Introduction to Machine Learning for Environmental Science

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This 2-day workshop introduces core concepts of machine learning including common algorithms, standard workflows and key software libraries. The focus will be on supervised machine learning for regression and classification using a range of methods such as random forests and deep convolutional neural networks. The material will be taught through a mix of theory and practical examples across different environmental sciences such as meteorology and ecology.

Introduction

- Supervised ML
- Model training
- Examples, model evaluation

Tree-based methods

- Decision trees
- Random Forest, XGBoost

Neural Networks

Supervised machine learning

- We usually have an target (outcome) measurement that we wish to predict.
- The prediction should be based on a set of features (inputs).
- For example
    - predict future temperature based on current temperature, pressure and wind speed
    - predict occurrence of wildfire based on measures of heat, drought and wind
    - predict crop yield based on precipitation, temperature, soil nutrients, pests.
- The goal of supervised ML is to build a model that predicts outcomes based on available features in new, previously unseen situations.
- A "good" model is one that produces accurate predictions.

Regression and classification

- The nature of the target variable determines the type of ML problem.
- Regression: Predicting quantitative outcomes.
    - For example: temperature in degrees, crop yield in tonnes, number of sharks, precipitation amount in mm
- Classification: Predicting categorical outcomes.
    - For example: wildfire occurrence, temperature below zero, precipitation type (rain/snow/hail), precipitation amount none/low/medium/high

Function approximation

- A ML model is a prediction rule that translates one or more features $x_1, x_2, \dots$ into an estimate $\hat{y}$ of the target y.
- The prediction rule is usually calculated by a specific mathematical function

$$\hat{y} = f(x_1, x_2, \dots)$$

- The function $f(\dots)$ usually includes one or many parameters $\theta_1, \theta_2, \dots$ that control how the function translates inputs to outputs.
- Defining the feature vector $\boldsymbol{x} = (x_1, x_2, \dots)$ and parameter vector $\boldsymbol{\theta} = (\theta_1, \theta_2, \dots)$ a ML model is often compactly written as

$$\hat{y} = f(\boldsymbol{x}; \boldsymbol{\theta})$$

Training data

- Supervised ML works by "learning from examples".
- Training data set is a set of input-output examples

$$S = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$$

  where
  - $\boldsymbol{x}_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,k})$ is the feature vector (containing k features) in the i-th example
  - y_i is the outcome in the i-th example
  - n is the sample size
- The training data set S is used to build our prediction model to predict a new outcome y^* based on a feature vector $\boldsymbol{x}^*$.

Empirical loss minimisation

- Model training is achieved by
  - trying to find model parameters $\boldsymbol{\theta}$ such that
  - the model outputs $\hat{y}_1, ..., \hat{y}_n$ calculated from $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$
  - are as "close" as possible to the training targets $y_1, \dots, y_n$
  - where closeness is measured by the loss function $L(\hat{y}, y)$

$$\hat{\boldsymbol{\theta}} = \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$$

- The trained model can then be used to make predictions $\hat{y}^*$ for new outcomed y^* based on new feature vectors $\boldsymbol{x}^*$

$$\hat{y}^* = f(\boldsymbol{x}^*; \hat{\boldsymbol{\theta}})$$

In summary ...

To train a ML model by empirical loss minimisation we need:

- a training data set S containing n examples of inputs and corresponding outcomes
- a model function with trainable parameters $\boldsymbol{\theta}$ that translates inputs $\boldsymbol{x}$ into an output $\hat{y}$
- a loss function that quantifies how close model output $\hat{y}$ is to the target outcome y
- a mechanism to find parameters that minimise the loss

Example: Linear regression

- Training features $x_1, \dots, x_n$ are temperatures at different times $t_1, \dots, t_n$
- Training targets $y_1, \dots, y_n$ are temperatures a short time Δ later $t_1 + \Delta, \dots, t_n + \Delta$
- Model function is a linear function with intercept θ_1 and slope θ_2, such that

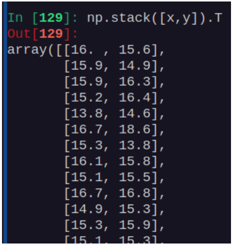
$$\hat{y} = f(x; \boldsymbol{\theta}) = \theta_1 + \theta_2 \cdot x$$

- Our loss function is the squared-error loss

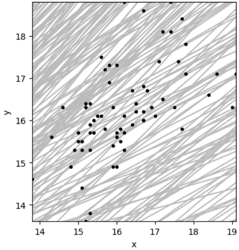
$$L(\hat{y}, y) = (\hat{y} - y)^2$$

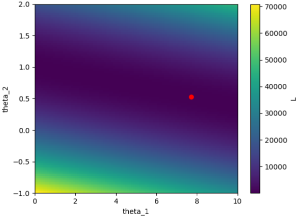
- Optimisation: exaustive search over a grid of parameter values (don't do this in practice!)

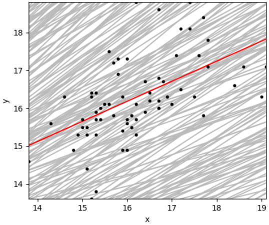
Example: Linear regression

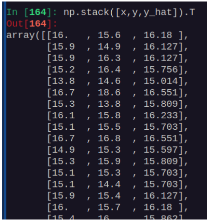


```
In [129]: np.stack([x,y]).T
Out[129]:
array([[16. , 15.6],
       [15.9, 14.9],
       [15.9, 16.3],
       [15.2, 16.4],
       [13.8, 14.6],
       [16.7, 18.6],
       [15.3, 13.8],
       [16.1, 15.8],
       [15.1, 15.5],
       [16.7, 16.8],
       [14.9, 15.3],
       [15.3, 15.9],
       [15.1, 15.3],
```





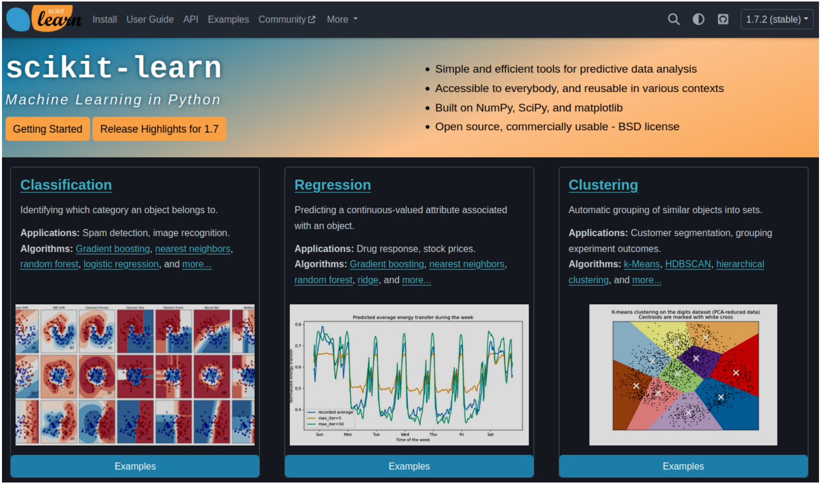




```
In [164]: np.stack([x,y,y_hat]).T
Out[164]:
array([[16.   , 15.6  , 16.18 ],
       [15.9  , 14.9  , 16.127],
       [15.9  , 16.3  , 16.127],
       [15.2  , 16.4  , 15.756],
       [13.8  , 14.6  , 15.014],
       [16.7  , 18.6  , 16.551],
       [15.3  , 13.8  , 15.809],
       [16.1  , 15.8  , 16.233],
       [15.1  , 15.5  , 15.703],
       [16.7  , 16.8  , 16.551],
       [14.9  , 15.3  , 15.597],
       [15.3  , 15.9  , 15.809],
       [15.1  , 15.3  , 15.703],
       [15.1  , 14.4  , 15.703],
       [15.9  , 15.4  , 16.127],
       [16.   , 15.7  , 16.18 ],
       [15.4  , 16.   , 15.862],
```

Machine Learning in python with `scikit-learn`

`https://scikit-learn.org`



scikit-learn

Machine Learning in Python

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying which category an object belongs to.

Applications: Spam detection, image recognition.
Algorithms: Gradient boosting, nearest neighbors, random forest, logistic regression, and more...

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, stock prices.
Algorithms: Gradient boosting, nearest neighbors, random forest, ridge, and more...

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, grouping experiment outcomes.
Algorithms: k-Means, HDBSCAN, hierarchical clustering, and more...

K-means clustering on the digits dataset (PCA-reduced data)
Centroids are marked with white cross
Examples

Linear Regression in Scikit-Learn

```
import numpy as np
from sklearn.linear_model import LinearRegression

# load file
t7110 = np.loadtxt("t7110.dat", comments="#")

# extract features (july temperatures) and targets (august temperatures)
x = t7110[:, 7]
y = t7110[:, 8]

# sklearn expects k features to be stored in a 2d array with k columns
x = x.reshape(-1, 1)

# initialise a linear regression model
model = LinearRegression()

# fit the model to data
model.fit(x, y)

# extract parameter estimates from fitted model
theta_hat = np.array([model.intercept_, model.coef_[0] ])

# calculate predictions in training data
y_hat = model.predict(x)

# calculate predictions on new data
x_new = np.linspace(15, 20, 100).reshape(-1,1)
y_new = model.predict(x_new)
```

How good is my model?

- The model outputs $\hat{y}_1, \ldots, \hat{y}_n$ be compared to the targets $y_1, \ldots, y_n$ using a suitable error metric.
- For example root mean squared error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}$$

- Our model has $RMSE \approx 0.9$ – Is that "good"?
- Getting $RMSE > 0$ means our model is not perfect, but how bad is it?
- To judge whether the model is useful we should compare it to a suitable benchmark.

Benchmarking

- A benchmark model (or reference model) for performance evaluation is usually one or several of
  - An alternative (competing) model for the same target.
  - Climatology (constant mean):

$$\hat{y}_i^{(clim)} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

  - Persistence (last available observation of the target); here:

$$\hat{y}_i^{(pers)} = x_i$$

  - Any other simple estimate of the target that could be calculated with reasonable effort given the same inputs as our model.
  - In fact, linear regression itself is often a good reference to benchmark more complicated ML model.

Skill scores

- Given a suitable error metric, we calculate
  - S: the error of our model (averaged over a test data set)
  - S_{ref}: the mean error of our chosen reference model
  - S_{perf}: the mean error or a hypothetical perfect model that outputs $\hat{y}_i = y_i$ each time; (usually $S_{perf} = 0$)
- The skill score of our model relative to the benchmark is then defined as

$$Skill = \frac{S_{ref} - S}{S_{ref} - S_{perf}}$$

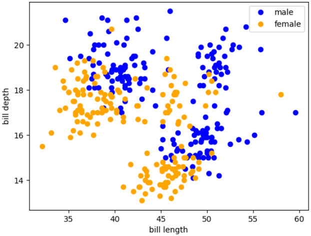
- $Skill \leq 0$: Our model is not better than the benchmark.
- $Skill \in (0, 1)$: Our model improves over the benchmark.
- $Skill = 1$: Our model is perfect.

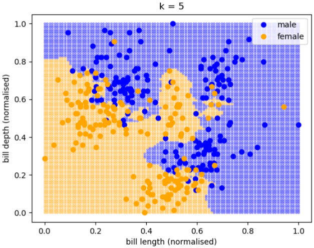
Example: k-nearest-neighbor classification

- given an input $\boldsymbol{x}^*$ find the k closest features $\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(k)}$ in the training data, and the corresponding outcomes $y^{(1)}, \dots, y^{(k)}$
- "closeness" between the feature vectors $\boldsymbol{x}^{(i)}$ and $\boldsymbol{x}^{(j)}$ is defined in terms of the Euclidean distance $\sqrt{\sum_m (x_m^{(i)} - x_m^{(j)})^2}$
- predict $\hat{y}^*$ as the majority vote over $y^{(1)}, \dots, y^{(k)}$
- ties are resolved by picking the outcome class lowest value or alphabetical rank

Example: k-nearest-neighbor classification

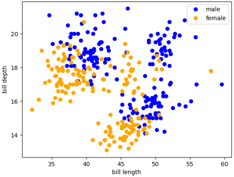
- For illustration we use data from the "Palmer Penguin" data.
- Features are penguins' bill length (x_1) and bill depth (x_2) and outcome (y) is the penguin's sex (male or female).
- The kNN classifier ($k = 5$) separates the x_1/x_2 plane into regions for "female" and "male", separated by a decision boundary.

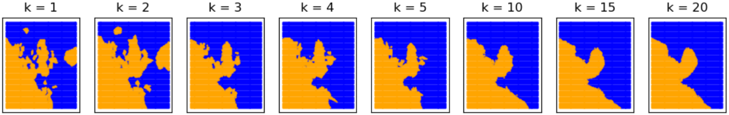




Example: k-nearest-neighbor classification

- The parameter k controls the "roughness" of the classifier.
- Larger values of k produce smoother decision boundaries.

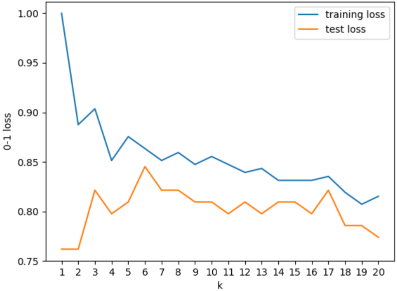




- Is k a trainable parameter that can be selected by empirical loss minimisation?

Example: k-nearest-neighbor classification

- Split the data randomly into training and test data set:
  - Only the training data set is used by the kNN classifier.
  - Training and test data are used separately to calculate the 0-1 loss (aka accuracy, aka proportion correct) of the classifier.



- The training accuracy is perfect for $k = 1$ (Why?) and goes down as k increases.
- The test accuracy is best for $k \approx 6$.

- The neighborhood parameter k can be optimised by loss minimisation, but should use a different data set than the one used to define the kNN classifier.

In-sample vs Out-of-sample error

- Our goal is to train a model that generalises well to new data.
- Loss on training data (in-sample error) is too optimistic because the model has seen the data.
- Overfitting: A model achieves very low training loss by "regurtitating" the training data, including any noise and accidental patterns. Overfitted models generalise poorly to new data.
- Loss on previously unseen data (out-of sample error) is what we are really interested in.
- It is good practice to remove a fraction of data (e.g. 20%) during training and use only for model testing.

Further reading

- Linear algebra for least squares regression.
- Alternative loss functions
- Multiple linear regression for multiple inputs.
- Logistic regression for classification.
- Radius-neighborhood classifier and other neighborhood methods.
- Neighborhood methods for missing data imputation.
- Uncertainty estimation: Resampling methods, bootstrapping.

Introduction

- Supervised ML
- Model training
- Examples, model evaluation

Tree-based methods

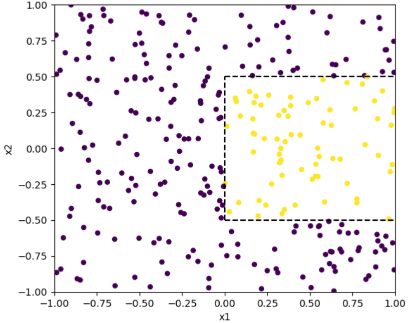
- Decision trees
- Random Forest, XGBoost

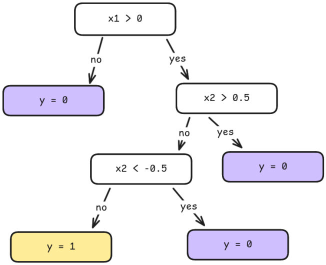
Neural Networks

Background

- Tree-based methods are simple and powerful function approximation methods.
- During training, the feature space is split up into rectangular regions.
- The model's prediction within each rectangular region is a constant.

Decision tree example





Decision tree terminology

- Split: Partitioning data based on a feature and threshold value
- Node: a point in the tree where a decision is made
- Root node: first split in the tree
- Internal/decision node: Any node that performs a split
- Leaf node: Final node that outputs a prediction
- Depth: Number of decision levels from Root node to leaves
- Impurity: Measure how mixed the classes are
- Information gain: Reduction in impurity after a split

Training a decision tree

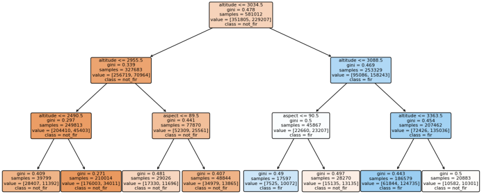
```
from sklearn.tree import DecisionTreeClassifier

# initialise decision tree with set maximum depth
clf = DecisionTreeClassifier(max_depth=10)

# X: shape (n_samples, n_features)
# y: shape (n_samples,) with 0/1 encoded class label

# train decision tree
clf.fit(X, y)
```

Decision tree for tree cover classification

Data set (plot), no code required it's on previous slide, decision surface

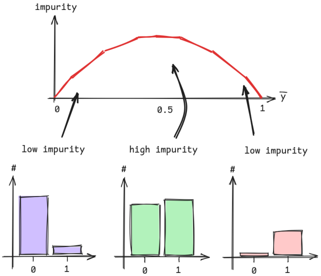
Visualising trained decision trees

```
from sklearn import tree
clf = DecisionTreeClassifier(
        max_depth=3)
clf.fit(X, y)
plt.figure(figsize=(10, 6))
tree.plot_tree(clf,
  feature_names=["altitude",
                 "aspect"],
  class_names=["not_fir",
               "fir"],
  filled=True,
  rounded=True,
  fontsize=8)
plt.show()
```



Finding features and thresholds for splitting

- Gini impurity and entropy are measures of impurity, disorder, indeterminism.
- Binary data: $\boldsymbol{y} = (y_1, \ldots, y_n) = (0, 0, 1, 0, 1, \ldots)$.
- Summarise $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.



- Gini impurity: $G(\boldsymbol{y}) = 1 - \bar{y}^2 - (1 - \bar{y})^2$
- Entropy: $H(\boldsymbol{y}) = \bar{y} \log \bar{y} + (1 - \bar{y}) \log(1 - \bar{y})$

Maximising Information Gain

- We apply threshold-splitting of the data wrt one feature.
- This separates the data $\boldsymbol{y}$ into $\boldsymbol{y}_{left}$ and $\boldsymbol{y}_{right}$ of sizes n_{left} and n_{right}.
- The impurity of the split data set is calculated by

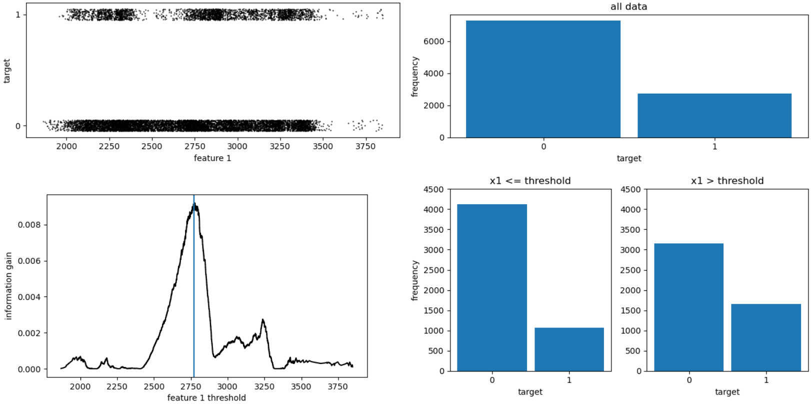
$$G(\boldsymbol{y}_{left}, \boldsymbol{y}_{right}) = \frac{n_{left}}{n} G(\boldsymbol{y}_{left}) + \frac{n_{right}}{n} G(\boldsymbol{y}_{right})$$

- The impurity reduction (or "information gain") caused by the split is given by

$$IG = G(\boldsymbol{y}) - G(\boldsymbol{y}_{left}, \boldsymbol{y}_{right})$$

- The feature/threshold combination that yields the highest information gain is selected.

Maximising Information Gain



Random Forest

- A RF is an ensemble of decision trees.
- Each tree is trained on random subsets of training data and input features.
- Each tree makes a prediction and the forest aggregates them.
  - Classification: Majority vote
  - Regression: Average
- Improves robustness and avoids overfitting compared to single decision tree.

Example

MORE HERE: show code, example data, single tree vs RF decision surfaces

Boosting

- In ensemble methods (such as RF), each classifier (tree) is independently trained and optimised for maximum accuracy.
- A boosting algorithm trains a chain of weak classifiers sequentially.
- Core algorithm:
    - train a simple model
    - calculate its errors over the training data
    - train the next model to take the same inputs but predict the previous model's errors
    - repeat, then aggregate all models (often with weights)
- Throughtout the sequence the model is improved by gradually refining the prediction.

Gradient Boosting, XGBoost

- Gradients of the loss function $g_i = \frac{\partial L(\hat{y}_i, y_i)}{\partial \hat{y}_i}$ approximate errors.
- Changing $\hat{y}_i$ proportional to $-g_i$ will decrease the loss.
- In gradient boosting, each tree predicts the negative gradient $\frac{\partial L(\hat{y}, y)}{\partial \hat{y}}$ of the previous tree
- XGBoost is a popular library for Gradient Boosting
- MORE HERE

OLD Background: Measuring surprise

- Shannon and Weaver (1948) developed a mathematical theory of communication
- As part of this they needed a mathematical measure of "surprise" after observing the outcome of a random variable, which has n possible outcomes with probabilities $p_1, \ldots, p_n$
- Based on simple considerations (additivity, continuity) they showed that if outcome k is observed, the only reasonable measure of surprise is

$$-\log_2 p_k$$

- A high-probability outcome is less surprising than a low-probability outcome.

OLD Background: Entropy

- Entropy is the negative expected surprise

$$H(p_1, \ldots, p_n) = \sum_{i=1}^{n} p_i \log_2 p_i$$

- Entropy is a summary measure of uncertainty or information content of a probability distribution.
- The higher entropy, the more "deterministic" a distribution is.
- TODO: A few bar plots of distributions with their entropy values.

OLD Background: Empirical entropy

- Given a set of values $S = (y_1, \dots, y_n)$ where each y_i is either 0 or 1
- From S we estimate the probability that $y_i = 1$ by

$$\hat{p} = \frac{1}{n} \sum_{i=1}^{n} y_i$$

- The probability that $y_i = 0$ is then estimated by $1 - \hat{p}$.
- We calculate the empirical binary entropy of the sample S as the entropy of the distribution $(\hat{p}, 1 - \hat{p})$

$$H(S) = \hat{p} \log_2 \hat{p} + (1 - \hat{p}) \log_2 (1 - \hat{p})$$

OLD Decision stump

- We have a data set of input/output pairs $S = \{(x_i, y_i)\}_{i=1}^n$ where
- $x_i \in \mathbb{R}$ are continuous inputs (eg temperature) and
- $y_i \in \{0, 1\}$ are binary outputs (eg rain occurrence)
- We want to find a threshold τ to "optimally separate" the data set S into S_l and S_r by

$$S_l = \{(x_i, y_i) : x_i < \tau\} \quad S_r = \{(x_i, y_i) : x_i > \tau\}$$

- How to choose the threshold? What does "optimally separate" mean here?

OLD Decision stump

- After setting the threshold τ a fraction $q_l = \frac{|S_l|}{|S|}$ of data ends up left of the threshold and $q_r = \frac{|S_r|}{|S|}$ on the right
- Each set has its individual empirical entropy $H(S_l)$ and $H(S_r)$
-

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Artificial neuron (Perceptron)

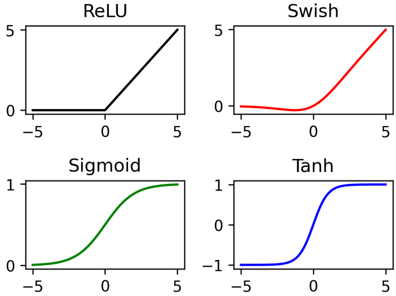
- An artificial neuron (perceptron) is a function

$$y = f(\boldsymbol{x}; \boldsymbol{w}, b) = \varphi\left(w_1 \cdot x_1 + \cdots + w_k \cdot x_k + b\right)$$

- where
  - $\boldsymbol{x} = (x_1, \ldots, x_k)$ is the k-dimensional input vector
  - y is the 1-dimensional output of the neuron
  - $\boldsymbol{w} = (w_1, \ldots, w_k)$ is the k-dimensional vector of weights
  - b is the bias
  - $\varphi(\cdot)$ is the activation function

Activation functions

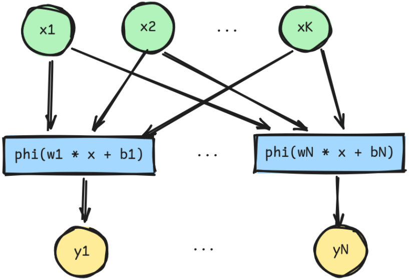
- Typical activation functions:
  - ReLU (Rectifier): $\varphi(x) = max(0, x)$
  - Sigmoid: $\varphi(x) = 1/(1 + e^{-x})$
  - Swish: $\varphi(x) = x/(1 + e^{-x})$
  - Tanh: $\varphi(x) = (e^{x} - e^{-x})/(e^{x} + e^{-x})$



Single-layer perceptron

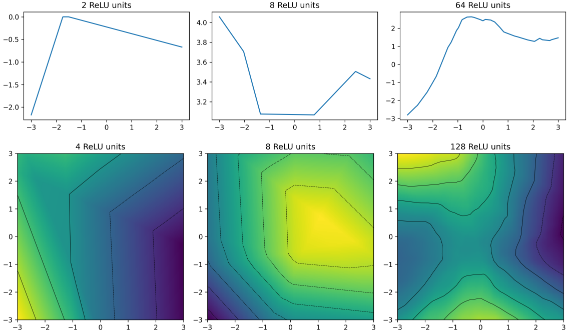
- multiple perceptrons (each with different weights and biases) calculating their outputs in parallel

$$y_i = \varphi\left(\boldsymbol{w}_i^T \boldsymbol{x} + b_i\right)$$



Examples

Examples of randomly initialised 1d and 2d single layer perceptrons with increasing numbers of neurons, illustrating increasing flexibility and "expressive power".



Terminology

Multilayer perceptron

The Keras API

Simple data example

Model summary

Loss functions

crossentropy-loss for classification, squared-error loss for regression

Gradient descent

Backpropagation

Stochastic gradient descent

Optimiser hyperparameters

Monitoring performance

learning curves, restarting training runs

Spatial data: 2d convolution

The channel dimension

Convolutional neural network

Encoder-Decoder architecture

Example: Weather image classification

Cross-validation, early stopping

Dropout

Further Reading

- Sensitivity analysis, interpretability
- Fine-tuning for new outputs/objectives
- Speeding up NNs: Quantisation, layer-wise optimisation
- MORE HERE