A brief overview, comparison and practical applications of machine learning models

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ASAS-NANP Pre-Conference Symposium
ASAS-CSAS-WSASAS Virtual Annual Meeting & Trade Show,
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ONTARIO AGRICULTURAL COLLEGE
DEPARTMENT OF ANIMAL BIOSCIENCES

Summary

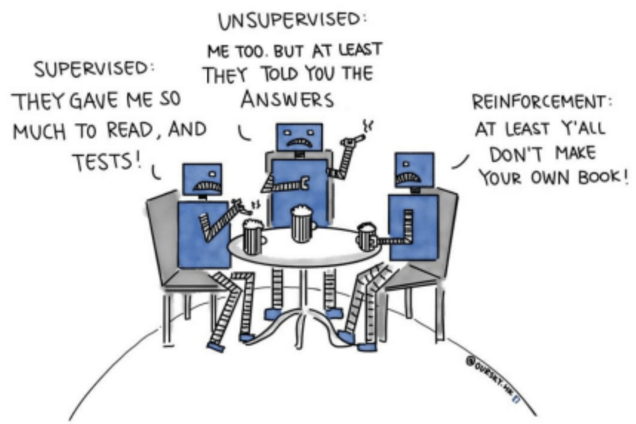
- Machine Learning – general notions
- Types of problems
  - Classification
    - Decision trees
    - Artificial neural networks
  - Regression
  - Clustering
    - K-Nearest Neighbour
  - Dimensionality reduction
- Developing ML models (practical considerations)
- Follow-up Hands-on/Demo Workshop

Learning

"Learning is any process by which a system improves performance from experience."

[Herbert Simon (1916-2001), American economist, political scientist and cognitive psychologist]

- Types of learning
  - **Supervised** (inductive) learning
    - Training data includes desired outputs
    - E.g.: classification problems
  - **Unsupervised** learning
    - Training data does not include desired outputs
    - E.g.: clustering problems
  - Semi-supervised learning (hybrid)
    - Training data includes a few desired outputs
  - Reinforcement learning
    - Rewards from sequence of actions
    - E.g.: intelligent robots



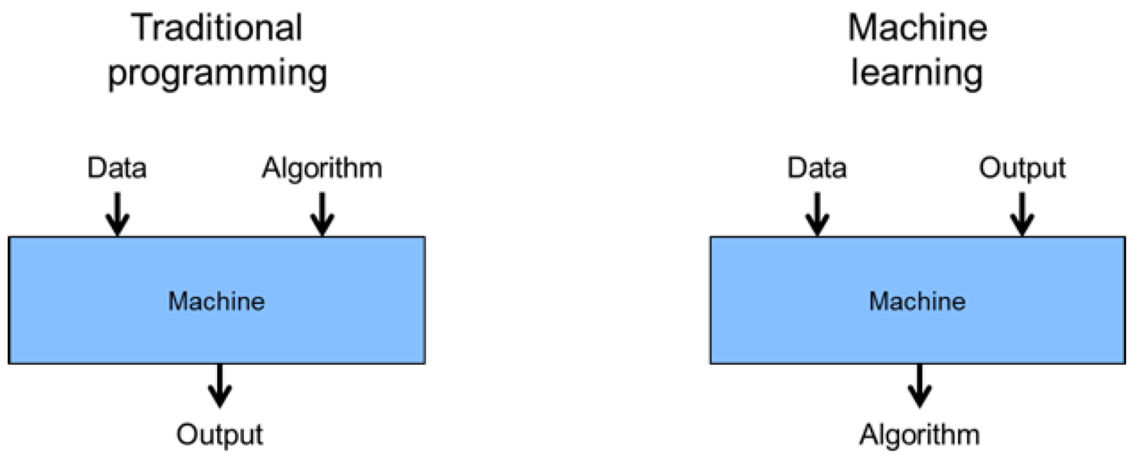
Machine learning https://me.me/

Machine learning (ML)

- The field of machine learning in concerned with the question of how to construct computer programs that automatically improve with experience.

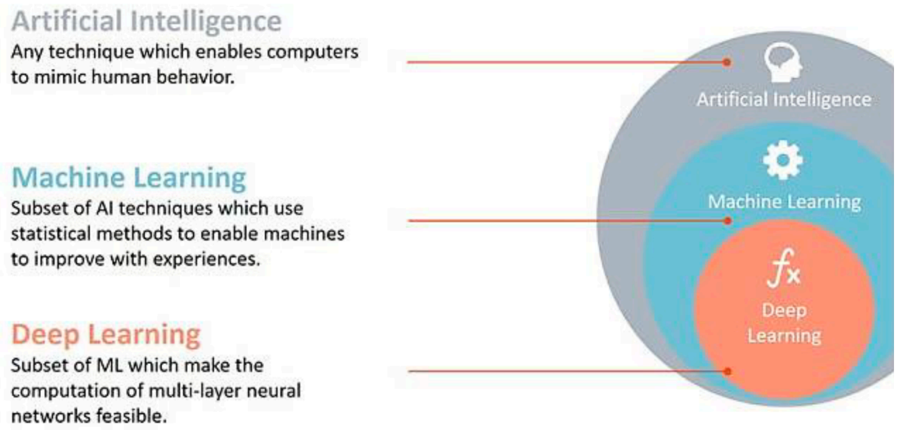
Tom Mitchell, Machine Learning (1997)

- Get computers to program themselves

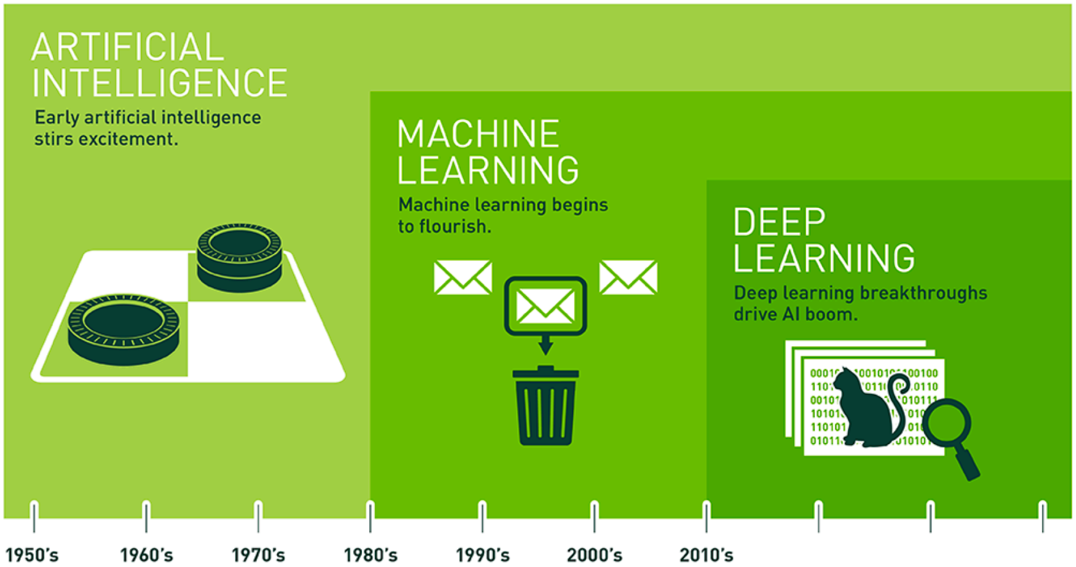


https://dzone.com/articles/what-everyone-should-know-about-machine-learning

Context

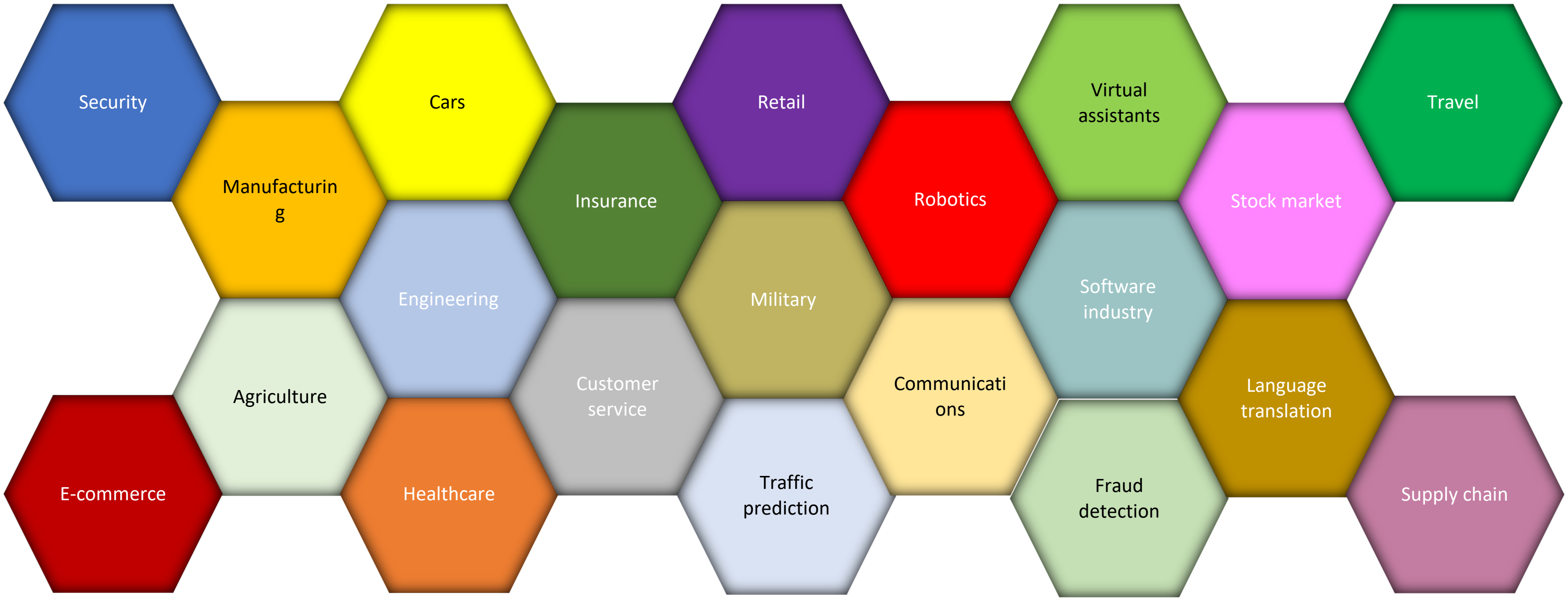


https://www.kdnuggets.com/2017/07/rapidminer-ai-machine-learning-deep-learning.html



https://blogs.nvidia.com/blog/2016/07/29/whats-difference-artificial-intelligence-machine-learning-deep-learning-ai/

Applications of ML



How does it work?

- **Step 1:** The user provides the learning system with **examples** of the concept to be learned or plain **data**.

- **Step 2:** The learning system algorithm **infers/builds** a characteristic **model** from these examples.

- **Step 3:** The **model is used to predict** quickly and with high accuracy whether or not future **novel instances** follow the model.

When to use machine learning?

- When there are patterns in the data
- When we can not figure out the functional relationships mathematically
- When we have a lot of (unlabeled) data
  - Labeled training sets are harder to find or generate
  - Data is in high-dimension
    - High dimension “features”
    - Example: sensor data
  - Want to “discover” lower-dimension representations
    - Dimensionality reduction

Inspired from: https://datatracker.ietf.org/meeting/92/materials/slides-92-sdnrg-0

The Ultimate Goal of ML

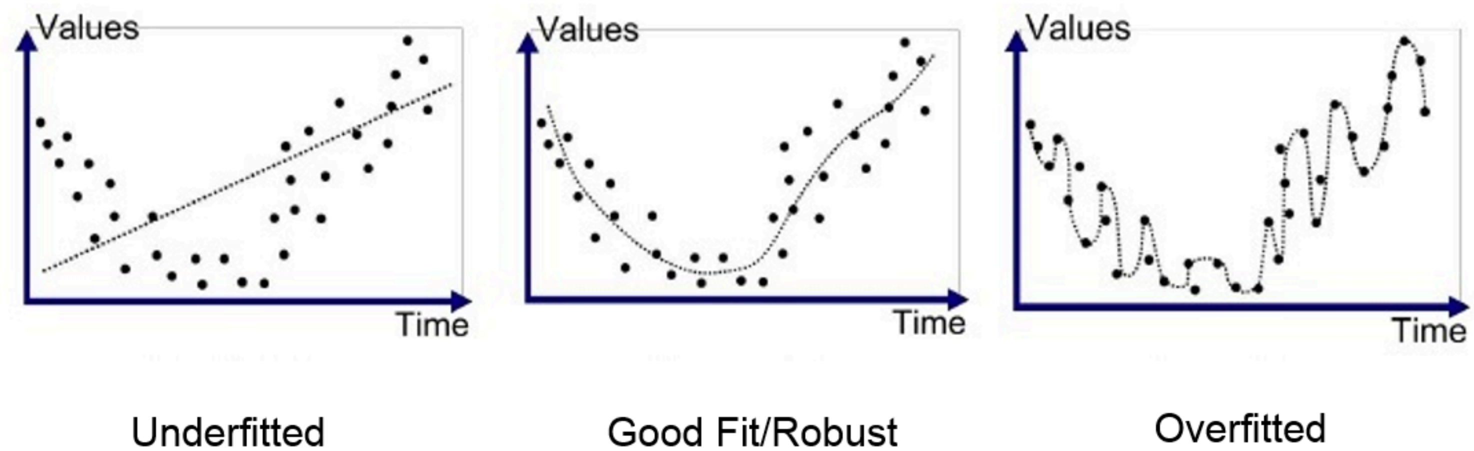
- **Generalization:** the ability of a trained model to fit unseen instances

Training set (labels known)

Test set (labels unknown)

cs.brown.edu/courses/cs143/2013/lectures/17.ppt

Generalization

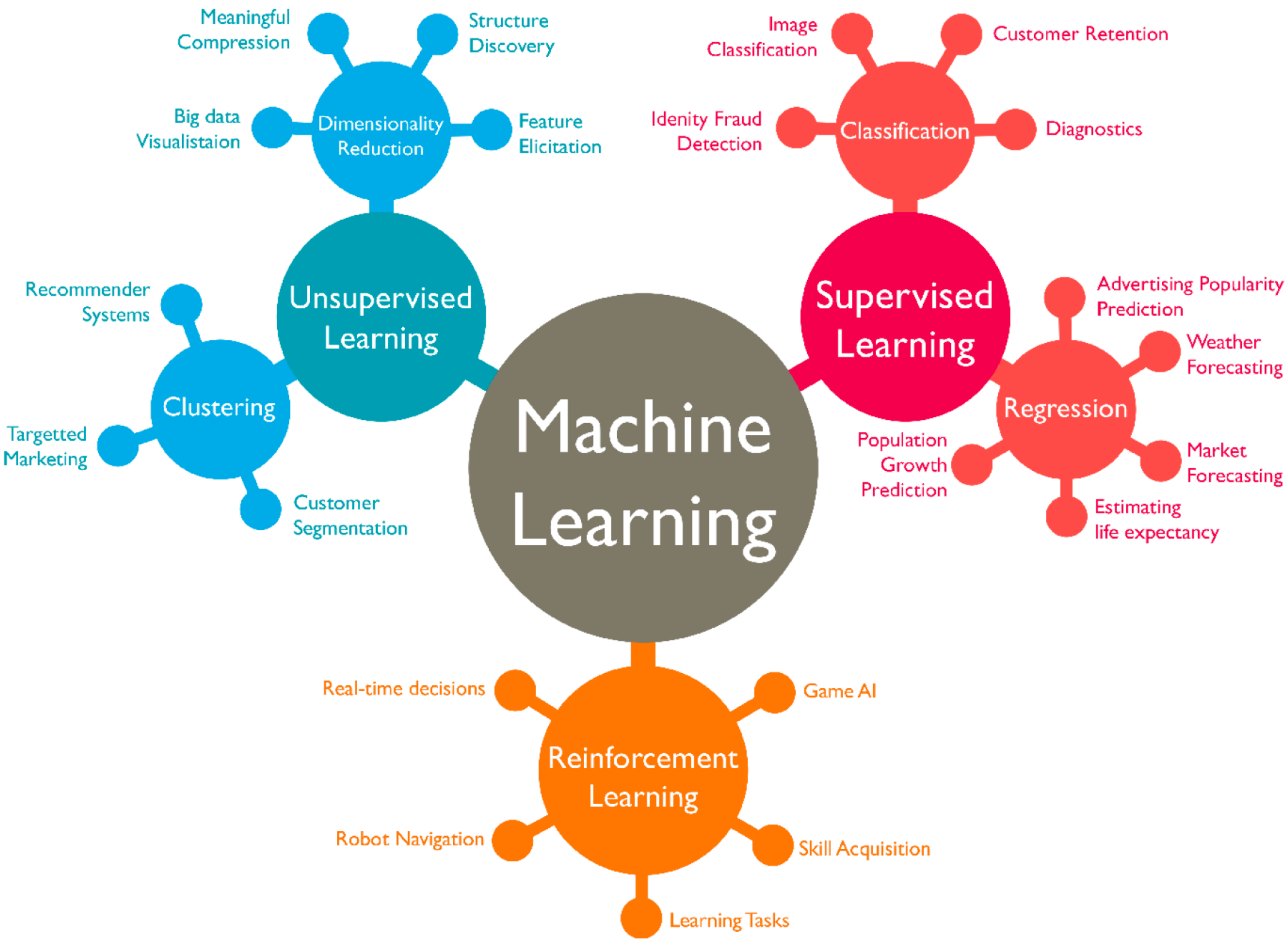


https://medium.com/greyatom/what-is-underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6803a989c76

- **Underfitting:** model is too "simple" to represent all the relevant class characteristics
  - High bias and low variance
  - High training error and high test error

- **Overfitting:** model is too "complex" and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - Low training error and high test error

Types of problems solved by ML



https://www.wordstream.com/blog/ws/2017/07/28/machine-learning-applications

Types of problems solved by ML

LEARNING TYPES

DATA TYPES

	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Classification

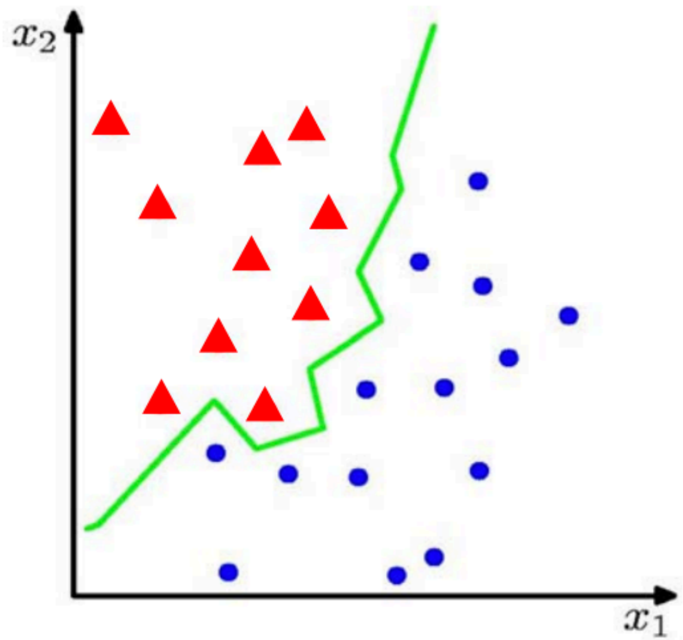
LEARNING TYPES

DATA TYPES	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Classification

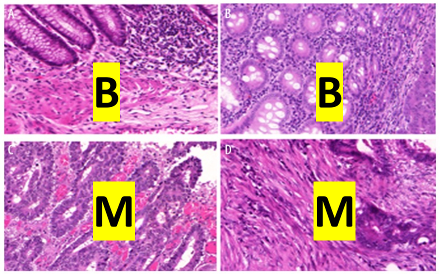
- Given a set of observations:
  - *($input_i$, $output_i$)* pairs, where $output_i \in \{c_1, c_2, \ldots\}$

- Find a function *f*, such that: $f(input_i) = output_i$



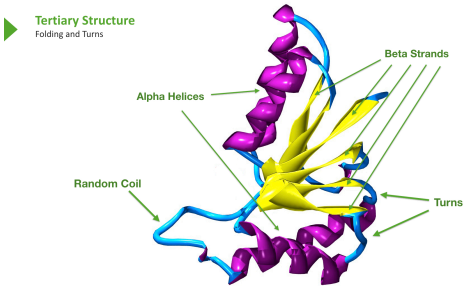
Classification Problem Examples

- Classify tumors as malign or benign



https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6154116/

- Classify protein secondary structures as α-helices, β-sheets, coils or turns



http://oregonstate.edu/instruct/bb450/450material/OutlineMaterials/4_5Proteins.html

- Classify mushrooms as edible or poisonous

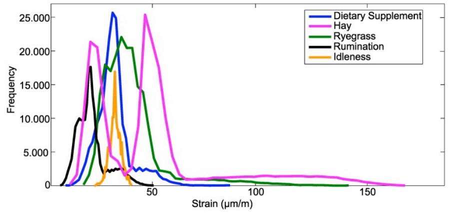
"Destroying Angel" Mushrooms

Edible Puffball Mushrooms

https://www.ck12.org/book/Biology-%252528CA-DTI3%2525292/r3/section/14.5/

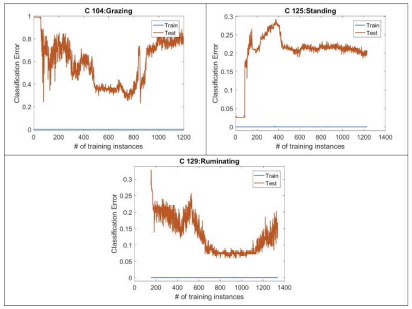
Classification Problem Examples

- Classify ruminants chewing patterns



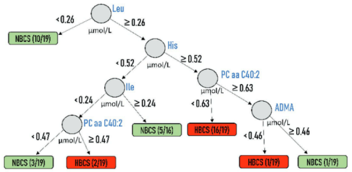
Pegorini et al., 2015: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4701289/

- Classify cattle behaviour based on ear tag, collar and halter sensors



Rahman et al., 2018: https://www.sciencedirect.com/science/article/pii/S2214317317301099

- Classify cattle BCS based on metabolite profiles



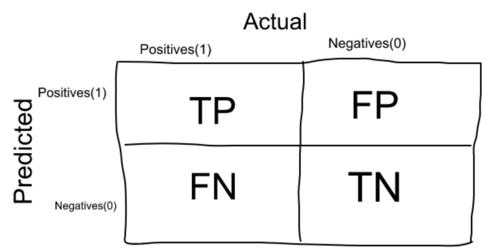
Ghaffari et al., 2019: https://www.journalofdairyscience.org/article/S0022-0302(19)30838-0/abstract#

Performance evaluation protocol

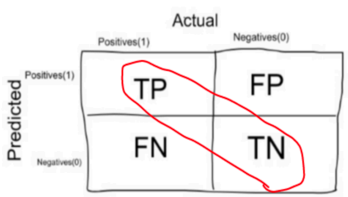
- Split the data into: training, testing (and validation)
  - Fixed split approach
    - E.g. 70% training, 30% testing
  - Cross-validation approach (k-fold)

- Choose evaluation metrics
- Perform measurements over n runs (n>= 1)

Performance evaluation measures

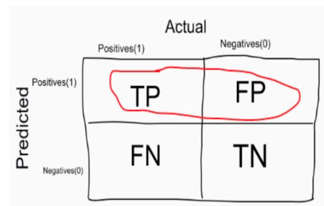


Confusion Matrix



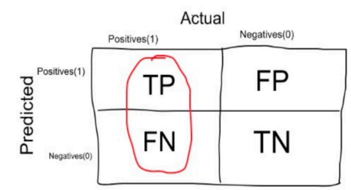
$$\text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

Use when data is balanced.



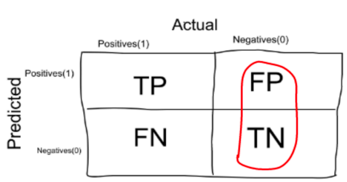
$$\text{Precision} = \frac{TP}{TP + FP}$$

Use to minimize FP.



$$\text{Sensitivity or Recall} = \frac{TP}{TP + FN}$$

Use to minimize FN.



$$\text{Specificity} = \frac{TN}{TN + FP}$$

The opposite of Recall

$$F1_{score} = \frac{2 \times precission \times recall}{precision + recall}$$

Great if it equals 1 and not good if it is 0.

+ 100 or more:

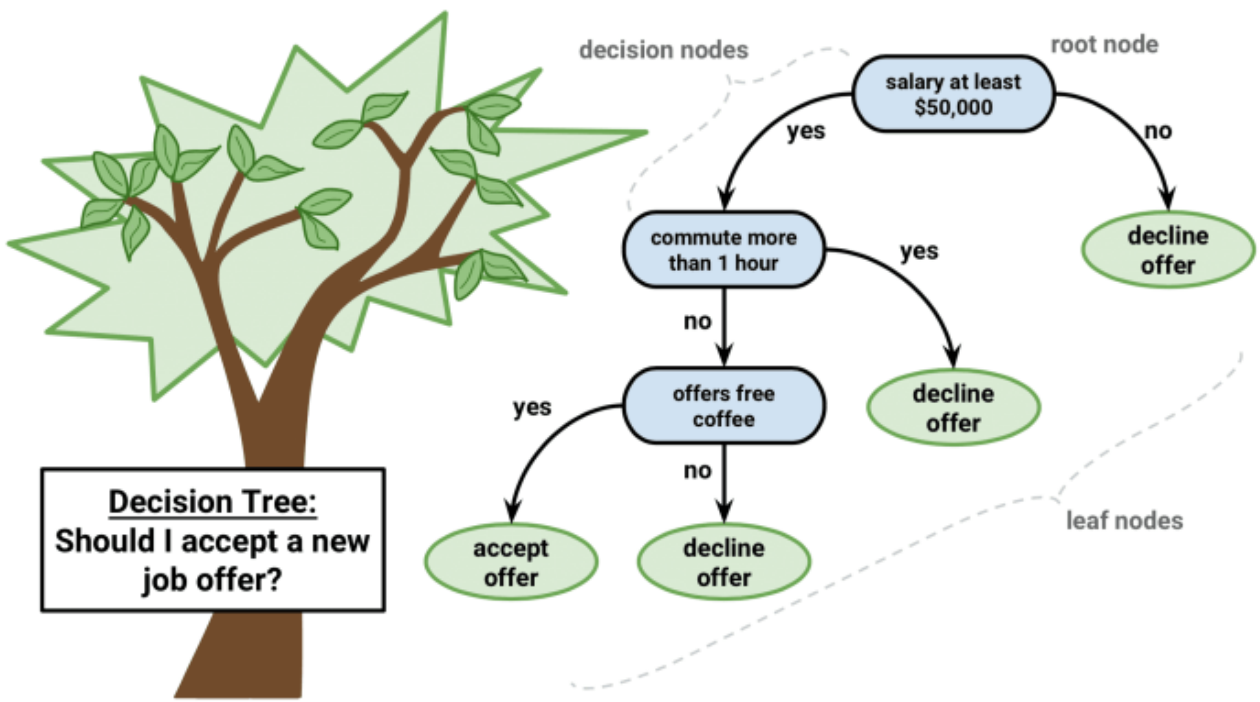
- **TPR, TDR**
- **FPR, FDR**
- **PPV, NPV**
- **MCC**
- **…**

Classification methods

- **Tree-based:**
  - **Random Forest** [Breiman 2001],
  - **J48** [Quinlan 1993]
- **Bayesian:**
  - **Naïve Bayes** [Clark & Niblett, 1989]
- **Boosting:**
  - **AdaBoost** [Freund & Schapire, 1996]
- **Kernel-based:**
  - **SVM** [Ben-Hur et al., 2001]
- **Rule-based:**
  - **Decision Table** [Kohavi 1995]
- **Artificial neural networks**
  - **Multi-layer Perceptron** [Rosenblatt 1961]
  - **RNN** [Rumelhart 1986],
- **Deep learning:**
  - **CNN** [Fukushima 1980;LeCun 1998]
- Etc.

Decision Trees

- A flow chart-like topology (a tree)
- Each internal node represents a test on an attribute
- Each branch represents an outcome of a test
- Leaf nodes represent class labels (if used for classification)



Decision Tree classifier, **Image credit:** http://www.packtpub.com

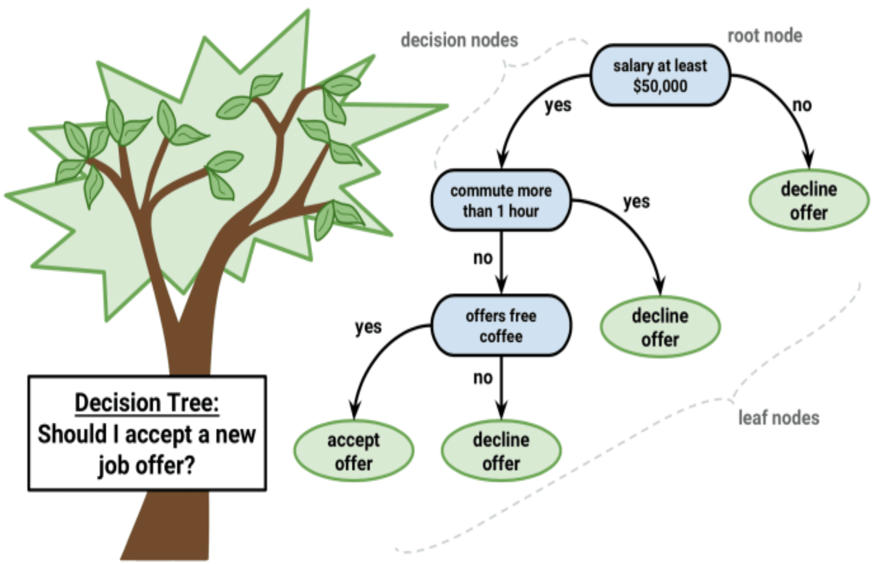
Decision Trees vs. Linear Models

- **Choose linear models if** the relationship between dependent & independent variables is well approximated by a linear model.

- **Choose a decision tree model if** there is a high non-linearity & complex relationship between dependent & independent variables.

- **Choose a decision tree model if** you need to build a model which is easy to explain to people. Decision tree models are even simpler to interpret than linear regression!

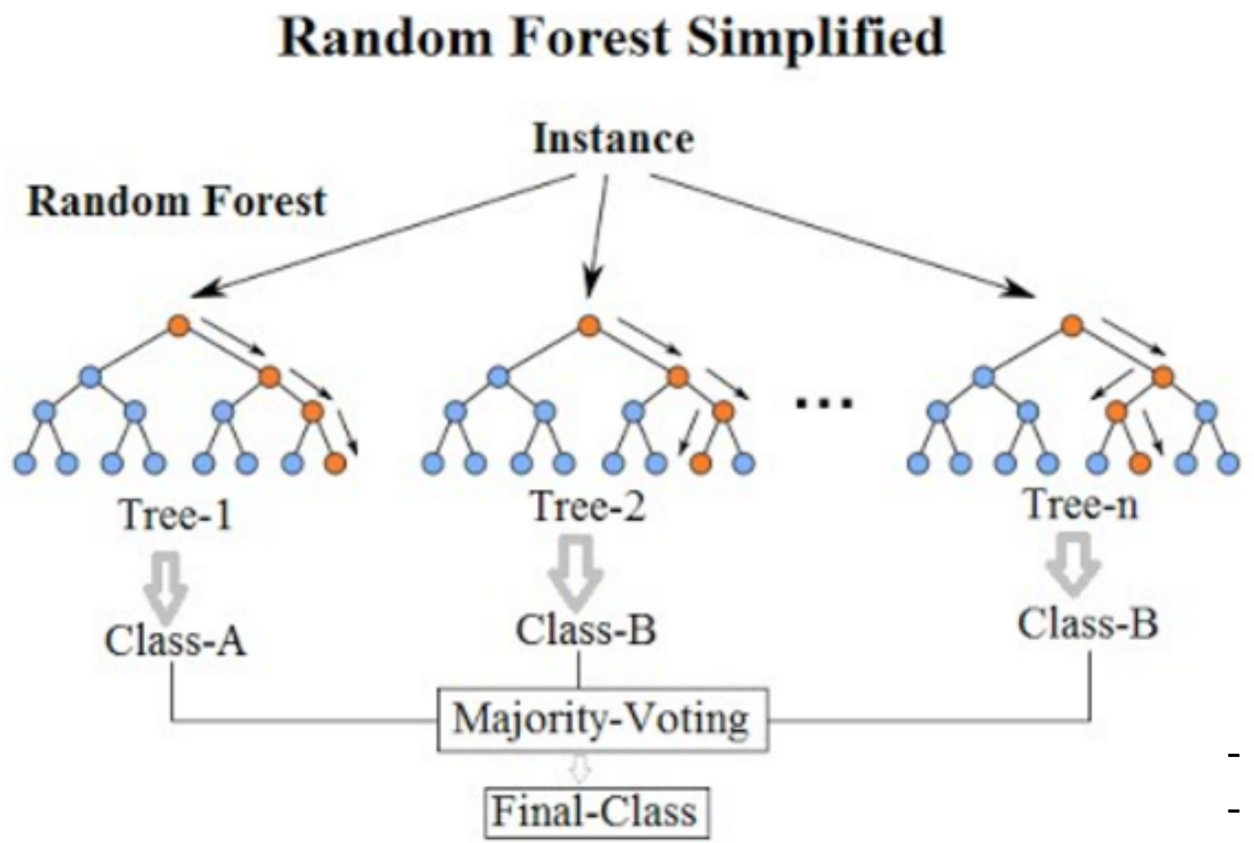
Decision Trees vs. Linear Models



Decision Tree classifier, **Image credit:** http://www.packtpub.com

$$\mathbf{F(s,d,c)} = \begin{cases} 0 & s < 50000. \\ 0 & s \geq 50000 \; and \; d > 1 \\ 0 & s \geq 50000 \; and \; d < 1 \; and \; c = 0 \\ 1 & otherwise \end{cases}$$

Random Forests



https://commons.wikimedia.org/wiki/File:Random_forest_diagram_complete.png

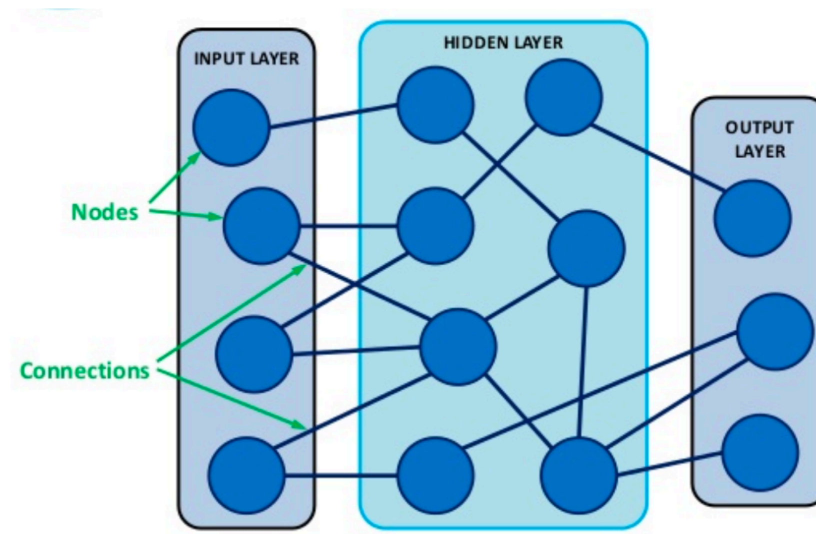
Bagging / bootstrap aggregation
Random sub-samples of the data

Option: **feature bagging**

- Decorrelate the data
- Reduce the impact of strong predictor variables

Artificial Neural Networks (ANN)

- An ANN is a biologically inspired computational model.
- ANNs attempt to mimic the functionality of the human brain.
- An ANN contains:
  - Processing elements (neurons)
  - Connections (between neurons)
  - Training & recall algorithms
- Important feature: network layout



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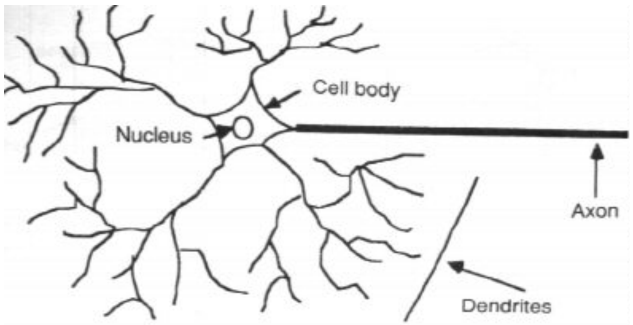
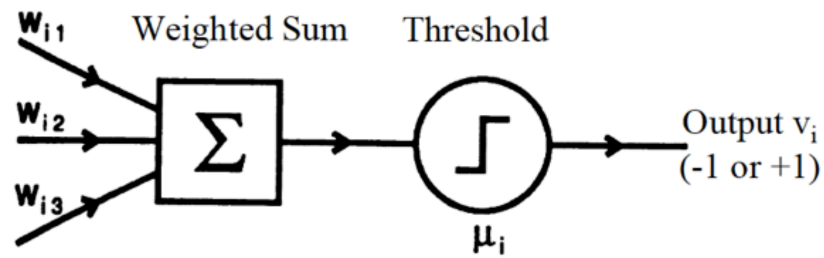
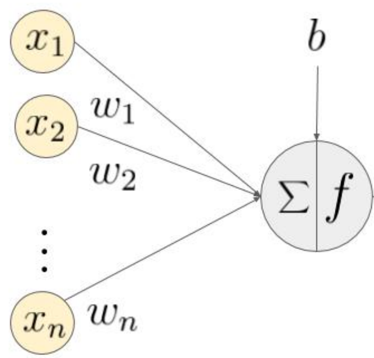
Artificial Neuron





- First model (**the perceptron**) was developed by Rosenblatt in 1957.
- **Idea**:

input data



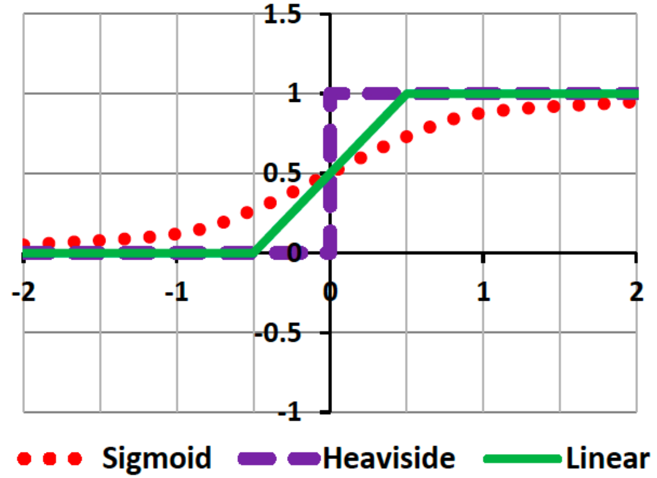
$$f\left(b + \sum_{i=1}^{n} x_i w_i\right)$$

An example of a neuron showing the input (x_1 - x_n), their corresponding weights (w_1 - w_n), a bias (b) and the activation function f applied to the weighted sum of the inputs.

https://www.learnopencv.com/understanding-feedforward-neural-networks/

The Perceptron

- **Input signals**:
  - Continuous or discrete values fed from previous neurons
  - Each input associated with a Weight
- **Integration Function**:
  - Usually a weighted summation function
  - Threshold/Bias regulates result of Integration Function
  - Output is called *neuron net input*
- **Activation/Transfer Function**:
  - Usually a non linear function
  - Output interval [0,1] or [-1,1]
  - Output values continuous or discrete



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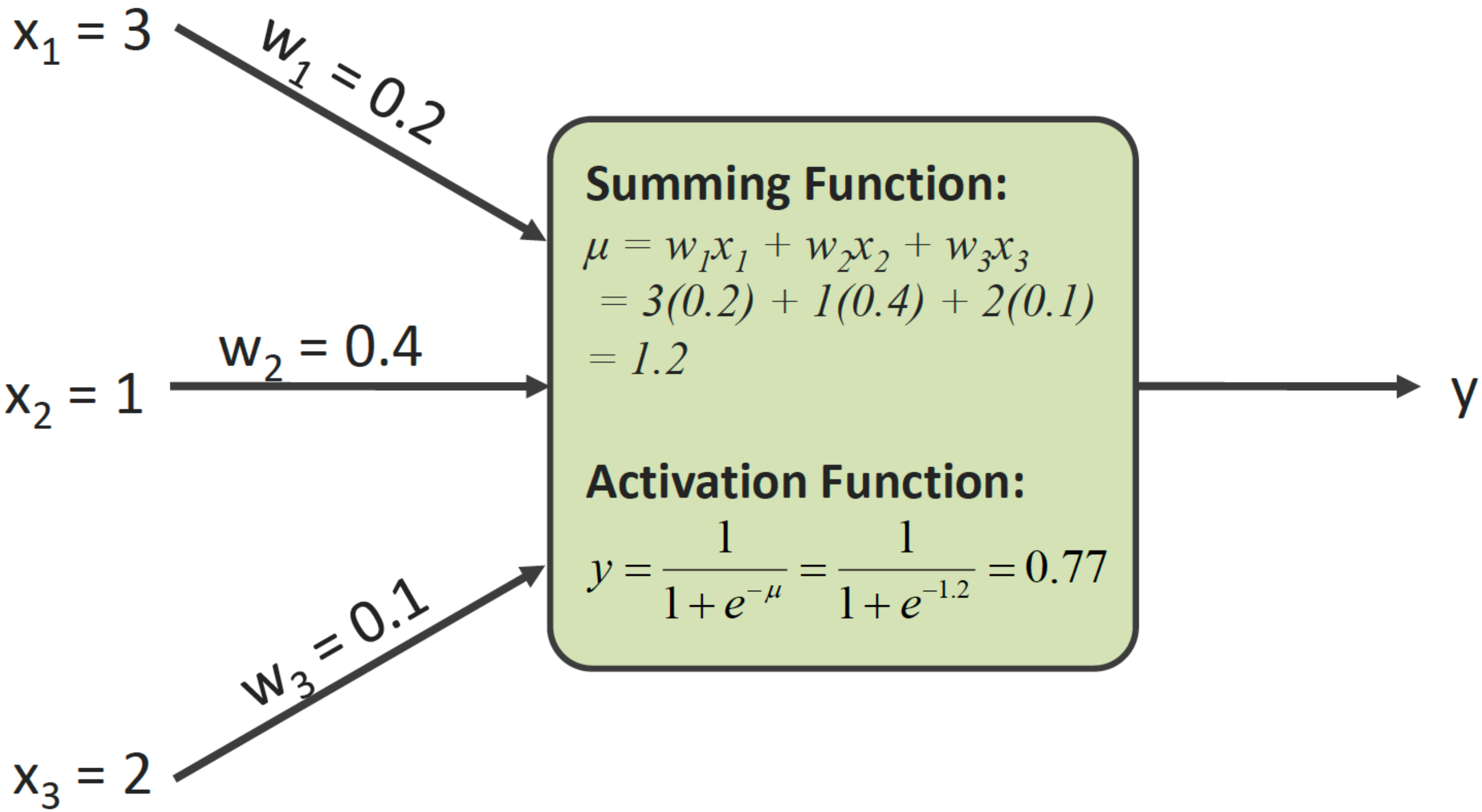
Perceptron Example



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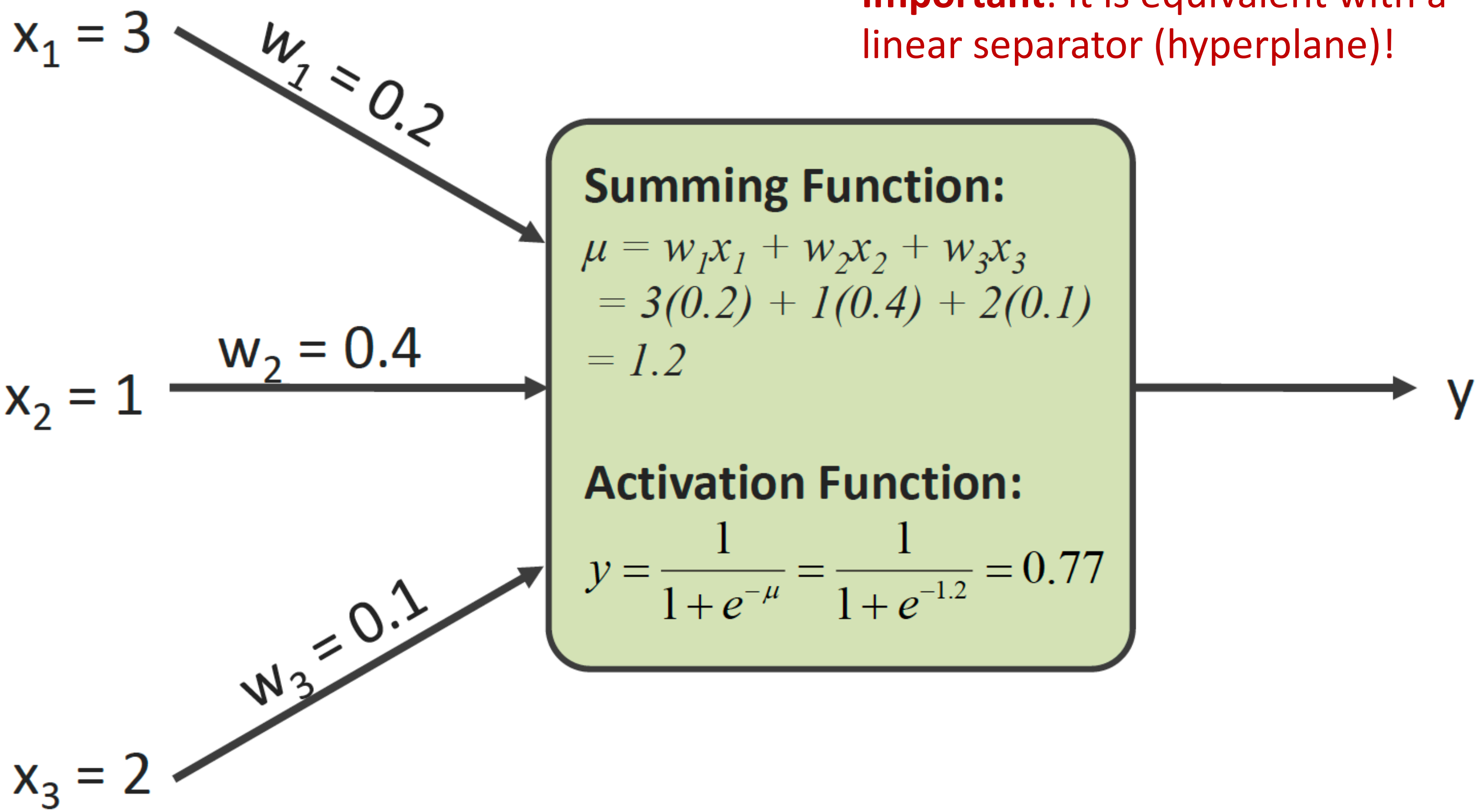
Perceptron Example

Important: It is equivalent with a linear separator (hyperplane)!



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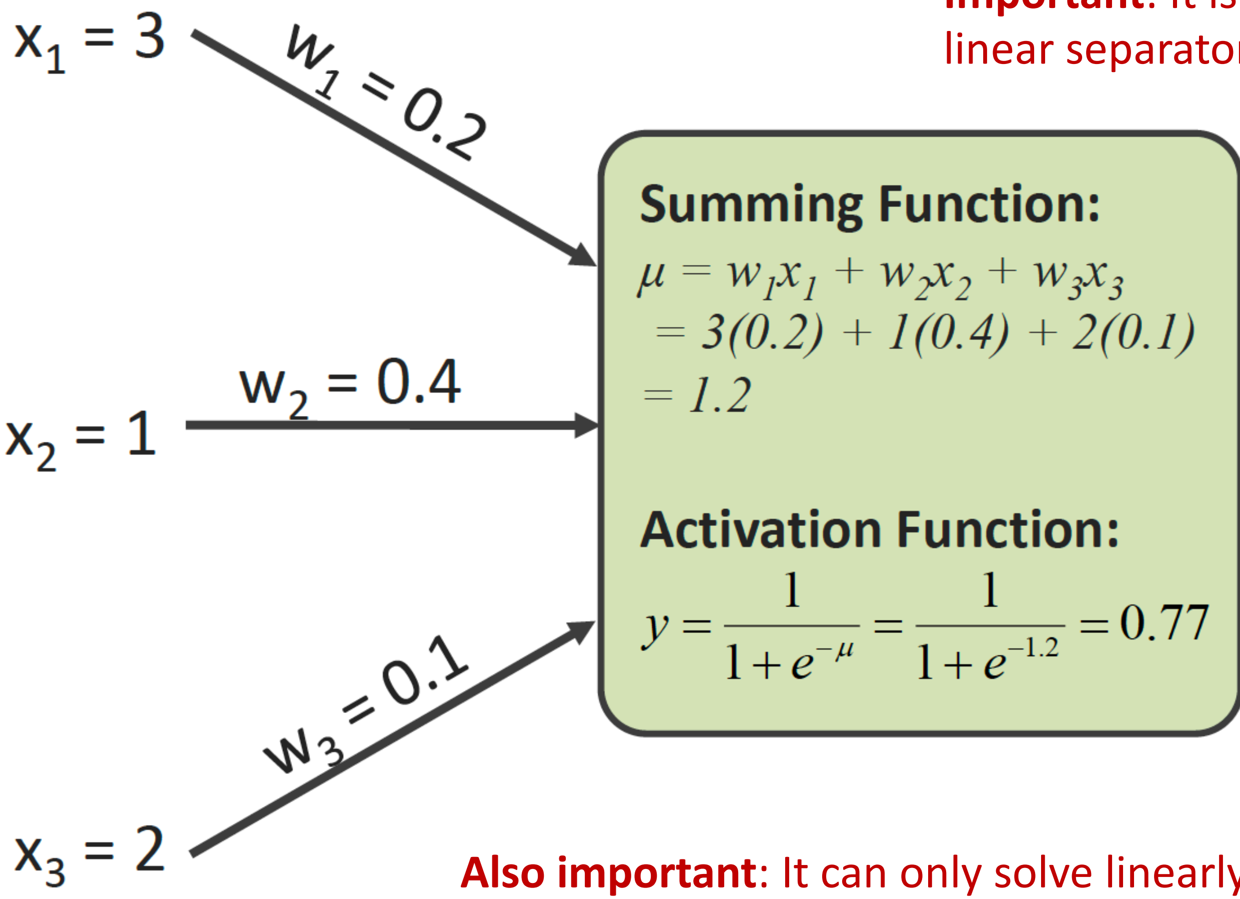
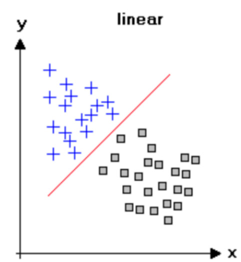
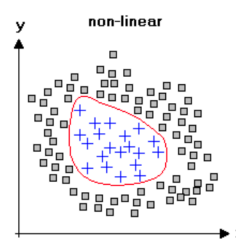


y



OK



NOT OK

Also important: It can only solve linearly separable problems.

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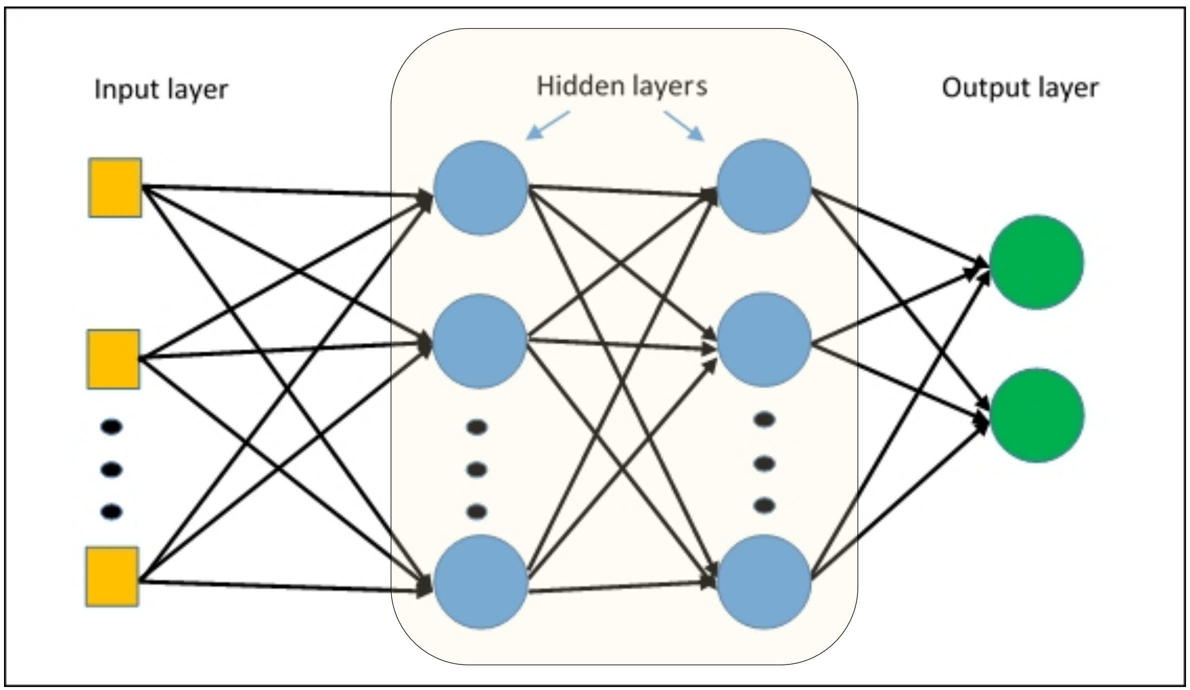
Multilayer Perceptron (MLP)

- Solution: 1980's – Multilayer perceptrons can solve non-linear separable problems



https://www.oreilly.com/library/view/getting-started-with/9781786468574/ch04s04.html

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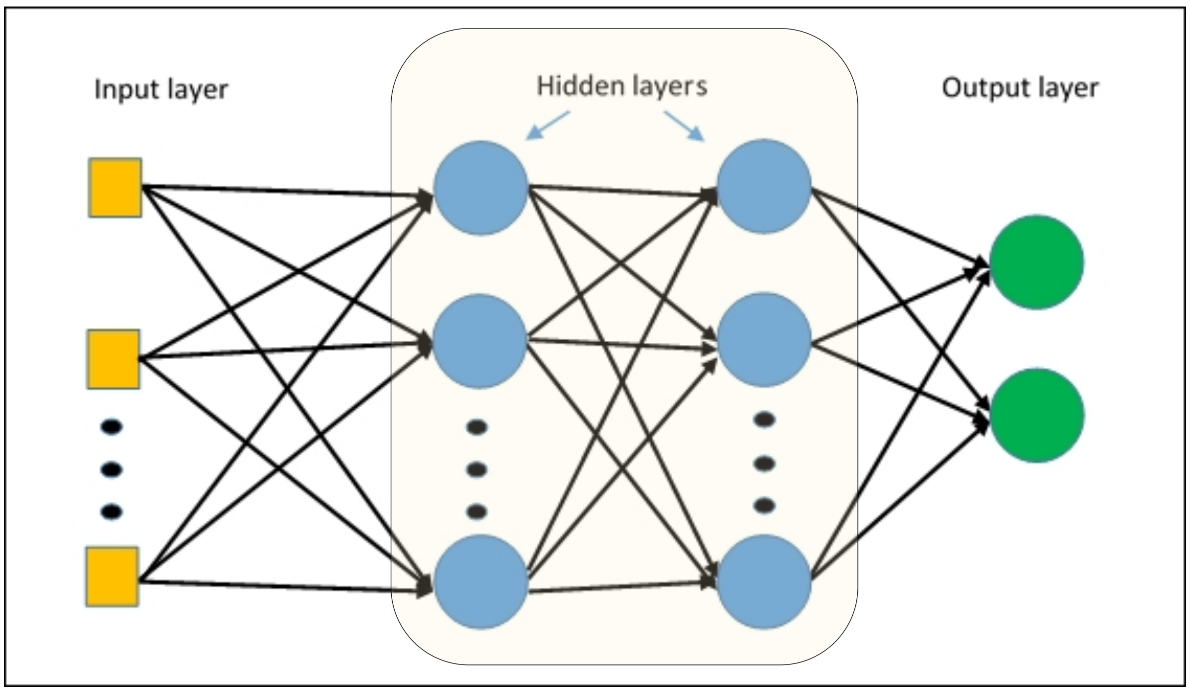

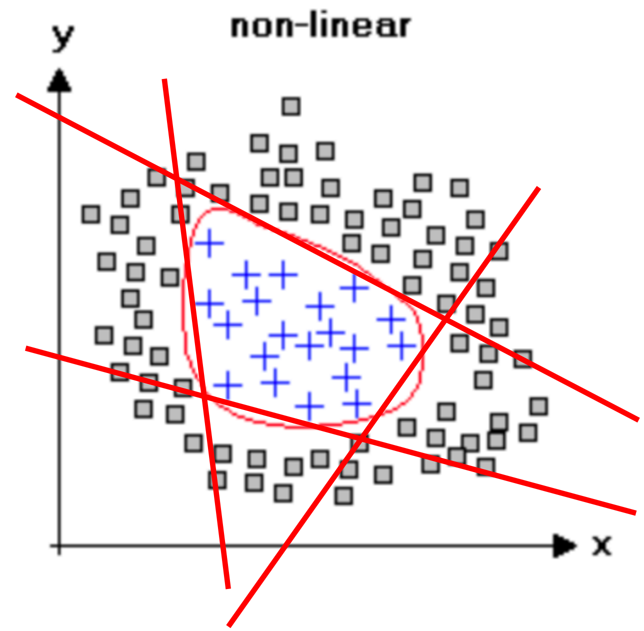

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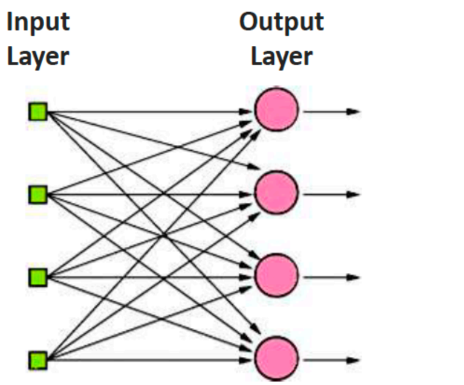
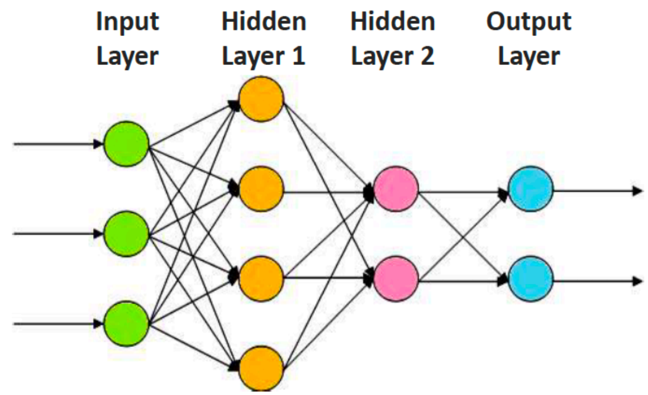
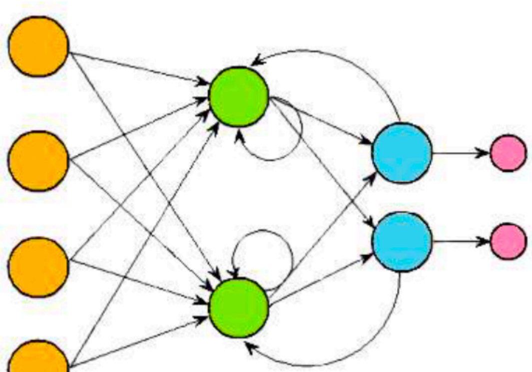
Examples of ANNs Topologies



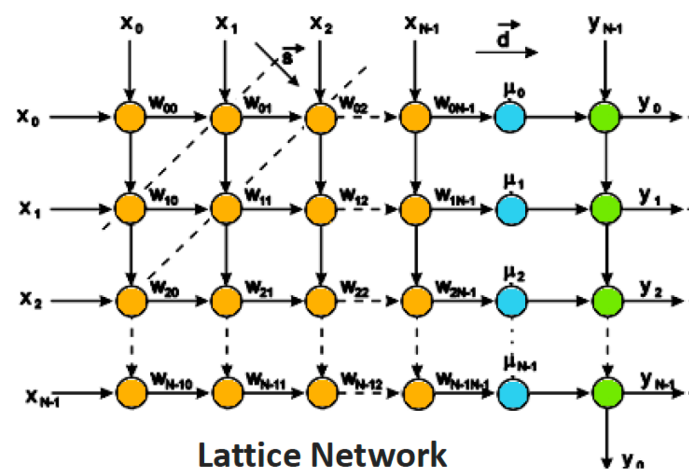
Single Layer Feedforward Network



Multi- Layer Feedforward Network



Recurrent Network



Lattice Network

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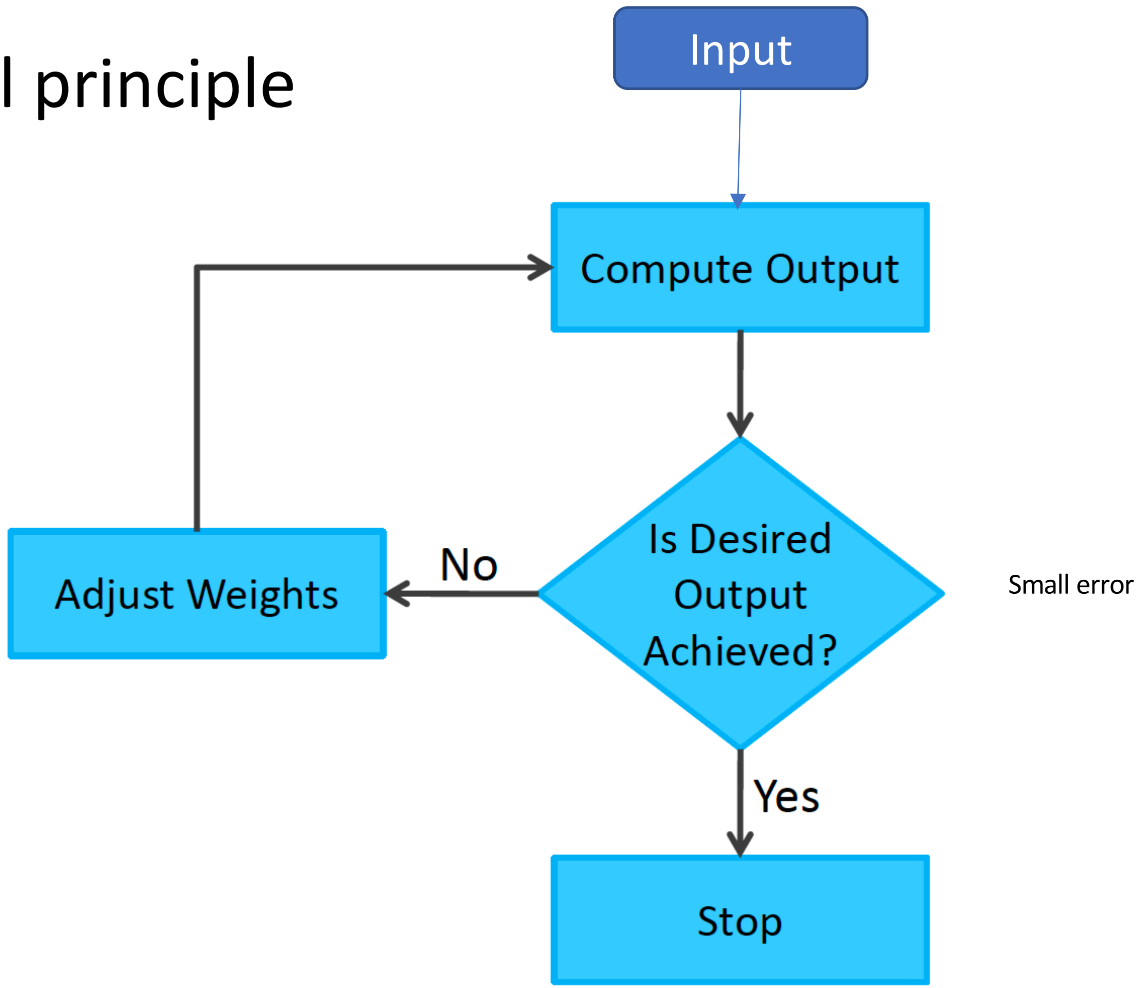
How do ANNs "Learn"?

- **Initialize the weights** (w_0, w_1, …, w_k)
  - Typically with random values
- **Adjust the weights** in such a way that the output of ANN is consistent with class labels of training examples
  - Error function: $$E = \sum_i \left[Y_i - f(w_i, X_i) \right]^2$$
  - **Find the weights** w_i's that **minimize** the above **error function** and adjust them proportionally with the error
    - e.g., gradient descent, backpropagation algorithm

ANN Supervised Learning

- General principle



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What Are ANNs Used For?

- **Classification**: Assigning each object to a known specific class
- **Clustering**: Grouping together objects similar to each other
- **Pattern Association**: Presenting of an input sample triggers the generation of specific output pattern
- **Function approximation**: Constructing a function generating almost the same outputs from input data as the modeled process
- **Optimization**: Optimizing function values subject to constraints
- **Forecasting**: Predicting future events on the basis of past history
- **Control**: Determining values for input variables to achieve desired values for output variables

https://www.slideshare.net/purneshaloni5/14-mohsin-dalvi-artificial-neural-networks-presentation-46777890

When to Use ANN?

- Input is high-dimensional discrete or raw-valued
- Output is discrete or real-valued
- Output is a vector of values
- Possibly noisy data
- The form of the target function is unknown
- Human readability of the result is not important

Regression

LEARNING TYPES

DATA TYPES

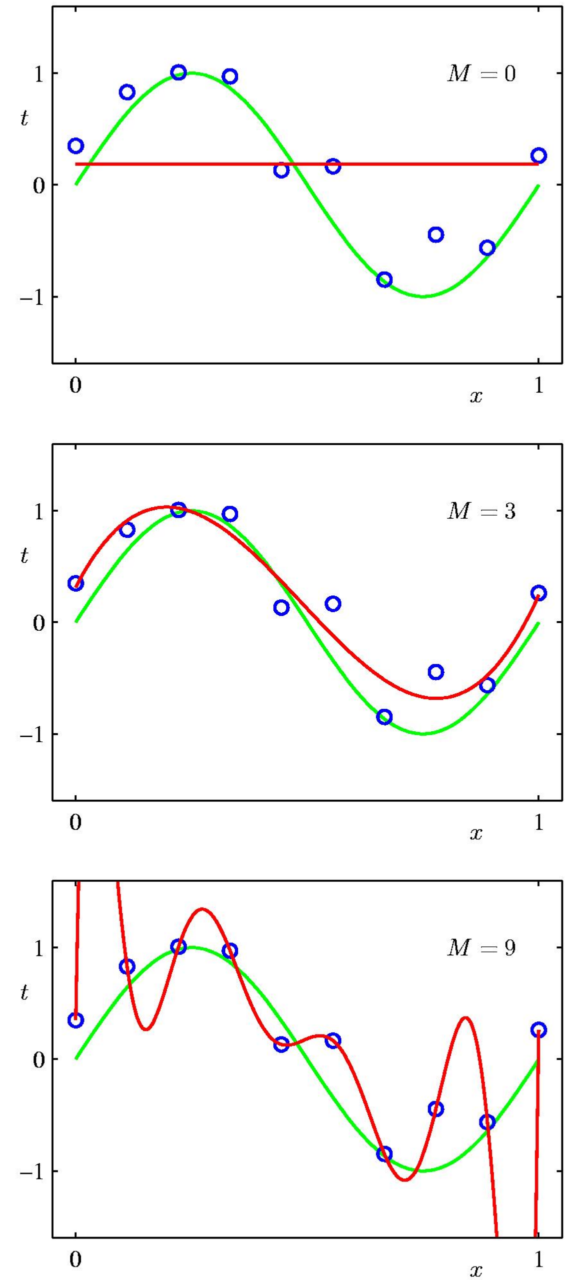
	Supervised Learning	*Unsupervised Learning*
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Regression

- **Regression** is a technique that is used to predict values of a desired target quantity when the target quantity is **continuous**.
  - **Note**: In classification, the target quantity is discrete.

- **Multiple methods**: linear, higher-order (quadratic, polynomial), least-squares, Bayesian, non-linear, logistic, ANN, DT, Generalized Linear Models (GLMs), …

- **Note**: Most methods for classification work for regression, too, with some modifications.



Performance evaluation protocol

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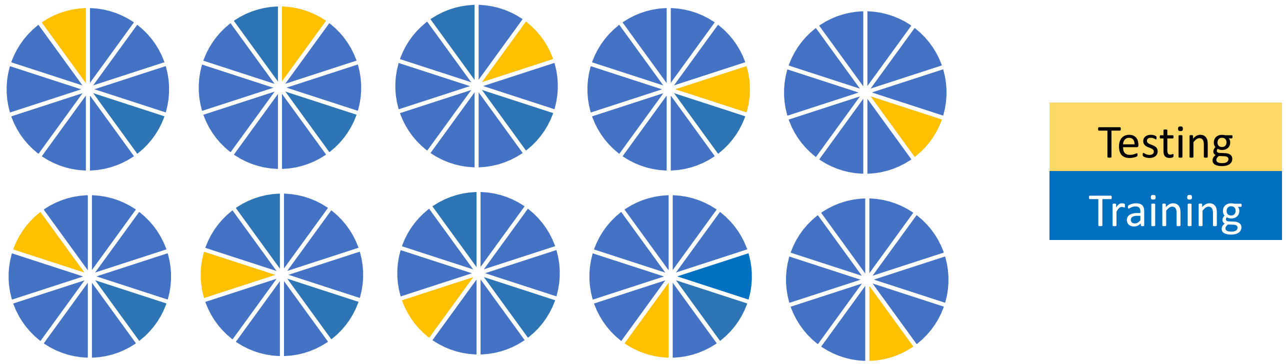
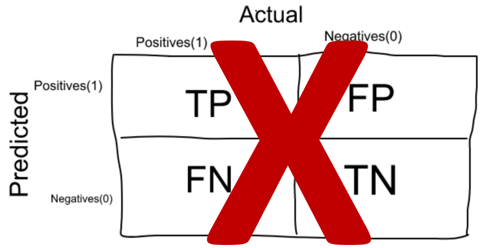
  - Fixed split approach
    - E.g. 70% training, 30% testing
  - Cross-validation approach (k-fold)



- Choose evaluation metrics
- Perform measurements over n runs (n>= 1)

Performance evaluation

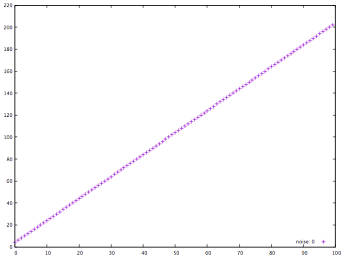


Confusion Matrix

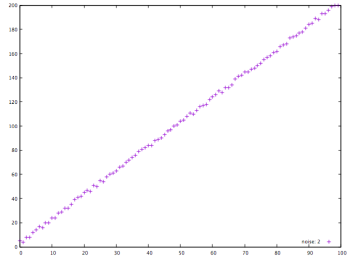
- Correlation coefficients (Pearson, Spearman, Kendall, …)
- Error functions
  - Mean absolute error
  - Mean absolute log error
  - Mean absolute perc. error
  - Root mean squared error
  - Root mean square log error
  - Root mean square perc. error
  - Root relative squared error
  - Relative absolute error
- …

Regression via multiple methods

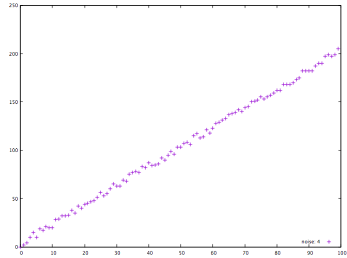
f(x) = 2x + 3 + Ɛ



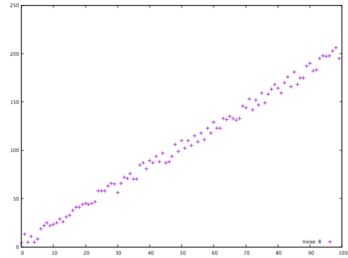
Ɛ = 0



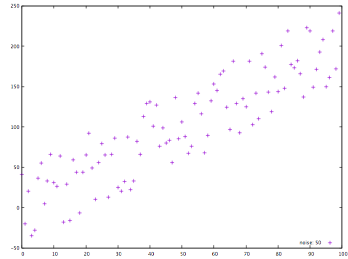
Ɛ ∈ [-2 .. +2]



Ɛ ∈ [-4 .. +4]



Ɛ ∈ [-8 .. 8]



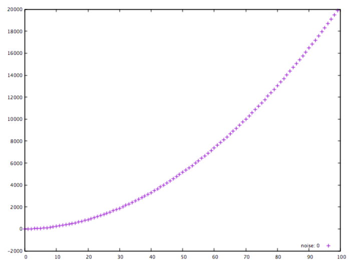
Ɛ ∈ [-50 .. 50]

Method	Ɛ = 0	Ɛ ∈ [-2 .. 2]	Ɛ ∈ [-4 .. 4]	Ɛ ∈ [-8 .. 8]	Ɛ ∈ [-50 .. 50]
Linear regression	**1.0000** 0.0000	**0.9998** 1.0805	**0.9992** 2.3775	**0.9968** 4.6496	**0.8803** 30.6469
Random Forest	**0.9998** 1.7155	**0.9996** 1.9921	**0.9986** 3.1983	**0.9953** 5.6982	**0.8173** 38.2657
ANN - MLP	**0.9995** 1.7715	**0.9993** 2.1454	**0.9985** 3.2222	**0.9967** 4.6653	**0.8740** 31.4028
Decision Table	0.9940 6.3388	0.9938 6.4299	0.9926 7.0318	0.9900 8.1663	0.8542 33.7570

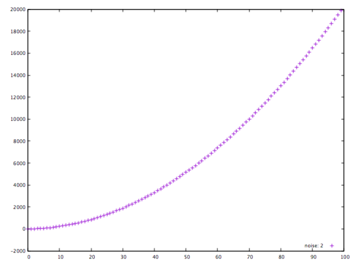
Pearson CCs & Root Mean Squared Errors (RMSE), n=100

Regression via multiple methods

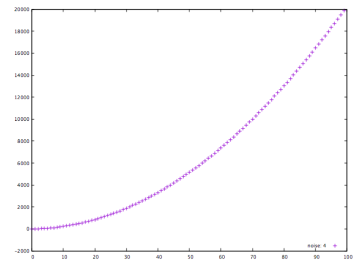
$f(x) = 2x^2 + 3x - 4 + \mathcal{E}$



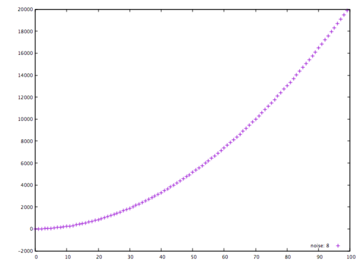
$\mathcal{E} = 0$



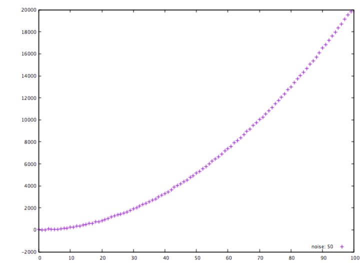
$\mathcal{E} \in$ [-2 .. +2]



$\mathcal{E} \in$ [-4 .. +4]



$\mathcal{E} \in$ [-8 .. 8]



$\mathcal{E} \in$ [-50 .. 50]

Method	$\mathcal{E} = 0$	$\mathcal{E} \in$ [-2 .. 2]	$\mathcal{E} \in$ [-4 .. 4]	$\mathcal{E} \in$ [-8 .. 8]	$\mathcal{E} \in$ [-50 .. 50]
Linear regression	0.9673 1520.0160	0.9673 1519.9055	0.9673 1519.8631	0.9673 1520.1075	0.9672 1521.9613
Random Forest	**0.9997** **190.2147**	**0.9997** **189.5386**	**0.9997** **188.0553**	**0.9997** **188.6072**	**0.9997** **185.6985**
ANN - MLP	**0.9997** **140.1311**	**0.9997** **142.1857**	**0.9998** **132.8442**	**0.9996** **161.0289**	**0.9998** **132.2034**
Decision Table	**0.9924** **737.0877**	**0.9924** **737.2094**	**0.9924** **736.5606**	**0.9924** **737.2194**	**0.9924** **734.9757**

Pearson CCs & Root Mean Squared Errors (RMSE)), n=100

Regression via multiple methods

$f(x,y,z,t) = 5x - 2\cos(y) + 3z^2/\mathrm{sqrt}(t) + \varepsilon$

Method	$\varepsilon = 0$	$\varepsilon \in [-2 .. 2]$	$\varepsilon \in [-4 .. 4]$	$\varepsilon \in [-8 .. 8]$	$\varepsilon \in [-50 .. 50]$
Linear regression	0.9415 29906.8719	0.9415 29906.6893	0.9415 29906.9306	0.9415 29906.2115	0.9415 29902.6757
Random Forest	**0.9997** **2935.4949**	**0.9997** **2935.3471**	**0.9997** **2934.9531**	**0.9997** **2935.7517**	**0.9997** **2921.3079**
ANN - MLP	**0.9999** **1399.9571**	**0.9998** **1558.516**	**0.9999** **1445.3883**	**0.9999** **1392.7396**	**0.9999** **1374.299**
Decision Table	**0.9907** **12059.6908**	**0.9907** **12059.7739**	**0.9907** **12059.4813**	**0.9907** **12059.8852**	**0.9907** **12062.0892**

Pearson CCs & Root Mean Squared Errors (RMSE)), n=100

Clustering

LEARNING TYPES

DATA TYPES

	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Clustering

- The most common **unsupervised learning** method

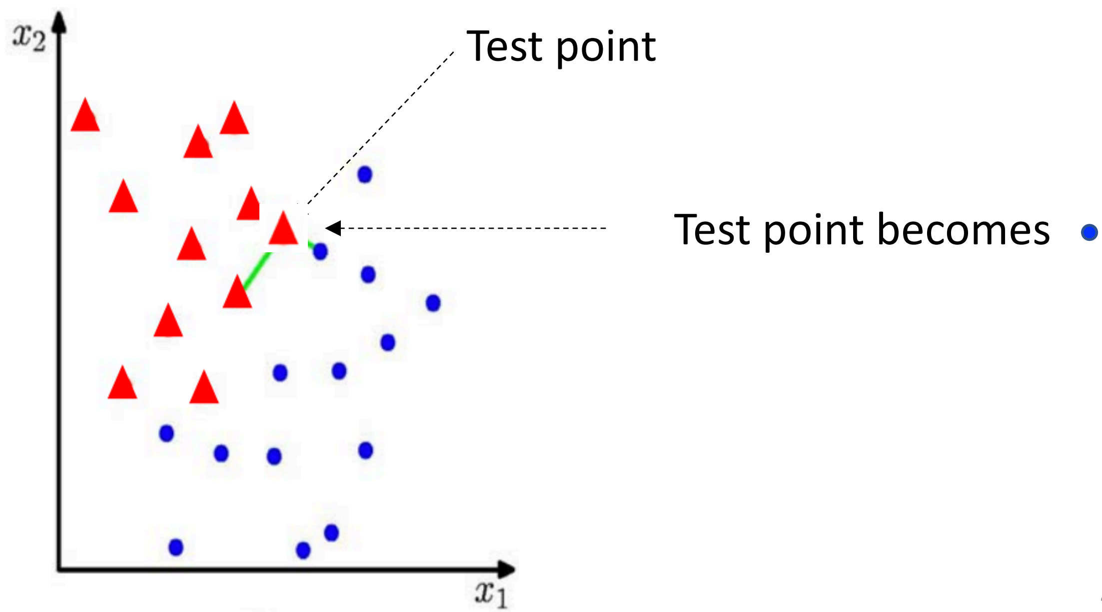
- Used for exploratory data analysis to:
  - Find hidden patterns in data
  - Find groupings in data

- Plethora of methods: KNN, K-means, hierarchical (e.g. neighbour joining), Gaussian mixture models, HMMs, self-organizing neural network maps (SOMs), …

K-Nearest Neighbour (KNN)

- For each test data point (that needs to be assigned a class), find the k-nearest labeled points in the data

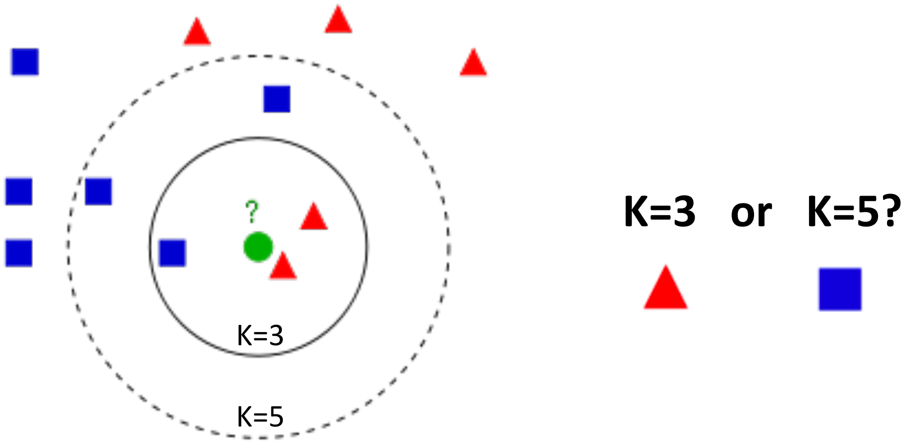
- The test point gets the class label of the majority



K-Nearest Neighbour (KNN)

- **Advantages:**
  - Simple and effective
  - Works on multi-class classification problems, too
  - Only a single parameter to tune (K)

- **Disadvantages:**
  - Accuracy depends on the distance metric
  - Sensitive to: the local structure of the data (skewed distributions), outliers, missing data



Dimensionality Reduction

LEARNING TYPES

DATA TYPES	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Dimensionality Reduction

- Reduce the number of variables to be considered in future analysis

- Why?
  - Quicker and more accurate results from ML methods
  - Easier to visualize the data
  - Sometimes real relationships in the data are described by only a few dimensions (the rest is noise)

- A plethora of methods is available
  - **Types**: local, global and ensemble-like
  - Most of them rely on nearest-neighbour relations
  - **Examples**: PCA, manifold learning, ANN, ISOMAP, Diffusion mapping, Maximum variance unfolding, Locally Linear Embedding (LLE), Laplacian eigenmaps, Hessian LLE, Local Tangent Space Analysis, Ensemble trees, Random Forests, …

ML in Livestock

sensors
MDPI

Review

Machine Learning in Agriculture: A Review

Konstantinos G. Liakos [1], Patrizia Busato [2], Dimitrios Moshou [1,3], Simon Pearson [4] and Dionysis Bochtis [1,*]

1 Institute for Bio-Economy and Agri-Technology (IBO), Centre of Research and Technology—Hellas (CERTH), 6th km Charilaou-Thermi Rd, GR 57001 Thessaloniki, Greece; k.liakos@certh.gr (K.G.L.); dmoshou@auth.gr (D.M.)

Animal Health Research Reviews

cambridge.org/ahr

Review

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A review of traditional and machine learning methods applied to animal breeding

Shadi Nayeri[1], Mehdi Sargolzaei[2,3] and Dan Tulpan[1]

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Abstract

The current livestock management landscape is transitioning to a high-throughput digital era where large amounts of information captured by systems of electro-optical, acoustical, mechanical, and biosensors is stored and analyzed on a daily and hourly basis, and actionable decisions are made based on quantitative and qualitative analytic results. While traditional animal breed-

Animal Behaviour 124 (2017) 203–220

Contents lists available at ScienceDirect

Animal Behaviour

journal homepage: www.elsevier.com/locate/anbehav

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Review

Applications of machine learning in animal behaviour studies

John Joseph Valletta [a,*], Colin Torney [a], Michael Kings [b], Alex Thornton [b], Joah Madden [c]

[a] Centre for Mathematics and the Environment, University of Exeter, Penryn Campus, Penryn, U.K.
[b] Centre for Ecology and Conservation, University of Exeter, Penryn Campus, Penryn, U.K.
[c] Centre for Research in Animal Behaviour, University of Exeter, Exeter, U.K.

Computers and Electronics in Agriculture 162 (2019) 531–542

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

ELSEVIER

Livestock vocalisation classification in farm soundscapes

James C. Bishop[a,b,*], Greg Falzon[a,b], Mark Trotter[c], Paul Kwan[b], Paul D. Meek[d,e]

[a] University of New England – Precision Agriculture Research Group (PARG), Armidale, NSW, Australia
[b] University of New England, School of Science and Technology, Armidale, NSW, Australia
[c] Institute for Future Farming Systems, CQUniversity, Rockhampton, QLD, Australia
[d] NSW Department of Primary Industries, PO Box 530, Coffs Harbour, NSW, Australia
[e] University of New England, School of Environmental and Rural Science, Armidale, NSW, Australia

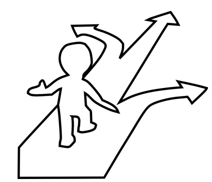
Developing an ML model from Scratch - Process

- **Clearly define the problem**
  - Objective, desired inputs and outputs
  - Is ML appropriate (good/best choice) for the problem?
- **Gather the data**
- **Prepare the data**
  - CLEAN THE DATA (if possible)
  - Re-format the data (image, txt, audio, etc. → tabular)
  - Deal with missing values, categorical vs. numerical values (encoding, scaling), …
  - Feature selection (use meaningful features) → dimensionality reduction (e.g. PCA, …)
  - Shuffle data if needed and if it makes sense (not temporal data)
  - Data splitting: training, testing, validation
- **Choose the evaluation measures**
  - Dependent on the type of problem (classification, regression, …)
  - Note: You can only improve what you can measure!!!
- **Choose an evaluation protocol**
  - fixed split, k-fold cross validation, …
- **Think about over- and under-fitting your data and how to avoid it**
- **Explore models before selecting one or more → Hands-on workshop using Weka**
  - Ideally with minimum programming effort
- **Choose one or more promising models**
- **Tune the chosen models (hyper-parameter optim.) to optimize performance**
  - Grid search, random search, etc.

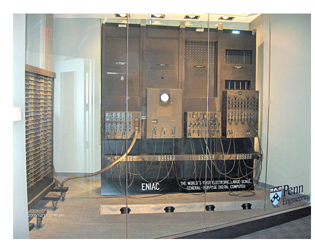
Developing an ML model from Scratch – Practical Considerations

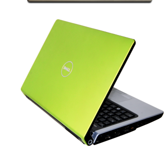
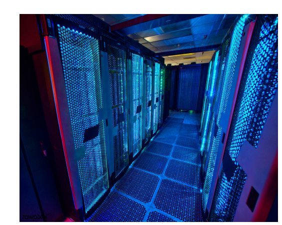
- **Feature selection**
    - Future model use vs. “theoretical beauty” (publication worthiness)

- **Model implementation**
    - Results variability depending on implementations
    - Saving a model is sometimes problematic



- **Model training, testing & deployment**
    - Dependency on hardware, OS and software



Hands-on/Demo Workshop

- Need to install Weka: https://www.cs.waikato.ac.nz/ml/weka/

- Use `Tools`→`Package Manager` to install all models
  - Takes approximately ~15 min and requires a lot of mouse clicks
  - *Note: Do not worry about warning messages. Some external packages are not compatible with the latest version of Weka.*

- Detailed instructions and materials:

  http://animalbiosciences.uoguelph.ca/~dtulpan/conferences/asas2020_mlworkshop/

  Or **https://tinyurl.com/yyx8p473**

References

- Theoretical ML
  - Books (Free):
    - Kubat (2017): An Introduction to Machine Learning
    - James et al. (2017): An Introduction to Statistical Learning
    - Hastie et al. (2017): The Elements of Statistical Learning
    - Leskovec et al. (2017): Mining of Massive Datasets
  - Books (Not Free)
    - Murphy (2012): Machine Learning: a Probabilistic Perspective
    - Marsland (2009): Machine Learning: an Algorithmic Perspective

- Practical ML
  - https://towardsdatascience.com/machine-learning-general-process-8f1b510bd8af

- Online tutorials
  - https://www.tutorialandexample.com/machine-learning-tutorial/

- Libraries and software tools
  - Weka
  - KNIME,
  - Python: scikit-learn, PyTorch, Keras
  - JavaScript: TensorFlow
  - R: caret
  - Apache: Mahout
  - RapidMiner

Thank you

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CDN Canadian Dairy Network

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