An Introduction to Machine Learning

Lecture 3

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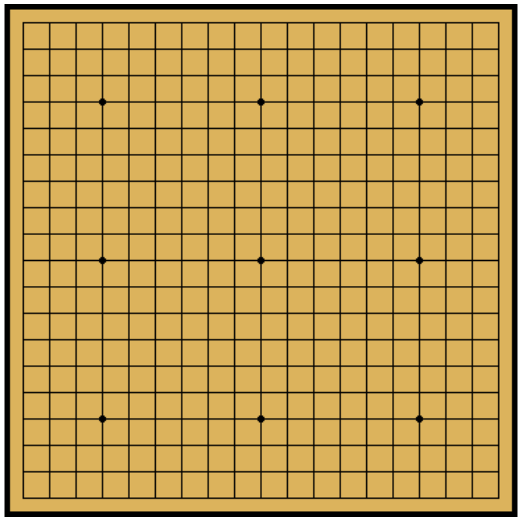
Topics

- Introduction
- A Bit of Theory
- Boosted Decision Trees
- Neural Networks
- The Future of Machine Learning

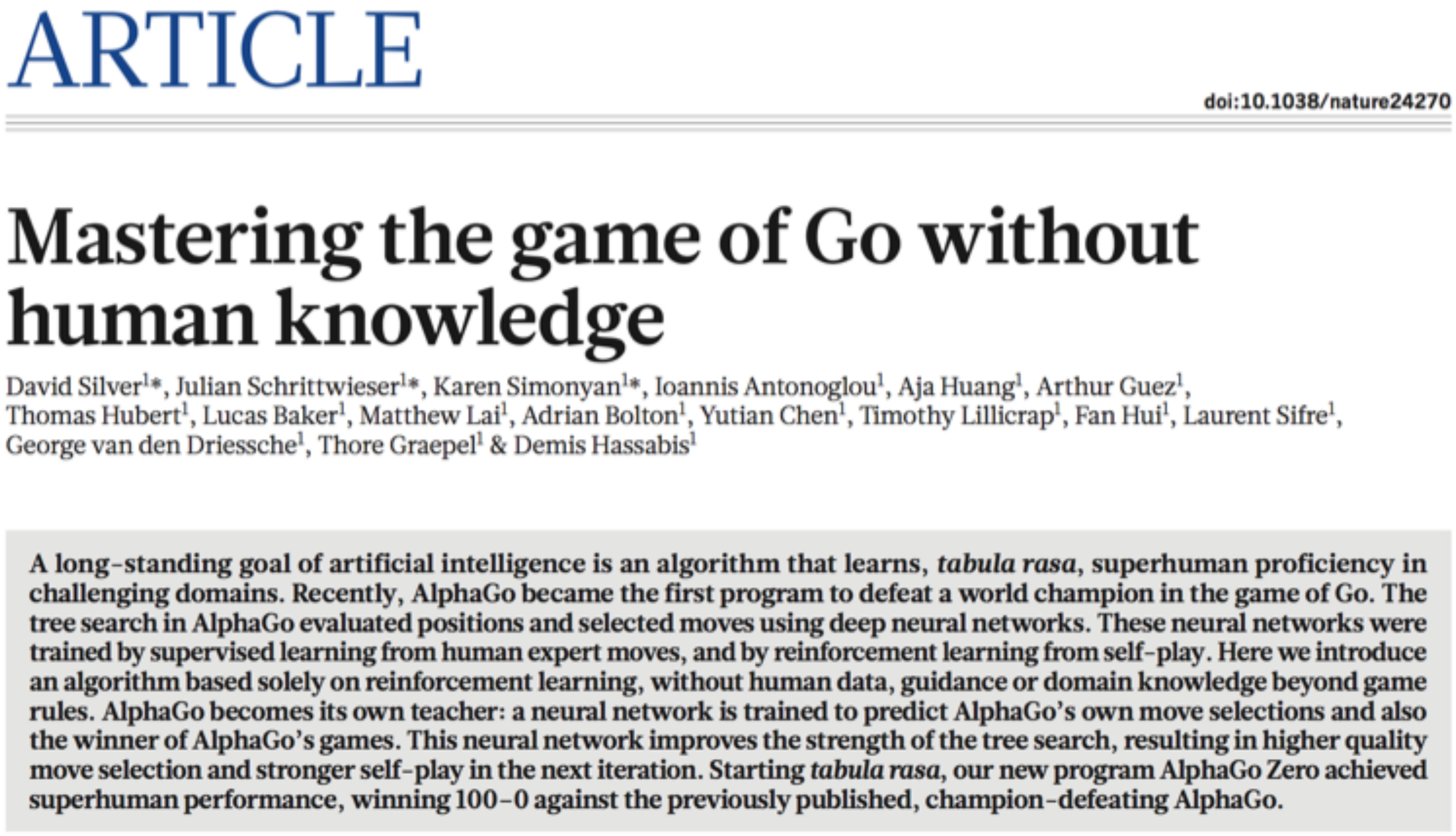
INTRODUCTION

AlphaGo 4, Homo Sapiens 1

2016 – Google’s AlphaGo program beats Go champion Lee Sodol.



Photograph: Yonhap/Reuters



ARTICLE

doi:10.1038/nature24270

Mastering the game of Go without human knowledge

David Silver[1]*, Julian Schrittwieser[1]*, Karen Simonyan[1]*, Ioannis Antonoglou[1], Aja Huang[1], Arthur Guez[1], Thomas Hubert[1], Lucas Baker[1], Matthew Lai[1], Adrian Bolton[1], Yutian Chen[1], Timothy Lillicrap[1], Fan Hui[1], Laurent Sifre[1], George van den Driessche[1], Thore Graepel[1] & Demis Hassabis[1]

A long-standing goal of artificial intelligence is an algorithm that learns, *tabula rasa*, superhuman proficiency in challenging domains. Recently, AlphaGo became the first program to defeat a world champion in the game of Go. The tree search in AlphaGo evaluated positions and selected moves using deep neural networks. These neural networks were trained by supervised learning from human expert moves, and by reinforcement learning from self-play. Here we introduce an algorithm based solely on reinforcement learning, without human data, guidance or domain knowledge beyond game rules. AlphaGo becomes its own teacher: a neural network is trained to predict AlphaGo's own move selections and also the winner of AlphaGo's games. This neural network improves the strength of the tree search, resulting in higher quality move selection and stronger self-play in the next iteration. Starting *tabula rasa*, our new program AlphaGo Zero achieved superhuman performance, winning 100–0 against the previously published, champion-defeating AlphaGo.

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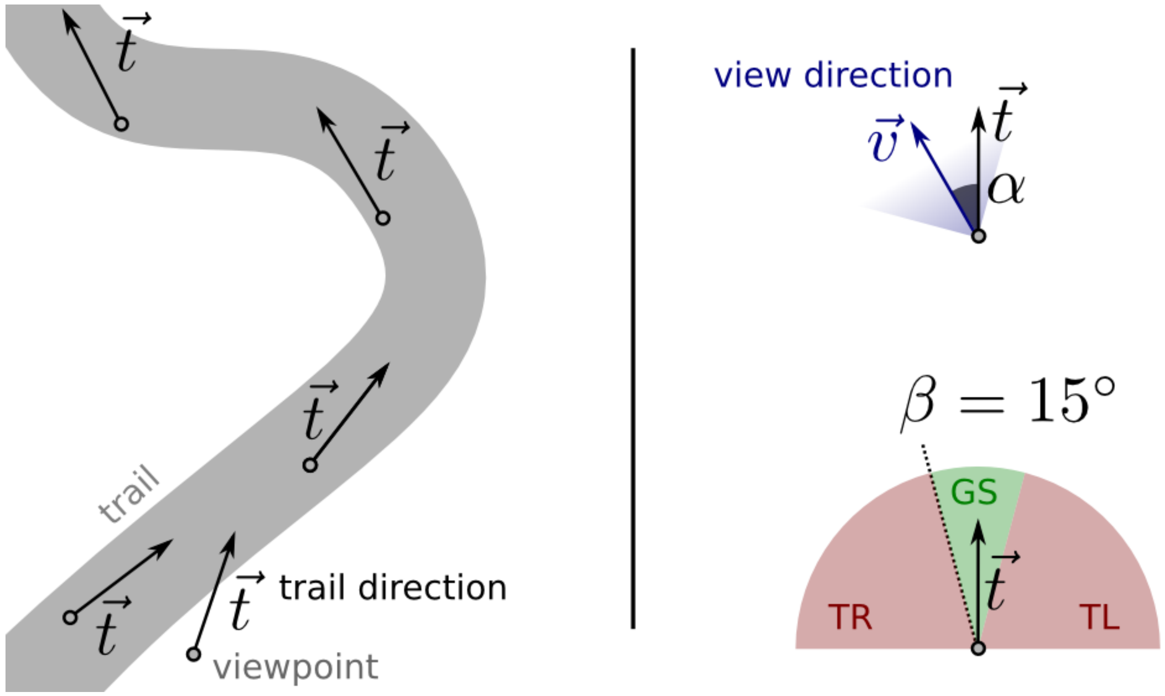
Follow the Yellow Brick Road!

Giusti *et al.* treat the problem of trail navigation as a classification problem!

Data: 8 hours of 1920 x 1080 30fps video using 3 GoPro cameras.



IEEE Robotics and Automation Letters (Volume: 1, Issue: 2, July 2016)

What is Machine Learning?

The use of computer-based algorithms for constructing useful *models* of data.

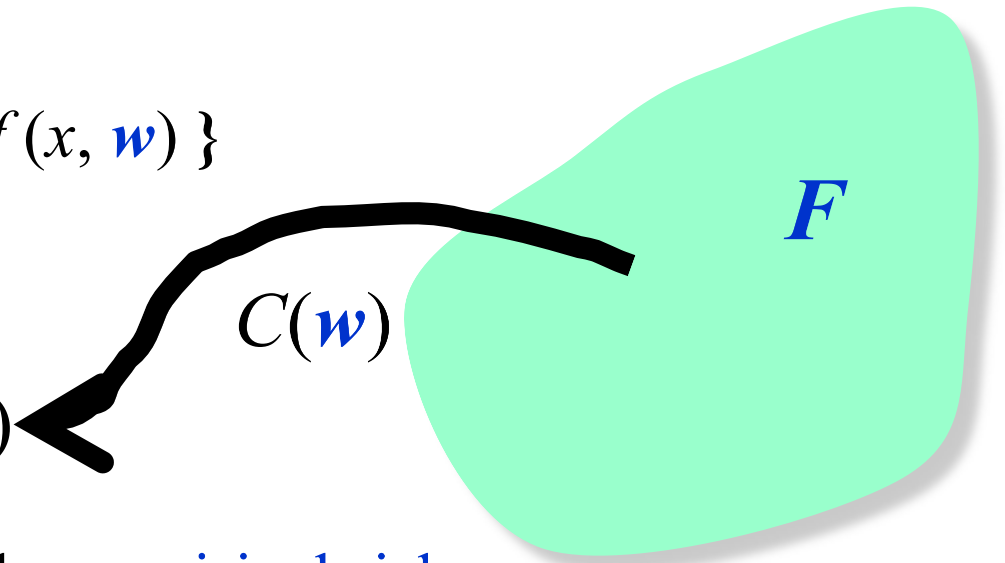
Machine learning algorithms fall into five broad categories:

1. Supervised Learning
2. Semi-supervised Learning
3. Unsupervised Learning
4. Reinforcement Learning
5. Generative Learning

Machine Learning

Choose

Function space	$F = \{ f(x, \mathbf{w}) \}$
Constraint	C
Loss function*	L



$f(x, \mathbf{w}^*)$

Method

Find $f(x)$ by minimizing the empirical risk

$$R(f) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(x_i, \mathbf{w}))$$

subject to the constraint $C(\mathbf{w})$

*The loss function measures the cost of making a bad choice of function from the function space.

Machine Learning

Many methods use the

quadratic loss $L(y, f) = (y - f)^2$

and choose $f(x, w^*)$ by minimizing the

constrained empirical risk (that is, the average loss)

$$R(f) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(x_i, w)) + C(w)$$

Machine Learning

Minimization via Gradient Descent

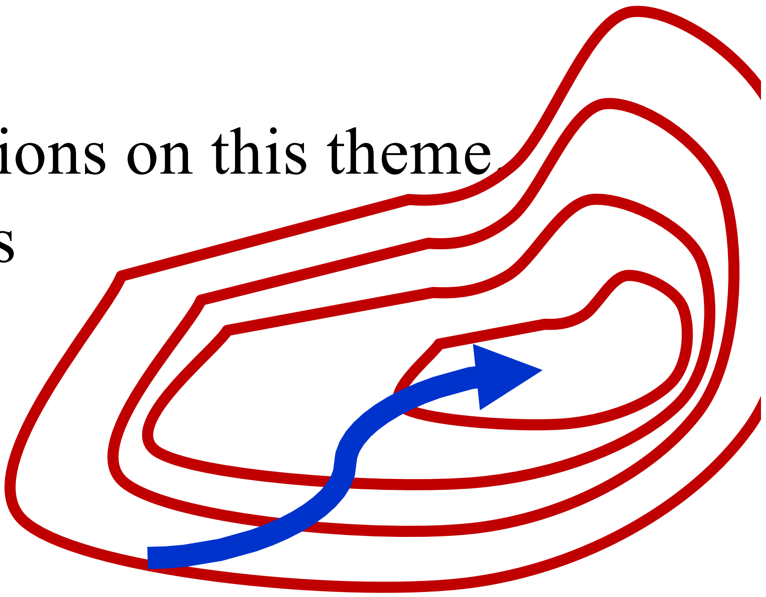
A "loss function" defines a "landscape" in the space of parameters, or equivalently in the *space of functions*.

The goal is to find the lowest point in the landscape, usually by moving in the direction of the local *negative* gradient:

$$w_i \leftarrow w_i - \rho \frac{\partial R(w)}{\partial w_i}$$

Most minimization algorithms are variations on this theme.

Stochastic Gradient Descent (SGD), uses random subsets of the training data to provide *noisy* estimates of the gradient.



A BIT OF THEORY

Minimizing Quadratic Loss

Consider the quadratic risk function in the limit $N \to \infty$

$$R(w) = \frac{1}{N}\sum_{i=1}^{N}(y_i - f(x_i, w))^2 + C(w)$$

$$\to \int dx \int dy \big(y - f(x, w)\big)^2 p(y, x)$$

$$= \int dx\, p(x)\left[\int dy (y - f)^2 p(y|x)\right]$$

where $p(y|x) = p(y, x)/p(x)$ and where we have assumed the influence of the constraint (in this limit) is negligible.

R is a *functional* $R[f]$ of $f(x, w)$, that is, R depends on (infinitely) many values of f.

Minimizing Quadratic Loss

If we change the function $\boldsymbol{f}$ by a small *arbitrary* function $\boldsymbol{\delta f}$ a small change

$$\delta R = 2\int dx\, p(x)\boldsymbol{\delta f}\left[\int dy (y - f) p(y|x)\right]$$

will be induced in R. In general, $\delta R \neq 0$.

But, if the function $\boldsymbol{f}$ is flexible enough we shall be able to reach the minimum of R, where $\boldsymbol{\delta R = 0}$.

This is to hold for all variations $\boldsymbol{\delta f}$ and for all values of $\boldsymbol{x}$.

This can happen if the quantity in brackets is ***zero***, that is, if

$$\boxed{f(x) = \int y\, p(y \mid x)\, dy}$$

Classification

Recall that Bayes' theorem is

$$p(y|x) = \frac{p(x\,|y)\,p(y)}{\int p(x\,|y)\,p(y)dy}$$

Now, let's assign the target value $\boldsymbol{y} = \mathbf{1}$ to objects of class $\boldsymbol{s}$ and target value $\boldsymbol{y} = \mathbf{0}$ to objects of class $\boldsymbol{b}$.

Then

$$\boxed{\begin{aligned} f(x) &= \int y\,p(y\,|\,x)\,dx = p(1|x) \\ &\equiv p(\boldsymbol{s}|x) \end{aligned}}$$

That is, the function approximates the class probability.

Classification

In 1990*, the result

$$f(x) = p(s|x) = \frac{p(x|s)p(s)}{p(x|s)p(s) + p(x|b)p(b)}$$

was derived in the context of neural networks. But, the result is, in fact, *independent of the nature of the function* $f(x, \boldsymbol{w})$ *provided that*:

1. we have sufficient training data ***T*** and
2. we have a sufficiently flexible function $f(x, \boldsymbol{w})$.

* Ruck et al., *IEEE Trans. Neural Networks* 4, 296-298 (1990); Wan, *IEEE Trans. Neural Networks* 4, 303-305 (1990);

Richard and Lippmann, *Neural Computation.* 3, 461-483 (1991)

Classification

If $p(s) = p(b)$, we arrive at the discriminant

$$D(x) = \frac{p(x|s)}{p(x|s) + p(x|b)} \equiv \frac{s(x)}{s(s) + b(x)}$$

This is an extremely useful result because it suggests many potential machine learning applications.

Ask me during discussion sessions!

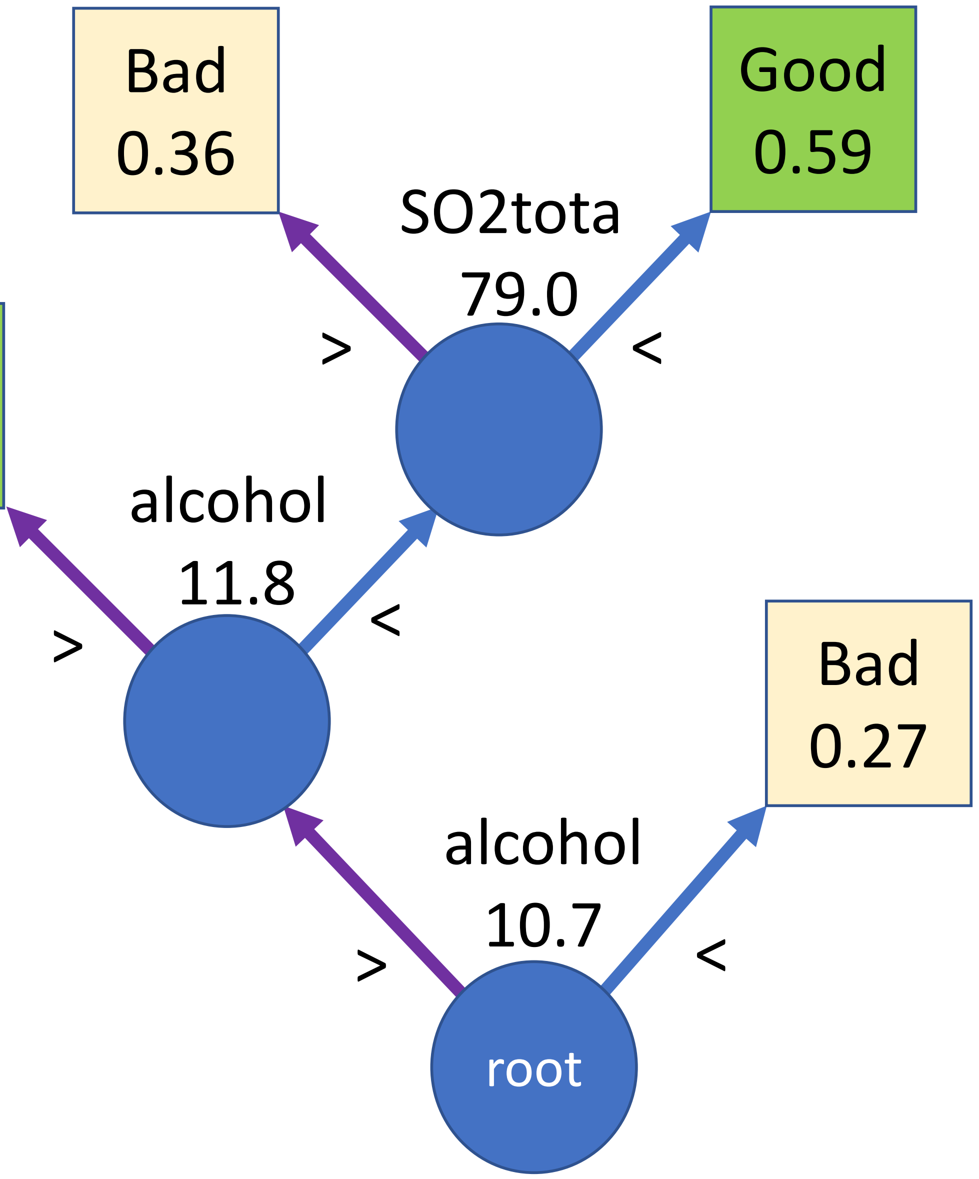
BOOSTED DECISION TREES

Decision Trees

Decision tree:
a sequence of if then else statements.

Basic idea: recursively partition the space into regions of diminishing *impurity*.

This is a simple example of an automated wine taster…more details later.

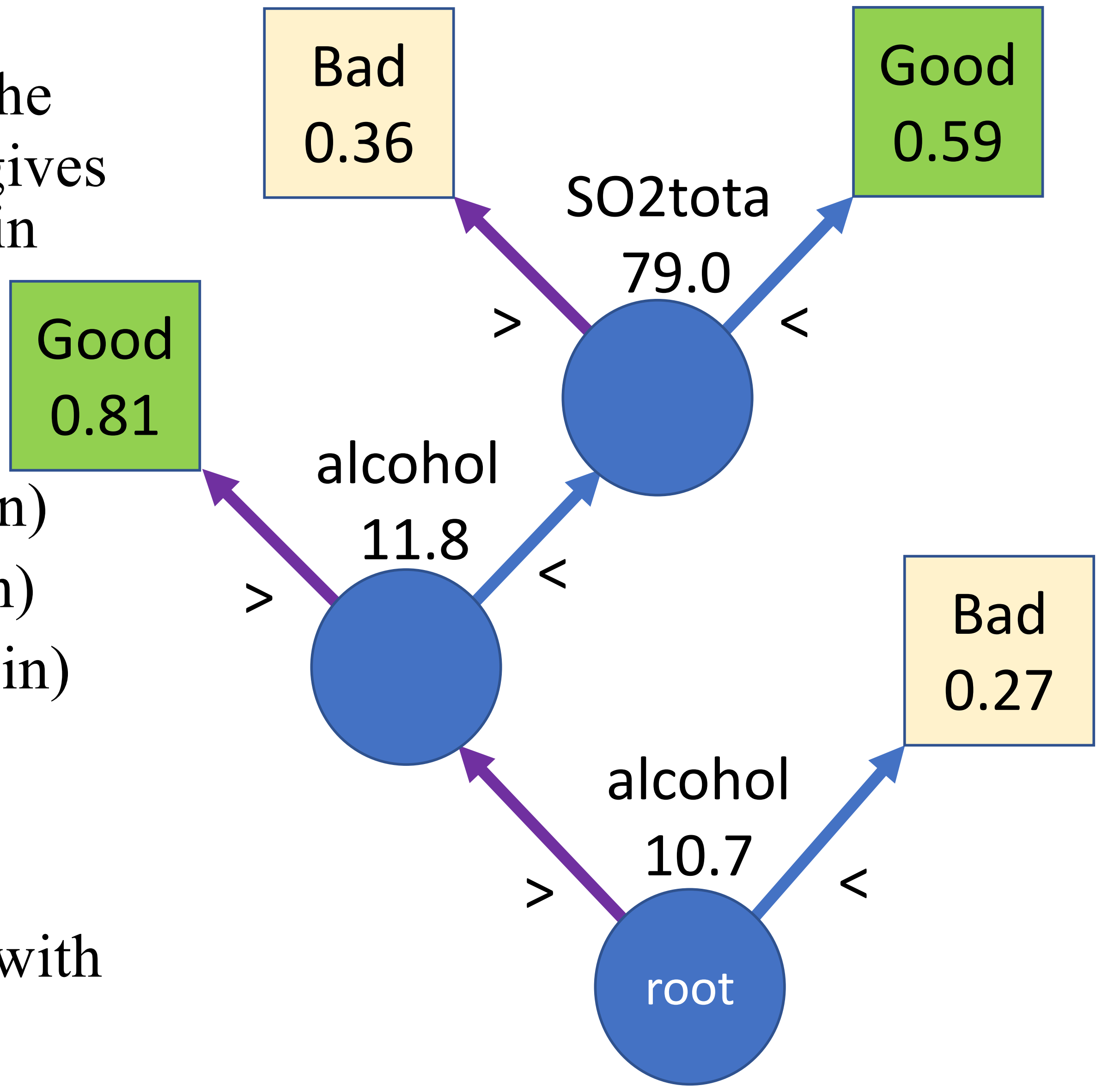


Decision Trees

For each variable, find the partition ("cut") that gives the greatest *decrease* in impurity:

Impurity (parent bin)
– **Impurity** ("left"-bin)
– **Impurity** ("right"-bin)

Then, choose the best partition among all partitions, and repeat with each child bin.



Decision Trees

The most common impurity measure is the Gini index (Corrado Gini, 1884-1965):

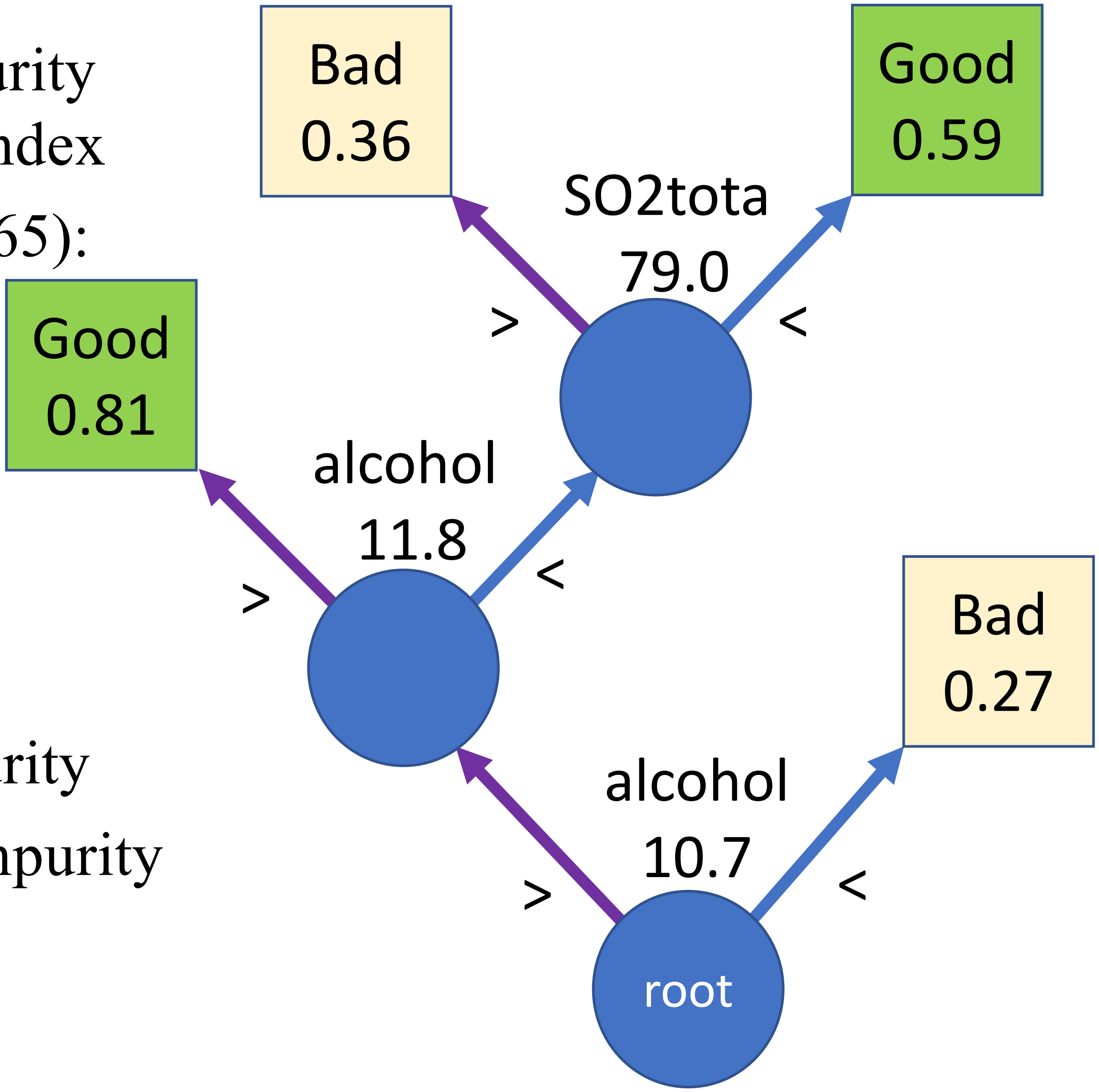
Gini index = $p\,(1 - p)$

where p is the purity

$p = S\,/\,(S + B)$

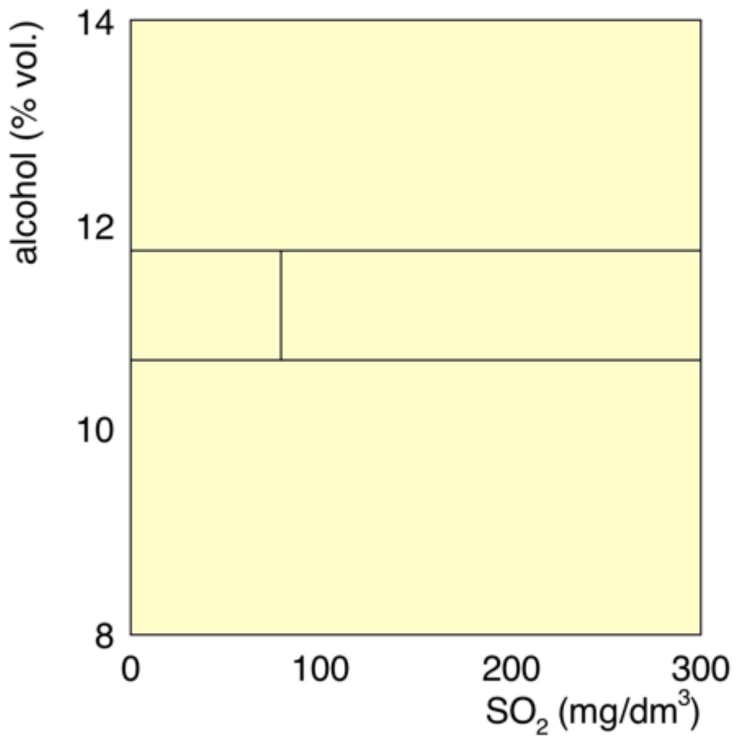
$p = 0$ or 1 = maximal purity

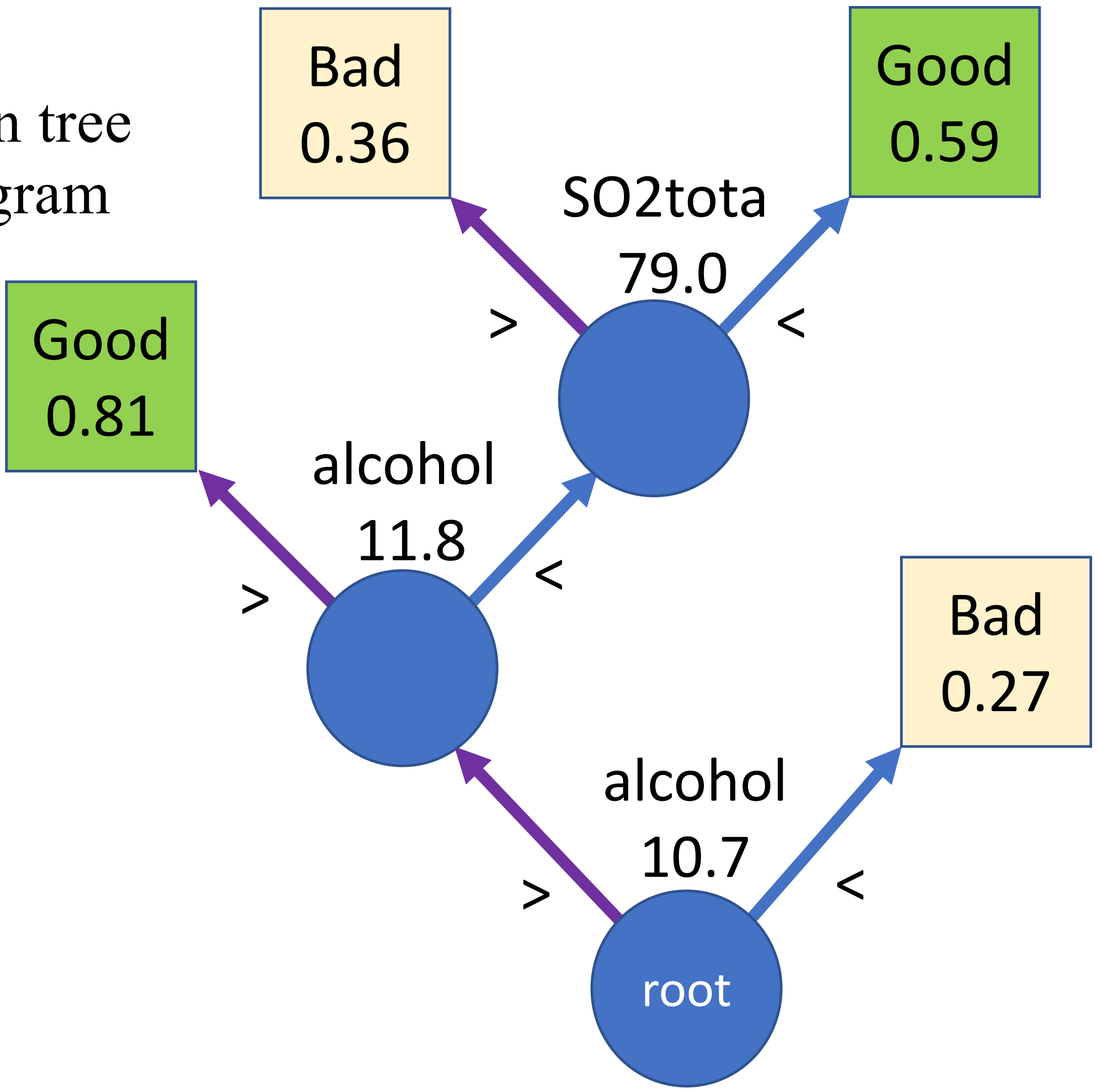
$p = 0.5$ = maximal impurity



Decision Trees

Geometrically, a decision tree is a *d-dimensional* histogram in which the bins are created *recursively*.

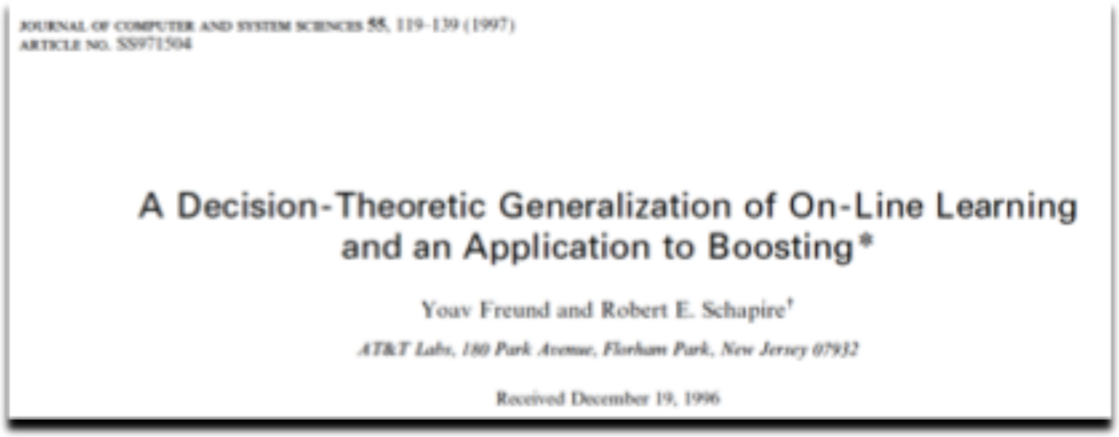




A Silk Purse from a Sow's Ear!

In 1997, AT&T researchers Freund and Schapire [Journal of Computer and Sys. Sci. **55** (1), 119 (1997)] showed that it was possible to build highly effective classifiers by combining a large number of mediocre ones!

The Freund-Schapire algorithm, which they called AdaBoost, was the first successful method to *boost* (i.e., enhance) the performance of poorly performing classifiers by *averaging* their outputs.



JOURNAL OF COMPUTER AND SYSTEM SCIENCES 55, 119–139 (1997)
ARTICLE NO. SS971504

A Decision-Theoretic Generalization of On-Line Learning and an Application to Boosting*

Yoav Freund and Robert E. Schapire†

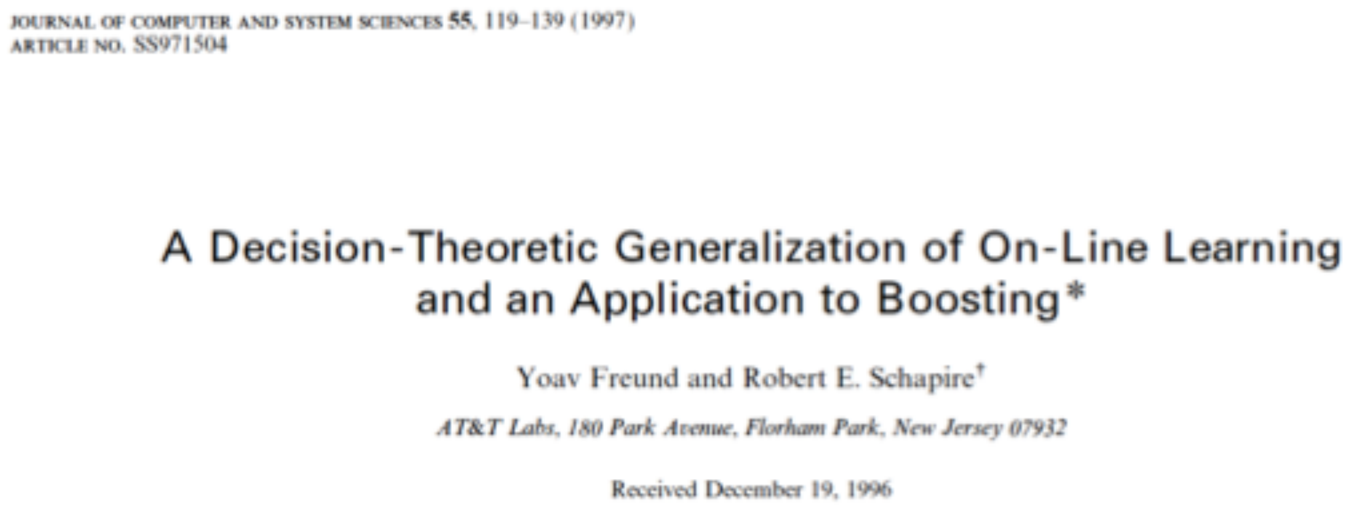
AT&T Labs, 180 Park Avenue, Florham Park, New Jersey 07932

Received December 19, 1996

Ensemble Methods

In 1997, AT&T researchers Y. Freund and R.E. Schapire [Journal of Computer and Sys. Sci. **55** (1), 119 (1997)], showed that it was possible to build highly effective classifiers by combining many weak ones!

This was the first successful method to improve (i.e., *boost*) the performance of poorly performing classifiers by averaging them.



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Ensemble Methods

Suppose you have an **ensemble** of classifiers $f\,(x, w_k)$, which, individually, perform only marginally better than random guessing. Such classifiers are called **weak learners**.

It is possible to build highly effective classifiers by *averaging* their outputs:

$$f(x) = a_0 + \sum_{n=1}^{N} a_n\, f(x_n, w_n)$$

Jerome Friedman & Bogdan Popescu (2008)

Ensemble Methods

The most popular methods (used mostly with decision trees) are:

• Bagging:	each tree is trained on a bootstrap* sample drawn from the training set
• Random Forest:	bagging with randomized trees
• Boosting:	each tree trained on a different reweighting of the training set

*A bootstrap sample is a sample of size N drawn, *with replacement*, from another of the same size. Duplicates can occur and are allowed.

Adaptive Boosting

The **AdaBoost** algorithm of Freund and Schapire uses decision trees $f(x, \mathbf{w})$ with weights $\mathbf{w}$ assigned to each object to be classified, and each assigned a target value of either $\mathbf{y = +1}$, or $\mathbf{-1}$, e.g., +1 for signal, –1 for background.

The value assigned to each leaf of $f(x, \mathbf{w})$ is also ± 1.

Consequently, for object $\boldsymbol{n}$, associated with values (y_n, x_n)

$f(x_n, \mathbf{w})\, y_n > 0$	for a correct classification
$f(x_n, \mathbf{w})\, y_n < 0$	for an incorrect classification

Y. Freund and R.E. Schapire. Journal of Computer and Sys. Sci. **55** (1), 119 (1997)

Adaptive Boosting

Initialize weights $\boldsymbol{w}$ in training set (e.g., setting each to **1/*N***)

for *k* = 1 to *K*:

1. Create a decision tree $f\,(x, \boldsymbol{w})$ using the current weights.
2. Compute its error rate $\boldsymbol{\varepsilon}$ on the ***weighted*** training set.
3. Compute $\boldsymbol{\alpha} = \ln\,(1 - \boldsymbol{\varepsilon})\,/\,\boldsymbol{\varepsilon}$ and store as $\boldsymbol{\alpha}_k = \boldsymbol{\alpha}$
4. Update each weight $\boldsymbol{w_n}$ in the training set as follows: $\boldsymbol{w_n} = \boldsymbol{w_n} \exp[-\boldsymbol{\alpha}_k\, f\,(x_n, \boldsymbol{w})\, y_n]$ /A, where A is a normalization constant such that $\sum \boldsymbol{w_n} = 1$. Since $f\,(x_n, \boldsymbol{w})\, y_n < 0$ for an incorrect classification, the weight of misclassified objects is ***increased***.

At the end, compute the average $f\,(x) = \sum \alpha_k\, f\,(x, \boldsymbol{w}_\mathbf{k})$

Y. Freund and R.E. Schapire. Journal of Computer and Sys. Sci. **55** (1), 119 (1997)

Adaptive Boosting

AdaBoost is a highly non-intuitive algorithm. However, soon after its invention, Friedman, Hastie and Tibshirani showed that the algorithm is mathematically equivalent to minimizing the following average loss function

$$R(F) = \int p(x, y) \exp(-y\, F(x)\, dx\, dy$$

where $F(x) = \sum_{n=1}^{N} a_n\, f(x_n, w_n)$,

Minimizing this loss function yields

$$D(x) = \text{logistic}(2F) = 1/(1 + \exp(-2\, F(x))$$

which can be interpreted as a probability, even though F cannot!

J. Friedman, T. Hastie and R. Tibshirani, "Additive logistic regression: a statistical view of boosting," The Annals of Statistics, 28(2), 377-386, (2000)

EXAMPLE: WINE TASTING

Wine Tasting

Wine tasting is big business. But, can a machine do it?
In principle, yes, if we can establish the physical attributes that define "good" wine, such as this one for **$117,000** a bottle!

Wine Tasting

We’ll use AdaBoost to build a classifier that can distinguishes good wines from bad wines

from

Vinho Verde

in Portugal.

.

🟩 Vinho Verde
🟥 Douro
SPAIN
porto
PORTUGAL
lisboa

Wine Tasting

Let's define a good wine as one with expert rating ≥ 0.6 on a scale from 0 to 1, where **1** is a wine from Heaven and **0** is a wine from Hell!

We'll use data from

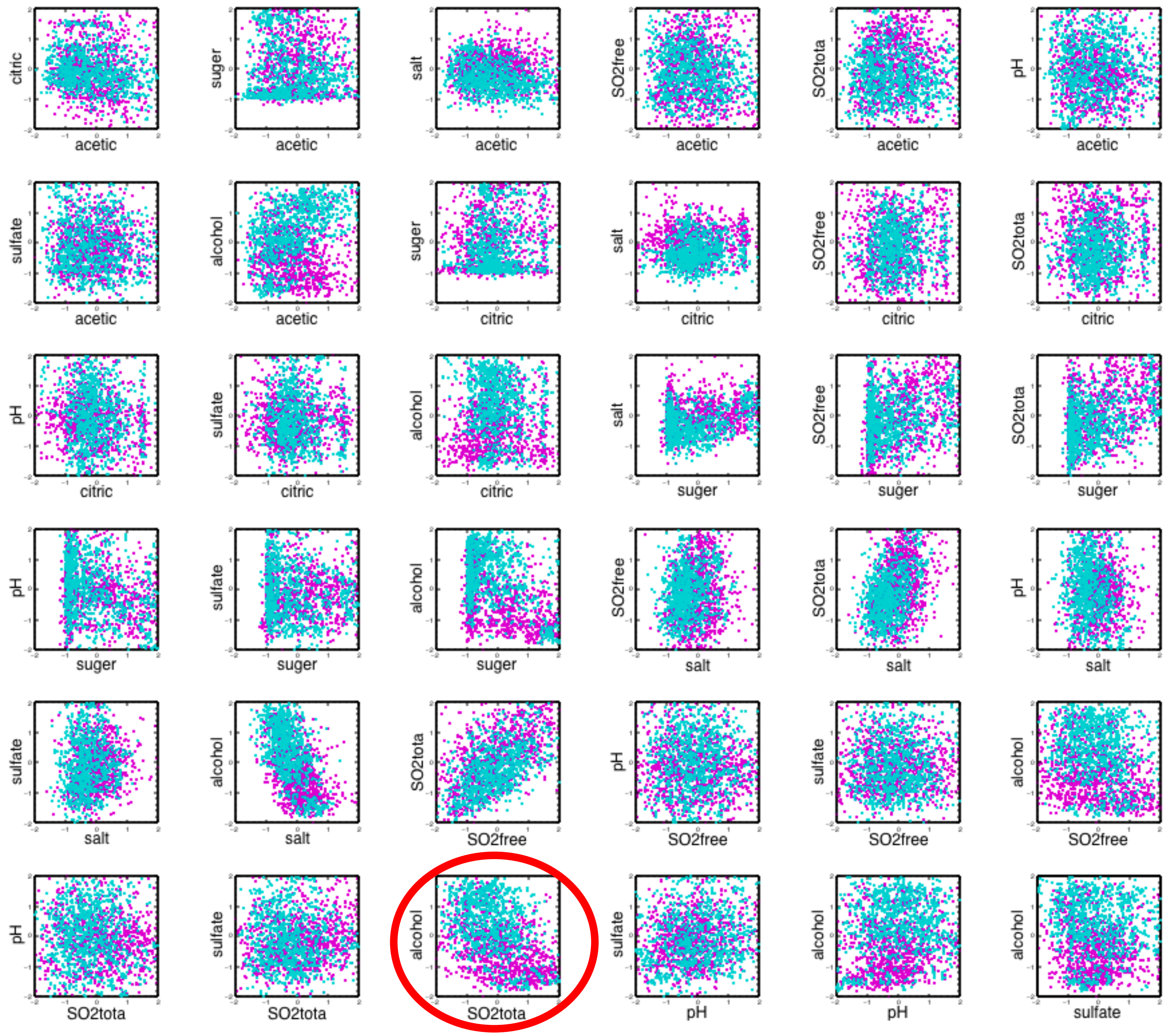
Cortez *et al.**

* P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis. Modeling wine preferences by data mining from physicochemical properties. In Decision Support Systems, Elsevier, 47(4):547-553. ISSN: 0167-9236

Wine Tasting: Data

Data: [Cortez *et al.*, 2009].

variables	**description**
acetic	acetic acid
citric	citric acid
sugar	residual sugar
salt	NaCl
SO2free	free sulfur dioxide
SO2tota	total sulfur dioxide
pH	pH
sulfate	potassium sulfate
alcohol	alcohol content
quality	(between 0 and 1)


citric
acetic
suger
acetic
salt
acetic
SO2free
acetic
SO2tota
acetic
pH
acetic
sulfate
acetic
alcohol
acetic
suger
citric
salt
citric
SO2free
citric
SO2tota
citric
pH
citric
sulfate
citric
alcohol
citric
salt
suger
SO2free
suger
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SO2free
pH
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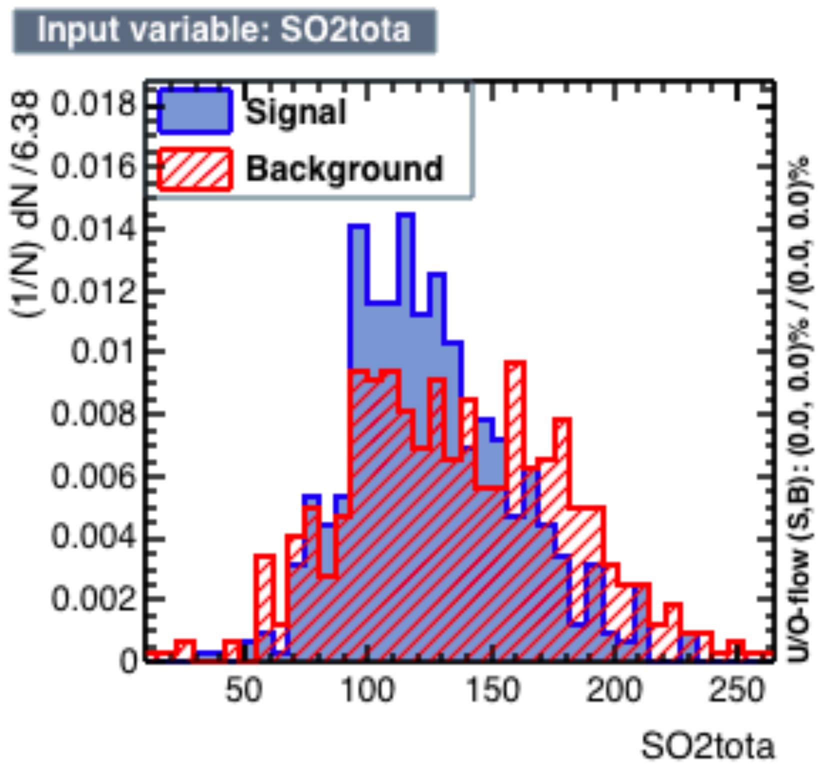
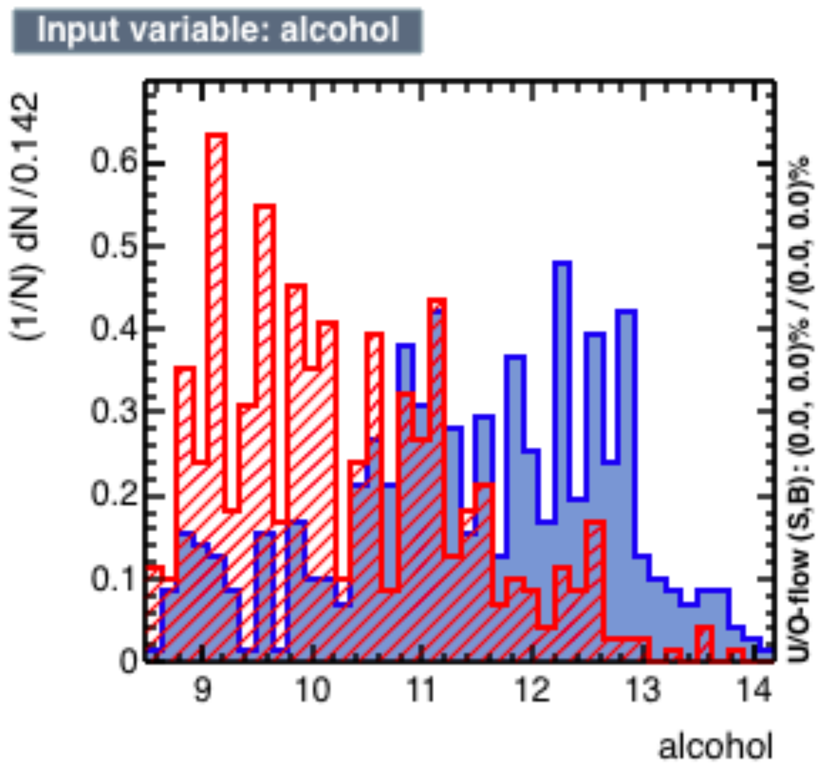
Wine Tasting: Variables

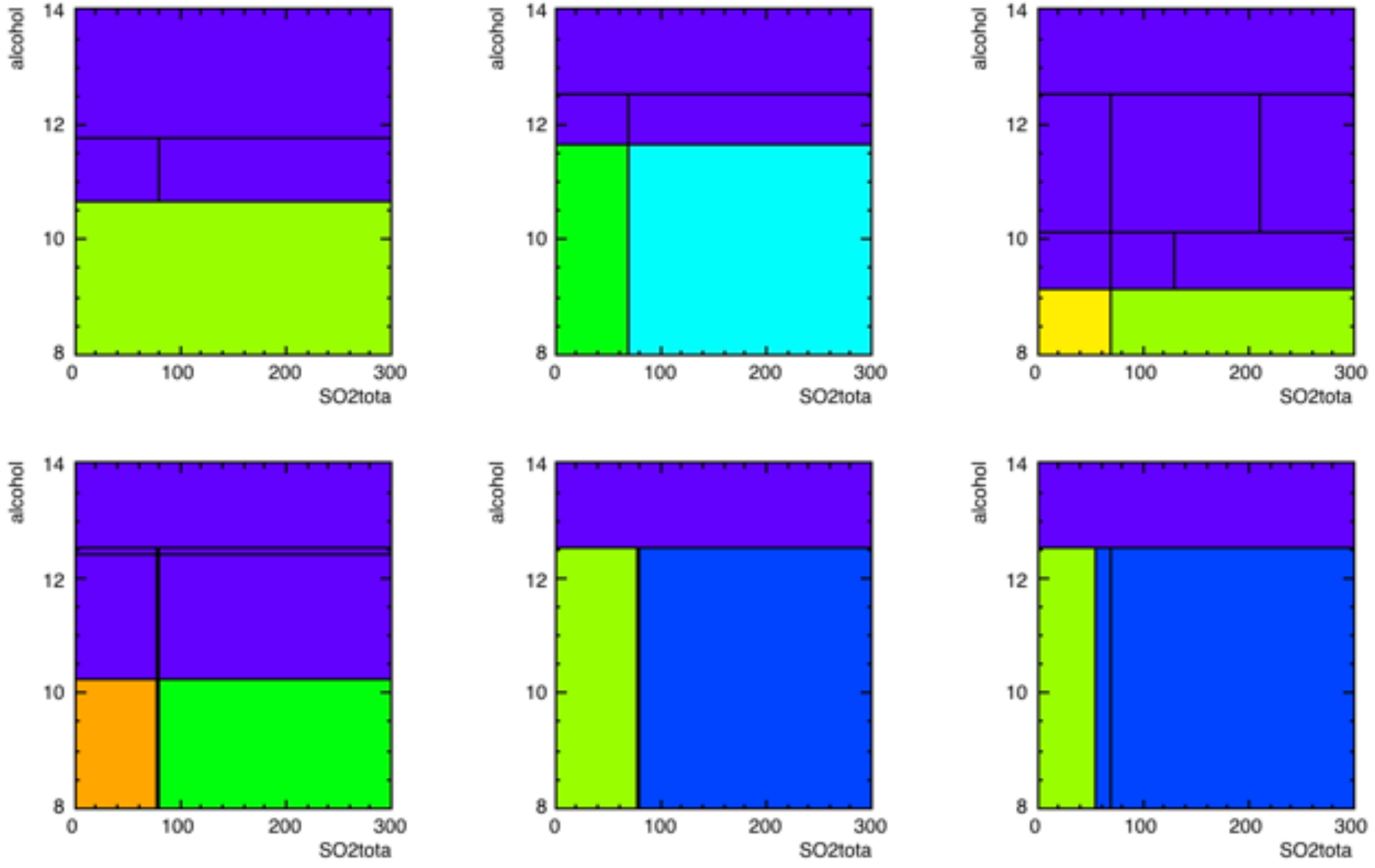
Variables:

- SO2tota: the total sulfur dioxide content (mg/dm^3)
- alcohol: alcohol content (% volume)





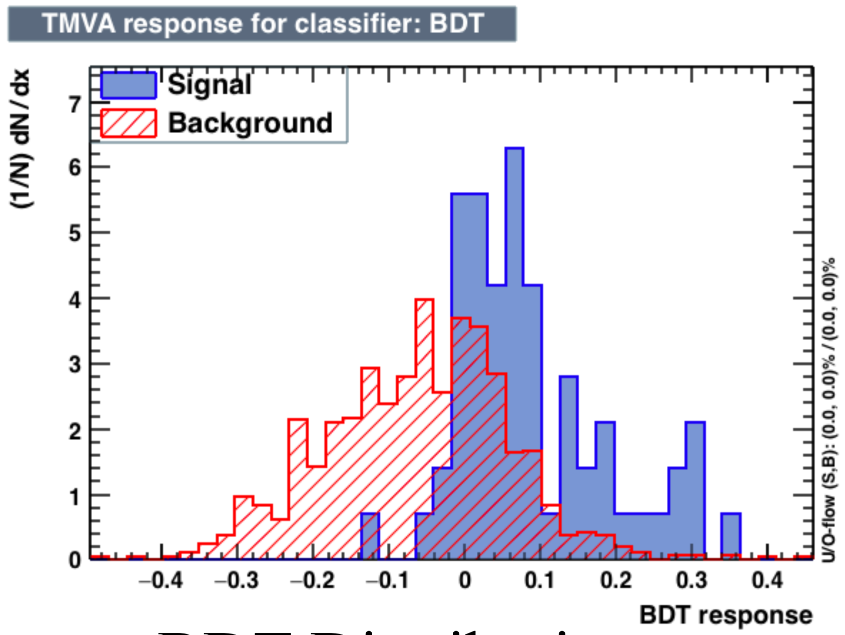
Wine Tasting: First 6 Decision Trees

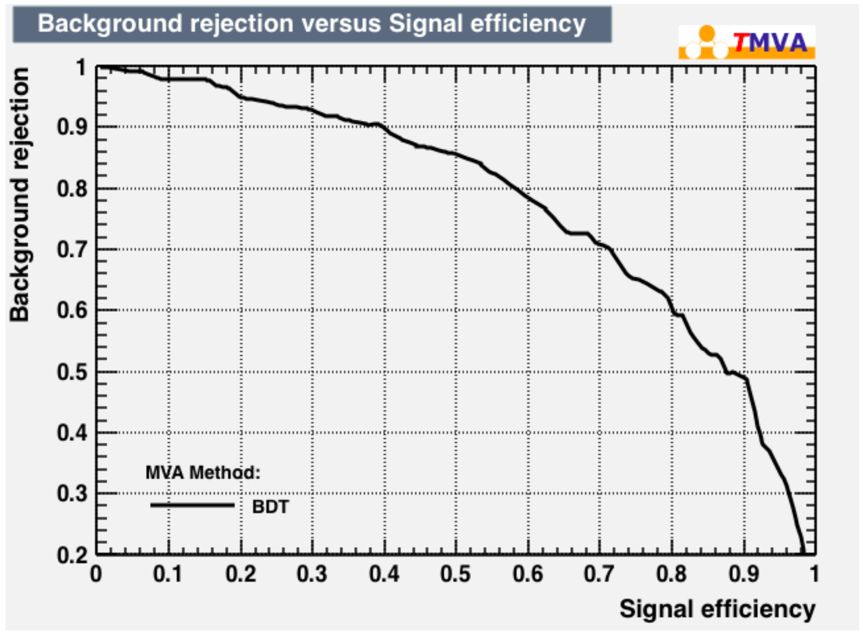


Wine Tasting: Results

x = SO2tota

y = alcohol





BDT Distribution

$$BDT(x,y) = \sum_{k=0}^{99} \alpha_k f(x,y,w_k)$$

Fraction of bad wine rejected for a given fraction of good wine accepted.

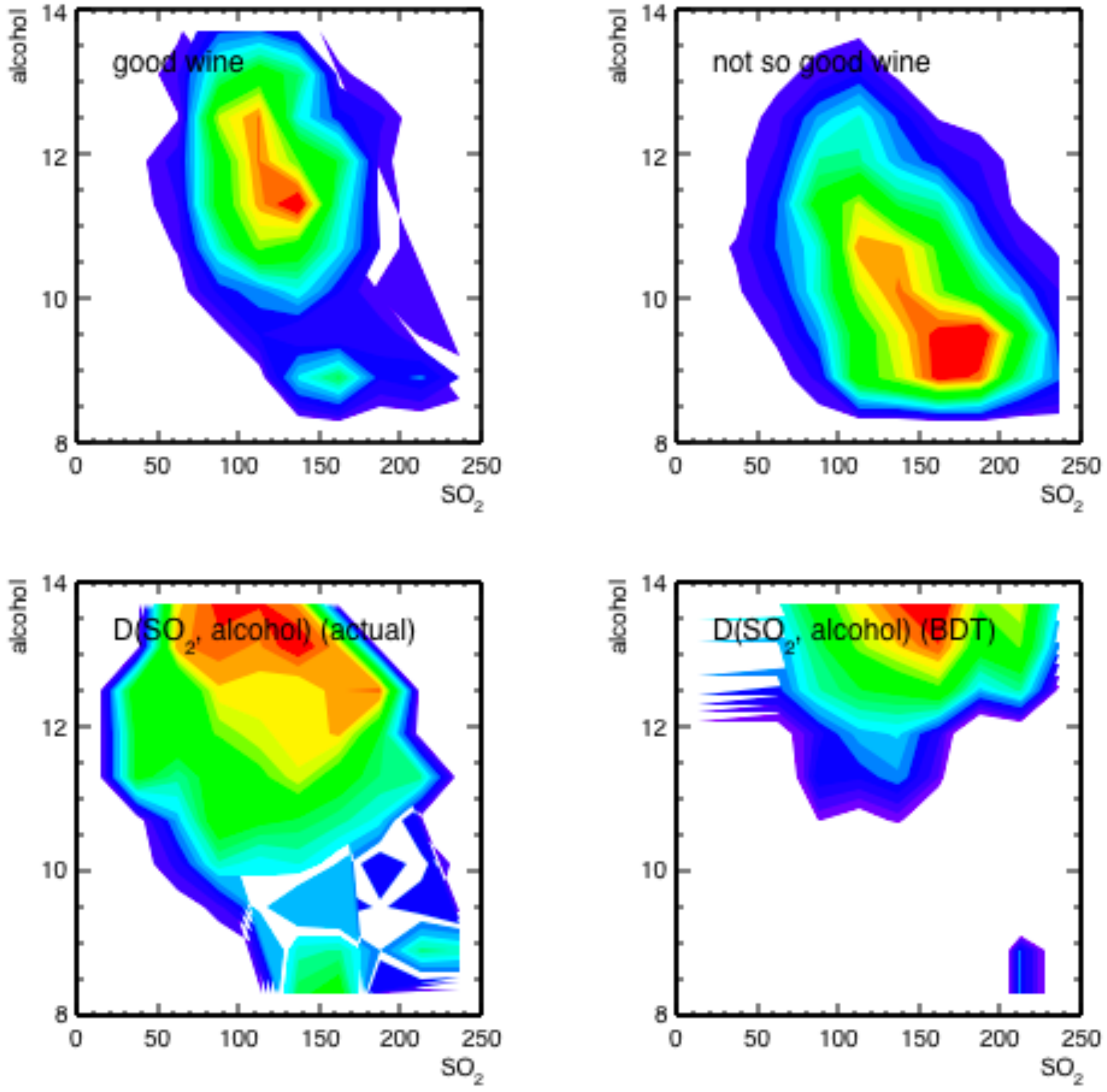
Wine Tasting: Results

The upper figures are density plots of the training data.

The lower plots are approximations of the discriminant

$D(x, y)$

The left, uses 2-D histograms, the right uses the BDT.



NEURAL NETWORKS

A Bit of History: Hilbert's 13th Problem

(One version of Problem 13): Prove

that it is *impossible* to do the following:

$f(x_1,\ldots,x_n) = F(\, g_1(x_{(1)},\ldots, x_{(m)}),\ldots, g_k(x_{(1)},\ldots, x_{(m)}))$

for $m < n$ for all n.

In 1957, Kolmogorov proved that it *was* possible with $m = 3$.

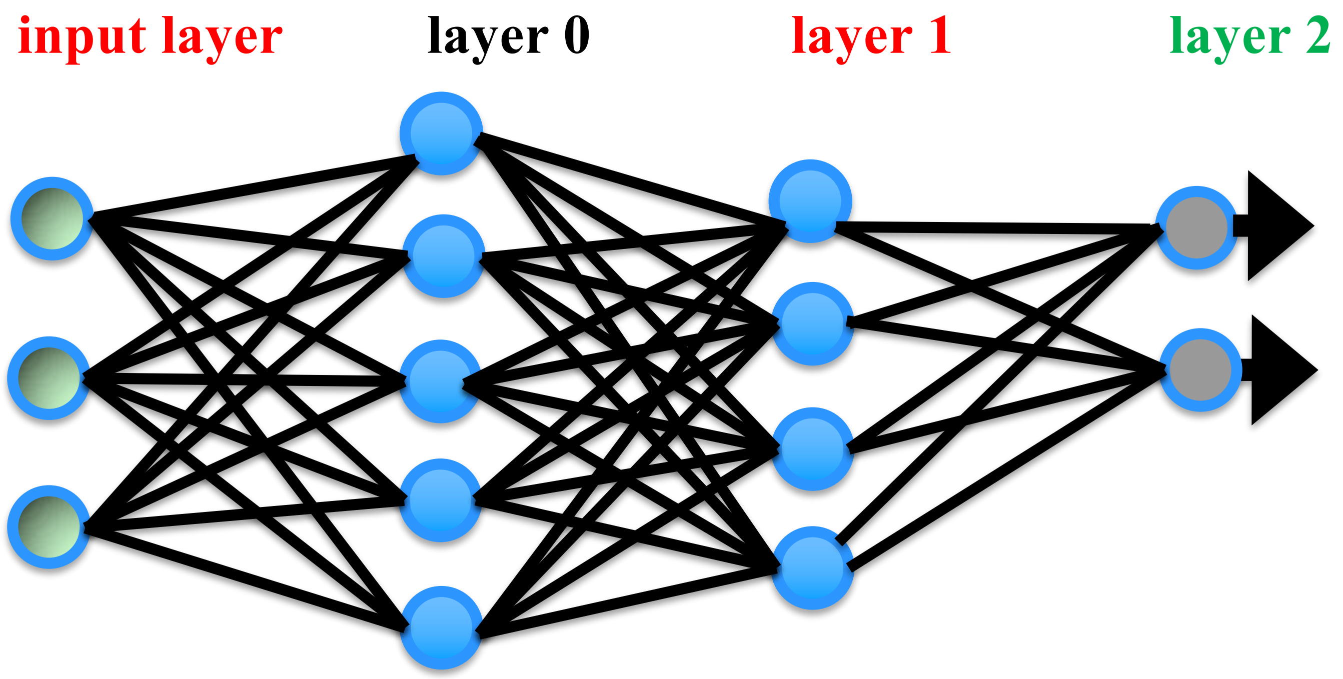
Today, we know that functions of the form

$$f_k(x,w) = \boldsymbol{a_k} + \sum_{j=1}^{H} \boldsymbol{w_{kj}} \boldsymbol{h}\left(\boldsymbol{b_j} + \sum_{i=1}^{I} \boldsymbol{w_{ji}} x_i \right)$$

can provide arbitrarily accurate approximations of real functions of *I* real variables.

(Hornik, Stinchcombe, and White, *Neural Networks* **2**, 359-366 (1989))

Deep Neural Networks



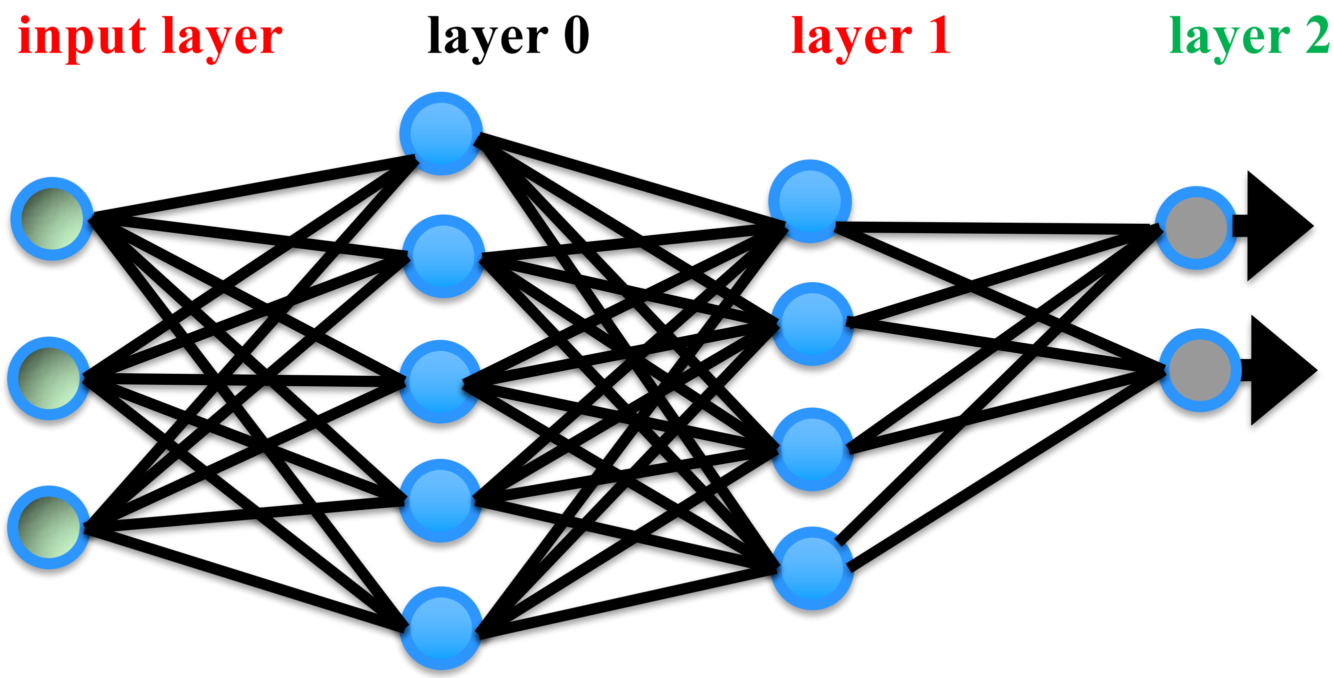
$\boldsymbol{x}$

$\boldsymbol{h}(\mathbf{b}_0 + \mathbf{w}_0\boldsymbol{x})$

$\boldsymbol{h}(\mathbf{b}_1 + \mathbf{w}_1\boldsymbol{h}_1)$

$\mathbf{o} = \boldsymbol{g}(\mathbf{b}_2 + \mathbf{w}_2\boldsymbol{h}_2)$

Deep Neural Networks



A 3-layer DNN

$$o = g(\boldsymbol{b_2} + \boldsymbol{w_2} h(\boldsymbol{b_1} + \boldsymbol{w_1} h(\boldsymbol{b}_0 + \boldsymbol{w_0} x)))$$

$h(z)$ = ReLU(z) [= max(0, z)], tanh(z)

g(z) = Identity(z), logistic(z) = 1/[1 + exp(-z)]

Deep Neural Networks

- In 2006, University of Toronto researchers Hinton, Osindero, and Teh (HOT*) succeeded in training a deep neural network for the first time. Each layer was trained to produce a representation of its inputs that served as the training data for the next layer. Then the entire network was adjusted using gradient descent.

- This breakthrough seemed to provide compelling evidence that the training of deep neural networks requires careful initialization of parameters and sophisticated machine learning algorithms.

* Hinton, G. E., Osindero, S. and Teh, Y. (HOT), A fast learning algorithm for deep belief nets, Neural Computation 18, 1527-1554.

Deep Neural Networks

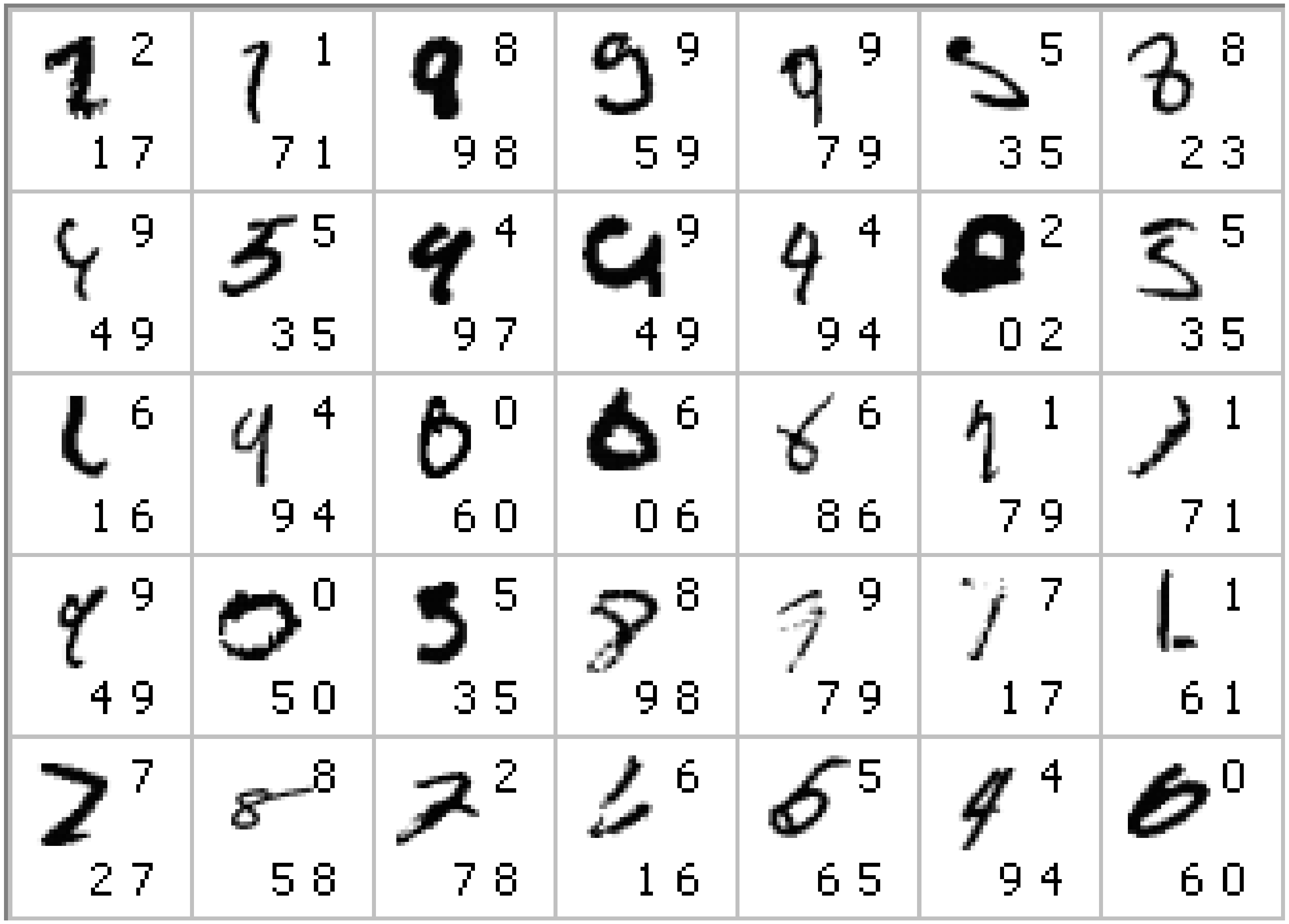
- But, in 2010, Ciresan *et al.** showed that such cleverness was not needed! The authors succeeded in training a DNN with architecture (784, 2500, 2000, 1500, 1000, 500, 10) that classified the hand-written digits in the MNIST database.

- The database comprises 60,000 $28 \times 28 = 784$ pixel images for training and validation, and 10,000 for testing.

- The error rate of their ~12-million parameter DNN was 35 images out of 10,000. The misclassified images are shown on the next slide.

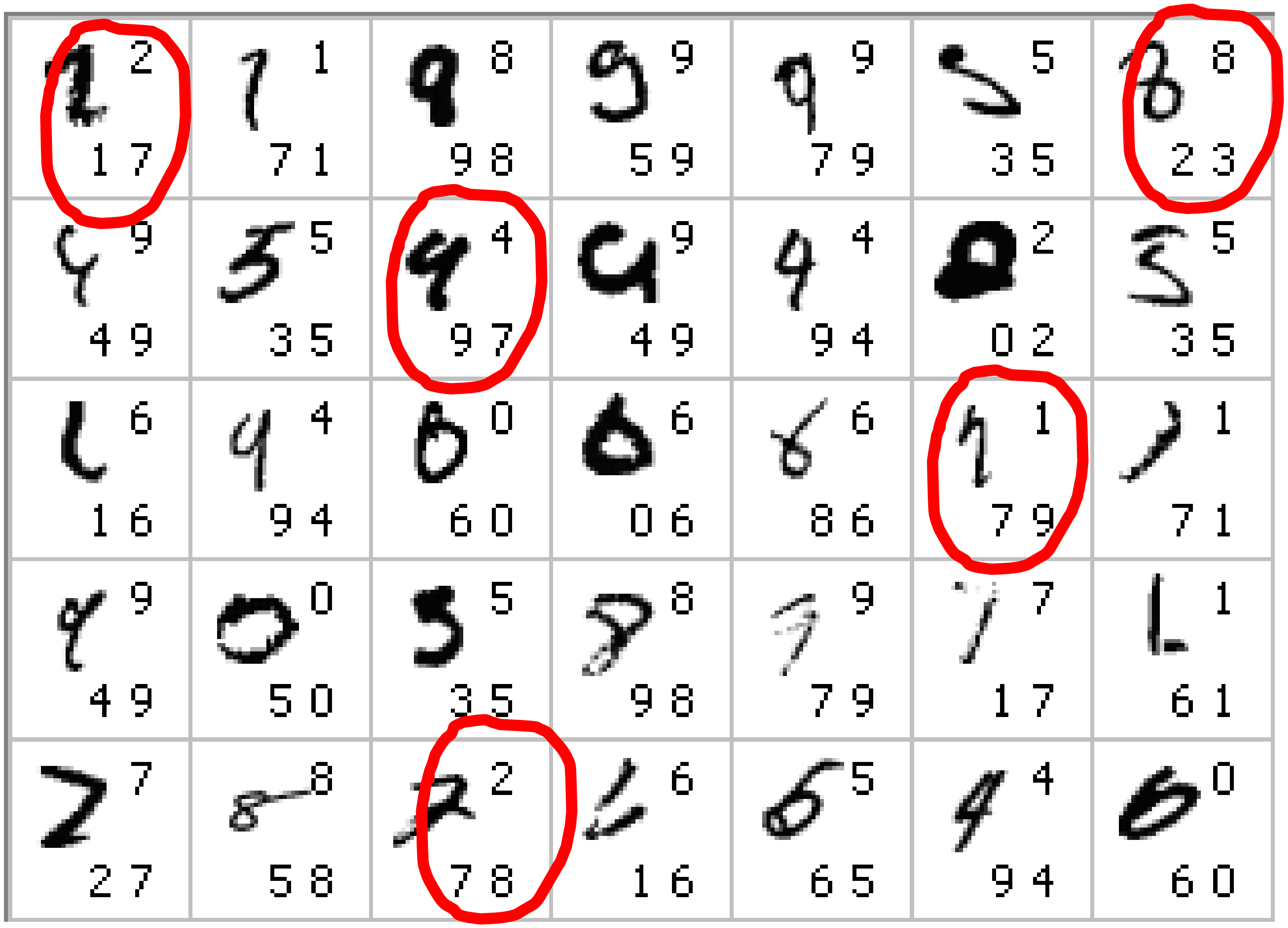
* Cireşan DC, Meier U, Gambardella LM, Schmidhuber J. , Deep, big, simple neural nets for handwritten digit recognition. Neural Comput. 2010 Dec; 22 (12): 3207-20. http://yann.lecun.com/exdb/mnist/

Deep Neural Networks



Upper right: correct answer; lower left answer of highest DNN output; lower right answer of next highest DNN output.

(784, 2500, 2000, 1500, 1000, 500, 10)

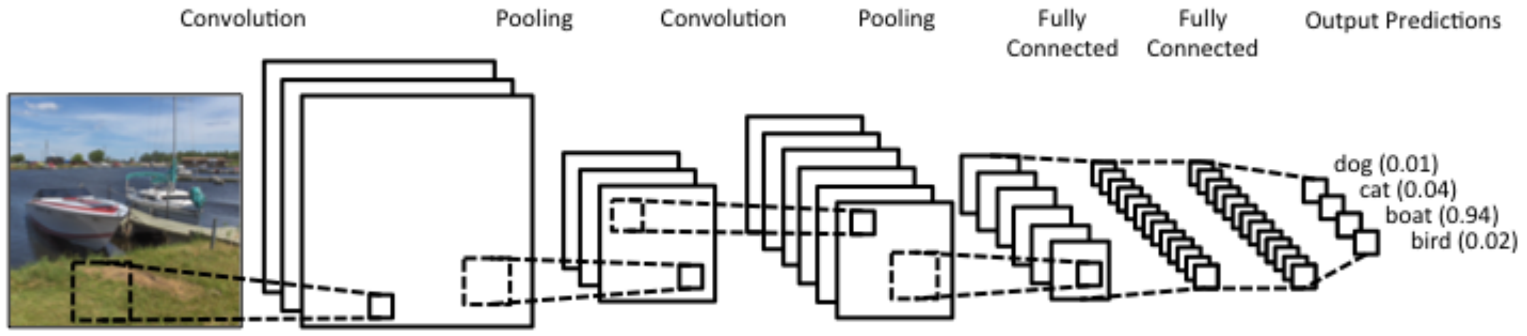


Upper right: correct answer; lower left answer of highest DNN output; lower right answer of next highest DNN output.

Convolutional Neural Networks

Many of the remarkable breakthroughs in tasks such as face recognition use a type of DNN called a convolutional neural network (CNN).

CNNs are *functions* that compress data and classify objects using their compressed representations via a standard fully connected NN. The compression dramatically reduces the dimensionality of the space to be searched.



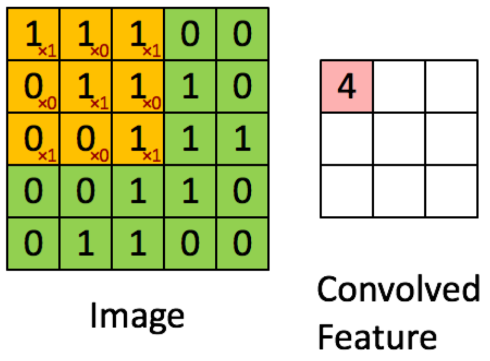
Source: https://www.clarifai.com/technology

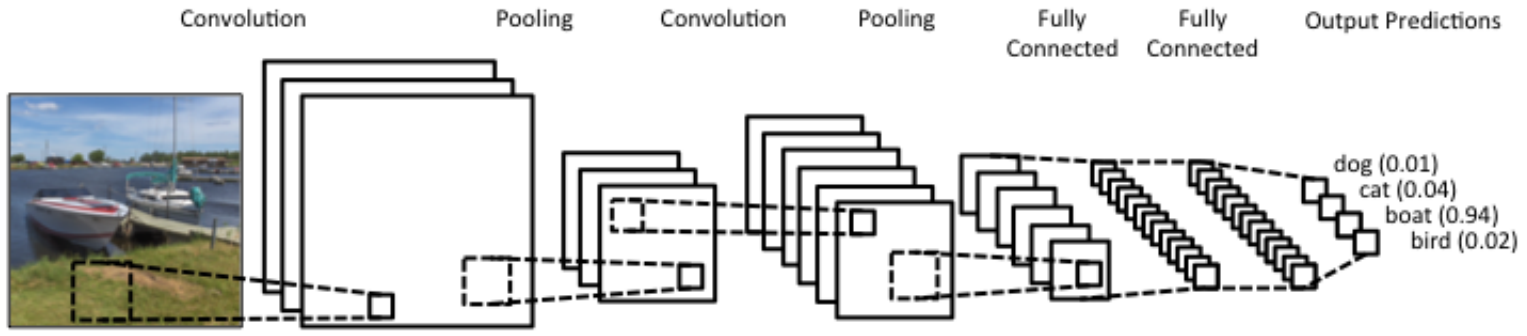
Convolutional Neural Networks

A CNN comprises three types of processing layers: 1. convolution, 2. pooling, and 3. classification.

1. **Convolution layers**

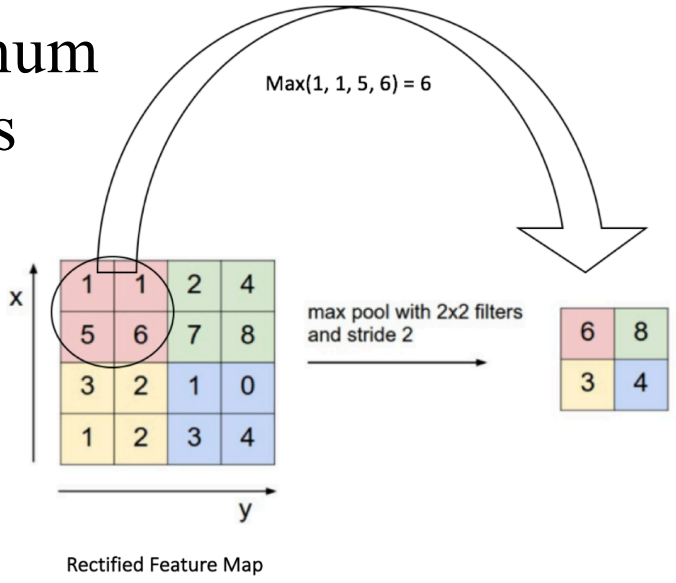
   The input layer is "convolved" with one or more matrices using element-wise products that are then summed. In this example, since the sliding matrix fits 9 times, we compress the input from a 5 x 5 to a to a 3 x 3 matrix.

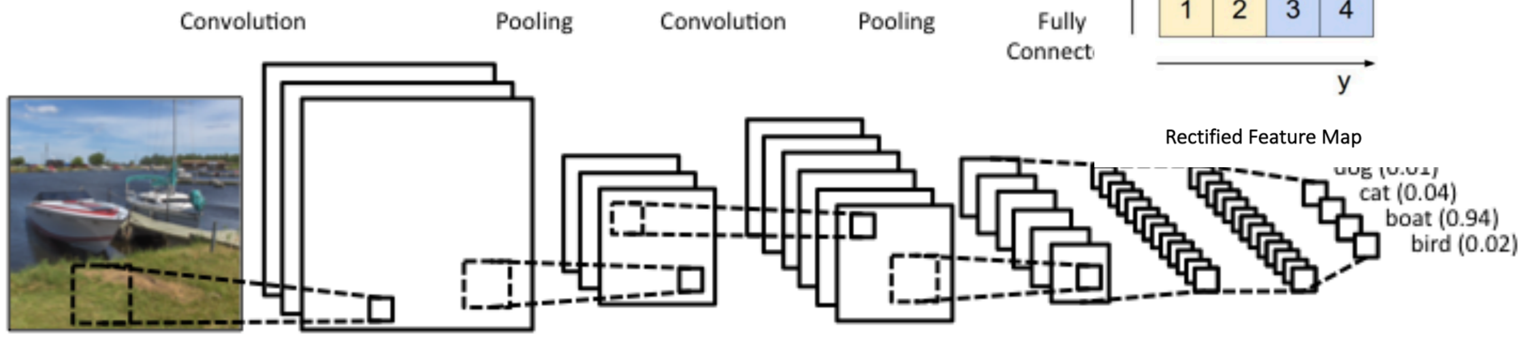




Convolutional Neural Networks

2. **Pooling Layers**
   After convolution, and a pixel by pixel non-linear map (using, e.g., the function $y = \max(0, x) = \mathrm{ReLU}(x)$) a coarse-graining of the layer is performed called max pooling in which the maximum values within a series of small windows are selected and become the output of a pooling layer.



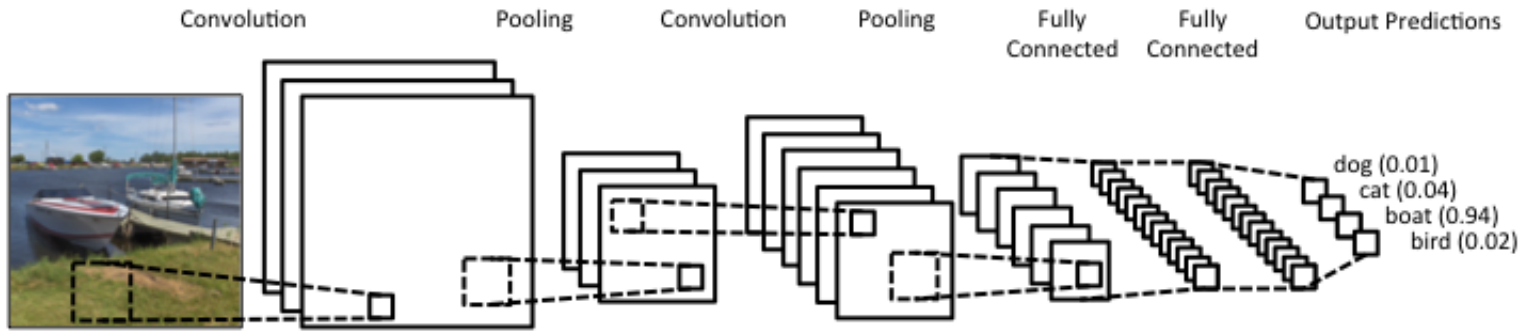


Convolutional Neural Networks

3. Classification Layers

After an alternating sequence of convolution and pooling layers, the outputs go to a standard neural network, either shallow or deep. The final outputs correspond to the different classes and like all flexible classifiers, a CNN approximates,

$$p(C_k|x) = p(x|C_k)p(C_k) / \sum_{m=1}^{M} p(x|C_m)p(C_m)$$



THE FUTURE OF MACHINE LEARNING

McKinsey&Company

MCKINSEY GLOBAL INSTITUTE

A FUTURE THAT WORKS: AUTOMATION, EMPLOYMENT, AND PRODUCTIVITY

JANUARY 2017

EXECUTIVE SUMMARY

“Almost half the activities people are paid almost $16 trillion in wages to do in the global economy have the potential to be automated by adapting currently demonstrated technology, according to our analysis of more than 2,000 work activities across 800 occupations.”

McKinsey & Company,
A FUTURE THAT WORKS: AUTOMATION, EMPLOYMENT, AND PRODUCTIVITY
Executive Summary January 2017

The Future of Machine Learning

By 2056, the following might be in routine use:

1. personal predictive medical systems
2. personal tutors
3. autonomous physician's assistant
4. autonomous house servant
5. autonomous pet sitter
6. autonomous vehicles that can drive safely in Italy!

The potential of AI is vast and exciting.

But it is argued (e.g, Bill Gates, Elon Musk, the late Stephen Hawking) that the *dangers* are also potentially vast: AI autonomous, self-aware, soldiers, AI micro-drone swarms….