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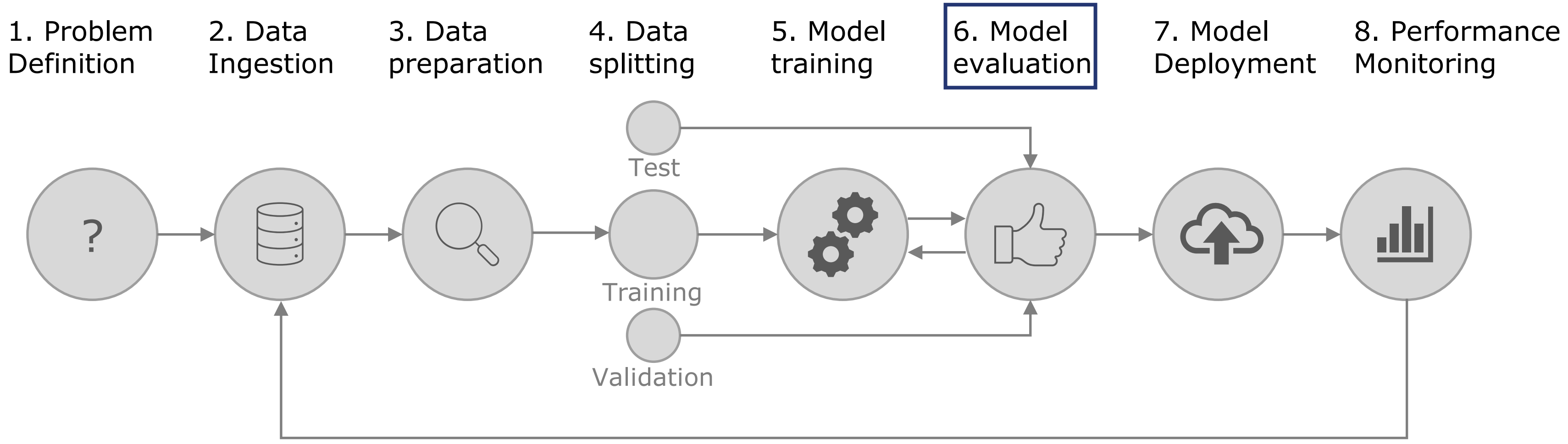
# Machine Learning, Artificial Intelligence, and Big Data Analytics (IL, 4th Semester)

Lecture 2

# Focus of this lecture



# Topics of today

- How to evaluate a ML model
- Coding:
  - Loading data
  - Manipulating with data.table
  - Data splitting and model evaluation

# Evaluating a model

## What to use for evaluating a **regression** model?

- MAE $= \frac{1}{n}\sum_{i=1}^{n}|e_i|$ ← Just the average absolute error (0 means perfect fit)
- MAPE $= \frac{1}{n}\sum_{i=1}^{n}\left|\frac{e_i}{y_i}\right|$ ← The average error in relation to the actual values (0% means perfect fit)
- RMSE $= \sqrt{\frac{1}{n}\sum_{i=1}^{n}|e_i^2|}$ ← The average error but penalizes larger errors more severely (0 means perfect fit)
- $R^2$-score $= 1 - \frac{RSS}{TSS}$ ← The degree to which the model explains the variance in the data
  (1 means perfect fit. 0 is no better than the mean. <0 is worse than the mean)

- Very easy to compute. R, Python, and Julia also provide built-in functions and usually include these metrics in the model object (from the training data).
- You should know these from the statistics lecture!
- What about **classification**?

# Evaluating a model

## What to use for evaluating a **Classification** model?

- Back to the spam detection example

| Actual | Prediction |
|---|---|
| No spam | Spam |
| No spam | No spam |
| No spam | Spam |
| No spam | No spam |
| No spam | No spam |
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### Confusion Matrix

Predicted

| Actual | | 1 | 0 |
|---|---|---|---|
| | 1 | True positive | False Negative |
| | 0 | False Positive | True negative |

# Evaluating a model

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### Confusion Matrix

Predicted

Actual

| | 1 | 0 |
|---|---|---|
| **1** | True positive | False Negative |
| **0** | False Positive | True negative |

| | Spam | No spam |
|---|---|---|
| **Spam** | 4 | 1 |
| **No spam** | 2 | 3 |

# Evaluating a model

## What to use for evaluating a **Classification** model?

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|---|---|
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### Confusion Matrix

Predicted

| Actual | | **1** | **0** |
|---|---|---|---|
| | **1** | True positive | False Negative |
| | **0** | False Positive | True negative |

| | **Spam** | **No spam** |
|---|---|---|
| **Spam** | 4 | 1 |
| **No spam** | 2 | 3 |

**Accuracy**: What fraction does it get right
(#TP+#TN)/#Total

**Precision**: When it says 1 how often is it right Sensitivity
#TP/(#TP+#FP)

**Recall**: What fraction of 1s does it get right specificity
#TP/(#TP+#FN)

**FP Rate**: What fraction of 0s are called 1s
#FP/(#FP+#TN)

**FN Rate**: What fraction of 1s are called 0s
#FN/(#TP+#FN)

**F1-Score**: $2 * \frac{precision*recall}{precision+recall}$

0.7 is acceptable, very impotant metric

# Evaluating a model

## What to use for evaluating a **Classification** model?

- Back to the spam detection example

| **Actual** | **Prediction** |
|---|---|
| No spam | Spam |
| No spam | No spam |
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| No spam | No spam |
| No spam | No spam |
| Spam | No spam |
| Spam | Spam |
| Spam | Spam |
| Spam | Spam |
| Spam | Spam |

### Confusion Matrix

Predicted

| Actual | | **1** | **0** |
|---|---|---|---|
| | **1** | True positive | False Negative |
| | **0** | False Positive | True negative |

| | **Spam** | **No spam** |
|---|---|---|
| **Spam** | 4 | 1 |
| **No spam** | 2 | 3 |

**Accuracy**: What fraction does it get right
(#TP+#TN)/#Total = 7/10 = 70%

**Precision**: When it says 1 how often is it right
#TP/(#TP+#FP) = 4/6 = 66%

**Recall**: What fraction of 1s does it get right
#TP/(#TP+#FN) = 4/5 = 80%

**FP Rate**: What fraction of 0s are called 1s
#FP/(#FP+#TN) = 2/5 = 40%

**FN Rate**: What fraction of 1s are called 0s
#FN/(#TP+#FN) = 1/5 = 20%

**F1-Score**: $2 * \frac{precision*recall}{precision+recall}$ = 0.72

# Evaluating a model

## The importance of looking at different metrics

- Imagine the following

| Actual | Prediction |
|---|---|
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| Spam | No spam |
| Spam | Spam |

Predicted

| Actual | | Spam | No spam |
|---|---|---|---|
| | Spam | TP=1 | FN=1 |
| | No spam | FP=0 | TN=8 |

**Accuracy**: What fraction does it get right
(#TP+#TN)/#Total = 9/10 = 90%

**Precision**: When it says 1 how often is it right
#TP/(#TP+#FP) = 1/1 = 100%

**FP Rate**: What fraction of 0s are called 1s
#FP/(#FP+#TN) = 0%

# Evaluating a model

## The importance of looking at different metrics

- Imagine the following

| Actual | Prediction |
|---|---|
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
| No spam | No spam |
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Predicted

| Actual | | **Spam** | **No spam** |
|---|---|---|---|
| | **Spam** | TP=1 | FN=1 |
| | **No spam** | FP=0 | TN=8 |

**Accuracy**: What fraction does it get right
(#TP+#TN)/#Total = 9/10 = 90%

**Precision**: When it says 1 how often is it right
#TP/(#TP+#FP) = 1/1 = 100%

**Recall**: What fraction of 1s does it get right
#TP/(#TP+#FN) = 1/2 = 50%

**FP Rate**: What fraction of 0s are called 1s
#FP/(#FP+#TN) = 0%

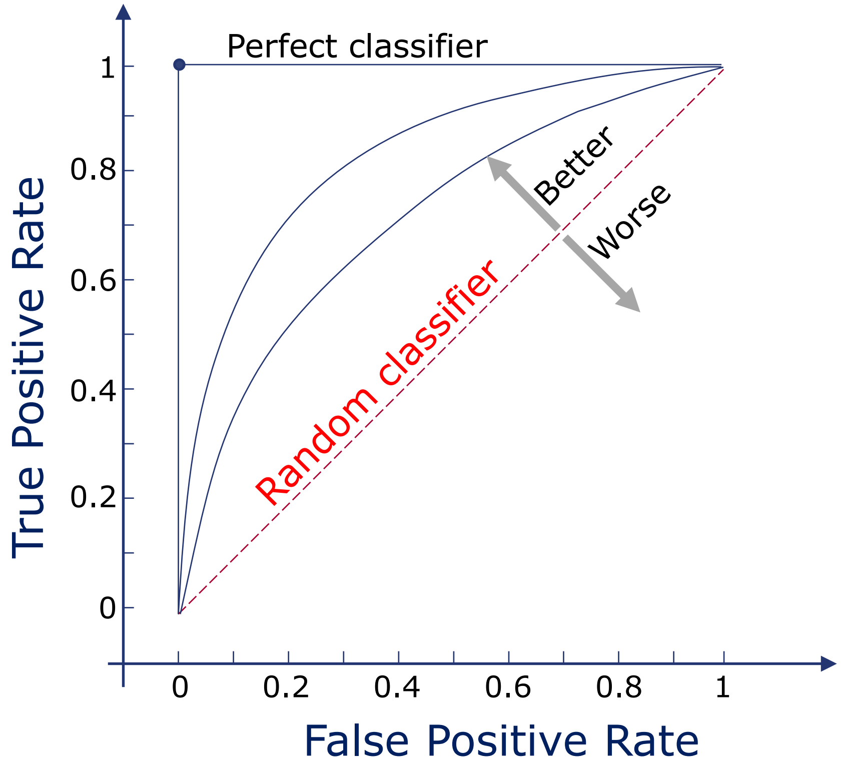
**FN Rate**: What fraction of 1s are called 0s
#FN/(#TP+#FN) = 1/2 = 50%

**F1-Score**: $2 * \frac{precision * recall}{precision + recall}$ = 0.66

# The ROC curve and the AUC

- Comparing binary classifiers
- True Positive vs. False Positive at various thresholds

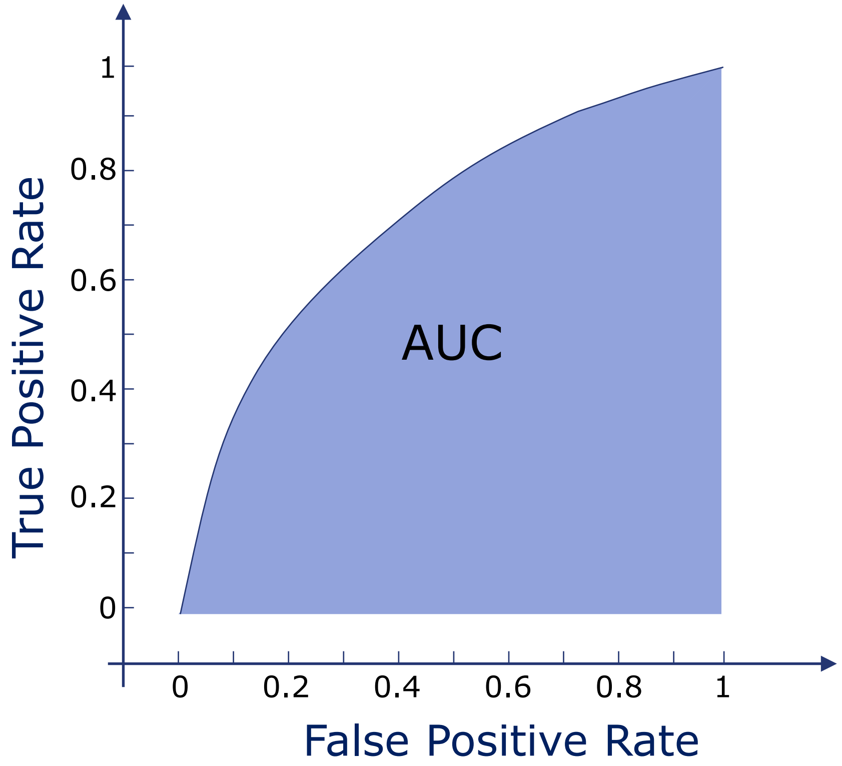
ROC is the visuzualization of the



# The ROC curve and the AUC

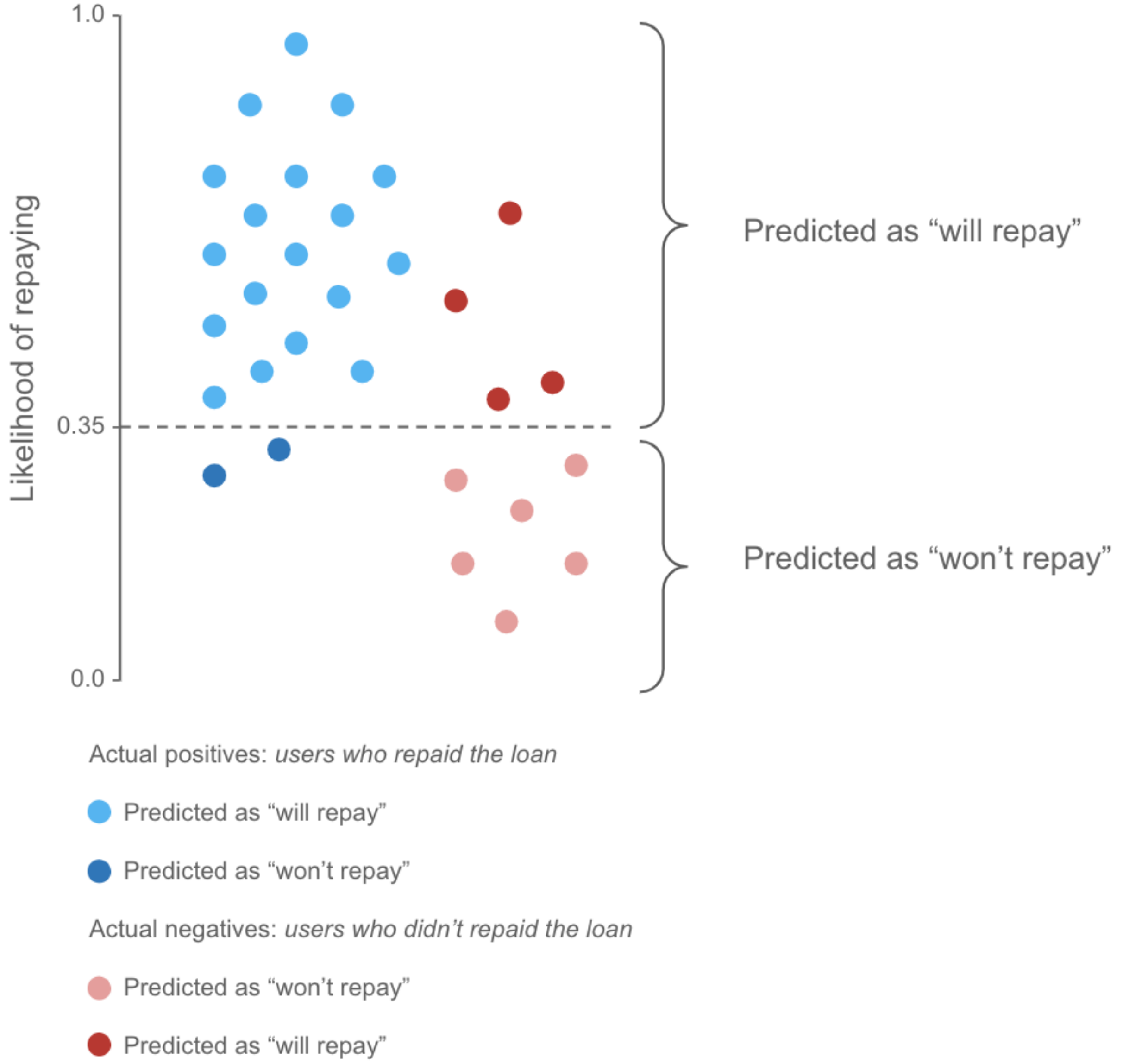
- Comparing binary classifiers
- True Positive vs. False Positive at various thresholds

- 0 < AUC < 1
- The larger the better

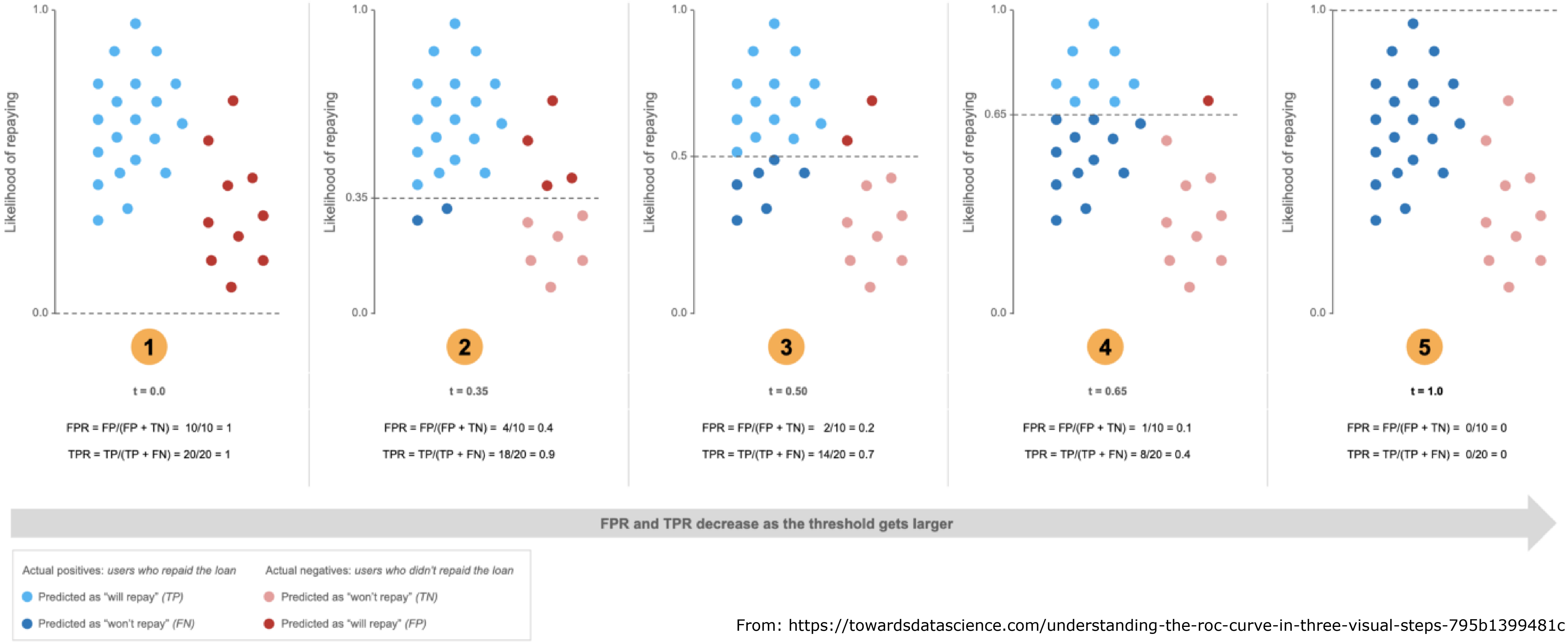


# ROC example

https://towardsdatascience.com/understanding-the-roc-curve-in-three-visual-steps-795b1399481c



# ROC example

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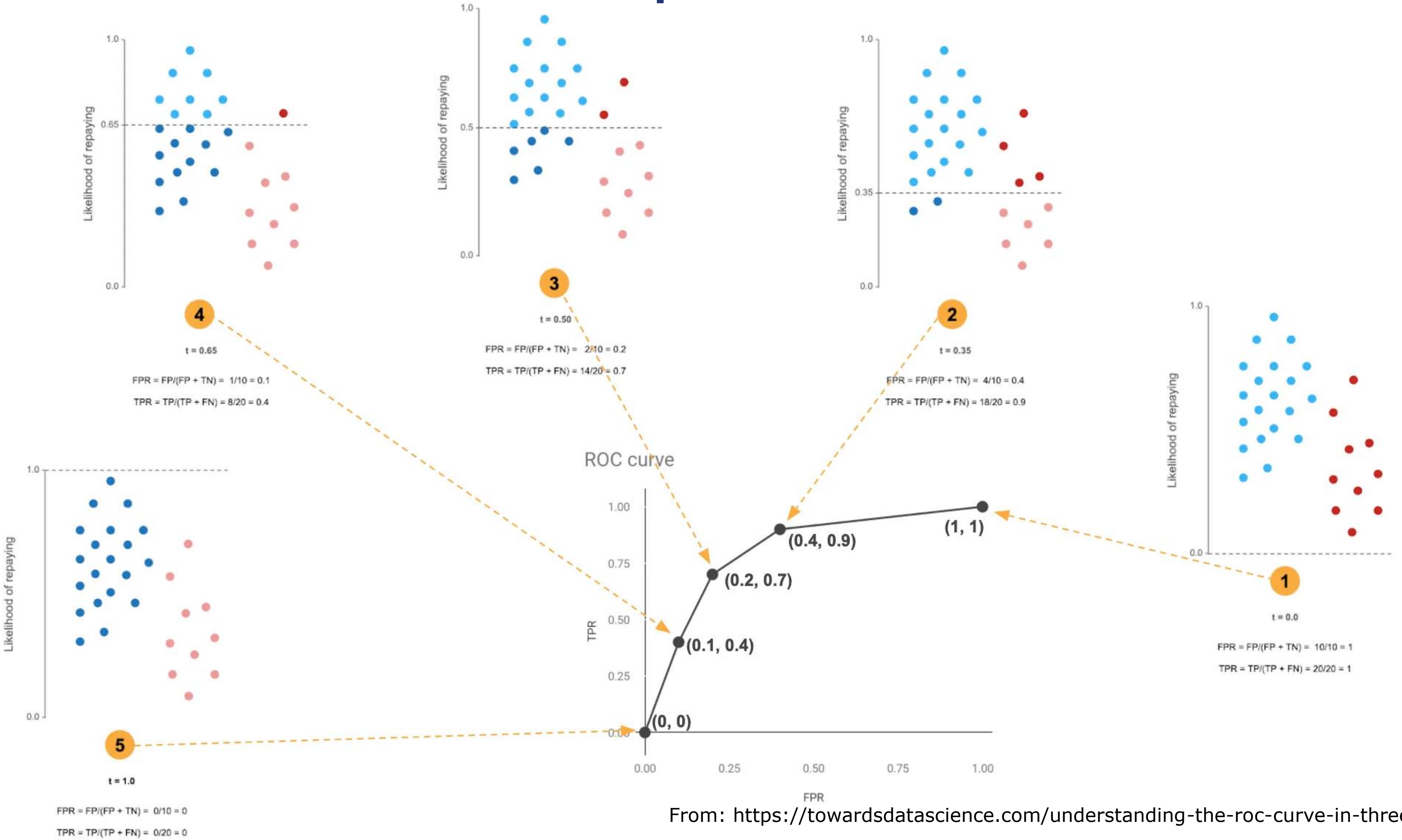
# ROC example




From: https://towardsdatascience.com/understanding-the-roc-curve-in-three-visual-steps-795b1399481c

# Evaluating a model

## Summary

| Metric | Formula | Meaning | Visual look | range |
|---|---|---|---|---|
| Accuracy | (#TP+#TN)/#Total | What fraction does it get right | **TP** FN / FP **TN** ÷ **TP** **FN** / **FP** **TN** | 0-1 |
| Precision | #TP/(#TP+#FP) | When it says 1 how often is it right | **TP** FN / FP TN ÷ **TP** FN / **FP** TN | 0-1 |
| Recall/ Sensitivity | #TP/(#TP+#FN) | What fraction of 1s does it get right (True Positive Rate – TPR) | **TP** FN / FP TN ÷ **TP** **FN** / FP TN | 0-1 |
| Specificity | #TN/(#TN+#FP) | What fraction of 0s does it get right (True Negative Rate – TNR) | TP FN / FP **TN** ÷ TP FN / **FP** **TN** | 0-1 |
| FP Rate | #FP/(#FP+#TN) | What fraction of 0s are called 1s | TP FN / **FP** TN ÷ TP FN / **FP** **TN** | 0-1 |
| FN Rate | #FN/(#TP+#FN) | What fraction of 1s are called 0s | TP **FN** / FP TN ÷ **TP** **FN** / FP TN | 0-1 |
| F1-score | $2 * \frac{precision * recall}{precision + recall}$ | How "good" are precision and recall | | 0-1 |

# Things you should know

- What is underfit/overfit. What is the bias-variance tradeoff. How do they relate?
- How does cross-validation work.
- What is bootstrapping and bagging.
- How to evaluate a regression or a classification model
  - RMSE, MAE, …
  - Accuracy, Precision, Recall,…
  - Interpret a ROC curve

- It continues in R

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# Feedback round

- Scan the barcode from your mobile phone

**OR**

- go to http://sli.do and insert this code: 19651

and follow my instructions.

# Exercise 1
## Overfit

1. **Load** the dataset wines.csv (or any other regression dataset from here – i.e., Regression task, numerical variables)
2. **Explore and visualize the dataset** (e.g., how many observations? How many features? Missing values? Are some features irrelevant?)
3. Crete a regression model (i.e., for wine: the quality by using density, chlorides, and volatile acidity).
    1. Split the data into training and test set
    2. Create a linear regression model and polynomial models with increasing degree.
    3. What’s the MAE, the RMSE, and the MAPE on the training and test set for all the models?
    4. When does the model start overfitting? Which degree would you choose?

- **Due date: March 12th, 23.59 CET (Late submission +1week, 6 pts)**
- Comment code and results (or write a notebook).
- Use R or Python