

# IMUVA

## ALGORITHMIC LEARNING

### **Analysis, Algebra and Geometry**

S. Xambó

UPC & IMTech

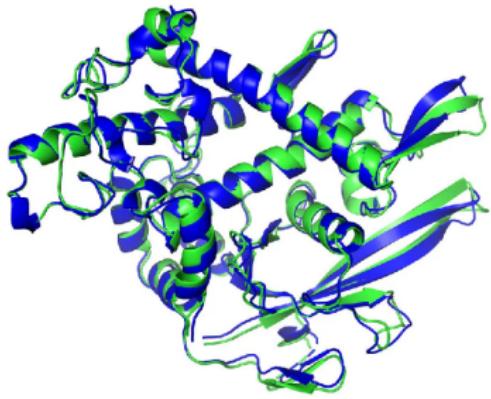
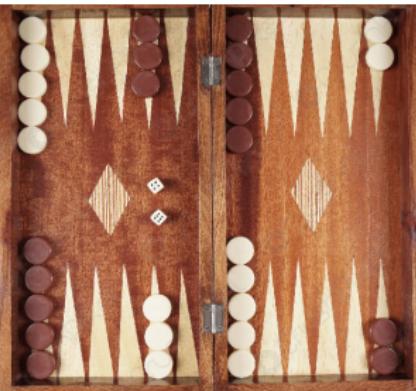
12/11/2021

Interest is Geometric Algebra, Physics, Effective computations, Image processing, Computer Vision:

[1], [2], [3], [4], [5], [6], [7], [8]\*, [9], [10]\*, [11], [12]\*\*, [13]\*\*, [14]\*, [15], [16], [17], [18], [19], [20], [21], [22], [23]\*\*, [24], [25], [26], [27].

A pivotal shift in my interests was meeting [Eduardo U. Moya](#) at the [AGACSE 2015](#) conference in Barcelona, but it was not until the [ICCA11](#) conference in Ghent [17], in August 2017, that we started talking about *the role of GA in DL* and how to go about implementing the *computational aspects*. At that time he was visiting the BSC and we have been collaborating since then ([24] is the first outcome). Later we presented joint work at the [ICIAM-2019](#) MS on “*Systems, patterns, and data engineering with geometric calculi*” which has appeared this year as two chapters of the Springer volume with the same title. Currently he is “[Director de IA](#) de la Coordinación General de Innovación del Estado de Jalisco” (México).

Another momentous influence has been the preparation of [27] with [Joan Bruna](#), followed by our collaboration in this [BGSM](#) course.



Chess, Backgammon, Go, Console games, Protein folding, ...

Beethoven's Unfinished 10th Symphony Brought to Life by Artificial Intelligence (Scientific American, October 15, 2021).

**Water Werzowa:** I dare to say that nobody knows Beethoven as well as the AI, did—as well as the algorithm.

I think music, when you hear it, when you feel it, when you close your eyes, it does something to your body. Close your eyes, sit back and be open for it, and I would love to hear what you felt after.

"The new model suggests the partnership between neuroscience and AI could also move beyond our understanding of each one alone and instead find the general principles that are necessary for brains and machines to be able to learn anything at all." QM21-10-18.

NEURAL NETWORKS

## Neuron Bursts Can Mimic Famous AI Learning Strategy

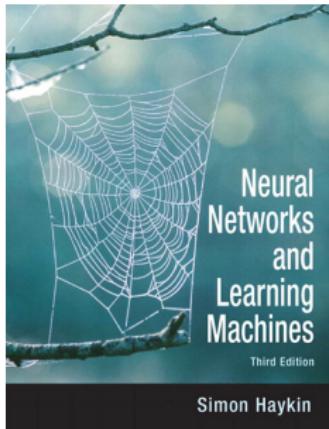
*A new model of learning centers on bursts of neural activity that act as teaching signals --- approximating backpropagation, the algorithm behind learning in AI.*



Allison Whitten

Source: Nature neuroscience

Reference: [28], *Learning representations by back-propagating errors*, Nature-86-10-09.



Shai Shalev-Shwartz and Shai Ben-David

# UNDERSTANDING MACHINE LEARNING

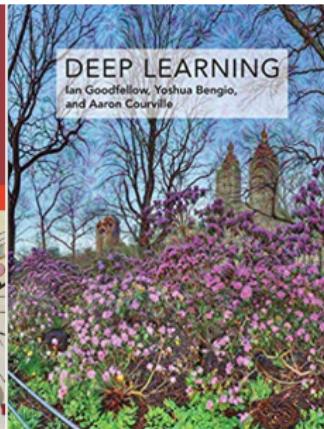
FROM THEORY TO ALGORITHMS



Neural  
Networks  
and  
Learning  
Machines

Third Edition

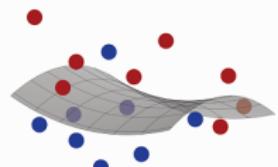
Simon Haykin



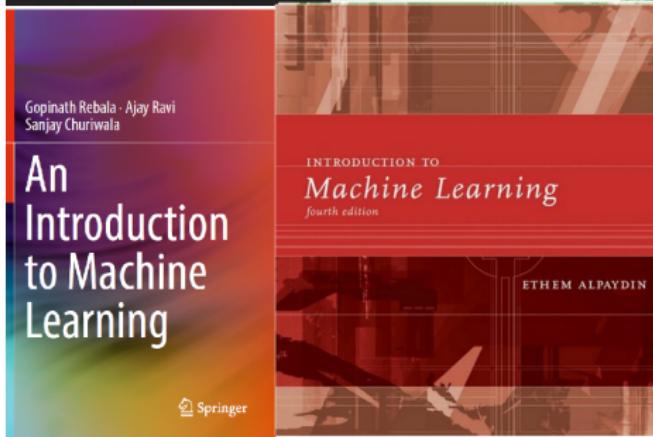
# DEEP LEARNING

Ian Goodfellow, Yoshua Bengio,  
and Aaron Courville

Foundations of  
Machine Learning second edition



Mehryar Mohri,  
Afshin Rostamizadeh,  
and Ameet Talwalkar



An  
Introduction  
to Machine  
Learning

Springer

INTRODUCTION TO  
*Machine Learning*

fourth edition

ETHEM ALPAYDIN

Learning Theory from First Principles  
Draft

François Fleuret  
Georgia Institute of Technology

June 28, 2011

The Principles of Deep Learning Theory  
*An Axiomatic Theory Approach to Understanding Neural Networks*

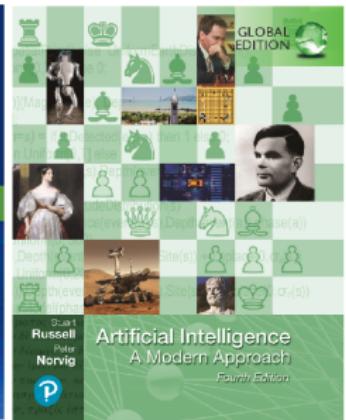
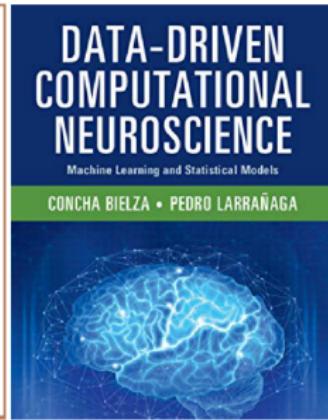
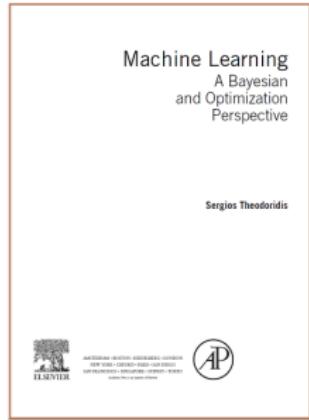
David A. Rosenberg and Shie Yekhanin

Joint research in collaboration with

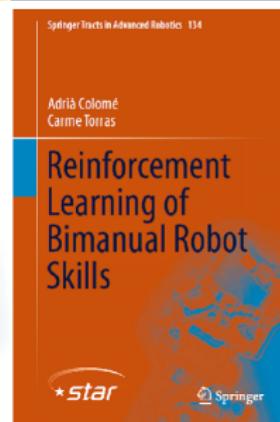
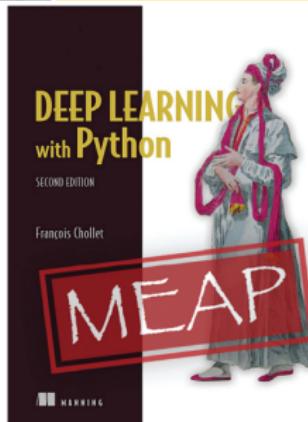
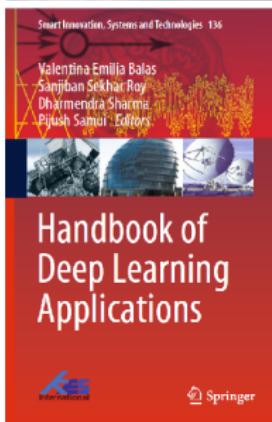
Doris Hahn

drosenst@mit.edu, shieyekhanin@gmail.com

## Bayesian approaches



# Applications



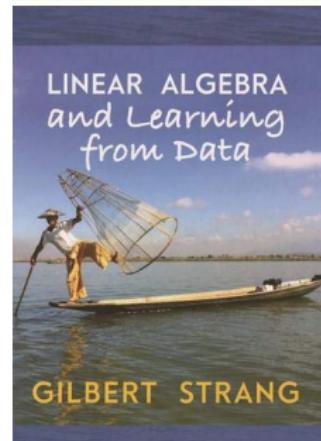
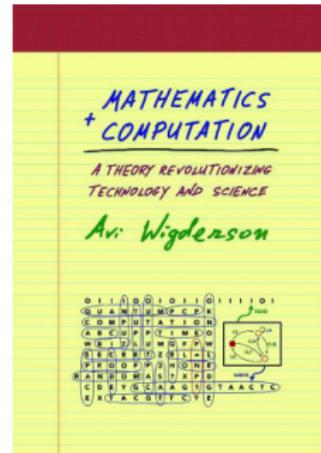
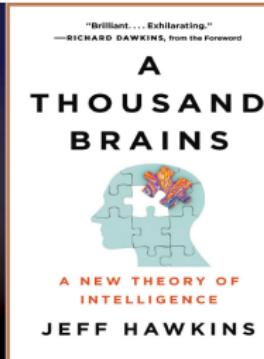
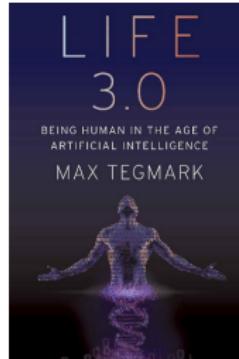
The many facets of the symbiosis

Mathematics & Computation are appraised in [29] (wigderson-2019).

In particular, Chapter 17 is devoted to computational learning theory.

See also the extensive survey [30] and, with a more popular style, Marr's blog [31].

Another useful reference is [32] (strang-2019).



## Bayes rule

Learning from experience is neatly encoded, in probabilistic terms, by the *Bayes-Laplace rule*:

$$P(Y|X) = P(Y)K(X, Y),$$

where  $K(X, Y) = P(X \cap Y)/P(X)P(Y)$  is symmetric ( $K(X, Y) = K(Y, X)$ ), which tells us how to modify our *prior* belief in  $Y$ ,  $P(Y)$ , to the belief  $P(Y|X)$  *posterior* to having observed  $X$ .

When  $K > 1$  ( $K < 1$ ), our belief is *increased* (*decreased*), and in any case it may be construed as a *learning* on  $Y$  produced by the observation of  $X$ .

The condition  $K = 1$  is equivalent to say that  $X$  and  $Y$  are independent, and in this case the belief in  $Y$  is unaffected by whether or not  $X$  occurs.

The Bayes–Laplace rule is the basis for *prediction models* of many sorts, as for example in weather forecasting.

Aimed at finding *hidden structure in data*,  $\mathcal{D} = \{x^1, \dots, x^m\}$ .

**$k$ -Means.** This algorithm groups unlabeled data  $\mathcal{D}$  in  $k$  classes:

- (1) Select  $k$  vectors  $z^1, \dots, z^k \in \mathcal{D}$  at random.
- (2) Assign each  $x^j \in \mathcal{D}$  to the first  $z^i$  nearest to  $x^j$  (initial groups).
- (3) Update each  $z^i$  to the *centroid* (or *mean*) of the  $z^i$  group.
- (4) Iterate (2) and (3) until the  $z^i$  are stable (up to a *tolerance*).

The associated *cluster predictor* assigns  $x$  to the first nearest  $z^i$ .

**$k$ -NN** (nearest neighbors). Let  $\mathcal{D} = \{(x^1, y^1), \dots, (x^m, y^m)\}$  be a labeled set and  $k$  a positive integer. The label predictor of the  $k$ -NN algorithm assigns a vector  $x$  to the mode of  $y^{j_1}, \dots, y^{j_k}$ , where  $x^{j_1}, \dots, x^{j_k}$  are the nearest neighbors of  $x$  from among  $x^1, \dots, x^m$ .

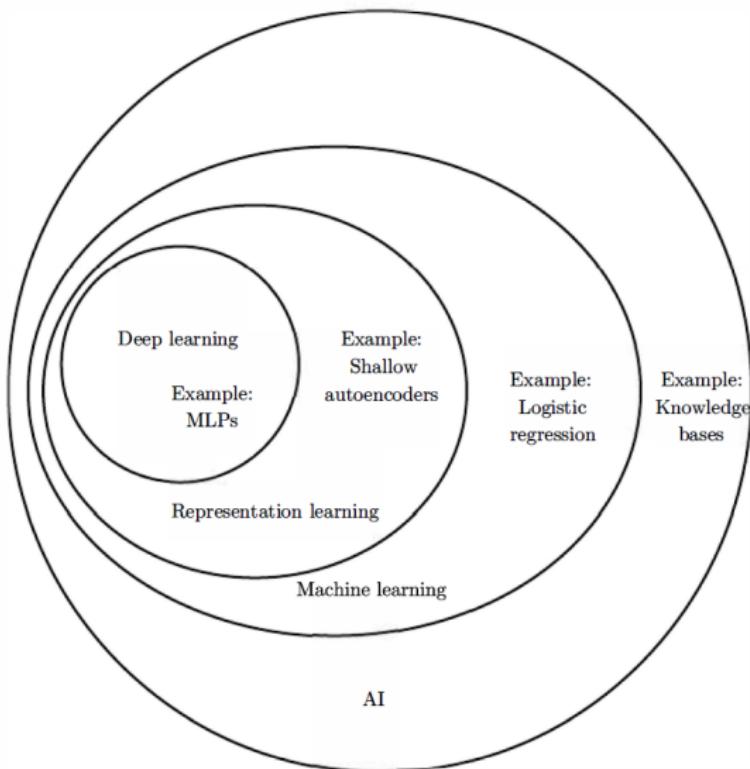
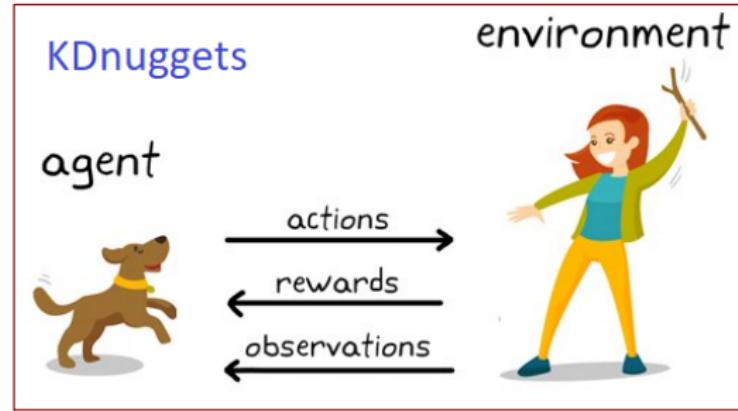
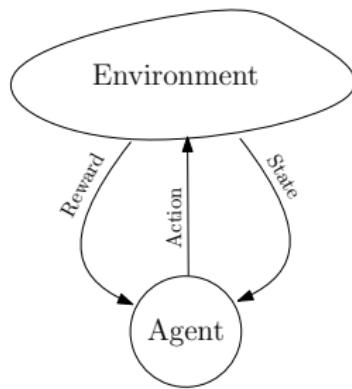


Figure 2.1: Inclusion relations:  $DL \subset RL \subset ML (AL) \subset AI$  (cf. [33]).

## Algorithm learns to *react* to an *environment*

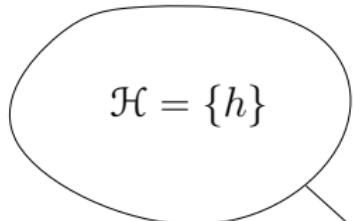


"We demonstrate how by using a *reinforcement learning algorithm*, the deep cross-entropy method, *one can find explicit constructions and counterexamples to several open conjectures in extremal combinatorics and graph theory*.

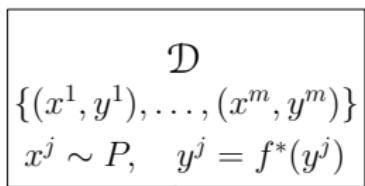
Amongst the conjectures we refute are a question of Brualdi and Cao about maximizing permanents of pattern avoiding matrices, and several problems related to the adjacency and distance eigenvalues of graphs." [34, Abstract].

An interesting feature is that in some cases the learning algorithm does not produce directly a counterexample but graphs which are close to refuting the conjecture; these graphs have a special structure and give a very clear indication about where to search for counterexamples. See IMTech NL01, p. 20 ([https://imtech.upc.edu/en/communication/nesletter/nl01\\_web.pdf](https://imtech.upc.edu/en/communication/nesletter/nl01_web.pdf)).

Hypothesis space<sup>3</sup>



Data, expert tables<sup>2</sup>



World – Observer<sup>1</sup>



Error measure<sup>4</sup>



Learner/LA<sup>5</sup>



Prediction rule<sup>6</sup>

$$y = h(x)$$

<sup>1</sup> *Urbi et Orbi* engraving (Flammarion). **Tycho Brahe** (observer model): He experienced the solar eclipse of 21 August 1560 [he was 15], and was greatly impressed by the fact that it *had been predicted, although the prediction based on current observational data was a day off*. He realized that *more accurate observations* would be **the key to making more exact predictions**. <sup>2</sup> **Ephemeris**: Tables of planet and comet positions over time.

<sup>3</sup> *Inductive bias*. Greeks: circles around Earth. <sup>4</sup> *Loss, risk, regret*. How close are predictions to observations?

<sup>5</sup> Learner model (Kepler): Ellipses with a focus at the Sun. Today: Learning algorithm. <sup>6</sup> Hopefully,  $h \approx f^*$ .

Set of objects  $x^j, j \in [m]$  (*dataset*).

Want to predict values  $y^j$  provided by a *supervisor* or *expert* in such a way that for objects  $x$  not in the dataset the value  $y$  corresponding to  $x$  is predicted with high probability (*generalization* capacity).

*Hypothesis space*: a space of parameterized functions,

$$\mathcal{H} = \{h_w\}_{w \in W}.$$

**Problem**: to find  $w \in W$  such that  $h_w(x^j) \approx y^j$ .

**Method**: If the criterion for fitness depends on a function  $\ell(h(x), y)$  (*local cost*), we transfer the problem to finding  $w$  that minimizes  $\sum_j \ell(h_w(x^j), y^j)$  (*empirical cost* or *risk*):

$$\operatorname{argmin}_w \sum_j \ell(h_w(x^j), y^j).$$

This is the *empirical risk minimization* rule, **ERM**.

Supervised learning has two main modalities:

*Classification*: When the set  $\mathcal{Y}$  is finite. In this case its elements are usually called *labels* or *classes*.

*Regression*: When the set  $\mathcal{Y}$  is the set  $\mathbb{R}$  of real numbers.

In *linear regression*,  $\mathcal{H}$  is the space of functions of the form

$$h(x) = w_1x_1 + \cdots + w_nx_n = w \cdot x$$

and the local cost is usually  $(h(x) - y)^2$ .

*Logistic regression* is linear regression of the function  $\log \frac{p}{1-p}$ ,  $p \in [0, 1]$ . If  $w$  is a solution, then  $p = 1/(1 + e^{-w \cdot x})$ .

In AL, a useful model of a *neuron* is depicted in Fig. 3.1:

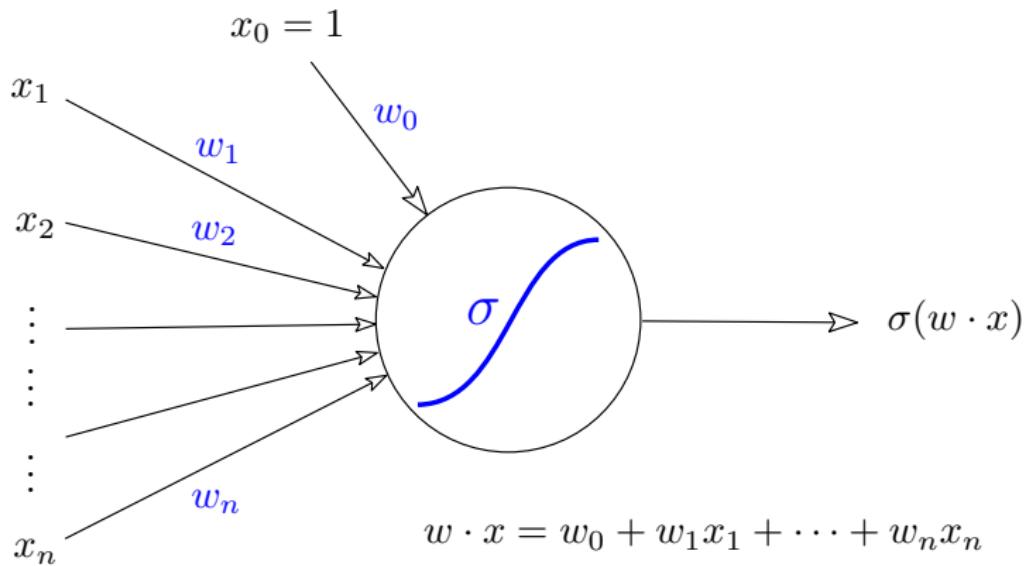


Figure 3.1: Scheme of a neuron. The neuron's output depends on the weights  $w$  and on  $\sigma$  (*activation function*), and this functionality is represented by the decorated circle.

In mathematical terms, a neuron is a function

$$x \mapsto f_w(x) = \sigma(x \cdot w), \quad (1)$$

where  $w \in \mathbb{R}^n$  (*weights* or *parameters*) and  $\sigma$  is a *sigmoid* function (called *activation function*), like for instance the *logistic function*  $\sigma(t) = (1 + e^{-t})^{-1}$ , in which case the neuron computes a *logistic regression*.

Augmenting  $x$  with  $x_0 = 1$  and providing an extra weight  $w_0$  (called the *bias*), the neuron computes  $\sigma(w_0 + w_1 x_1 + \dots + x_n w_n)$ .

To display separately the bias and the other weights, we may write  $f_{w,w_0}$  or some similar notation.

A *neural network* (NN) can be construed as a *composition of neurons* according to a graph of connections called the *architecture* of the net.

Here we will consider the case of *directed graphs* and thus leaving aside nets based on undirected graphs such as *Boltzmann machines*. Nor will we discuss networks with feedback (those having closed paths), such as the *Hopfield networks*.

The standard architecture of a NN is a directed graph structured in *layers*  $L_j$ , as illustrated in Figure 4.1, and its *functional signature* can be condensed as a chain:

$$\mathcal{N} : \text{Input} \xrightarrow{f_1} L_0 \xrightarrow{f_2} L_1 \xrightarrow{\dots} L_{d-1} \xrightarrow{f_d} L_d \rightarrow \text{Output} \quad (2)$$

The integer  $d$  is the *depth* of the net. Conventionally, the net is *deep* if  $d > 2$ , and *shallow* otherwise. The layers  $L_1, \dots, L_{d-1}$  are considered to be *hidden*, while the input and output layers ( $L_0$  and  $L_d$ ), are *visible*.

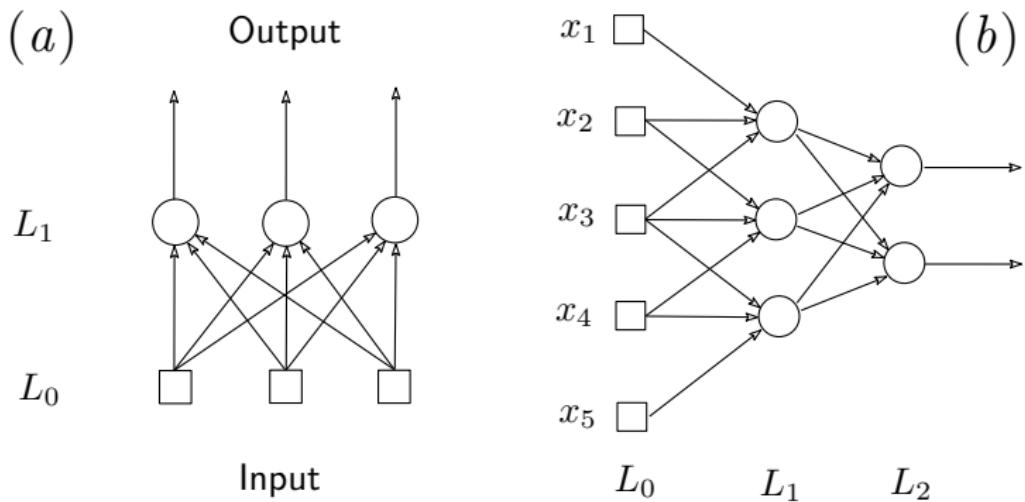


Figure 4.1: (a) Neural network with no hidden neurons and *fully connected*. (b) Network with a hidden layer  $L_1$  of three neurons fully connected to the two output neurons of  $L_2$ . The input layer,  $L_0$ , is only partially connected to  $L_1$ .

The quantities  $x_j$  and  $w_j$  used in the neuron model introduced in equation (1) are real numbers. But we can imagine that they are entities of an algebraic structure  $\mathcal{A}$  sufficient to guarantee that the expression  $x \cdot w = x_1 w_1 + \dots + x_n w_n$ , and an activation function  $\sigma : \mathcal{A} \rightarrow \mathcal{A}$ , make sense.

For example,  $\mathcal{A}$  can be a real algebra of finite dimension and  $\sigma$  the function of an ordinary sigmoid applied component-wise (with respect to a fixed basis of the algebra). We thus arrive at the concept of  *$\mathcal{A}$ -neuron* and, connecting neurons as we have done before, to the notion of  *$\mathcal{A}$ -neural network*, or  *$\mathcal{A}$ -NN*.

Another generalization is to replace  $x$  and  $w$  with more general data structures, such as  *$\mathcal{A}$ -arrays* (or *tensors*), and the product  $x \cdot w$  by a suitable operation  $x \star w$ . Among these operations, the most commonly used are certain bilinear products, such as *cross-correlation*, as well as nonlinear ones, such as *max-pooling*.

Thus the conventional (artificial) neurons and neural networks are **R**-neurons and **R**-neuronal networks.

Beyond real numbers, among the most immediate concrete cases of algebras **A** we can mention **C** (complex numbers), **H** (quaternions), **O** (octonions), an algebra of matrices **R(n)**, or a geometric algebra  $\mathcal{G} = \mathcal{G}_{r,s}$  of signature  $(r,s)$ . N

To simplify the terminology, we will talk about real, complex, quaternionic (QNN), octonionic (ONN), matrix (MNN), and geometric (GNN) networks, respectively.

One advantage of  $\mathcal{A}$ -neurons is that the number of (real) weights they require decreases in inverse proportion to  $d = \dim \mathcal{A}$ . The argument is based on the simple observation that  $w \in \mathcal{A}$  counts for  $d$  real weights, whereas both  $x$  and  $x' = x \star w$  count for  $d$  real parameters each and hence we need  $d^2$  real weights to connect them.

Another advantage is that the algebraic structure of  $\mathcal{A}$  can be regarded as a resource for describing and implementing AL algorithms, a point that is particularly relevant when  $\mathcal{A}$  is a geometric algebra on account of its intimate connection with the geometry of its geometric space.

**Remark.** This is not unlike the use of finite fields as alphabets for coding information, for being able to sum, multiply and divide alphabet symbols turns out to represent a great bonus with respect to a set with no structure.

Besides the further references provided henceforth, we find that the text [35] is a remarkably inspiring early reference for most of the topics discussed in this section. In particular, it studies complex NNs in chapter 2 and QNNs in chapter 5. It also features interesting applications of these algebras to predict chaotic time series (chapter 6) and to robotics (chapter 7).

Perhaps the most important idea of these networks is that they can exploit the phase properties of complex numbers.

At the beginning of the study of these networks, the contributions of Hirose and his school stand out. They focus on signal processing, with collections such as [36] (2003) and treated as [37] (2009), or [38] (2012; a second edition of a book of the same title and author published in 2006), and the collection of ten articles collected in [39] (2013), of which the first stands out, by Hirose himself (the editor of the volume), with the title *Application fields and fundamental merits of complex-valued neural networks*.

The text [40] belongs to the same circle, which illustrates with very convincing graphic experiments the value of considering the phase.

More recently we have [41] (2016), on complex convolutional networks; [42] (2017), focused on image classification; [43] (2017), where the emphasis is on deep networks; and [44] (2018), which provides an assessment of complex networks in real signal classification tasks.

Finally we mention [45], which reveals the significance of complex networks from other points of view, particularly that of deep AL, an “umbrella term for emerging techniques that attempt to generalize deep (structured) neural models to non-Euclidean domains such as graphs and varieties.”

The interest of these networks comes from the relation that the quaternions keep with the group of rotations of the ordinary Euclidean space, a relation especially transparent in terms of  $\mathbf{H} = \mathcal{G}_3^+$ , for the expression  $\underline{h}(x) = h x \bar{h}$ ,  $h \in \mathbf{H}$  non-zero, is a vector and  $\underline{h}$  is a similarity of ratio  $|h|^2$  (a rotation if  $h$  is unitary).

Another reason is that quaternions have three phases and that these phases can be used to extract valuable information from the signals to be processed.

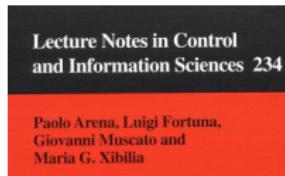
Research in QNNs also comes from long ago, even before that of complex networks. We refer to [46] and [47] for relevant historical information regarding what is called *Clifford's analysis*, especially in relation to Fourier and wavelet transforms in a quaternionic context and their generalization to the geometric context.

In the origin of the more specific topic we are considering, we find Gerald Sommer and his collaborators: [48] (generalization of Gabor filters) and [49] (generalization of the real multilayer perceptron, cf. [50]).

The report [51] presents a quaternion wavelet theory “for image analysis and processing” and [52] an overview of the properties and applications of quaternion networks up to that point.

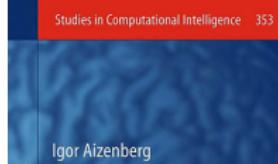
In the last decade, research on **QNNs** has continued both on the applied and theoretical fronts.

The article [53] deals with the quaternionic multilayer perceptron. **Hopfield QNNs** and their rotation invariance are investigated in [54]. In the works [55] and [56], the **QNNs** are applied to the comprehension of the spoken language. Deep **QNNs** are studied in [57] and convolutional ones in [58]. Finally [59] presents a quaternionic version of capsule networks aimed at processing point clouds in Euclidean space and in [24] a new **QNN** deterministic layer is introduced that provides contrast invariance and sensitivity to rotation angles using quaternionic Gabor functions and Hilbert transforms, while in [25] the authors use the Riesz transform in the quaternion monogenic representation to propose a novel deterministic convolution layer in the Fourier domain robust to contrast and haze changes in image classification.



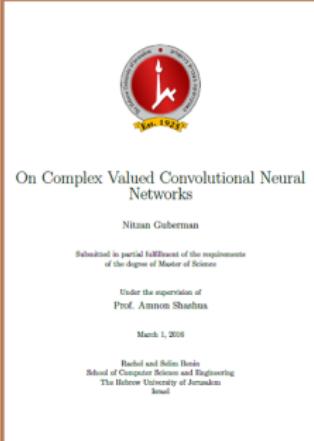
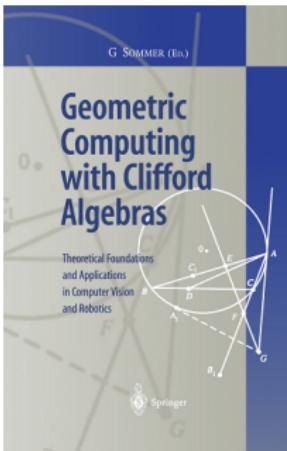
## Neural Networks in Multidimensional Domains

Fundamentals and New Trends in Modelling and Control



Igor Aizenberg

## Complex-Valued Neural Networks with Multi-Valued Neurons



## On Complex Valued Convolutional Neural Networks

Nitzaa Guberman

Submitted in partial fulfillment of the requirements  
of the degree of Master of Science

Under the supervision of  
Prof. Amnon Shashua

March 1, 2005

Racheli and Reuven Bein  
School of Computer Science and Engineering  
The Hebrew University of Jerusalem  
Israel



## A Theory of Neural Computation with Clifford Algebras

Dissertation

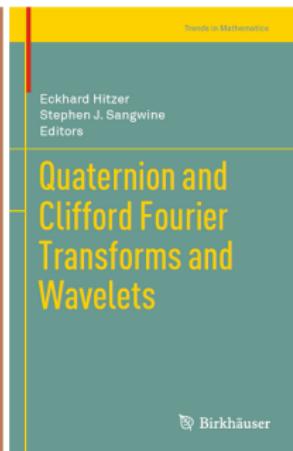
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Doktor der Ingenieurwissenschaften  
(Dr.-Ing.)

der Technischen Fakultät

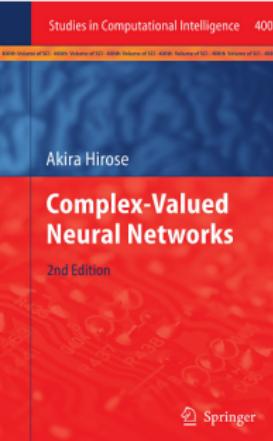
der Christian-Albrechts-Universität zu Kiel

Sven Bachthäuser

Kiel  
2005



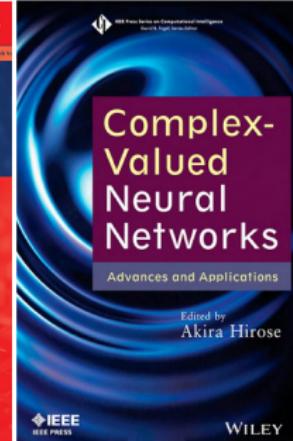
## Quaternion and Clifford Fourier Transforms and Wavelets



Akira Hirose

## Complex- Valued Neural Networks

2nd Edition



## Complex- Valued Neural Networks

Advances and Applications

Edited by  
Akira Hirose

WILEY

Interestingly, the study of **GNNs** began even before that of **QNNs**, as in [60], and G. Sommer was a strong proponent of this inquiry at the beginning of the millennium with works such as [61], in which he developed the theoretical foundations that served him well for problems such as artificial vision and robotics; [62], dedicated to a  $\mathcal{G}$ -version of the multilayer perceptron; [63] and [64], which develop the notion of *monogenic signal*. A culmination of these efforts was Sven Buchholz's thesis, [65], which should be considered, as its title indicates, a theory of neuronal computation with geometric algebras. As a sample of applications, we cite [66] (image segmentation), [67] (support vectors in the geometric context), the volumes [68] (geometric computing for wavelet transforms, artificial vision, learning, control and action) and [69] (geometric computing in engineering and computer science), [70] (use of geometric algebra for edge detection in color images), [71] (clustering methods based on the conformal geometric algebra  $\mathcal{G}_{4,1}$ ), and [72] (treatment of multispectral images with geometric algebra). We end with [73] and [74], a 2-volume set of what should be a systematic treatment on these developments, but see also [75] and [76].

In the recent article [77], convolutional octonion networks are constructed and applied to **CIFAR-10** and **CIFAR-100** image classification. According to the authors, they have better convergence and accuracy than other networks applied to the same tasks.

Octonions have also been successfully applied to *dictionary learning*, as for instance in [78], an approach that can in fact be formulated for more general algebras, including geometric ones, as in [79].

Another recent example is the case when  $\mathcal{A}$  is the algebra of *commutative quaternions*,  $\mathbf{H}^c = \langle \mathbf{1}, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3 \rangle$ . They were introduced by C. Segre in 1892 (see [80]) and can be defined by the relations  $\mathbf{i}_1^2 = \mathbf{i}_3^2 = -1$ ,  $\mathbf{i}_2^2 = 1$ ,  $\mathbf{i}_1 \mathbf{i}_2 \mathbf{i}_3 = -1$ . These imply that  $\mathbf{i}_1 \mathbf{i}_2 = \mathbf{i}_2 \mathbf{i}_1 = \mathbf{i}_3$ ,  $\mathbf{i}_2 \mathbf{i}_3 = \mathbf{i}_3 \mathbf{i}_2 = \mathbf{i}_1$ ,  $\mathbf{i}_3 \mathbf{i}_1 = \mathbf{i}_1 \mathbf{i}_3 = -\mathbf{i}_2$ , and hence  $\mathbf{H}^c$  is commutative. This algebra has been revived in [81] at the level of what, in our notations, would be called  $\mathbf{H}^c$ -neurons.

Finally let us have a look to the recent paper [82]. In its Abstract we read:

Our work considers a richer set of objects for activations and weights, and undertakes a comprehensive study of alternative algebras as number representations by studying their performance on two challenging problems: large-scale image classification using the [ImageNet](#) dataset and language modeling using the [enwiki8](#) and [WikiText-103](#) datasets. We denote this broader class of models as AlgebraNets. Our findings indicate that the conclusions of prior work, which explored neural networks constructed from **C** (complex numbers) and **H** (quaternions) on smaller datasets, do not always transfer to these challenging settings. However, our results demonstrate that there are alternative algebras which deliver better parameter and computational efficiency compared with **R**. We consider **C**, **H**, **M**<sub>2</sub>(**R**) (the set of  $2 \times 2$  real-valued matrices), **M**<sub>2</sub>(**C**), **M**<sub>3</sub>(**R**), **M**<sub>4</sub>(**R**), dual numbers and the **R**<sup>3</sup> cross product. Additionally, we note that multiplication in these algebras has higher compute density than real multiplication, a useful property in situations with inherently limited parameter reuse such as auto-regressive inference and sparse neural networks.

These are all  $\mathcal{A}$ -NNs. Are they GNNs?

By our comments on the isomorphism class of  $\mathcal{G}_{r,s}$ , this is certainly the case for  $2\mathbf{R} \simeq \mathcal{G}_{1,0}$ ,<sup>1</sup>  $\mathbf{C} \simeq \mathcal{G}_{0,1}$ ,  $\mathbf{R}(2) \simeq \mathcal{G}_{2,0}$ ,  $\mathbf{H} \simeq \mathcal{G}_{0,2} = \mathcal{G}_{3,0}^+$ ,  $\mathbf{C}(2) \simeq \mathcal{G}_{1,2}$ , and  $\mathbf{R}(4) \simeq \mathcal{G}_{2,2}$ .

The exceptions are  $\mathbf{R}(3)$  and  $(\mathbf{R}^3, \times)$ , as their dimensions are not powers of 2. Note, however, that the nature of the latter is also geometric, as the cross product is the Hodge dual of their wedge product, which lives in  $\mathcal{G}_{3,0}$ . See also [35, Ch. 3] (on [Vectorial NNs](#)).

To remark also that although the octonions are not a geometric algebra, they are nevertheless a subalgebra of  $\mathcal{G}_{0,7}$  (see [83, §7.4]).

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<sup>1</sup> $2\mathbf{R} = \mathbf{R} \oplus \mathbf{R}$  is the algebra of dual numbers, and in general  $2\mathcal{A} = \mathcal{A} \oplus \mathcal{A}$ . By  $\mathcal{A}(n)$ , or  $M_n(\mathcal{A})$ , we denote the algebra of  $n \times n$  matrices with entries in  $\mathcal{A}$ .

In this section we try to establish some connections between what has been said or hinted before and possible lines of inquiry in the area of AL by means of what can be described, in a broad sense, as *geometric calculi*. Our comments will refer to the following topics:

- AL of mathematical structures.
- Other faces of geometric AL.
- Robotics.
- Computational resources and techniques.
- Recent advances on  $k$ -NN (*nearest neighbors*).
- Other liaisons.

A compelling illustration of this theme is reported in [84].

In our view, it represents a line of research that may be promising for AL with geometric calculi as well. Quote from the Abstract:

Neural networks have a reputation for being better at solving statistical or approximate problems than at performing calculations or working with symbolic data. In this paper, we show that they can be surprisingly good at more elaborated tasks in mathematics, such as *symbolic integration* and solving *differential equations*. We propose a syntax for representing mathematical problems, and methods for generating large datasets that can be used to train sequence-to-sequence models. We achieve results that *outperform* commercial Computer Algebra Systems such as Matlab or Mathematica.

For other works of a similar potential, see [85] (on learning *algebraic structures*), [86] (the bearing of AL on current research in *number theory*), [87] (a kindred report in the realm of *physical sciences*, with many useful insights in various aspects of AL), [88] (“a foray into discrete analogues of Riemannian manifolds, providing a *rich interplay between combinatorics, geometry and theoretical physics*”), [89] (on finding *symbolic equations* that match a given dataset, with the surprising illustration of an “overdensity *equation for dark matter*”), [90] (showing that “neural networks can learn *advanced theorems and complex computations* without built-in mathematical knowledge”), [91] (a version of AL that learns *mappings between function spaces*, with impressive applications to partial differential equations).

Altogether, these works point out to novel avenues for inquiries in AL that are *transforming the understanding of science in general, and of mathematics in particular, in ways never seen hitherto*.

For people working in geometric algebra/calculus, it is natural to term **AL** as “geometric” if based on those formalisms. But **AL** researchers came up with a different use for this qualification, as in [92]:

[...] we consider the general question of how to construct deep architectures with small learning complexity on general non-Euclidean domains, which are typically unknown and need to be estimated from the data.

Even more explicit in these appraisals is [93]:

Geometric deep learning is an umbrella term for emerging techniques attempting to generalize (structured) deep neural models to non-Euclidean domains such as *graphs* and *manifolds*. The purpose of this paper is to overview different examples of geometric deep learning problems and present available solutions, key difficulties, applications, and future research directions in this *nascent field*.

Further evidence for the great potential of this paradigm can be gleaned in the survey [94], whose main thrust lies in *linking graph neural networks* and (neural) *symbolic computing*:

The need for improved *explainability*, interpretability and trust of *AI* systems in general demands *principled methodologies*, as suggested by neural-symbolic computing. In this paper, we review the state-of-the-art on the use of *GNNs* as a model of neural-symbolic computing.

We do not regard the two views of “geometric” that we are considering as antagonistic in any way, as in fact we sense that each can benefit from the other.

We have already mentioned the application of quaternions to robotics presented in [35, Ch. 7].

Among later texts, let us refer to the pioneer book [75], particularly chapters 2 and 7; Selig's treatise *Geometric fundamentals of robotics*, [95]; the collection [76], especially the papers in Part VIII (Geometry and Robotics), and the extensive compilation [68], especially Part IV (Geometric computing of *robot kinematics and dynamics*) and Part VI (Applications II: Robotics and *medical robotics*).

For recent summaries of robotics analyzed with *CGA*, see [19, Ch. 4] and [96].

Concerning **AL** in robotics, it has proceeded largely in parallel to the geometric developments, as witnessed by [97] (how machine learning has been applied to robotic path-planning and path-planning related concepts), the survey [98] (reinforcement learning in robotics; see also [99]), Lenz' **PhD** thesis [100], and the surveys [101] (**DL** techniques for mobile robot applications), [102] (**DL** methods for robot vision), [103] (learning *control in robotics*).

It appears ever more clearly that advanced **AL** is playing a major role in robotics aimed at providing all sorts of *assisting services to humans*, as epitomized by the memoir [104].

In all these cases, *the opportunities for applying geometric methods to gain theoretical and applied advantages seem clearly plentiful, if only because of the many engineering aspects that concur in any such system.*

Currently, there is a wealth of software (frameworks) for deep learning (see [Comparison\\_of\\_deep-learning\\_software](#) in Wikipedia).

For example, [Tensorflow](#) (see [105]) provides

... an interface for expressing machine learning algorithms, and an implementation for executing such algorithms.

Most of them offer a [Python](#) interface and increasingly also a [Julia](#) interface, as for instance [Tensorflow](#). An interesting case is [Flux](#) (2017), which is pure [Julia](#) (framework and interface).

But as far as we know, none of these frameworks can deal with [GNNs](#) beyond [complex NNs](#).

On the other hand, there is a rich variety of systems that perform computations with geometric algebras (see, for example, the Software section in the Wikipedia [Geometric\\_algebra](#) article).

But again, and as far as we know, none offers a deep learning framework. By its design, the [Julia](#) system described in [106] has perhaps the highest potentiality to serve as a basis for developing such a framework.

A first step in this direction would be a framework supporting [QNN](#)s. Another useful resource is provided by [template libraries](#), as for instance [107].

The authors of [108] also express the view (end of §2.1), that

the theory [...] for many branches of *unsupervised learning* is still in its infancy.

For our inquiry, there are two main directions to look at.

One concerns recent advances in conventional (non-geometric) unsupervised learning, as for example [109], which orchestrates a powerful scenario for an automatic physicist with no supervision.

In our appraisal, there is much that can conceivably be transferred to other domains, like the strategies that it advocates and the algorithmic ways by which they are marshaled.

For other instances of a similar kind, see [110] (reconstruction of the *periodic table*), [111] (proposing “a family of biologically plausible artificial neural networks (NNs) for unsupervised learning”) and [112] (steps “towards the long-term goal of *machine-assisted scientific discovery from experimental data without making prior assumptions about the system*”).

The other direction is linking unsupervised learning with [GNNs](#).

Aside from contributions such as the innovative paper [71], which develops a clustering method based on [CGA](#), it appears to be a largely uncharted terrain.

Many of the ideas in the preceding paragraph may be relevant for these explorations.

In this, it may bear further fruits the [\*unsupervised learning of Lie group transformations\*](#) studied in [113] on account of its generality and the geometric character of Lie groups (cf. [18, §6.5]).

Earlier we have met layered *A*-NNs, but now it is convenient for us to allow more flexible architectures.

By adapting the conventional notions about **graph NNs** (cf. [114], [115]), we find that a suitable class, among many other possible generalizations, is formed by directed acyclic graphs  $(N, E)$  with no isolated nodes and endowed with (trainable) *weights*  $w_e \in \mathcal{A}$  ( $e \in E$ ) and, for each non-initial node  $n$ , (trainable) *biases*  $b_n \in \mathcal{A}$  and activation functions  $\sigma_n : \mathcal{A} \rightarrow \mathcal{A}$ .

The states of a node are in one-to-one correspondence with elements of  $a \in \mathcal{A}$ . The initial nodes are input nodes. For a non-initial node  $n$ , its state  $a_n$  is determined by the formula  $a_n = \sigma_n(b_n + \sum_{e: e_0=n} w_e a_{e_1})$ , where  $e_0$  and  $e_1$  are the nodes connected by the edge  $e$ .

The output of the net is given by the states of the terminal nodes produced by these rules.

In the layered  $A$ -NN, the initial (final) nodes are those of  $L_0$  ( $L_d$ ).

Let us also suggest that it may be productive, particularly in the case of **GNNs**, to allow that weights  $w$  be operators acting on states  $a$  according to suitable law  $w \star a$  (let us dub  $\star$ NNs these structures).

These notions draw some inspiration from [19, Ch. 5] and [116] (on oriented **CGA** and its application to *molecular distance geometry*), and actually it looks puzzling to see whether they could help in porting **AL** to bear on the problems tackled by molecular distance geometry (see the more specific comments on **AL** in Chemistry at the end of this section). In doing so, it is important to bear in mind early trailblazers on Clifford neurons such as [117], [118] and [119].

Other areas where the scheme may provide analytic and geometric advantages is in the treatment of *3D point clouds* (see the survey [120], and papers like [121], [122], [123]), as well as in devising more powerful *capsule nets*: see [124], [125], [126], [127].

Of these, only the latter operates with complex numbers. Since CapsNets process elementary patterns, they should benefit from drawing ideas about *pattern theories*, say in the sense of the monograph [128], and also to enhance *explainability* along the lines of [129].

A few hints on the aptness of  $\star$ NNs to properly deal with *invariance* and *covariance* properties are in order.

These concepts always refer to the action of some group. If a group  $G = \{g\}$  acts on a set  $\mathcal{X}$ , a function  $f(x)$  is *invariant* under this action if  $f(g \cdot x) = f(x)$  for all  $x \in \mathcal{X}$  and  $g \in G$ .

Similarly, if  $G$  also acts on a set  $\mathcal{Y}$ , a map  $f : \mathcal{X} \rightarrow \mathcal{Y}$  is *covariant* (or *equivariant*) with respect to the actions of  $G$  in  $\mathcal{X}$  and  $\mathcal{Y}$  if  $f(g \cdot x) = g \cdot f(x)$  for all  $x \in \mathcal{X}$  and  $g \in G$ .

Note that an invariant function  $f$  is covariant if we let the action of  $G$  act trivially on the range of  $f$ , so that  $g \cdot f(x) = f(x)$  for all  $x \in \mathcal{X}$ .

The main reason in the context of AL to care about  $G$ -covariance is that no *data augmentation* is required to recognize features in arbitrary  $G$ -poses, as in [130] for discrete groups of rigid motions.

Let us go back to AL for Chemistry. We note a perceptible  $\star$  character of the networks studied in works such as [131], [132], [133], [134], [135], which motivates a careful study of their contributions from the  $\star$ NN point of view.

See also the collection [136] and especially the paper [137], in which the relevant group is  $SE(3)$ , the group of distance-preserving transformations of the ordinary Euclidean space. The main claim is that the authors “directly verify that the performance gains are connected with the unique  *$SE(3)$ -equivariant convolution architecture* of the new model”.

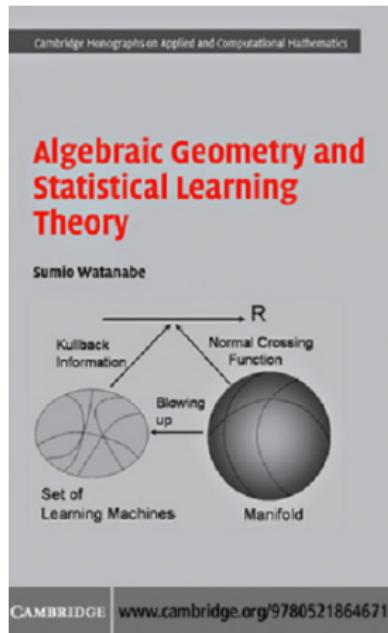
Even closer to the spirit of our disquisition is [138], as for us geometric algebras are optimally suited for the treatment of tensors in the sense of this paper, and many other geometric entities and formalisms as well.

By the way, we note that the AlgebraNets that we have seen before are special cases of  $\star$ NNs, and that they have been mainly applied to classification problems, but more research could uncover properties and applications based on their geometric character.

We end with a few remarks on the scattering transforms (a special kind of [CNN](#)) introduced in [139] and further studied in [140] (for graph networks), [141] and [142]. The computational side of this transform has produced the system [143].

Altogether, it would be worthwhile to define and study a geometric scattering transform based on the geometric algebra wavelet theory first introduced in [144] and further exploited in [51] (for quaternions), the collection [145] (particularly the paper by P. Cerejeiras, M. Ferreira, and U. Kähler), and [47].

It would also be gainful to devise a scattering transform network that could be trained, both in the conventional sense and in the geometric realm just mentioned, and a computational platform that could deal with both.



CAMBRIDGE [www.cambridge.org/9780521864671](http://www.cambridge.org/9780521864671)

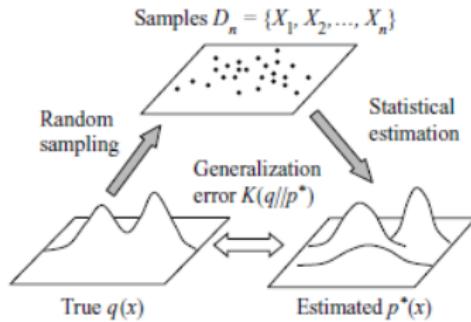


Fig. 1.1. Statistical learning

In this book, we study a method which employs a parametric probability density function. A conditional probability density function  $p(x|w)$  of  $x \in \mathbb{R}^N$  for a given parameter  $w \in W$  is called a learning machine or a statistical model, where  $W$  is the set of all parameters. Sometimes the notation  $p(x|w) = p_w(x)$  is used.

Enjoy reading, thinking, writing, speaking, living!

Thank you!

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For me, the most surprising aspect of these winning algorithms is that its authors are not experts in the games, nor on the chemistry of proteins for that matter.

In some sense they are not unlike the infinite variety of tools invented by humanity that extend the human capacities beyond the biological nature. Any tool can serve to illustrate this: the fire and the wheel; hammers and anvils; screws and screwdrivers; bicycles, cars, planes and submarines; photography, movies and digital cameras; and so on. Among the tools, there is the outstanding class of scientific instruments, like lenses, telescopes, microscopes, or the detectors of gravitational waves.

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## General

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- [151] (roberts-yaida-hanin-2021)

## Bayesian approaches

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- [153] (patel-nguyen-baraniuk-2015)
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## Applications

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## Sketch of GA

The reason for using geometric algebras is that their formalism is optimally adapted to express the geometric facts of any *linear geometric space*, that is, of a real vector space  $E = E_{r,s}$  endowed with a metric (a bilinear symmetric real-valued product  $x \cdot x'$ ,  $x, x' \in E$ ) of signature  $(r, s)$ . The most direct way to introduce the geometric algebra  $\mathcal{G}_{r,s}$  of this space, one that is arguably the closest to the ideas on which W. K. Clifford (1845-1879) based his creation, is that Grassmann's exterior algebra of  $E, \Lambda E$ , has *a unique bilinear associative product* with unit 1 (called *geometric product* by Clifford himself) such that

$$xa = x \cdot a + x \wedge a \quad (x \in E, a \in \Lambda E), \quad (3)$$

where  $x \cdot a = i_x(a)$  (the contraction of  $x$  with  $a$ ).



Since  $i_x$  is the unique skew derivation of  $\Lambda E$  such that  $i_x(x') = x \cdot x'$  for any  $x' \in E$ , the formula (3) shows how to multiply any multivector  $a$  by any vector  $x$  on the left.

In fact, *the formula suffices for the calculation of any product of multivectors* because of the following reasoning.

By bilinearity, it is enough to know how to multiply a non-zero exterior product  $b = x_1 \wedge \cdots \wedge x_r$  ( $r \geq 2$ ) of vectors  $x_1, \dots, x_r$  (such products are called *r-blades*) by an arbitrary multivector  $a$ .

We can further assume that  $x_1, \dots, x_r$  are *pair-wise orthogonal*, for the space  $\langle x_1, \dots, x_r \rangle$  has orthogonal bases and the exterior product of any such basis is equal, up to a multiplicative constant, to  $b$ .

Finally we have that  $x_1 \cdots x_r = b$  (by induction on  $r$  we may assume that  $x_2 \cdots x_r = x_2 \wedge \cdots \wedge x_r$ , and then  $x_1 x_2 \cdots x_r = x_1 (x_2 \wedge \cdots \wedge x_r) = x_1 \wedge x_2 \wedge \cdots \wedge x_r$  because  $x_1 \cdot (x_2 \wedge \cdots \wedge x_r) = 0$ ). So  $ba = x_1 \cdots x_r a$ , which can be determined by  $r$  applications of (3).

Now the *geometric algebra*  $\mathcal{G}_{r,s}$  is the exterior algebra  $\Lambda E_{r,s}$  enriched with the geometric product (this structure is also known as *Clifford's algebra*). It is clear then that it has dimension  $2^n$ , where  $n = r + s = \dim E$ .

Note that the equation (3) shows that the linear grading of  $\mathcal{G}_{r,s}$ , which is in fact a grading with respect to the exterior product, *is not a grading with respect to the geometric product*.

But the decomposition  $\mathcal{G} = \mathcal{G}^+ \oplus \mathcal{G}^-$  into *even* ( $\mathcal{G}^+$ ) and *odd* ( $\mathcal{G}^-$ ) grade components is a grading mod 2 *also with respect to the geometric product* (ultimately this is derived from the equation (3), by which the product of two vectors is resolved as the sum of a scalar, which has grade 0, and a bivector, which has grade 2).

In particular,  $\mathcal{G}^+$  is a subalgebra.



The isomorphisms  $\mathcal{G}_{1,0} \simeq \mathbb{R} \oplus \mathbb{R}$ ,  $\mathcal{G}_{0,1} \simeq \mathcal{G}_{2,0}^+ \simeq \mathbb{C}$ ,  $\mathcal{G}_{2,0} \simeq \mathbb{R}(2)$ , or  $\mathcal{G}_{0,2} \simeq \mathcal{G}_{3,0}^+ \simeq \mathbb{H}$ , easy to derive directly, are in fact examples of a general trend (cf. [18]):

$\mathcal{G}_{r,s}$  is isomorphic to a matrix algebra  $F_\nu(m)$ , where  $\nu = s - r \pmod{8}$ ,  $F_\nu = \mathbb{R}, \mathbb{C}, \mathbb{H}, 2\mathbb{H}, \mathbb{H}, \mathbb{C}, \mathbb{R}, 2\mathbb{R}$  for  $\nu = 0, 1, 2, 3, 4, 5, 6, 7$ , and  $\dim(F_\nu)m^2 = 2^n$ . For example,  $\mathcal{G}_{1,3} = F_2(m) = \mathbb{H}(2)$ .

Of these isomorphisms, those that most closely connect algebra with geometry are  $\mathbb{C} = \mathcal{G}_{2,0}^+ \simeq \mathbb{C}$  and  $\mathbb{H} = \mathcal{G}_{3,0}^+ \simeq \mathbb{H}$  in the case of the Euclidean plane and space, respectively (of  $\mathbb{C}$  and  $\mathbb{H}$  we say that they are the *geometric* complex numbers and quaternions, respectively, since they emerge directly from the geometry and not from ad hoc definitions as the usual ones for  $\mathbb{C}$  and  $\mathbb{H}$ ).

For samples of various applications of geometric algebra, see [18, 19] and their bibliographies. For a discussion of a broader perspective of geometric algebra and its applications, see [161] (especially Ch. 1).