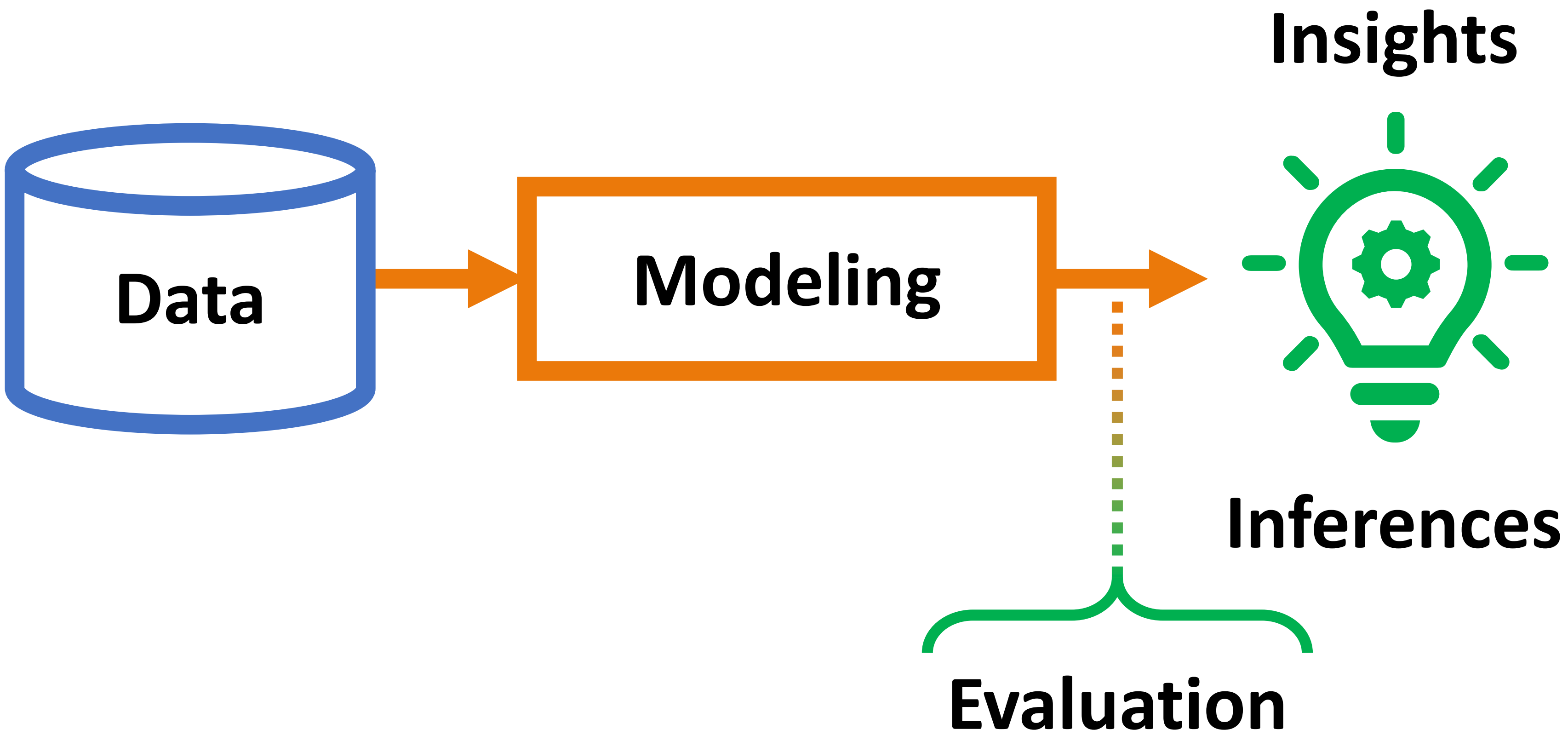
Data Processing

8 A

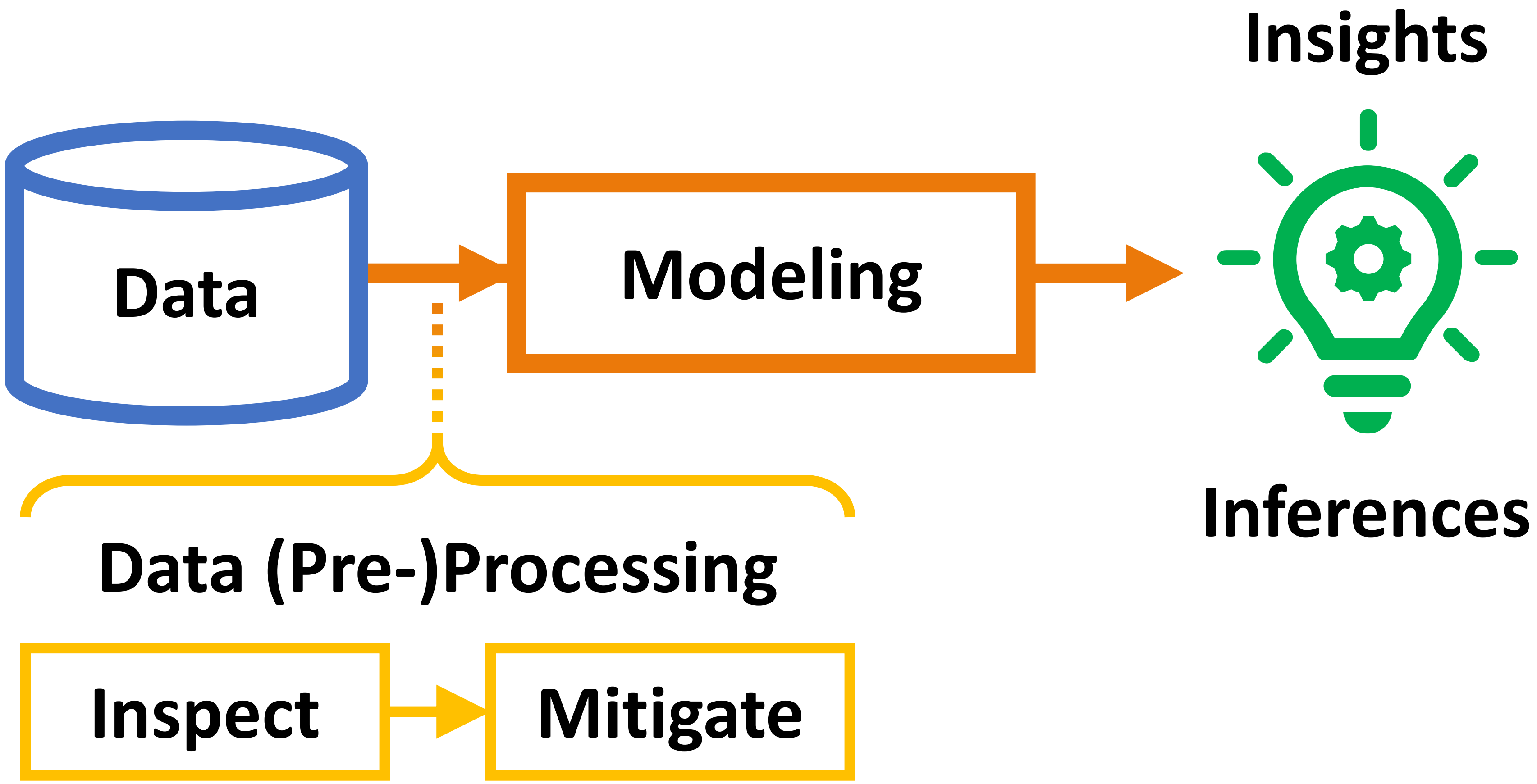
CS 3244
Machine Learning

NUS National University of Singapore | Computing

Machine Learning Pipeline



Machine Learning Pipeline



W08 Pre-Lecture Task

Read

1. Discover Feature Engineering, How to Engineer Features and How to Get Good at It by Jason Brownlee
2. 8 Tactics to Combat Imbalanced Classes in Your Machine Learning Dataset by Jason Brownlee

Task

1. Identify cases of **bad data** in machine learning
2. Propose **mitigation strategies**

   Tip: you can your own projects too; you don't have to be correct
3. Post a 1–2 sentence answer to the topic in your tutorial group: #tg-xx

Pre-Lecture Activity for this week

1. Identify cases of **bad data** in machine learning
2. Propose **mitigation strategies**

1 — Bad data could include statistical noise and errors. To mitigate this, do data cleaning.

2 — Bad data could be when there are too many irrelevant features, which can be mitigated by selecting only the most important features, or by feature extraction where several features are combined into a single feature that is more relevant.

3 — High dimensional features
   a. Since the dataset is made up of raw images, each image is represented by a 256 x 256 x 3 array of numbers which, if simply flattened without much feature engineering, will result in 196608 dimensions. This will be an issue as the model will not only suffer from the curse of high dimensionality, it will also take extremely long to train.
   b. **Mitigation:** I plan to find different ways to reduce the dimensionality of the dataset during the pre-processing phase and choose the one that gives the best results.

4 — To mitigate the problem of imbalanced data, we could try to generate synthetic samples of the minority class. We could also try to change our performance metric to take into account the imbalance of our dataset. For example, the Cohen's Kappa can provide a classification accuracy normalised by the imbalance of the classes in the data. To reduce the noise in the dataset, we could resample or collect more data.

There are many different cases of bad data such as imbalanced data, missing data or error/mistakes in the collected data etc.

Mitigation strategies for such cases of bad data could include resampling the data, collecting more data or in some cases even just dropping the erroneous/missing data

4 — https://www.reuters.com/article/us-amazon-com-jobs-automation-insight-idUSKCN1MK08G
Here is an example of how imbalanced data can cause real-world harms. Amazon fed in the resumes of people who were hired at amazon to create a model to screen applicants. However, since the men outnumbered the women in the training data, the model learned a hypothesis that was skewed on favour of male applicants. This shows how if one is not careful with the composition of the training data in a deployed model, it can lead to real-world harms. Possible methods to combat this could be to feed the model fictional female candidates to try to make the classes more even, and thus make the predictions less skewed.

U.S.
Amazon scraps secret AI recruiting tool that showed bias against women (43 kB)

Issues identified:
1. Erroneous data
2. Irrelevant data
3. High dimensionality
4. Imbalanced data
5. Missing data

5 — One common case of bad data is data with a lot of missing values. Some ways to mitigate this are to delete the data (either likewise or pairwise deletion) or to impute the missing values (e.g. replace the data with mean, median, or mode, or do regression to get the "predicted" values)

Week 08: Learning Outcomes

Data **Issues**

1. Linear Separability
2. Curse of Dimensionality
3. Imbalanced Data

Issue Template

1. **What** is the issue?
2. **Why** is it a problem?
3. **When** would it happen?
4. **How** to **check** for it?
5. **How** to **mitigate** it?

Exercise W08b.1

For each issue, which of the following techniques can:

1) **Check** for the issue?

2) **Mitigate** the issue?

Issue	Check	Mitigate
Linear Separability		
Curse of Dimensionality		
Imbalanced Data		

1. Feature Engineering
2. Feature Extraction (extract new features)
3. Information Gain
4. Linear Discriminant Analysis (LDA)
5. Principle Components Analysis (PCA)
6. SMOTE
7. Support Vector Machine
8. Visualize Histogram
9. Visualize Scatterplot

Emote (react) in Slack #general channel <u>one or more options</u> (MRQ) for each issue

For each issue, which of the following techniques can:

1) **Check** for the issue?
2) **Mitigate** the issue?

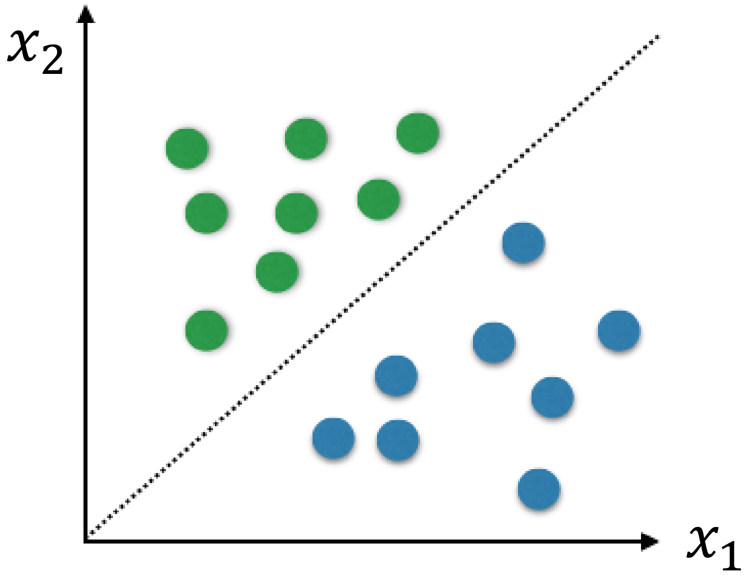
Issue	Check	Mitigate
Linear Separability	9 Visualize Scatterplot 7 Support Vector Machine 4 5 Check Basis Vectors (with LDA, PCA)	1 Feature Engineering 2 Feature Extraction 4 5 Matrix Factorization (with LDA, PCA)
Curse of Dimensionality	8 Visualize Histogram (of distances)	3 Feature Selection (using Information Gain) 4 5 Dimensionality Reduction (with LDA, PCA)
Imbalanced Data	8 Visualize Histogram	6 SMOTE

Linear Separability

NUS National University of Singapore | Department of Computer Science
School of Computing

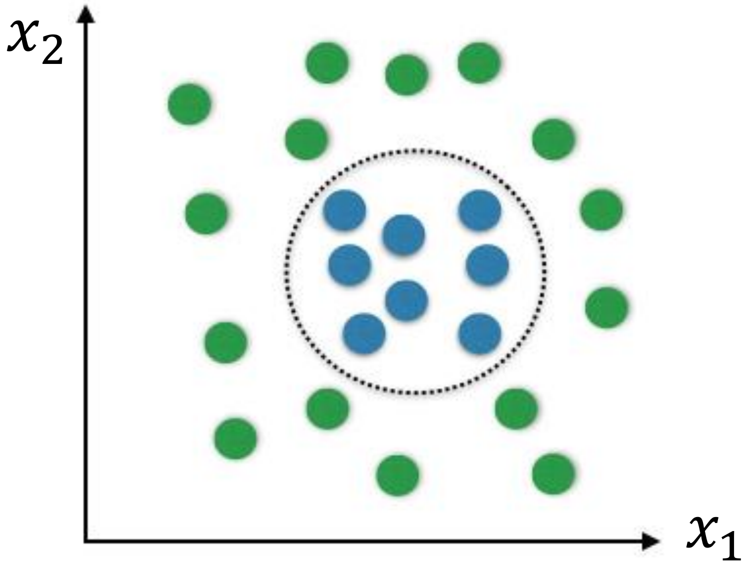
Linearly Separable?

Yes



$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Not without data processing



How to make linearly separable?

$$\boldsymbol{x}' = \begin{pmatrix} (x_1 - \bar{x}_1)^2 \\ (x_2 - \bar{x}_2)^2 \end{pmatrix} = (\boldsymbol{x} - \bar{\boldsymbol{x}})^\top (\boldsymbol{x} - \bar{\boldsymbol{x}})$$

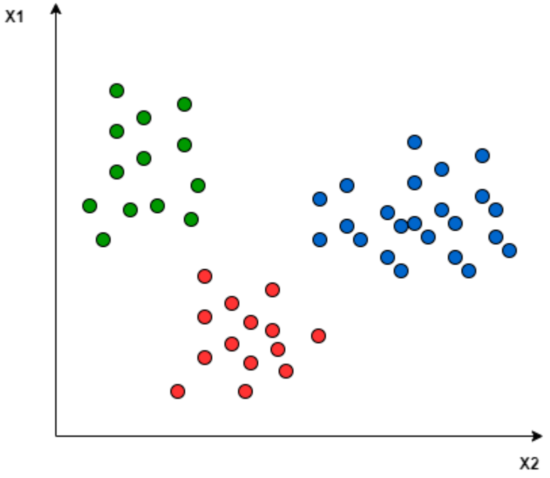
Feature Engineering!

Image Credit: Sebastian Raschka

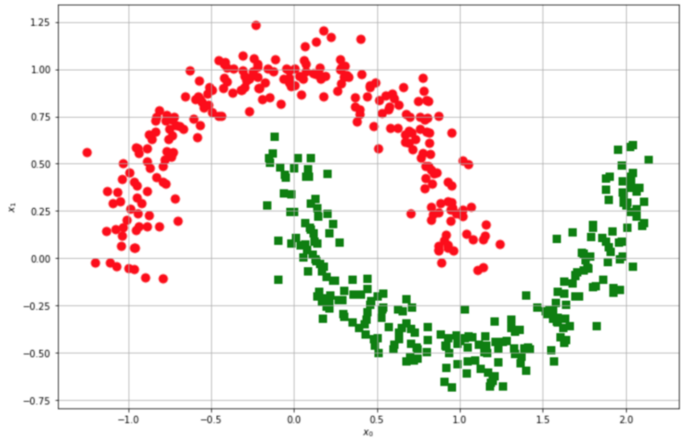
Which of the following is:

1. Is Linearly separable (📏:straight_ruler:)?
2. Can it be made Linearly Separable (➰:curly_loop:)? How? (Write in **thread**)

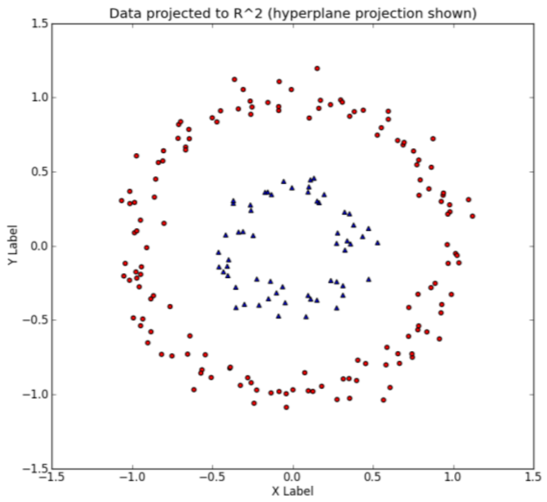
a)



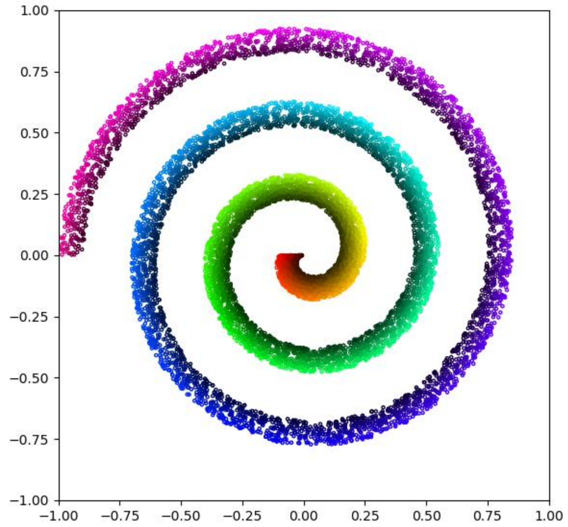
b)



c)

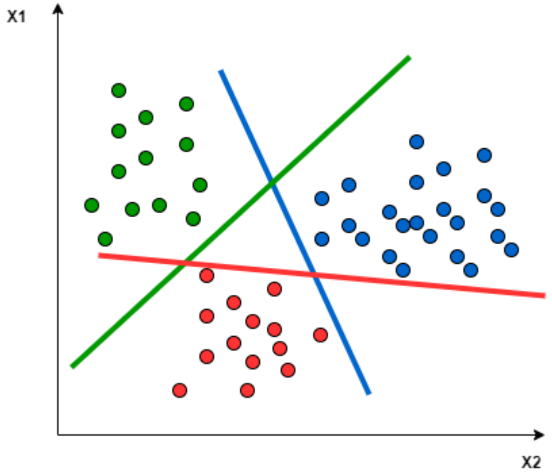


d)

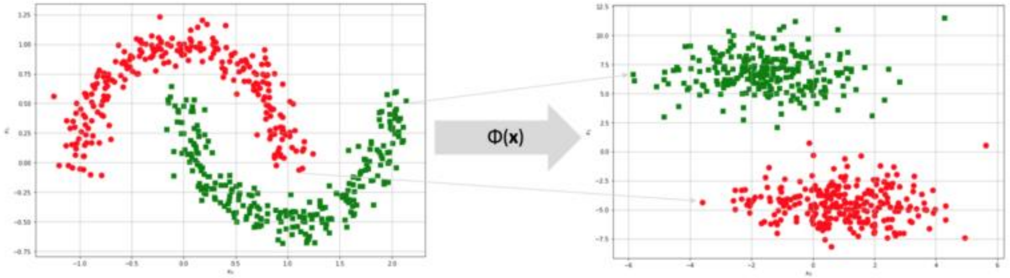


Which of the following is:
1. Is Linearly separable (📏:straight_ruler:)?
2. Can it be made Linearly Separable (➰:curly_loop:)? How? (Write in **thread**)

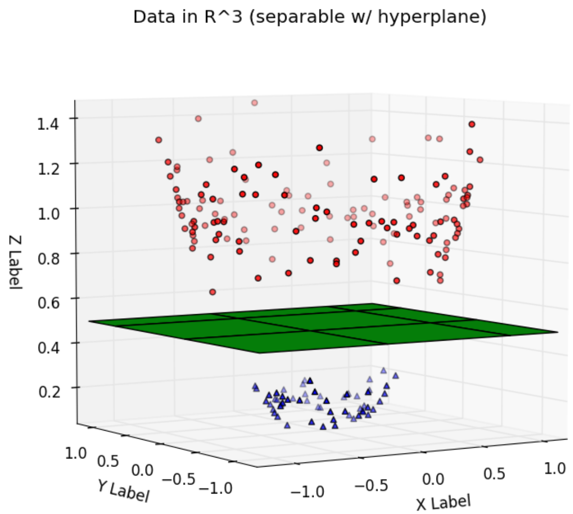
a) ➰📏



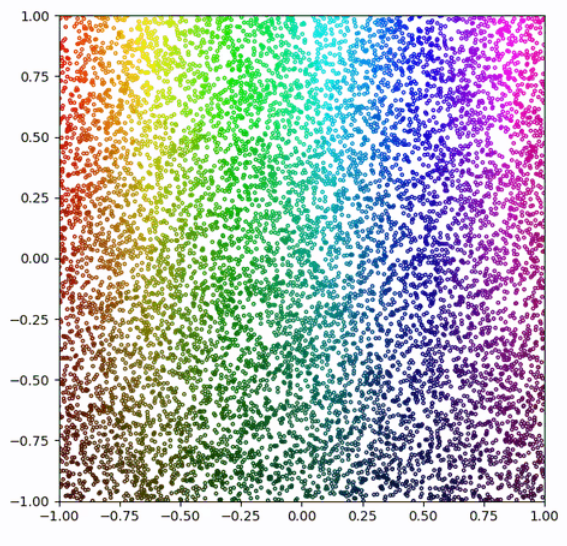
b) ➰



c) ➰



d) ➰



Issue: Linear Separability

1. **What** is the issue?
    1. Many models assume that data features are **linearly** separable
    2. Does your data satisfy this **assumption**?
2. **Why** is it a problem?
    1. Irrelevant features will be uninformative to train the model to discriminate between prediction labels
    2. If features are not linearly separable, you cannot learn a good **linear model**
    3. Need to use more complex models
3. **When** would it happen?
    1. Most of the time, for “fresh” unprocessed data.
    2. Especially for unstructured (non-tabular) data, e.g., images, time, text

Issue: Linear Separability

4. **How** to **check** for it?
   1. Visualize
      - 2D: **Scatterplot** of x_1 by x_2 graph
      - >2D: **Scatterplot Matrix**
      - 500 dimensions?

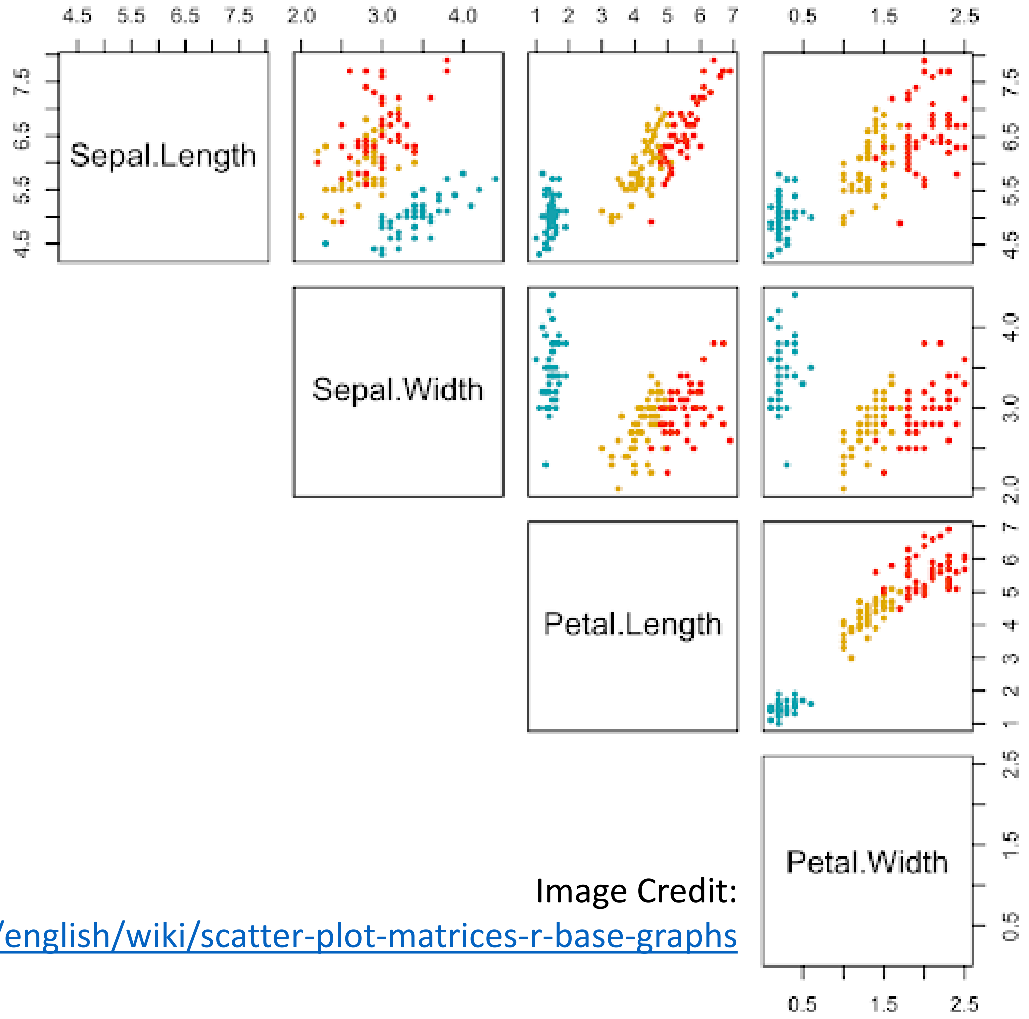


Image Credit:
http://www.sthda.com/english/wiki/scatter-plot-matrices-r-base-graphs

Issue: Linear Separability

4. **How** to **check** for it?
   1. Visualize
   2. Computational metrics
      1. Linear SVM [W04b]

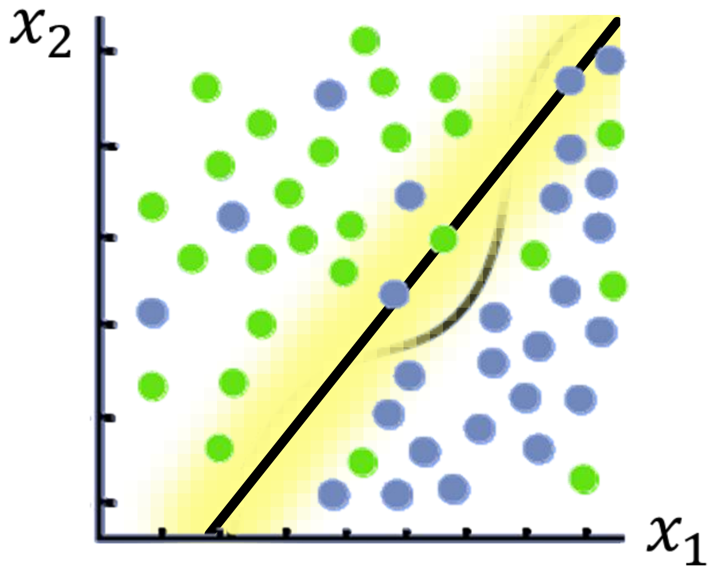


Image Credit:
http://www.sthda.com/english/wiki/scatter-plot-matrices-r-base-graphs

Cost Function w Slack Variables

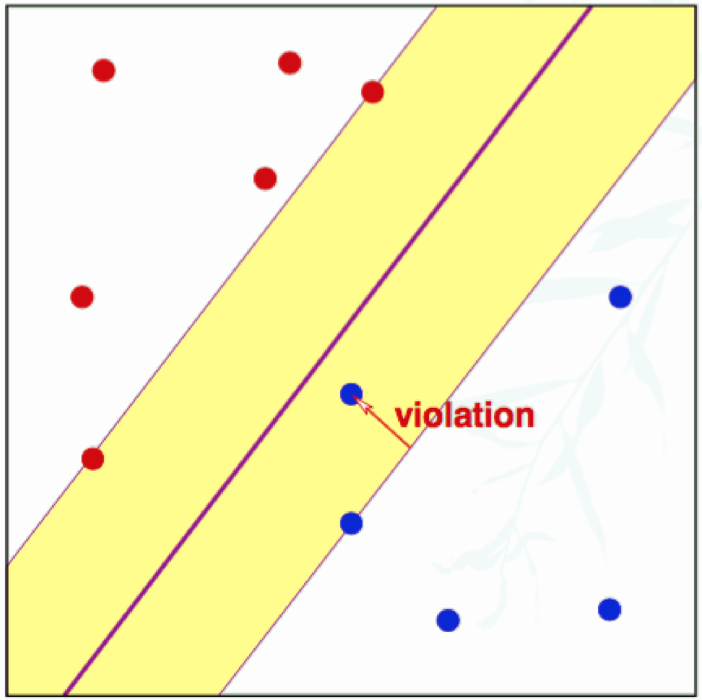
Margin violation: $y^{(*)}\left(\boldsymbol{\theta}^\top \mathbf{x}^{(*)} + b\right) \geq 1$ fails

Quantify this:

$y^{(*)}\left(\boldsymbol{\theta}^\top \mathbf{x}^{(*)} + b\right) \geq 1 - \xi^{(*)}$
where $\xi^{(*)} \geq 0$

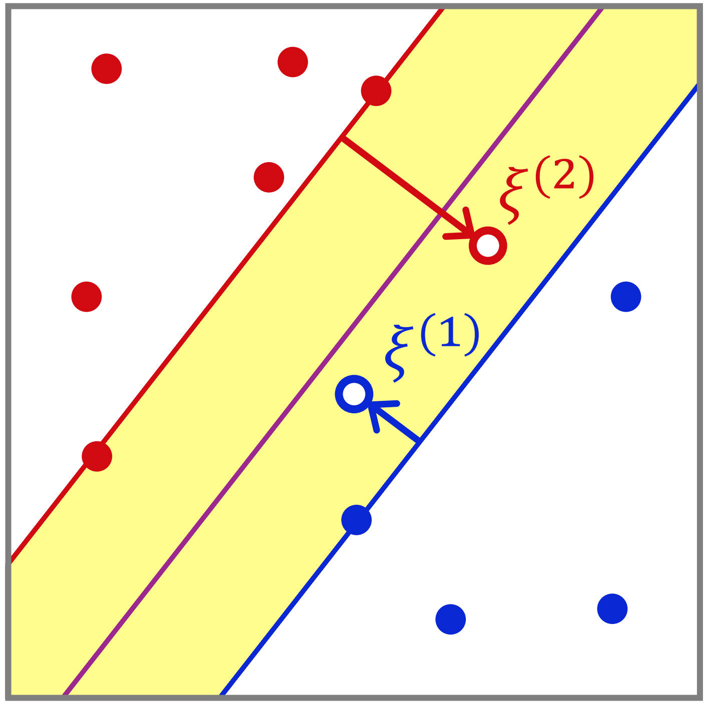
Slack variable: Soft error on $(x^{(*)}, y^{(*)})$

Total violation: $\sum_{j=1}^{m} \xi^{(j)}$



Testing Linear Separability with Linear Soft-Margin SVM

- Each $\xi^{(j)}$ is the **distance** that the misclassified point j is from its correct margin
- Total violation: $\sum_{j=1}^{m} \xi^{(j)}$
- Calculating the **total violation** indicates how **linearly separable** the data is in terms of its features
- Higher violation => Less linearly separable



Further Reading: https://towardsdatascience.com/support-vector-machines-soft-margin-formulation-and-kernel-trick-4c9729dc8efe

Issue: Linear Separability

4. **How** to **check** for it?
   1. Visualize
   2. Computational metrics
      1. Linear SVM [W04b]
      2. Reduce dimensions (LDA, PCA), then check separability (for separation by "diagonal planes")
      3. Others: Linear programming, Convex Hulls

Only these are **examinable**

Issue: Linear Separability

5. **How** to **mitigate** it?
   - Find useful features
     - Feature extraction (collect new features of your data)
   - Transformation of features
     - Feature Engineering (e.g., $\boldsymbol{x} \to \boldsymbol{x}^{\mathbf{2}}$)
     - Change Basis Vectors (e.g., PCA, LDA)
     - Kernel trick (e.g., for kernel SVM [W04b])
     - Feature Learning (e.g., Neural Networks [W09/10])

Issue: Linear Separability

5. **How** to **mitigate** it?
   - Find useful features
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   - Transformation of features
     - Feature Engineering (e.g., $x \rightarrow x^2$)
     - **Change Basis Vectors (e.g., PCA, LDA)**
     - Kernel trick (e.g., for kernel SVM [W04b])
     - Feature Learning (e.g., Neural Networks [W09/10])

Vector Spaces and Basis Vectors

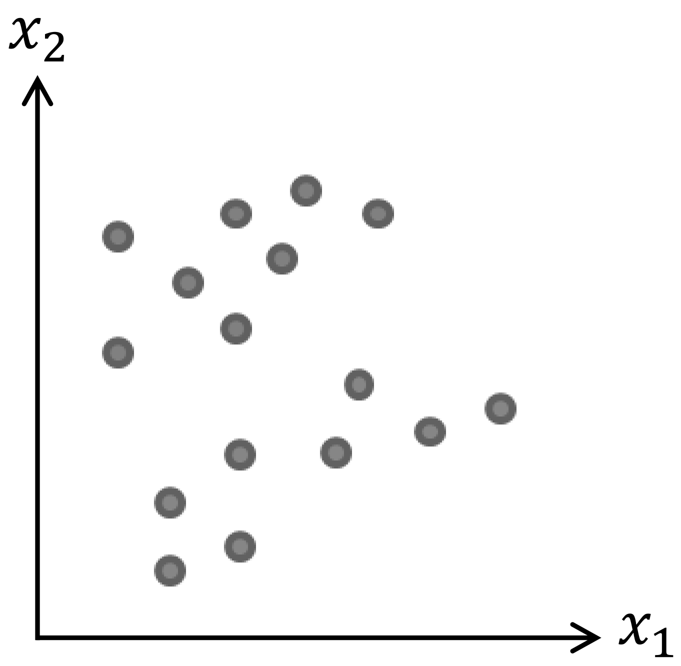


Image Credit: https://nirpyresearch.com/classification-nir-spectra-linear-discriminant-analysis-python/

Vector Spaces and Basis Vectors

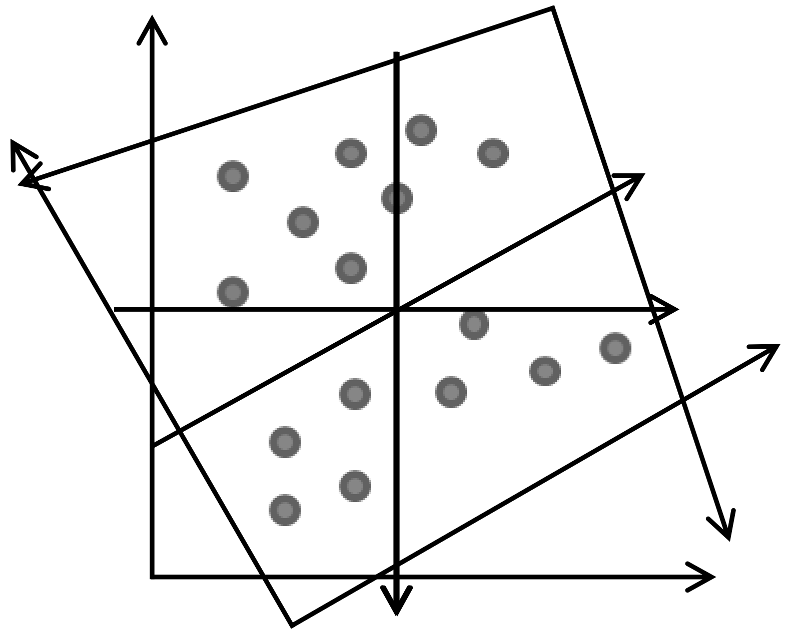
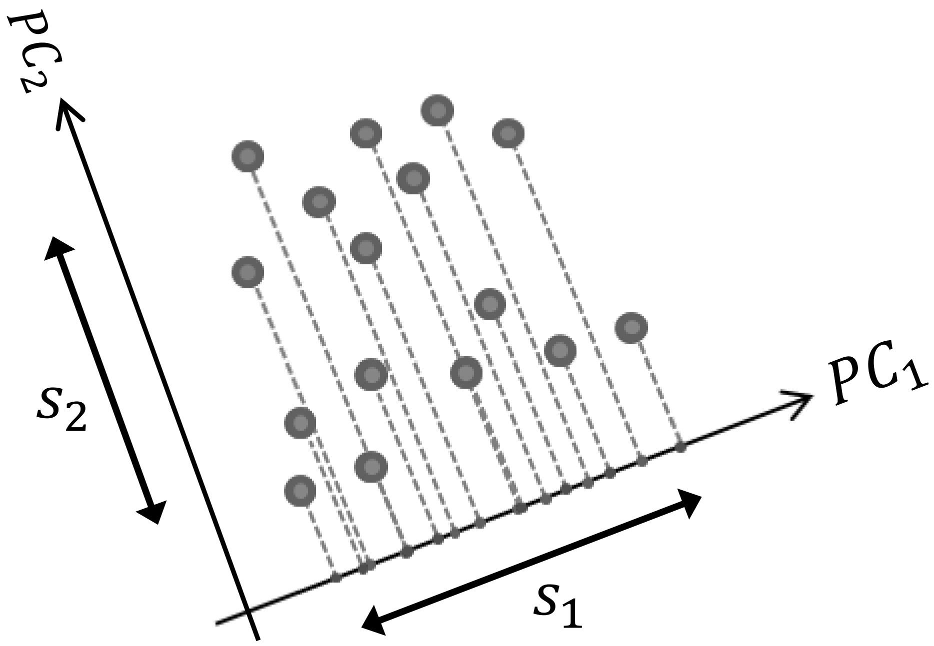


Image Credit: https://nirpyresearch.com/classification-nir-spectra-linear-discriminant-analysis-python/

Principal Component Analysis (PCA)

What axis best **describes the variation** in the data?



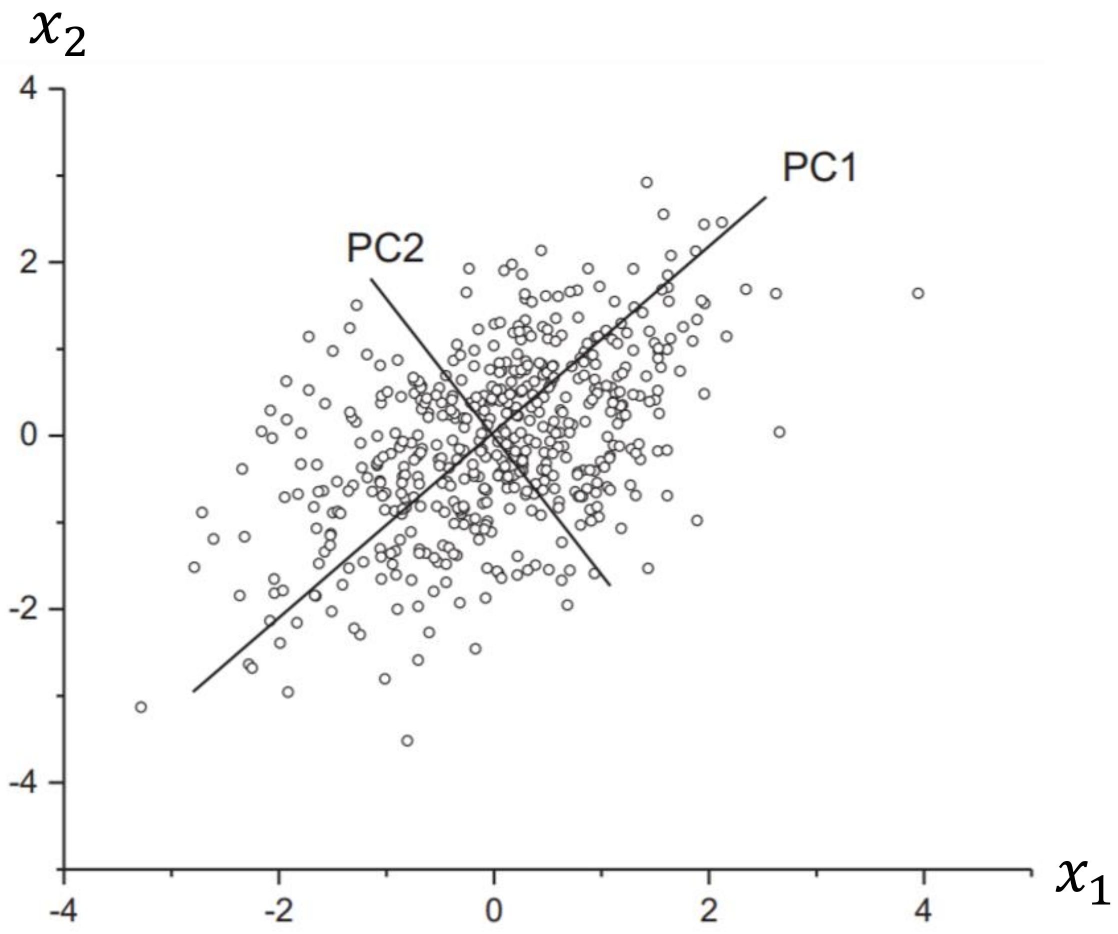
$$\begin{pmatrix}x_1\\x_2\end{pmatrix} \xrightarrow{\text{PCA Projection}} \begin{pmatrix}PC_1\\PC_2\end{pmatrix}$$

$$s_1 > s_2$$

$$\begin{pmatrix}PC_1\\PC_2\end{pmatrix} \xrightarrow{\text{Reduce Dimensions}} (PC_1)$$

Further reading:
[PCA 1: the basics - simply explained] by [TileStats],
[StatQuest: Principal Component Analysis (PCA), Step-by-Step] by [StatQuest with Josh Starmer]
Image Credit: https://nirpyresearch.com/classification-nir-spectra-linear-discriminant-analysis-python/

Principal Component Analysis (PCA)



$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \xrightarrow[]{\text{PCA Projection}} \begin{pmatrix} PC_1 \\ PC_2 \end{pmatrix}$$

$$s_1 > s_2$$

$$\begin{pmatrix} PC_1 \\ PC_2 \end{pmatrix} \xrightarrow{\text{Reduce Dimensions}} (PC_1)$$

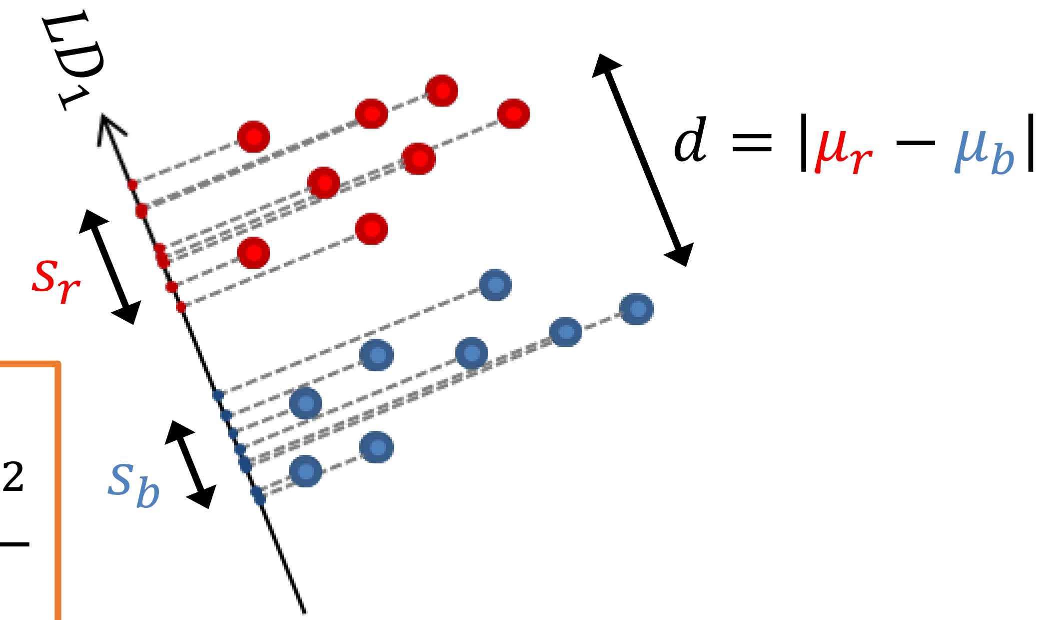
Image Credit: https://ekamperi.github.io/mathematics/2021/02/23/pca-limitations.html

Linear Discriminant Analysis (LDA)

What axis best **distinguishes classes** in the data?

Maximize

$$F = \frac{|\mu_r - \mu_b|^2}{s_r^2 + s_b^2}$$



Further reading: Linear discriminant analysis (LDA) - simply explained by TileStats,
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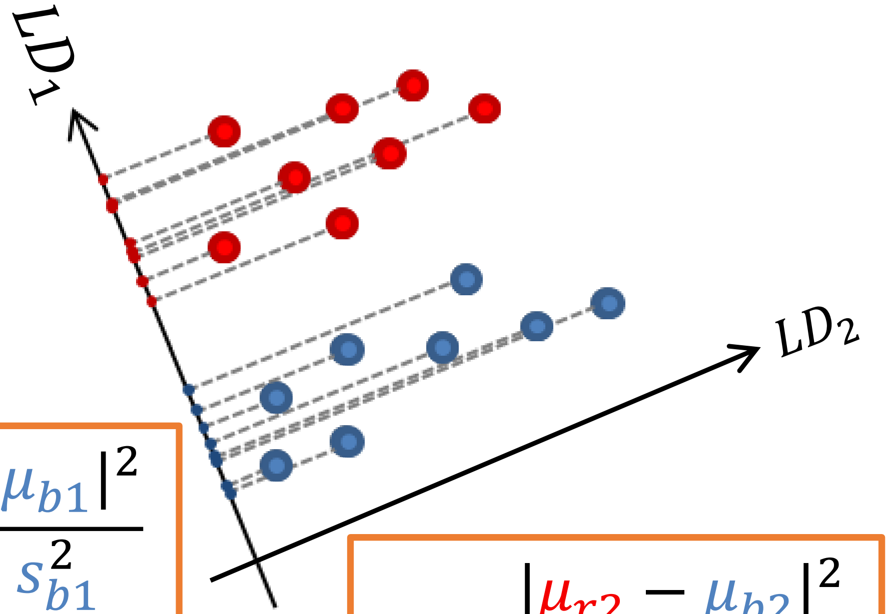
Image Credit: https://nirpyresearch.com/classification-nir-spectra-linear-discriminant-analysis-python/

Linear Discriminant Analysis (LDA)



$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \xrightarrow{\text{LDA Projection}} \begin{pmatrix} LD_1 \\ LD_2 \end{pmatrix}$$

$$F_1 > F_2$$

$$F_1 = \frac{|\mu_{r1} - \mu_{b1}|^2}{s_{r1}^2 + s_{b1}^2}$$

$$F_2 = \frac{|\mu_{r2} - \mu_{b2}|^2}{s_{r2}^2 + s_{b2}^2}$$

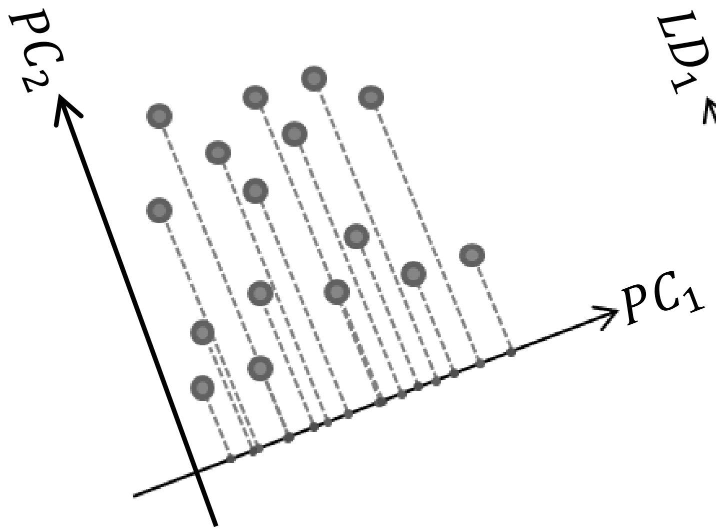
$$\begin{pmatrix} LD_1 \\ LD_2 \end{pmatrix} \xrightarrow{\text{Reduce Dimensions}} (LD_1)$$

Further reading: Linear discriminant analysis (LDA) - simply explained by TileStats,
StatQuest: Linear Discriminant Analysis (LDA) clearly explained by StatQuest with Josh Starmer
Image Credit: https://nirpyresearch.com/classification-nir-spectra-linear-discriminant-analysis-python/

PCA and LDA

PCA

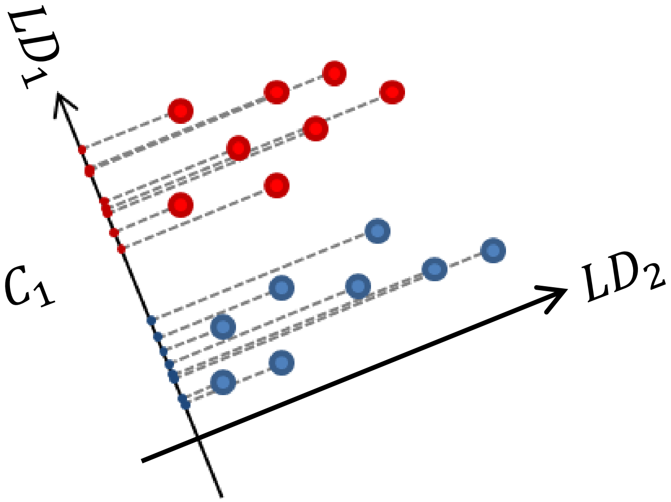
Maximize Data Variance



Good for
dimensionality reduction
for supervised regression

LDA

Maximize Class Separation



Good for
dimensionality reduction
for supervised classification
and unsupervised learning

Steps

- All axes are orthogonal (independent)

1. **Identify** basis vectors
2. **Rank** basis vectors by importance
3. **Truncate** selection of basis vectors
   - Keeps more important features
   - Performs dimensionality reduction


Questions!

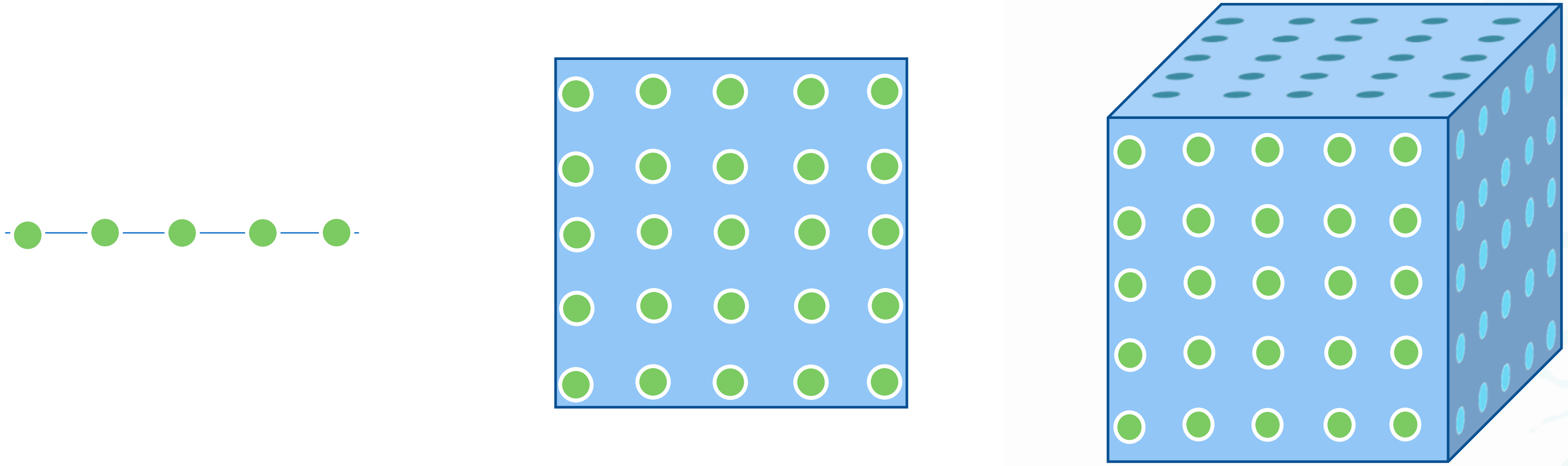
Curse of Dimensionality

Sparsity with high dimensions

$m = 5$
$n = 1$

$m = 25$
$n = 2$

$m = 125$
$n = 3$



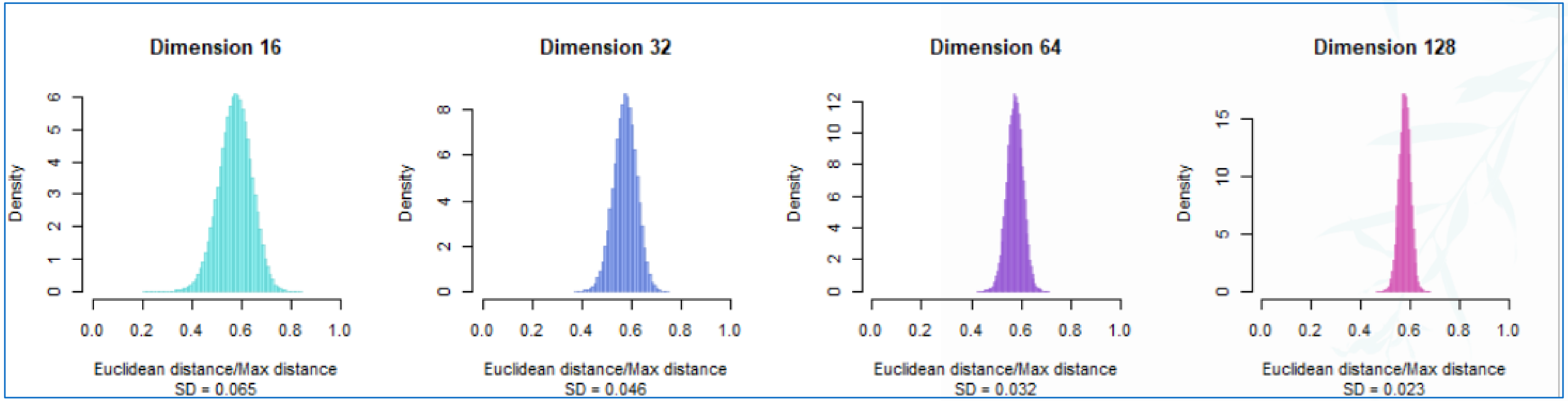
Sparsity problem: maintaining density of samples depends on exponential growth of the data

Chart illustration idea: Stanford CS229N

Curse of Dimensionality

In high dimensional space, most points are nearly the same distance away.

The result: learners that depend on distance break down in high dimensions.



https://stats.stackexchange.com/questions/451027/mathematical-demonstration-of-the-distance-concentration-in-high-dimensions

Issue: Curse of Dimensionality

1. **What** is the issue?
    1. Too many **features**; many more features than instances
2. **Why** is it a problem?
    1. Data too sparse to inform about true decision boundary (for classification) => Too easy to fit a model on sparse training data => Overfitting
    2. Distances are too similar (bad for kNN [W02], clustering [W11])
3. **When** would it happen?
    1. Extracted more features than data instances (i.e., $n \gtrsim m$)
    2. Unstructured data (e.g., features as image pixels, sensor readings)

Issue: Curse of Dimensionality

4. **How** to **check** for it?

- Visualize histogram of **distances** (check for **variance** σ^2)

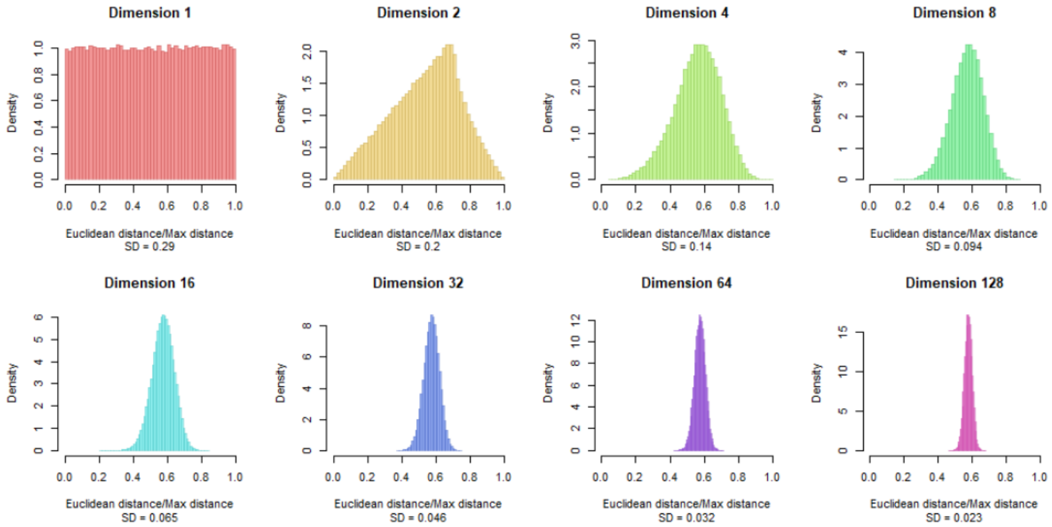


Image Credit: https://www.mygreatlearning.com/blog/understanding-curse-of-dimensionality/

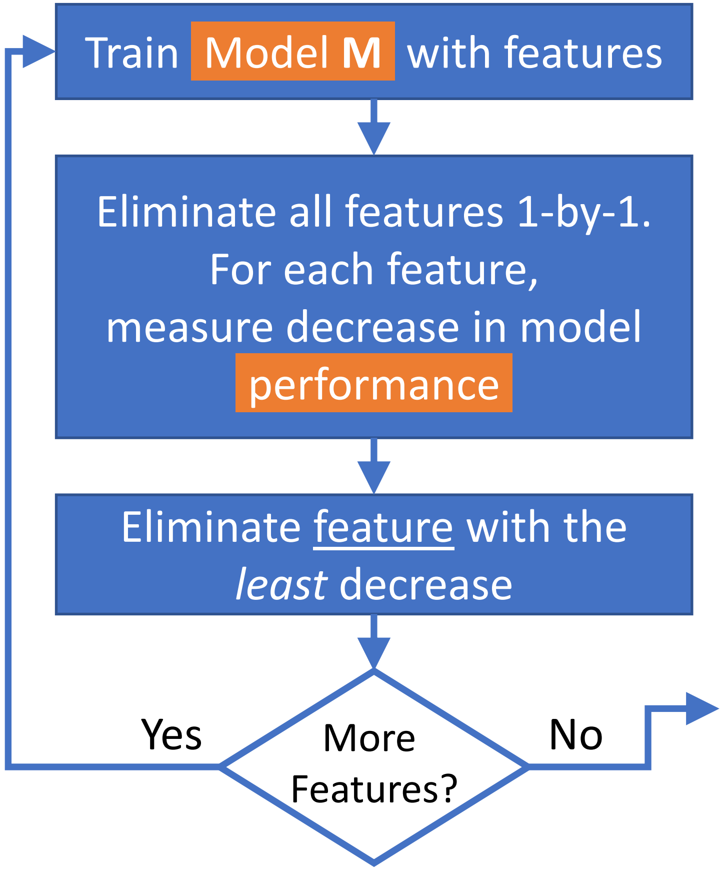
Generally tedious to analyze this; just aim for: $n < m/5$

Issue: Curse of Dimensionality

5. **How** to **mitigate** it?
   - Feature Selection
     - Wrapper methods
     - Filter methods

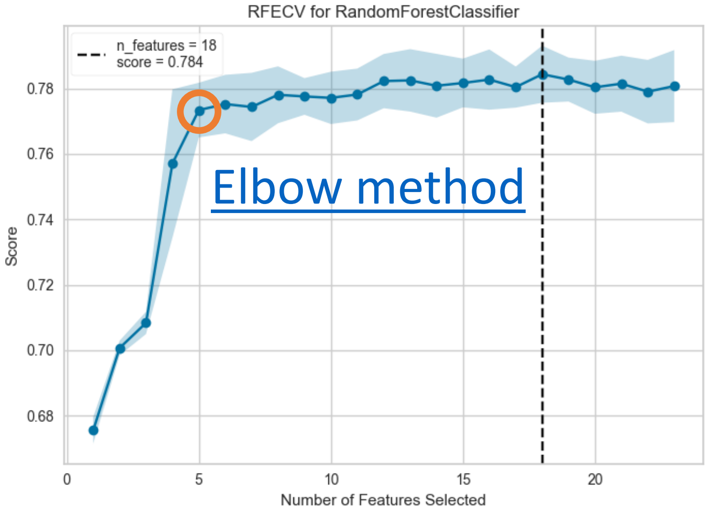
Issue: Curse of Dimensionality

5. **How** to **mitigate** it?
    - Feature Selection
        - **Wrapper methods** (e.g., [RFE]())
        - Filter methods



Recursive Feature Elimination (RFE)

Image Credit: https://www.scikit-yb.org/en/latest/api/model_selection/rfecv.html



Issue: Curse of Dimensionality

5. **How** to **mitigate** it?

- Feature Selection
  - Wrapper methods
  - **Filter methods**
    - Mutual Information = Information Gain [W03b]
    - Correlation

Recap W03a (slides 22-28)

Information gain

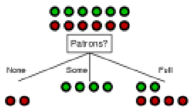
A chosen feature x_i divides the example set S into subsets $S_1, S_2, \dots, S_c$ according to the C_i distinct values for x_i.
The entropy then reduces to the entropy of the subsets $S_1, S_2, \dots, S_c$:

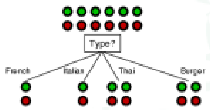
$$\text{remainder}(S, x_i) = \sum_{j=1}^{C_i} \frac{|S_j|}{|S|} H(S_j)$$

Information Gain (IG; "reduction in entropy") from knowing the value of x_i.
Choose the attribute with the largest IG:

$$\boxed{\text{IG}(S, x_i) = H(S) - \text{remainder}(S, x_i)}$$

For the training set at the root,
$p = n = 6,\ H\left(\frac{6}{12}, \frac{6}{12}\right) = 1$ bit.





Consider the attributes *Patrons* and *Type*:

$$IG(\textit{Patrons}) = 1 - \left[\frac{2}{12} H(0,1) + \frac{4}{12} H(1,0) + \frac{6}{12} H\left(\frac{2}{6}, \frac{4}{6}\right)\right] = 0.541 \text{ bits}$$

$$IG(\textit{Type}) = 1 - \left[\frac{2}{12} H\left(\frac{1}{2}, \frac{1}{2}\right) + \frac{2}{12} H\left(\frac{1}{2}, \frac{1}{2}\right) + \frac{4}{12} H\left(\frac{2}{4}, \frac{2}{4}\right) + \frac{4}{12} H\left(\frac{2}{4}, \frac{2}{4}\right)\right] = 0 \text{ bits}$$

Patrons has the highest IG, and so is chosen by DTL as the root.

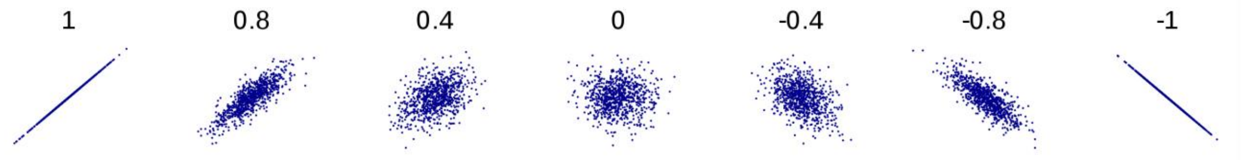
Further Reading: https://machinelearningmastery.com/feature-selection-with-real-and-categorical-data/, https://towardsdatascience.com/feature-selection-for-machine-learning-3-categories-and-12-methods-6a4403f86543

Issue: Curse of Dimensionality

5. **How** to **mitigate** it?

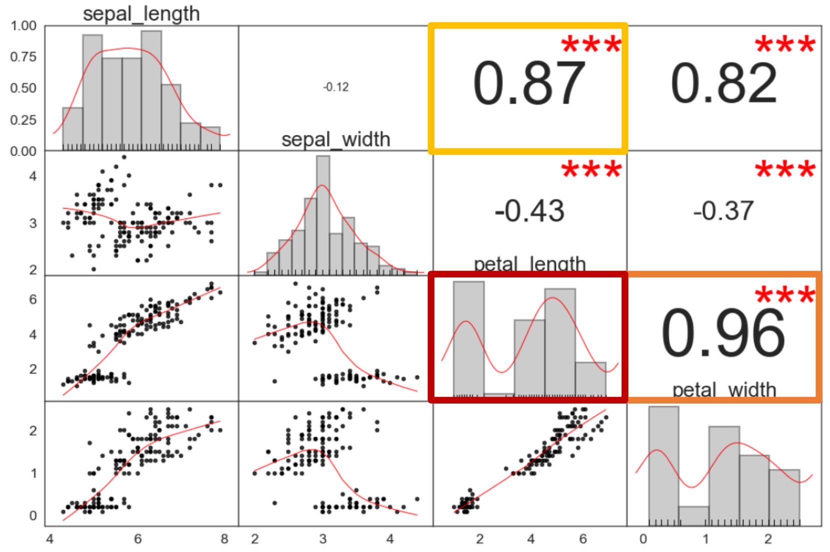
- Feature Selection
  - Wrapper methods
  - **Filter methods**
    - Mutual Information
    - <u>Correlation</u>

Pearson Correlation Coefficient



Higher **magnitude** => more **correlated**. $r > 0.7$ is very **high**.
Further reading: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient

Pearson Correlation Coefficients
for Iris (flower) dataset



`petal_length` is highly correlated to **`petal_width`** and **`sepal_length`**
=> Should remove, due to redundancy

Issue: Curse of Dimensionality

5. **How** to **mitigate** it?
   - Feature Selection
   - Dimensionality Reduction
     - Linear Matrix Factorization (e.g., PCA, LDA)
     - Non-linear Manifold Learning (e.g., SOM, MDS, t-SNE, UMAP)
     - Deep Auto-Encoders

Only these are **examinable**

Further reading:
https://machinelearningmastery.com/dimensionality-reduction-for-machine-learning/

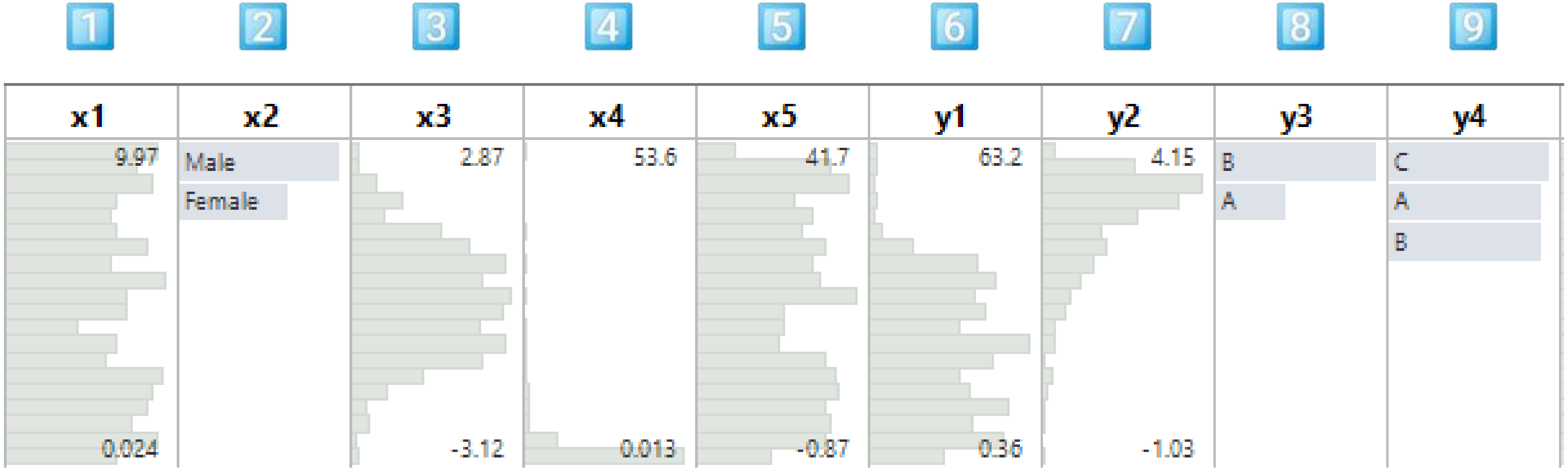
Benefits of Feature Selection

- Avoid Curse of Dimensionality
- Faster model training (optimizing fewer parameters on fewer features)
- Fewer features to read => easier to interpret

Imbalanced Data

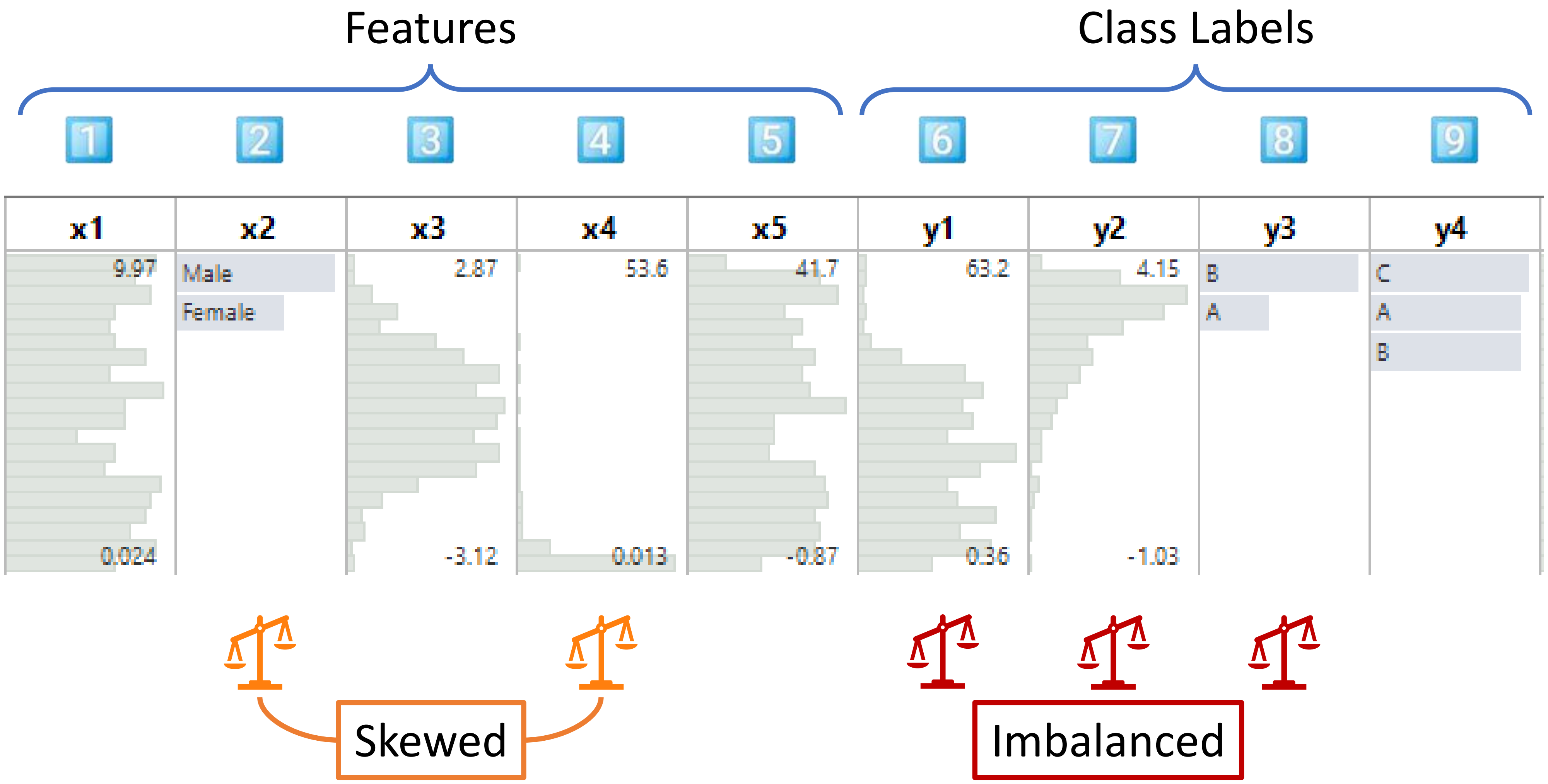
Department of Computer Science
School of Computing

Which of the following variables (columns) are imbalanced?



Emote (react) in Slack #general channel <u>one or more options</u> (MRQ)

Which of the following variables (columns) are imbalanced?



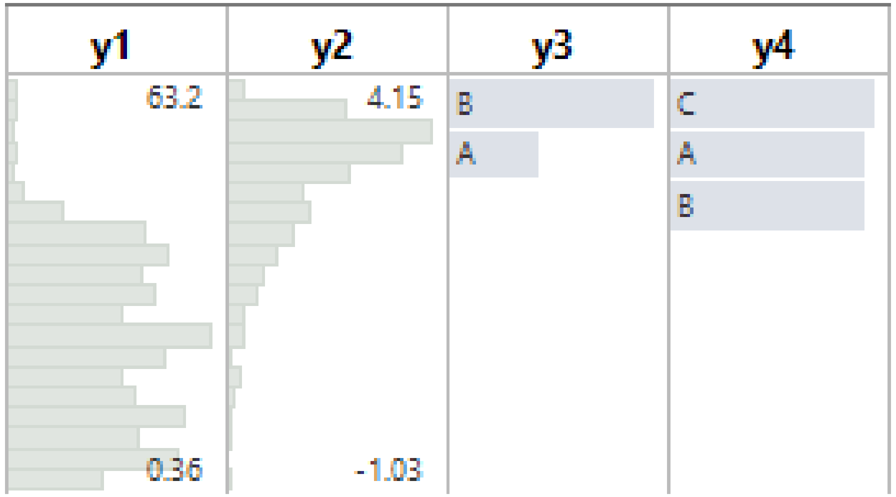
Issue: Imbalanced Data

1. **What** is the issue?
    1. Values not evenly distributed in feature
    2. Data may be skewed
2. **Why** is it a problem?
    1. Evaluation metrics become misleading to interpret [W07b]
    2. Models overfit to majority class
3. **When** would it happen?
    1. When events unevenly occur (e.g., rare cancer)
    2. When data collection is uneven (e.g., only positive survey respondents)

Issue: Imbalanced Data

4. How to **check** for it?

- Visualize **histogram** or **bar chart** of feature values



Issue: Imbalanced Data

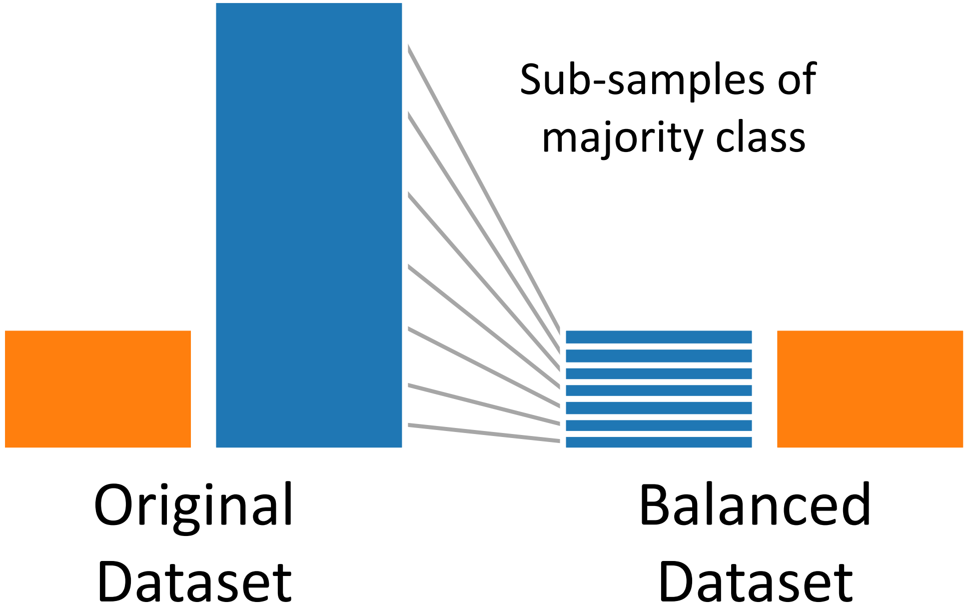
5. **How** to **mitigate** it?
   - Collect more data instances
   - Resample instances (e.g., Undersampling, Oversampling, SMOTE)

Further reading:
https://machinelearningmastery.com/dimensionality-reduction-for-machine-learning/

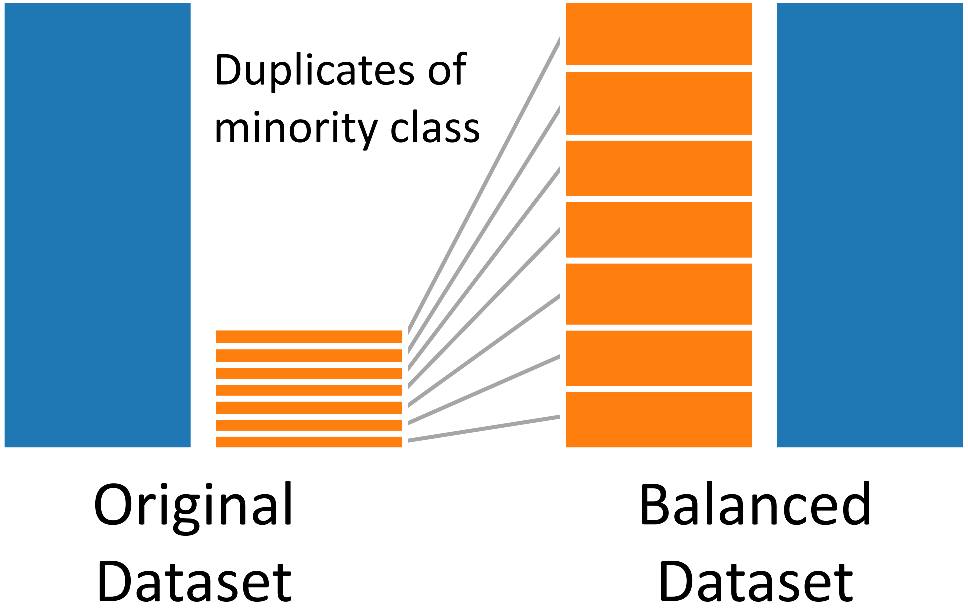
Data Resampling

Image credit: https://www.analyticsvidhya.com/blog/2020/07/10-techniques-to-deal-with-class-imbalance-in-machine-learning/

Undersampling

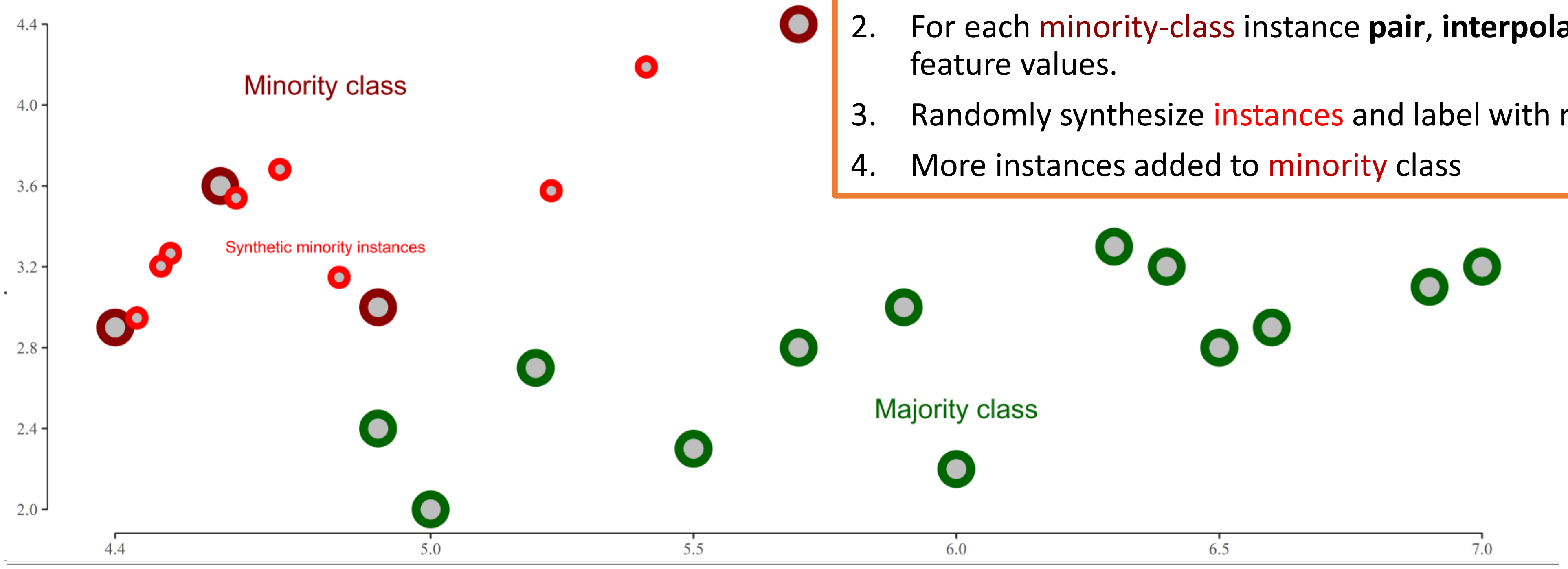


Oversampling



Data leakage (snooping): remember to **first split** dataset to train–test, then **resample** train and test datasets separately

Synthetic Minority Oversampling Technique (SMOTE)

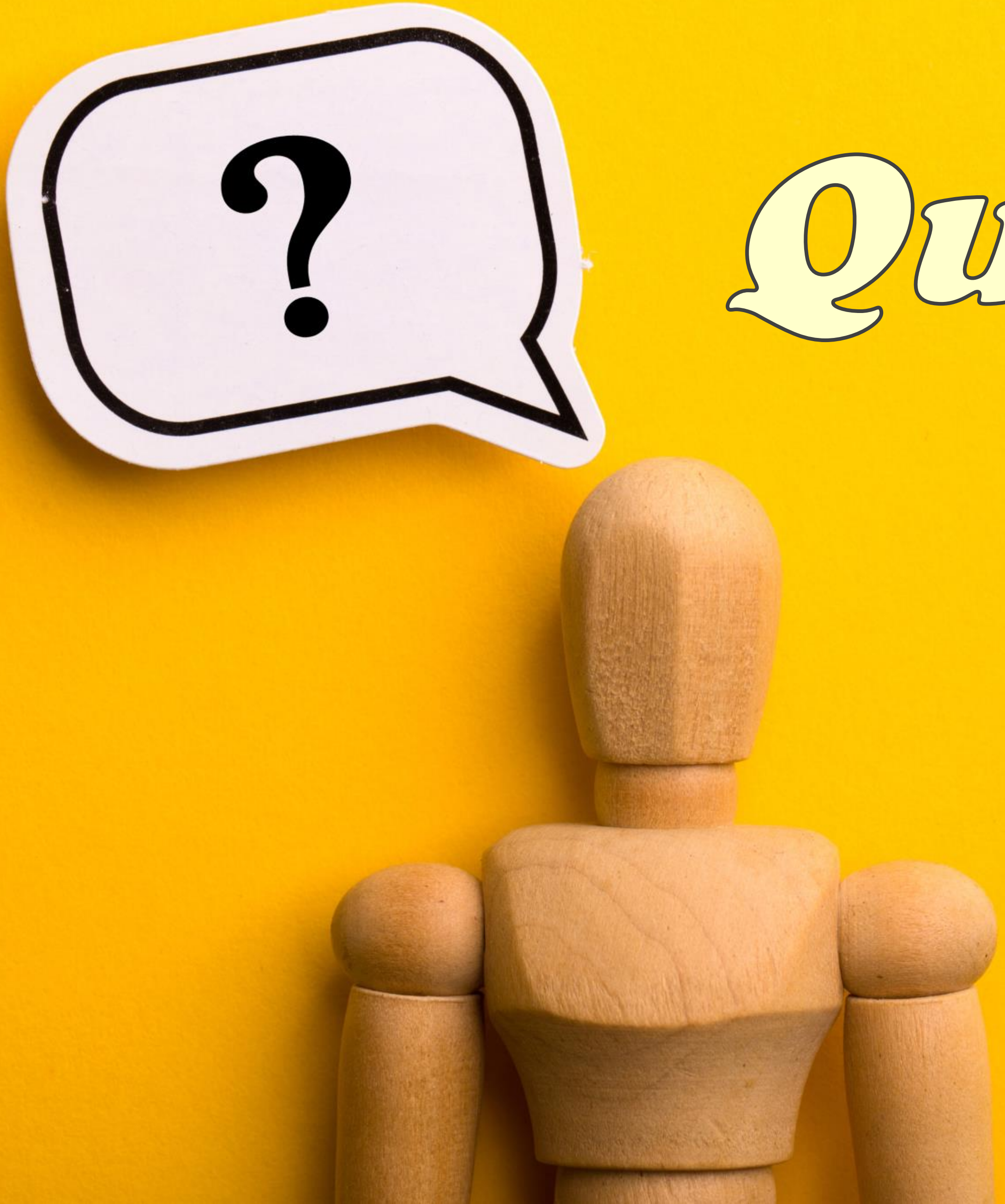


Steps

1. Consider minority and majority instances in vector space.
2. For each minority-class instance **pair**, **interpolate** their feature values.
3. Randomly synthesize instances and label with minority class
4. More instances added to minority class

Image Credit: https://www.quora.com/Can-you-explain-me-SMOTE-Synthetic-Minority-Over-sampling-Technique-in-simple-terms

Questions!



Wrapping Up

What did we learn this week?

Data **Issues**

1. Linear Separability
2. Curse of Dimensionality
3. Imbalanced Data

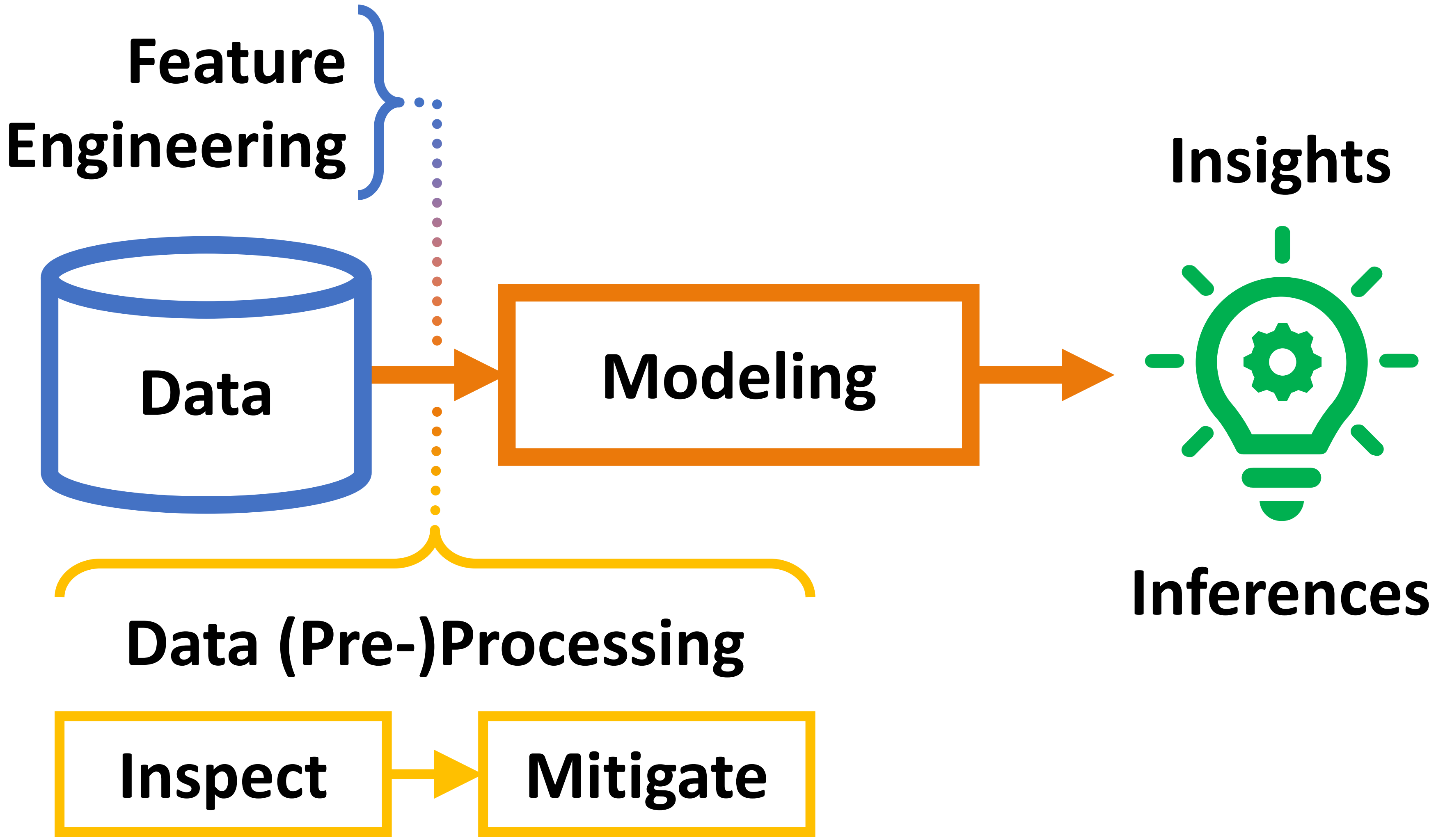
Issue Template

1. **What** is the issue?
2. **Why** is it a problem?
3. **When** would it happen?
4. **How** to **check** for it?
5. **How** to **mitigate** it?

Mitigations

1. Linear PCA, LDA
   (for Linear Separability, Dimensionality Reduction)
2. Feature Selection
   (Recursive Feature Elimination, Correlation, Mutual Information)
3. Resampling
   (Undersampling, Oversampling, SMOTE)

Machine Learning Pipeline



On Thursday: Feature Engineering