Week 3

Machine Learning and Big Data - DATA622

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K-Nearest Neighbor

Classify data according to its k-closest neighbors

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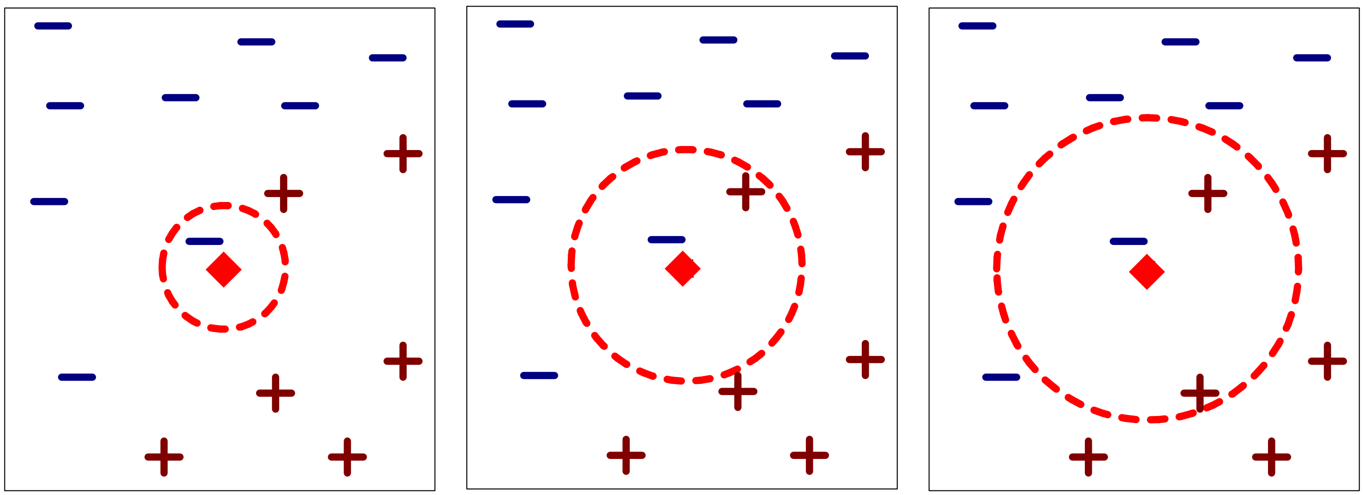
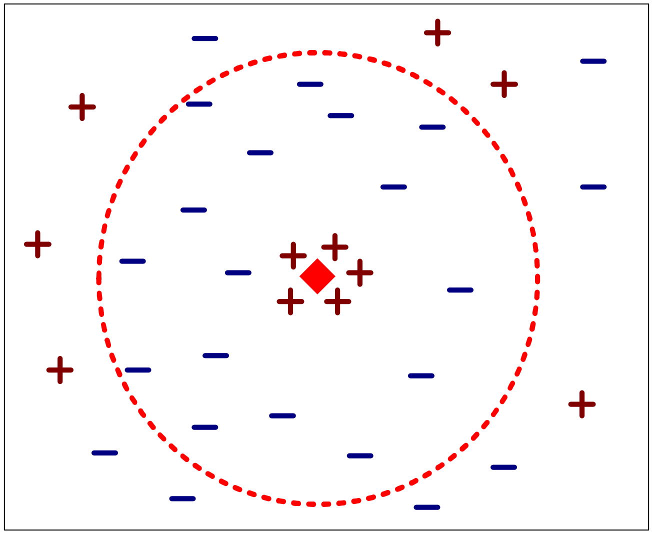
k-Nearest Neighbor (KNN)



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

Choice of k

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other



Rule of thumb:

$$k = \sqrt{N}$$

N: number of training points

Lazy Learning

- Lazy Learning
  - Simply stores training data and delays processing (“lazy evaluation”) until given an input
  - Uses Euclidean distance (straight line, where all dimensions are linear & scaled similarly)
- Eager Learning
  - Given a set of training set, constructs a classification model before inference (prediction)
  - New input uses the classification model (usually the training data is not stored)

- Lazy: Less time in training but more time in inference (prediction)
- Eager: More time in training but less time in inference

PC1

Source: Guide to Intelligent Data Science, Berthold et al

Principal Component Analysis (PCA)

Dimension reduction technique based on maximum variance in data.

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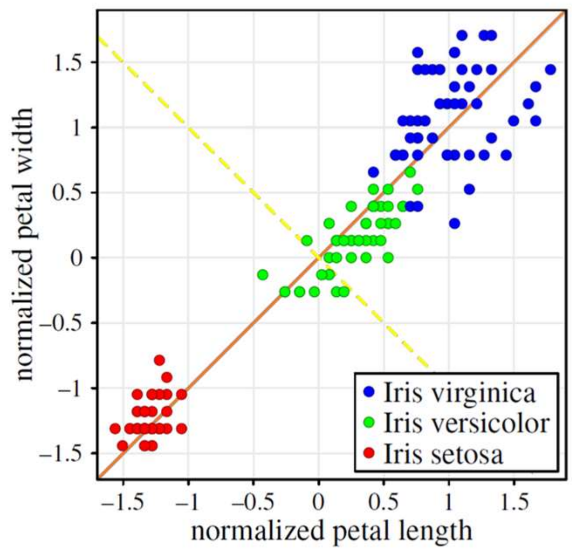
Principal Component Analysis (PCA)

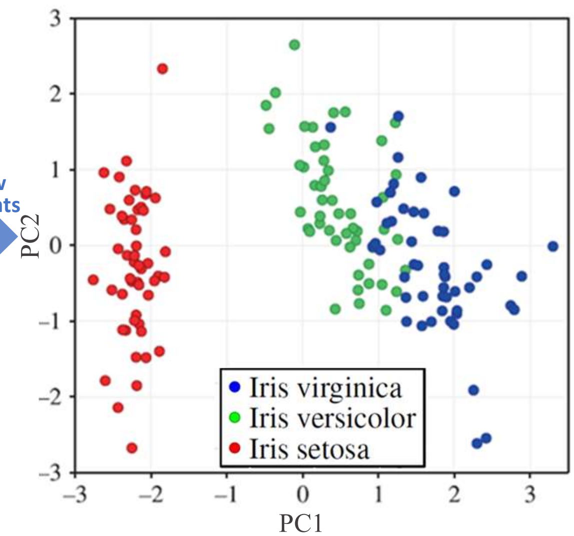
- Dimensionality reduction technique
- Project data from the high-dimensional space to a lower-dimensional space
- Criteria: Maximize data variance to construct principal components

Steps:
1. Construct a line in the direction of maximum variance in data (PC1 = orange line)
2. Next component is orthogonal to the previous component (PC2 = yellow line)

Repeat for as many PC as you need.

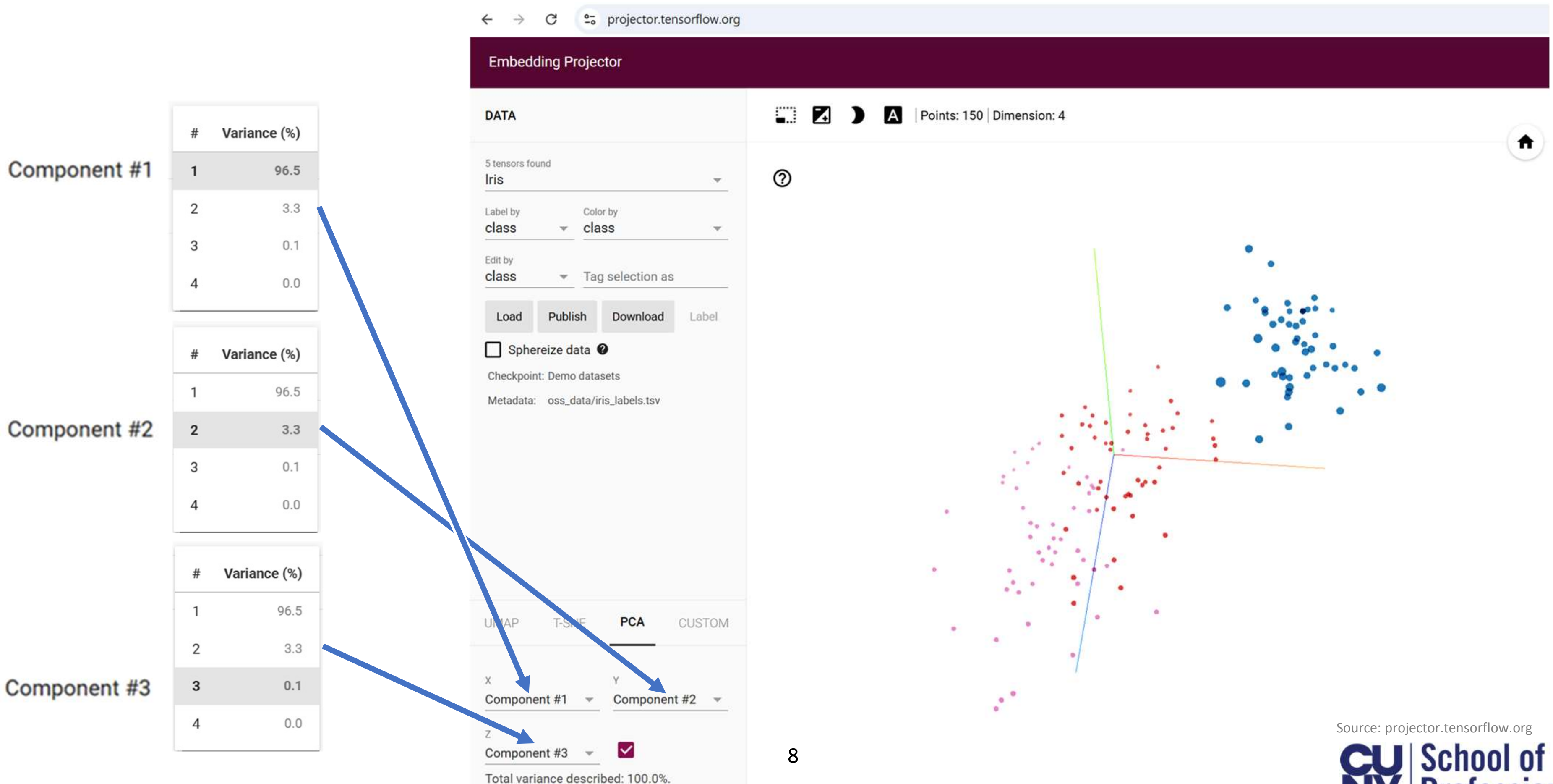


Replot onto new components



Source: Guide to Intelligent Data Science, Berthold et al

Visualization Example



Source: projector.tensorflow.org

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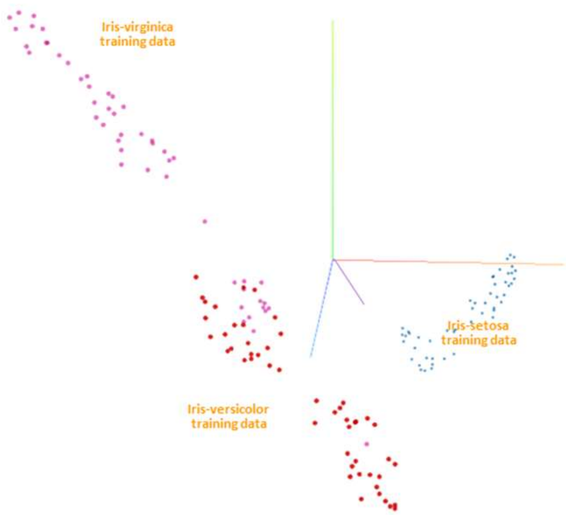
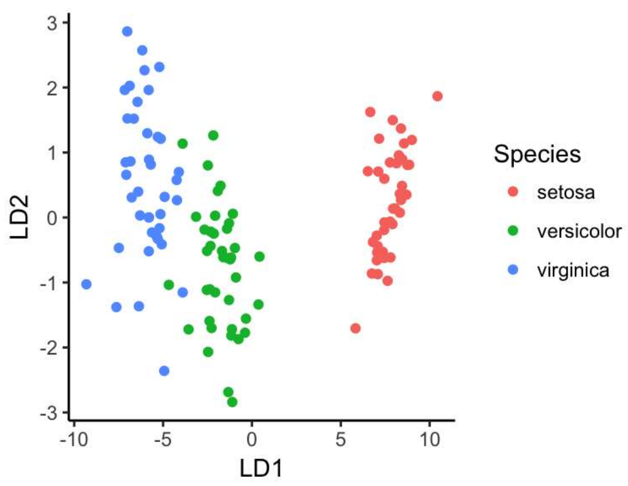
Example: Iris data set

4-dimensional input space



PCA

2-components (2-dimensions)

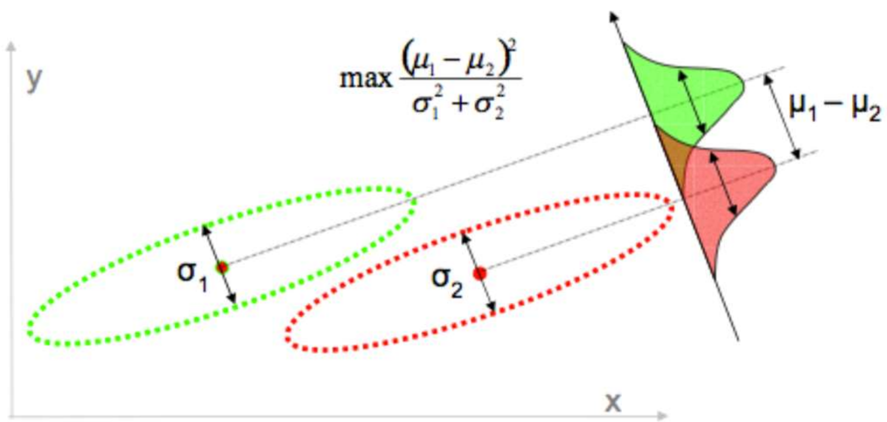


Linear Discriminant Analysis (LDA)

Dimension reduction technique based on maximizing distance between means <u>and</u> minimizing spread.

Linear Discriminant Analysis (LDA)

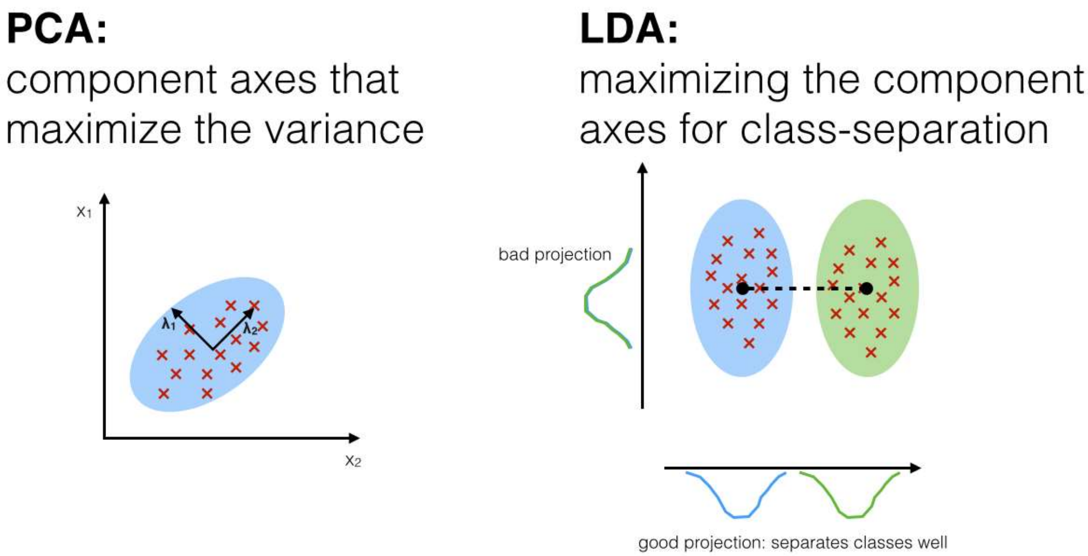
- Dimensionality reduction approach
- Two criteria are used by LDA to create a new axis:
    1. Maximize the distance between means of the two classes.
    2. Minimize the variation (spread) within each class.



Source: Victor Lavrenko

PCA vs LDA

	PCA	LDA
Transformation	Linear	Linear
Supervised vs Unsupervised	Un-supervised	Supervised
Objective	Capture variability by finding principal components	Separate classes by identifying a lower dimension which has better discriminatory power
Type	Component: maximize the variance <u>in the data</u>	Discriminant: maximize the separation <u>between classes</u>
Compute requirements	Low	High
Use-cases	Visualization (and classification)	Any classification



PC1

Source: Guide to Intelligent Data Science, Berthold et al

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PCA vs LDA

- Discriminants (LDA) maximize the separation between classes
- Components (PCA) maximize the variance in the data
- Dimensionality reduction technique
- Project data from the high-dimensional space to a lower-dimensional space
- Criteria: Maximize data variance to construct principal components

PC1

Source: Guide to Intelligent Data Science, Berthold et al

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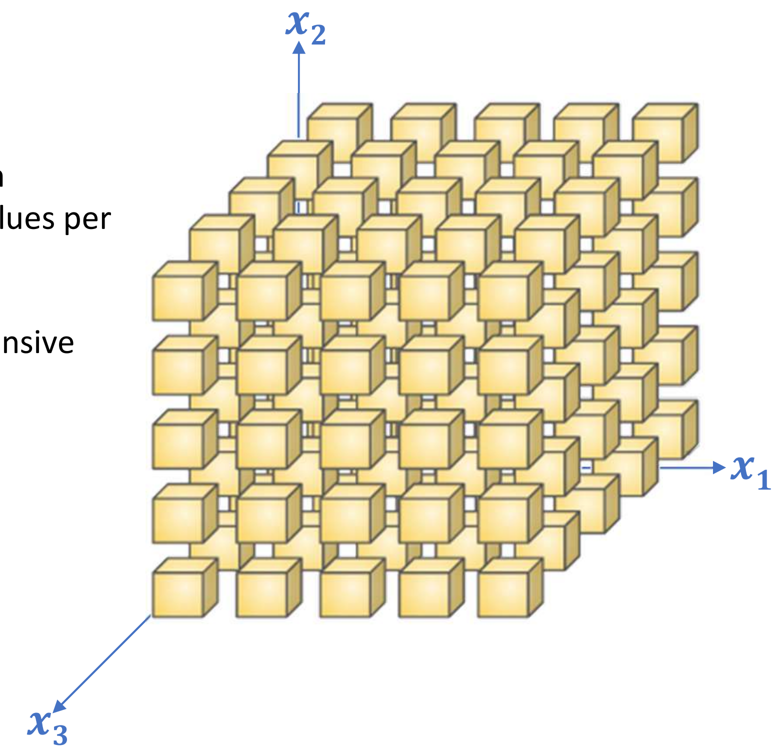
Curse of Dimensionality

As dimensions increase, the data we need to generalize grows exponentially

Curse of dimensionality

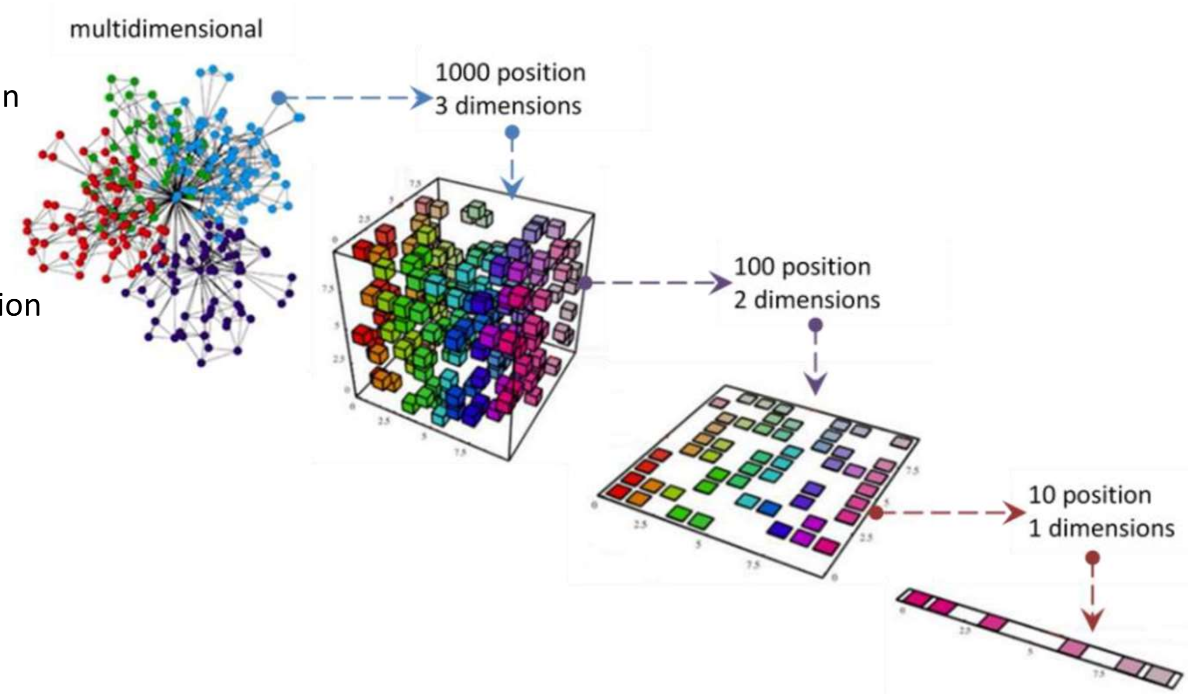
- The Iris data set has 150 instances in 4-dimensions: an average of ~3.5 values per dimension (3.5^4)
- Labeled data is hard to get and expensive (about $2/instance on average for outsourced labeling services)



Source: therbootcamp.github.io

Let’s look at the flip-side

- Dimension reduction results in information loss – important for pattern recognition
- Domain knowledge (understanding data and business context) helps minimize information loss during dimension reduction



Source: Liudmyla Poteriailo et al 2023 IOP Conf. Ser.: Earth Environ. Sci. 1189 012021

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Impact of the Curse of Dimensionality

Issues with too many dimensions:

- Data Sparsity
- Increased distance between points
- Higher computational cost
- Overfitting (due to too many features)
- Difficulty in Visualization & Interpretation
- Data needs grows with dimensions

PC1

Source: Guide to Intelligent Data Science, Berthold et al

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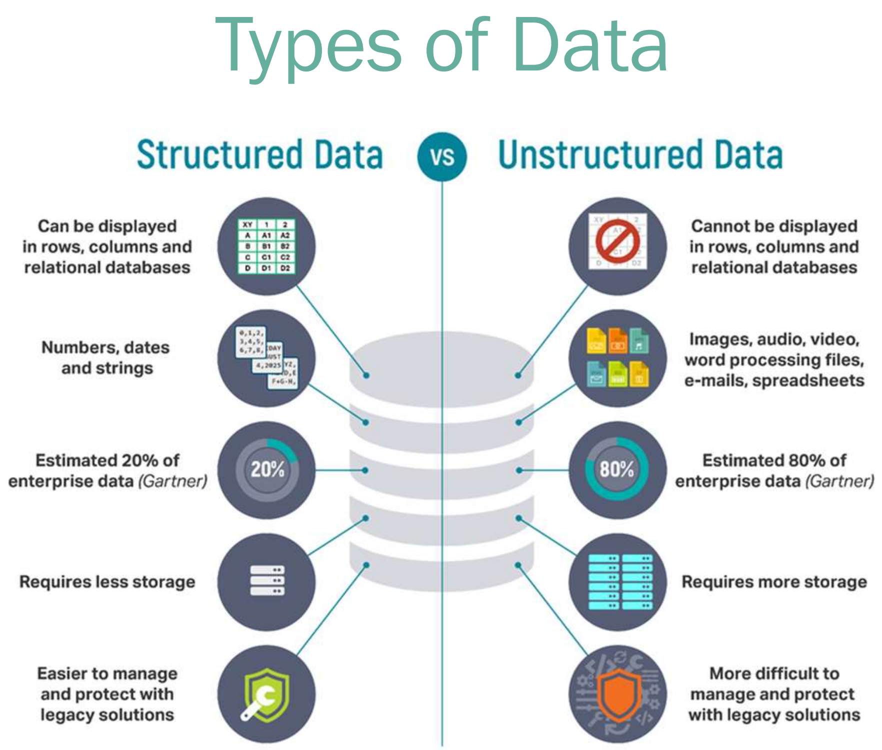
Data point-cloud

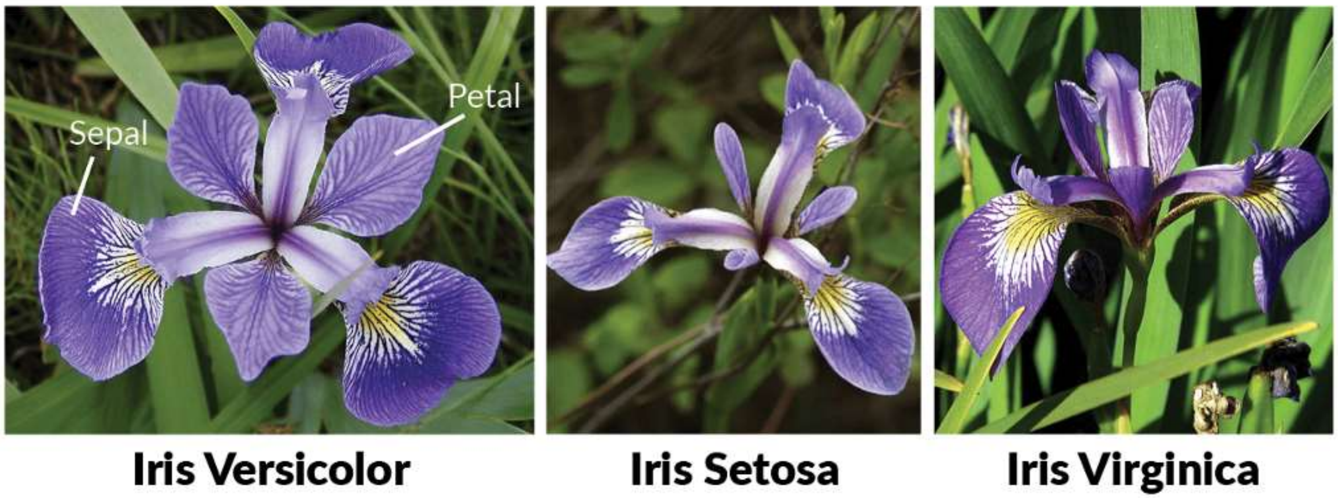
Tabular (structured) data can be plotted on an n-dimensional space (where n=number of input columns in the table). This creates a point-cloud of data points in the table (with each dot a line in the table). Unstructured data can also be plotted – but needs processing first.

Types of Data



Source: igneous.io

Example: Iris data set



Source: Fisher (1936) https://onlinelibrary.wiley.com/doi/epdf/10.1111/j.1469-1809.1936.tb02137.x

Iris data

Data is labeled (with 3 classes).

Features (inputs)

Labels

A single instance

Instance	Sepal Length (cm)	Sepal width (cm)	Petal legth (cm)	Petal width (cm)	Class
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5	3.6	1.4	0.2	Iris-setosa
5	5.4	3.9	1.7	0.4	Iris-setosa

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50	7	3.2	4.7	1.4	Iris-versicolor
51	6.4	3.2	4.5	1.5	Iris-versicolor
52	6.9	3.1	4.9	1.5	Iris-versicolor
53	5.5	2.3	4	1.3	Iris-versicolor
54	6.5	2.8	4.6	1.5	Iris-versicolor
55	5.7	2.8	4.5	1.3	Iris-versicolor
56	6.3	3.3	4.7	1.6	Iris-versicolor

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100	6.3	3.3	6	2.5	Iris-virginica
101	5.8	2.7	5.1	1.9	Iris-virginica
102	7.1	3	5.9	2.1	Iris-virginica
103	6.3	2.9	5.6	1.8	Iris-virginica
104	6.5	3	5.8	2.2	Iris-virginica
105	7.6	3	6.6	2.1	Iris-virginica

Labels (output) will have 3 classes

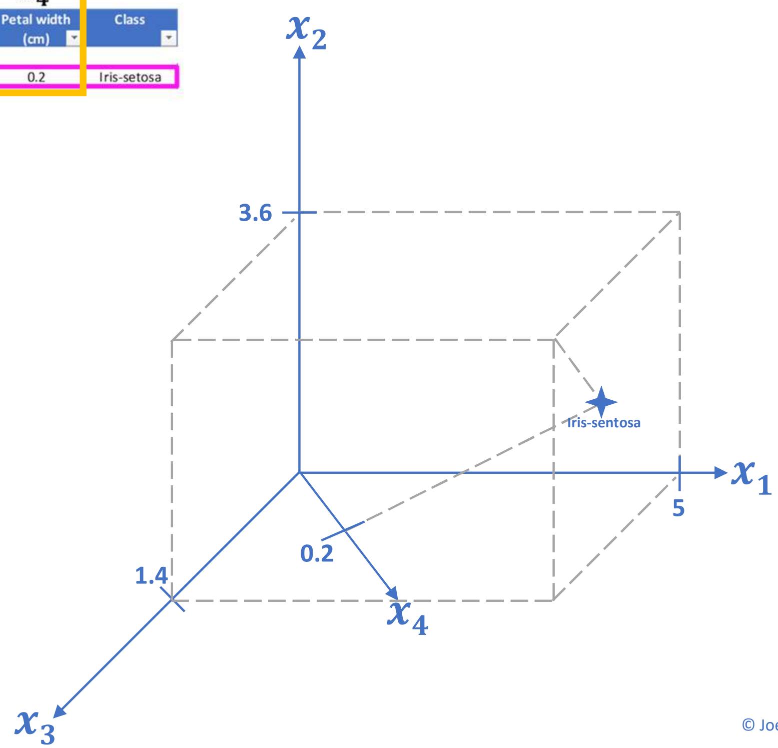
There are 4 features (inputs): x_1, x_2, x_3 & x_4

Features (“Independent inputs”)

A single instance

	x_1	x_2	x_3	x_4	
Instance	Sepal Length (cm)	Sepal width (cm)	Petal legth (cm)	Petal width (cm)	Class
1	5	3.6	1.4	0.2	Iris-setosa

- Every feature is a dimension
  4 features = 4 dimensions
- An instance is a single point in that 4-dimensional space
- All of the data forms a point- cloud in that 4-dimensional space



Demo

projector.tensorflow.org

One-hot encoding

- ML requires numbers: labels must be converted to numbers
- Each class (type of label must be its own dimension)
- The value in each dimension conveys the probability it is of that class
- Training Data Labels always have a probability of 1 (100%) i.e. they are the “Ground Truth”

Labels → **One-Hot Encoding** → **Labels**

$(y_1, y_2, y_3) = (1,0,0)$

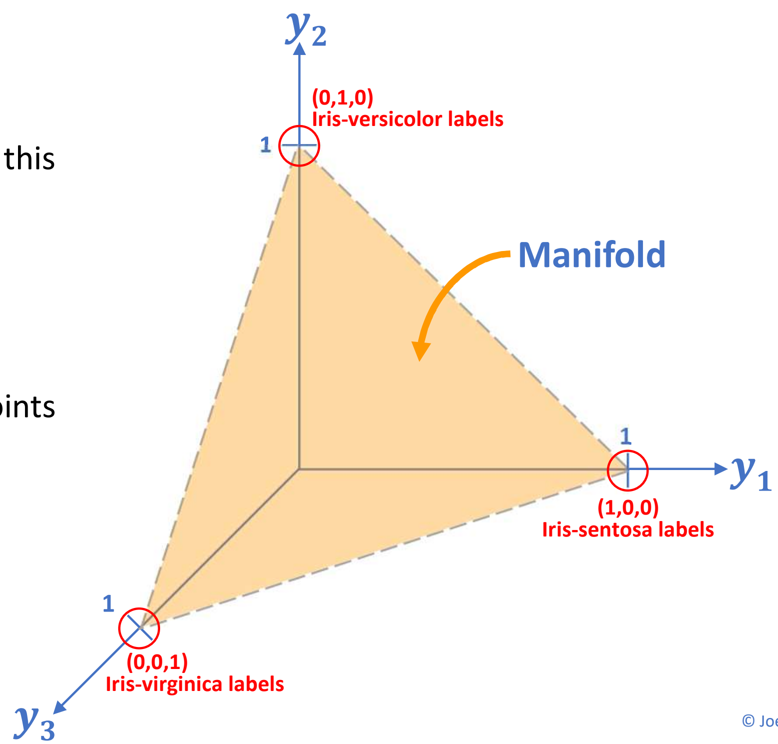
$(0,1,0)$

$(0,0,1)$

Class	Class1 iris-setosa	Class2 iris-versicolo	Class3 iris-virginica
Iris-setosa	1	0	0
Iris-setosa	1	0	0
Iris-setosa	1	0	0
Iris-setosa	1	0	0
Iris-setosa	1	0	0
Iris-setosa	1	0	0
• • •		• • •	
Iris-versicolor	0	1	0
Iris-versicolor	0	1	0
Iris-versicolor	0	1	0
Iris-versicolor	0	1	0
Iris-versicolor	0	1	0
Iris-versicolor	0	1	0
Iris-versicolor	0	1	0
• • •		• • •	
Iris-virginica	0	0	1
Iris-virginica	0	0	1
Iris-virginica	0	0	1
Iris-virginica	0	0	1
Iris-virginica	0	0	1
Iris-virginica	0	0	1

Solution Manifold

- The number of dimensions = number of classes. In this case 3 dimensions.
- A Label (or prediction) is one data-point in that 3-dimensional space
- Probabilities of all classes add up to 1 (100%) so points lie on a manifold
- Only labels have values of 1



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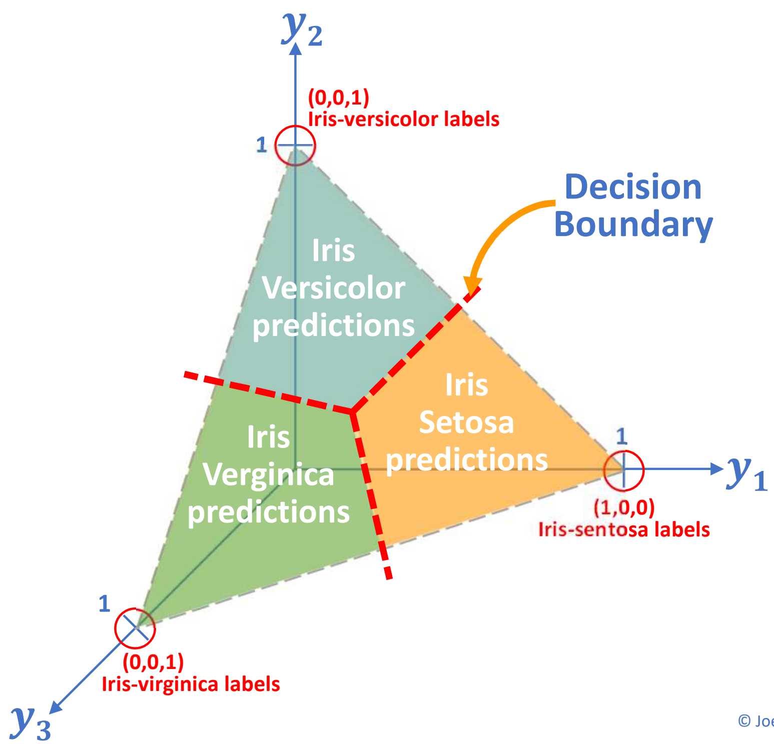
Decision Boundary

- A decision boundary separates the classes.
- For 2 classes the decision boundary is typically 0.5 (when probability of either class is 50%)
- It may be linear or non-linear



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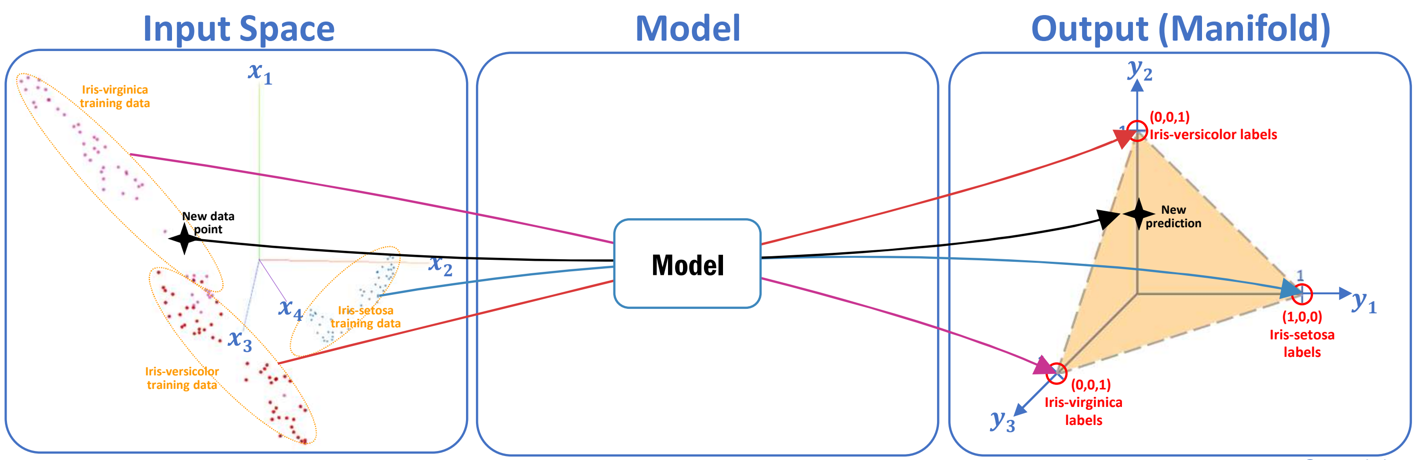
Putting it together

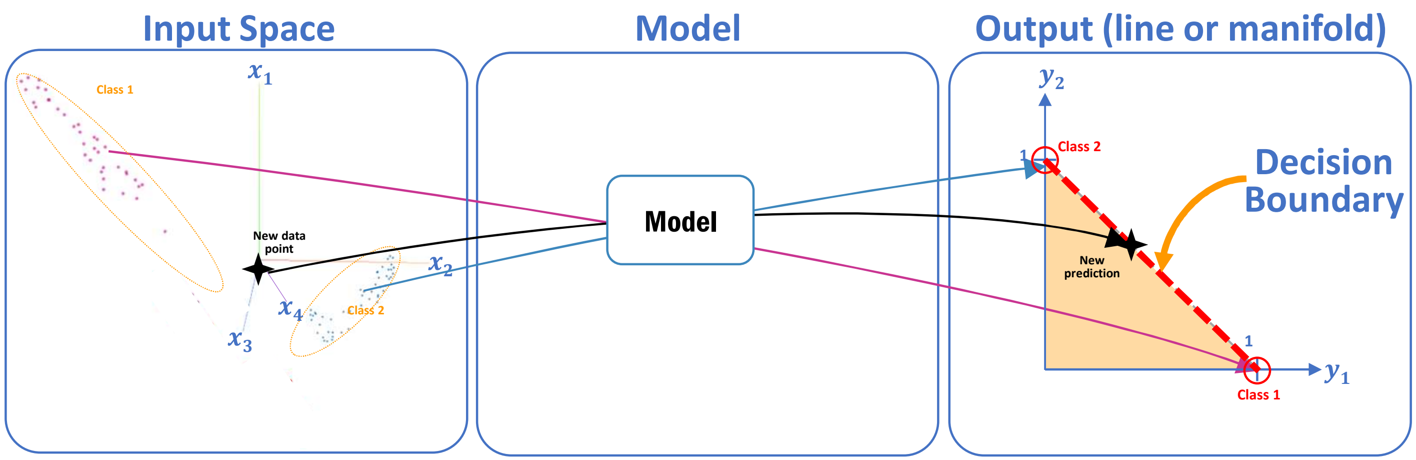
Three class results in a 3-dimensional output space, with the prediction landing on a line where: p($\boldsymbol{y_1}$) + p ($\boldsymbol{y_2}$) + p ($\boldsymbol{y_3}$) = 1



Supervised Machine Learning. Simplified. Same caveats as before.

2 vs 3 classes

Two class results in a 2-dimensional output space, with the prediction landing on a line where: p($\boldsymbol{y_1}$) + p ($\boldsymbol{y_2}$) = 1



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