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Master in Data Science - Lesson 2

Introduction to Machine Learning

What is Machine Learning ?

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Definition

“Machine learning is the field of study that gives computers the ability to learn without being explicitly programmed”

Arthur L. Samuel, AI pioneer, 1959

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“Machine learning is the field of study that gives computers the ability to learn without being explicitly programmed”

Arthur L. Samuel, AI pioneer, 1959

Without ML	With ML
I have to explicitly encode computer behavior	Computers learn without direct involvement of programmer

What is a model?

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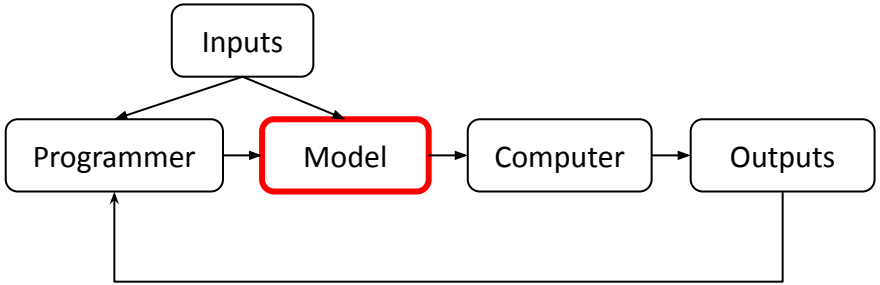
- In **physics** a *model*, it is a representation (simplified) of a system
  - It is much simpler and idealized than a real system
  - Eg. the shape of the Earth not actually a sphere, but we might treat it as one if we are designing a globe.

- In **machine learning**
  - A model is the output of a machine learning algorithm run on data.
  - definition by Tom Mitchell:
    - *"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E."*

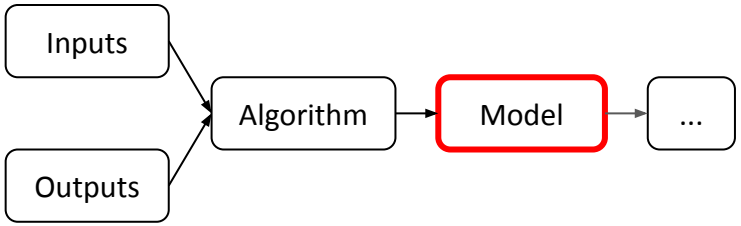
What is Machine Learning?

The paradigm shift

The Traditional Programming Paradigm

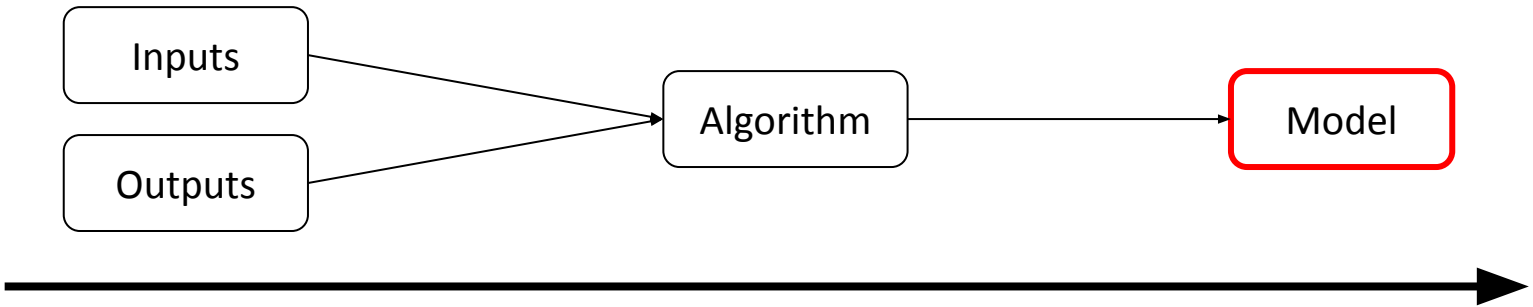


Machine Learning



What is Machine Learning?

The new paradigm



Data

Gets better with more training examples and bigger computers

Algorithm

Statistics
Optimization
Computer science

Program

Given examples (*training data*), make a machine learn how to predict on new samples, or discover patterns in data.

What is Machine Learning?

Model for predictive tasks

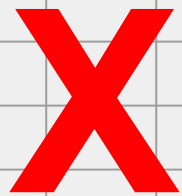
- I want to predict *Event E*.
  - Ideally, I would like to measure it, but because I can't measure it directly, the next best thing I can do is to predict it
  - Eg. As real estate agent I want to estimate (predict) if I sell this house (yes/no)

- I can observe **some** properties related to the Event E.
  - Eg. I can observe m^2, number of bedrooms, garage yes/no, garden yes/no, etc..
  - Eg. I can't measure house foundation, client's real budget, neighbour friendliness

What is Machine Learning?

Model for predictive tasks

x1	x2	x3	x4	x5	x6	x7	y
							0
							0
							0
							0
							1
							1
							1
							1



m^2, number of bedrooms, garage yes/no, garden yes/no

house foundation, client's real budget, neighbour friendliness

1 = yes
0 = no

- I can't directly measure **y**
- Using **x1**, **x2**, **x3**, **x4**, **x5**, **x6**, **x7** I would perfectly predict **y**
- I can observe (and measure) **x1**, **x2**, **x3**, **x4**
- I can't observe **x5**, **x6**, **x7**
- I use **x1**, **x2**, **x3**, **x4** to predict **y** (with some errors)

Variation is information (monovariate)

x	y
3	0
3	0
3	0
3	0
3	1
3	1
3	1
3	1

x gives no information to predict **y**

x	y
3	0
3	0
5	0
5	0
5	1
5	1
5	1
5	1

x gives some information to predict **y**

x	y
3	0
3	0
3	0
3	0
5	1
5	1
5	1
5	1

x gives perfect information to predict **y**

Variation is information (multivariate)

x1	x2	y
5	3	0
5	3	0
5	3	0
5	3	0
5	3	1
5	3	1
5	3	1
5	3	1

x1 and x2 give no information to predict **y**

x1	x2	y
2	1	0
2	3	0
8	6	0
8	6	0
8	6	1
2	4	1
2	5	1
2	5	1

x1 and x2 give some information to predict **y**

x1	x2	y
2	1	0
2	3	0
8	7	0
8	6	0
2	6	1
2	4	1
2	5	1
2	9	1

x1 and x2 give some information to predict **y**
(x1 = 2 & x2 > 3 ⟶ 1, else 0)

Structured vs unstructured data

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Structured Data

Set of numbers and labels organized in a tabular format

Databases
Spreadsheets

Semi-structured Data

Loosely organization with categories and meta tags

Emails by Sent / Inbox
Tweets and hashtags
Folders by topic

Unstructured Data

Unorganized data

Media posts, Emails
Video, Images
Speech, Sounds

Machine Learning Categories

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The 3 main Machine Learning categories

Supervised Learning

Labeled data
Direct feedback
Predict outcome
Predict future

Unsupervised Learning

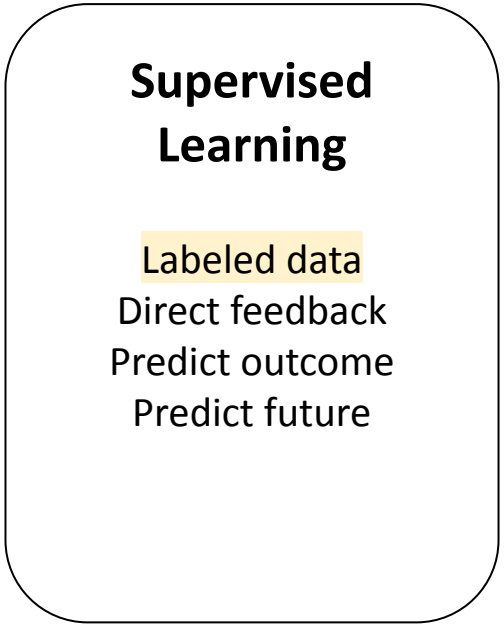
No labels
No feedbacks
Find hidden structures

Reinforcement Learning

Decision process
Reward system
Learn series of action

The 3 main Machine Learning categories

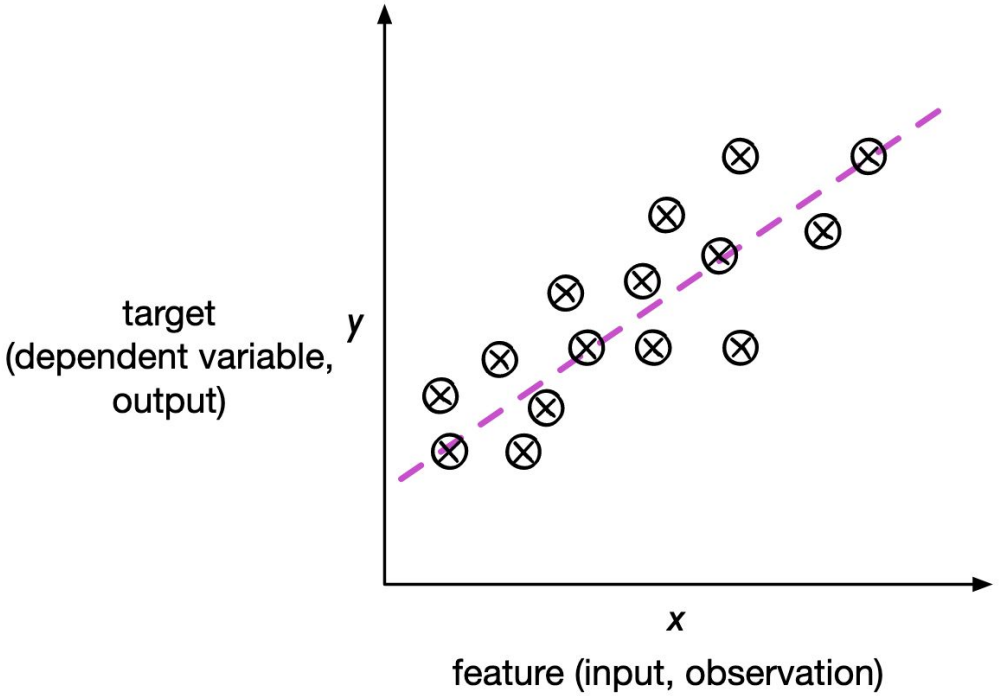
Supervised Learning



Regression

Numerical values

x	y
2	5
4	6
7	10
3	5
..	..



Source: Raschka and Mirjalily (2019). *Python Machine Learning, 3rd Edition*

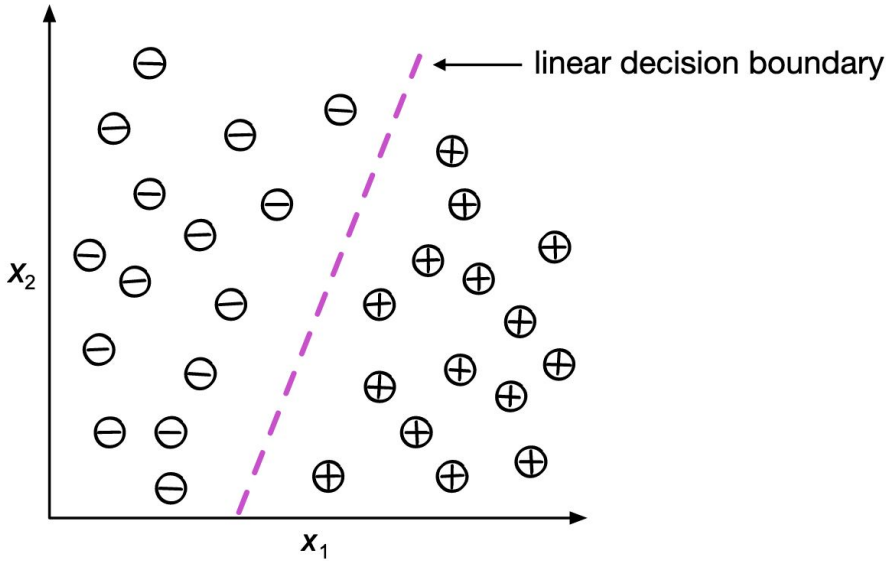
Classification

Categorical values

x1	x2	y
2	5	-
4	10	-
7	-2	+
3	8	+
..	..	..

What are the class labels (y's)?

Binary classification example with two *features* ("independent" variables, predictors)



Source: Raschka and Mirjalily (2019). *Python Machine Learning, 3rd Edition*

Ranking

- Correct order matter

>

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The 3 main Machine Learning categories > Supervised Learning

Ordinal Regression

- Correct label matter
  - Eg. Modeling of human levels of preference (from "very poor" to "excellent")

>

>

★★★★★ ★★★ ★

The 3 main Machine Learning categories

Unsupervised Learning

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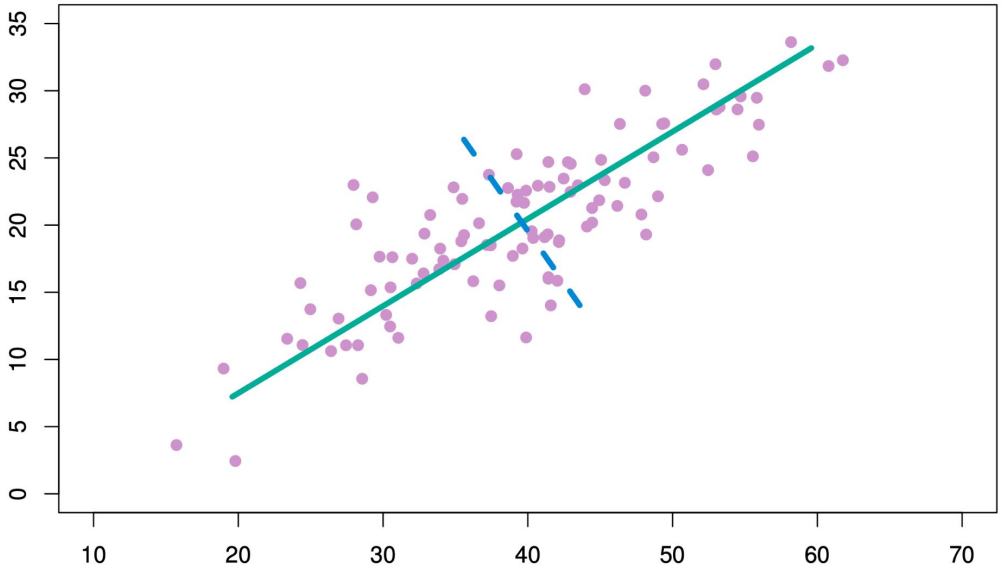
Unsupervised Learning

No labels
No feedbacks
Find hidden structures

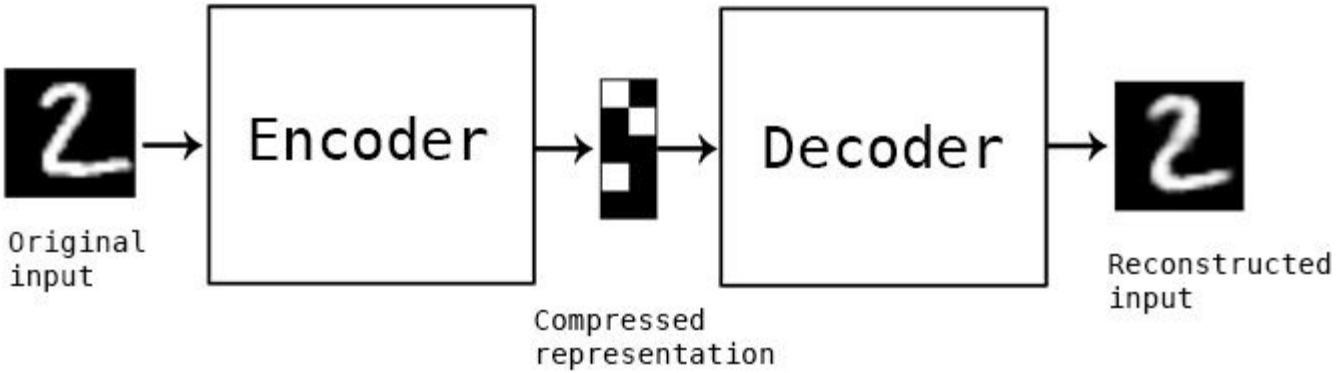
Dimensionality Reduction - PCA

x1	x2
2	5
4	10
7	-2
3	8
..	..



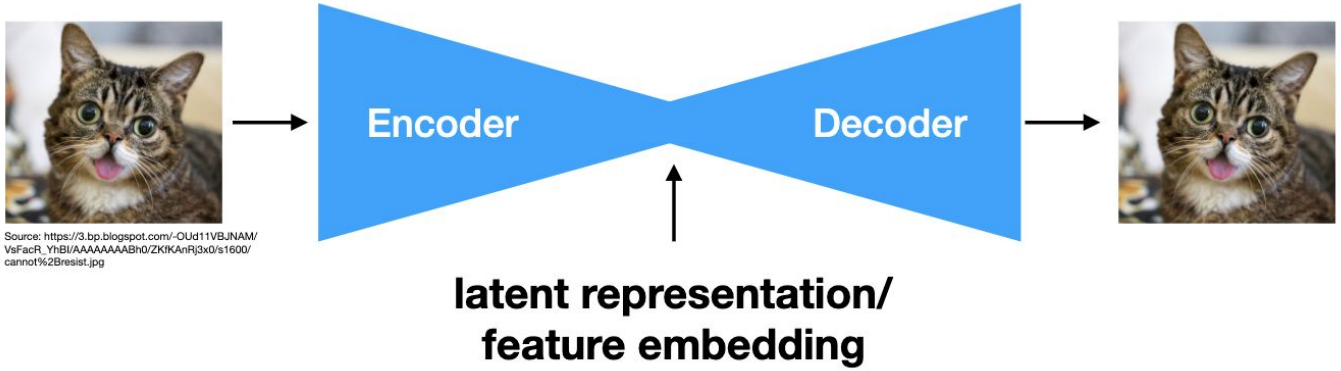
- Maximize the variance of projection along each component
- Minimize the reconstruction error (of the original data)

Dimensionality Reduction - Autoencoders



https://blog.keras.io/building-autoencoders-in-keras.html

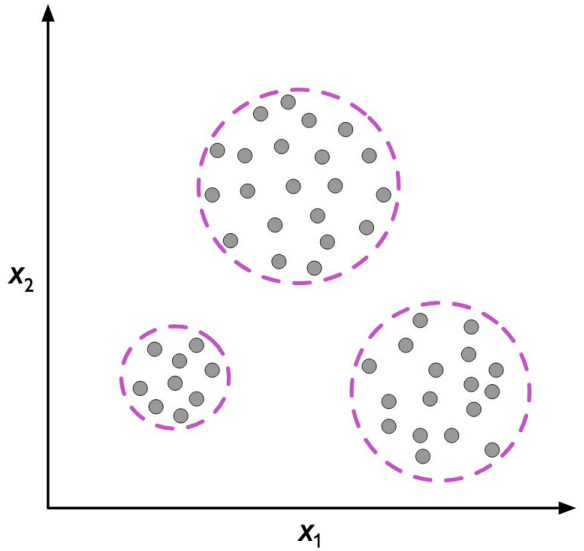
Dimensionality Reduction - Autoencoders



Source: https://3.bp.blogspot.com/-OUd11VBJNAM/VsFacR_YhBI/AAAAAAAABh0/ZKfKAnRj3x0/s1600/cannot%2Bresist.jpg

Clustering

Assigning group memberships to unlabelled examples (instances, data points)



Source: Raschka and Mirjalily (2019). *Python Machine Learning, 3rd Edition*

The 3 main Machine Learning categories

Reinforcement Learning

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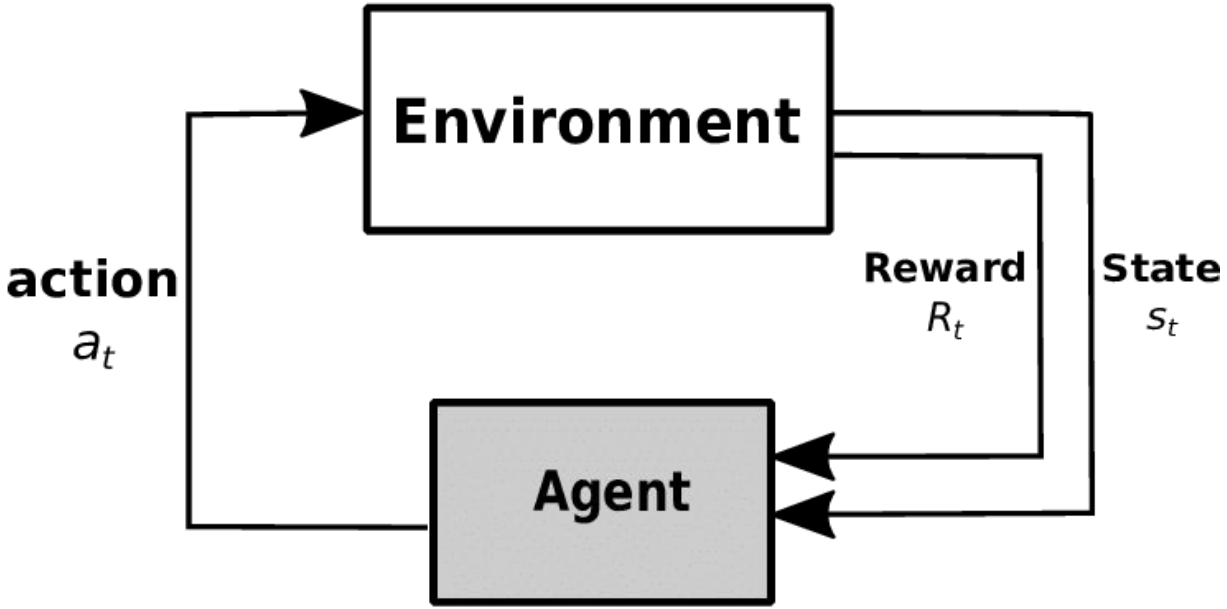
Reinforcement Learning

Decision process
Reward system
Learn series of actions

Reinforcement Learning

Overview



Reinforcement Learning

Lane following task

https://neptune.ai/blog/reinforcement-learning-applications

Terminology & Notation

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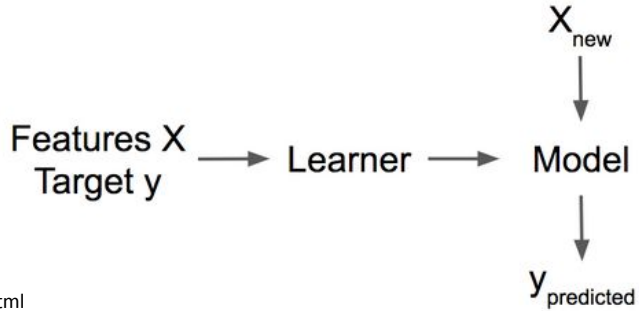
Terminology & Notation

Learner & Model

- A **Learner** or **Machine Learning Algorithm** is the program used to learn a machine learning model from data. Another name is "inducer" (e.g. "tree inducer").

- A **Machine Learning Model** is the learned program that maps inputs to predictions. This can be a set of weights for a linear model or for a neural network. Other names for the rather unspecific word "model" are "predictor" or - depending on the task - "classifier" or "regression model". In formulas, the trained machine learning model is called f^ or f^(x).



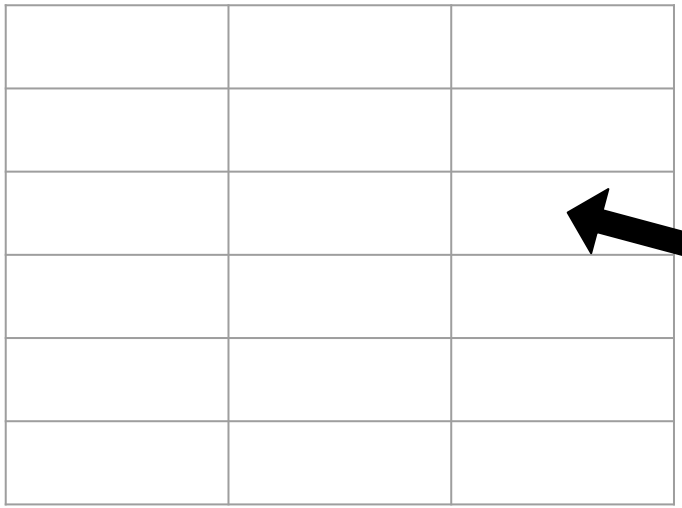
https://christophm.github.io/interpretable-ml-book/terminology.html

Terminology & Notation

Structured data

- Columns
- Variables
- Features
- Predictors

- Observations
- Instances
- Rows
- Entries
- Records



- Data point
- Value

Terminology

- **Supervised learning**: learn function to map input x (features) to output y (targets)
- **Structured data**: databases, spreadsheets/csv files
- **Unstructured data**: features like image pixels, audio signals, text sentences
- **Training example**, synonymous to observation, training record, training instance, training sample (in some contexts, sample refers to a collection of training examples)
- **Feature**, synonymous to predictor, variable, independent variable, input, attribute, covariate
- **Target**, synonymous to outcome, ground truth, output, response variable, dependent variable, (class) label (in classification)
- **Output /Prediction**, use this to distinguish from targets; here, means output from the model

Terminology & Notation

Supervised learning notation

"training examples"

Training set: $\mathcal{D} = \{\langle \mathbf{x}^{[i]}, y^{[i]} \rangle, i = 1, \ldots, n\},$

Unknown function: $f(\mathbf{x}) = y$

Hypothesis: $h(\mathbf{x}) = \hat{y}$

sometimes *t* or *o*

Classification

Regression

$h : \mathbb{R}^m \to \mathcal{Y}, \quad \mathcal{Y} = \{1, \ldots, k\}$

$h : \mathbb{R}^m \to \mathbb{R}$

Terminology & Notation

Data representation

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

Feature vector

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix}$$

Design Matrix

$$\mathbf{X} = \begin{bmatrix} x_1^{[1]} & x_2^{[1]} & \cdots & x_m^{[1]} \\ x_1^{[2]} & x_2^{[2]} & \cdots & x_m^{[2]} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{[n]} & x_2^{[n]} & \cdots & x_m^{[n]} \end{bmatrix}$$

Design Matrix

Machine Learning Pipeline

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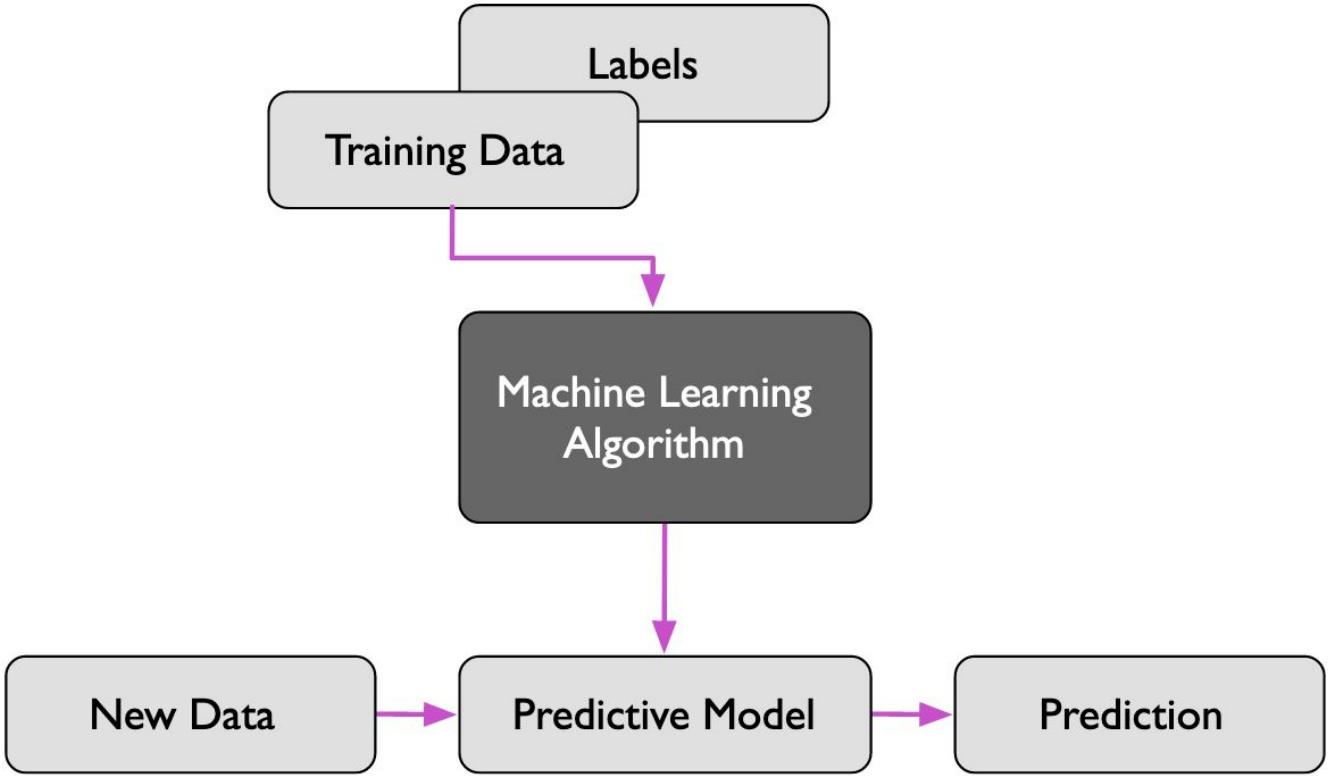
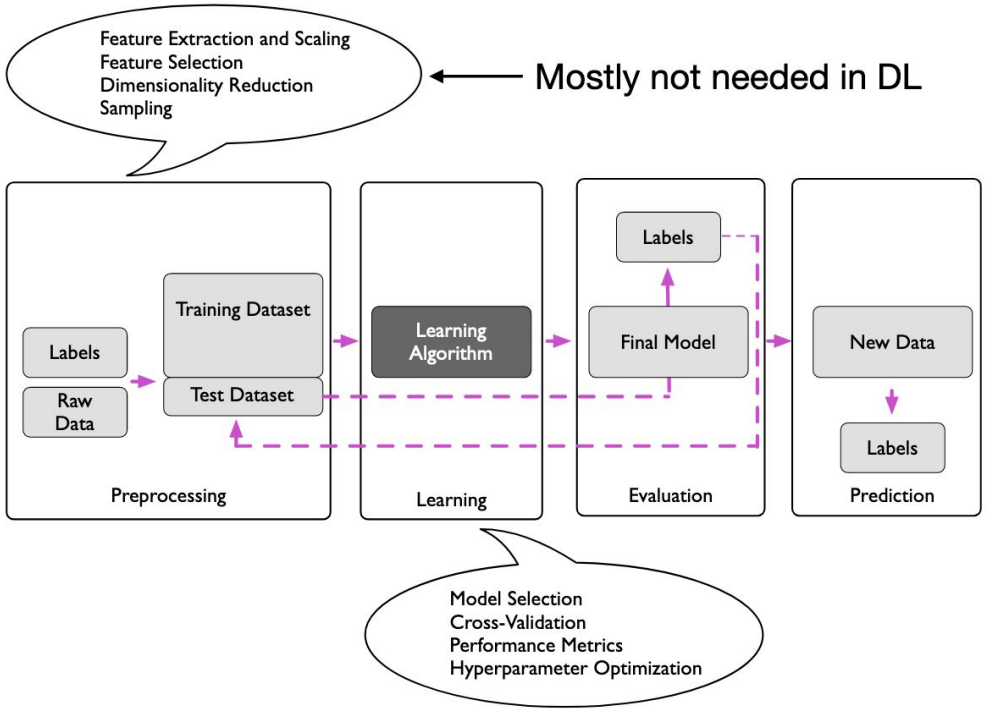
Machine Learning Pipeline

Supervised Learning Workflow



Machine Learning Pipeline

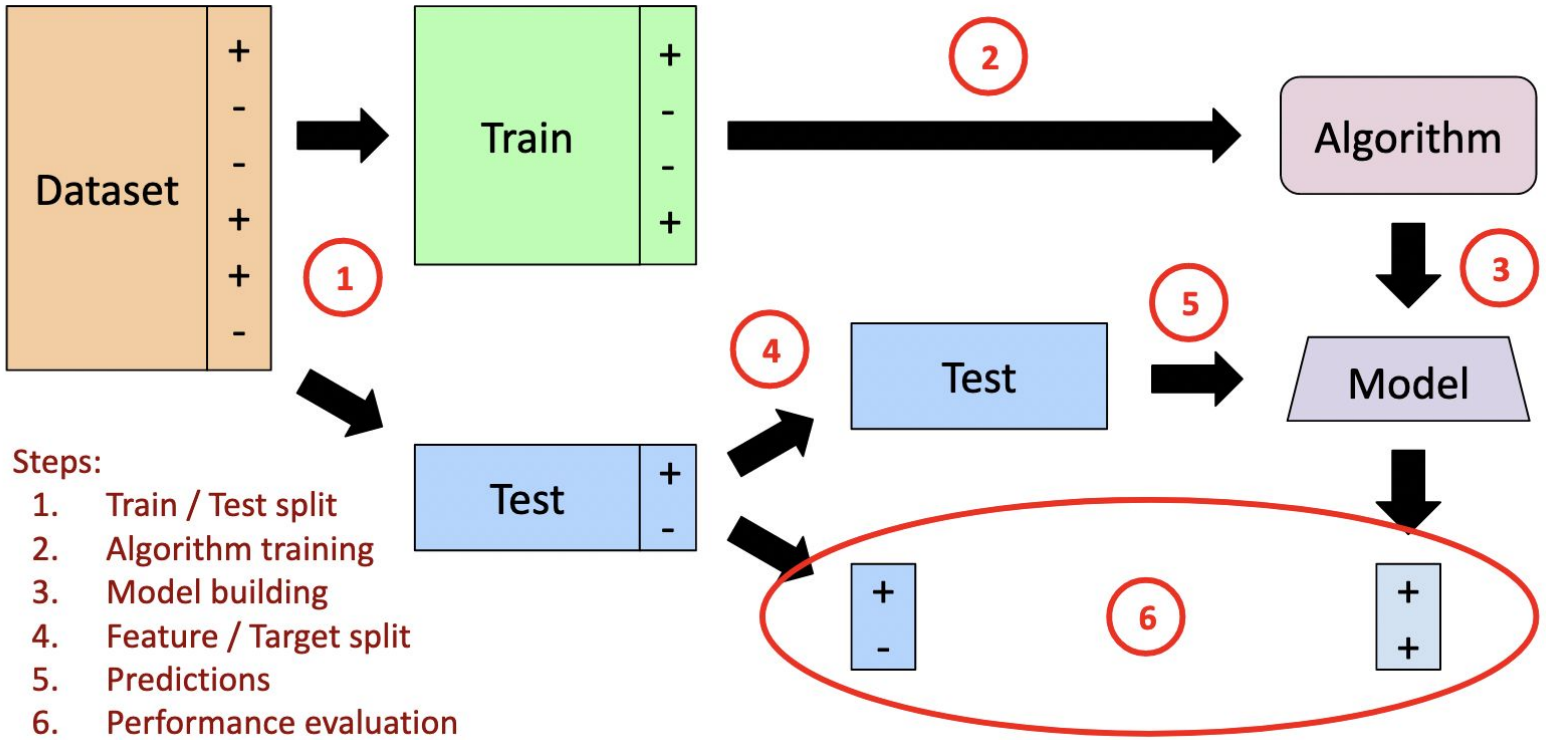
Supervised Learning Workflow (more details)



Source: Raschka and Mirjalily (2019). *Python Machine Learning, 3rd Edition*

Machine Learning Pipeline

Training and Test dataset

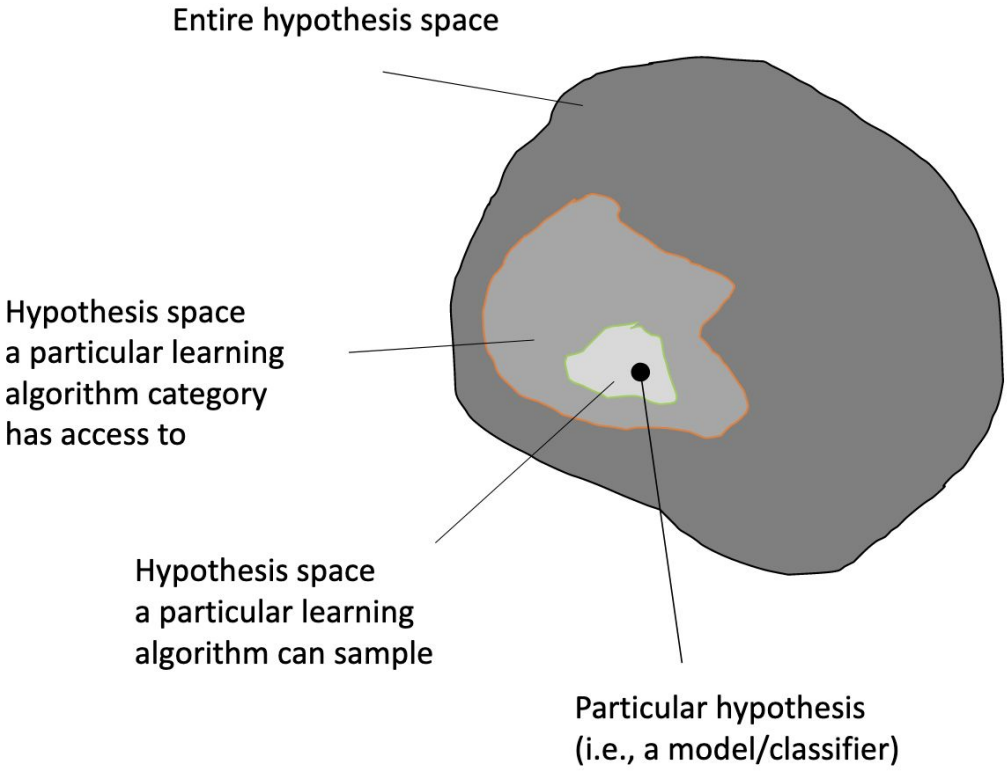


Steps:

1. Train / Test split
2. Algorithm training
3. Model building
4. Feature / Target split
5. Predictions
6. Performance evaluation

Machine Learning Pipeline

Hypothesis space



Machine Learning Pipeline

5 steps to address Machine Learning problems

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1. Define problem to solve
2. Get data
3. Choose machine learning algorithm
4. Choose optimization metric for the model
    - Cost function / Loss function
5. Choose evaluation metric(s)

Learning

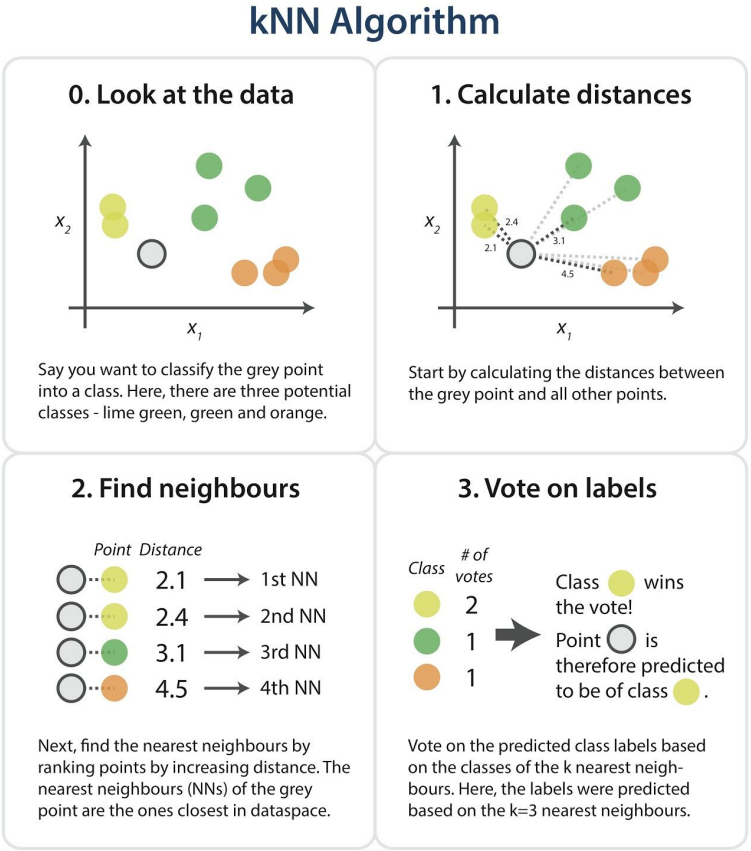
Learning = Representation + Evaluation + Optimization

(Pedro Domingos, A Few Useful Things to Know about Machine Learning
https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf)

Machine Learning Pipeline

The first model: kNN

- **k-nearest neighbour (kNN)** classifies new instances by grouping them together with the most similar cases
- kNN is a type of supervised machine learning (though somewhat confusingly, in kNN there is no explicit training phase; see lazy learning)
- The kNN task can be broken down into 3 main tasks (see image)



Conclusion

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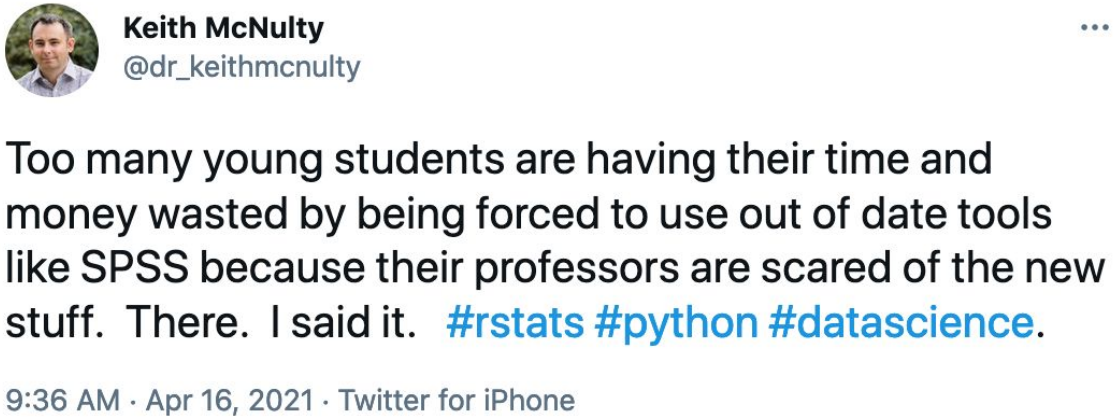
Conclusion

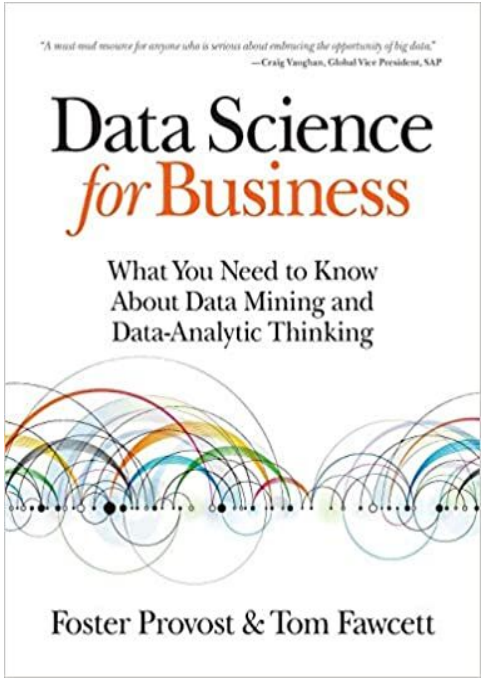
ML is a field in constant evolution

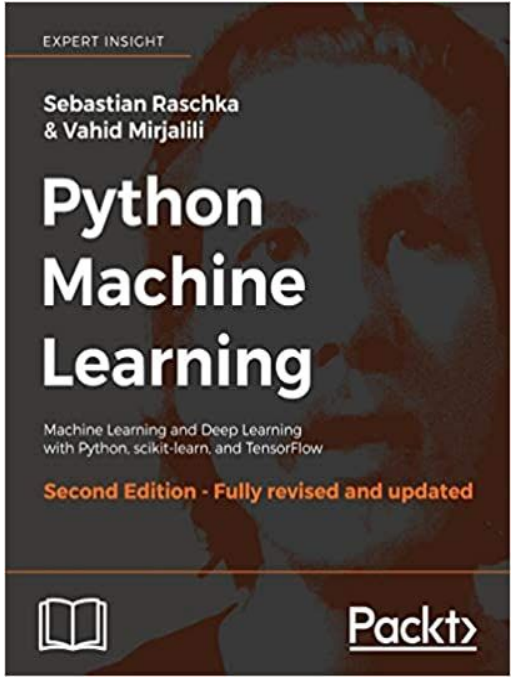


https://twitter.com/dr_keithmcnulty/status/1382870396408627202

Conclusion

Suggested readings





Conclusion

Suggested videos

Ted talk

Conclusion

Sources

- Sebastian Raschka - STAT 453: Intro to Deep Learning - 2020 slides
- Implementing your own k-nearest neighbour algorithm using Python
- The missing semester https://missing.csail.mit.edu/2020/
- https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html#sklearn.neighbors.KNeighborsClassifier

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Buono Studio!

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