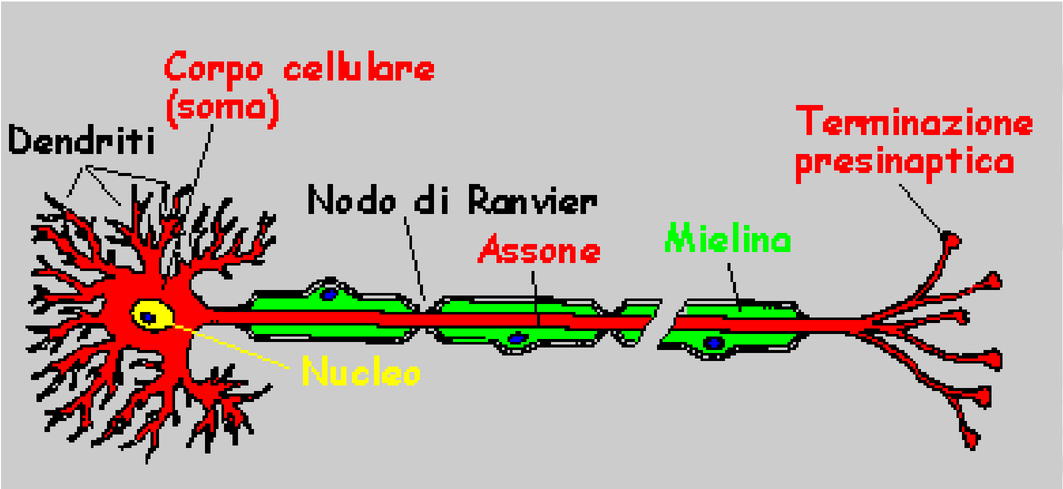
Artificial Neural Networks (ANN)

ANN emulate the Neural Network of the brain

- Human brain contains 10 billion neurons approx. Each one connected, at least, to other 10.000 neurons.
- Signals are transmitted through the neurons

Input

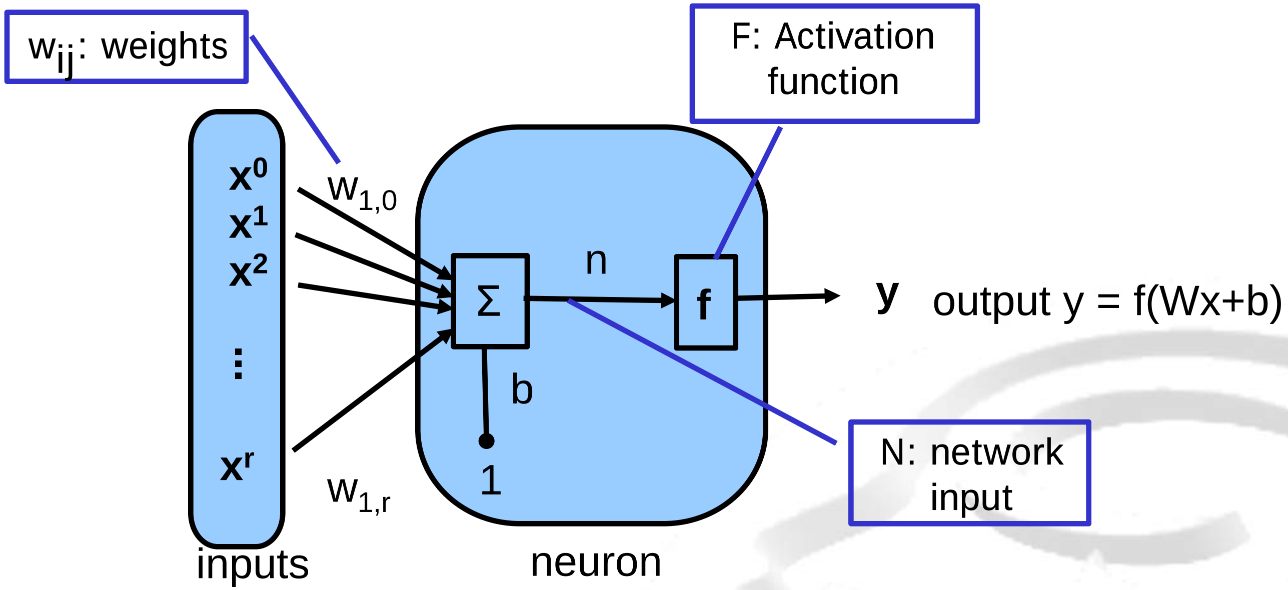


Output

Signal

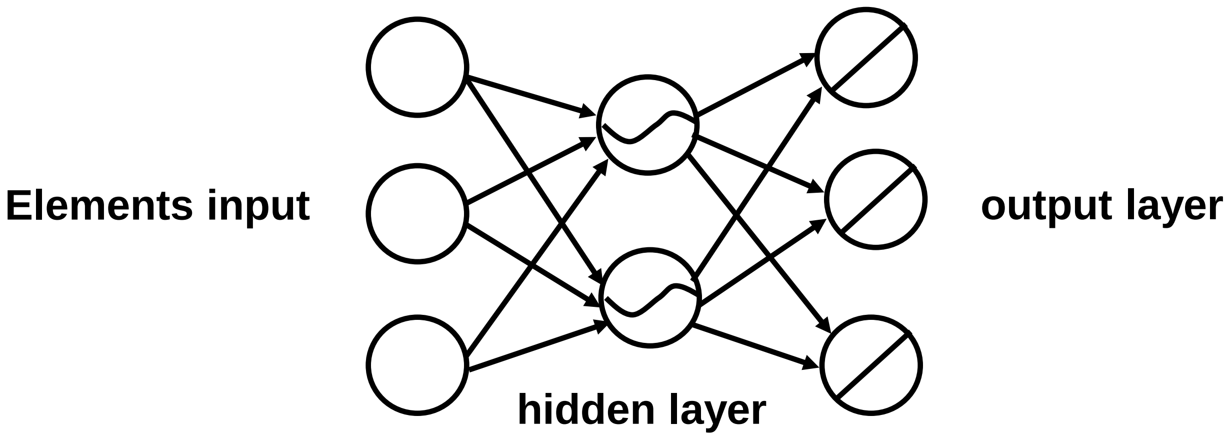
Artificial Neural Networks (ANN)

A simple model of one artificial neuron



Artificial Neural Networks (ANN)

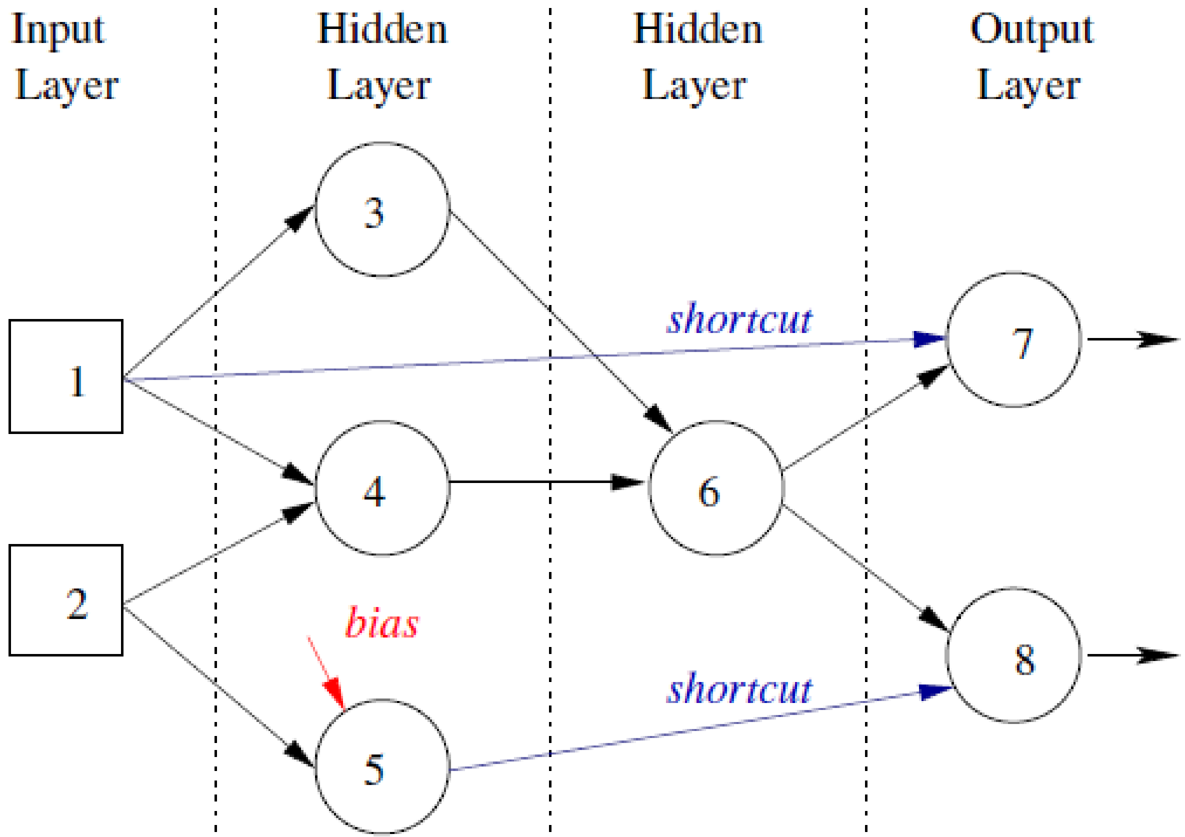
Structure of a multi-layer network



- Brain properties emulated by ANNs:
  - Parallel and Distributed Computation
  - Dense connection of basic units
  - Connections can be modified through experience
  - Learning is constant

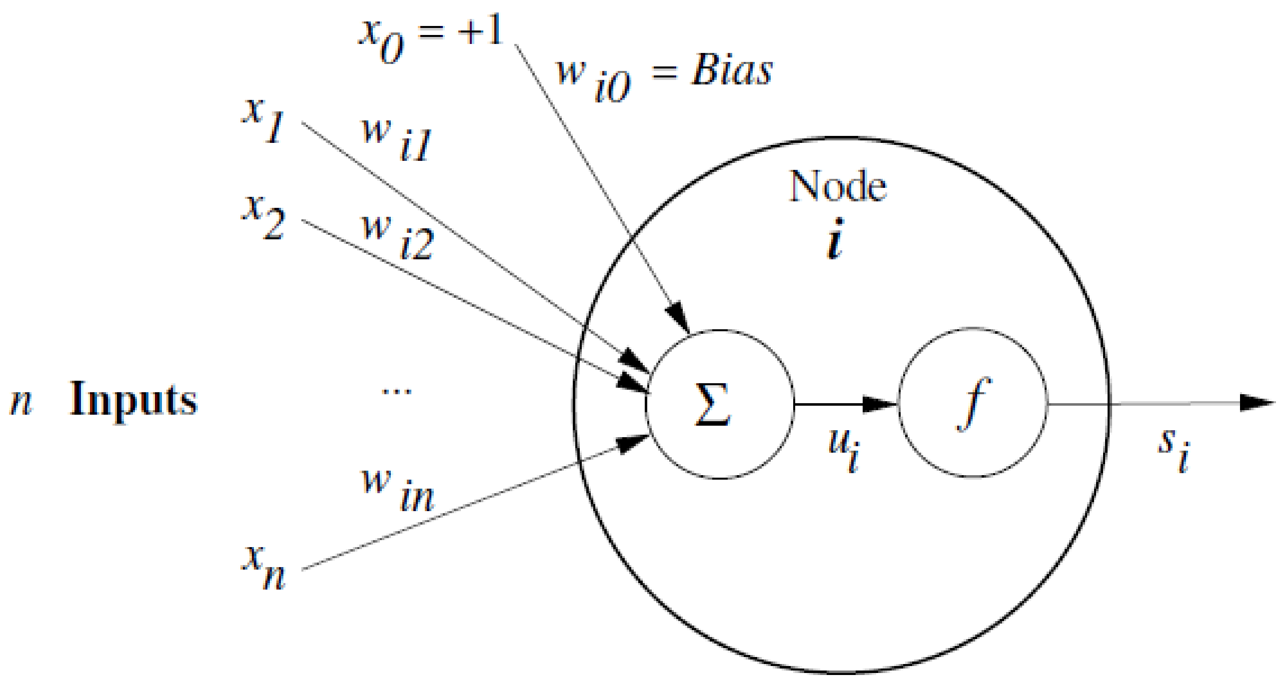
Multilayer Perceptrons (MLPs) [Bishop, 1995][Haykin, 2009]

- Most popular Neural Network type;
- Uses **feedforward** connections and nodes are organized in **layers**;



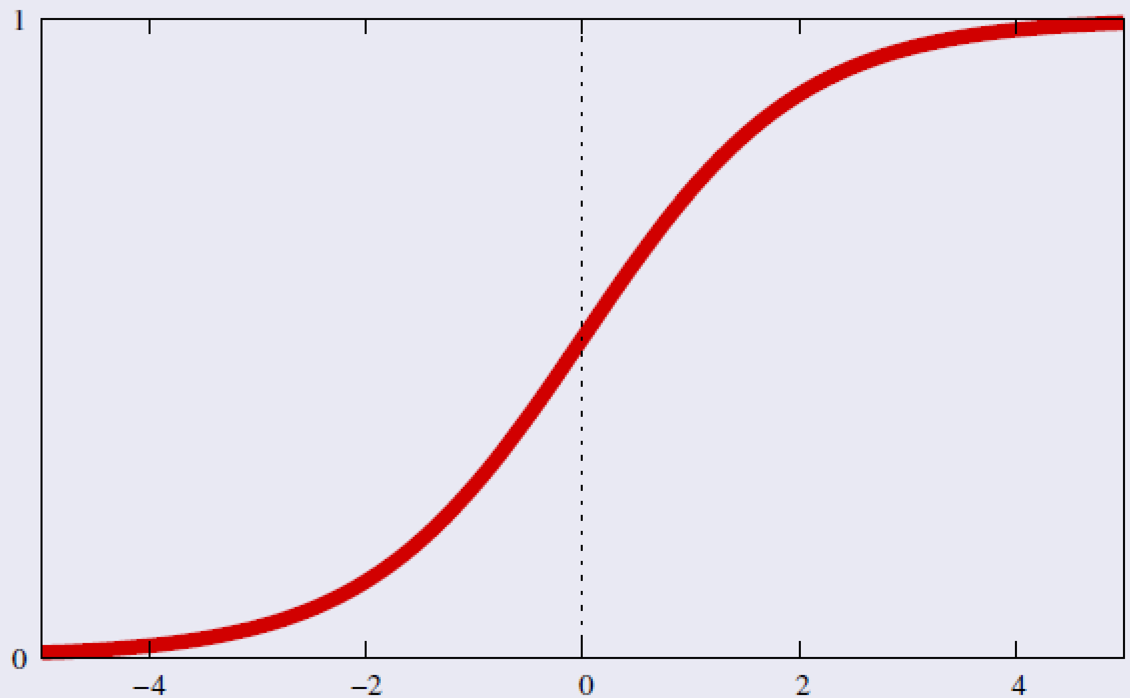
Multilayer Perceptrons (MLPs) [Bishop, 1995][Sarle, 2005]

- Feedforward neural network where each node **outputs** an activation function applied over the weighted sum of its **inputs**:
  $s_i = f(w_{i,0} + \sum_{j \in I} w_{i,j} \times s_j)$

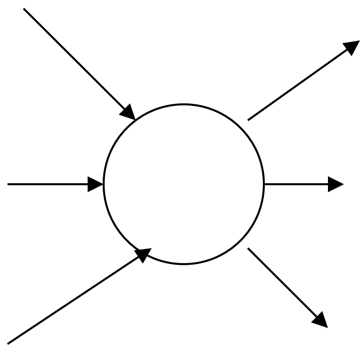


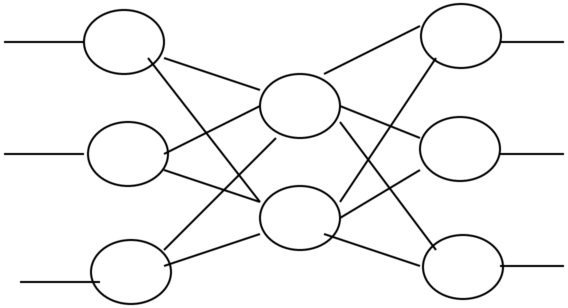
Activation functions

- Linear: $y = x$;
- Tanh: $y = tanh(x)$;
- **Logistic** or Sigmoid (most used): $y = \frac{1}{1+e^{-x}}$;



Artificial Neural Networks (ANN)





- Coding or Training Step
- Decoding or Classification Step
- Perceptrons, Backpropagation technique and Kohonen Maps.

- **Popularity** - the most used Neural Network, with several software tools available;
- **Universal Approximators** - general-purpose models, with a huge number of applications (e.g. classification, regression, forecasting, control or reinforcement learning);
- **Nonlinearity** - when compared to other data mining techniques (e.g. multiple regression) MLPs often present a higher predictive accuracy;
- **Robustness** - good at ignoring irrelevant inputs and noise;
- **Explanatory Knowledge** - Difficult to explain when compared with other algorithms (e.g. decision trees), but it is possible to extract knowledge from trained MLPs (e.g. if-then rules, sensitivity analysis);

- 6 UCI classification (AUC% values) and regression tasks (RRSE% values):

	WEKA		R/rminer	
Task	**NN**	**SVM**	**NN**	**SVM**
balance	97.5±0.2	88.1±0.2	**99.5**±0.1	98.9±0.2
cmc	71.4±0.3	63.8±0.3	**73.9**±0.0	72.9±0.2
german	73.5±0.7	67.2±0.7	76.3±0.8	**77.9**±0.5
heart	85.6±1.2	83.7±0.4	88.5±1.4	**90.2**±0.4
house-votes	98.6±0.2	95.7±0.3	98.0±0.5	**99.2**±0.1
sonar	89.2±1.3	76.6±1.8	87.4±0.9	**95.6**±0.8
abalone	72.7±2.1	69.9±0.1	**64.0**±0.1	66.0±0.1
auto-mpg	44.3±3.4	44.5±0.3	37.4±3.1	**34.8**±0.4
concrete	46.5±1.4	65.6±0.2	**31.8**±0.4	35.9±0.5
housing	49.9±3.0	55.2±0.4	**38.3**±1.6	40.1±1.3
servo	46.1±4.5	84.0±0.4	**40.8**±6.0	44.9±1.5
white	91.3±3.1	85.5±0.1	79.0±0.3	**76.1**±0.6

- Set initial model configuration details (e.g. number of hidden layers of MLP, SVM kernel type).

Common MLP setup (e.g. R tool):

- Often, it is better to perform **one** classification/regression task per model;
- The number of input nodes is defined by the task;
- Use of one hidden layer of H nodes with logistic functions;
- **Binary classification**: one output node with logistic function;
- **Multi-class classification**: N_C output linear nodes ($f(x) = x$) and and the softmax function is used to transform these outputs into class probabilities;
- **Regression**: one linear output neuron.

Gradient-descent [Riedmiller, 1994]:

- **Backpropagation (BP)** - most used, yet may be slow;
- Other algorithms: **Backpropagation with Momentum**; **QuickProp**; **RPROP**; **BGFS**, **Levenberg-Marquardt**, ...

Evolutionary Computation [Rocha et al., 2007]

- May overcome local minima problems;
- Can be applied when no gradient information is available (reinforcement learning).

- The MLP weights are randomly initialized within small ranges (e.g. [-0.7;0.7]);
- Each training may converge to a different (local) minima;

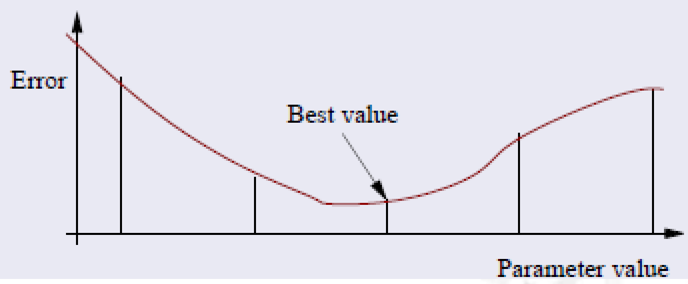
Solutions

- Use of N_R **multiple** trainings, selecting the *MLP* with lowest error;
- Use an **ensemble** with N_R MLPs, where the final output is given as the average of the MLPs.

- Powerful learners (MLP, SVM) have several hyperparameters that need to be set/tuned;
- Such parameters can be set using: heuristic rules, simple grid-search or more advanced optimization algorithms (e.g. Evolutionary Computation) [Rocha et al., 2007];

Grid-Search

- One (or more) parameters are scanned through a given range;
- Range example for MLP hidden nodes: $H \in \{0,2,4,...,20\}$;
- Variants: two-level greedy grid-search (search at the first level and then a second pass is taken, using a smaller range and step).



Confusion matrix [Kohavi and Provost, 1998]

- Matches the **predicted** and **actual** values;
- The 2×2 *confusion matrix*:

$\downarrow$ **actual** \ **predicted** $\rightarrow$	**negative**	**positive**
negative	**TN**	*FP*
positive	*FN*	**TP**

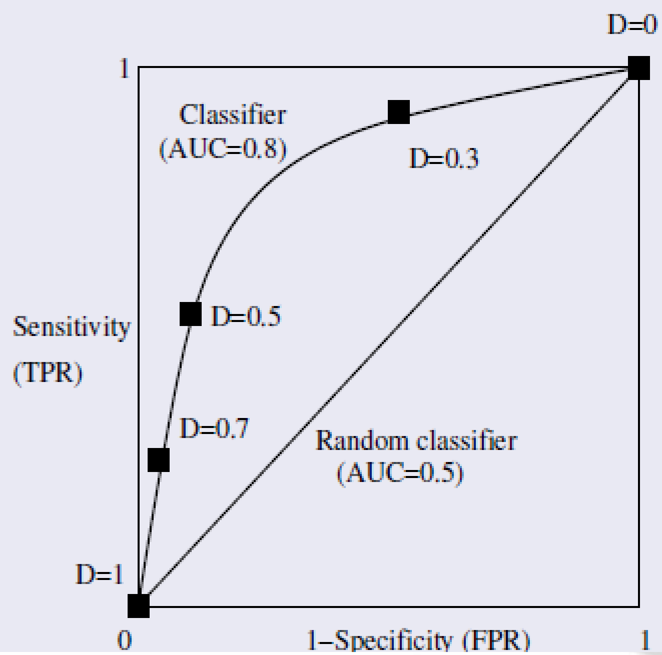
- Three accuracy measures can be defined:
  - the **Accuracy** $= \frac{TN+TP}{TN+FP+FN+TP} \times 100\ (\%)$ (use if FP/FN costs are equal);
  - TPR or **Sensitivity** (*Type II Error*) $= \frac{TP}{FN+TP} \times 100\ (\%)$;
  - TNR or **Specificity** (*Type I Error*) ; $= \frac{TN}{TN+FP} \times 100\ (\%)$
- The higher, the better (the ideal value is 100%);

- Multi-class confusion matrix example [Cortez et al., 2009]:

Actual class	Red wine predictions					White wine predictions				
	4	5	6	7	8	4	5	6	7	8
3	1	7	2	0	0	0	2	17	0	0
4	**1**	36	15	1	0	**19**	55	88	1	0
5	3	**514**	159	5	0	7	**833**	598	19	0
6	0	194	**400**	44	0	4	235	**1812**	144	3
7	0	10	107	**82**	1	0	18	414	**441**	7
8	0	0	10	8	**0**	0	3	71	43	**59**
9						0	1	3	2	0

Receiver Operating Characteristic (ROC) [Fawcett, 2006]

- Shows the behavior of a 2 class classifier ($y \in [0, 1]$) when varying a decision parameter $D \in [0, 1]$ (e.g. True if $y > 0.5, D = 0.5$);
- The curve plots $FPR = 1 - TNR$ ($x-$axis) vs TPR (Sensitivity);
- Global performance measured by the **Area Under the Curve (AUC)**: $AUC = \int_0^1 ROC\, dD$ (the perfect AUC value is 1.0).



Given a dataset with the function pairs $x_1 \rightarrow y_1, \cdots, x_N \rightarrow y_N$, we can compute:

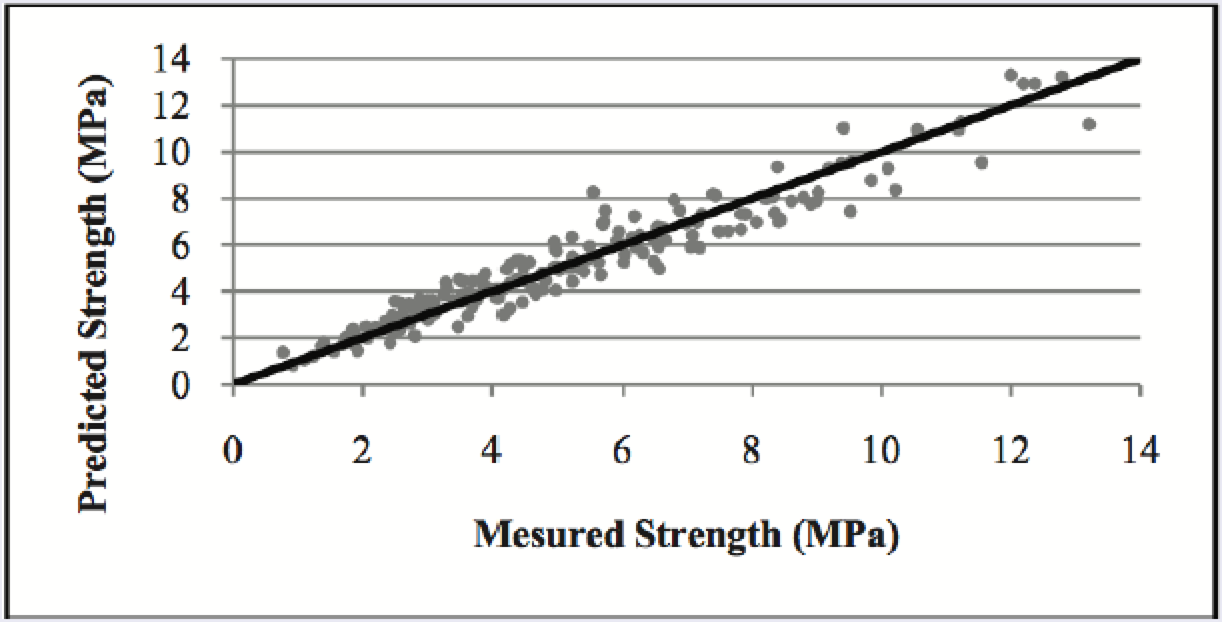
Error metrics

- **Mean Absolute Error/Deviation (MAE)**: $MAE = \frac{\sum_{i=1}^{N}|e_i|}{N}$
- **Sum Squared Error (SSE)**: $SSE = \sum_{i=1}^{N} e_i^2$
- **Mean Squared Error (MSE)**: $MSE = \frac{SSE}{N}$
- **Root Mean Squared Error (RMSE)**: $RMSE = \sqrt{MSE}$
- **Relative Absolute Error** (RAE, scale independent): $RAE = MAE/MAE_{\text{baseline}} \times 100\ (\%)$, where baseline often denotes the average predictor.
- **Relative Squared Error** (RSE, scale independent): $RSE = SSE/SSE_{\text{baseline}} \times 100\ (\%)$

- The lower, the better (ideal value is 0).

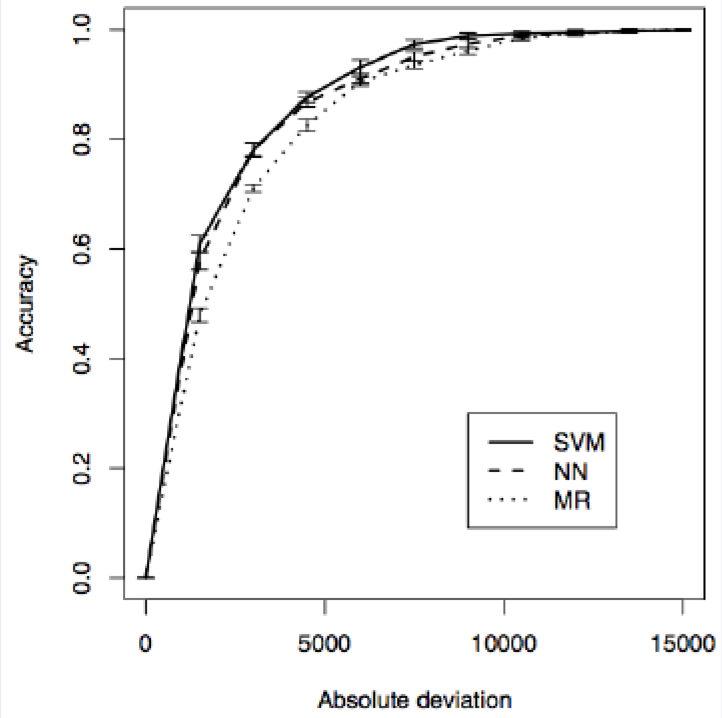
Scatter plot: desired (x-axis) vs predicted (y-axis) values

- Used to assess the prediction quality of a regression model;
- The perfect fit is the diagonal line;
- Civil engineering application example [Tinoco et al., 2009]:



Regression Error Characteristic (REC) curves [Bi and Bennett, 2003]

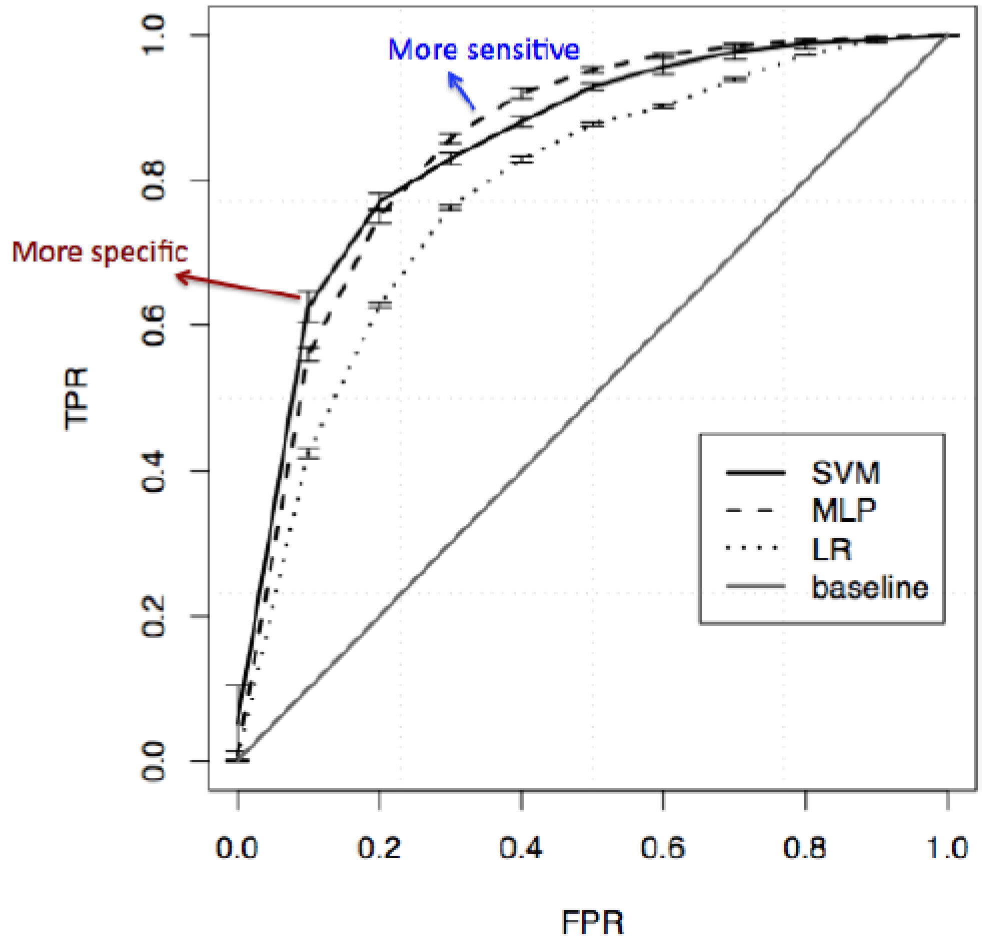
- Used to compare several regression models;
- The curve plots the error tolerance (absolute deviation, x-axis) versus the percentage of points predicted within the tolerance (y-axis);



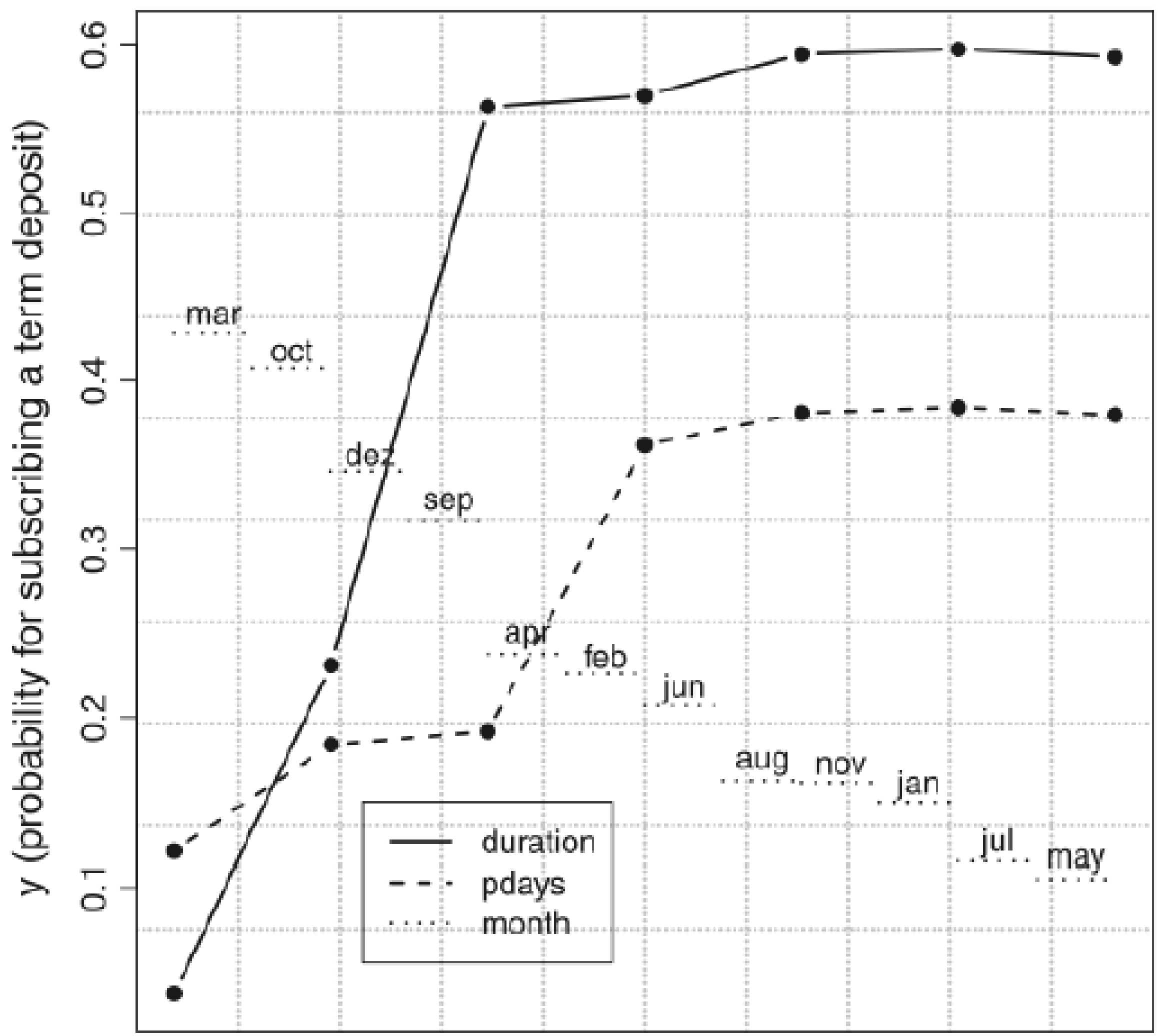
- The aim is to assess if the DM model meets the **business goals** and if it is **interesting**.

- **Interestingness**: does the model makes sense to the domain experts and unveils useful or challenging information?
- **Business impact**: by using such model, what is the gain achieved?

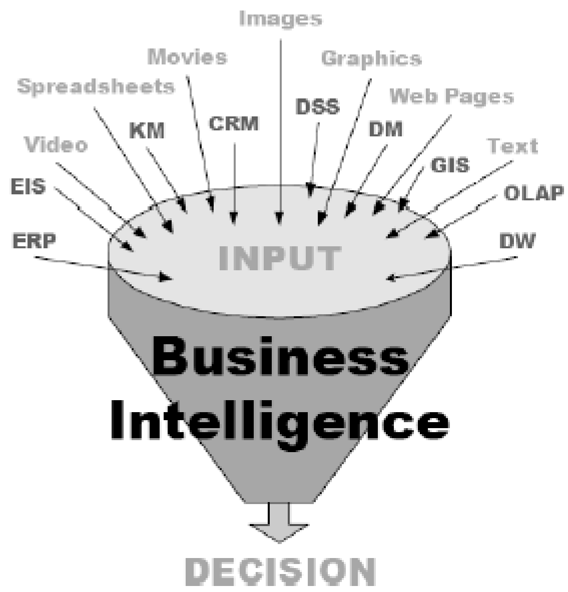
- Business impact example: ROC Curve and benefit-cost analysis (FPR-TPR trade-off).



Visualization of Input Effect: VEC curve (Bank Marketing)



- BI systems often use DM (for knowledge extraction and **prediction**).



Adaptive Business Intelligence (ABI) [Michalewicz et al., 2006]