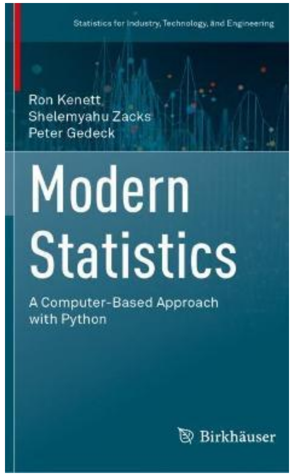
A Biomed Data Analyst Training Program

Supervised (and some unsupervised) learning

Professor Ron S. Kenett



Statistics for Industry, Technology, and Engineering

Ron Kenett
Shelemyahu Zacks
Peter Gedeck

Modern Statistics

A Computer-Based Approach with Python

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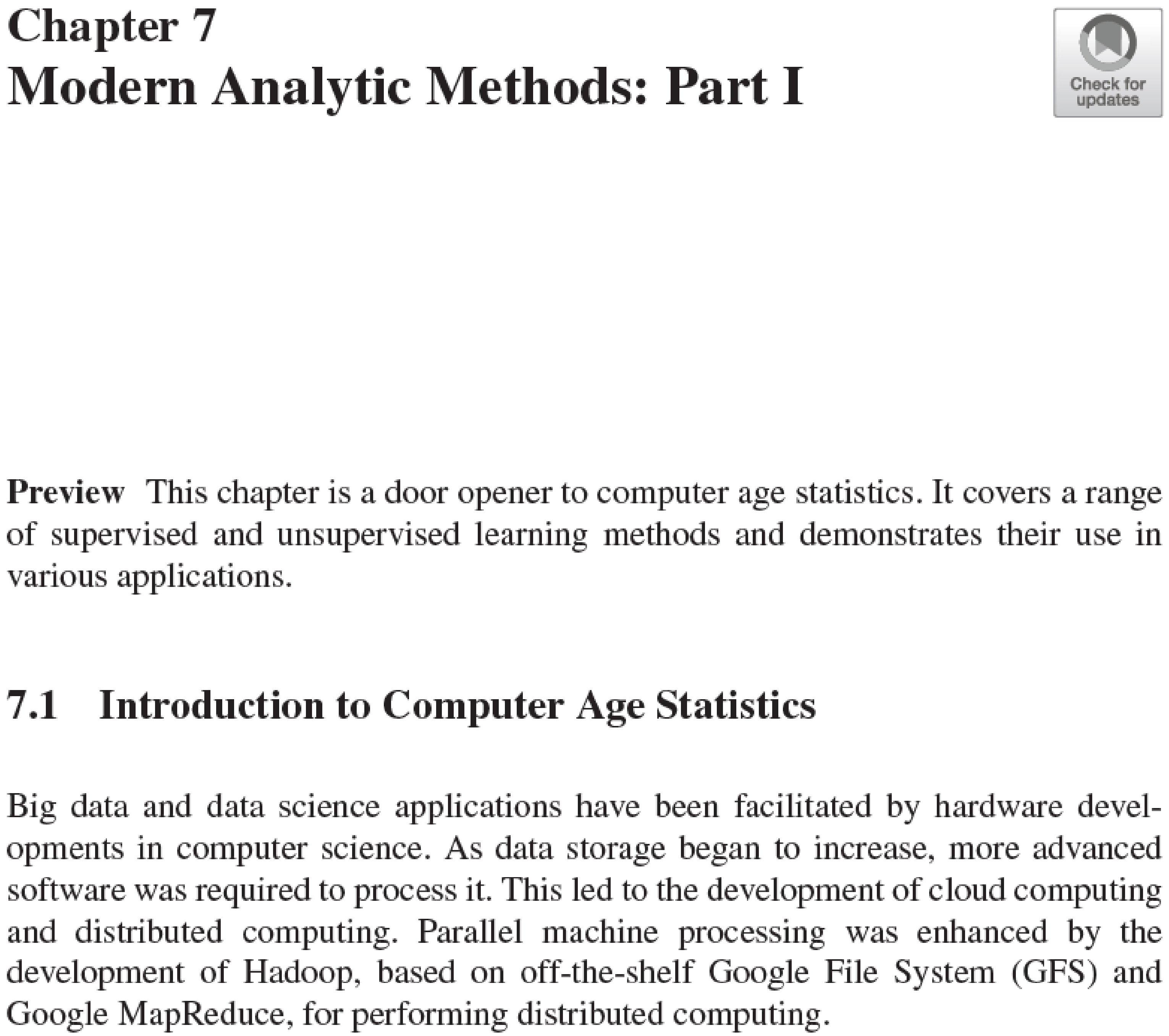
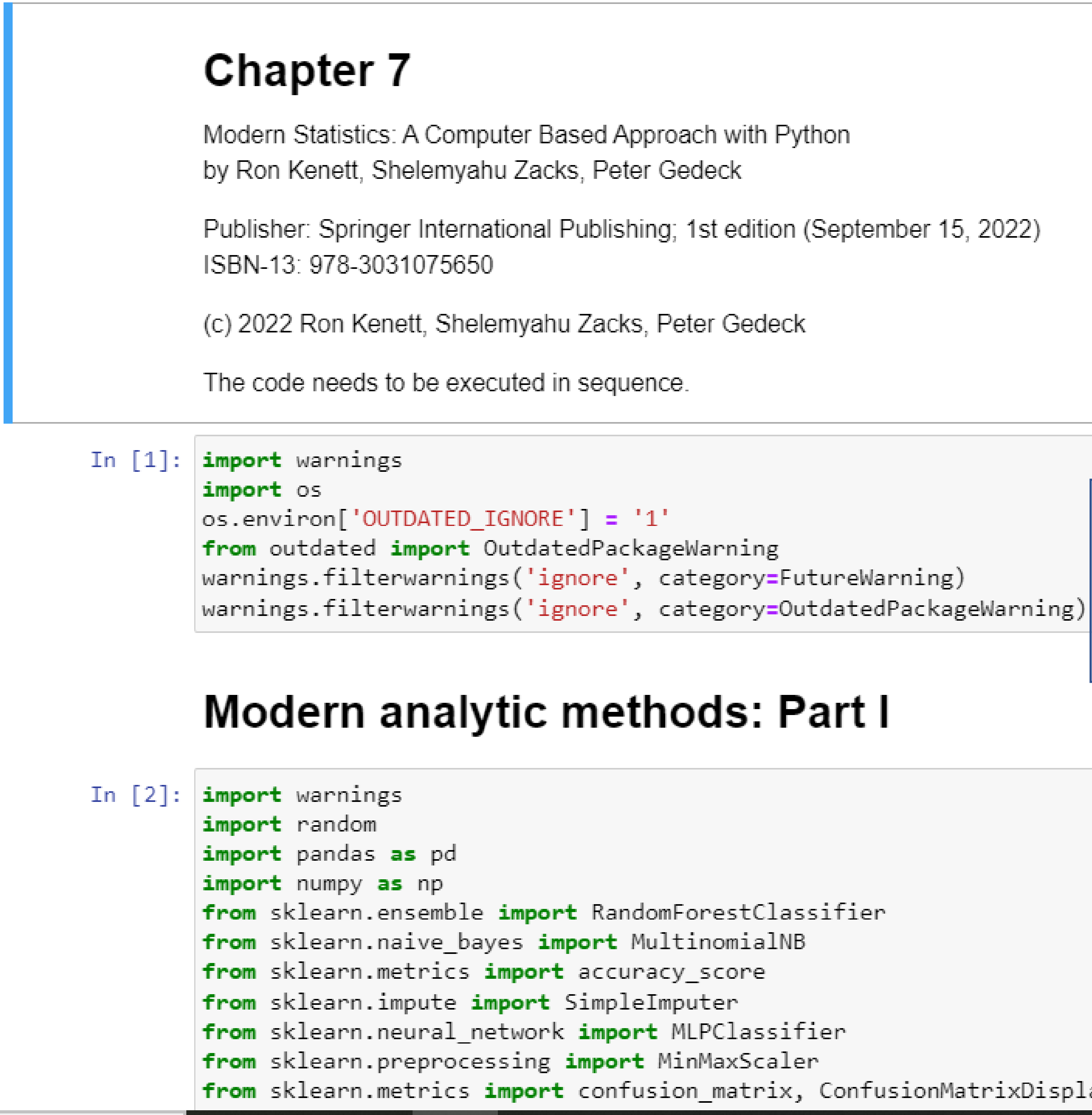


Chapter 7
Modern Analytic Methods: Part I

Preview This chapter is a door opener to computer age statistics. It covers a range of supervised and unsupervised learning methods and demonstrates their use in various applications.

7.1 Introduction to Computer Age Statistics

Big data and data science applications have been facilitated by hardware developments in computer science. As data storage began to increase, more advanced software was required to process it. This led to the development of cloud computing and distributed computing. Parallel machine processing was enhanced by the development of Hadoop, based on off-the-shelf Google File System (GFS) and Google MapReduce, for performing distributed computing.



Chapter 7

Modern Statistics: A Computer Based Approach with Python
by Ron Kenett, Shelemyahu Zacks, Peter Gedeck

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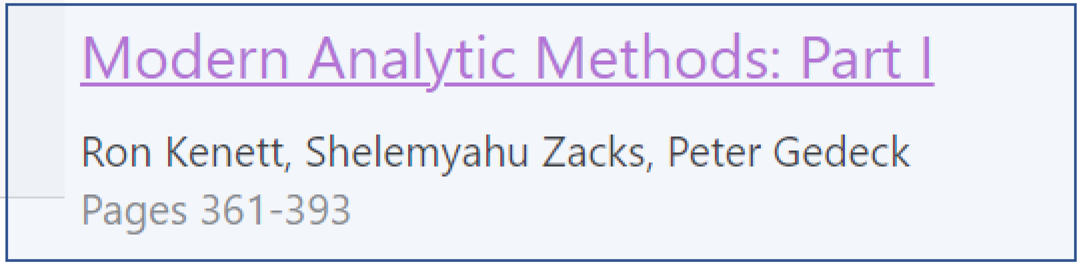
ISBN-13: 978-3031075650

The code needs to be executed in sequence.

In [1]:
```
import warnings
import os
os.environ['OUTDATED_IGNORE'] = '1'
from outdated import OutdatedPackageWarning
warnings.filterwarnings('ignore', category=FutureWarning)
warnings.filterwarnings('ignore', category=OutdatedPackageWarning)
```

Modern analytic methods: Part I

In [2]:
```
import warnings
import random
import pandas as pd
import numpy as np
from sklearn.ensemble import RandomForestClassifier
from sklearn.naive_bayes import MultinomialNB
from sklearn.metrics import accuracy_score
from sklearn.impute import SimpleImputer
from sklearn.neural_network import MLPClassifier
from sklearn.preprocessing import MinMaxScaler
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay
```



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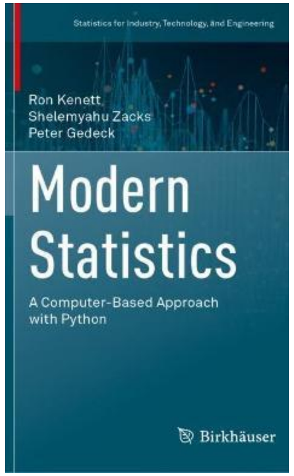

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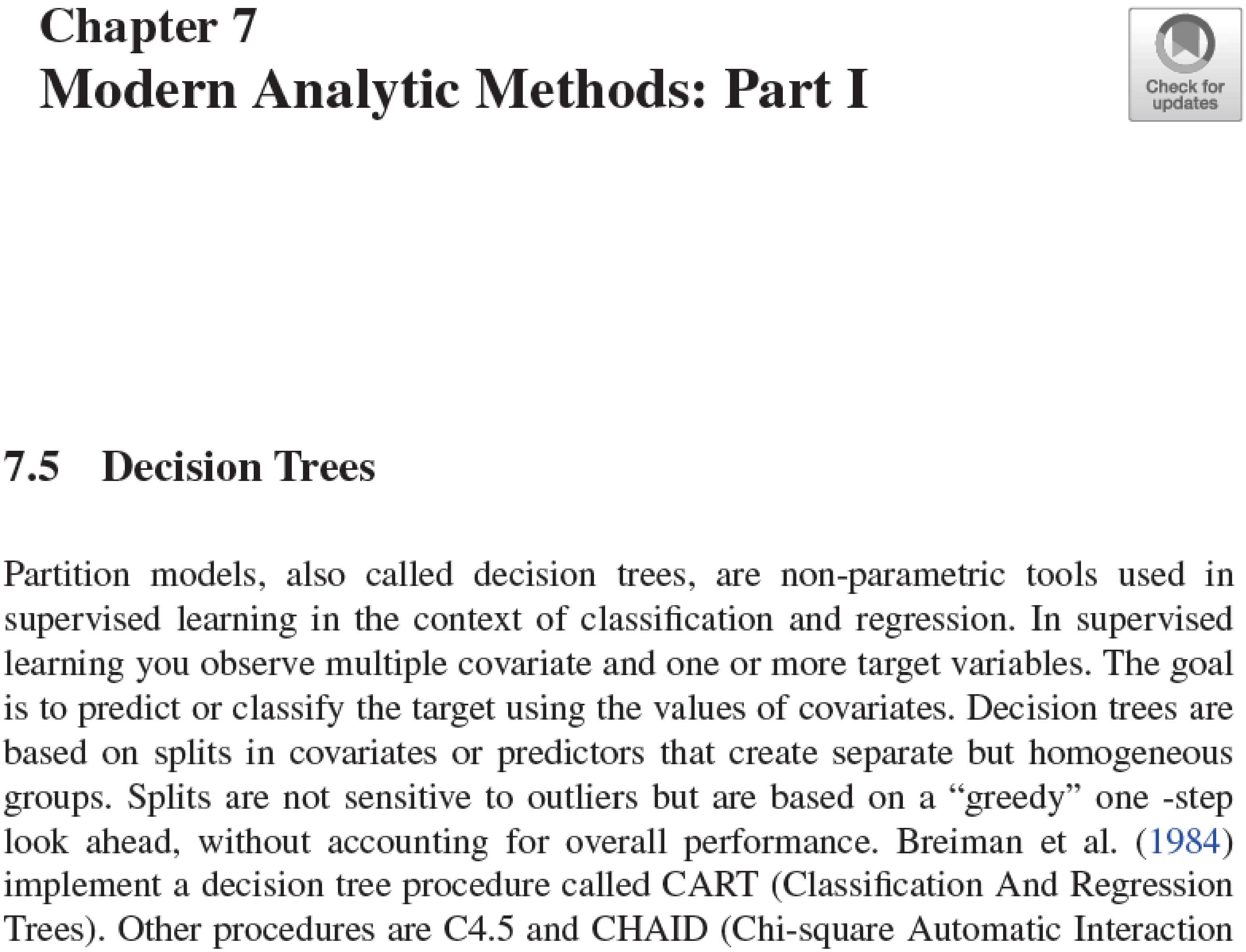
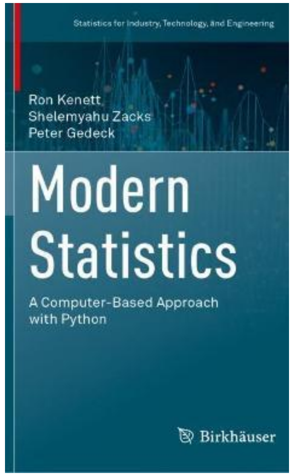


Chapter 7
Modern Analytic Methods: Part I

7.5 Decision Trees

Partition models, also called decision trees, are non-parametric tools used in supervised learning in the context of classification and regression. In supervised learning you observe multiple covariate and one or more target variables. The goal is to predict or classify the target using the values of covariates. Decision trees are based on splits in covariates or predictors that create separate but homogeneous groups. Splits are not sensitive to outliers but are based on a "greedy" one -step look ahead, without accounting for overall performance. Breiman et al. (1984) implement a decision tree procedure called CART (Classification And Regression Trees). Other procedures are C4.5 and CHAID (Chi-square Automatic Interaction



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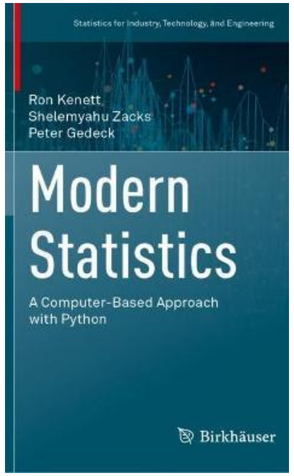
Example 7.2 Data set **SENSORS.csv** consists of 174 measurements from 63 sensors tracking performance of a system under test. Each test generates values for these 63 sensors and a status determined by the automatic test equipment. The distribution of the test results is presented in Fig. 7.5. Our goal is to predict the outcome recorded by the testing equipment, using sensor data. The test results are coded as Pass (corresponding to “Good,” 47% of the observations) and Fail (all other categories, marked in grey). The column **Status** is therefore a dichotomized version of the column **Test result**.

```
sensors = mistat.load_data('SENSORS.csv')
dist = sensors['testResult'].value_counts()
dist = dist.sort_index()
ax = dist.plot.bar(color='lightgrey')
ax.patches[dist.index.get_loc('Good')].set_facecolor('black')
plt.show()
```



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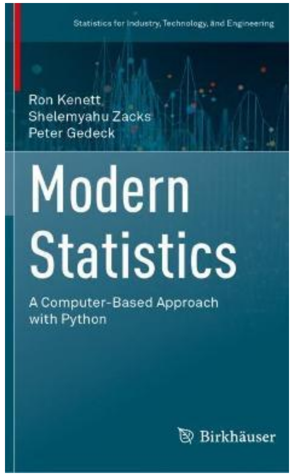
The goal is to predict the outcome recorded by the testing equipment, using sensor data. We can use `scikit-learn` for this. It has decision tree implementations for classification and regression. Here, we create a classification model for Pass-Fail using the 67 sensors.

```
from sklearn.tree import DecisionTreeClassifier, plot_tree, export_text

predictors = [c for c in sensors.columns if c.startswith('sensor')]
outcome = 'status'
X = sensors[predictors]
y = sensors[outcome]

# Train the model
clf = DecisionTreeClassifier(ccp_alpha=0.012, random_state=0)
clf.fit(X, y)

# Visualization of tree
plot_tree(clf, feature_names=list(X.columns))
plt.show()
```



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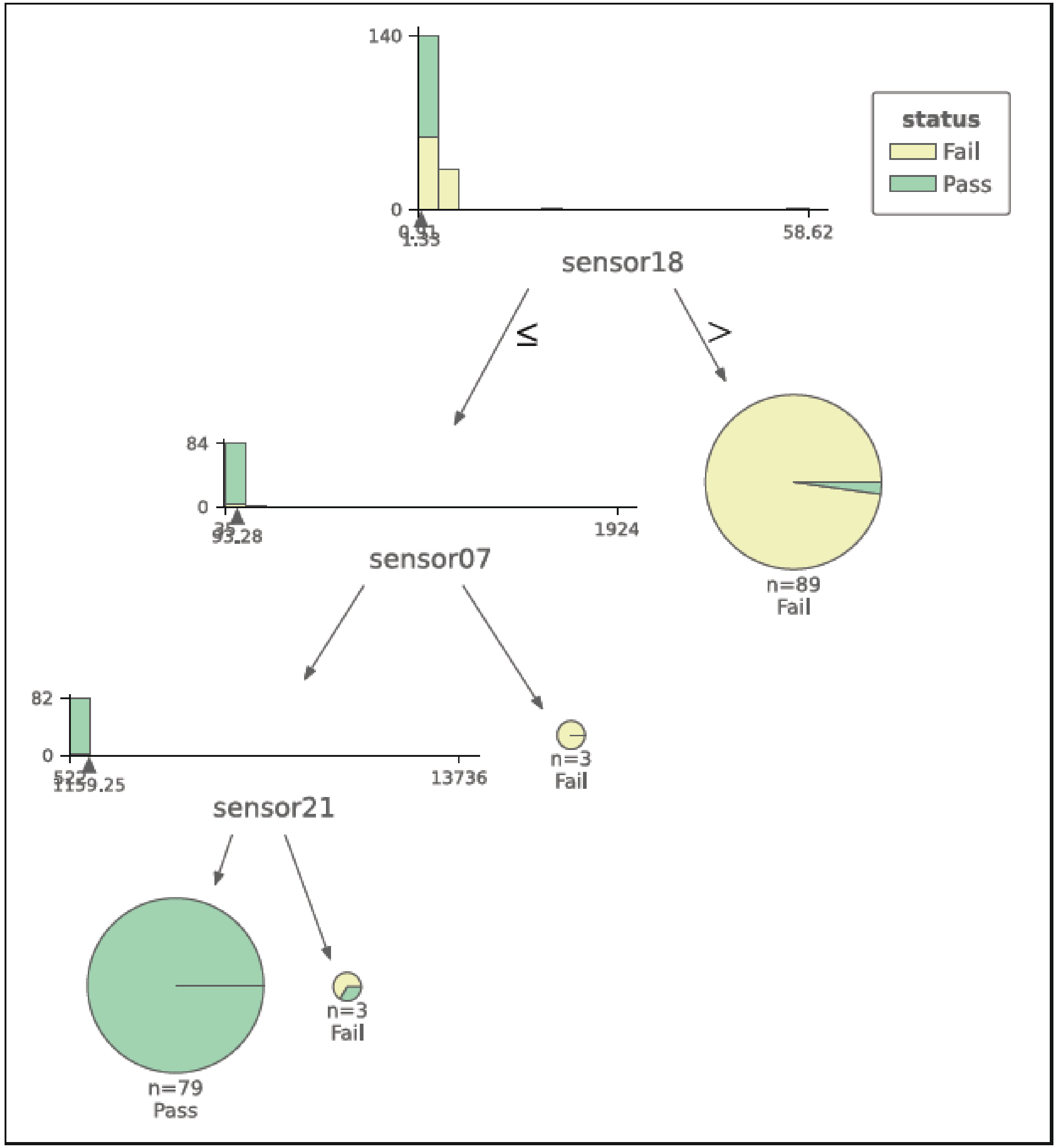
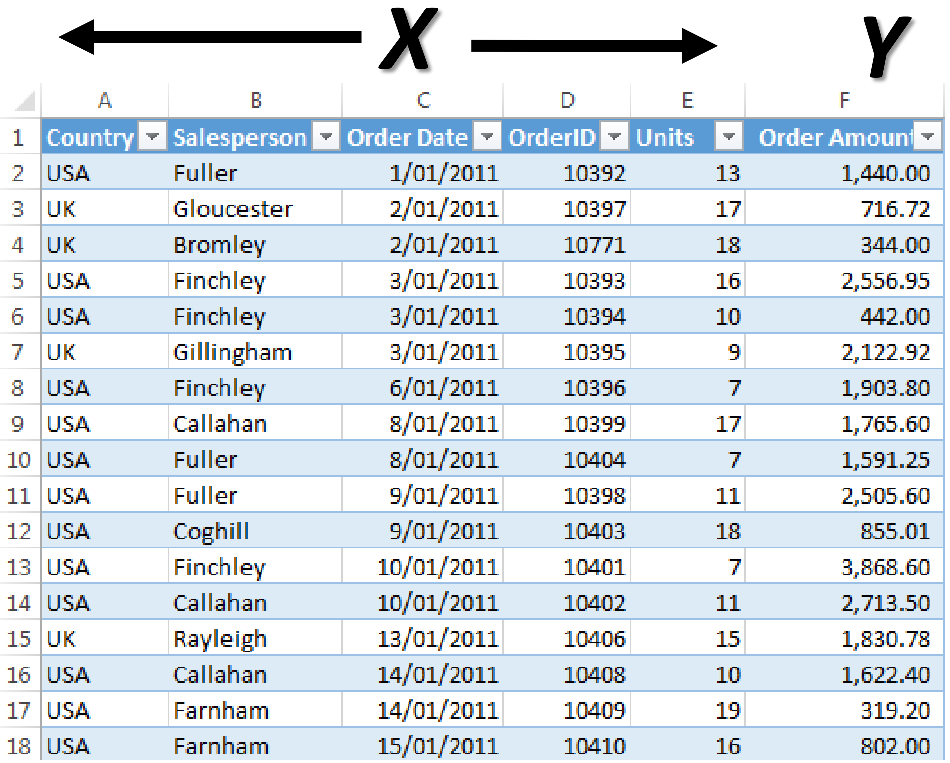
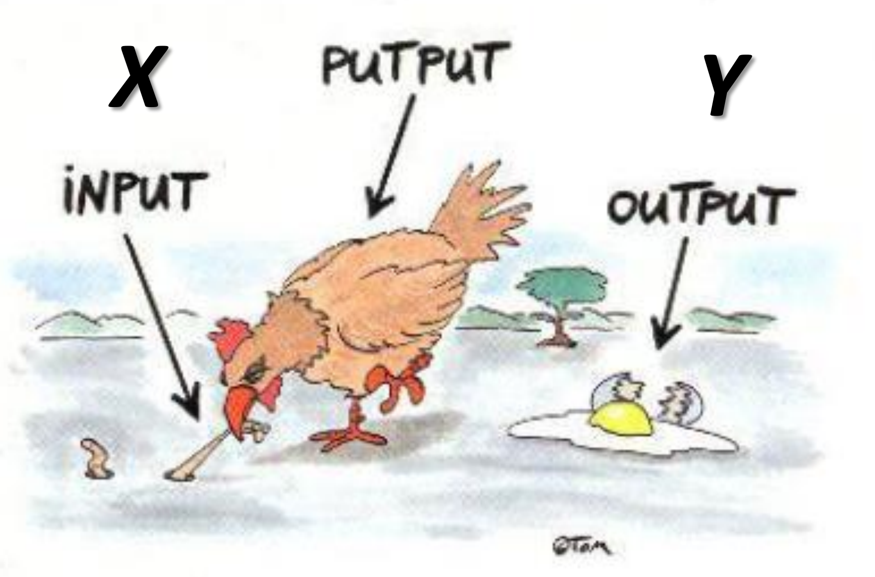


Fig. 7.7 Decision tree visualization of classification tree

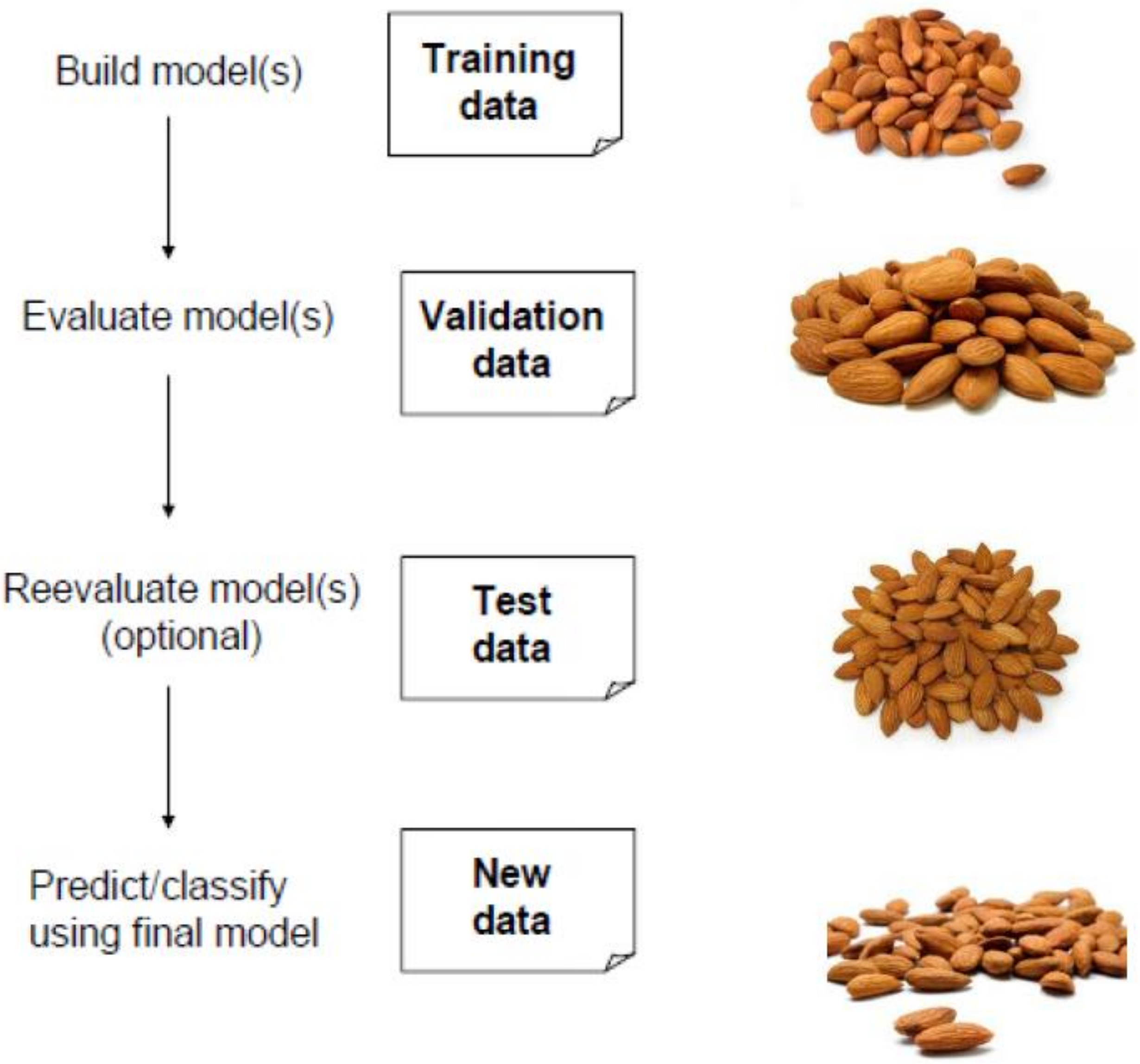
Supervised Learning



	A	B	C	D	E	F
1	Country	Salesperson	Order Date	OrderID	Units	Order Amount
2	USA	Fuller	1/01/2011	10392	13	1,440.00
3	UK	Gloucester	2/01/2011	10397	17	716.72
4	UK	Bromley	2/01/2011	10771	18	344.00
5	USA	Finchley	3/01/2011	10393	16	2,556.95
6	USA	Finchley	3/01/2011	10394	10	442.00
7	UK	Gillingham	3/01/2011	10395	9	2,122.92
8	USA	Finchley	6/01/2011	10396	7	1,903.80
9	USA	Callahan	8/01/2011	10399	17	1,765.60
10	USA	Fuller	8/01/2011	10404	7	1,591.25
11	USA	Fuller	9/01/2011	10398	11	2,505.60
12	USA	Coghill	9/01/2011	10403	18	855.01
13	USA	Finchley	10/01/2011	10401	7	3,868.60
14	USA	Callahan	10/01/2011	10402	11	2,713.50
15	UK	Rayleigh	13/01/2011	10406	15	1,830.78
16	USA	Callahan	14/01/2011	10408	10	1,622.40
17	USA	Farnham	14/01/2011	10409	19	319.20
18	USA	Farnham	15/01/2011	10410	16	802.00



Data Stratification



Build model(s)

Training data

Evaluate model(s)

Validation data

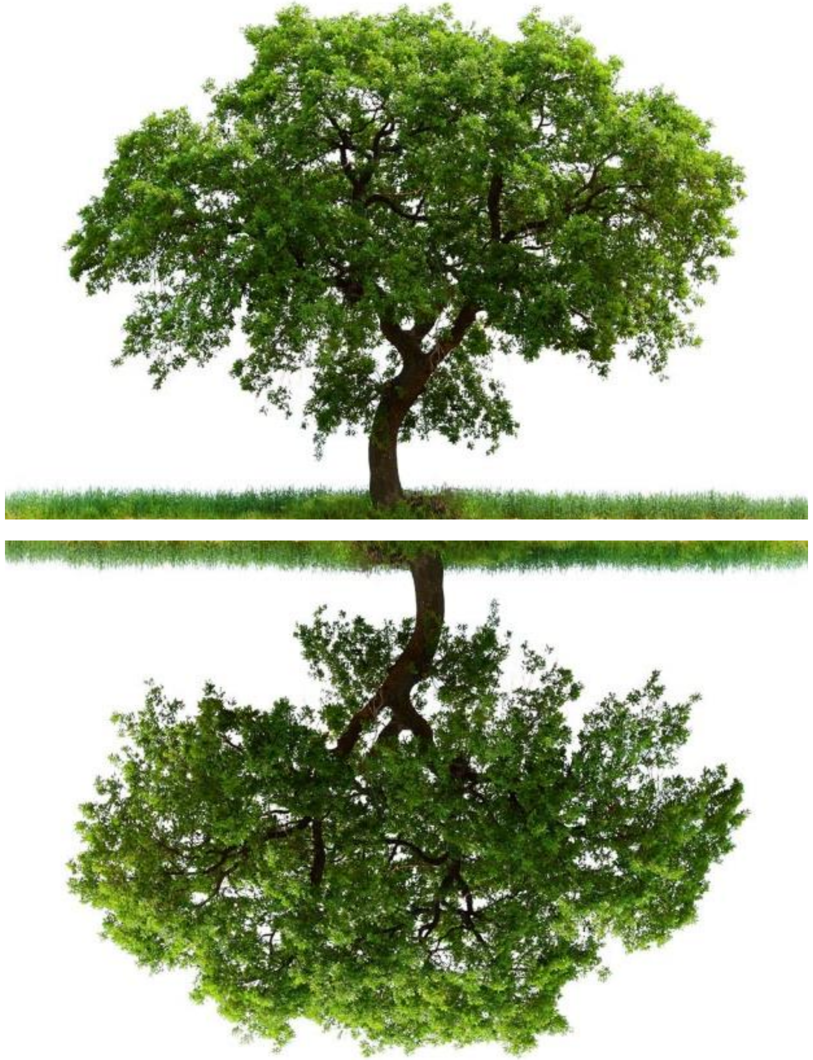
Reevaluate model(s) (optional)

Test data

Predict/classify using final model

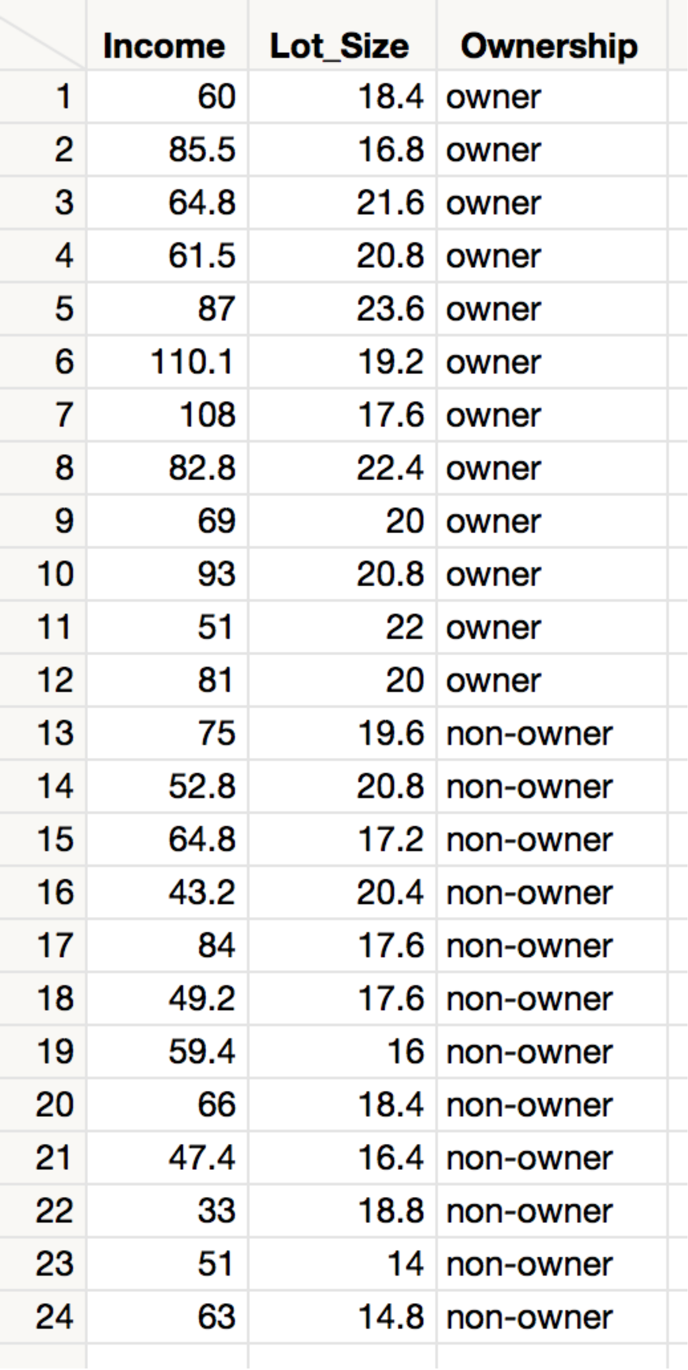
New data

Decision Trees



Income

Lot size



	Income	Lot_Size	Ownership
1	60	18.4	owner
2	85.5	16.8	owner
3	64.8	21.6	owner
4	61.5	20.8	owner
5	87	23.6	owner
6	110.1	19.2	owner
7	108	17.6	owner
8	82.8	22.4	owner
9	69	20	owner
10	93	20.8	owner
11	51	22	owner
12	81	20	owner
13	75	19.6	non-owner
14	52.8	20.8	non-owner
15	64.8	17.2	non-owner
16	43.2	20.4	non-owner
17	84	17.6	non-owner
18	49.2	17.6	non-owner
19	59.4	16	non-owner
20	66	18.4	non-owner
21	47.4	16.4	non-owner
22	33	18.8	non-owner
23	51	14	non-owner
24	63	14.8	non-owner

Splitting on Continuous Variables

- Order records according to one variable, say lot size
- Split at the first value
- Measure the dissimilarity between the two subsets
- Split at the next value, and continue
- Repeat for the other variable(s)
- For all variables, the split value that drives the greatest dissimilarity in propensities (or probabilities) is selected as the split point

Shmueli, G., Bruce, P., Stephens, M. and Patel, N. (2016) Data Mining for Business Analytics: Concepts, Techniques, and Applications with JMP Pro, Wiley, USA https://www.wiley.com/en-us/Data+Mining+for+Business+Analytics%3A+Concepts%2C+Techniques%2C+and+Applications+with+JMP+Pro-p-9781118877524

Splitting on Categorical Variables

- Examine all possible ways in which the categories can be split.
- E.g., nominal categories A, B, C can be split 3 ways

  {A} and {B, C}

  {B} and {A, C}

  {C} and {A, B}

- With many categories, # of potential splits becomes huge

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Splitting on Categorical Variables

- For ordinal data (ordered categories) there is an option for the splits to respect ordering
- Example: An ordinal predictor takes on the values 1, 2, 3, or 4
- The data can be split 3 ways:

{1} and {2, 3, 4}

{1, 2} and {3, 4}

{1, 2, 3} and {4}

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Gini Index

Gini Index for rectangle *A* containing *m* records

$$I(A) = 1 - \sum_{k=1}^{m} p_k^2$$

p = proportion of cases in rectangle *A* that belong to class *k*

- I(A) = 0 when all cases belong to same class
- Max value when all classes are equally represented (= 0.50 in binary case)

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Entropy

p = proportion of cases (out of *m*) in rectangle *A* that belong to class *k*

$$entropy\ (A) = -\sum_{k=1}^{m} p_k\, log_2(p_k)$$

- Entropy ranges between 0 (most pure) and $\log_2(m)$ (equal representation of classes)

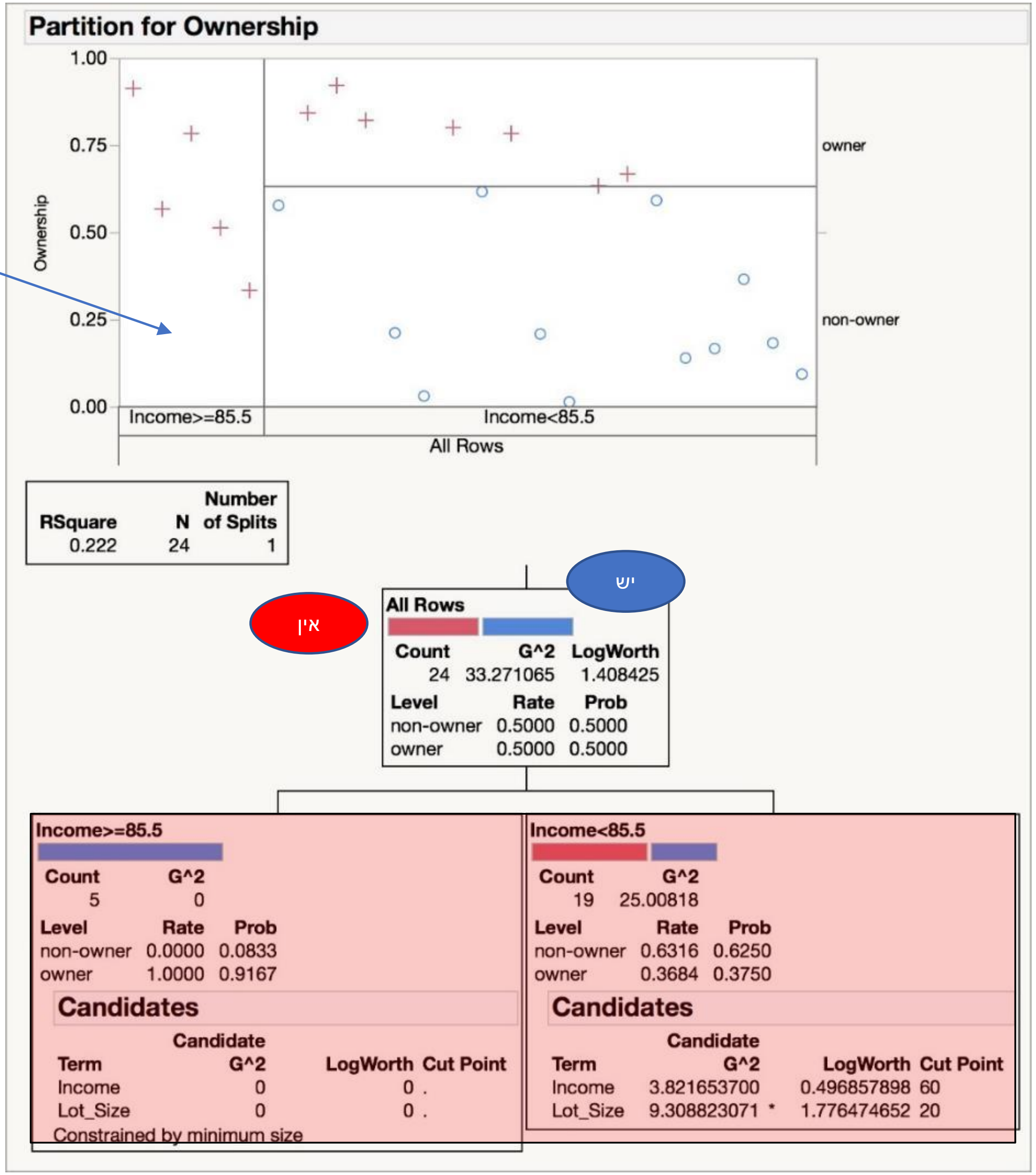
Shmueli, G., Bruce, P., Stephens, M. and Patel, N. (2016) Data Mining for Business Analytics: Concepts, Techniques, and Applications with JMP Pro, Wiley, USA https://www.wiley.com/en-us/Data+Mining+for+Business+Analytics%3A+Concepts%2C+Techniques%2C+and+Applications+with+JMP+Pro-p-9781118877524

Impurity and Recursive Partitioning

- Obtain overall impurity measure (weighted avg. of individual rectangles)
- At each successive stage, compare this measure across all possible splits in all variables
- Choose the split that reduces impurity the most
- Chosen split points become nodes on the tree

Shmueli, G., Bruce, P., Stephens, M. and Patel, N. (2016) Data Mining for Business Analytics: Concepts, Techniques, and Applications with JMP Pro, Wiley, USA https://www.wiley.com/en-us/Data+Mining+for+Business+Analytics%3A+Concepts%2C+Techniques%2C+and+Applications+with+JMP+Pro-p-9781118877524

Rectangle A



Partition for Ownership

RSquare	N	Number of Splits
0.222	24	1

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All Rows

Count	G^2	LogWorth
24	33.271065	1.408425

Level	Rate	Prob
non-owner	0.5000	0.5000
owner	0.5000	0.5000

Income>=85.5

Count	G^2
5	0

Level	Rate	Prob
non-owner	0.0000	0.0833
owner	1.0000	0.9167

Candidates

Term	Candidate G^2	LogWorth	Cut Point
Income	0	0	.
Lot_Size	0	0	.

Constrained by minimum size

Income<85.5

Count	G^2
19	25.00818

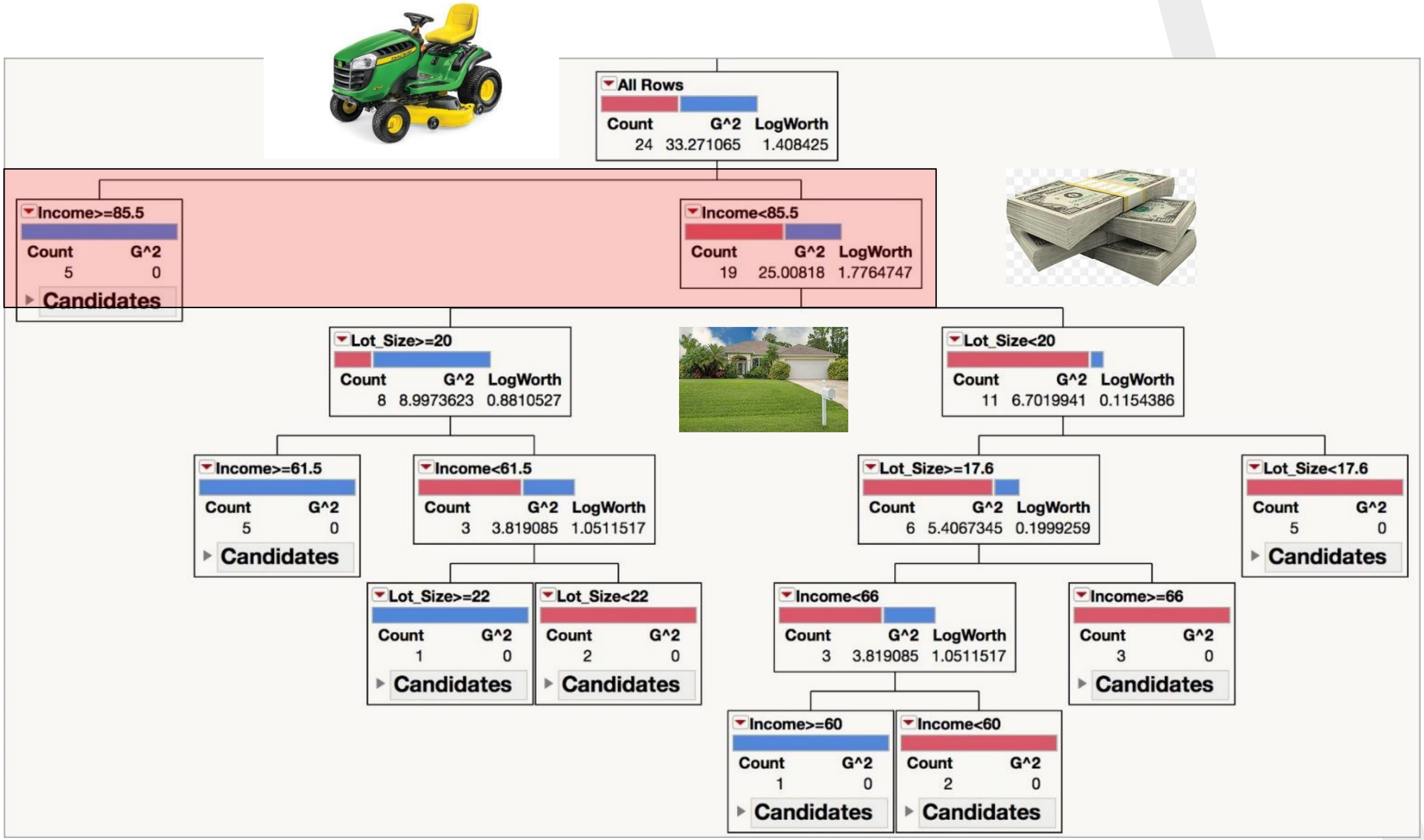
Level	Rate	Prob
non-owner	0.6316	0.6250
owner	0.3684	0.3750

Candidates

Term	Candidate G^2		LogWorth	Cut Point
Income	3.821653700		0.496857898	60
Lot_Size	9.308823071	*	1.776474652	20

Gini and Entropy measures are not available in JMP. JMP uses measures of dissimilarity (G^2 and Sum of Squares) rather than measures of impurity

Income



All Rows

Count	G^2	LogWorth
24	33.271065	1.408425

Income>=85.5

Count	G^2
5	0

Candidates

Income<85.5

Count	G^2	LogWorth
19	25.00818	1.7764747

Lot_Size>=20

Count	G^2	LogWorth
8	8.9973623	0.8810527

Lot_Size<20

Count	G^2	LogWorth
11	6.7019941	0.1154386

Income>=61.5

Count	G^2
5	0

Candidates

Income<61.5

Count	G^2	LogWorth
3	3.819085	1.0511517

Lot_Size>=17.6

Count	G^2	LogWorth
6	5.4067345	0.1999259

Lot_Size<17.6

Count	G^2
5	0

Candidates

Lot_Size>=22

Count	G^2
1	0

Candidates

Lot_Size<22

Count	G^2
2	0

Candidates

Income<66

Count	G^2	LogWorth
3	3.819085	1.0511517

Income>=66

Count	G^2
3	0

Candidates

Income>=60

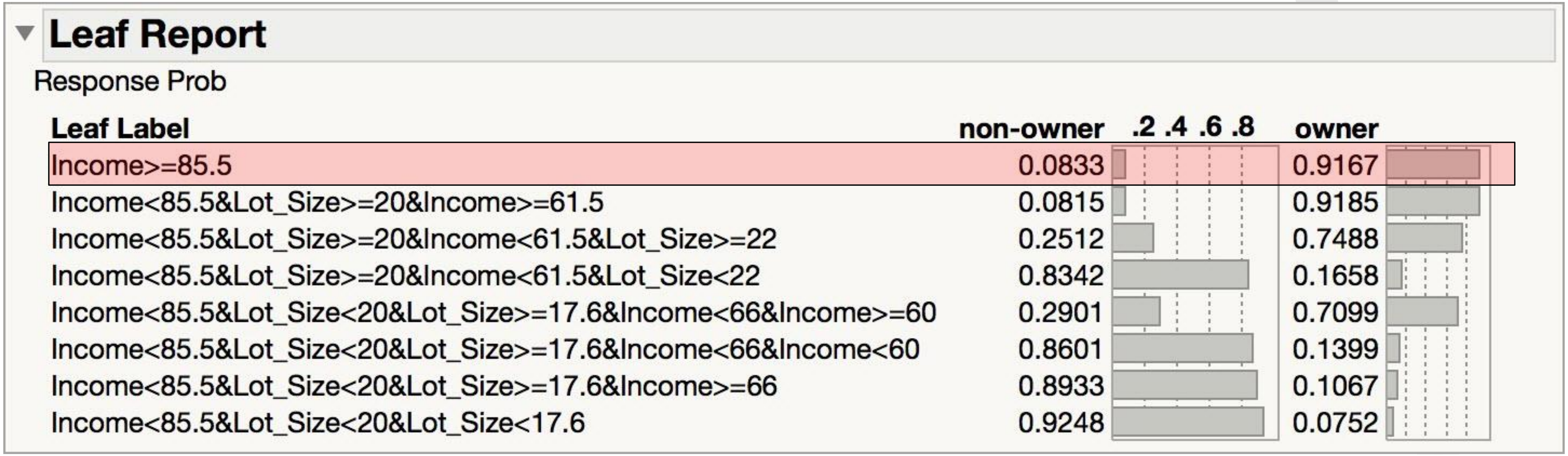
Count	G^2
1	0

Candidates

Income<60

Count	G^2
2	0

Candidates



Leaf Report

Response Prob

Leaf Label	non-owner	owner
Income>=85.5	0.0833	0.9167
Income<85.5&Lot_Size>=20&Income>=61.5	0.0815	0.9185
Income<85.5&Lot_Size>=20&Income<61.5&Lot_Size>=22	0.2512	0.7488
Income<85.5&Lot_Size>=20&Income<61.5&Lot_Size<22	0.8342	0.1658
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income<66&Income>=60	0.2901	0.7099
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income<66&Income<60	0.8601	0.1399
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income>=66	0.8933	0.1067
Income<85.5&Lot_Size<20&Lot_Size<17.6	0.9248	0.0752

Tree Structure

- Split points become nodes on the tree
- Leaves are the terminal nodes (there are no further splits)
- Read down tree to derive the decision rule

  E.g., Income < 85.5, Lot Size is >= 20, and Income >=61.5 , the probability that a household is an owner is 0.9185.

- Records within each node are from the training data (validation data are not used in building the tree)
- Default cutoff = 0.5 is used for classification

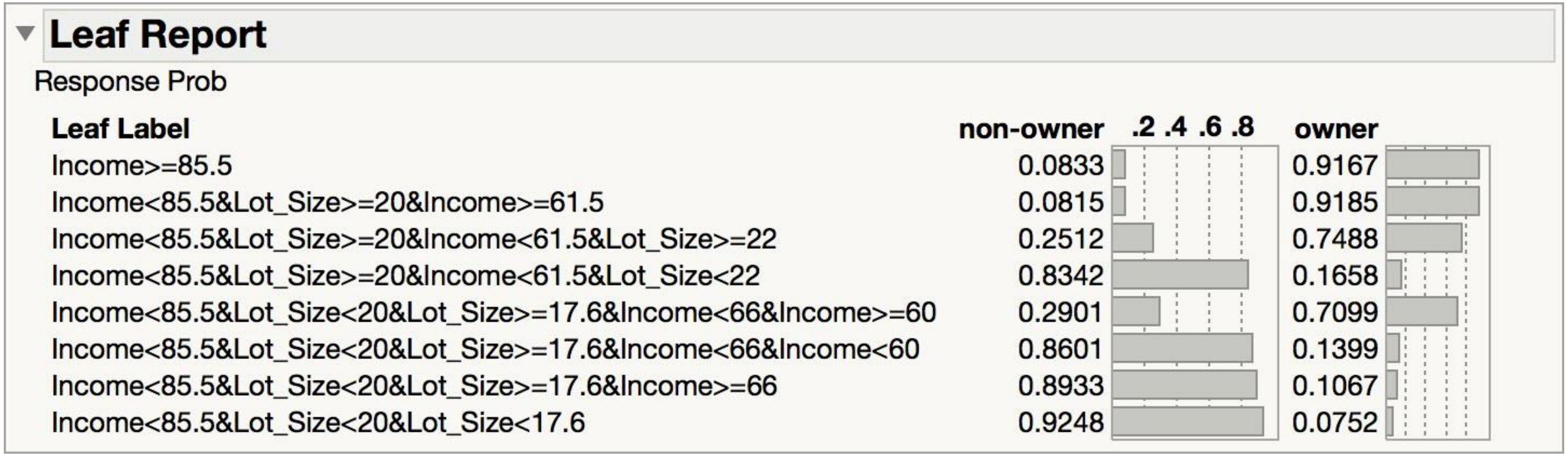
  In the previous example, the record would be classified as an owner.

The Riding Mowers

The leaf report provides a summary the splits

It displays the rules for classifying outcomes

For example, If Income < 85.5, Lot Size is < 17.6, the probability that a household is an owner is 0.0752. This record will be classified as a non-owner.



Response Prob

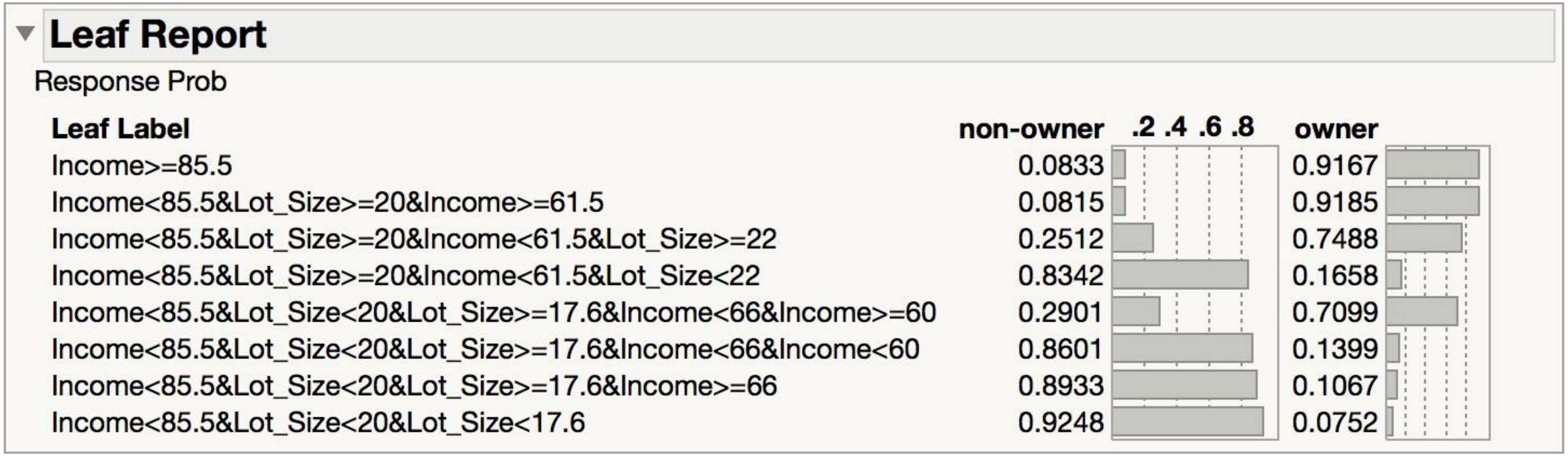
Leaf Label	non-owner	owner
Income>=85.5	0.0833	0.9167
Income<85.5&Lot_Size>=20&Income>=61.5	0.0815	0.9185
Income<85.5&Lot_Size>=20&Income<61.5&Lot_Size>=22	0.2512	0.7488
Income<85.5&Lot_Size>=20&Income<61.5&Lot_Size<22	0.8342	0.1658
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income<66&Income>=60	0.2901	0.7099
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income<66&Income<60	0.8601	0.1399
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income>=66	0.8933	0.1067
Income<85.5&Lot_Size<20&Lot_Size<17.6	0.9248	0.0752

$$\text{Prob}_i = \frac{n_i + \text{prior}_i}{\sum(n_i + \text{prior}_i)}$$

where the summation is across all response levels; n_i is the number of observations at the node for the i^{th} response level; and prior_i is the prior probability for the i^{th} response level, calculated as follows:

$$\text{prior}_i = \lambda p_i + (1-\lambda)P_i$$

where p_i is the prior_i from the parent node, P_i is the Prob_i from the parent node, and λ is a weighting factor currently set at 0.9.



Leaf Report

Response Prob

Leaf Label	non-owner	owner
Income>=85.5	0.0833	0.9167
Income<85.5&Lot_Size>=20&Income>=61.5	0.0815	0.9185
Income<85.5&Lot_Size>=20&Income<61.5&Lot_Size>=22	0.2512	0.7488
Income<85.5&Lot_Size>=20&Income<61.5&Lot_Size<22	0.8342	0.1658
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income<66&Income>=60	0.2901	0.7099
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income<66&Income<60	0.8601	0.1399
Income<85.5&Lot_Size<20&Lot_Size>=17.6&Income>=66	0.8933	0.1067
Income<85.5&Lot_Size<20&Lot_Size<17.6	0.9248	0.0752

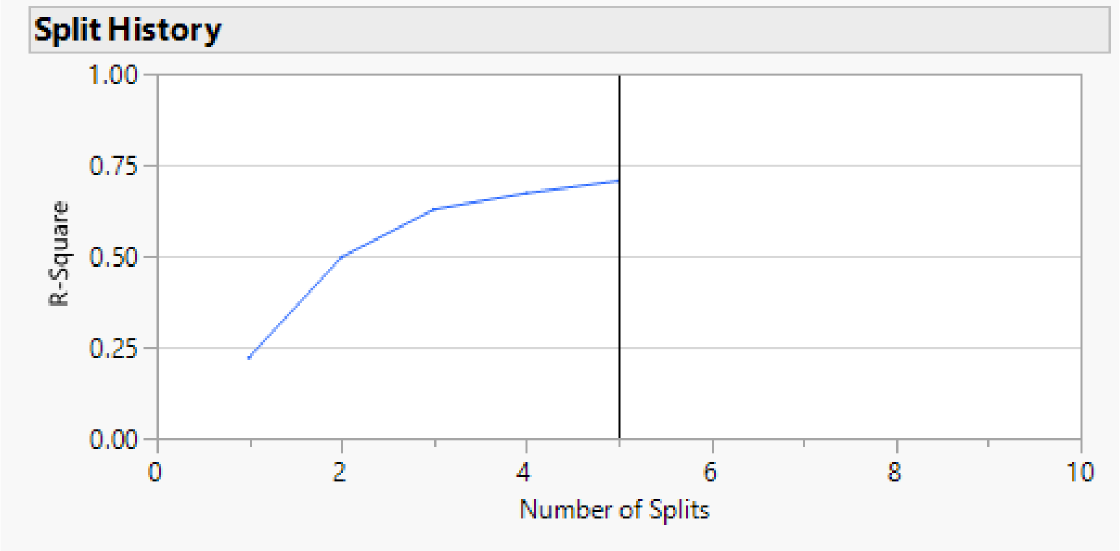
Stopping Tree Growth

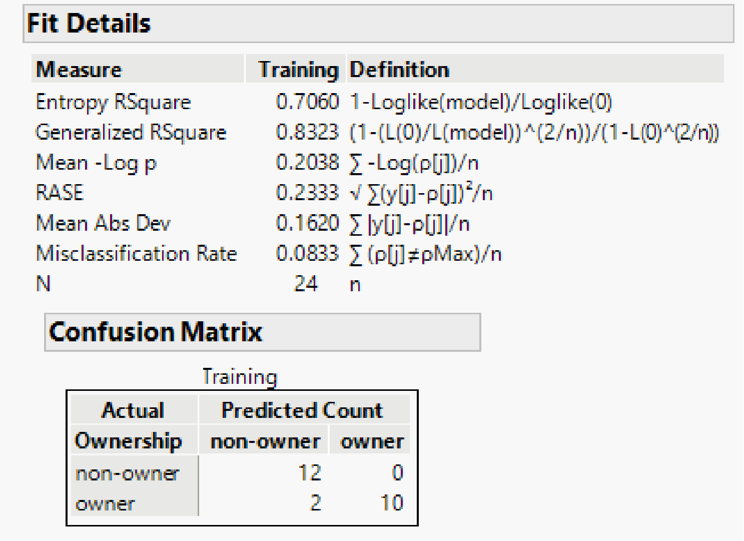
Natural end of process is 100% purity in each leaf

This **overfits** the data, which end up fitting noise in the data

Overfitting leads to low predictive accuracy of new data

Past a certain point, the error rate for the validation data starts to increase





Fit Details

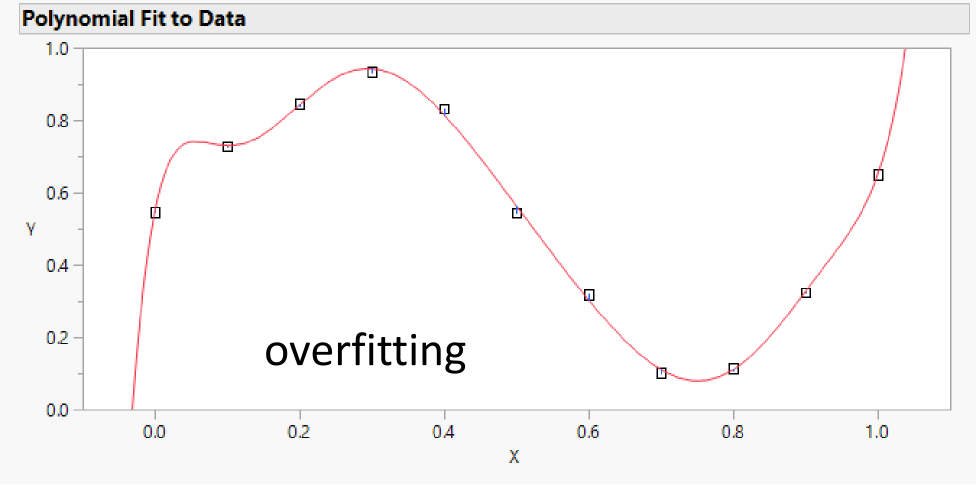
Measure	Training	Definition
Entropy RSquare	0.7060	1-Loglike(model)/Loglike(0)
Generalized RSquare	0.8323	(1-(L(0)/L(model))^(2/n))/(1-L(0)^(2/n))
Mean -Log p	0.2038	∑ -Log(ρ[j])/n
RASE	0.2333	√ ∑(y[j]-ρ[j])^2/n
Mean Abs Dev	0.1620	∑ |y[j]-ρ[j]|/n
Misclassification Rate	0.0833	∑ (ρ[j]≠ρMax)/n
N	24	n

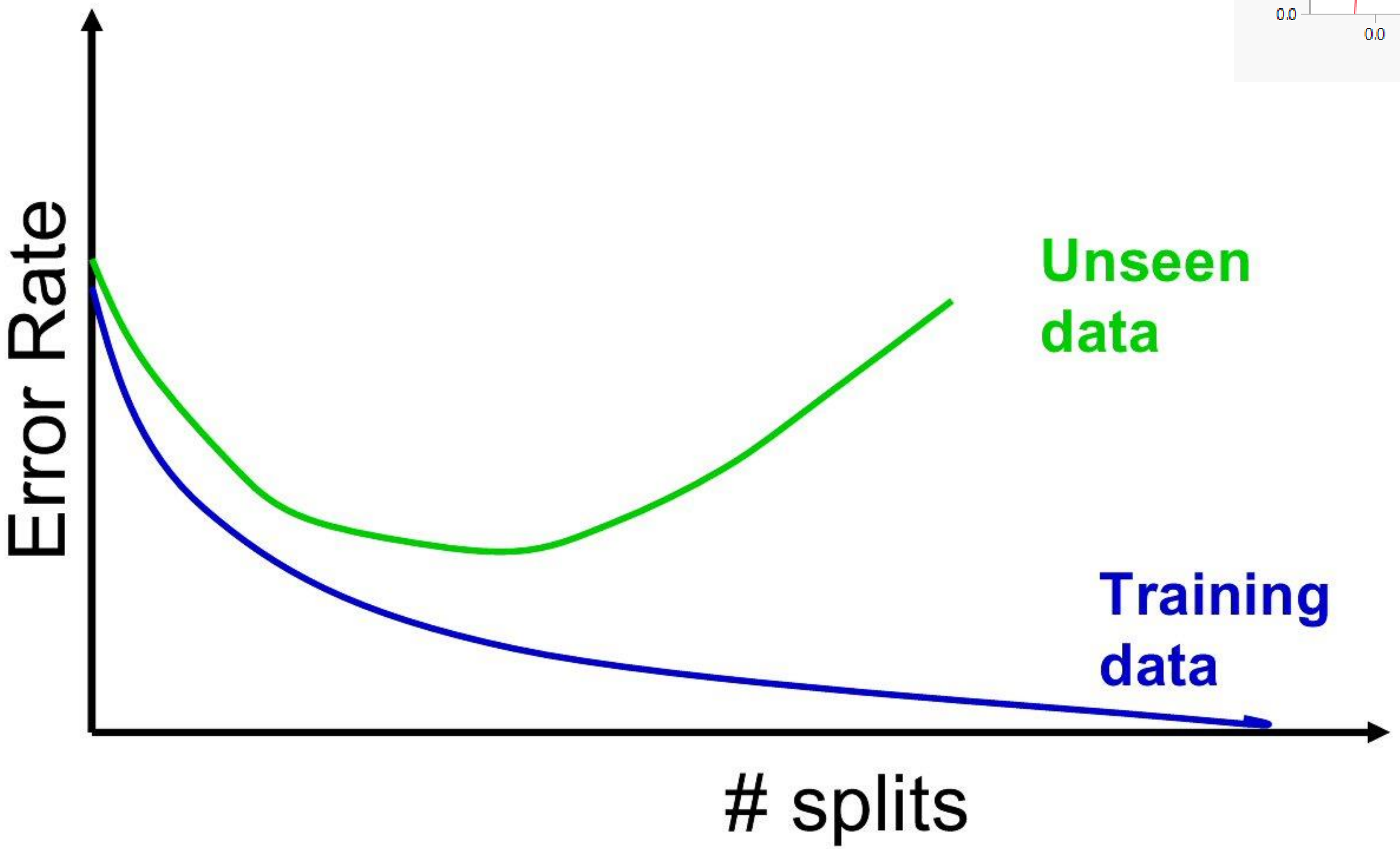
Confusion Matrix

Training

Actual	Predicted Count	
Ownership	non-owner	owner
non-owner	12	0
owner	2	10

Full Tree Error Rate





CART - Classification and regression trees

- CART lets tree grow to full extent, then prunes it back
- Idea is to find that point at which the validation error begins to rise
- Generate successively smaller trees by pruning leaves
- At each pruning stage, multiple trees are possible
- Use *cost complexity* to choose the best tree at that stage

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Cost Complexity

$$CC(T) = Err(T) + \alpha\, L(T)$$

CC(T) = cost complexity of a tree

Err(T) = proportion of misclassified records

L(T) – size of tree

α = penalty factor attached to tree size (set by user)

Among trees of given size, choose the one with lowest CC

Do this for each size of tree

CART - Classification and regression trees

- Nonparametric (no probabilistic assumptions)
- Automatically performs variable selection
- Uses any combination of continuous/discrete variables
    - Very nice feature: ability to automatically bin massively categorical variables into a few categories (zip code, business class, make/model…)
- Invariant to monotonic transformations of predictive variable
- Unlike regression, not sensitive to outliers in predictive variables

CART Overview

- Classification and Regression Trees are an easily understandable and transparent method for predicting or classifying new records
- A tree is a graphical representation of a set of rules
- Trees must be pruned to avoid over-fitting of the training data
- As trees do not make any assumptions about the data structure, they usually require large samples

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CHAID - Chi-squared automatic interaction detector

- CHAID, older than CART, uses chi-square statistical test to limit tree growth
- Splitting stops when purity improvement is not statistically significant

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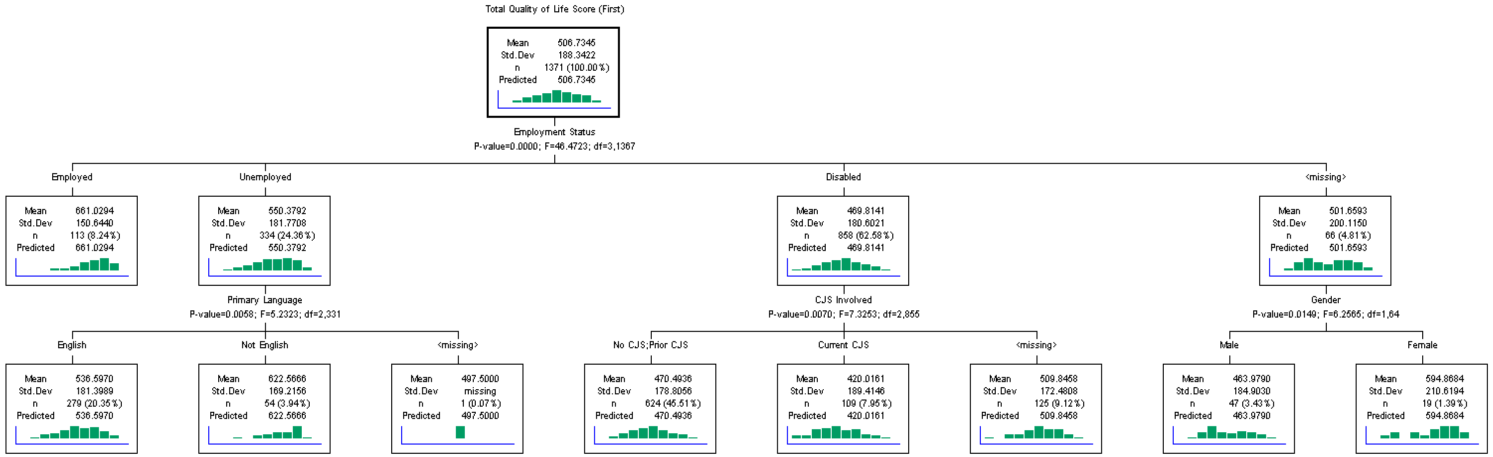
CHAID - Chi-squared automatic interaction detector

- CHAID is a non-binary decision tree.
- The decision or split made at each node is still based on a single variable, but can result in multiple branches.
- The split search algorithm is designed for categorical variables.



Classification Trees: CART versus CHAID

- At each split, the CHAID algorithm looks for the predictor variable that if split, most "explains" the category response variable. In order to decide whether to create a particular split based on this variable, the CHAID algorithm tests a hypothesis regarding dependence between the split variable and the categorical response (using the chi-squared test for independence). Using a pre-specified significance level, if the test shows that the split variable and the response are independent, the algorithm stops the tree growth. Otherwise, the split is created, and the next best split is searched. In contrast, the CART algorithm decides on a split based on the amount of homogeneity within class that is achieved by the split. The split is reconsidered based on considerations of over-fitting.

- CHAID is most useful for analysis, whereas CART is more suitable for prediction. In other words, CHAID should be used when the goal is to describe or understand the relationship between a response variable and a set of explanatory variables, whereas CART is better suited for creating a model that has high prediction accuracy of new cases.

Limiting Tree Size

JMP uses a combination of limiting tree growth and pruning the tree after it has grown

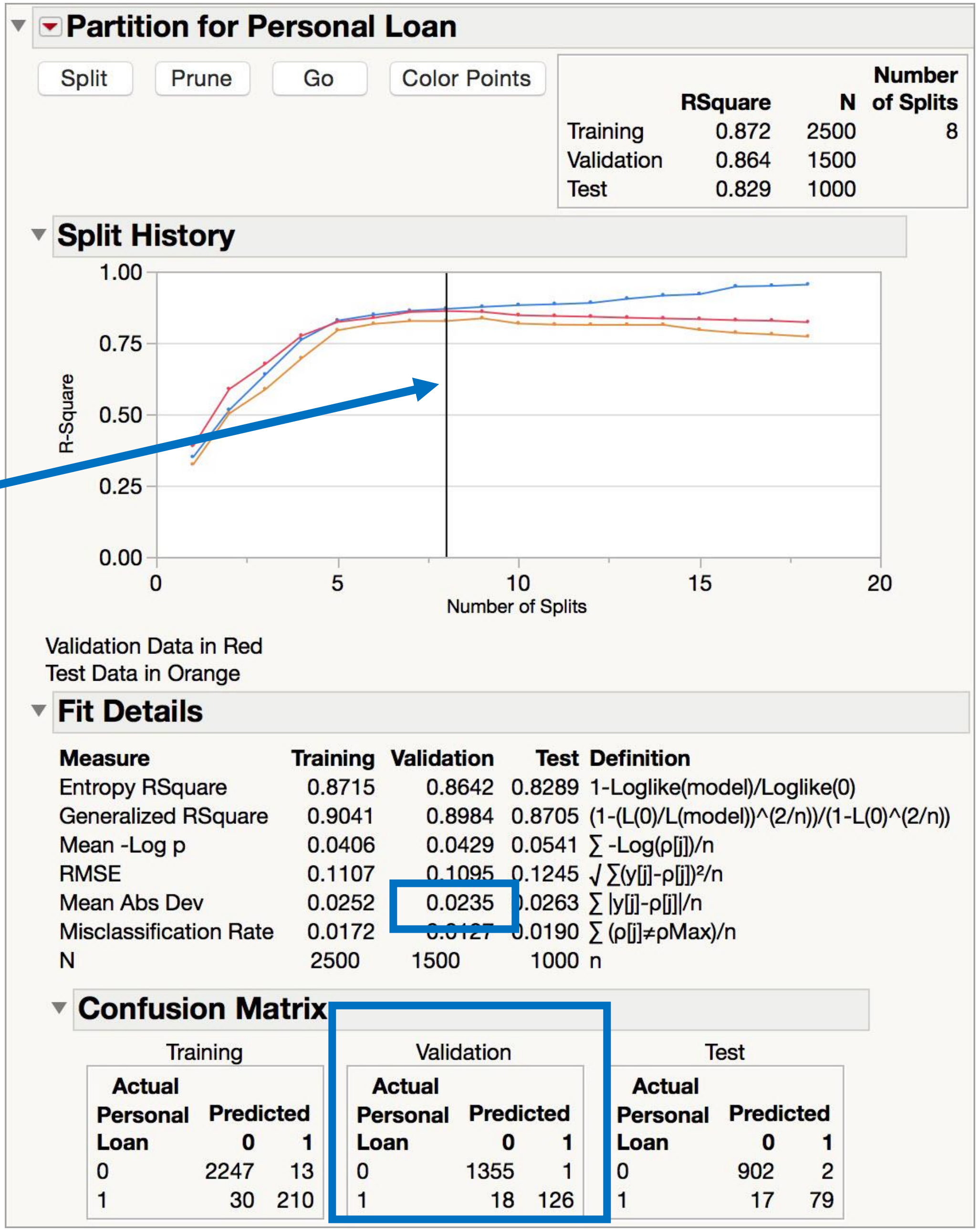
- **Minimum Split Size**: Controls the minimum number of records in terminal nodes
- **Validation**: The tree is grown, and pruned back to maximize the RSquare on the validation data

When validation is used, the "Go" option automates tree growth and pruning

The tree with the maximum Validation Rsquare has 8 splits

The tree is grown to 18 splits, and is pruned back to 8 splits

Validation error rate and confusion matrix for the final tree (cutoff for classification = 0.50)



Partition for Personal Loan

	RSquare	N	Number of Splits
Training	0.872	2500	8
Validation	0.864	1500	
Test	0.829	1000	

Validation Data in Red
Test Data in Orange

Fit Details

Measure	Training	Validation	Test	Definition
Entropy RSquare	0.8715	0.8642	0.8289	1-Loglike(model)/Loglike(0)
Generalized RSquare	0.9041	0.8984	0.8705	(1-(L(0)/L(model))^(2/n))/(1-L(0)^(2/n))
Mean -Log p	0.0406	0.0429	0.0541	∑ -Log(ρ[j])/n
RMSE	0.1107	0.1095	0.1245	√ ∑(y[j]-ρ[j])²/n
Mean Abs Dev	0.0252	0.0235	0.0263	∑ |y[j]-ρ[j]|/n
Misclassification Rate	0.0172	0.0127	0.0190	∑ (ρ[j]≠ρMax)/n
N	2500	1500	1000	n

Confusion Matrix

Training

Actual Personal Loan	Predicted 0	Predicted 1
0	2247	13
1	30	210

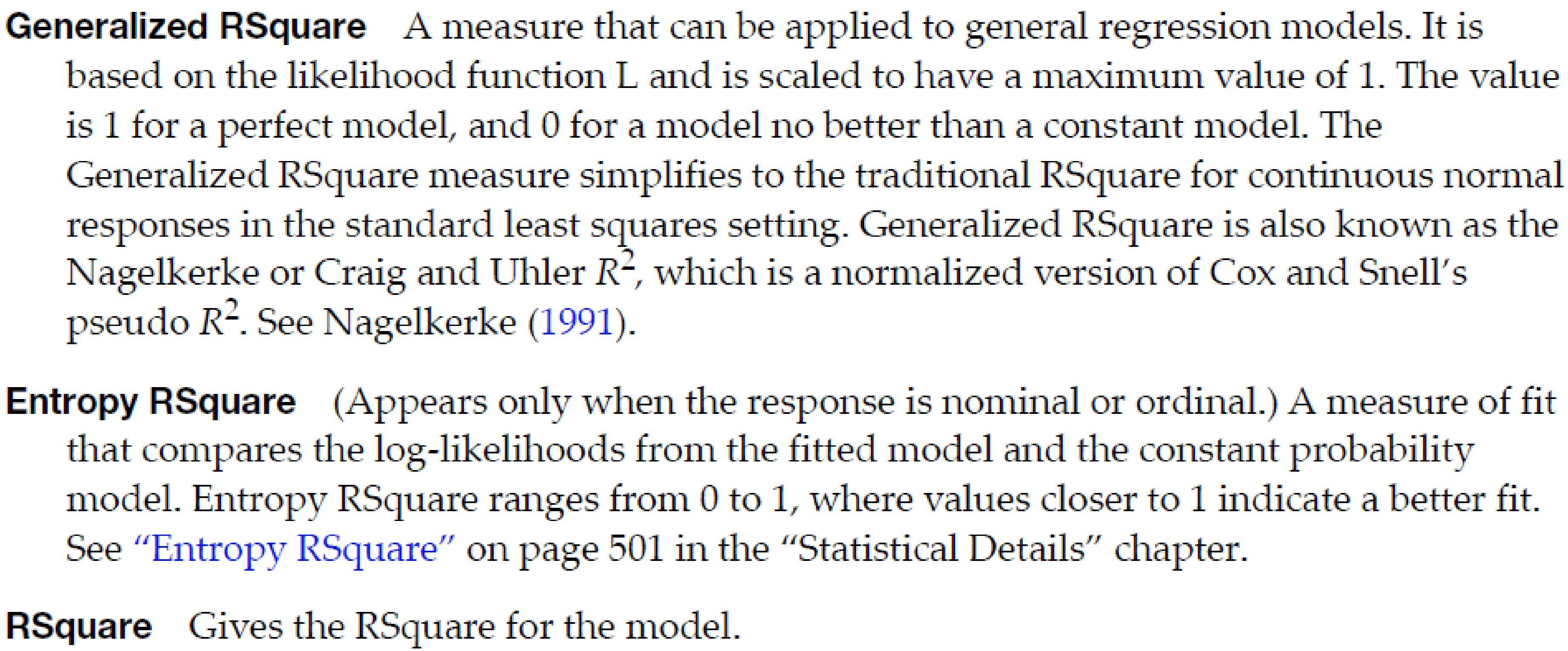
Validation

Actual Personal Loan	Predicted 0	Predicted 1
0	1355	1
1	18	126

Test

Actual Personal Loan	Predicted 0	Predicted 1
0	902	2
1	17	79

Validation

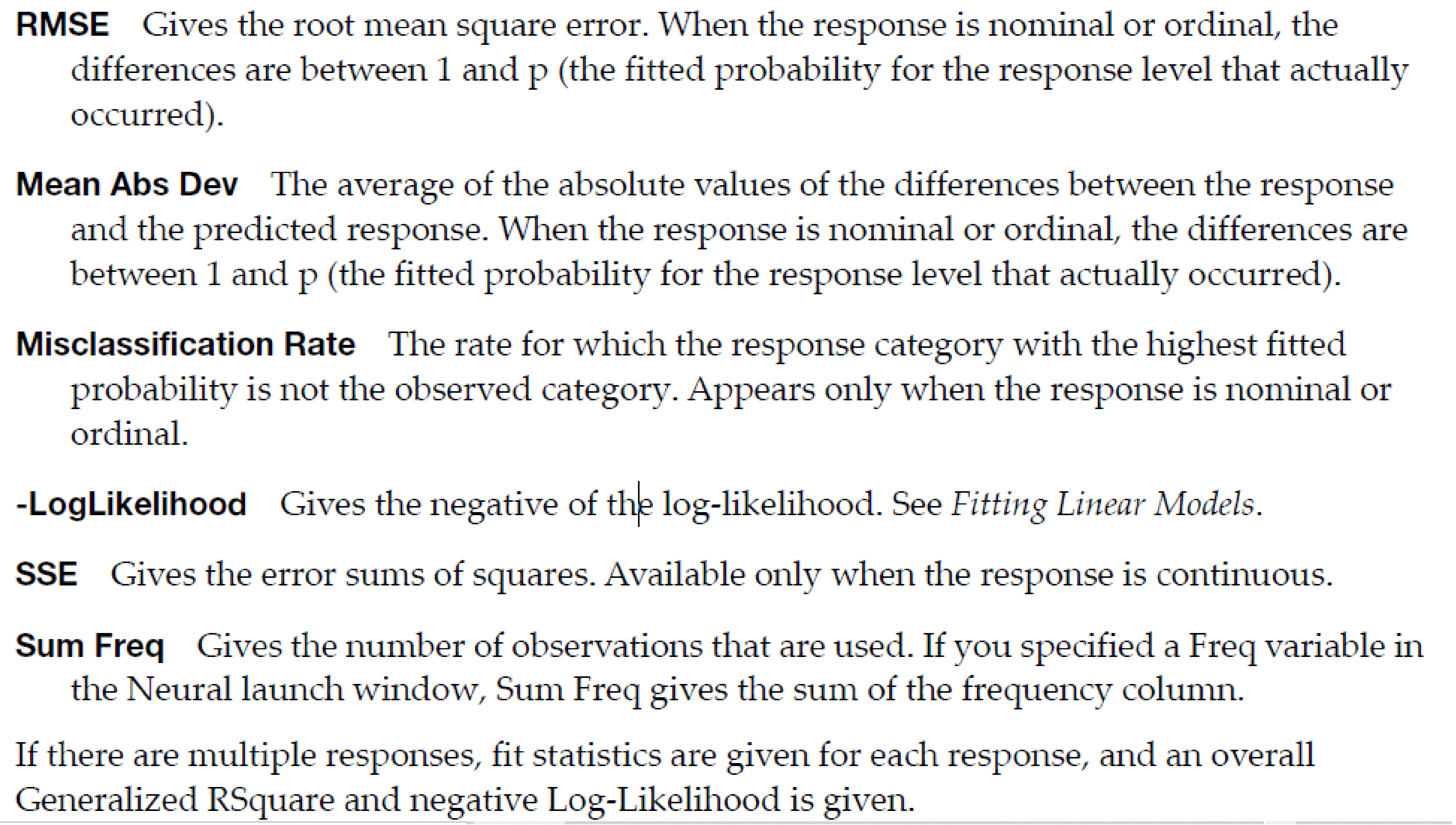


Generalized RSquare A measure that can be applied to general regression models. It is based on the likelihood function L and is scaled to have a maximum value of 1. The value is 1 for a perfect model, and 0 for a model no better than a constant model. The Generalized RSquare measure simplifies to the traditional RSquare for continuous normal responses in the standard least squares setting. Generalized RSquare is also known as the Nagelkerke or Craig and Uhler R^2, which is a normalized version of Cox and Snell's pseudo R^2. See Nagelkerke (1991).

Entropy RSquare (Appears only when the response is nominal or ordinal.) A measure of fit that compares the log-likelihoods from the fitted model and the constant probability model. Entropy RSquare ranges from 0 to 1, where values closer to 1 indicate a better fit. See "Entropy RSquare" on page 501 in the "Statistical Details" chapter.

RSquare Gives the RSquare for the model.

Validation



RMSE Gives the root mean square error. When the response is nominal or ordinal, the differences are between 1 and p (the fitted probability for the response level that actually occurred).

Mean Abs Dev The average of the absolute values of the differences between the response and the predicted response. When the response is nominal or ordinal, the differences are between 1 and p (the fitted probability for the response level that actually occurred).

Misclassification Rate The rate for which the response category with the highest fitted probability is not the observed category. Appears only when the response is nominal or ordinal.

-LogLikelihood Gives the negative of the log-likelihood. See *Fitting Linear Models*.

SSE Gives the error sums of squares. Available only when the response is continuous.

Sum Freq Gives the number of observations that are used. If you specified a Freq variable in the Neural launch window, Sum Freq gives the sum of the frequency column.

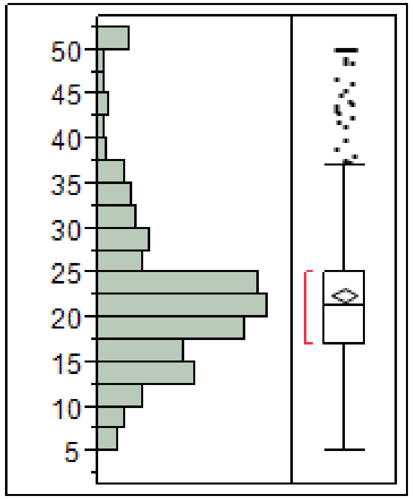
If there are multiple responses, fit statistics are given for each response, and an overall Generalized RSquare and negative Log-Likelihood is given.

Regression Trees for Prediction

- Used with continuous outcome variable
- Procedure like classification tree
- Many splits attempted, choose the one that maximizes the difference between subgroup means
- Difference measured as the sum of squared deviations
- Prediction is the **average** of the numerical target variable (rather than a probability)

Regression Trees

mvalue



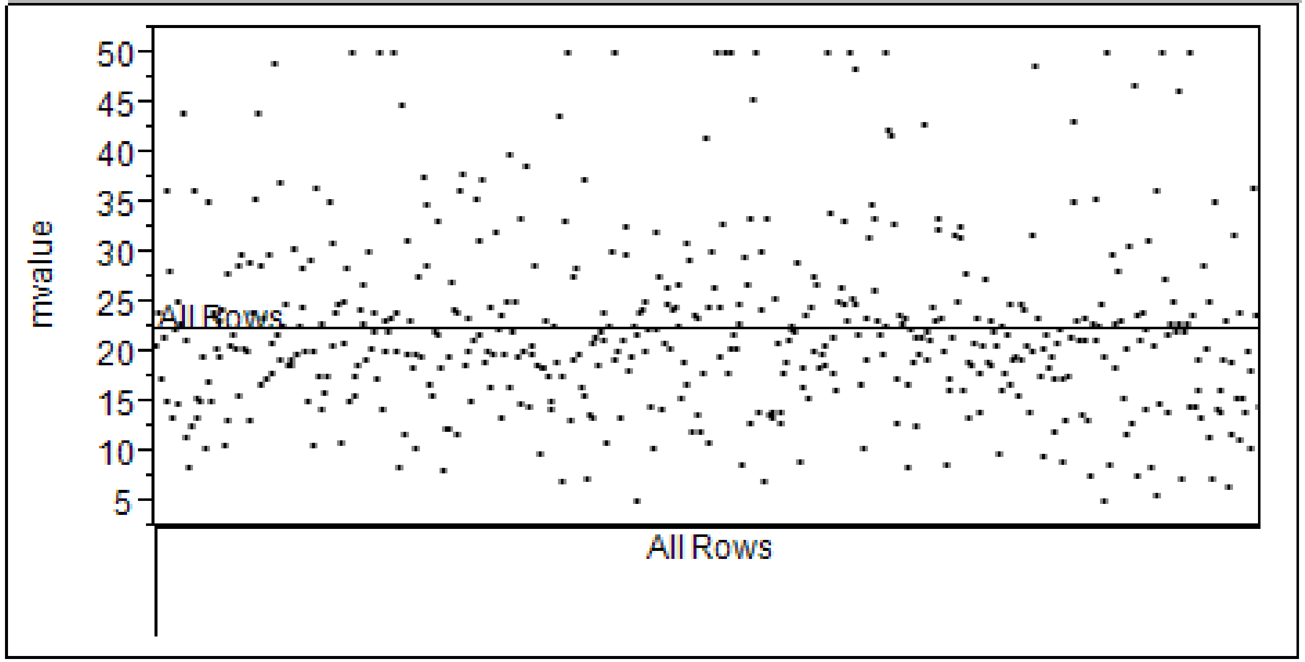
Quantiles

100.0%	maximum	50
99.5%		50
97.5%		50
90.0%		34.9
75.0%	quartile	25
50.0%	median	21.2
25.0%	quartile	16.95
10.0%		12.7
2.5%		8.235
0.5%		5.321
0.0%	minimum	5

Summary Statistics

Mean	22.532806
Std Dev	9.1971041
Std Err Mean	0.4088611
Upper 95% Mean	23.336085
Lower 95% Mean	21.729528
N	506

Partition for mvalue

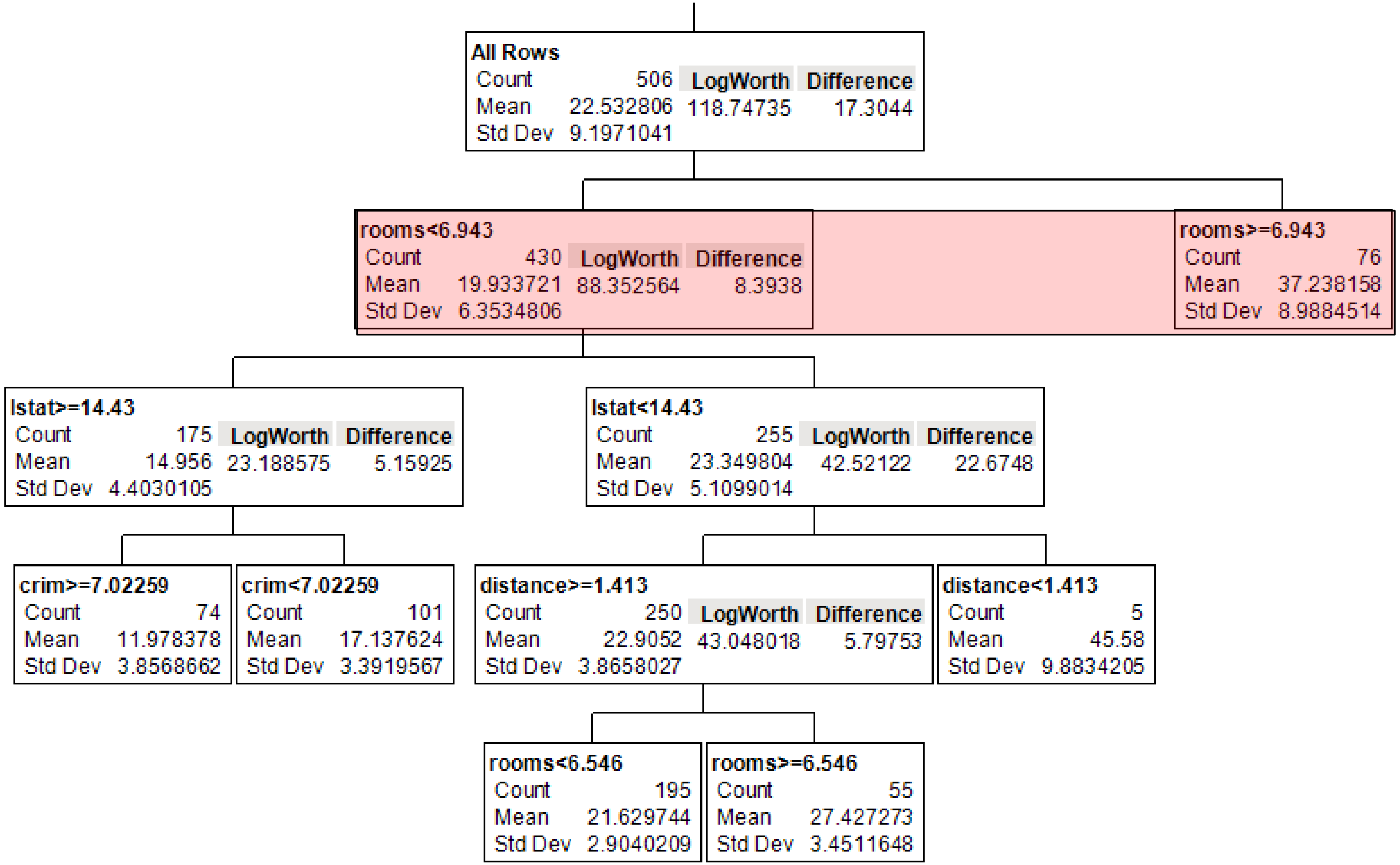


RSquare	RMSE	N	Number of Splits	AICc
0.000	.	506	0	0

All Rows

Count	506
Mean	22.532806
Std Dev	9.1971041

Regression Trees



All Rows

Count	506	LogWorth	Difference
Mean	22.532806	118.74735	17.3044
Std Dev	9.1971041		

rooms<6.943

Count	430	LogWorth	Difference
Mean	19.933721	88.352564	8.3938
Std Dev	6.3534806		

rooms>=6.943

Count	76
Mean	37.238158
Std Dev	8.9884514

lstat>=14.43

Count	175	LogWorth	Difference
Mean	14.956	23.188575	5.15925
Std Dev	4.4030105		

lstat<14.43

Count	255	LogWorth	Difference
Mean	23.349804	42.52122	22.6748
Std Dev	5.1099014		

crim>=7.02259

Count	74
Mean	11.978378
Std Dev	3.8568662

crim<7.02259

Count	101
Mean	17.137624
Std Dev	3.3919567

distance>=1.413

Count	250	LogWorth	Difference
Mean	22.9052	43.048018	5.79753
Std Dev	3.8658027		

distance<1.413

Count	5
Mean	45.58
Std Dev	9.8834205

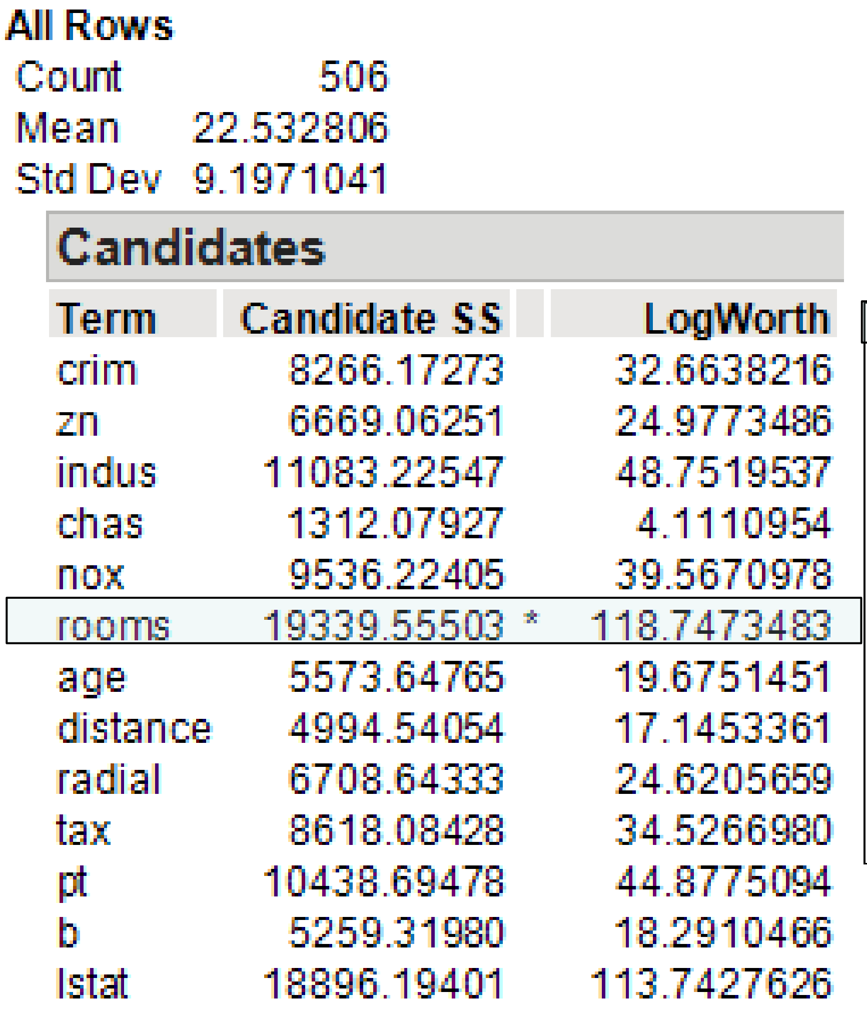
rooms<6.546

Count	195
Mean	21.629744
Std Dev	2.9040209

rooms>=6.546

Count	55
Mean	27.427273
Std Dev	3.4511648

Boston Housing Data

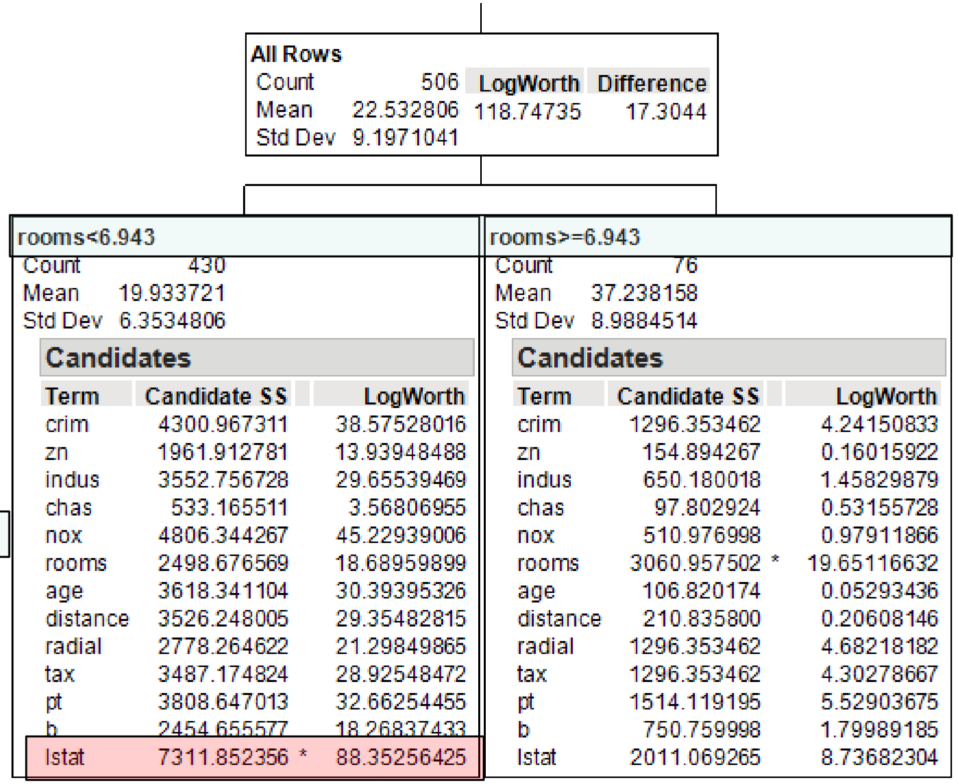


All Rows

Count	506
Mean	22.532806
Std Dev	9.1971041

Candidates

Term	Candidate SS		LogWorth
crim	8266.17273		32.6638216
zn	6669.06251		24.9773486
indus	11083.22547		48.7519537
chas	1312.07927		4.1110954
nox	9536.22405		39.5670978
rooms	19339.55503	*	118.7473483
age	5573.64765		19.6751451
distance	4994.54054		17.1453361
radial	6708.64333		24.6205659
tax	8618.08428		34.5266980
pt	10438.69478		44.8775094
b	5259.31980		18.2910466
lstat	18896.19401		113.7427626



All Rows

		LogWorth	Difference
Count	506		
Mean	22.532806	118.74735	17.3044
Std Dev	9.1971041		

rooms<6.943

Count	430
Mean	19.933721
Std Dev	6.3534806

Candidates

Term	Candidate SS		LogWorth
crim	4300.967311		38.57528016
zn	1961.912781		13.93948488
indus	3552.756728		29.65539469
chas	533.165511		3.56806955
nox	4806.344267		45.22939006
rooms	2498.676569		18.68959899
age	3618.341104		30.39395326
distance	3526.248005		29.35482815
radial	2778.264622		21.29849865
tax	3487.174824		28.92548472
pt	3808.647013		32.66254455
b	2454.655577		18.26837433
lstat	7311.852356	*	88.35256425

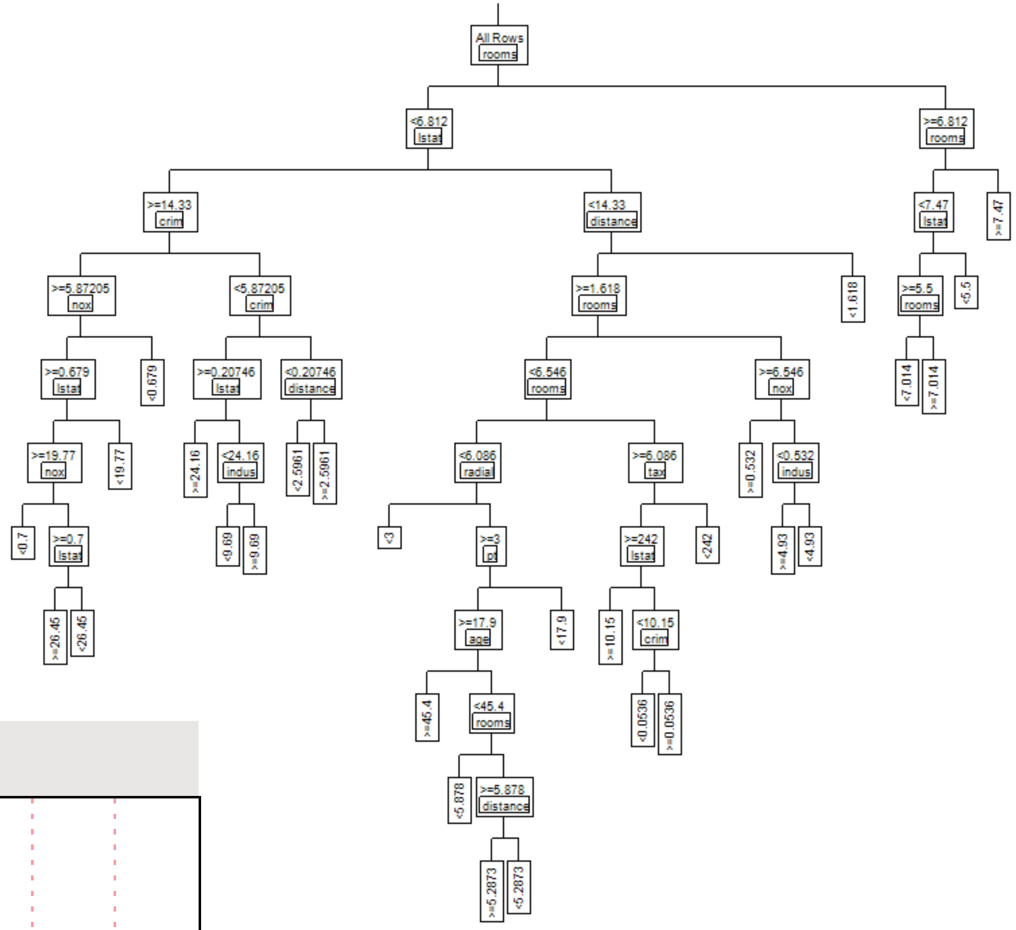
rooms>=6.943

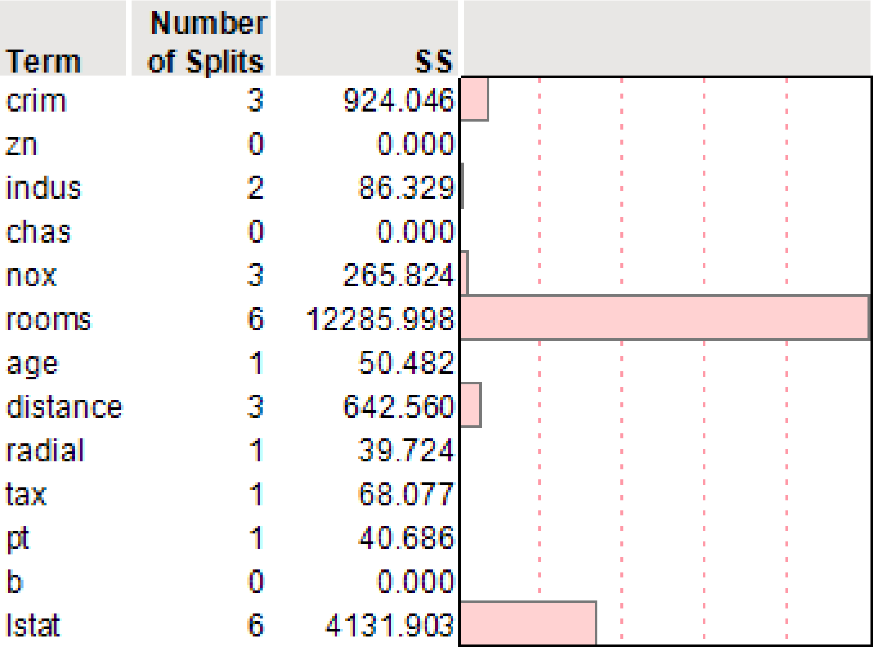
Count	76
Mean	37.238158
Std Dev	8.9884514

Candidates

Term	Candidate SS		LogWorth
crim	1296.353462		4.24150833
zn	154.894267		0.16015922
indus	650.180018		1.45829879
chas	97.802924		0.53155728
nox	510.976998		0.97911866
rooms	3060.957502	*	19.65116632
age	106.820174		0.05293436
distance	210.835800		0.20608146
radial	1296.353462		4.68218182
tax	1296.353462		4.30278667
pt	1514.119195		5.52903675
b	750.759998		1.79989185
lstat	2011.069265		8.73682304

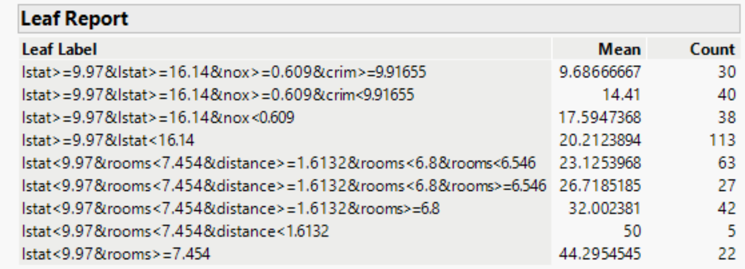
$-\log_{10}(p\text{-value})$





Term	Number of Splits	SS
crim	3	924.046
zn	0	0.000
indus	2	86.329
chas	0	0.000
nox	3	265.824
rooms	6	12285.998
age	1	50.482
distance	3	642.560
radial	1	39.724
tax	1	68.077
pt	1	40.686
b	0	0.000
lstat	6	4131.903

1. CRIM - per capita crime rate by town
2. ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
3. INDUS - proportion of non-retail business acres per town.
4. CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)
5. NOX - nitric oxides concentration (parts per 10 million)
6. RM - average number of rooms per dwelling
7. AGE - proportion of owner-occupied units built prior to 1940
8. DIS - weighted distances to five Boston employment centres
9. RAD - index of accessibility to radial highways
10. TAX - full-value property-tax rate per $10,000
11. PTRATIO - pupil-teacher ratio by town
12. B - 1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
13. LSTAT - % lower status of the population
14. MEDV - Median value of owner-occupied homes in $1000's



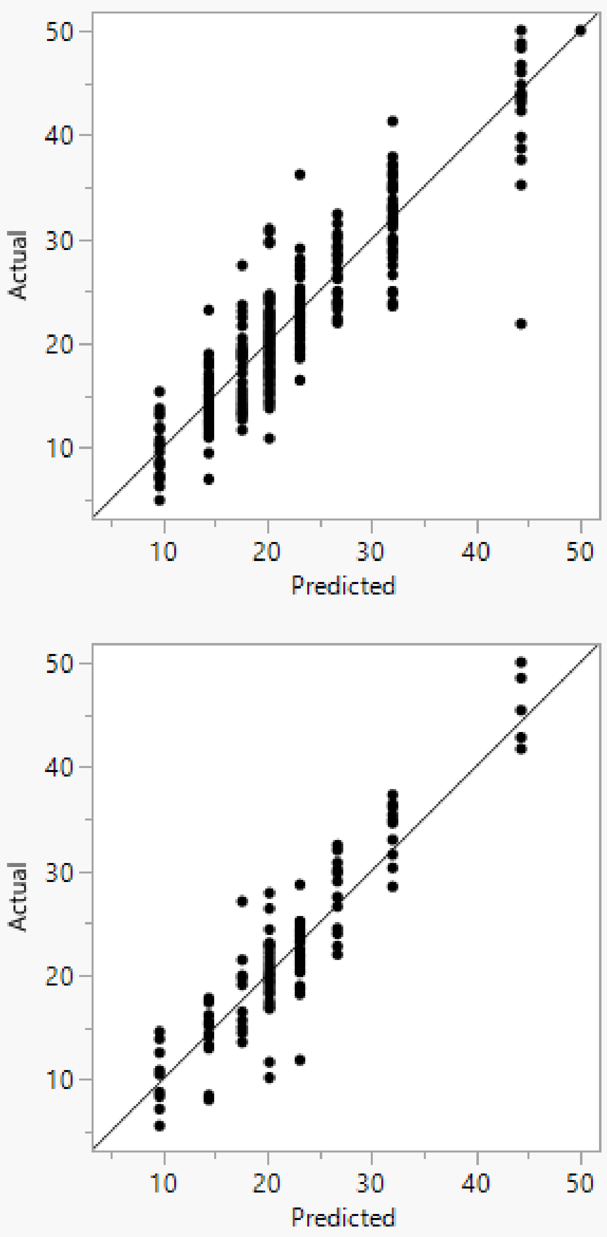
Leaf Report

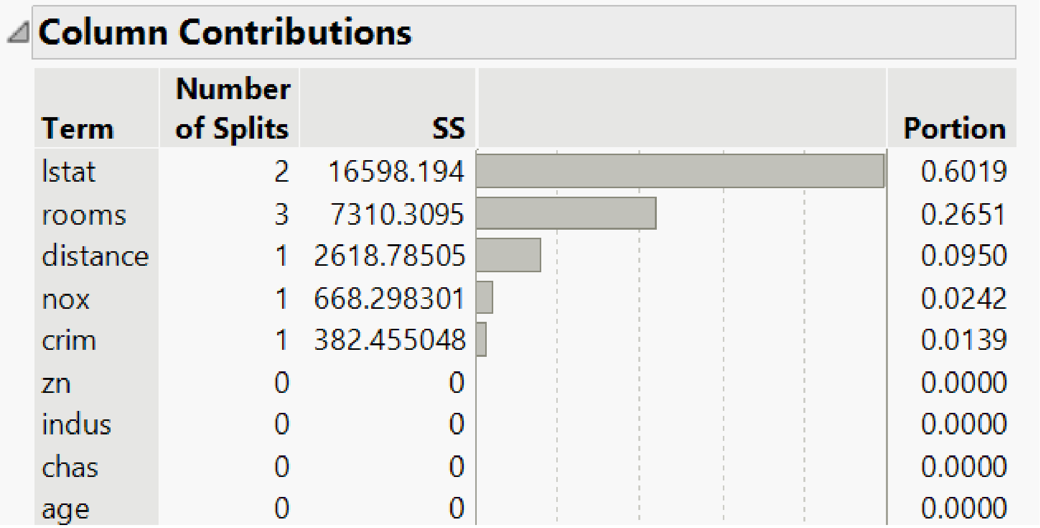
Leaf Label	Mean	Count
lstat>=9.97&lstat>=16.14&nox>=0.609&crim>=9.91655	9.68666667	30
lstat>=9.97&lstat>=16.14&nox>=0.609&crim<9.91655	14.41	40
lstat>=9.97&lstat>=16.14&nox<0.609	17.5947368	38
lstat>=9.97&lstat<16.14	20.2123894	113
lstat<9.97&rooms<7.454&distance>=1.6132&rooms<6.8&rooms<6.546	23.1253968	63
lstat<9.97&rooms<7.454&distance>=1.6132&rooms<6.8&rooms>=6.546	26.7185185	27
lstat<9.97&rooms<7.454&distance>=1.6132&rooms>=6.8	32.002381	42
lstat<9.97&rooms<7.454&distance<1.6132	50	5
lstat<9.97&rooms>=7.454	44.2954545	22

Actual by Predicted Plot

Training Set

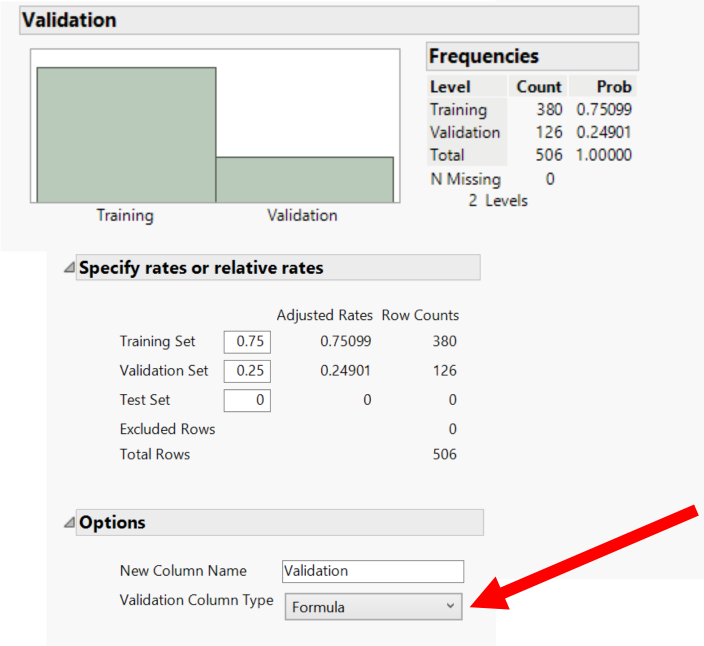
Validation Set





Column Contributions

Term	Number of Splits	SS		Portion
lstat	2	16598.194		0.6019
rooms	3	7310.3095		0.2651
distance	1	2618.78505		0.0950
nox	1	668.298301		0.0242
crim	1	382.455048		0.0139
zn	0	0		0.0000
indus	0	0		0.0000
chas	0	0		0.0000
age	0	0		0.0000



Validation

Frequencies

Level	Count	Prob
Training	380	0.75099
Validation	126	0.24901
Total	506	1.00000
N Missing	0	
2 Levels		

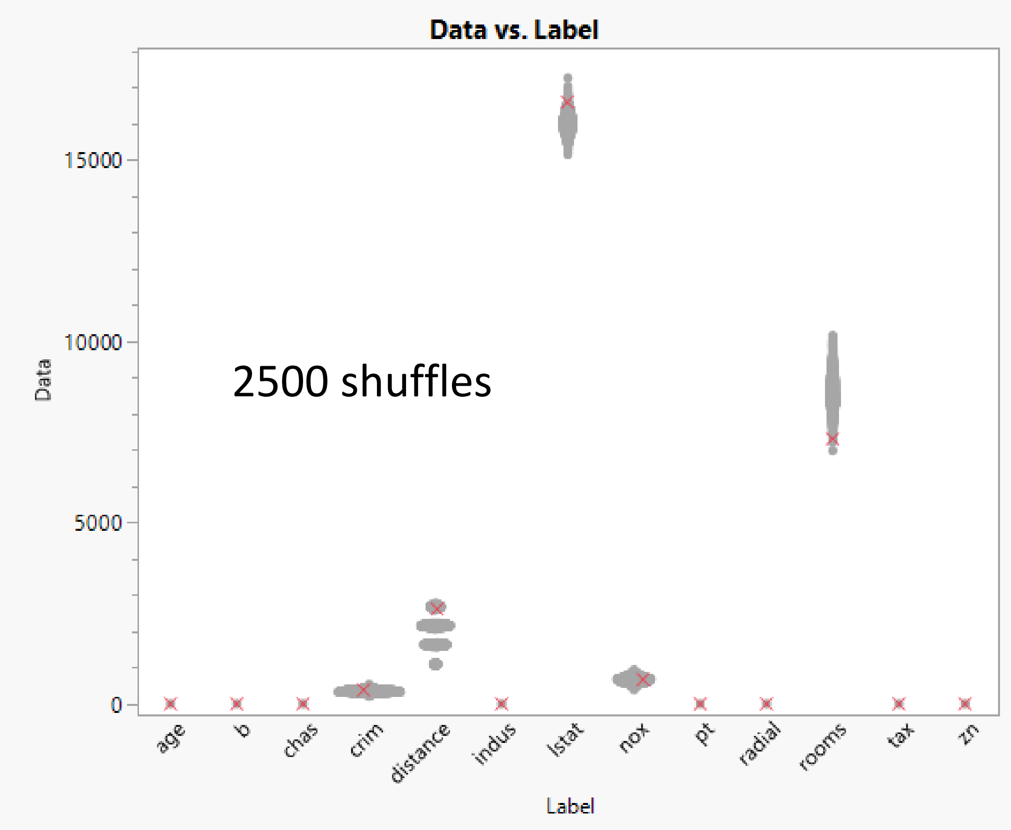
Specify rates or relative rates

		Adjusted Rates	Row Counts
Training Set	0.75	0.75099	380
Validation Set	0.25	0.24901	126
Test Set	0	0	0
Excluded Rows			0
Total Rows			506

Options

New Column Name: Validation

Validation Column Type: Formula



Data vs. Label

2500 shuffles

Advantages of Trees

- Easy to use, understand
- Produce rules that are easy to interpret & implement
- Variable selection & reduction is automatic
- Do not require the assumptions of statistical models
- Can work without extensive handling of missing data (this is an option in the Partition dialog in JMP)

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Disadvantages of Trees

- May not perform well where there is structure in the data that is not well captured by horizontal or vertical splits
- Since the process deals with one variable at a time, no way to capture interactions between variables

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Improving Trees

- Single trees may not have good predictive ability.
- Results from multiple trees can be combined to improve performance
- The resulting model is an “ensemble” model
- Two multi-tree approaches in JMP Pro:
    - **Bootstrap Forests** (a variant of Random Forests)
    - **Boosted Trees**

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Ensemble Tree Methods

- Bootstrap Forests (Random Forrest)

Grow many trees to bootstrapped versions of the training data and average them

- Boosted Trees (Boosting)

Repeatedly grow shallow trees to the residuals and build up an additive model consisting of a sum of trees

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Ensemble Tree Methods

Bootstrap Forests

1. A random sample is drawn with replacement from the data set (bootstrapping)
2. Predictors are randomly drawn from the candidate list of predictors
3. A small tree is fit (a “weak learner”)
4. The process is repeated
5. The final model is the average of all of the trees, producing a “Bootstrap aggregated” (or “bagged) model

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Ensemble Tree Methods

Boosted Trees

1. A simple (small) tree is fit to the data with a random sample of the predictors
2. The scaled residuals from this tree are calculated
3. A new simple tree is fit to these scaled residuals with another random sample of predictors
4. This process continues
5. The final boosted model is the sum of the models for the individual trees

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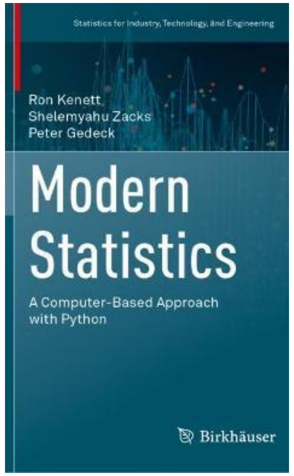


Statistics for Industry, Technology, and Engineering

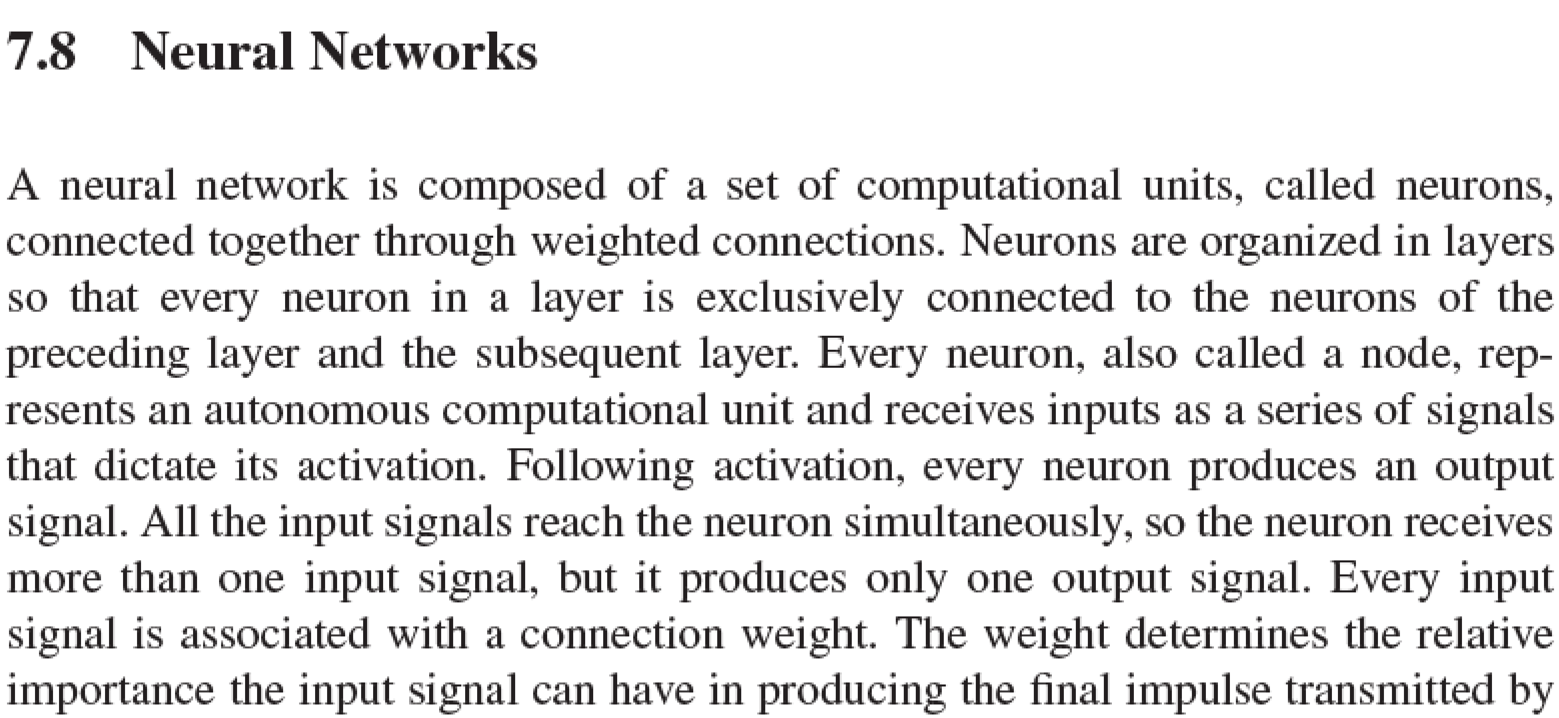
Ron Kenett
Shelemyahu Zacks
Peter Gedeck

Modern Statistics

A Computer-Based Approach with Python

Birkhäuser

Chapter 7
Modern Analytic Methods: Part I



7.8 Neural Networks

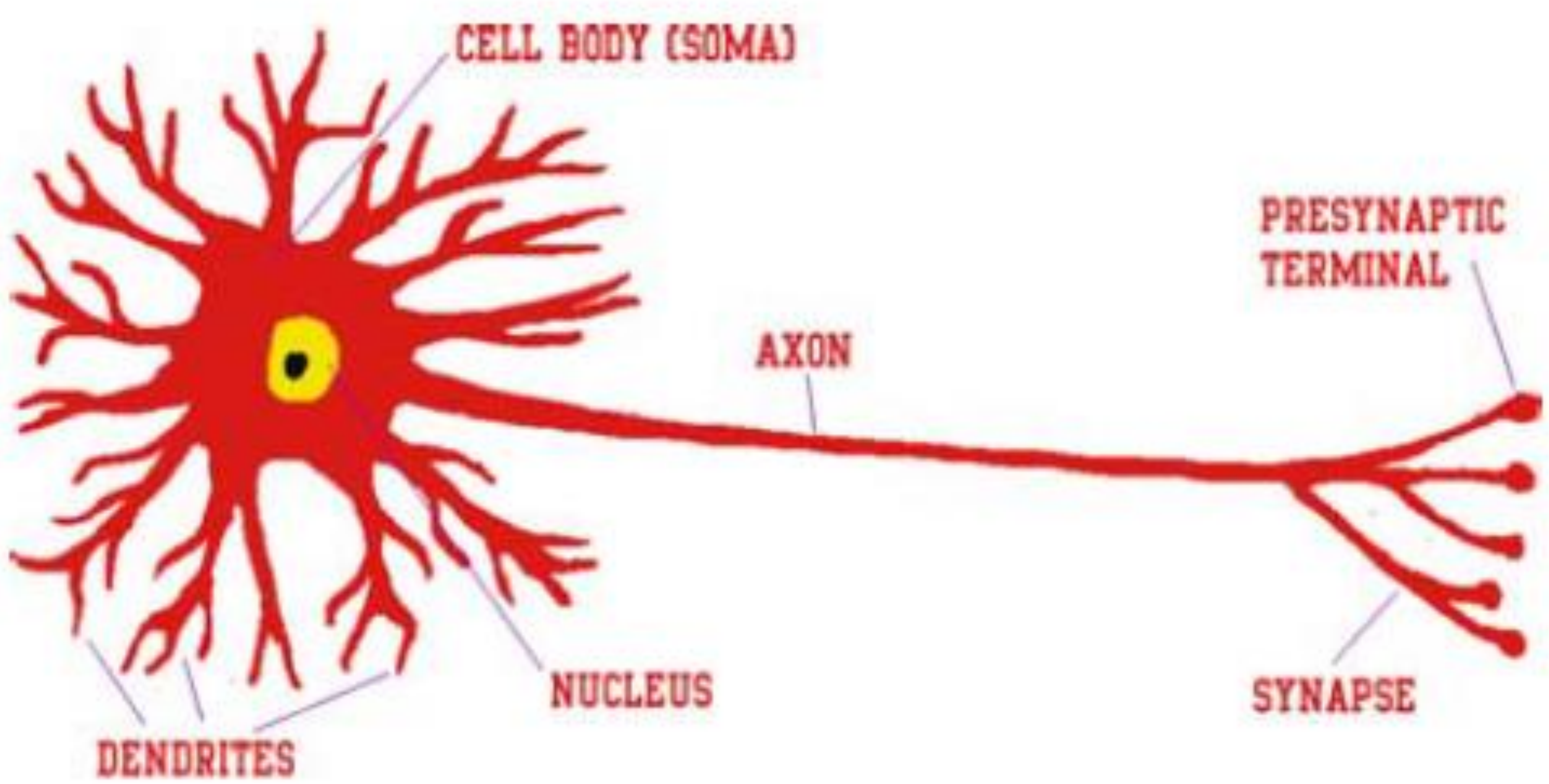
A neural network is composed of a set of computational units, called neurons, connected together through weighted connections. Neurons are organized in layers so that every neuron in a layer is exclusively connected to the neurons of the preceding layer and the subsequent layer. Every neuron, also called a node, represents an autonomous computational unit and receives inputs as a series of signals that dictate its activation. Following activation, every neuron produces an output signal. All the input signals reach the neuron simultaneously, so the neuron receives more than one input signal, but it produces only one output signal. Every input signal is associated with a connection weight. The weight determines the relative importance the input signal can have in producing the final impulse transmitted by

Neural networks: Basic Idea

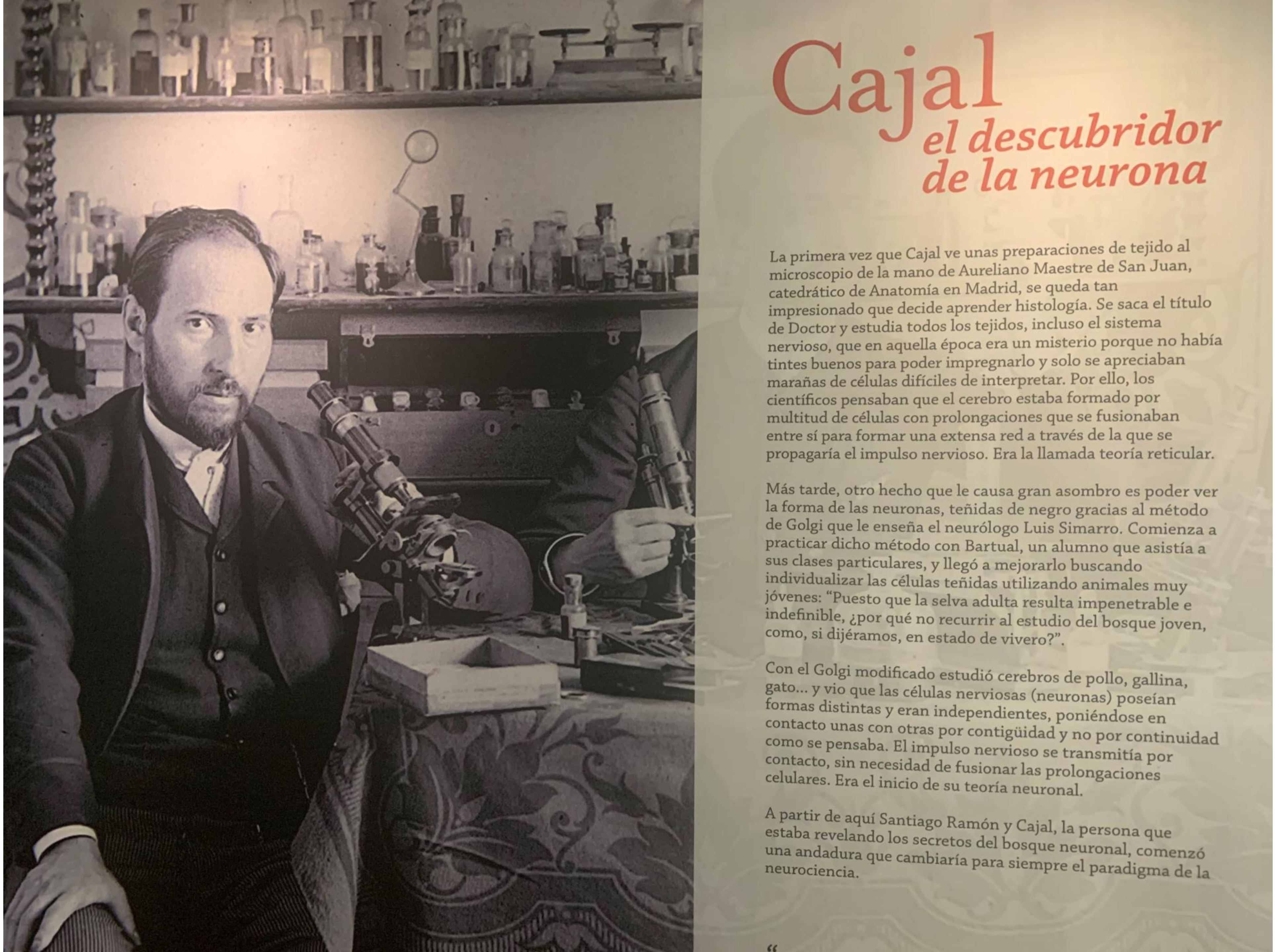
- Combine input information in a complex and flexible neural net “model”
- Model “coefficients” are continually tweaked in an iterative process
- The network’s interim performance in classification and prediction informs successive tweaks

Shmueli, G., Bruce, P., Stephens, M. and Patel, N. (2016) Data Mining for Business Analytics: Concepts, Techniques, and Applications with JMP Pro, Wiley, USA https://www.wiley.com/en-us/Data+Mining+for+Business+Analytics%3A+Concepts%2C+Techniques%2C+and+Applications+with+JMP+Pro-p-9781118877524

Neural Networks



Santiago Ramón y Cajal



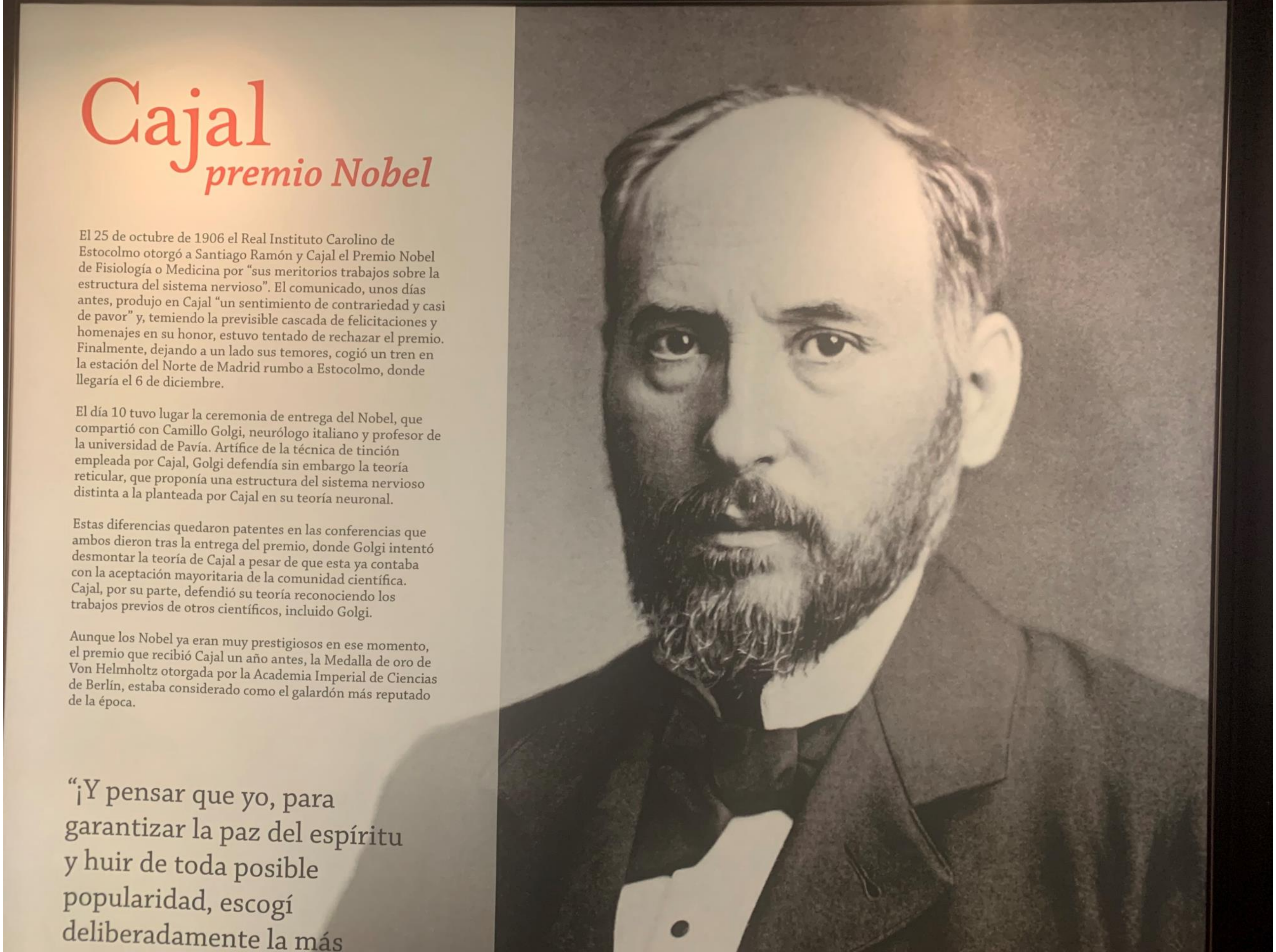
Cajal *el descubridor de la neurona*

La primera vez que Cajal ve unas preparaciones de tejido al microscopio de la mano de Aureliano Maestre de San Juan, catedrático de Anatomía en Madrid, se queda tan impresionado que decide aprender histología. Se saca el título de Doctor y estudia todos los tejidos, incluso el sistema nervioso, que en aquella época era un misterio porque no había tintes buenos para poder impregnarlo y solo se apreciaban marañas de células difíciles de interpretar. Por ello, los científicos pensaban que el cerebro estaba formado por multitud de células con prolongaciones que se fusionaban entre sí para formar una extensa red a través de la que se propagaría el impulso nervioso. Era la llamada teoría reticular.

Más tarde, otro hecho que le causa gran asombro es poder ver la forma de las neuronas, teñidas de negro gracias al método de Golgi que le enseña el neurólogo Luis Simarro. Comienza a practicar dicho método con Bartual, un alumno que asistía a sus clases particulares, y llegó a mejorarlo buscando individualizar las células teñidas utilizando animales muy jóvenes: "Puesto que la selva adulta resulta impenetrable e indefinible, ¿por qué no recurrir al estudio del bosque joven, como, si dijéramos, en estado de vivero?".

Con el Golgi modificado estudió cerebros de pollo, gallina, gato... y vio que las células nerviosas (neuronas) poseían formas distintas y eran independientes, poniéndose en contacto unas con otras por contigüidad y no por continuidad como se pensaba. El impulso nervioso se transmitía por contacto, sin necesidad de fusionar las prolongaciones celulares. Era el inicio de su teoría neuronal.

A partir de aquí Santiago Ramón y Cajal, la persona que estaba revelando los secretos del bosque neuronal, comenzó una andadura que cambiaría para siempre el paradigma de la neurociencia.



Cajal *premio Nobel*

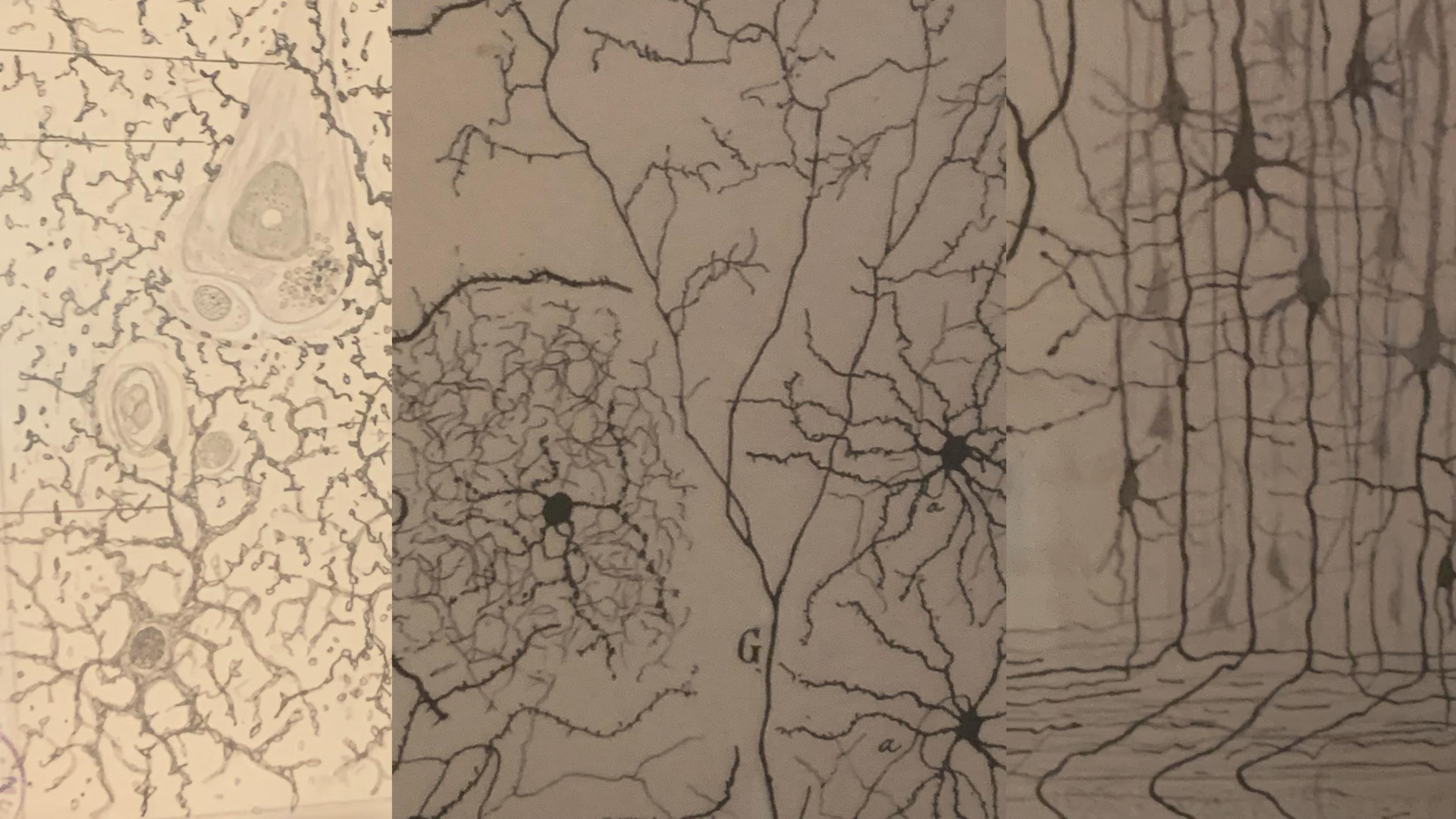
El 25 de octubre de 1906 el Real Instituto Carolino de Estocolmo otorgó a Santiago Ramón y Cajal el Premio Nobel de Fisiología o Medicina por "sus meritorios trabajos sobre la estructura del sistema nervioso". El comunicado, unos días antes, produjo en Cajal "un sentimiento de contrariedad y casi de pavor" y, temiendo la previsible cascada de felicitaciones y homenajes en su honor, estuvo tentado de rechazar el premio. Finalmente, dejando a un lado sus temores, cogió un tren en la estación del Norte de Madrid rumbo a Estocolmo, donde llegaría el 6 de diciembre.

El día 10 tuvo lugar la ceremonia de entrega del Nobel, que compartió con Camillo Golgi, neurólogo italiano y profesor de la universidad de Pavía. Artífice de la técnica de tinción empleada por Cajal, Golgi defendía sin embargo la teoría reticular, que proponía una estructura del sistema nervioso distinta a la planteada por Cajal en su teoría neuronal.

Estas diferencias quedaron patentes en las conferencias que ambos dieron tras la entrega del premio, donde Golgi intentó desmontar la teoría de Cajal a pesar de que esta ya contaba con la aceptación mayoritaria de la comunidad científica. Cajal, por su parte, defendió su teoría reconociendo los trabajos previos de otros científicos, incluido Golgi.

Aunque los Nobel ya eran muy prestigiosos en ese momento, el premio que recibió Cajal un año antes, la Medalla de oro de Von Helmholtz otorgada por la Academia Imperial de Ciencias de Berlín, estaba considerado como el galardón más reputado de la época.

"¡Y pensar que yo, para garantizar la paz del espíritu y huir de toda posible popularidad, escogí deliberadamente la más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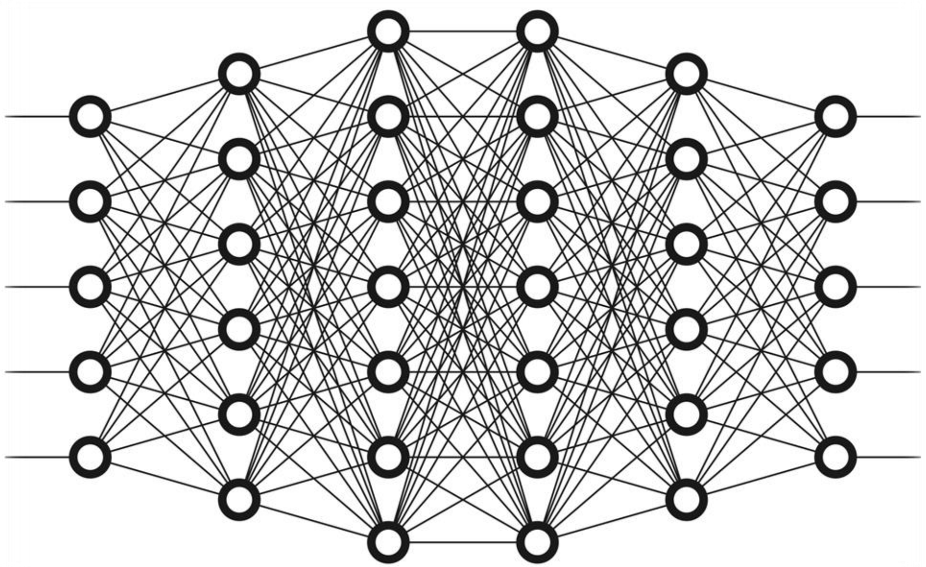
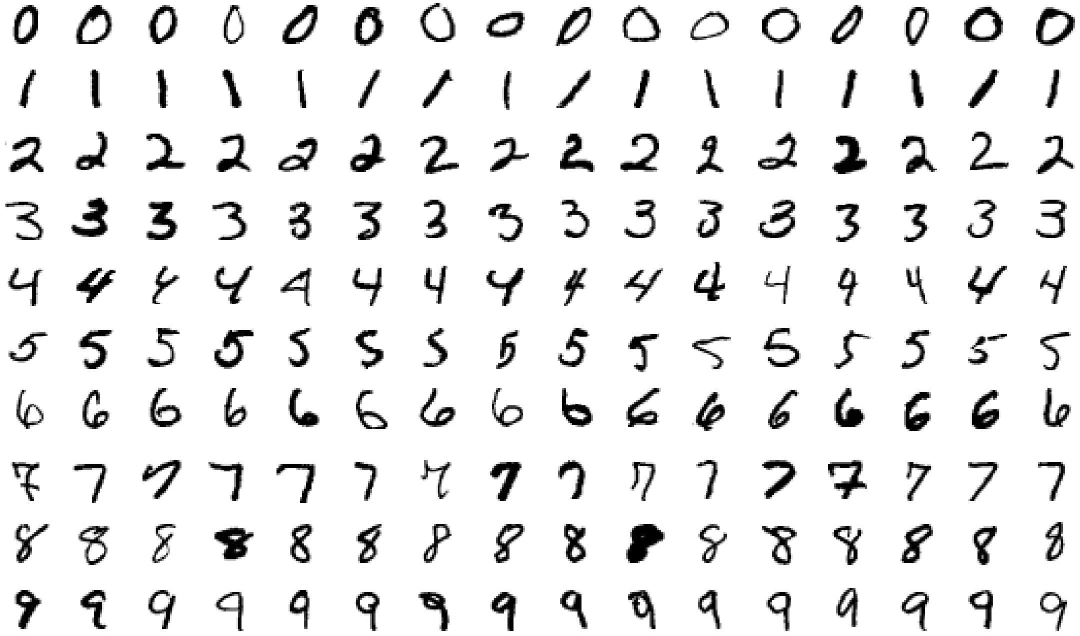
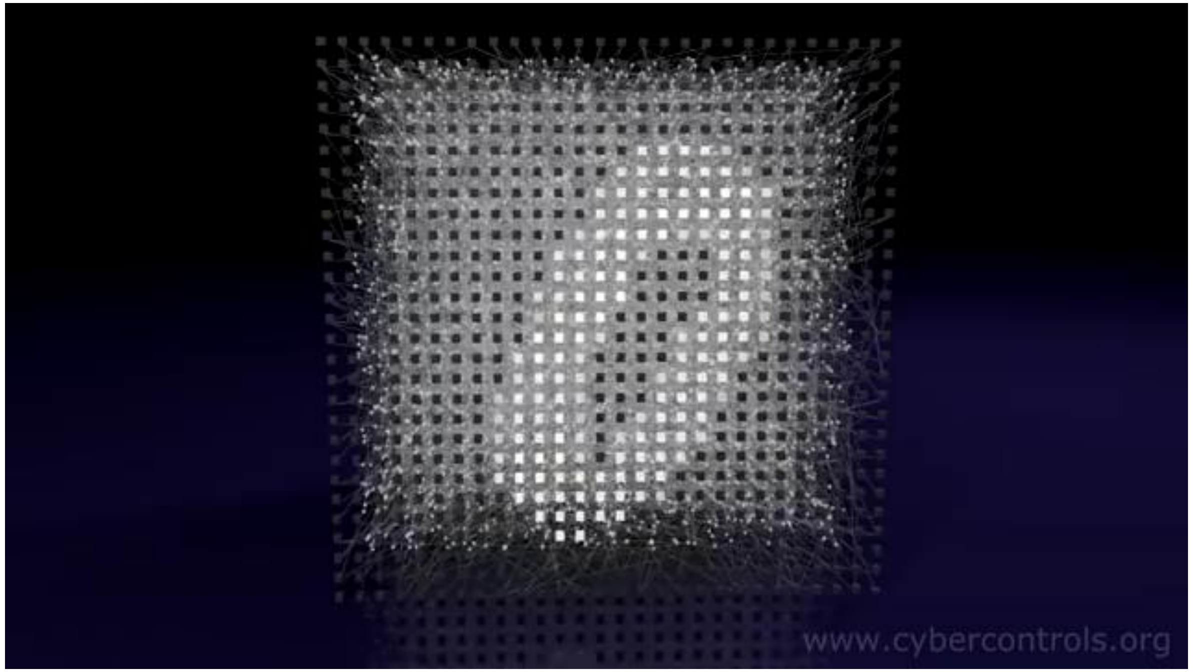
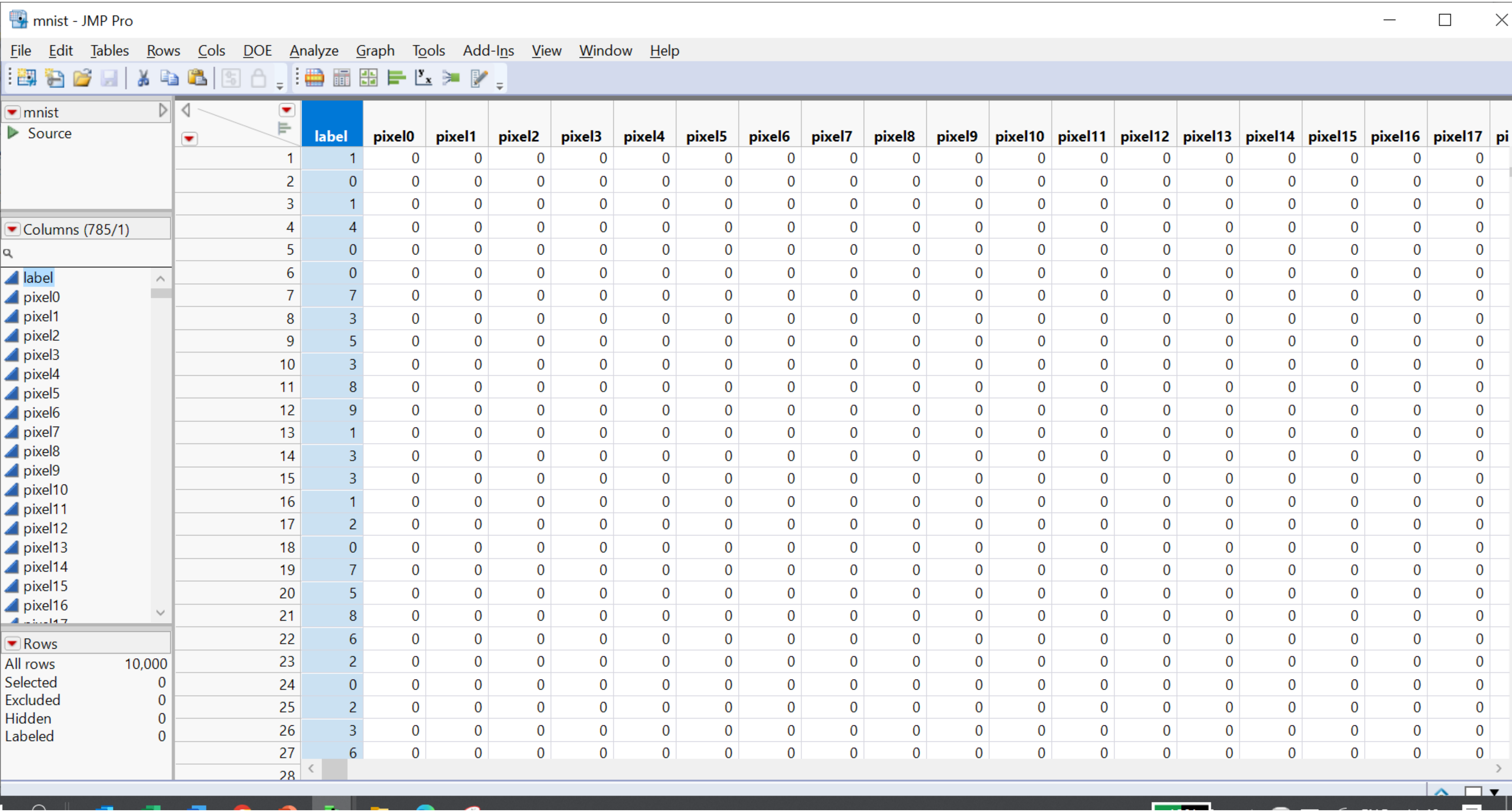


MNIST

Modified **N**ational **I**nstitute of **S**tandards and **T**echnology







mnist

Source

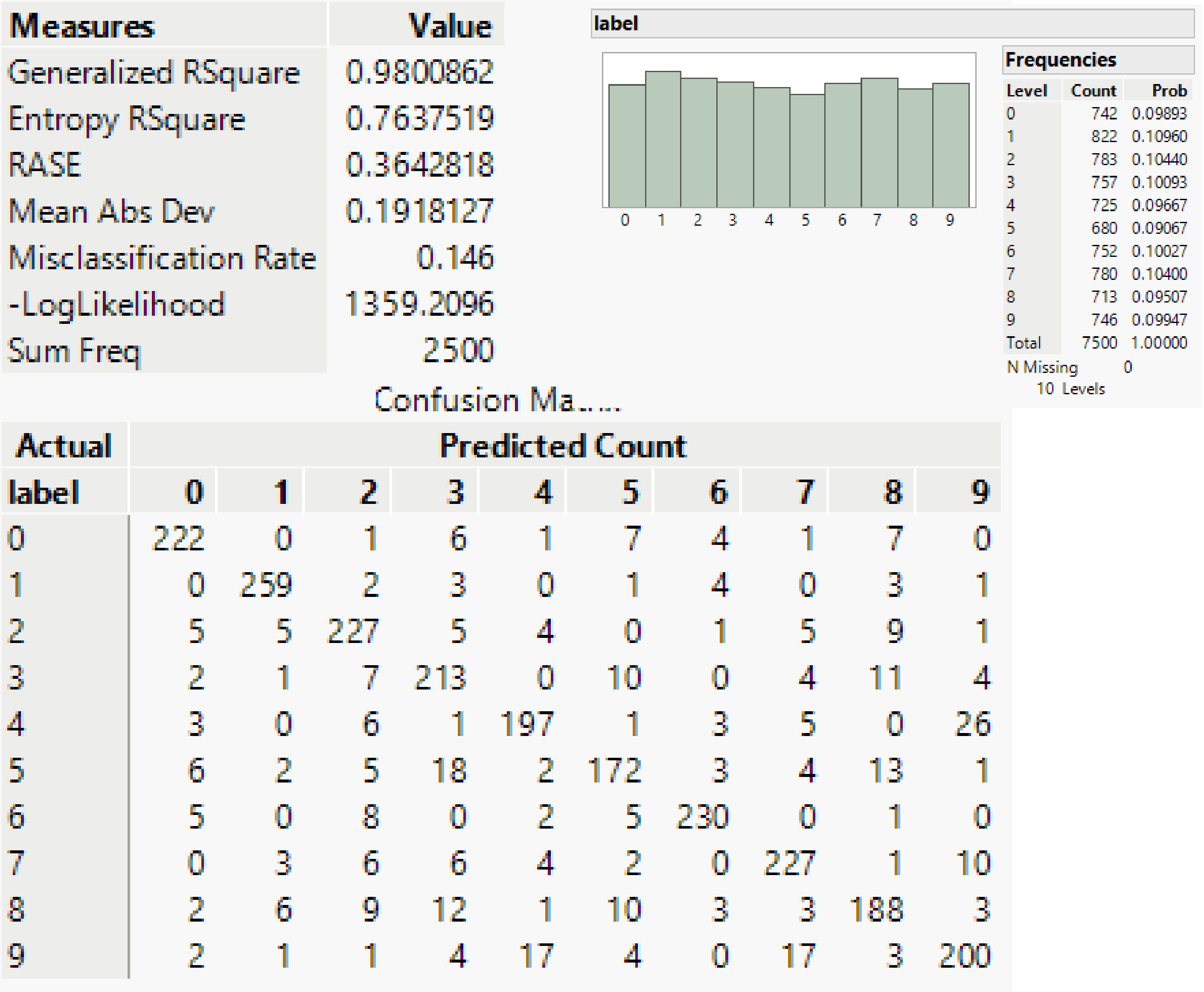
Columns (785/1)

label
pixel0
pixel1
pixel2
pixel3
pixel4
pixel5
pixel6
pixel7
pixel8
pixel9
pixel10
pixel11
pixel12
pixel13
pixel14
pixel15
pixel16

Rows

All rows	10,000
Selected	0
Excluded	0
Hidden	0
Labeled	0

	label	pixel0	pixel1	pixel2	pixel3	pixel4	pixel5	pixel6	pixel7	pixel8	pixel9	pixel10	pixel11	pixel12	pixel13	pixel14	pixel15	pixel16	pixel17	pi
1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
7	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
8	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
9	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
10	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
11	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
12	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
13	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
14	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
15	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
16	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
17	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
19	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
20	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
21	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
22	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
23	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
25	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
26	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
27	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
28																				



Measures	Value
Generalized RSquare	0.9800862
Entropy RSquare	0.7637519
RASE	0.3642818
Mean Abs Dev	0.1918127
Misclassification Rate	0.146
-LogLikelihood	1359.2096
Sum Freq	2500

label

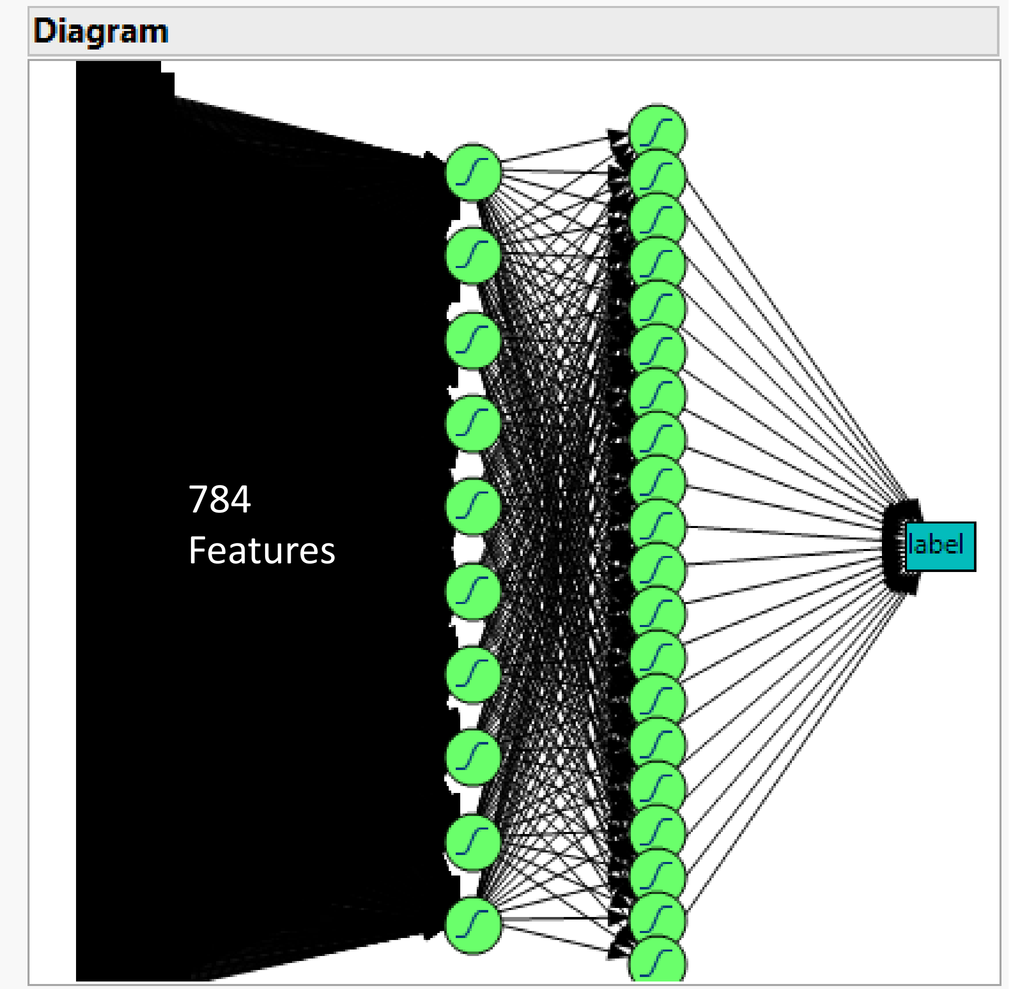
Frequencies

Level	Count	Prob
0	742	0.09893
1	822	0.10960
2	783	0.10440
3	757	0.10093
4	725	0.09667
5	680	0.09067
6	752	0.10027
7	780	0.10400
8	713	0.09507
9	746	0.09947
Total	7500	1.00000

N Missing 0
10 Levels

Confusion Ma.....

Actual	Predicted Count									
label	0	1	2	3	4	5	6	7	8	9
0	222	0	1	6	1	7	4	1	7	0
1	0	259	2	3	0	1	4	0	3	1
2	5	5	227	5	4	0	1	5	9	1
3	2	1	7	213	0	10	0	4	11	4
4	3	0	6	1	197	1	3	5	0	26
5	6	2	5	18	2	172	3	4	13	1
6	5	0	8	0	2	5	230	0	1	0
7	0	3	6	6	4	2	0	227	1	10
8	2	6	9	12	1	10	3	3	188	3
9	2	1	1	4	17	4	0	17	3	200

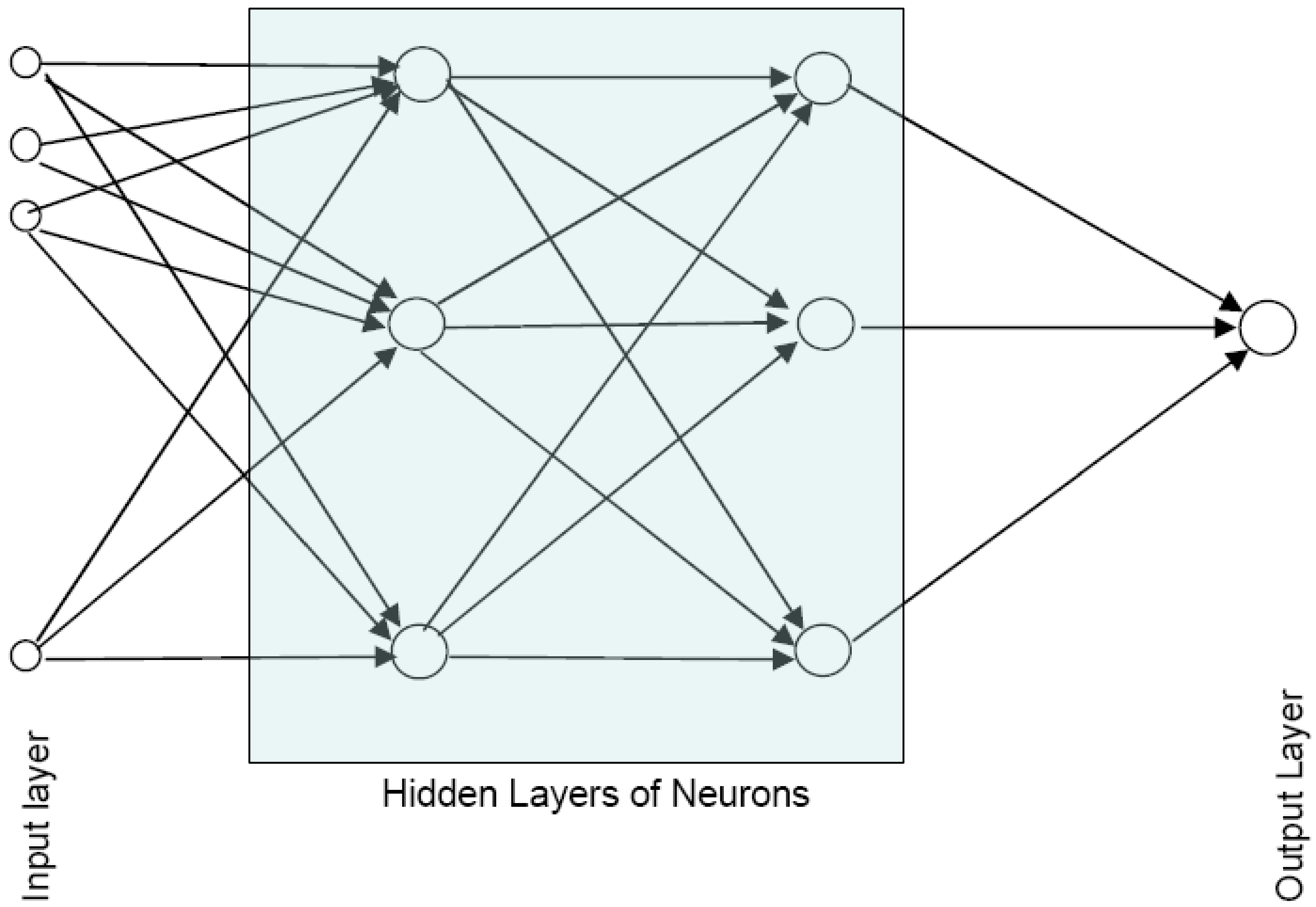


Diagram

Network Structure

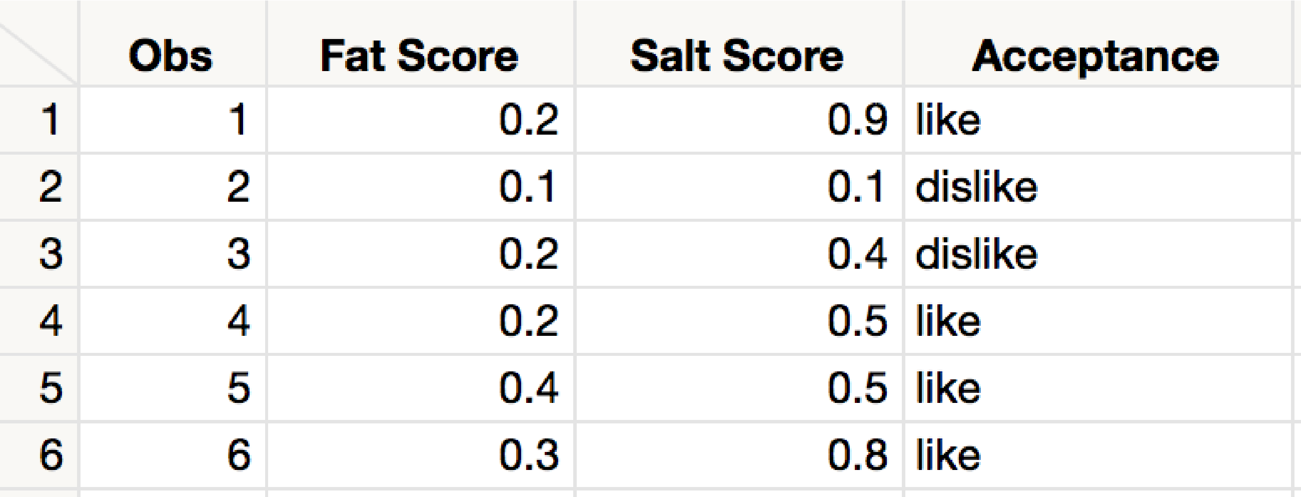
- Multiple layers
  - Input layer (raw observations)
  - Hidden layers
  - Output layer
- Nodes
- Weights (like coefficients, subject to iterative adjustment)
- Bias values (also like coefficients, but not subject to iterative adjustment)

Schematic Diagram



Tiny Example

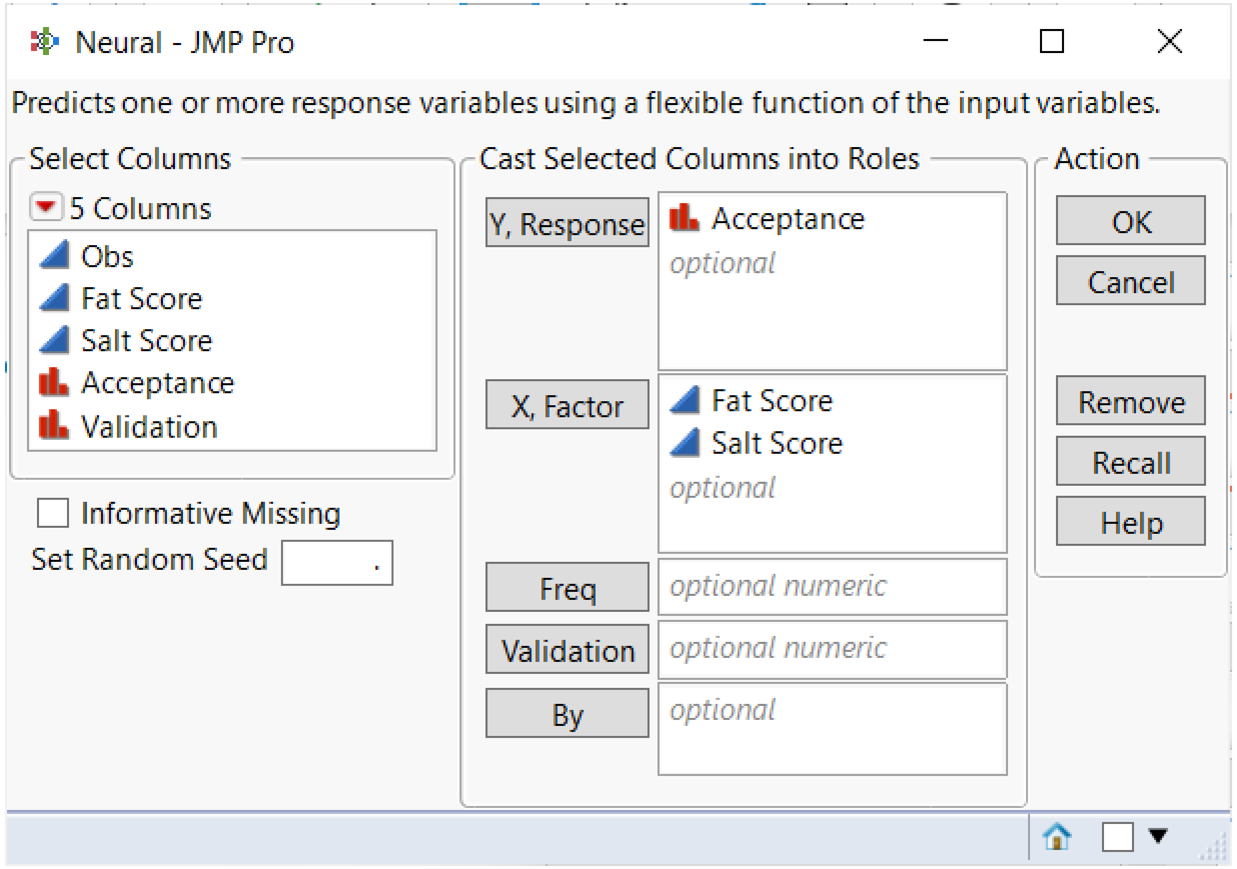
- Using fat and salt content to predict consumer acceptance of cheese



	Obs	Fat Score	Salt Score	Acceptance
1	1	0.2	0.9	like
2	2	0.1	0.1	dislike
3	3	0.2	0.4	dislike
4	4	0.2	0.5	like
5	5	0.4	0.5	like
6	6	0.3	0.8	like

Shmueli, G., Bruce, P., Stephens, M. and Patel, N. (2016) Data Mining for Business Analytics: Concepts, Techniques, and Applications with JMP Pro, Wiley, USA https://www.wiley.com/en-us/Data+Mining+for+Business+Analytics%3A+Concepts%2C+Techniques%2C+and+Applications+with+JMP+Pro-p-9781118877524

Tiny Example Neural Network



Neural - JMP Pro

Predicts one or more response variables using a flexible function of the input variables.

Select Columns

5 Columns

- Obs
- Fat Score
- Salt Score
- Acceptance
- Validation

□ Informative Missing

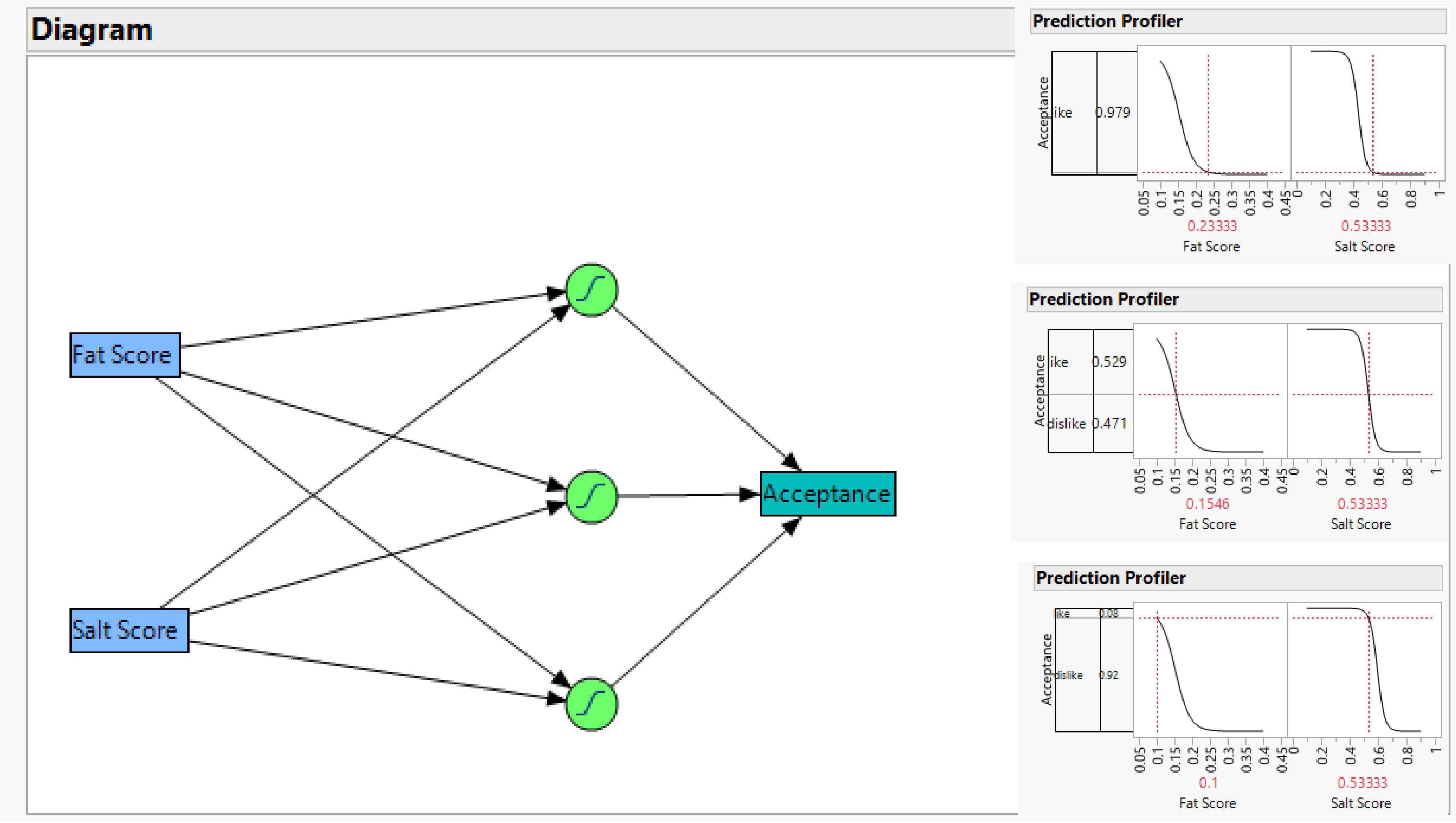
Set Random Seed .

Cast Selected Columns into Roles

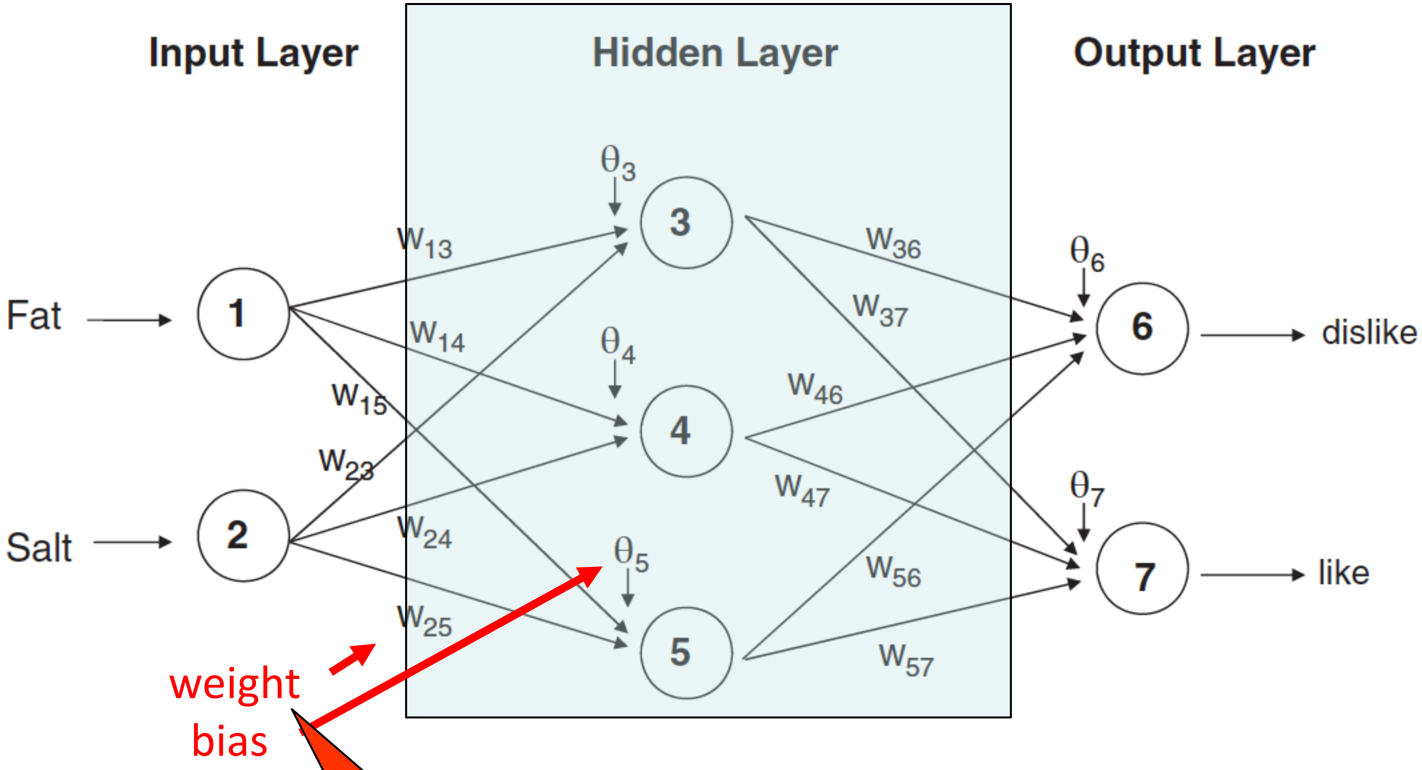
Y, Response: Acceptance

X, Factor: Fat Score, Salt Score

Tiny Example Neural Network



Tiny Example Neural Network



Initially set as ±0.005

The Input Layer

For input layer, input = output

E.g., for record #1:

Fat input = output = 0.2

Salt input = output = 0.9

Output of input layer = input into hidden layer

The Hidden Layer

In this example, hidden layer has 3 nodes

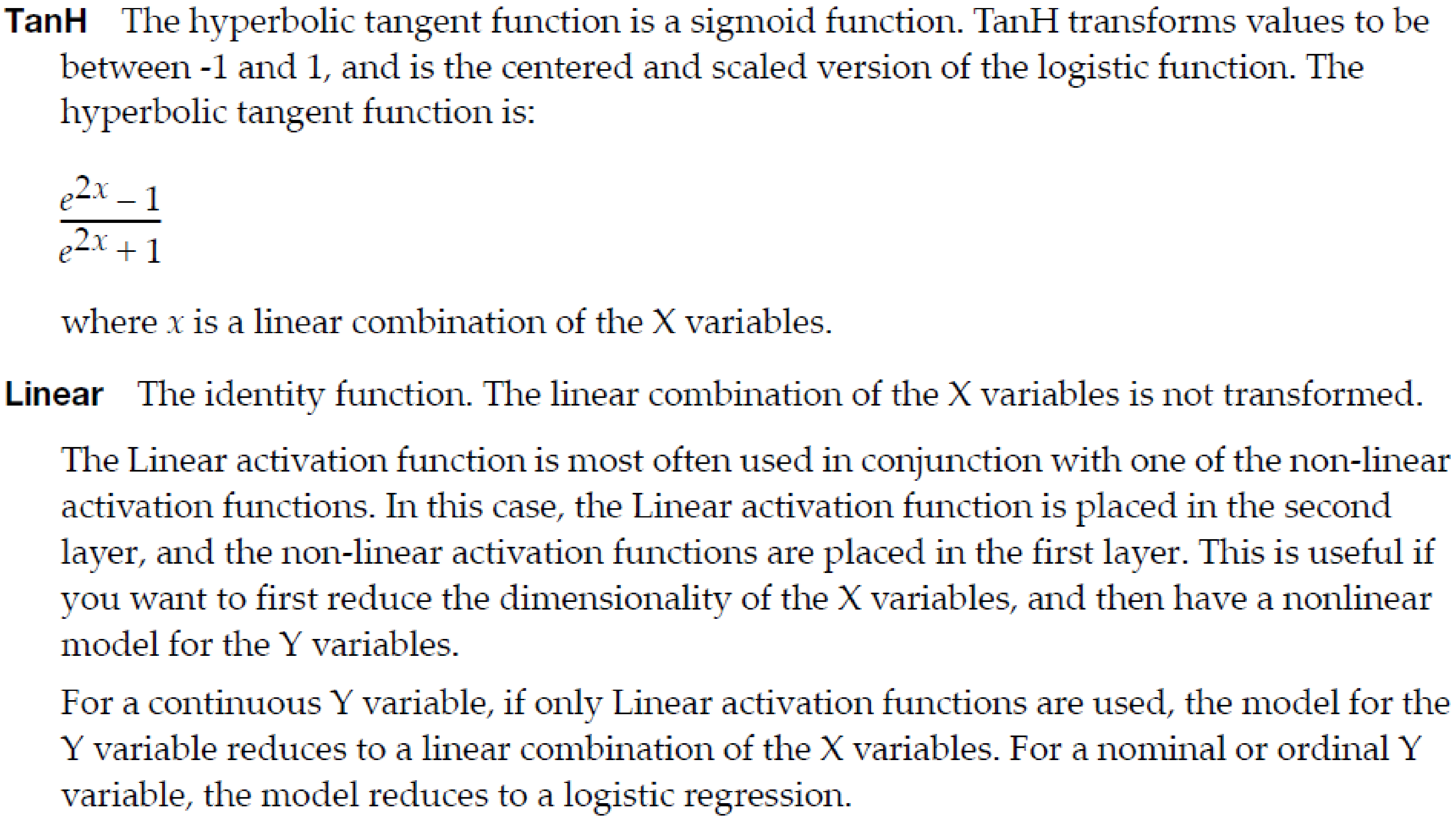
Each node receives as input the output of all input nodes

Output of each hidden node is a function of the weighted sum of inputs

$$output_j = g(\Theta_j + \sum_{i=1}^{p} w_{ij}\, x_i)$$

(The hidden layer function is also called an ”activation function”.)

The Hidden Layer



TanH The hyperbolic tangent function is a sigmoid function. TanH transforms values to be between -1 and 1, and is the centered and scaled version of the logistic function. The hyperbolic tangent function is:

$$\frac{e^{2x}-1}{e^{2x}+1}$$

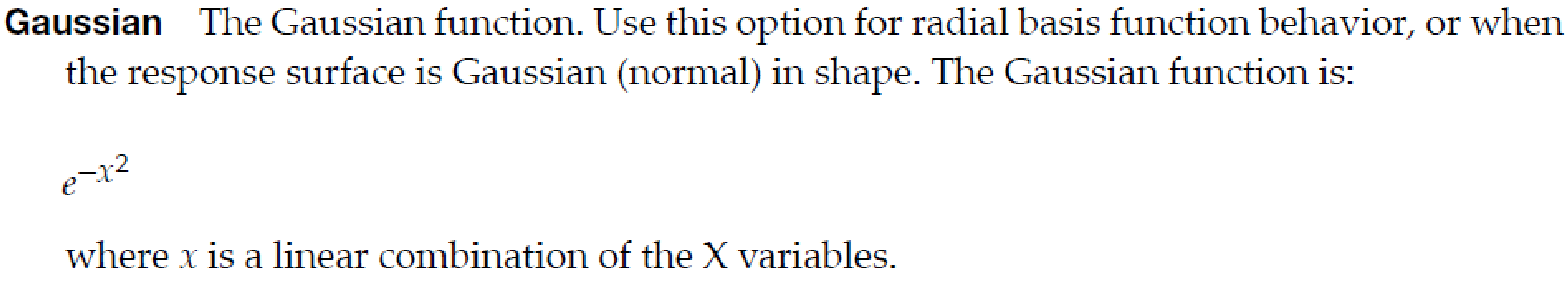
where x is a linear combination of the X variables.

Linear The identity function. The linear combination of the X variables is not transformed.

The Linear activation function is most often used in conjunction with one of the non-linear activation functions. In this case, the Linear activation function is placed in the second layer, and the non-linear activation functions are placed in the first layer. This is useful if you want to first reduce the dimensionality of the X variables, and then have a nonlinear model for the Y variables.

For a continuous Y variable, if only Linear activation functions are used, the model for the Y variable reduces to a linear combination of the X variables. For a nominal or ordinal Y variable, the model reduces to a logistic regression.

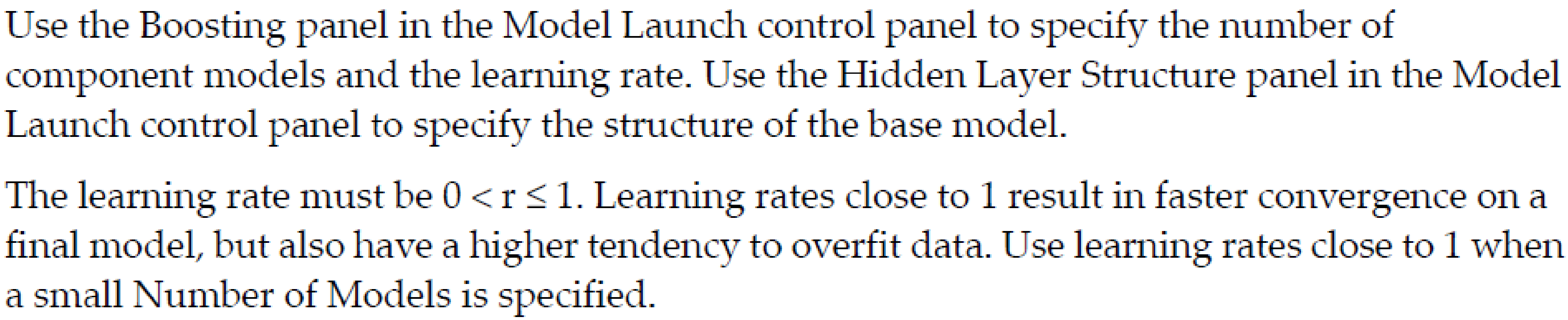
The Hidden Layer



Gaussian The Gaussian function. Use this option for radial basis function behavior, or when the response surface is Gaussian (normal) in shape. The Gaussian function is:

$$e^{-x^2}$$

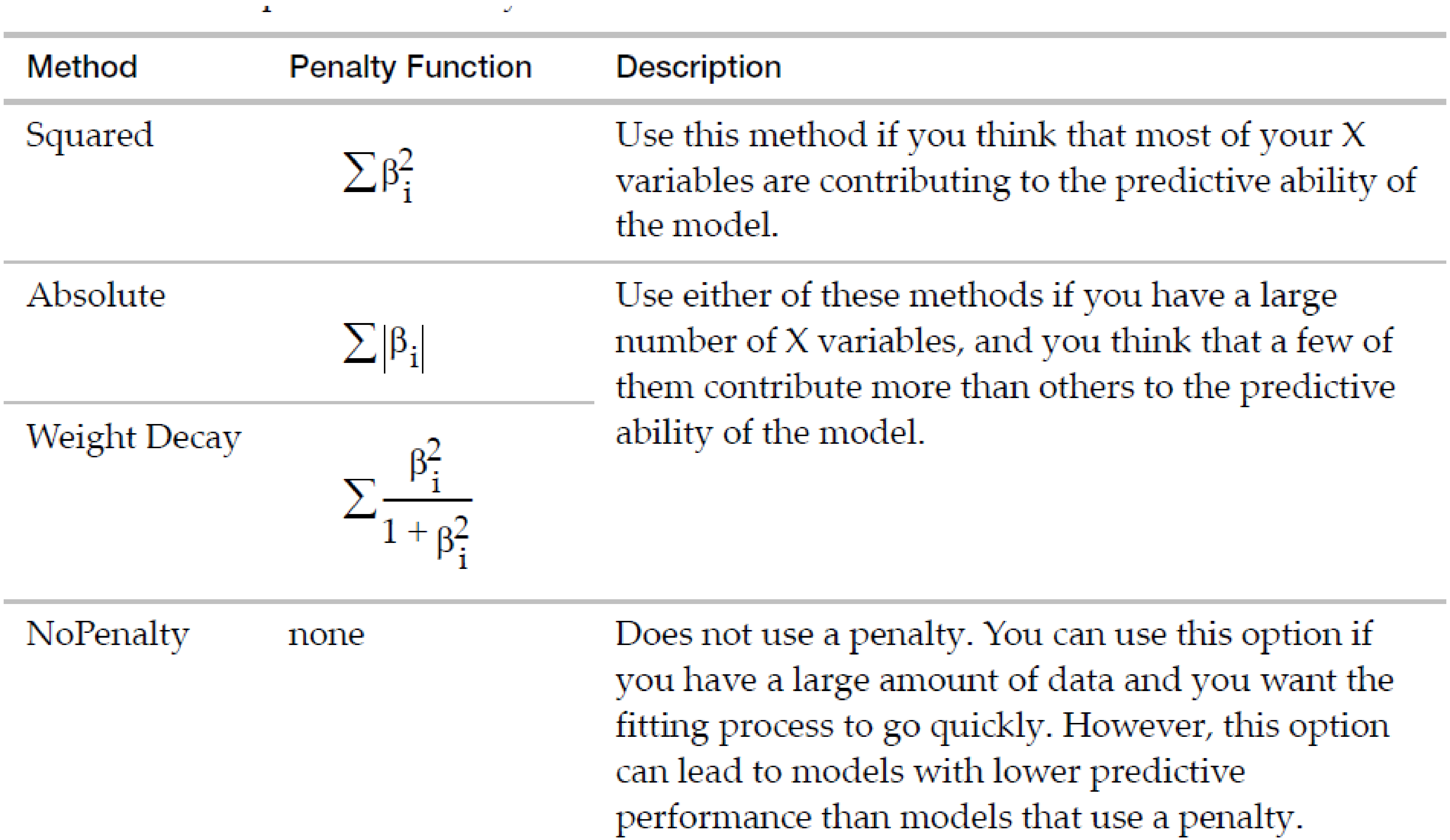
where x is a linear combination of the X variables.



Use the Boosting panel in the Model Launch control panel to specify the number of component models and the learning rate. Use the Hidden Layer Structure panel in the Model Launch control panel to specify the structure of the base model.

The learning rate must be $0 < r \leq 1$. Learning rates close to 1 result in faster convergence on a final model, but also have a higher tendency to overfit data. Use learning rates close to 1 when a small Number of Models is specified.

Options



Method	Penalty Function	Description
Squared	$\sum \beta_i^2$	Use this method if you think that most of your X variables are contributing to the predictive ability of the model.
Absolute	$\sum \lvert\beta_i\rvert$	Use either of these methods if you have a large number of X variables, and you think that a few of them contribute more than others to the predictive ability of the model.
Weight Decay	$\sum \frac{\beta_i^2}{1 + \beta_i^2}$	
NoPenalty	none	Does not use a penalty. You can use this option if you have a large amount of data and you want the fitting process to go quickly. However, this option can lead to models with lower predictive performance than models that use a penalty.

The Weights

The weights θ (theta) and *w* are typically initialized to random values in the range -0.05 to +0.05

- ➢JMP uses random normal starting weights

Equivalent to a model with random prediction (in other words, no predictive value)

These initial weights are used in the first round of training

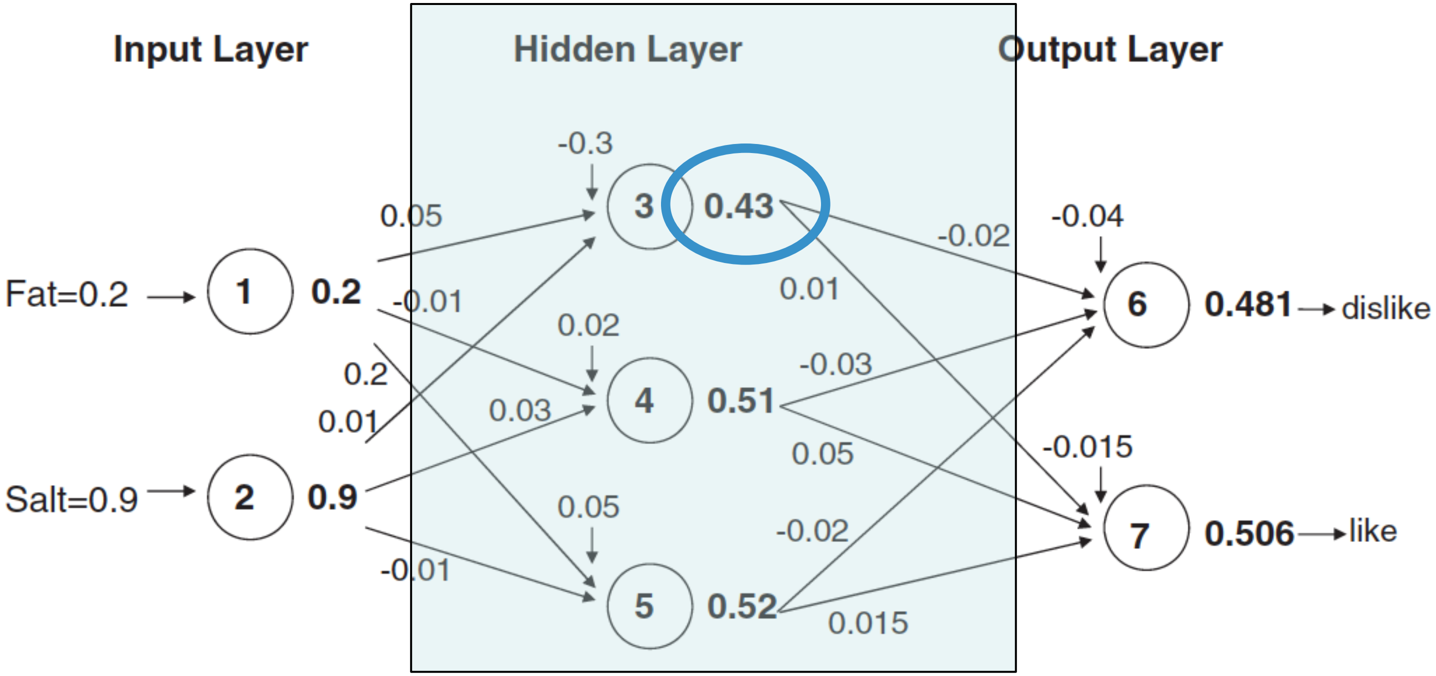
Output of Node 3, if *g* is a Logistic Function

$$output_j = g(\Theta_j + \sum_{i=1}^{p} w_{ij}\, x_i)$$

$$\text{Output}_j = g\left(\theta_j + \sum_{i=1}^{p} w_{ij}x_i\right) = \frac{1}{1+e^{-(\theta_j+\sum_{i=1}^{p} w_{ij}x_i)}}.$$

$$output_3 = \frac{1}{1+e^{-[-0.3+(0.05)(0.2)+(0.01)(0.9)]}} = \boxed{0.43}$$

Tiny Example Neural Weights



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Output Layer

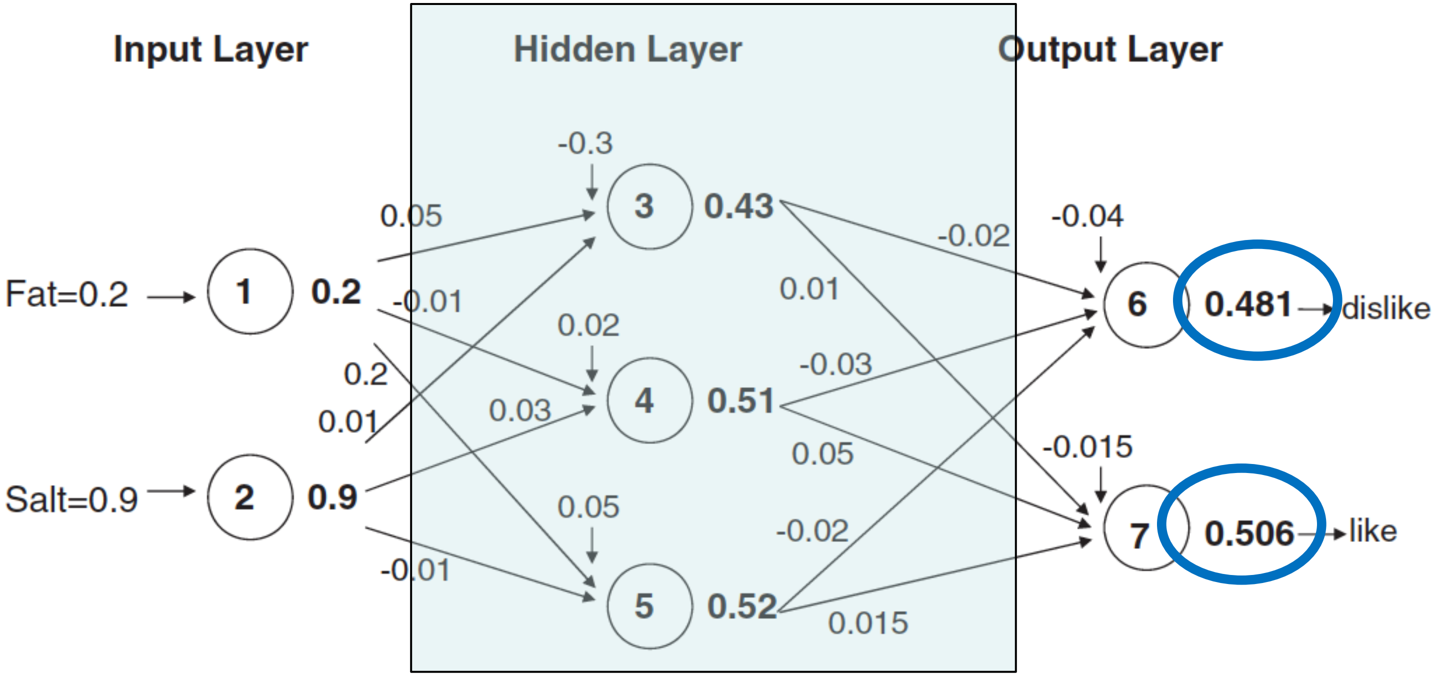
The output of the last hidden layer becomes input for the output layer

Uses same function as above, i.e. a function *g* of the weighted average

$$\text{Output}_6 = \frac{1}{1 + e^{-[-0.04+(-0.02)(0.43)+(-0.03)(0.51)+(0.015)(0.52)]}} = 0.481$$

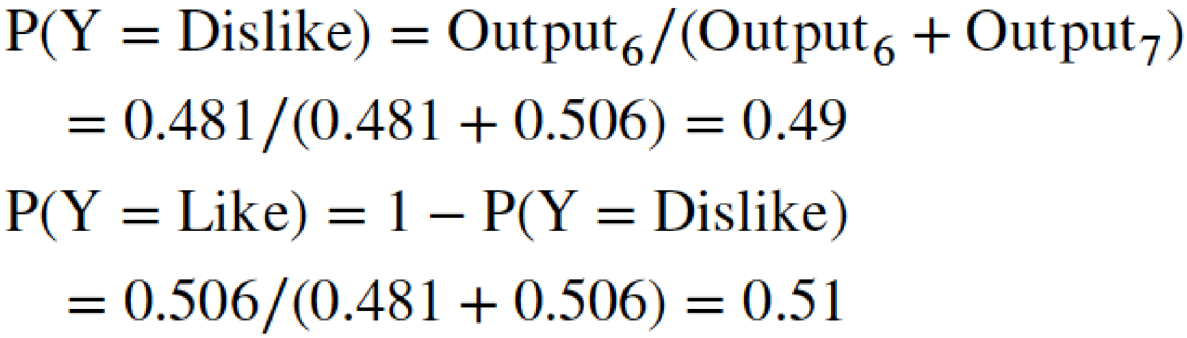
$$\text{Output}_7 = \frac{1}{1 + e^{-[-0.015+(0.01)(0.430)+(0.05)(0.507)+(0.015)(0.511)]}} = 0.506$$

Tiny Example Output Layer



Mapping the output to a classification

These values are normalized so they are propensities (which add up to 1.0).



$$\begin{aligned}
\mathrm{P}(\mathrm{Y} = \mathrm{Dislike}) &= \mathrm{Output}_6/(\mathrm{Output}_6 + \mathrm{Output}_7)\\
&= 0.481/(0.481 + 0.506) = 0.49\\
\mathrm{P}(\mathrm{Y} = \mathrm{Like}) &= 1 - \mathrm{P}(\mathrm{Y} = \mathrm{Dislike})\\
&= 0.506/(0.481 + 0.506) = 0.51
\end{aligned}$$

The default cutoff for classification is 0.5.

This first record would be classified as a Like.

Relation to Linear Regression

A net with a single output node and no hidden layers, where *g* is the identity function, takes the same form as a linear regression model

$$\hat{y} = \Theta + \sum_{\mathrm{i}=1}^{\mathrm{p}} \mathrm{w_i}\,\mathrm{x_i}$$

Initial Pass-Through Network

Goal: Find weights that yield best predictions

- The process we described above is repeated for all records
- At each record, compare prediction to actual
- Difference is the error for the output node
- Error is propagated back and distributed to all the hidden nodes and used to update their weights

Training the Model

Back Propagation of Error

- Output from output node k: $\hat{y}_k$
- Error associated with that node:

$$err_k = \boxed{\hat{y}_k(1 - \hat{y}_k)}(y_{k-}\hat{y}_k)$$

Note: this is like ordinary error, multiplied by a correction factor

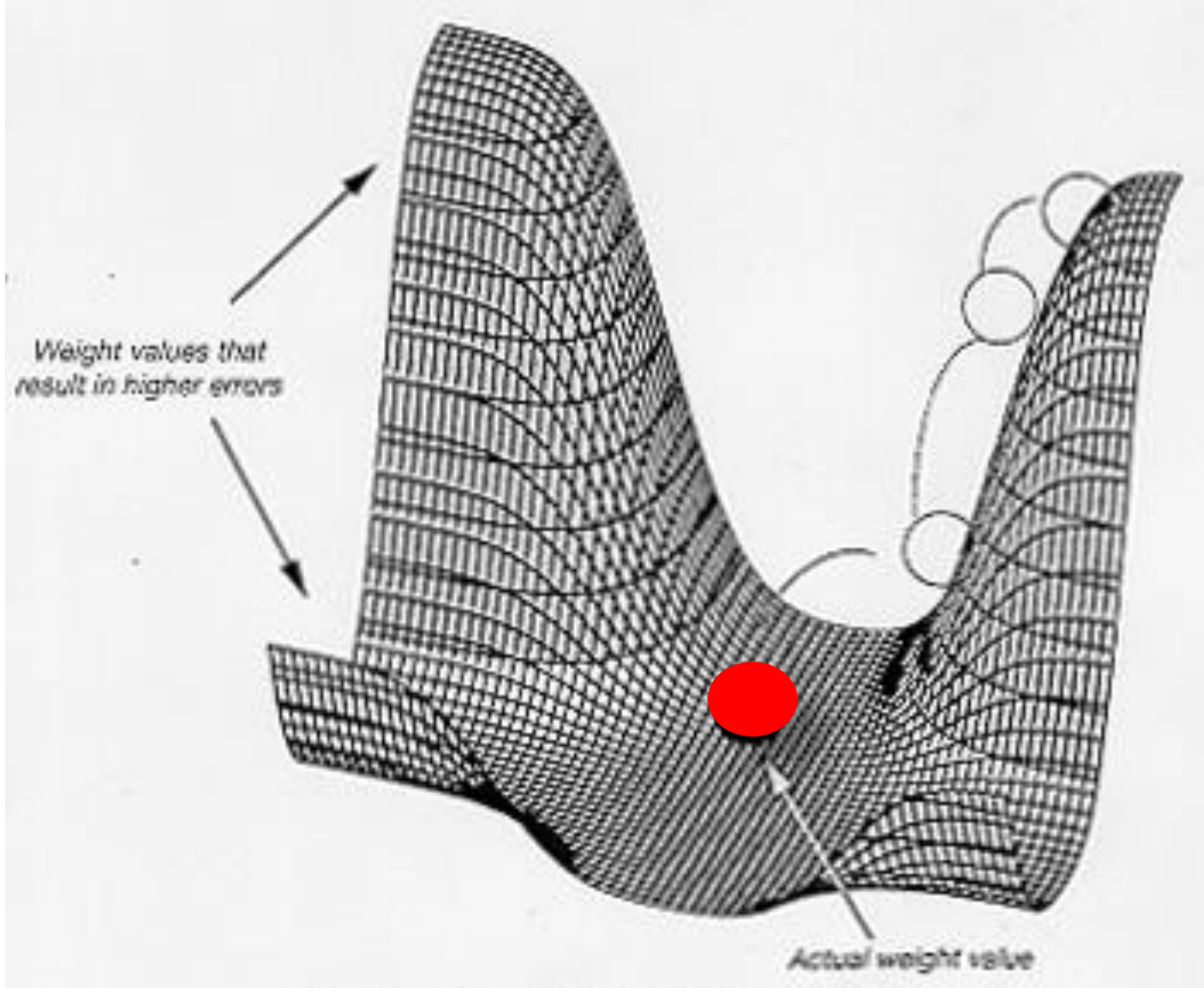
Error is Used to Update Weights

$$\theta_j^{new} = \theta_j^{old} + l\left(err_j\right)$$

$$\mathrm{w}_j^{new} = w_j^{old} + l(err_j)$$

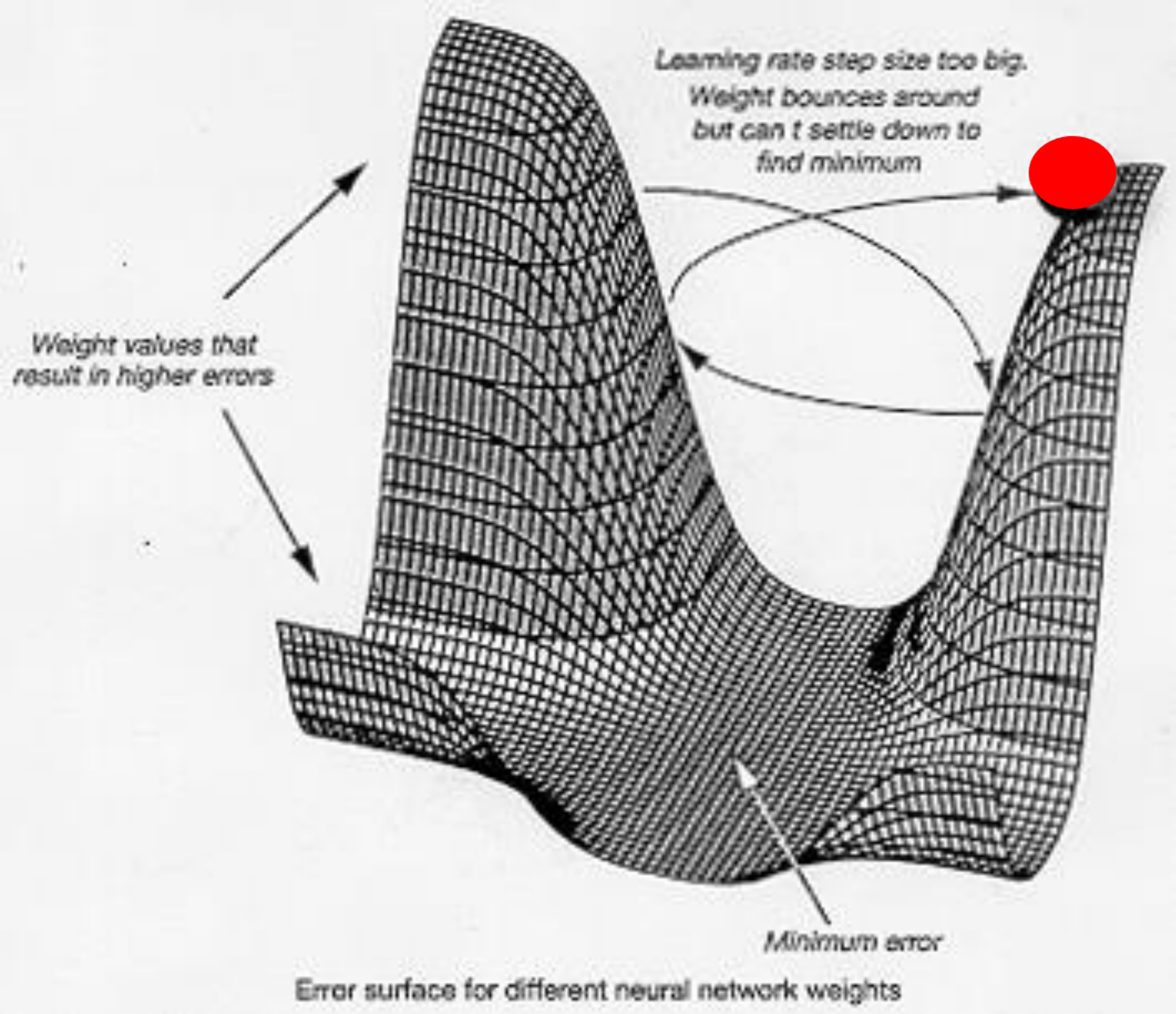
l = constant between 0 and 1, reflects the “learning rate” or “weight decay parameter”

Error is Used to Update Weights



Error surface for different neural network weights

Error is Used to Update Weights

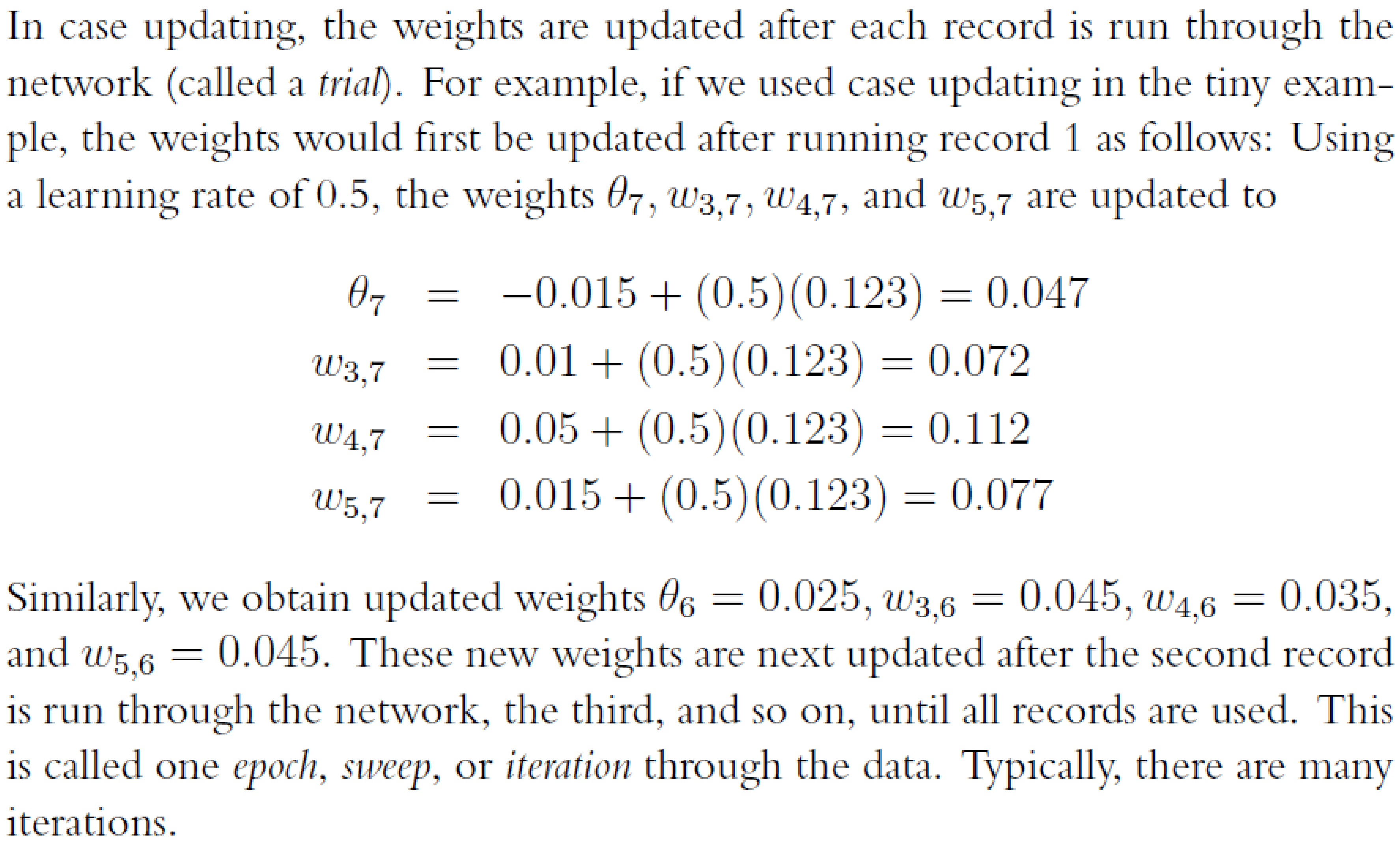


Error surface for different neural network weights

Case Updating

- Weights are updated after each record is run through the network
- Completion of all records through the network is one *epoch* (also called *sweep* or *iteration*)
- After one epoch is completed, return to first record and repeat the process

Case Updating



In case updating, the weights are updated after each record is run through the network (called a *trial*). For example, if we used case updating in the tiny example, the weights would first be updated after running record 1 as follows: Using a learning rate of 0.5, the weights $\theta_7, w_{3,7}, w_{4,7}$, and $w_{5,7}$ are updated to

$$\begin{aligned} \theta_7 &= -0.015 + (0.5)(0.123) = 0.047 \\ w_{3,7} &= 0.01 + (0.5)(0.123) = 0.072 \\ w_{4,7} &= 0.05 + (0.5)(0.123) = 0.112 \\ w_{5,7} &= 0.015 + (0.5)(0.123) = 0.077 \end{aligned}$$

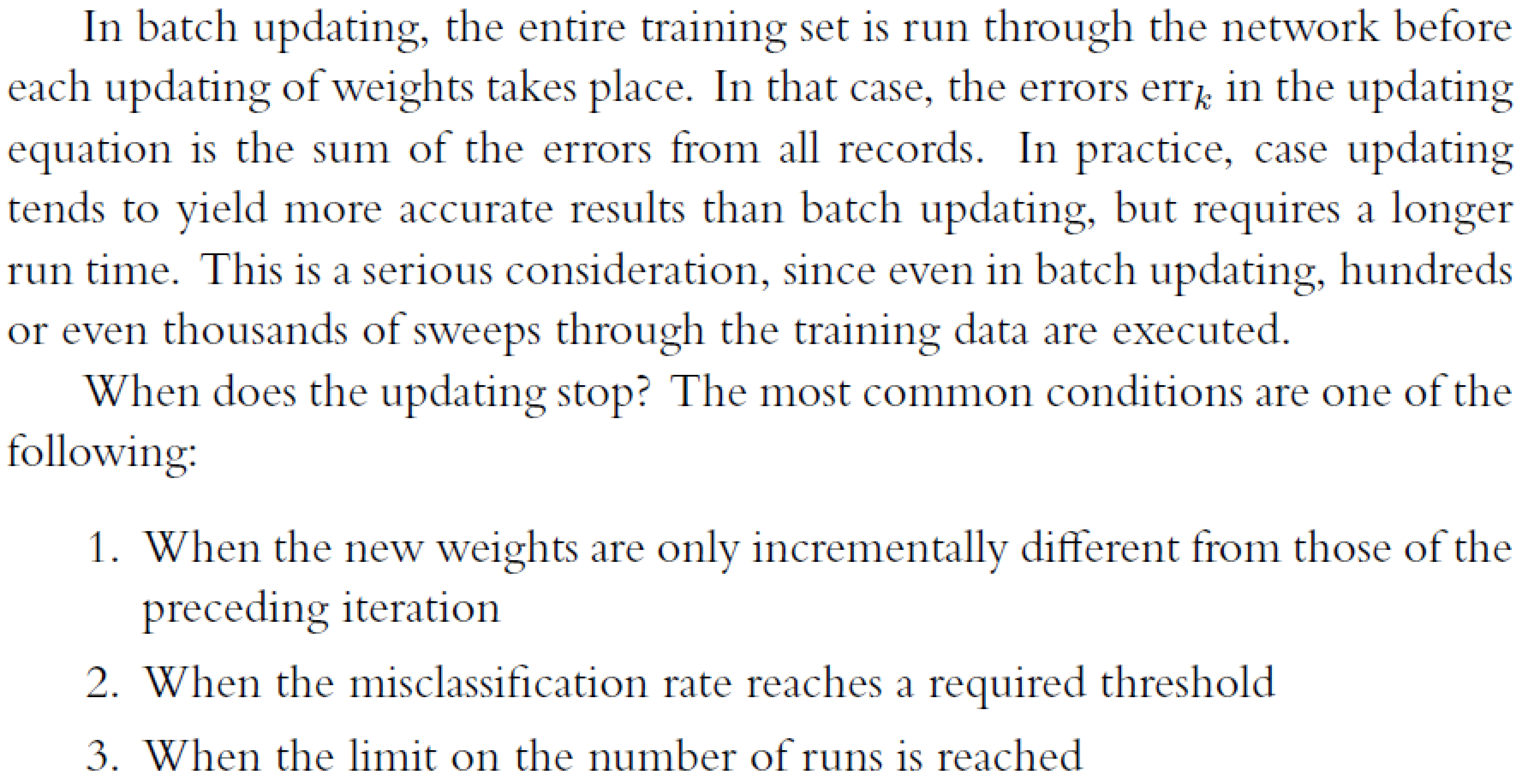
Similarly, we obtain updated weights $\theta_6 = 0.025$, $w_{3,6} = 0.045$, $w_{4,6} = 0.035$, and $w_{5,6} = 0.045$. These new weights are next updated after the second record is run through the network, the third, and so on, until all records are used. This is called one *epoch*, *sweep*, or *iteration* through the data. Typically, there are many iterations.

Batch Updating

- All records in the training set are fed to the network before updating takes place

- In this case, the error used for updating is the sum of all errors from all records

Batch Updating



In batch updating, the entire training set is run through the network before each updating of weights takes place. In that case, the errors err_k in the updating equation is the sum of the errors from all records. In practice, case updating tends to yield more accurate results than batch updating, but requires a longer run time. This is a serious consideration, since even in batch updating, hundreds or even thousands of sweeps through the training data are executed.

When does the updating stop? The most common conditions are one of the following:

1. When the new weights are only incrementally different from those of the preceding iteration
2. When the misclassification rate reaches a required threshold
3. When the limit on the number of runs is reached

Why It Works

- Big errors lead to big changes in weights

- Small errors leave weights relatively unchanged

- Over thousands of updates, a given weight keeps changing until the error associated with that weight is negligible, at which point weights change little

Common Criteria to Stop the Updating

- When weights change very little from one iteration to the next
- When the misclassification rate reaches a required threshold
- When a limit on runs is reached

Neural Model fitting

- One uses an algorithm that finds optimal values of weights and bias values that minimize a function of the combined errors (maximum likelihood)
- This approach produces similar results to back propagation, but
  - ➢Its generally much faster
  - ➢It can be used for both continuous and categorical responses

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Neural Model fitting

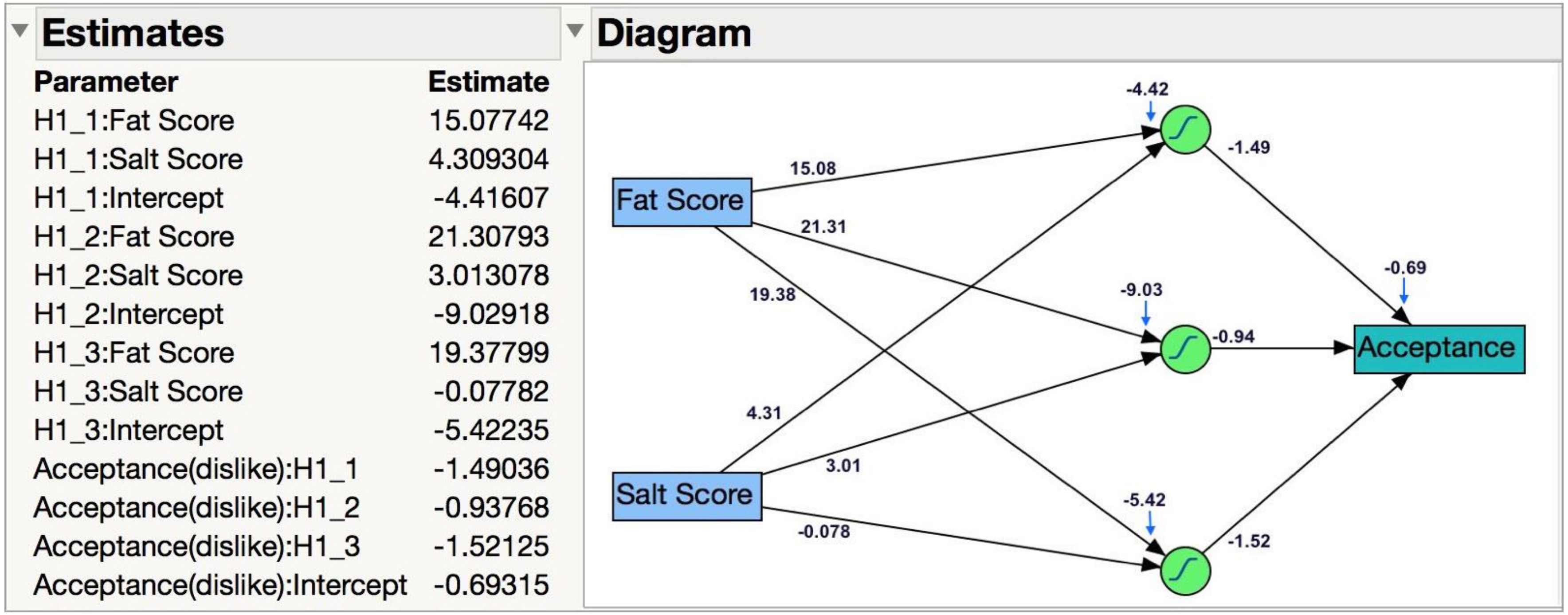
Neural models tend to overfit the data.

To avoid overfitting, one uses a **penalty parameter** and requires **crossvalidation**

The JMP Neural fitting process:

1. Set the penalty to 0
2. Use random normal weights for the starting values
3. Vary the penalty parameter
4. For each value of the penalty parameter, search for weights that minimize error
5. Select the model with the lowest crossvalidation error

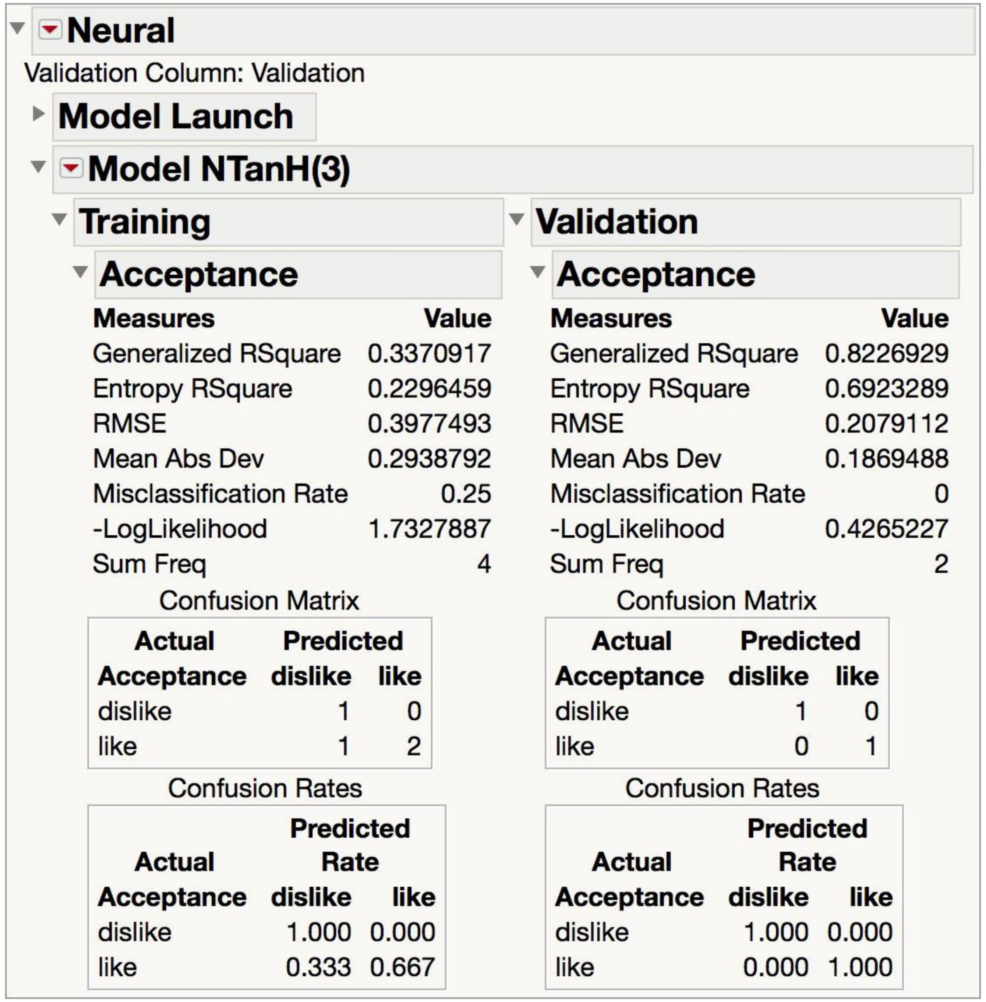
Tiny Example: Final Weights



Estimates

Parameter	Estimate
H1_1:Fat Score	15.07742
H1_1:Salt Score	4.309304
H1_1:Intercept	-4.41607
H1_2:Fat Score	21.30793
H1_2:Salt Score	3.013078
H1_2:Intercept	-9.02918
H1_3:Fat Score	19.37799
H1_3:Salt Score	-0.07782
H1_3:Intercept	-5.42235
Acceptance(dislike):H1_1	-1.49036
Acceptance(dislike):H1_2	-0.93768
Acceptance(dislike):H1_3	-1.52125
Acceptance(dislike):Intercept	-0.69315

Tiny Example: Fit Statistics



Validation Column: Validation

Training

Acceptance

Measures	Value
Generalized RSquare	0.3370917
Entropy RSquare	0.2296459
RMSE	0.3977493
Mean Abs Dev	0.2938792
Misclassification Rate	0.25
-LogLikelihood	1.7327887
Sum Freq	4

Confusion Matrix

Actual	Predicted	
Acceptance	dislike	like
dislike	1	0
like	1	2

Confusion Rates

	Predicted	
Actual	Rate	
Acceptance	dislike	like
dislike	1.000	0.000
like	0.333	0.667

Validation

Acceptance

Measures	Value
Generalized RSquare	0.8226929
Entropy RSquare	0.6923289
RMSE	0.2079112
Mean Abs Dev	0.1869488
Misclassification Rate	0
-LogLikelihood	0.4265227
Sum Freq	2

Confusion Matrix

Actual	Predicted	
Acceptance	dislike	like
dislike	1	0
like	0	1

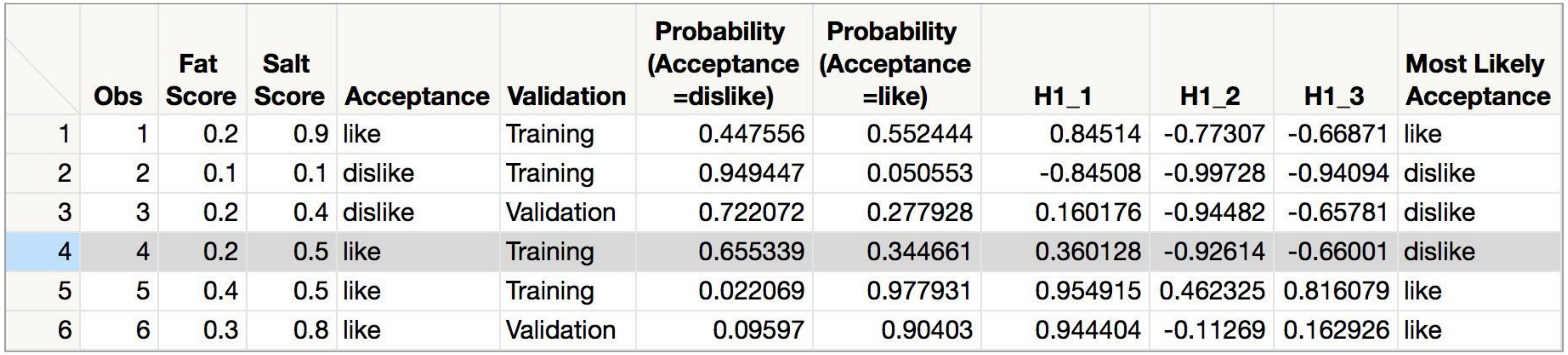
Confusion Rates

	Predicted	
Actual	Rate	
Acceptance	dislike	like
dislike	1.000	0.000
like	0.000	1.000

Tiny Example: Classifications

Estimated propensities and classifications

- One record in the training set was misclassified
- Both records in the validation set were correctly classified



	Obs	Fat Score	Salt Score	Acceptance	Validation	Probability (Acceptance =dislike)	Probability (Acceptance =like)	H1_1	H1_2	H1_3	Most Likely Acceptance
1	1	0.2	0.9	like	Training	0.447556	0.552444	0.84514	-0.77307	-0.66871	like
2	2	0.1	0.1	dislike	Training	0.949447	0.050553	-0.84508	-0.99728	-0.94094	dislike
3	3	0.2	0.4	dislike	Validation	0.722072	0.277928	0.160176	-0.94482	-0.65781	dislike
4	4	0.2	0.5	like	Training	0.655339	0.344661	0.360128	-0.92614	-0.66001	dislike
5	5	0.4	0.5	like	Training	0.022069	0.977931	0.954915	0.462325	0.816079	like
6	6	0.3	0.8	like	Validation	0.09597	0.90403	0.944404	-0.11269	0.162926	like

Specify Network Architecture

Number of hidden layers

- Most popular – one hidden layer

Number of nodes in hidden layer(s)

- More nodes capture complexity, but increase chances of overfit

Hidden Layer Activation Functions

- Combinations of three functions (TanH, Linear and Gaussian) can be applied in the hidden layers to add model complexity

User Inputs

Network Architecture, cont.

Number of tours

- How many times JMP restarts the model-fitting algorithm

“Learning Rate”

- Low values “downweight” the new information from errors at each iteration
- This slows learning, but reduces tendency to overfit to local structure

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Advantages

- Good predictive ability
- Can capture complex relationships
- No need to specify a model

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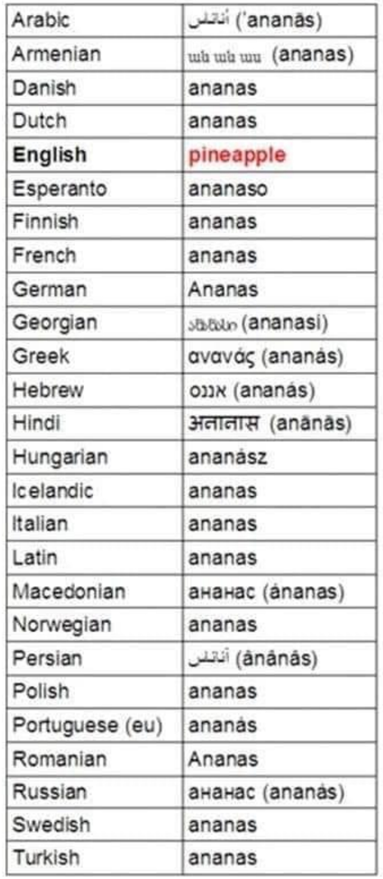
Disadvantages

- Considered a “black box” prediction machine, with no insight into relationships between predictors and outcome
- No variable-selection mechanism, so you have to exercise care in selecting variables
- Heavy computational requirements if there are many variables

Shmueli, G., Bruce, P., Stephens, M. and Patel, N. (2016) Data Mining for Business Analytics: Concepts, Techniques, and Applications with JMP Pro, Wiley, USA https://www.wiley.com/en-us/Data+Mining+for+Business+Analytics%3A+Concepts%2C+Techniques%2C+and+Applications+with+JMP+Pro-p-9781118877524

Unsupervised Learning



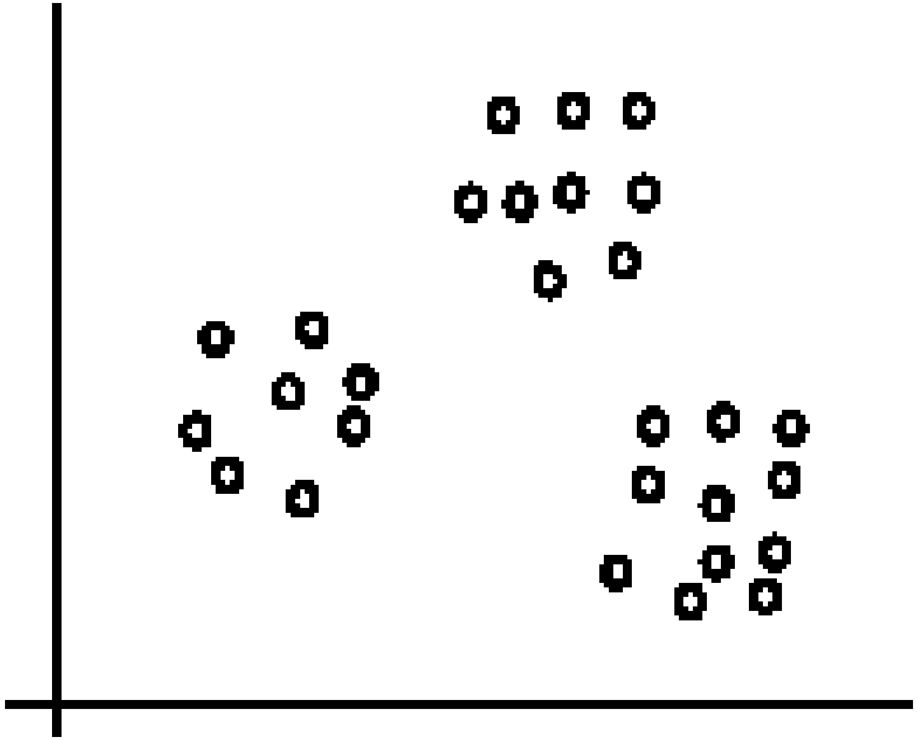
	Arabic	أناناس ('ananās)
	Armenian	անանաս (ananas)
	Danish	ananas
	Dutch	ananas
o_O	**English**	pineapple
	Esperanto	ananaso
	Finnish	ananas
	French	ananas
	German	Ananas
	Georgian	ანანასი (ananasi)
	Greek	ανανάς (ananás)
	Hebrew	אננס (ananás)
	Hindi	अनानास (anānās)
	Hungarian	ananász
	Icelandic	ananas
	Italian	ananas
	Latin	ananas
	Macedonian	ананас (ánanas)
	Norwegian	ananas
	Persian	آناناس (ânânâs)
	Polish	ananas
	Portuguese (eu)	ananás
	Romanian	Ananas
	Russian	ананас (ananás)
	Swedish	ananas
	Turkish	ananas

Clustering

- Clustering is a technique for finding similarity groups in data, called **clusters**. I.e.,
  - it groups data instances that are similar to (near) each other in one cluster and data instances that are very different (far away) from each other into different clusters.
- Clustering is often called an **unsupervised learning** task as no class values denoting an *a priori* grouping of the data instances are given, which is the case in supervised learning.

An illustration

- The data set has three natural groups of data points, i.e., 3 natural clusters.



Aspects of clustering

- A clustering algorithm
  - Partitional clustering
  - Hierarchical clustering
  - …
- A distance (similarity, or dissimilarity) function
- Clustering quality
  - Inter-clusters distance $\Rightarrow$ maximized
  - Intra-clusters distance $\Rightarrow$ minimized
- The quality of a clustering result depends on the algorithm, the distance function, and the application.

K-means clustering

- K-means is a partitional clustering algorithm
- Let the set of data points (or instances) *D* be

  $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_\mathrm{n}\}$,

  where $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ir})$ is a vector in a real-valued space $X \subseteq R^r$, and r is the number of attributes (dimensions) in the data.
- The *K*-means algorithm partitions the given data into *k* clusters.
  - Each cluster has a cluster **center**, called **centroid**.
  - *K* is specified by the user

K-means algorithm

Given *K*, the *K-means* algorithm works as follows:

1) Randomly choose *K* data points (seeds) to be the initial centroids, cluster centers

2) Assign each data point to the closest centroid

3) Re-compute the centroids using the current cluster memberships.

4) If a convergence criterion is not met, go to 2).

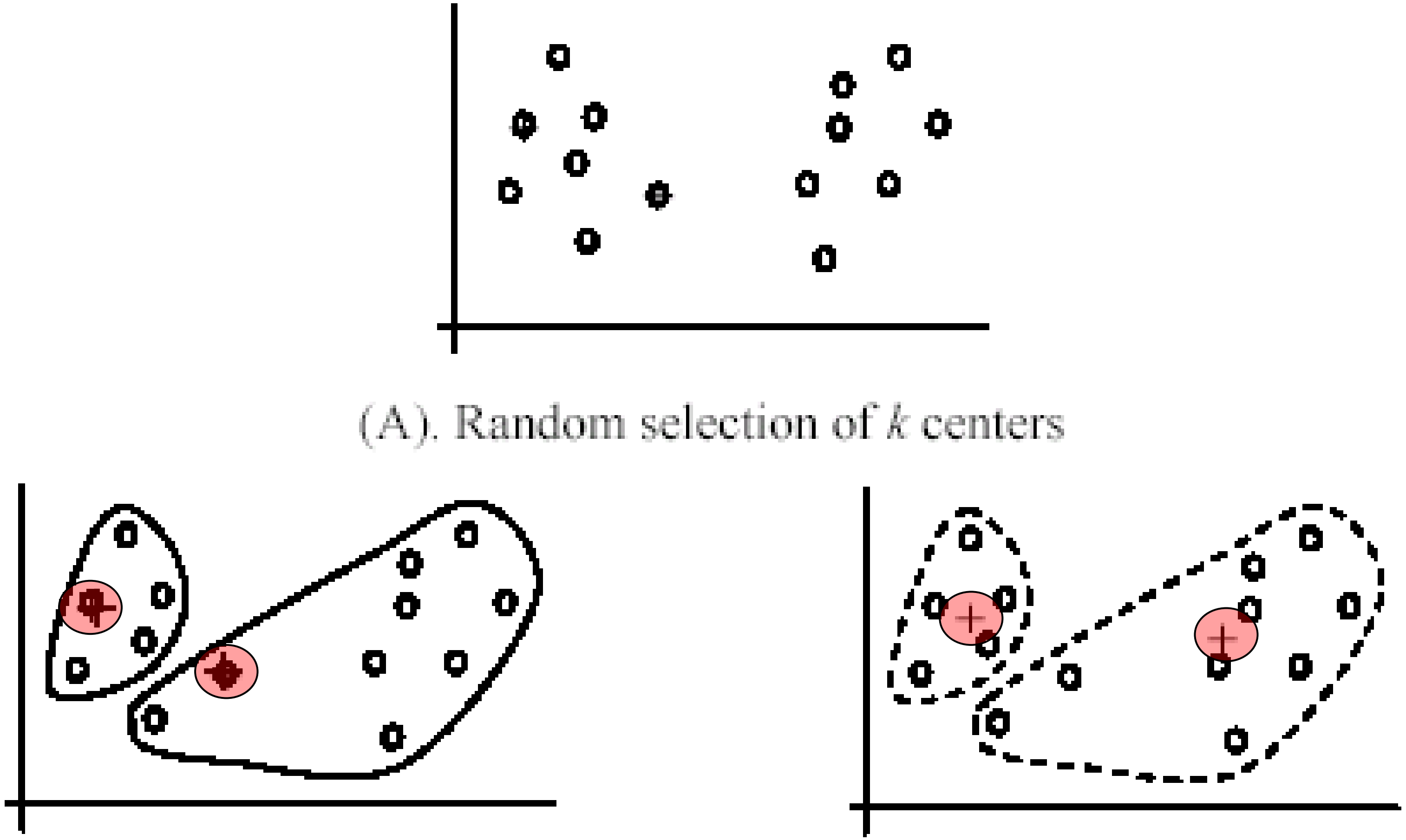
Stopping/convergence criterion

1. no (or minimum) re-assignments of data points to different clusters,
2. no (or minimum) change of centroids, or
3. minimum decrease in the **sum of squared error** (SSE),

$$SSE = \sum_{j=1}^{k} \sum_{\mathbf{x} \in C_j} dist(\mathbf{x}, \mathbf{m}_j)^2 \qquad (1)$$

- C_i is the *j*th cluster, $\mathbf{m}_j$ is the centroid of cluster C_j (the mean vector of all the data points in C_j), and *dist*(**x**, $\mathbf{m}_j$) is the distance between data point **x** and centroid $\mathbf{m}_j$.

An example

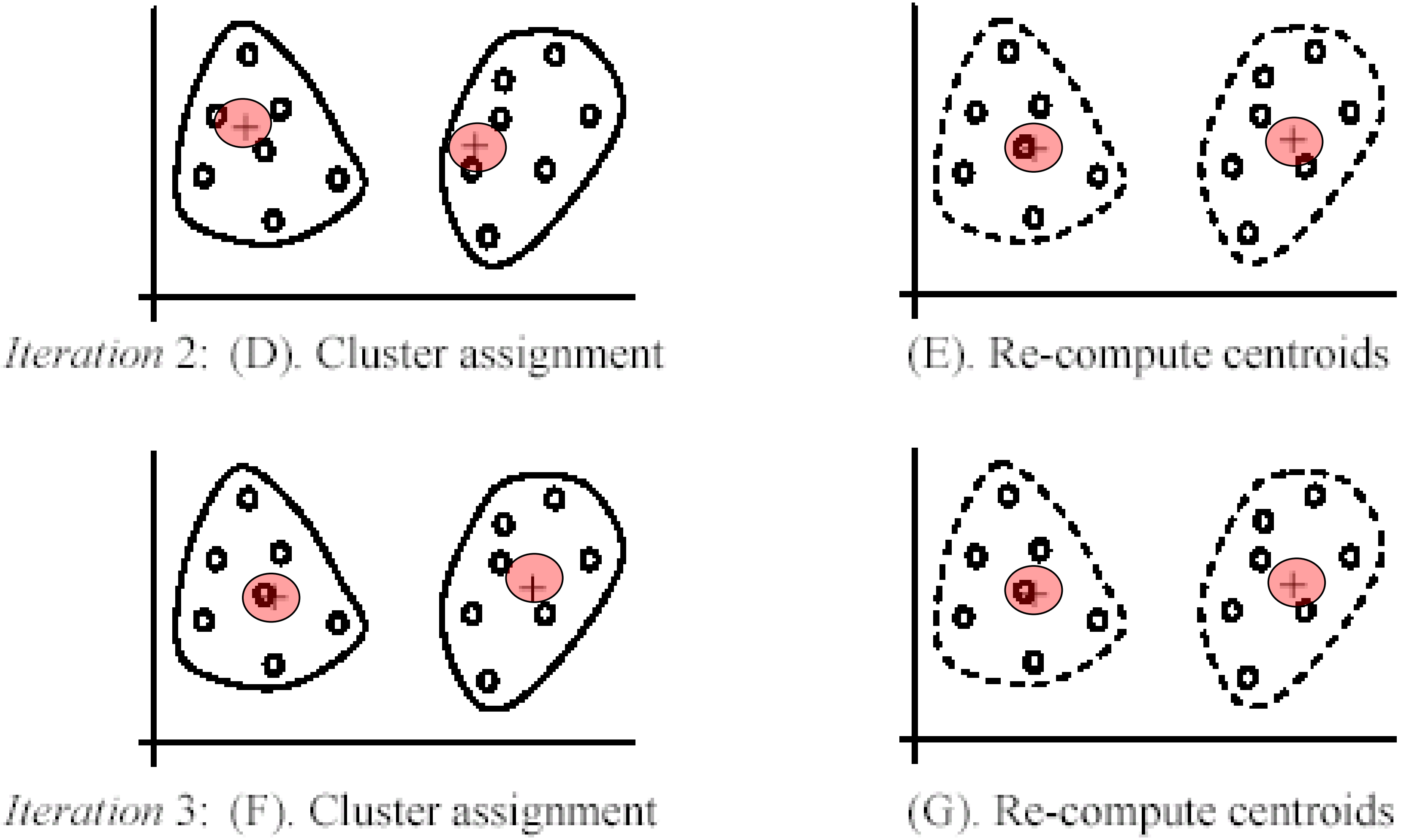


(A). Random selection of *k* centers

Iteration 1: (B). Cluster assignment

(C). Re-compute centroids

An example (cont …)



Iteration 2: (D). Cluster assignment

(E). Re-compute centroids

Iteration 3: (F). Cluster assignment

(G). Re-compute centroids

Strengths of K-means

- Strengths:
  - Simple: easy to understand and to implement
  - Efficient: Time complexity: $O(tkn)$,

    where n is the number of data points,

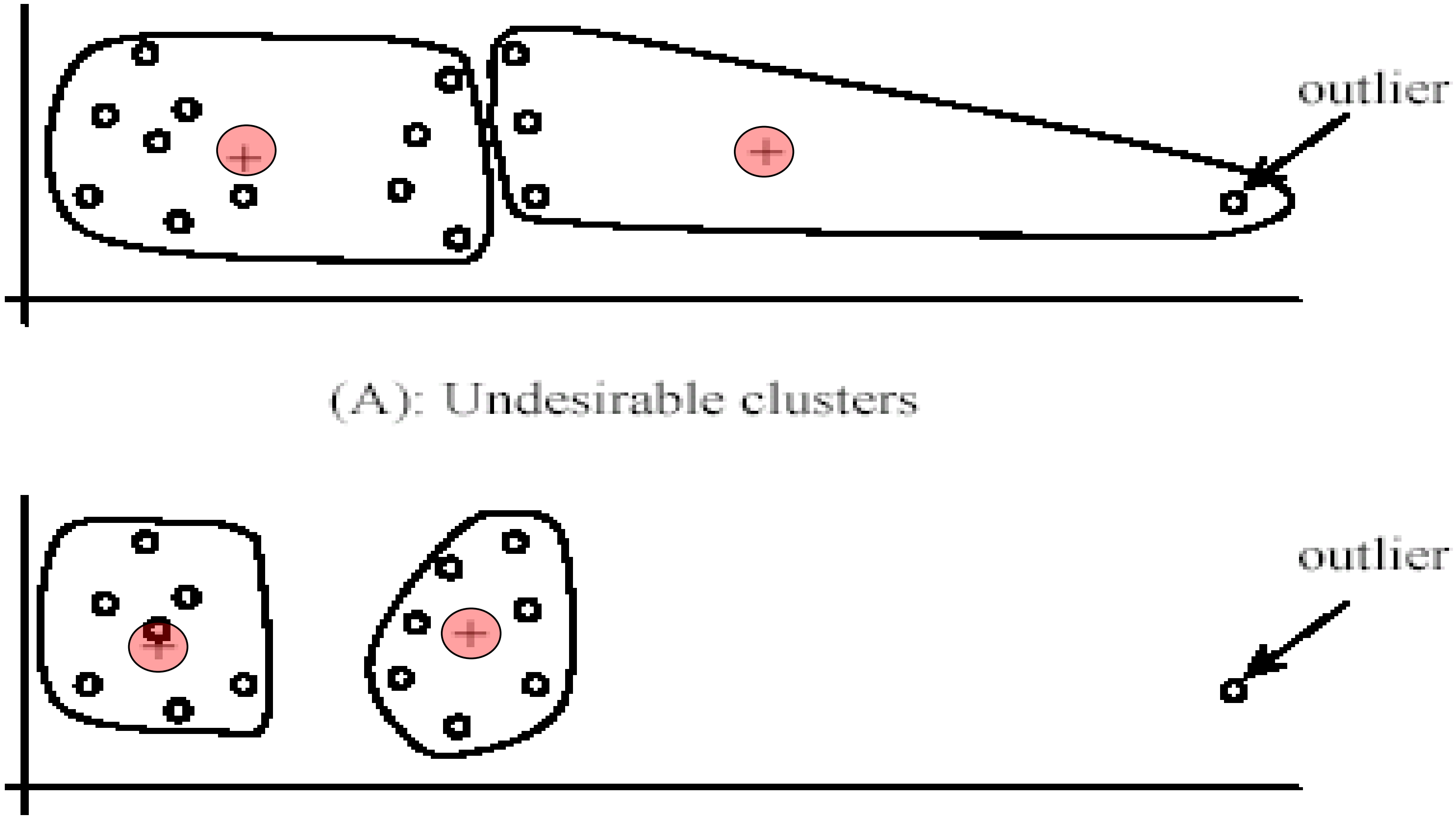
    K is the number of clusters, and

    t is the number of iterations.
  - Since both k and t are small. k-means is considered a linear algorithm.
- K-means is the most popular clustering algorithm.
- Note that: it terminates at a local optimum if SSE is used. The global optimum is hard to find due to complexity.

Weaknesses of K-means

- The algorithm is only applicable if the mean is defined.
    - For categorical data, *K*-mode - the centroid is represented by most frequent values.
- The user needs to specify *K*.
- The algorithm is sensitive to **outliers**
    - Outliers are data points that are very far away from other data points.
    - Outliers could be errors in the data recording or some special data points with very different values.

Weaknesses of K-means: Outliers



(A): Undesirable clusters

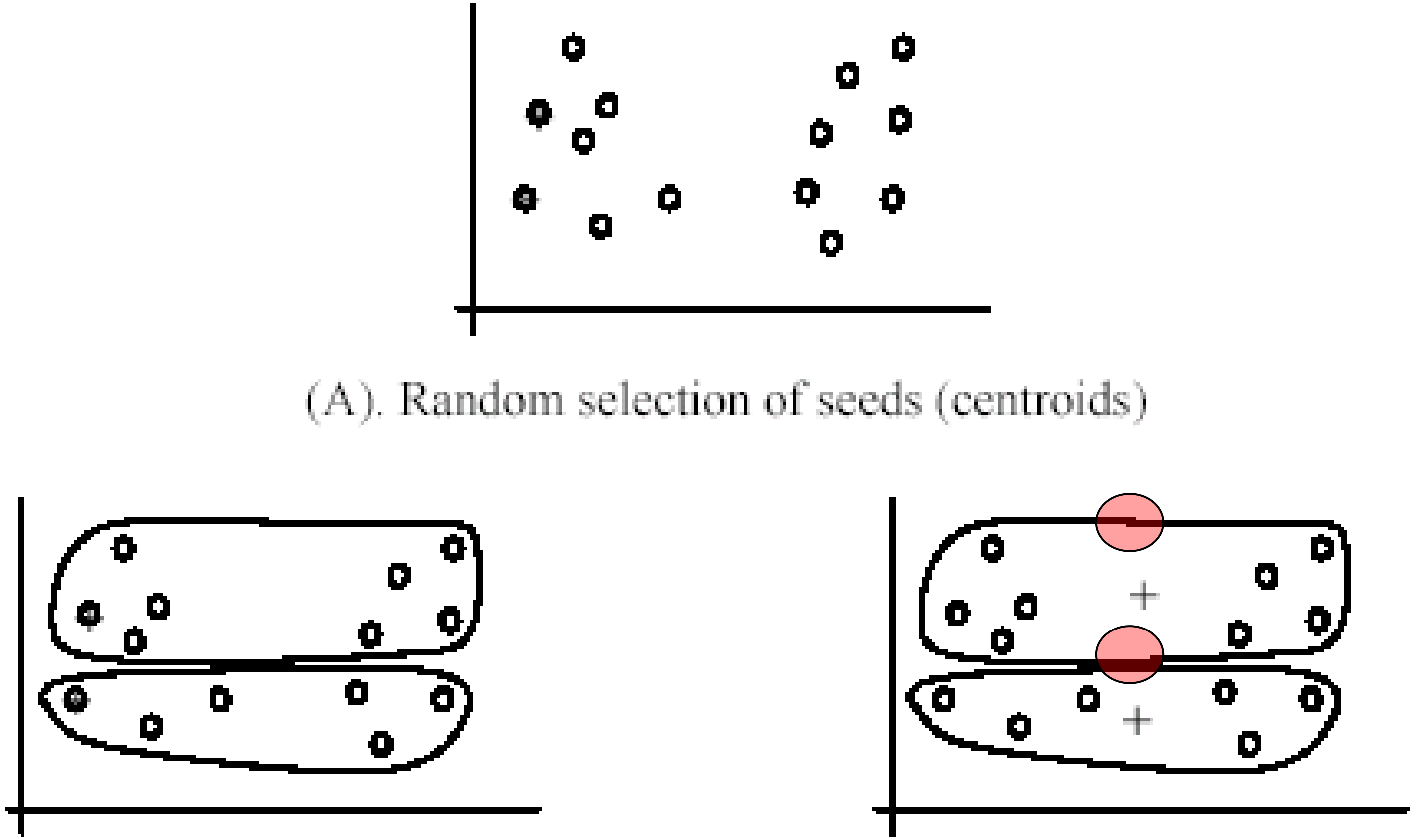
(B): Ideal clusters

Weaknesses of K-means: Outliers

- One method is to remove some data points in the clustering process that are much further away from the centroids than other data points.
    - Monitor possible outliers over a few iterations and then decide to remove them.
- Another method is to perform random sampling. Since in sampling we only choose a small subset of the data points, the chance of selecting an outlier is very small.
    - Assign the rest of the data points to the clusters by distance or similarity comparison, or classification

Weaknesses of K-means (cont …)

- The algorithm is sensitive to initial seeds.



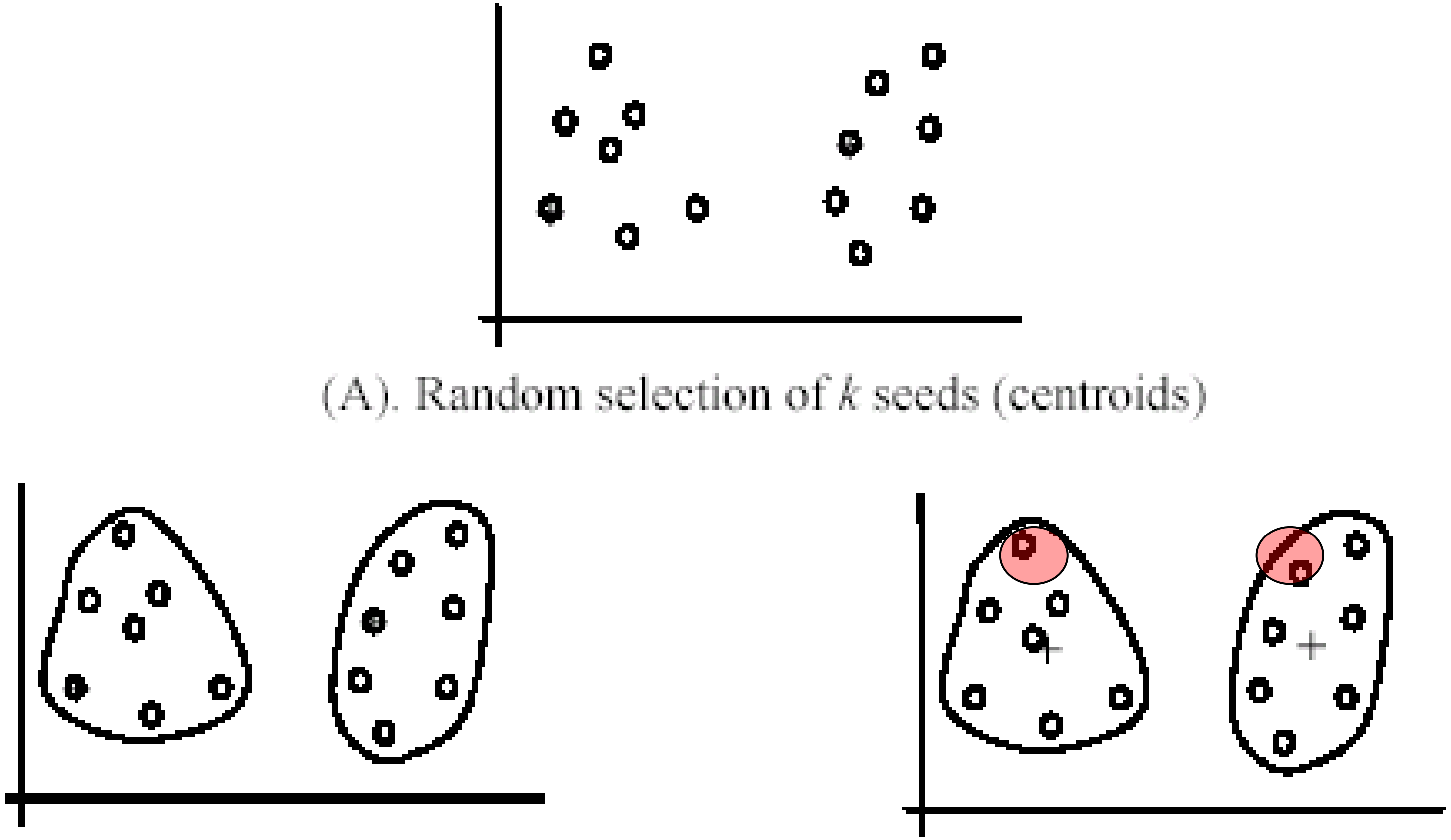
(A). Random selection of seeds (centroids)

(B). Iteration 1

(C). Iteration 2

Weaknesses of K-means (cont …)

- If we use different seeds: good results



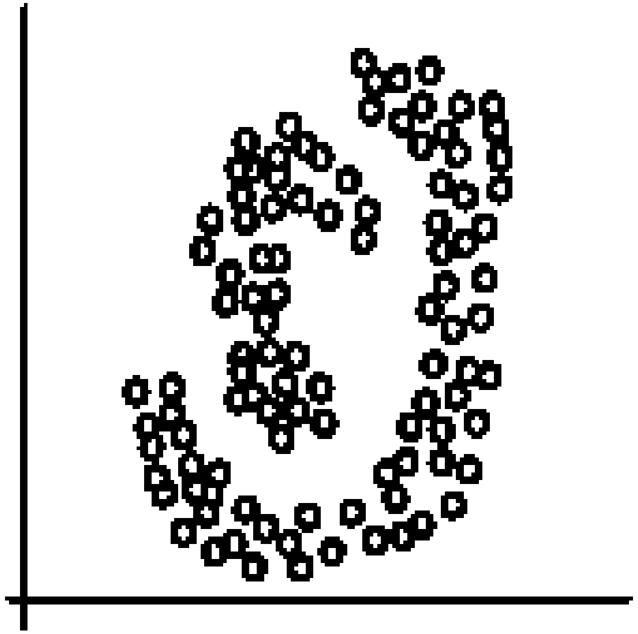
(A). Random selection of *k* seeds (centroids)

(B). Iteration 1

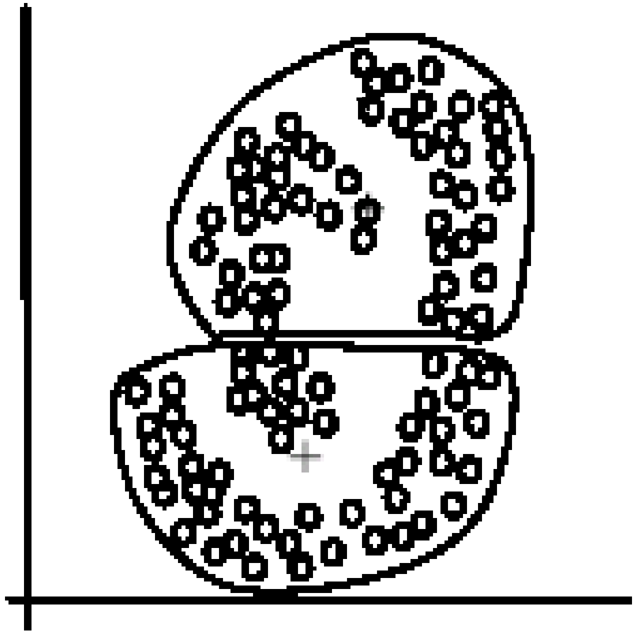
(C). Iteration 2

Weaknesses of K-means (cont …)

- The *k*-means algorithm is not suitable for discovering clusters that are not hyper-ellipsoids (or hyper-spheres).



(A): Two natural clusters



(B): *k*-means clusters

K-means summary

- Despite weaknesses, *K*-means is still the most popular algorithm due to its simplicity, efficiency and
    - other clustering algorithms have their own lists of weaknesses.
- No clear evidence that any other clustering algorithm performs better in general
    - although they may be more suitable for some specific types of data or applications.
- Comparing different clustering algorithms is a difficult task. No one knows the correct clusters!

Common ways to represent clusters

- Use the centroid of each cluster to represent the cluster.
  - compute the radius and
  - standard deviation of the cluster to determine its spread in each dimension

  - The centroid representation alone works well if the clusters are of the hyper-spherical shape.
  - If clusters are elongated or are of other shapes, centroids are not sufficient

Hierarchical methods

Agglomerative Methods

- Begin with n-clusters (each record its own cluster)
- Keep joining records into clusters until one cluster is left (the entire data set)
- Most popular

Divisive Methods

- Start with one all-inclusive cluster
- Repeatedly divide into smaller clusters

Distance between two records

Euclidean Distance is most popular:

$$d_{ij} = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}$$

Normalizing

Problem: Raw distance measures are highly influenced by scale of measurements

Solution: normalize (standardize) the data first

- Subtract mean, divide by std. deviation
- Also called **z-scores**

Other distance measures

- Correlation-based similarity
- Statistical distance (Mahalanobis)
- Manhattan distance (absolute differences)
- Maximum coordinate distance
- Gower’s similarity (for mixed variable types: continuous & categorical)

Minimum distance (Cluster A to Cluster B)

- Also called **single linkage**

- Distance between two clusters is the distance between the pair of records A_i and B_j that are closest

Maximum distance (Cluster A to Cluster B)

- Also called **complete linkage**

- Distance between two clusters is the distance between the pair of records A_i and B_j that are farthest from each other

Average distance

- Also called **average linkage**

- Distance between two clusters is the average of all possible pair-wise distances

Centroid distance

- Distance between two clusters is the distance between the two cluster centroids
- Centroid is the vector of variable averages for all records in a cluster

Ward’s method

- Considers loss of information when observations are clustered together
- Uses error sum of squares (ESS) to measure the difference between observations and the centroid
- The *Fast Ward* method in JMP is more efficient, and is used automatically for large data sets

The Hierarchical Clustering (using agglomerative method)

Steps:

1. Start with *n* clusters (each record is its own cluster)
2. Merge two closest records into one cluster
3. At each successive step, the two clusters closest to each other are merged

Dendrogram, from left to right, illustrates the process

Interpreting clusters

Goal: obtain meaningful and useful clusters

Caveats:

(1) Random chance can often produce apparent clusters

(2) Different cluster methods produce different results

Solutions:

- Obtain summary statistics
- Also review clusters in terms of variables **not** used in clustering
- Label the cluster (e.g. clustering of financial firms in 2008 might yield label like "midsize, sub-prime loser")

Desirable cluster features

Stability

- ➢Are clusters and cluster assignments sensitive to slight changes in inputs?
- ➢Are cluster assignments in partition B similar to partition A?

Separation

- ➢check ratio of between-cluster variation to within-cluster variation (higher is better)

K-Means clustering algorithm

1. Choose # of clusters desired, *K*
2. Start with a partition into K clusters

   Often based on random selection of k centroids

3. At each step, move each record to cluster with closest centroid
4. Recompute centroids, repeat step 3
5. Stop when moving records increases within-cluster dispersion

K-means algorithm: choosing K and initial partitioning

Choose *K* based on the how results will be used

- e.g., “How many market segments do we want?”

Also experiment with slightly different *K*’s

Initial partition into clusters can be random, or based on domain knowledge

- If random partition, repeat the process with different random partitions

Clustering overview

- Cluster analysis is an exploratory tool
- It is useful only when it produces **meaningful** clusters
- **Hierarchical** clustering gives visual representation of different levels of clustering
- **Non-hierarchical** clustering is computationally cheap and more stable (good with larger data sets); requires user to set *k*
- Can use both methods
- Be wary of chance results; data may not have definitive “real” clusters