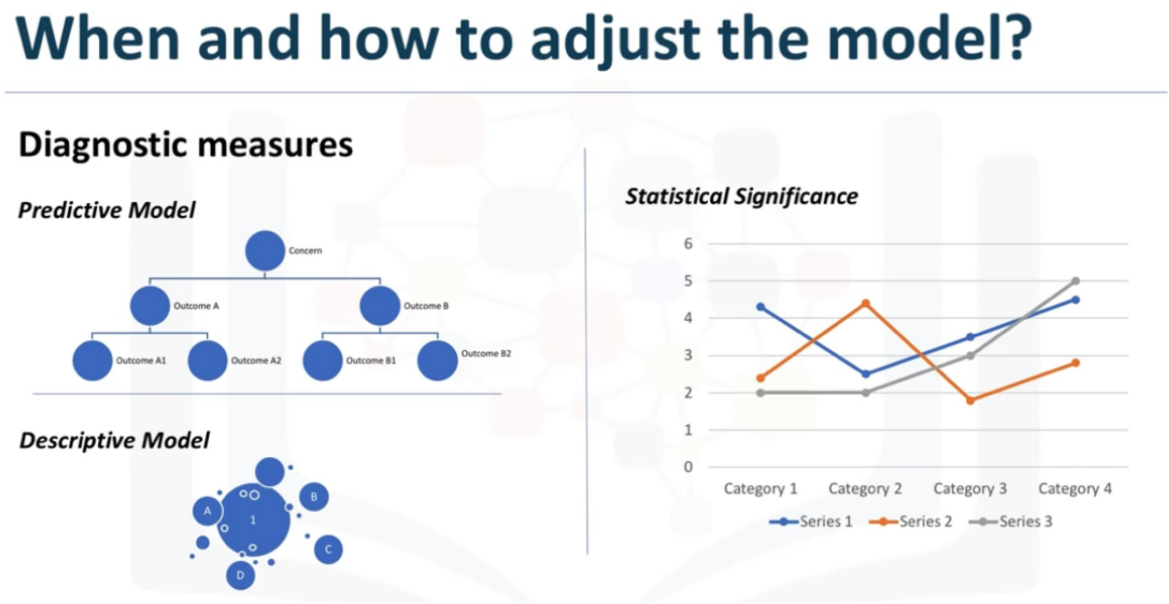


Model evaluation is performed during model development and before the model is deployed. Evaluation allows the quality of the model to be assessed but it's also an opportunity to see if it meets the initial request. Evaluation answers the question:

- Does the model used really answer the initial question or does it need to be adjusted?

Model evaluation can have two main phases.

1. The first is the **diagnostic measures phase**, which is used to ensure the model is working as intended. If the model is a predictive model, a decision tree can be used to evaluate if the answer the model can output, is aligned to the initial design. It can be used to see where there are areas that require adjustments. If the model is a descriptive model, one in which relationships are being assessed, then a testing set with known outcomes can be applied, and the model can be refined as needed.



2. The second phase of evaluation that may be used is **statistical significance testing**. This type of evaluation can be applied to the model to ensure that the data is being properly handled and interpreted within the model. This is designed to avoid unnecessary second guessing when the answer is revealed.

So now, let's go back to our case study so that we can apply the "Evaluation" component within the data science methodology. Let's look at one way to find the optimal model through a diagnostic measure based on tuning one of the parameters in model building. Specifically we'll see how to tune the relative cost of misclassifying yes and no outcomes. As shown in this table, four models were built with four different relative misclassification costs.

Case Study – Relative costs

Misclassification cost tuning

- Tune the relative misclassification costs
- Balance true-positive rate and false-positive rate for best model

Model	Relative Cost Y:N	True Positive Rate (Sensitivity)	Specificity (accuracy on N)	False Positive Rate (1 – Specificity)
1	1:1	0.45	0.97	0.03
2	1.5:1	0.60	0.92	0.08
3	4:1	0.68	0.85	0.15
4	9:1	0.97	0.35	0.65

As we see, each value of this model-building parameter increases the true-positive rate, or sensitivity, of the accuracy in predicting yes, at the expense of lower accuracy in predicting no, that is, an increasing false-positive rate.

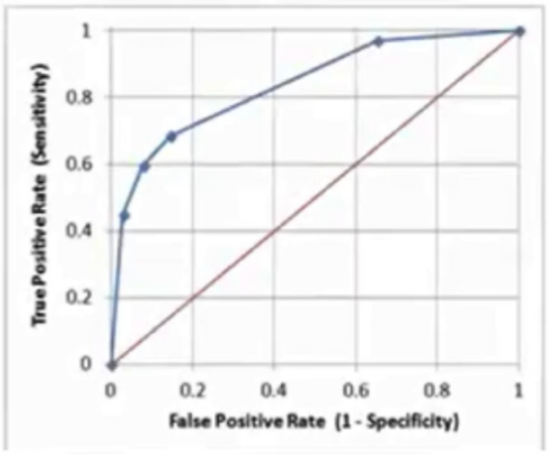
The question then becomes, **which model is best based on tuning this parameter?**

For budgetary reasons, the risk-reducing intervention could not be applied to most or all congestive heart failure patients, many of whom would not have been readmitted anyway. On the other hand, the intervention would not be as effective in improving patient care as it should be, with not enough high-risk congestive heart failure patients targeted. So, **how do we determine which model was optimal?**

Case Study – Using the ROC curve

Diagnostic tool for classification model evaluation

- Classification model performance
- True-Positive Rate vs False-Positive Rate
- Optimal model at maximum separation



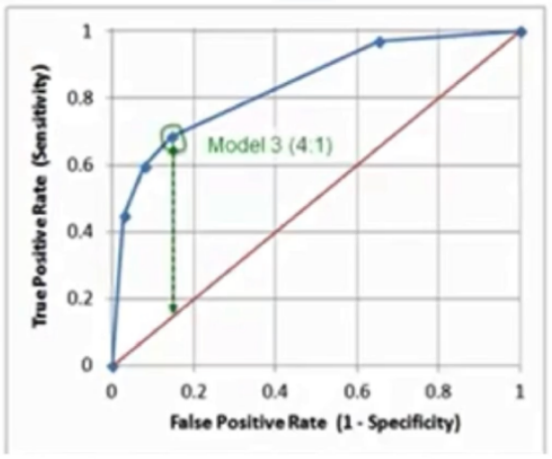
As you can see on this slide, the optimal model is the one giving the maximum separation between the blue ROC curve relative to the red base line. We can see that model 3, with a relative misclassification cost of 4-to-1, is the best of the 4 models. And just in case you were wondering, **ROC** stands for **receiver operating characteristic** curve, which was first developed during World War II to detect enemy aircraft on radar. It has since been used in many other fields as well. Today it is commonly used in machine learning and data mining.

The ROC curve is a useful diagnostic tool in determining the optimal classification model. This curve **quantifies how well a binary classification model performs**, declassifying the yes and no outcomes when some discrimination criterion is varied. In this case, the criterion is a relative misclassification cost.

Cost Study – Using the ROC curve

Diagnostic tool for classification model evaluation

- Classification model performance
- True-Positive Rate vs False-Positive Rate
- Optimal model at maximum separation



By plotting the true-positive rate against the false-positive rate for different values of the relative misclassification cost, the ROC curve helped in selecting the optimal model.