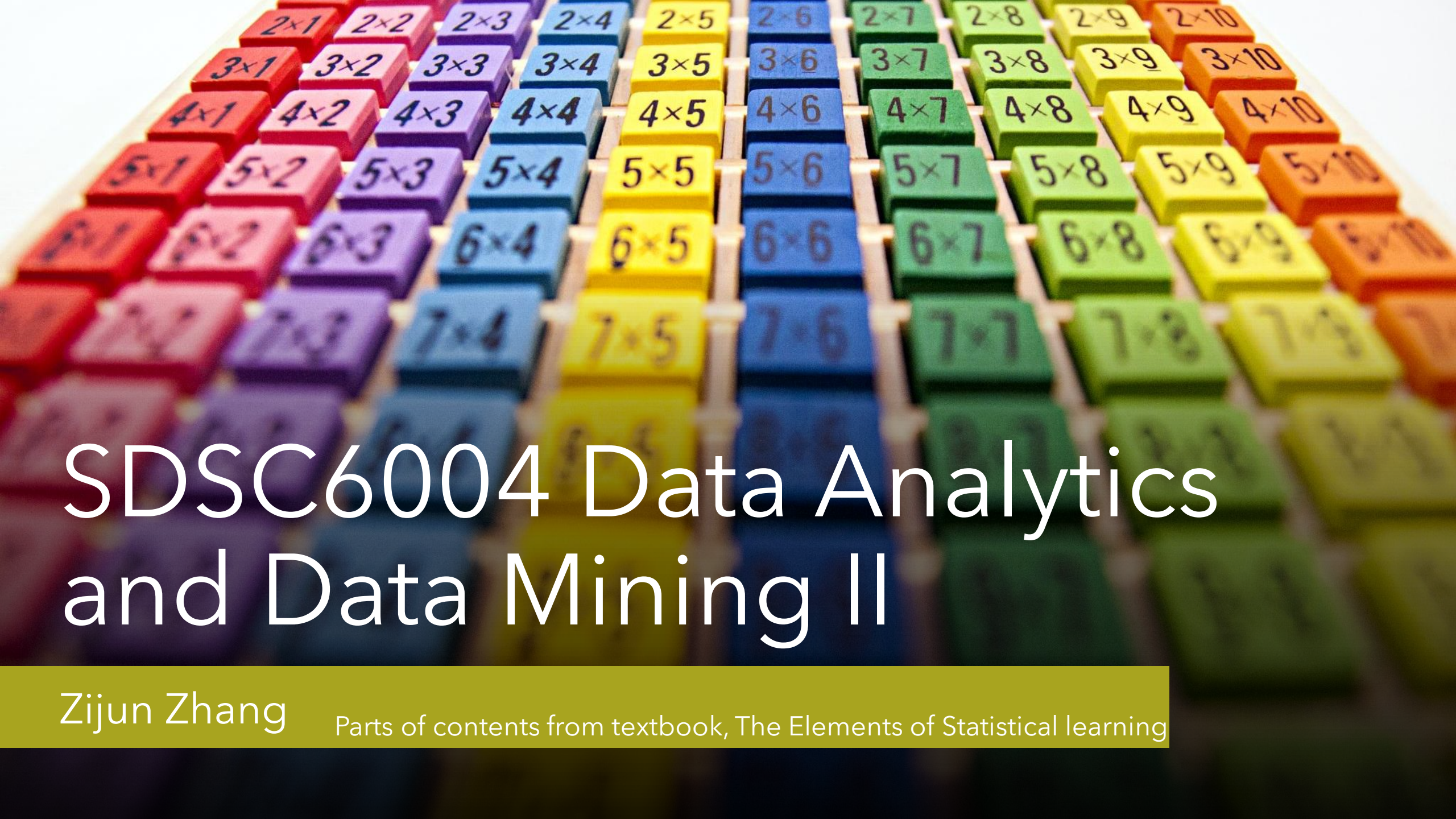


SDSC6004 Data Analytics and Data Mining II

Zijun Zhang

Parts of contents from textbook, The Elements of Statistical learning

Regression: Definition

- Given a collection of records (training set)
  - Each record is by characterized by a tuple ($\boldsymbol{x}$,y), where $\boldsymbol{x}$ is the attribute set and y is the numerical
- Task:
  - Learn a model which predicts the value of y based on the attribute set $\boldsymbol{x}$

Basic statistical regression methods

- Linear regression

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j. \qquad (3.1)$$

- Learning goal:

$$\beta = \text{argmin}_{\beta} \sum (f(X, \beta) - y)$$

Basic statistical regression methods

- Ridge

$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\text{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}. \qquad (3.41)$$

Basic statistical regression methods

- LASSO

$$\hat{\beta}^{\text{lasso}} = \underset{\beta}{\operatorname{argmin}} \left\{ \frac{1}{2} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}. \qquad (3.52)$$

Ridge v.s. Lasso

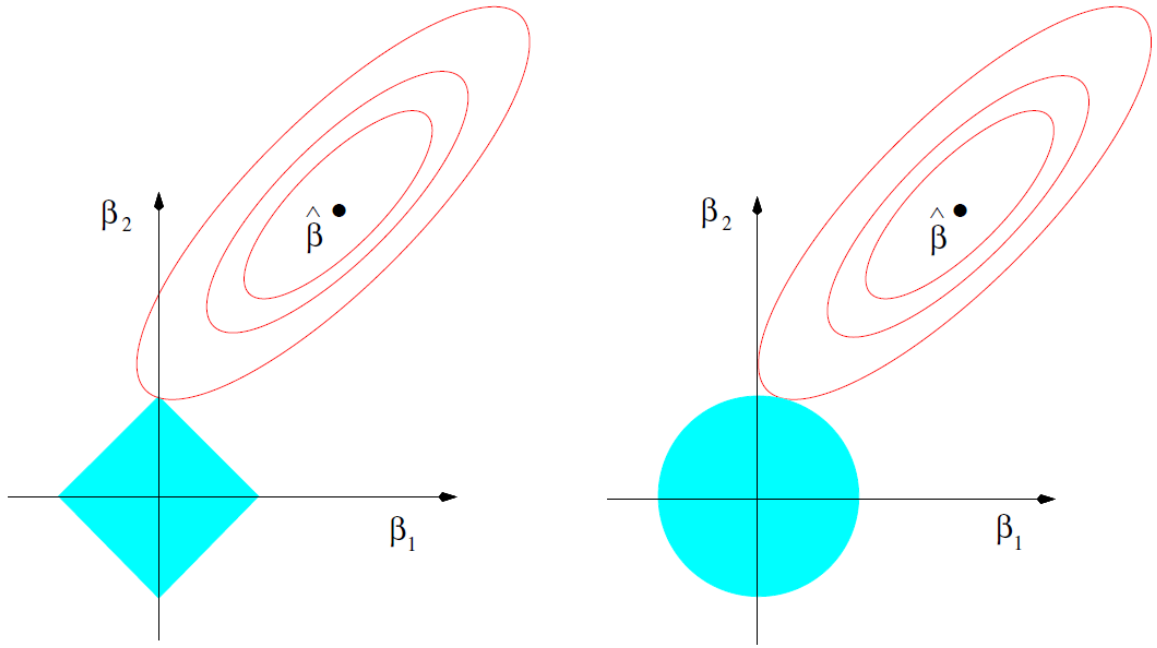


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

k Nearest Neighbor Regression

- Searching k nearest neighbors based on the value of k and the distance metric.
- Simply take the average of y of k nearest neighbors and use it as the estimated y of the target data.

$$\hat{f}(x) = \mathrm{Ave}(y_i | x_i \in N_k(x)) \qquad (6.1)$$

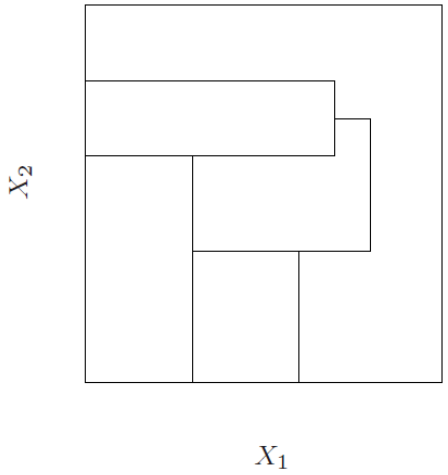
Regression Trees

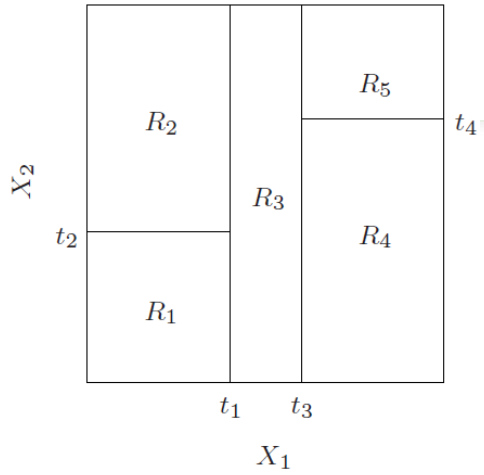
$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

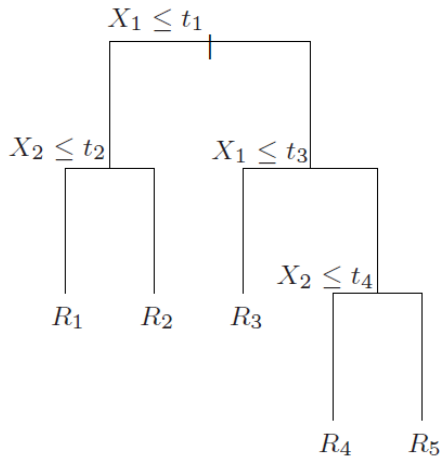
- Partition space of data
- Find the optimal split
- Taking the average of

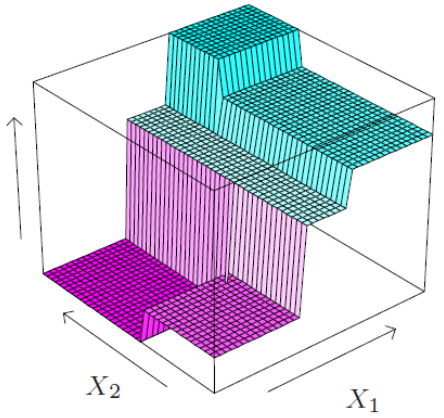
y of data points in nodes

of tree as the final estimates









Regression Trees

- A greedy split strategy and the split criteria

$$R_1(j,s) = \{X | X_j \leq s\} \text{ and } R_2(j,s) = \{X | X_j > s\}.$$

- which leads to

$$\min_{j,\, s} \left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right].$$

SVM Regression

- To find a linear function $f(x)=x'\beta+b$
- with the minimal norm value ($\beta'\beta$), which is formulated as

$$J(\beta)=1/2(\beta'\beta)$$

$$s.t.$$

$$\forall n:[y_n-(x_n'\beta+b)]\leq\varepsilon$$

It means to have all residuals less than ε.

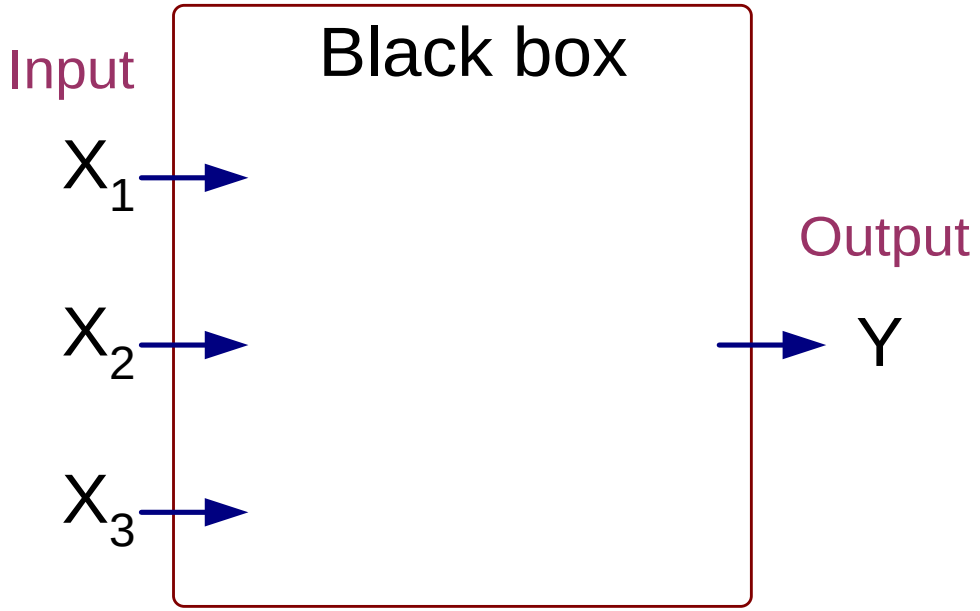
SVM Regression

- It is possible that the previous idea $f(x)$ might not exist
- We can introduce the slack variable ξ
- We can use kernels to project x to other planes $G(x_n, x)$, commonly considered kernels: Linear, Gaussian, Polynomial

Artificial Neural Networks

- Start with classification examples

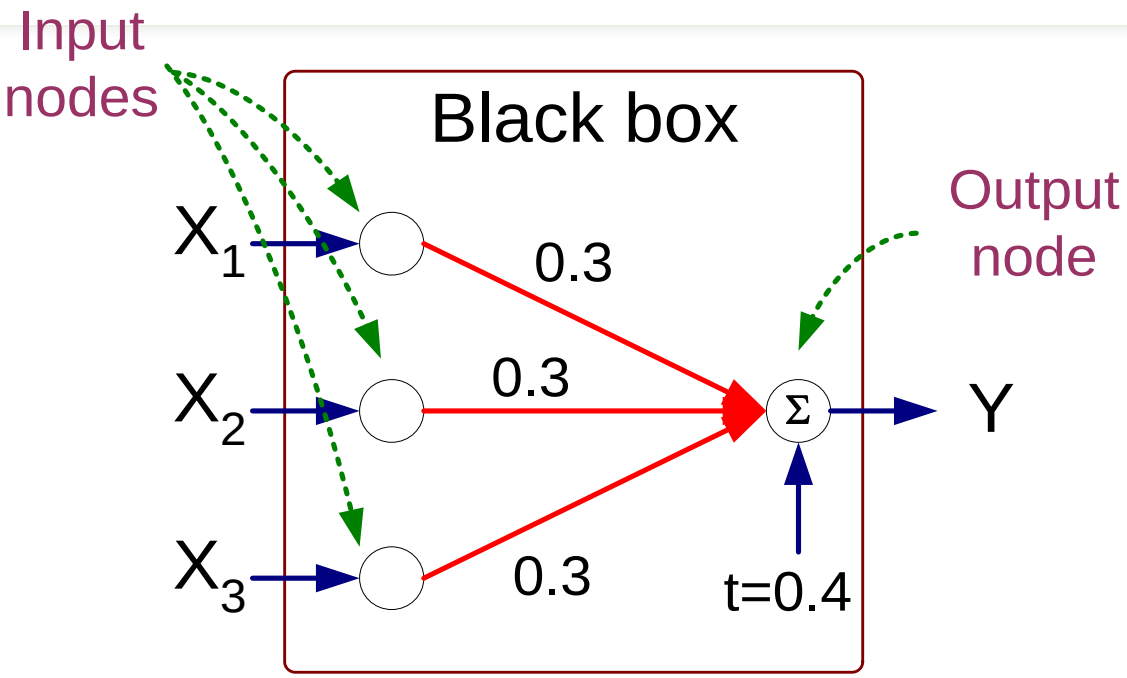
X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1



Output Y is 1 if at least two of the three inputs are equal to 1.

Artificial Neural Networks

X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1



$$Y = sign(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4)$$

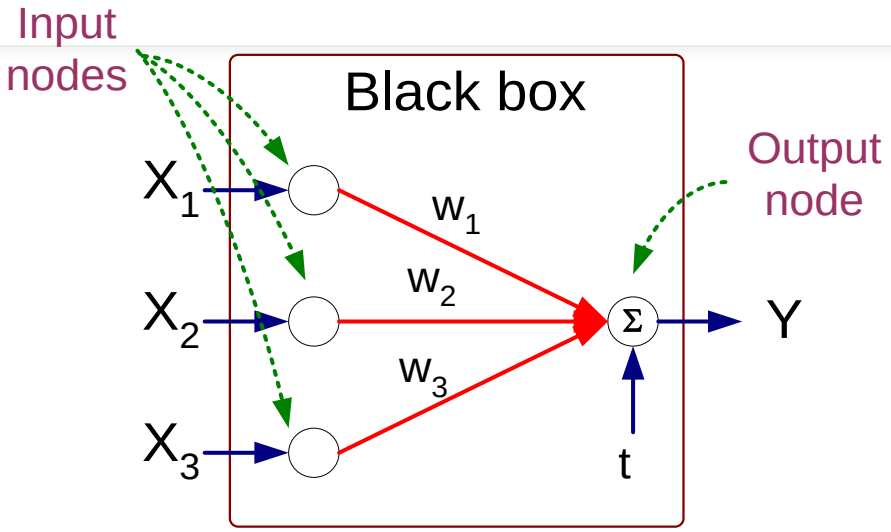
$$\text{where } sign(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0 \end{cases}$$

Artificial Neural Networks

- Model is an assembly of inter-connected nodes and weighted links

- Output node sums up each of its input value according to the weights of its links

- Compare output node against some threshold t

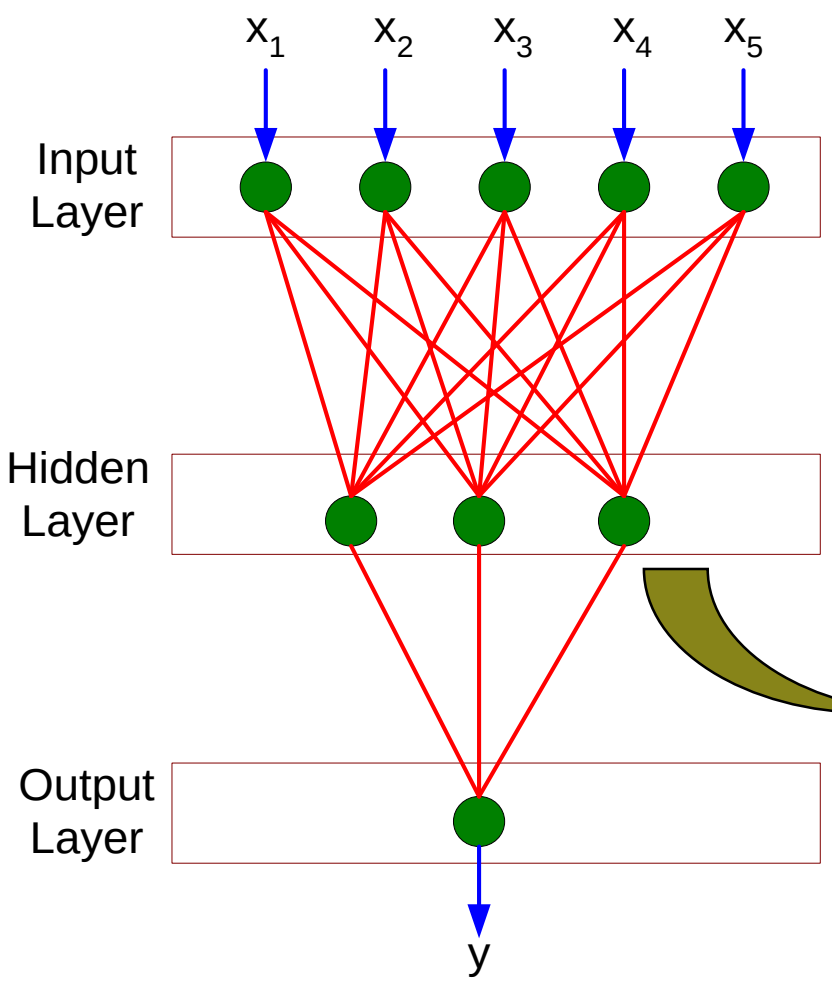


Perceptron Model

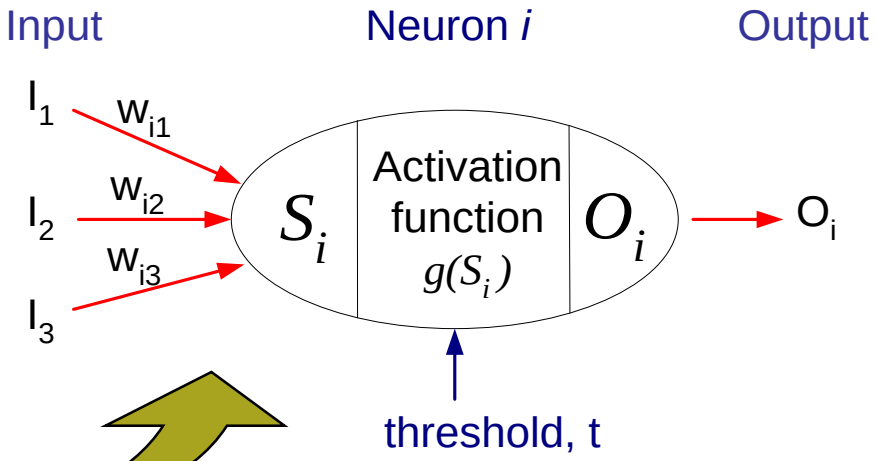
$$Y = sign(\sum_{i=1}^{d} w_i X_i - t)$$

$$= sign(\sum_{i=0}^{d} w_i X_i)$$

Artificial Neural Networks



General Network Structure



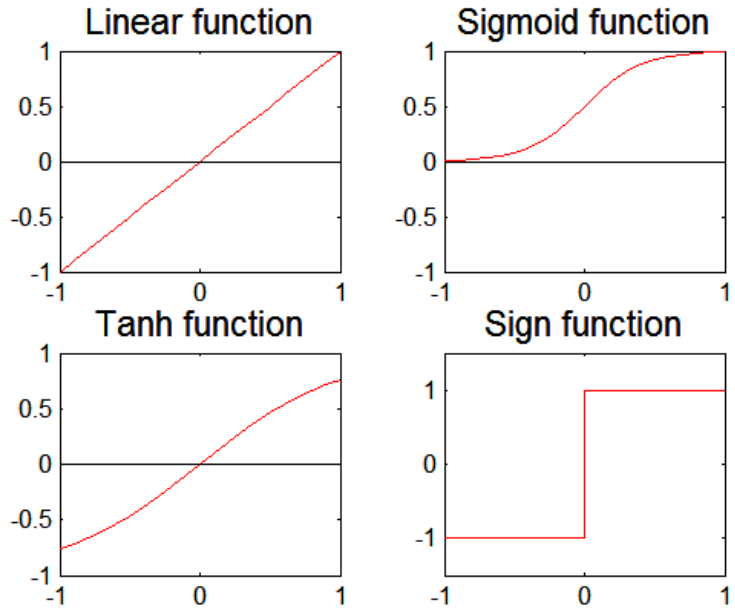
Training ANN means learning the weights of the neurons

Artificial Neural Networks

- Various types of neural network topology
  - single-layered network (perceptron) versus multi-layered network
  - Feed-forward versus recurrent network

- Various types of activation functions (f)

$$Y = f(\sum_i w_i X_i)$$



Perceptron

- Single layer network
  - Contains only input and output nodes
- Activation function: f = sign(w•x)
- Applying model is straightforward

$$Y = sign(0.3X_1 + 0.3X_2 + 0.3X_3 - 0.4)$$

$$\text{where } sign(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0 \end{cases}$$

- $X_1 = 1, X_2 = 0, X_3 = 1 \Rightarrow y = sign(0.2) = 1$

Perceptron Learning Rule

- Initialize the weights (w_0, w_1, …, w_d)
- Repeat
  - For each training example (x_i, y_i)
    - Compute f(w, x_i)
    - Update the weights:

$$w^{(k+1)} = w^{(k)} + \lambda\left[y_i - f\left(w^{(k)}, x_i\right)\right]x_i$$

- Until stopping condition is met

Perceptron Learning Rule

- Weight update formula:

$$w^{(k+1)} = w^{(k)} + \lambda\left[y_i - f(w^{(k)}, x_i)\right]x_i \;\; ; \;\; \lambda : \text{learning rate}$$

- Intuition:
  - Update weight based on error: $e = \left[y_i - f(w^{(k)}, x_i)\right]$
  - If y=f(x,w), e=0: no update needed
  - If y>f(x,w), e=2: weight must be increased so that f(x,w) will increase
  - If y<f(x,w), e=-2: weight must be decreased so that f(x,w) will decrease

Example of Perceptron Learning

$$w^{(k+1)} = w^{(k)} + \lambda\left[y_i - f(w^{(k)}, x_i)\right]x_i$$

$$Y = sign(\sum_{i=0}^{d} w_i X_i)$$

$$\lambda = 0.1$$

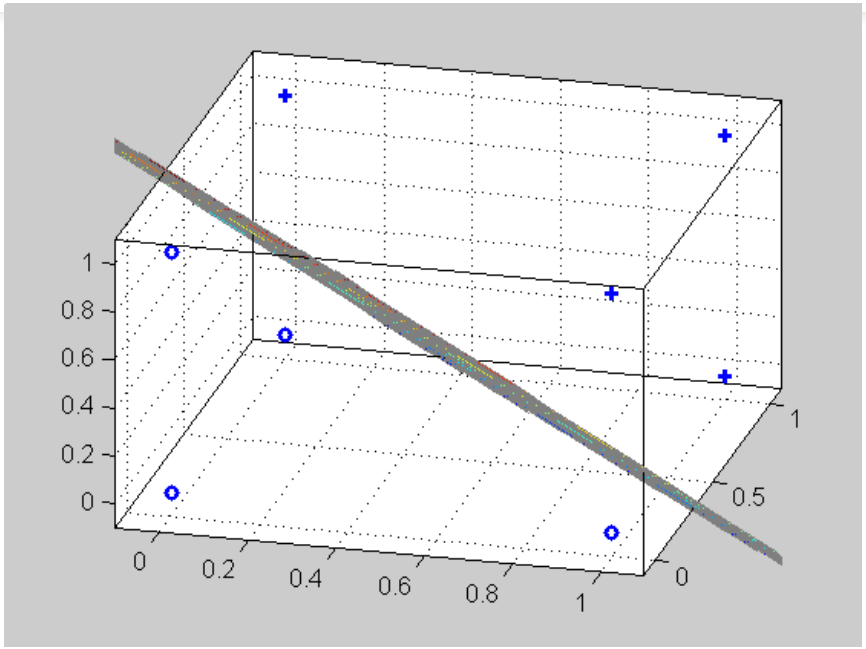
X_1	X_2	X_3	Y
1	0	0	-1
1	0	1	1
1	1	0	1
1	1	1	1
0	0	1	-1
0	1	0	-1
0	1	1	1
0	0	0	-1

	w_0	w_1	w_2	w_3
0	0	0	0	0
1	-0.2	-0.2	0	0
2	0	0	0	0.2
3	0	0	0	0.2
4	0	0	0	0.2
5	-0.2	0	0	0
6	-0.2	0	0	0
7	0	0	0.2	0.2
8	-0.2	0	0.2	0.2

Epoch	w_0	w_1	w_2	w_3
0	0	0	0	0
1	-0.2	0	0.2	0.2
2	-0.2	0	0.4	0.2
3	-0.4	0	0.4	0.2
4	-0.4	0.2	0.4	0.4
5	-0.6	0.2	0.4	0.2
6	-0.6	0.4	0.4	0.2

Perceptron Learning Rule

- Since f(w,x) is a linear combination of input variables, decision boundary is linear

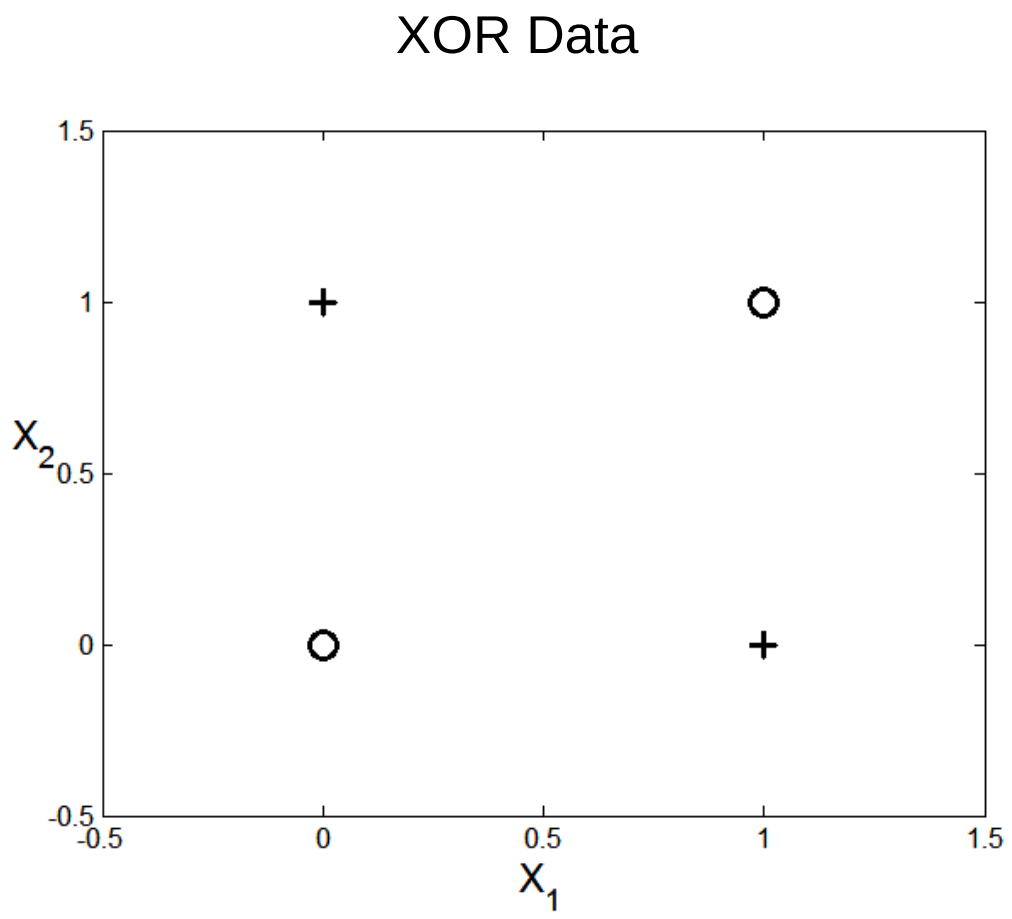


- For nonlinearly separable problems, perceptron learning algorithm will fail because no linear hyperplane can separate the data perfectly

Nonlinearly separable data

$$y = x_1 \oplus x_2$$

x_1	x_2	y
0	0	-1
1	0	1
0	1	1
1	1	-1

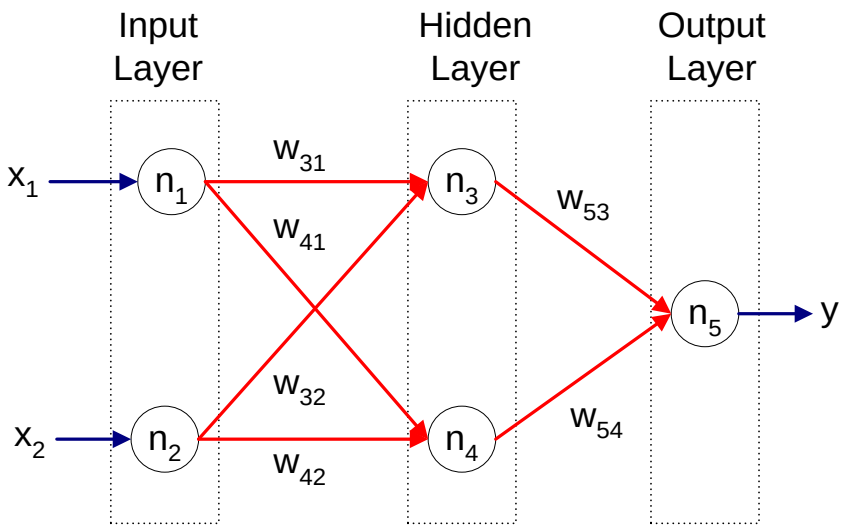


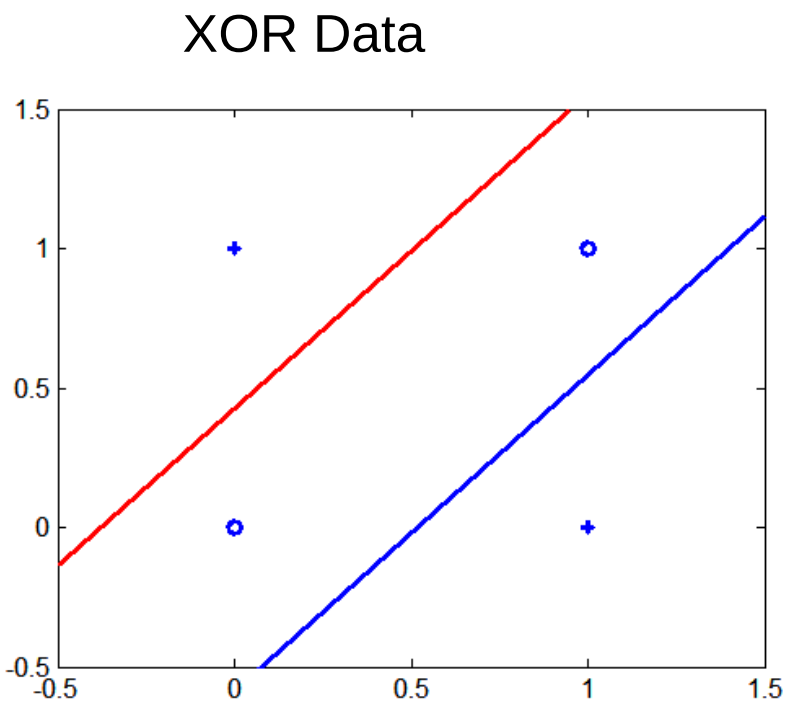
Multilayer Perceptron

- Hidden layers
  - intermediary layers between input & output layers
- More general activation functions (sigmoid, linear, etc)

Multilayer Perceptron

- Multi-layer neural network can solve any type of classification task involving nonlinear decision surfaces





Learning Multilayer Perceptron

- Can we apply perceptron learning rule to each node, including hidden nodes?
  - Perceptron learning rule computes error term e = y-f(w,x) and updates weights accordingly
    - Problem: how to determine the true value of y for hidden nodes?
  - Approximate error in hidden nodes by error in the output nodes
    - Problem:
      - Not clear how adjustment in the hidden nodes affect overall error
      - No guarantee of convergence to optimal solution

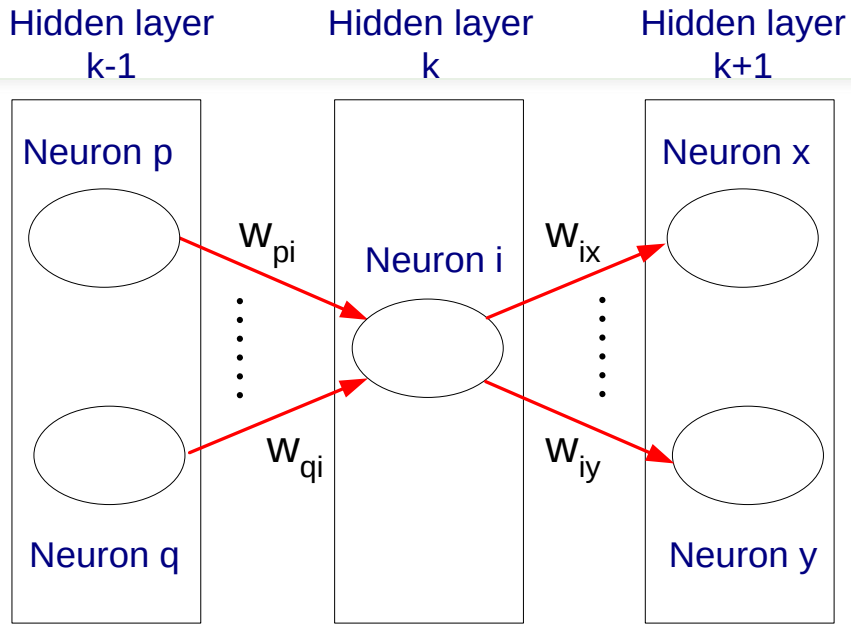
Gradient Descent for Multilayer Perceptron

- Weight update: $w_j^{(k+1)} = w_j^{(k)} - \lambda \frac{\partial E}{\partial w_j}$
- Error function: $E = \frac{1}{2}\sum_{i=1}^{N}\left(t_i - f(\sum_j w_j x_{ij}) \right)$
- Activation function f must be differentiable
- For sigmoid function: $w_j^{(k+1)} = w_j^{(k)} + \lambda \sum_i (t_i - o_i) o_i (1 - o_i) x_{ij}$
- Stochastic gradient descent (update the weight immediately)

Gradient Descent for Multilayer Perceptron

- For output neurons, weight update formula is the same as before (gradient descent for perceptron)

- For hidden neurons:



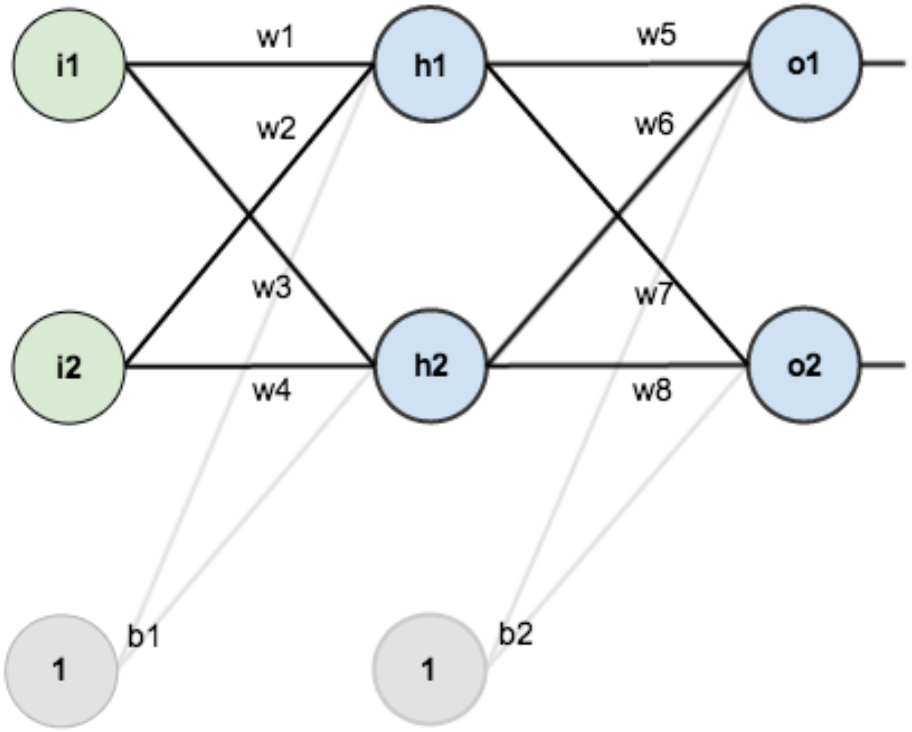
$$w_{pi}^{(k+1)} = w_{pi}^{(k)} + \lambda o_i (1 - o_i) \sum_{j \in \Phi_i} \delta_j w_{ij} x_{pi}$$

$$\text{Output neurons}: \delta_j = o_j (1 - o_j)(t_j - o_j)$$

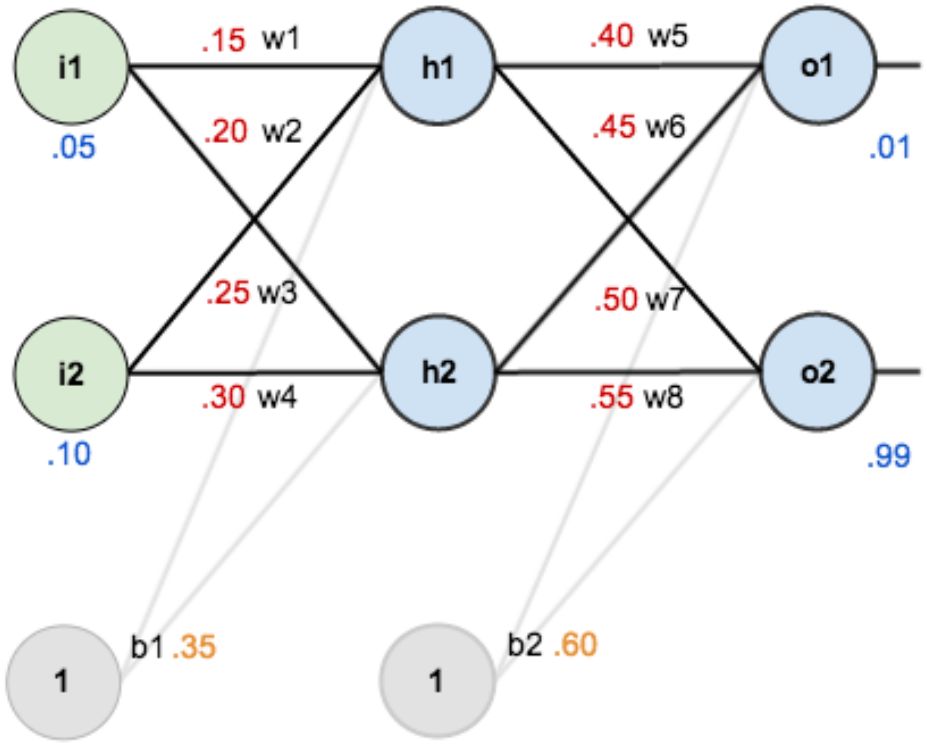
$$\text{Hidden neurons}: \delta_j = o_j (1 - o_j) \sum_{k \in \Phi_j} \delta_k w_{jk}$$

Backpropagation

A nice example offered by Matt Mazur



Given inputs 0.05 and 0.1, make NN output 0.01 and 0.99



Backpropagation

You want to make changes, first you need to check how it performs right now – Forward pass

$$net_{h1} = w_1 * i_1 + w_2 * i_2 + b_1 * 1$$

$$net_{h1} = 0.15 * 0.05 + 0.2 * 0.1 + 0.35 * 1 = 0.3775$$

Activation function: Logistic

$$out_{h1} = \frac{1}{1+e^{-net_{h1}}} = \frac{1}{1+e^{-0.3775}} = 0.593269992$$

$$out_{h2} = 0.596884378$$

Backpropagation

We next move to the output

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$net_{o1} = 0.4 * 0.593269992 + 0.45 * 0.596884378 + 0.6 * 1 = 1.105905967$$

Still activation function: Logistic

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}} = \frac{1}{1+e^{-1.105905967}} = 0.75136507$$

$$out_{o2} = 0.772928465$$

The forward pass completes

Backpropagation

Computing error:

$$E_{total} = \sum \frac{1}{2}(target - output)^2$$

$$E_{o1} = \frac{1}{2}(target_{o1} - out_{o1})^2 = \frac{1}{2}(0.01 - 0.75136507)^2 = 0.274811083$$

$$E_{o2} = 0.023560026$$

$$E_{total} = E_{o1} + E_{o2} = 0.274811083 + 0.023560026 = 0.298371109$$

Now we know where we are!

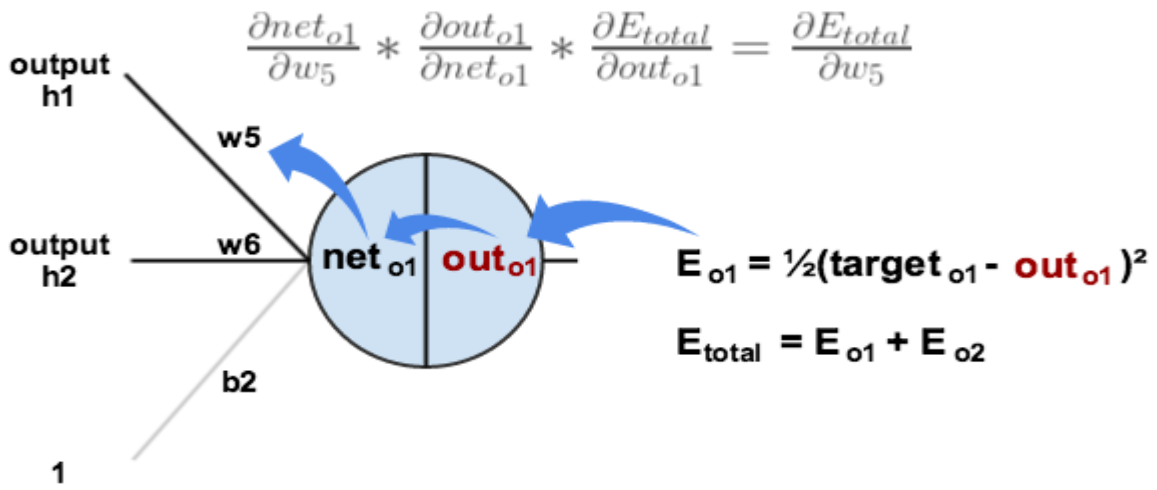
Backpropagation

Backwards pass – update weights of NN to make outputs closer to truths

Example: weight 5 $\frac{\partial E_{total}}{\partial w_5}$

A chain rule

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$



Backpropagation

Get the gradient step 1

$$E_{total} = \frac{1}{2}(target_{o1} - out_{o1})^2 + \frac{1}{2}(target_{o2} - out_{o2})^2$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = 2 * \frac{1}{2}(target_{o1} - out_{o1})^{2-1} * -1 + 0$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = -(target_{o1} - out_{o1}) = -(0.01 - 0.75136507) = 0.74136507$$

Backpropagation

Get the gradient step 2

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}}$$

$$\frac{\partial out_{o1}}{\partial net_{o1}} = out_{o1}(1 - out_{o1}) = 0.75136507(1 - 0.75136507) = 0.186815602$$

Get the gradient step 3

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$\frac{\partial net_{o1}}{\partial w_5} = 1 * out_{h1} * w_5^{(1-1)} + 0 + 0 = out_{h1} = 0.593269992$$

Backpropagation

- Take them together

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$

$$\frac{\partial E_{total}}{\partial w_5} = 0.74136507 * 0.186815602 * 0.593269992 = 0.082167041$$

$$w_5^+ = w_5 - \eta * \frac{\partial E_{total}}{\partial w_5} = 0.4 - 0.5 * 0.082167041 = 0.35891648$$

The similar procedure can be applied to w_6, w_7, w_8

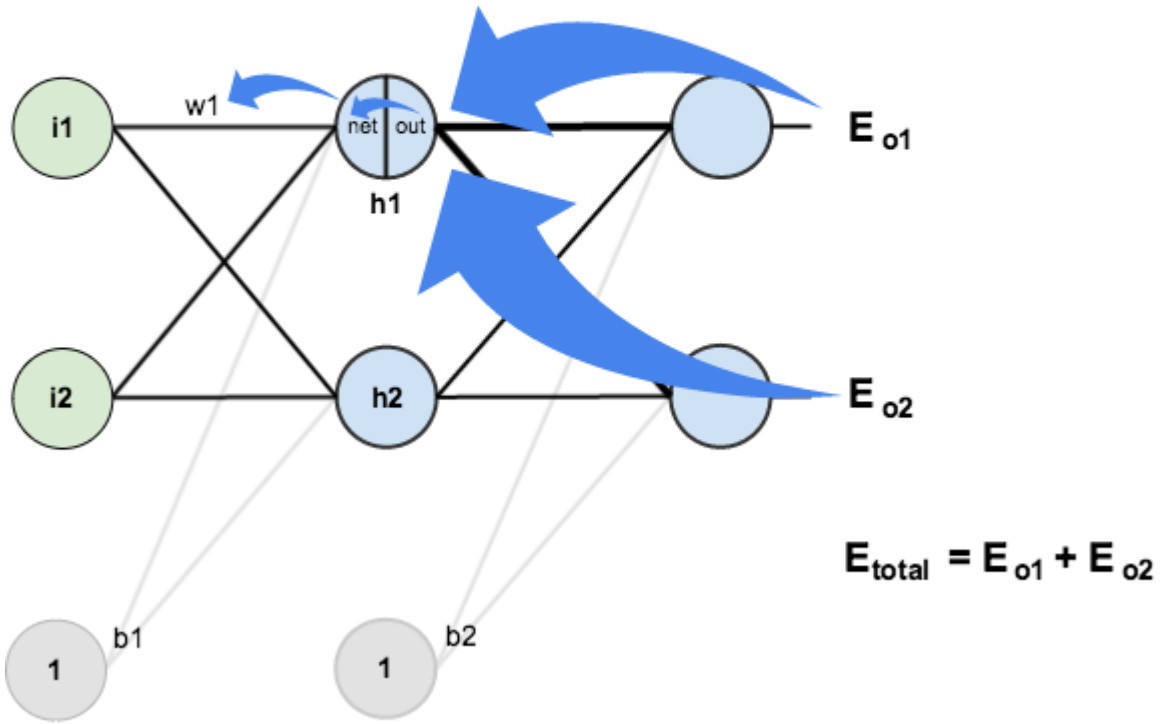
Backpropagation

- Hidden layer

weight update

$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}}$$



Backpropagation

Starting with

$$\frac{\partial E_{o1}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial out_{h1}}$$

$$\frac{\partial E_{o1}}{\partial net_{o1}} = \frac{\partial E_{o1}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} = 0.74136507 * 0.186815602 = 0.138498562$$

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$\frac{\partial net_{o1}}{\partial out_{h1}} = w_5 = 0.40$$

$$\frac{\partial E_{o1}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial out_{h1}} = 0.138498562 * 0.40 = 0.055399425$$

Backpropagation

- Similarly $\frac{\partial E_{o2}}{\partial out_{h1}} = -0.019049119$

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}} = 0.055399425 + -0.019049119 = 0.036350306$$

Next

$$out_{h1} = \frac{1}{1+e^{-net_{h1}}}$$

$$\frac{\partial out_{h1}}{\partial net_{h1}} = out_{h1}(1 - out_{h1}) = 0.59326999(1 - 0.59326999) = 0.241300709$$

Backpropagation

$$net_{h1} = w_1 * i_1 + w_3 * i_2 + b_1 * 1$$

$$\frac{\partial net_{h1}}{\partial w_1} = i_1 = 0.05$$

Put all together

$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\frac{\partial E_{total}}{\partial w_1} = 0.036350306 * 0.241300709 * 0.05 = 0.000438568$$

$$w_1^+ = w_1 - \eta * \frac{\partial E_{total}}{\partial w_1} = 0.15 - 0.5 * 0.000438568 = 0.149780716$$

Similar process apply to w_2, w_3, w_4

Design Issues in ANN

- Number of nodes in input layer
  - One input node per binary/continuous attribute
  - k or $\log_2$ k nodes for each categorical attribute with k values
- Number of nodes in output layer
  - One output for binary class problem
  - k or $\log_2$ k nodes for k-class problem
- Number of nodes in hidden layer
- Initial weights and biases

Characteristics of ANN

- Multilayer ANN are universal approximators but could suffer from overfitting if the network is too large
- Gradient descent may converge to local minimum
- Model building can be very time consuming, but testing can be very fast
- Can handle redundant attributes because weights are automatically learnt
- Sensitive to noise in training data
- Difficult to handle missing attributes

SDSC 6004

Laboratory Section – Data Mining with Weka

Why Weka?

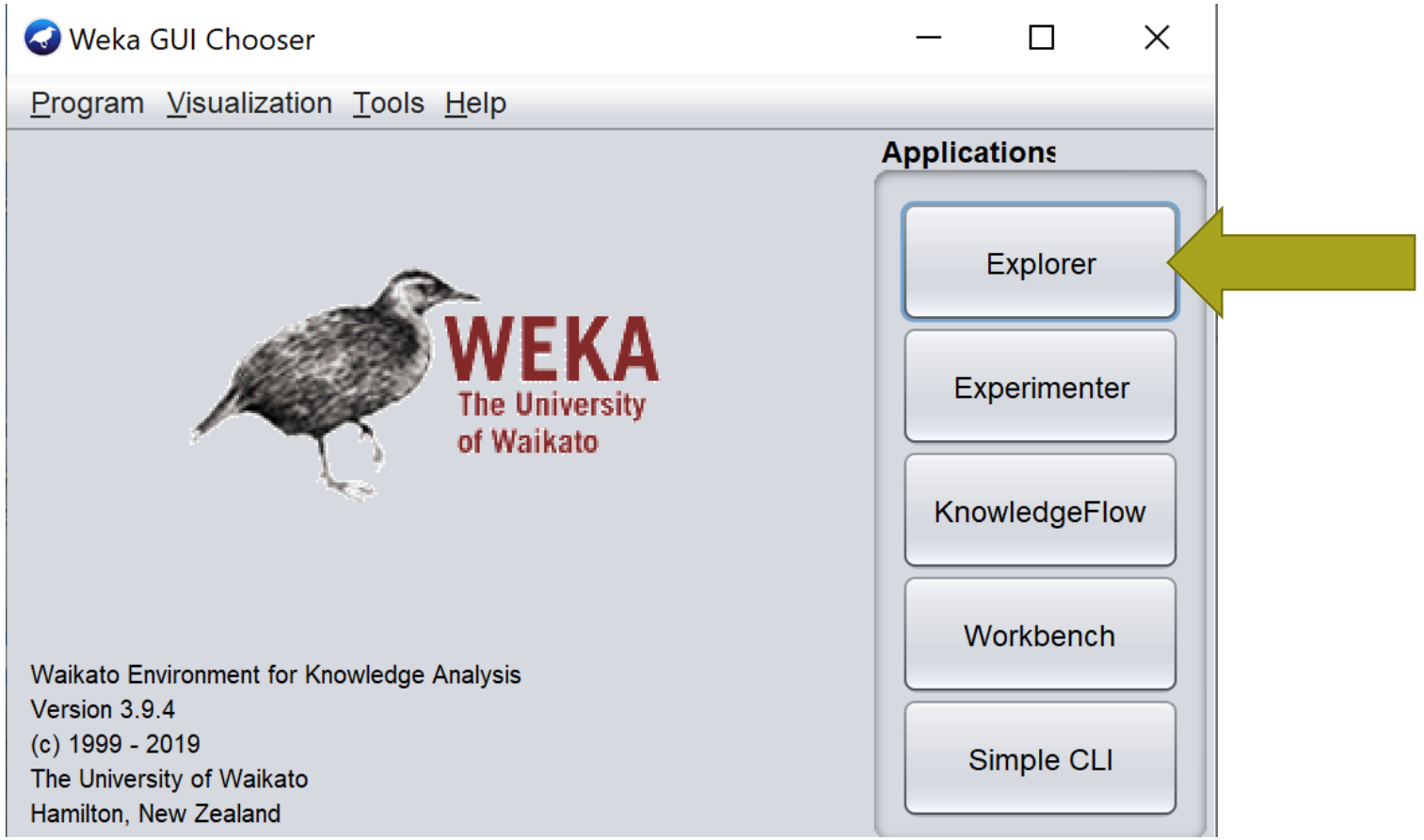
- A user-friendly free software
- It almost covers a full range of basic needs of data mining
- It offers classical algorithms in clustering, classification, and regression

How to get Weka

Link: https://www.cs.waikato.ac.nz/ml/weka/

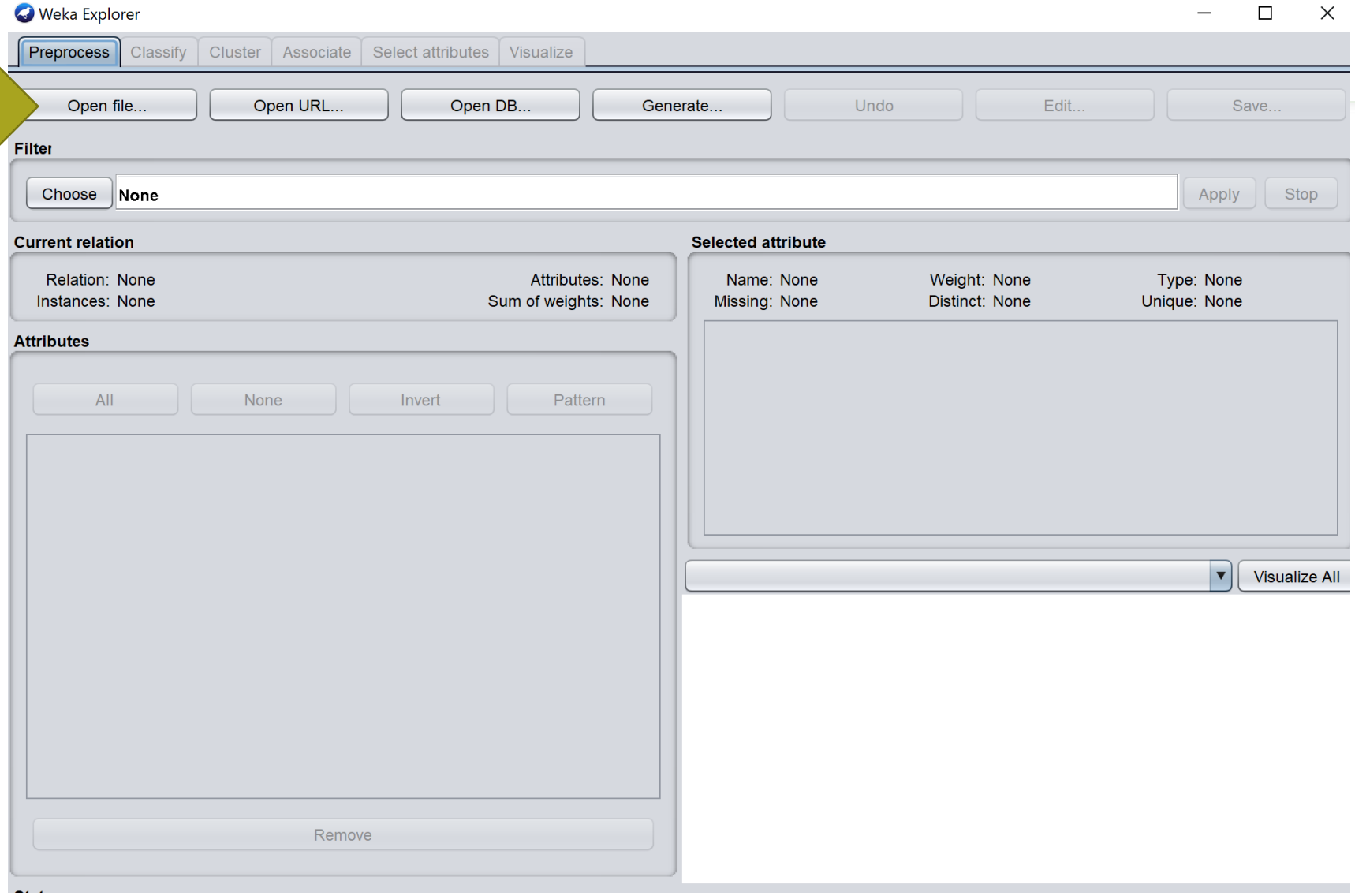
Select the correct version according to the specification of your operation systems, such as windows, Mac OS, Linux…

Weka Interface



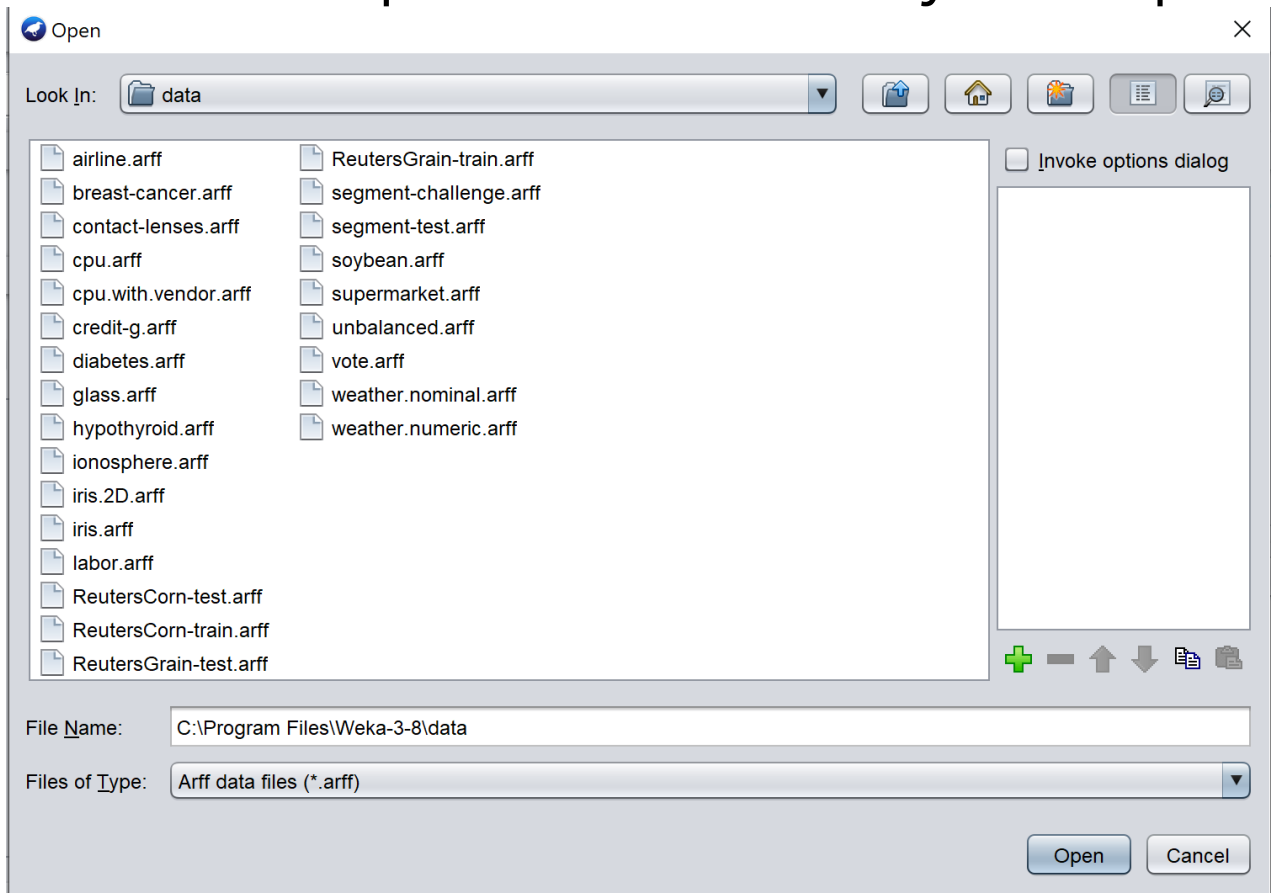
Weka Interface

Loading data via Open File



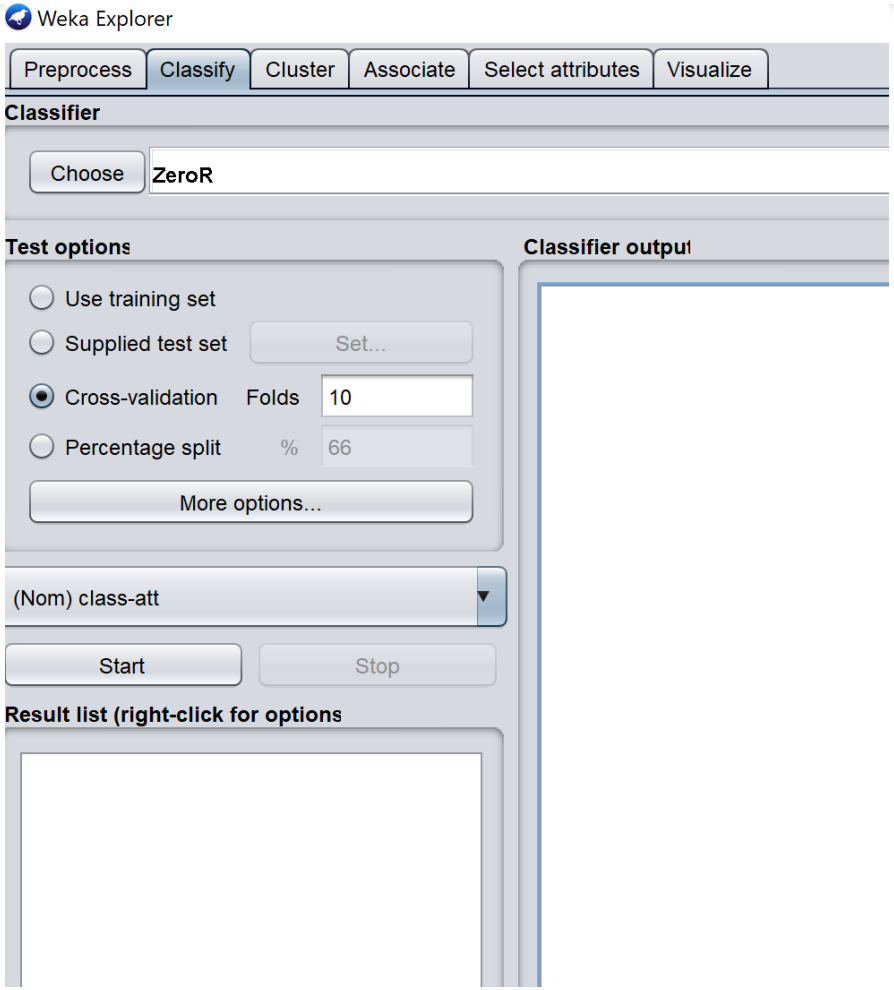
Weka Default Datasets

Weka has some example datasets for you to practice:



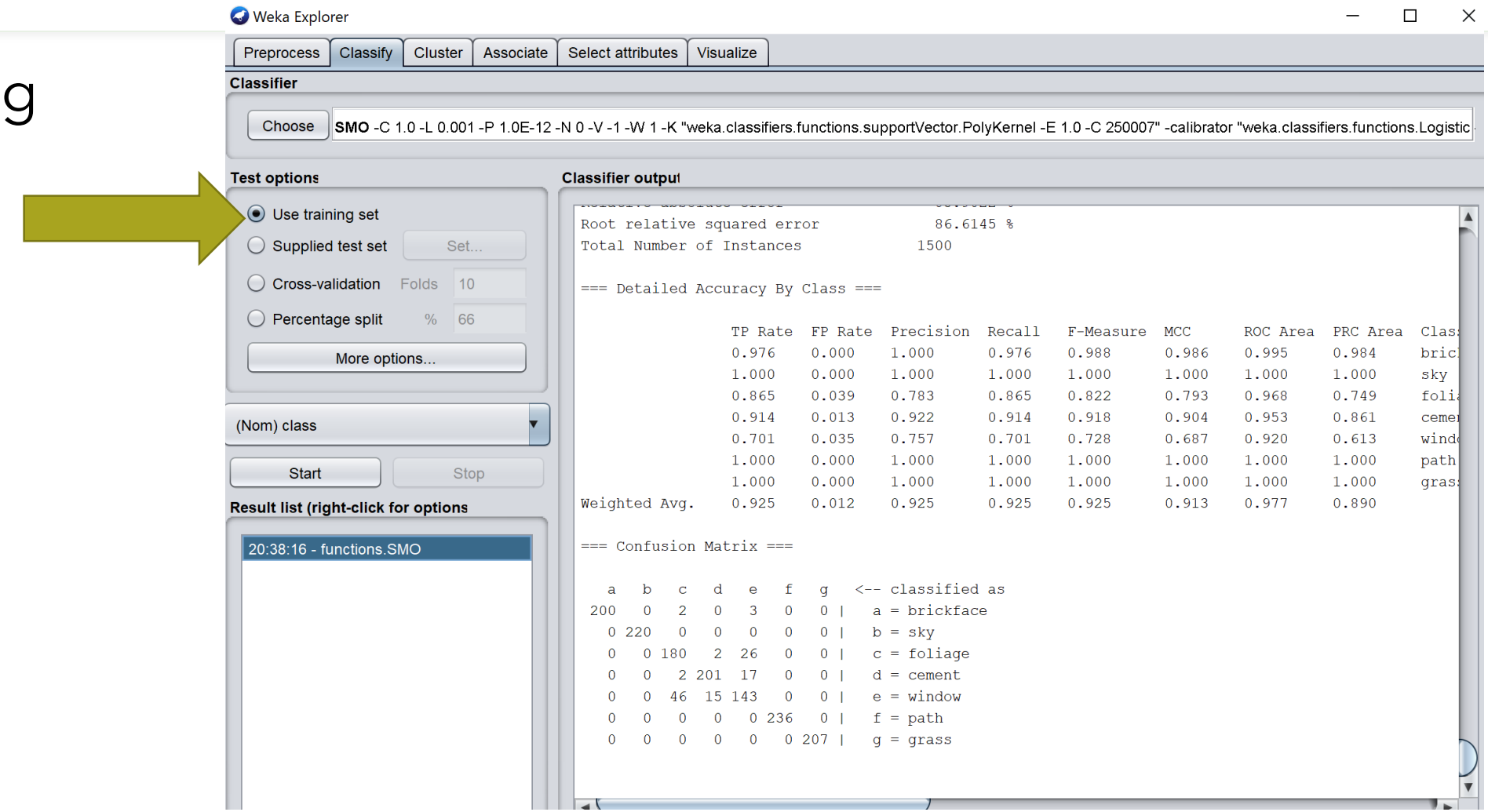
Weka Data Mining Options

All classification and regression are done under the tag Classify



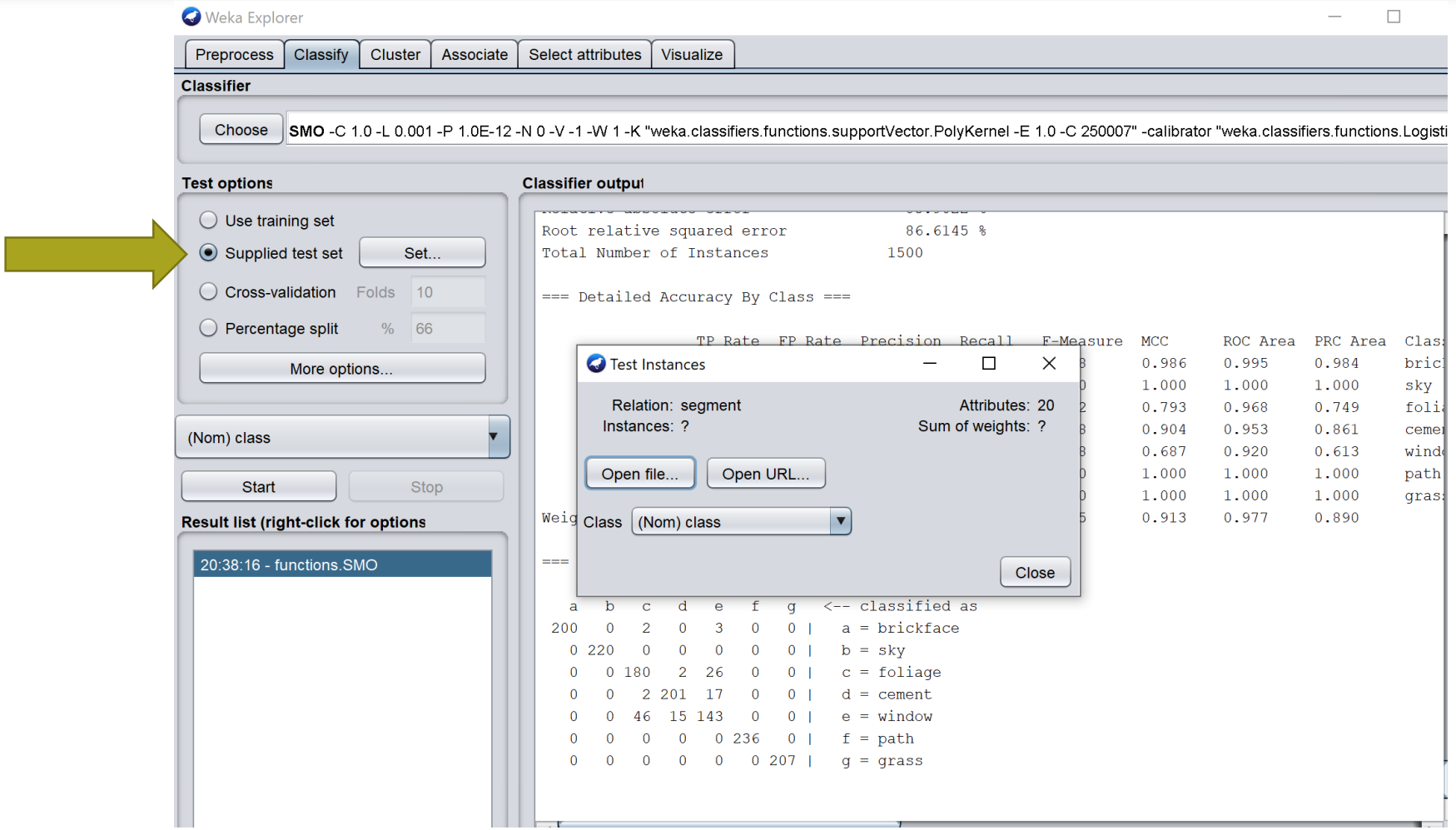
Weka Data Mining Process

Training



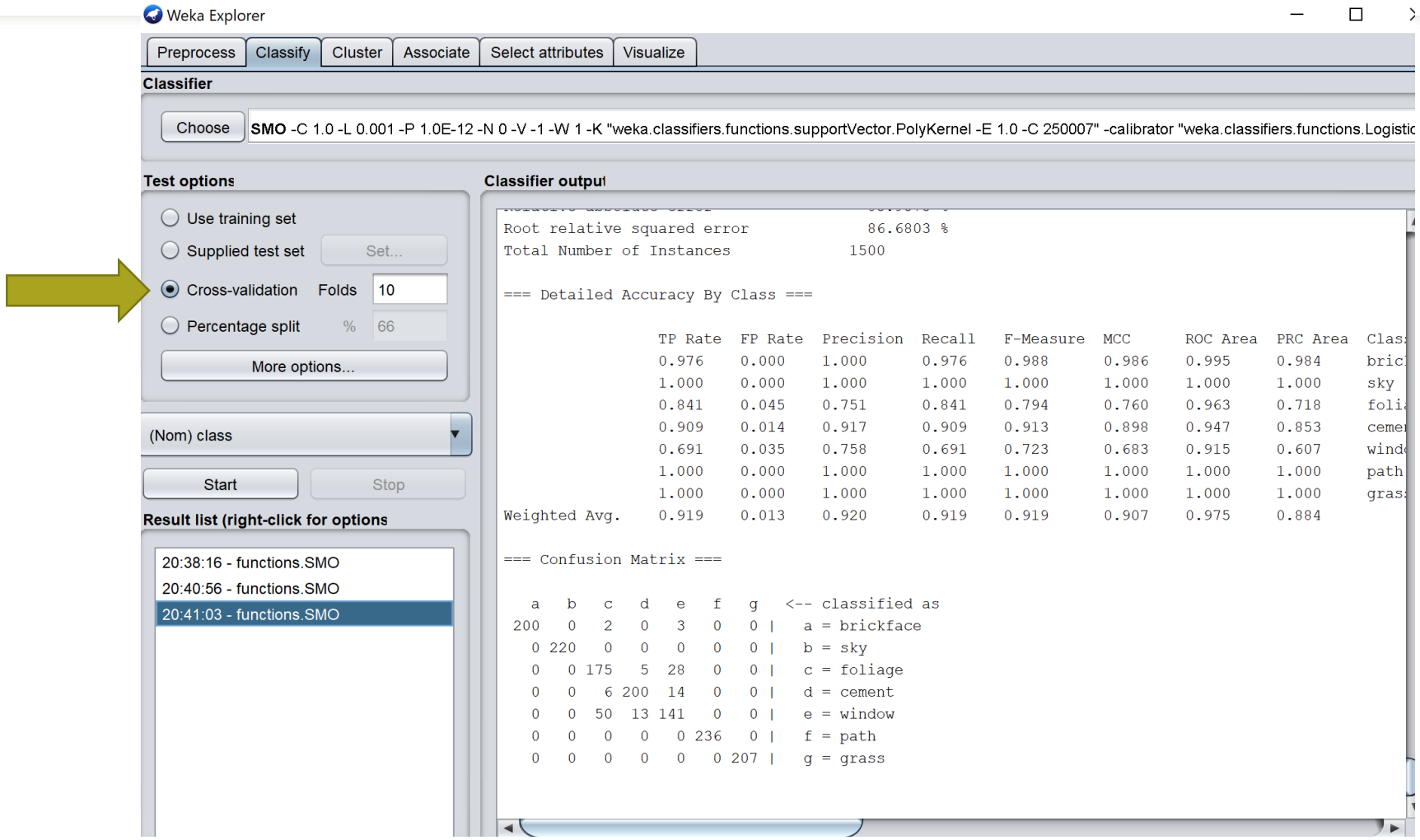
Weka Data Mining Process

Testing

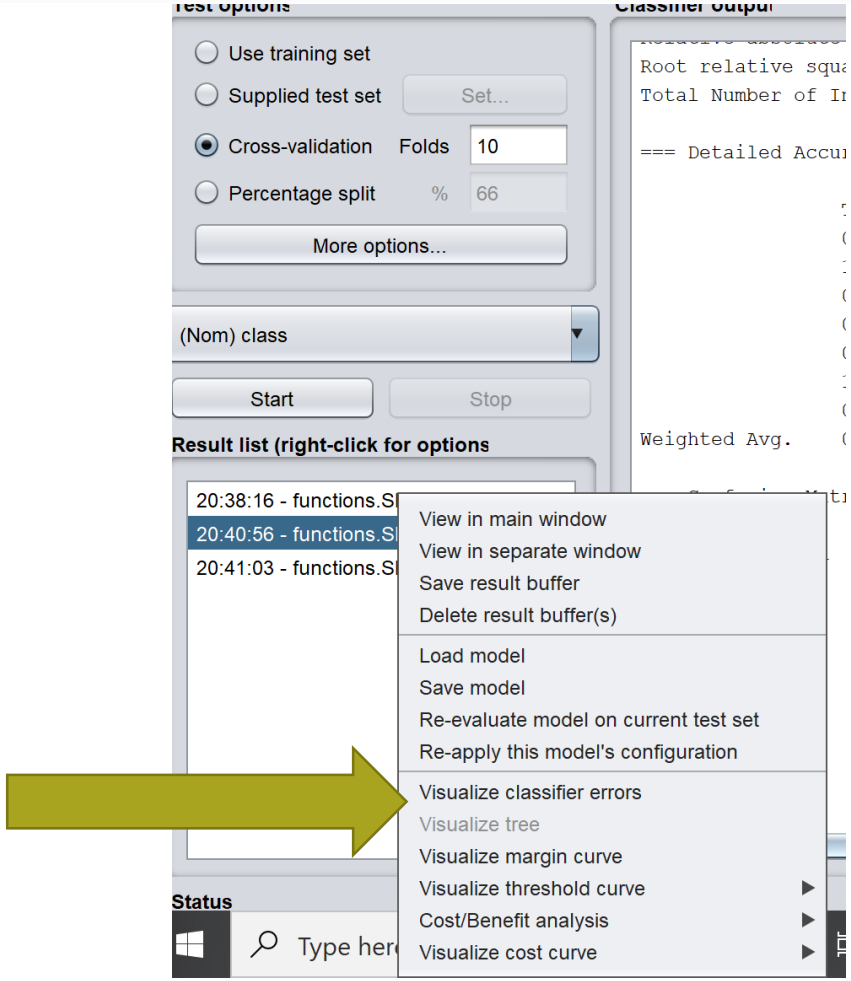


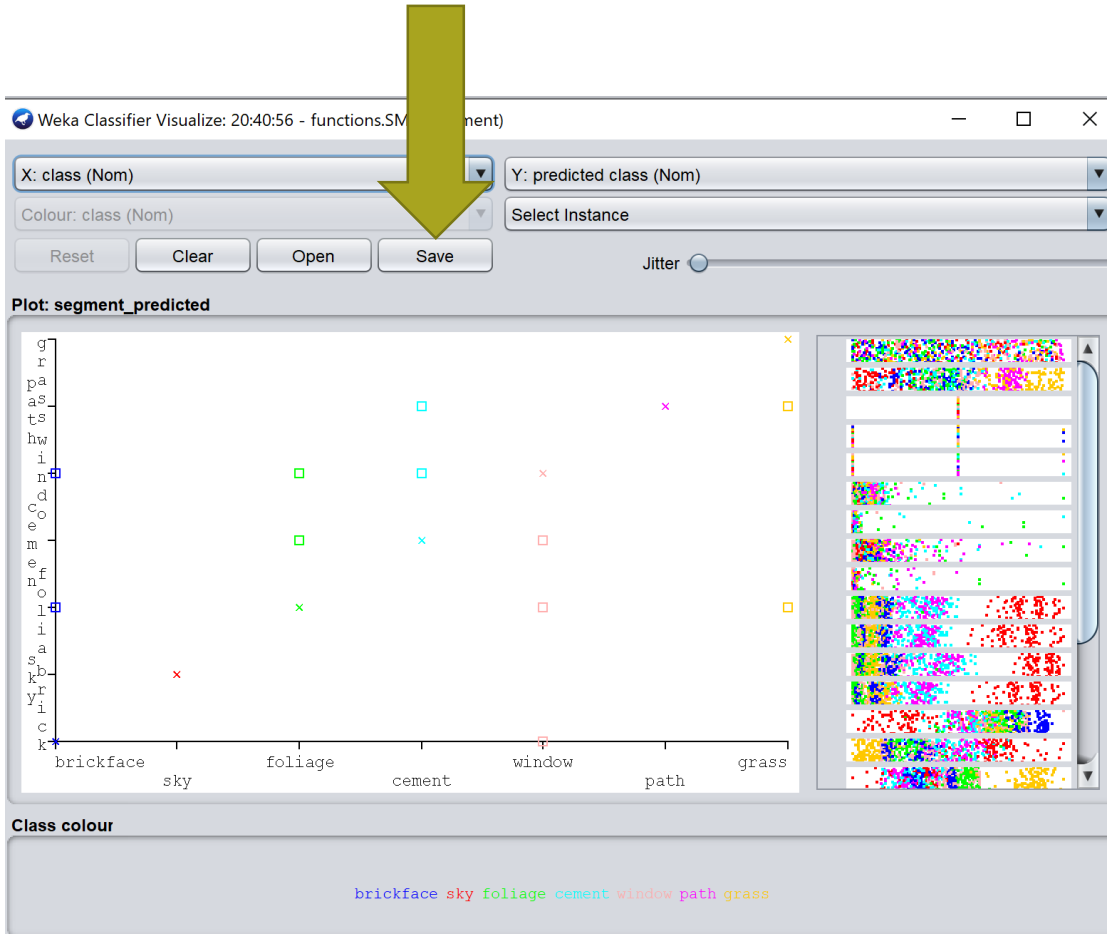
Weka Data Mining Process

10-fold cross validation



Weka Data Mining Results





Weka Data Mining

- Clustering…
- Feature selection…

Weka Data Mining