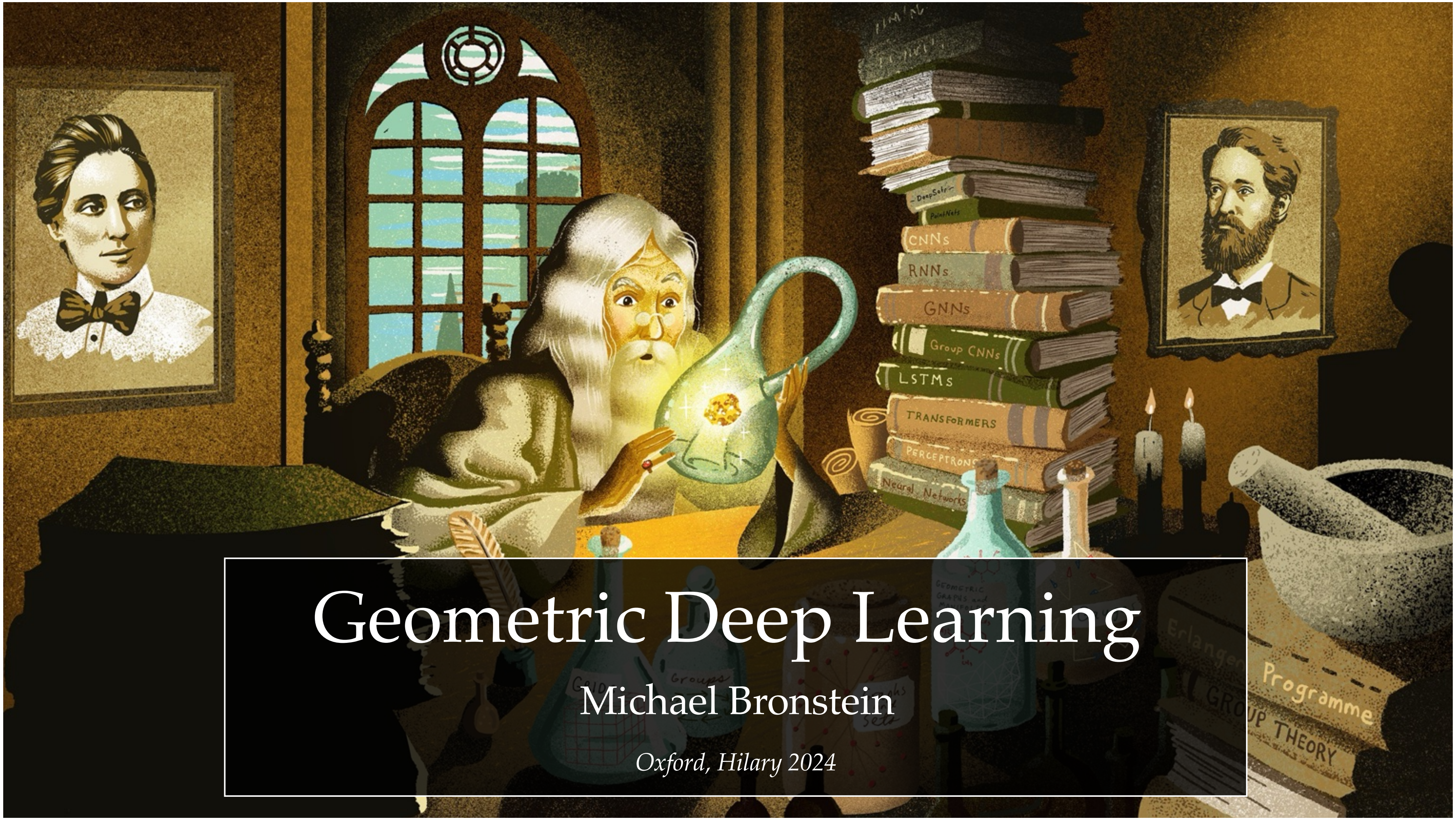
Geometric Deep Learning

Michael Bronstein

Oxford, Hilary 2024



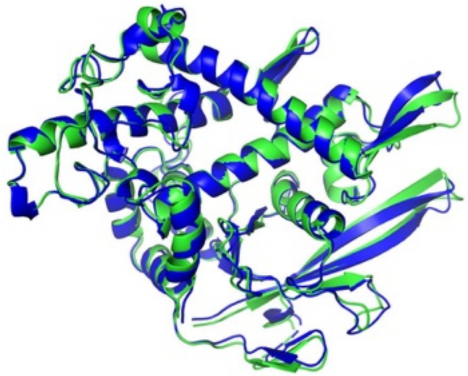
Autonomous driving

Generative art

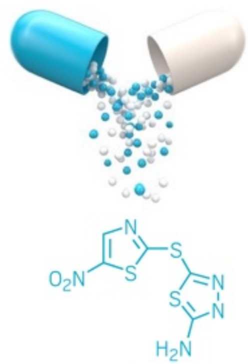
Robotics

Language processing

Speech recognition



Protein folding



Drug discovery

“[ML] is the new electricity”

—Andrew Ng (2017)

"There's a self-congratulatory feeling in the air. We say things like 'machine learning is the *new electricity*.' I'd like to offer an alternative metaphor: machine learning has become *alchemy*."

—Ali Rahimi at NIPS 2017

Image: Byron Eggenschwiler

Fundamental principles underlying deep learning architectures

"The knowledge of certain principles easily compensates the lack of knowledge of certain facts"

—Claude Adrien Helvétius

Symmetry

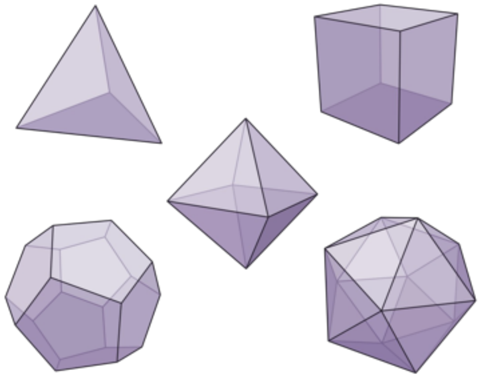
“Symmetry, as wide or as narrow as you may define its meaning, is one idea by which man through the ages has tried to comprehend and create order, beauty, and perfection”

H. Weyl

Weyl 1952

ON THE SHOULDERS OF GIANTS

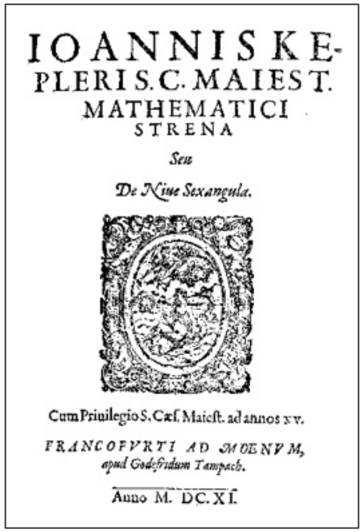
συμμετρία



Platonic solids

Plato

~370 BC



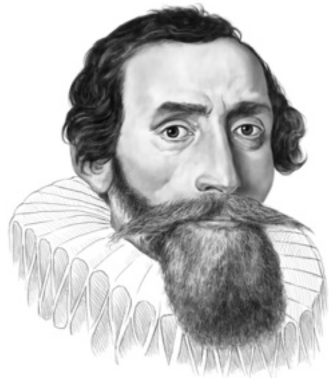
IOANNIS KE-
PLERI S.C. MAIEST.
MATHEMATICI
STRENA
Seu
De Nive Sexangula.

Cum Priuilegio S. Cæs. Maiest. ad annos xv.

FRANCOFVRTI AD MOENVM,
apud Godefridum Tampach.

Anno M. DC. XI.

"On the six-cornered snowflake"



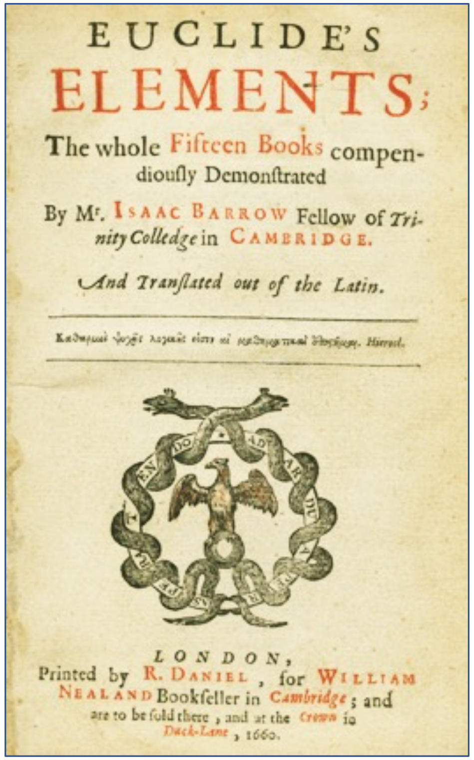
J. Kepler

1611

Marina Viazovska
2022 Fields Medal
8-dimensional sphere packing

Euclidean geometry

Fifth Postulate: "In a plane, given a line and a point not on it, at most one line parallel to the given line can be drawn through the point"


EUCLIDE'S
ELEMENTS;
The whole Fifteen Books compen-
diouſly Demonſtrated
By Mr. Isaac Barrow Fellow of Tri-
nity Colledge in Cambridge.
And Tranſlated out of the Latin.

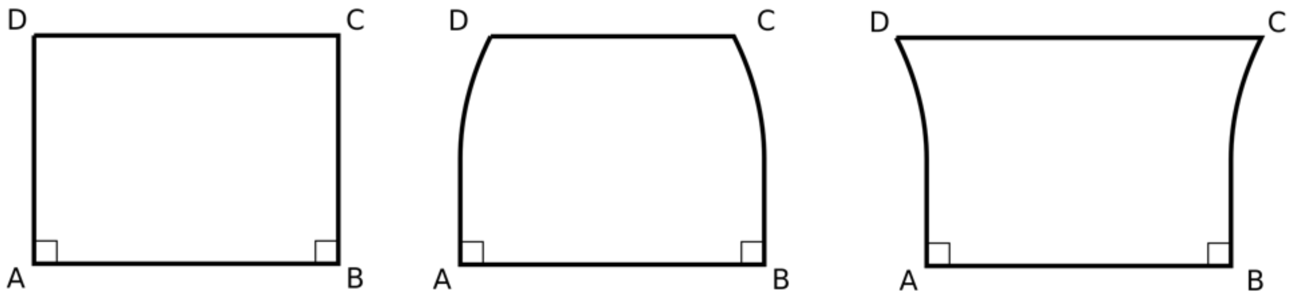
[illegible]

LONDON,
Printed by R. Daniel, for William
Nealand Bookſeller in Cambridge; and
are to be ſold there, and at the Crown in
Duck-Lane, 1660.

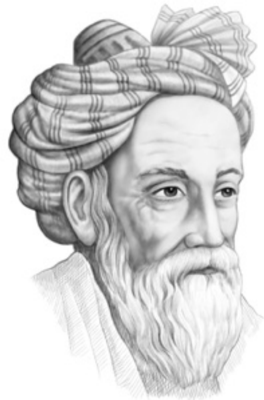

Euclid

~300 BC

Early attempts



Khayyam-Saccheri quadrilateral



Omar Khayyam

1077

"Three cases of angles in a quadrilateral: Fifth Postulate follows from the right-angle assumption"

Early attempts

Et hujus quidem (post multa, ne dicam omnia, conditionatè expensa) absolutam falsitatem in XXXIII. tandem ostendo, quia repugnantis naturæ lineæ rectæ, circa quam multa ibi interfero necessaria Lemmata . Tandem verò in præcedente Propositione absolutè demonstro sibi ipsi repugnantem hypothesin anguli acuti .

"repugnant to the nature of straight lines"
— Giovanni Saccheri

EUCLIDES
AB OMNI NÆVO VINDICATUS:
SIVE
CONATUS GEOMETRICUS
QUO STABILIUNTUR
Prima ipsa universæ Geometriæ Principia.
AUCTORE
HIERONYMO SACCHERIO
SOCIETATIS JESU
In Ticinensi Universitate Matheseos Professore.
OPUSCULUM
EX.MO SENATUI
MEDIOLANENSI
Ab Auctore Dicatum.
MEDIOLANI, MDCCXXXIII.
Ex Typographia Pauli Antonii Montani. *Superiorum permissu.*

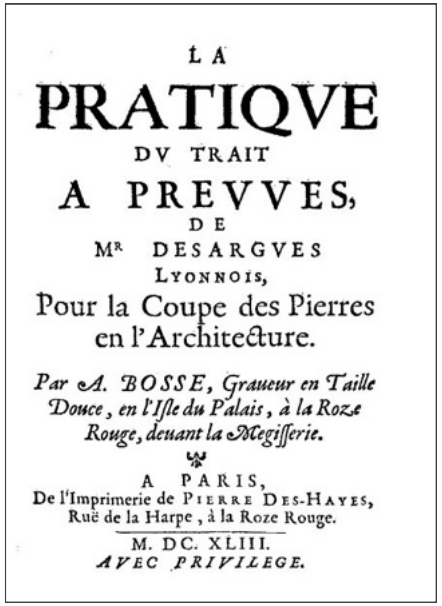
1736


ЄΥΚΛЄΙΔΗϹ

Projective Geometry

G. Desargues

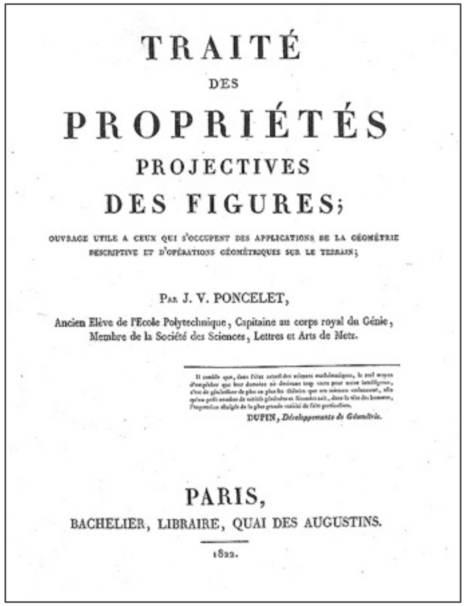
1643



LA
PRATIQVE
DV TRAIT
A PREVVES,
DE
M^R DESARGVES
LYONNOIS,
Pour la Coupe des Pierres
en l'Architecture.

Par A. BOSSE, Graueur en Taille Douce, en l'Isle du Palais, à la Roze Rouge, deuant la Megisserie.

A PARIS,
De l'Imprimerie de PIERRE DES-HAYES,
Ruë de la Harpe, à la Roze Rouge.
M. DC. XLIII.
AVEC PRIVILEGE.



TRAITÉ
DES
PROPRIÉTÉS
PROJECTIVES
DES FIGURES;

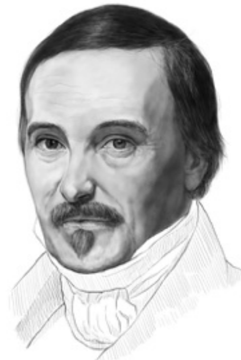
OUVRAGE UTILE A CEUX QUI S'OCCUPENT DES APPLICATIONS DE LA GÉOMÉTRIE DESCRIPTIVE ET D'OPÉRATIONS GÉOMÉTRIQUES SUR LE TERRAIN;

PAR J. V. PONCELET,

Ancien Elève de l'Ecole Polytechnique, Capitaine au corps royal du Génie, Membre de la Société des Sciences, Lettres et Arts de Metz.

DUPIN, *Développements de Géométrie.*

PARIS,
BACHELIER, LIBRAIRE, QUAI DES AUGUSTINS.
1822.



J. V. Poncelet

1822

"Projective geometry"

Desargues 1643; Poncelet 1822

"Non-Euclidean Geometry"

"I have discovered such wonderful things that I was amazed... out of nothing I have created a strange new world."

— Jánus Bolyai to his father

Bolyai's 1823 letter to his father

J. Bolyai

1823

Bolyai (1823) 1832

“Non-Euclidean Geometry”

“To praise it would amount to praising myself. For the entire content of the work...coincides almost exactly with my own meditations [in the] past thirty or thirty-five years.”

— Gauss to Farkas Bolyai

C. F. Gauss

~1800

“Non-Euclidean Geometry”

“In geometry I find certain imperfections which I hold to be the reason why this science […] can as yet make no advance from that state in which it came to us from Euclid. I consider […] the momentous gap in the theory of parallels, to fill which all efforts of mathematicians have so far been in vain.”

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О НАЧАЛАХЪ ГЕОМЕТРІИ (*).

(*Г. Лобачевскаго.*)

Кажется, трудность понятій увеличивается по мѣрѣ ихъ приближенія къ начальнымъ истинамъ въ природѣ; также какъ она возрастаетъ въ другомъ направленіи, къ той границѣ, куда стремится умъ за новыми познаніями. Вотъ почему трудности въ Геометріи дожны пренадлежать, вопервыхъ, самому предмету. Далѣе, средства, къ которымъ надобно прибѣгнуть чтобы достигнуть здѣсь послѣдней строгости, едва ли могутъ отвѣчать цѣли и простотѣ сего ученія. Тѣ, которые хотѣли удволетворить симъ требованіямъ, заключили себя въ такой тѣсной кругъ, что всѣ усилія ихъ не могли быть вознаграждены успѣхомъ. Наконецъ скажемъ и то, что со времени Нютона и Декарта, вся Математика, сдѣлавшись Аналитикой, пошла столь быстрыми шагами впередъ, что оставила далеко за собой то ученіе, безъ котораго могла уже об-

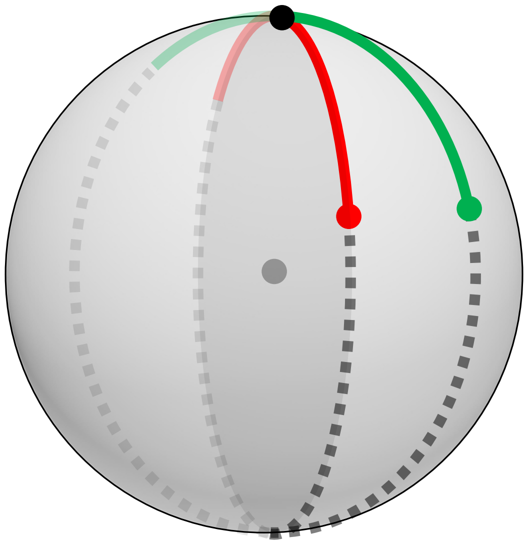
(*) Извлечено самимъ Сочинителемъ изъ разсужденія, подъ названіемъ: *Exposition succincte des principes de la Géometrie etc.*, читаннаго имъ въ засѣданіи Отдѣленія Физико-Математическихъ наукъ, 12 Февраля 1826 года.

N. Lobachevsky

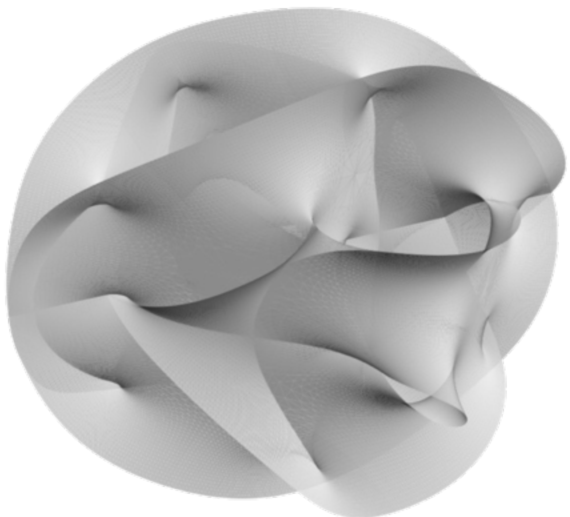
1829

Lobachevsky (1826) 1829

"Non-Euclidean Geometry"



Constant-curvature spherical geometry



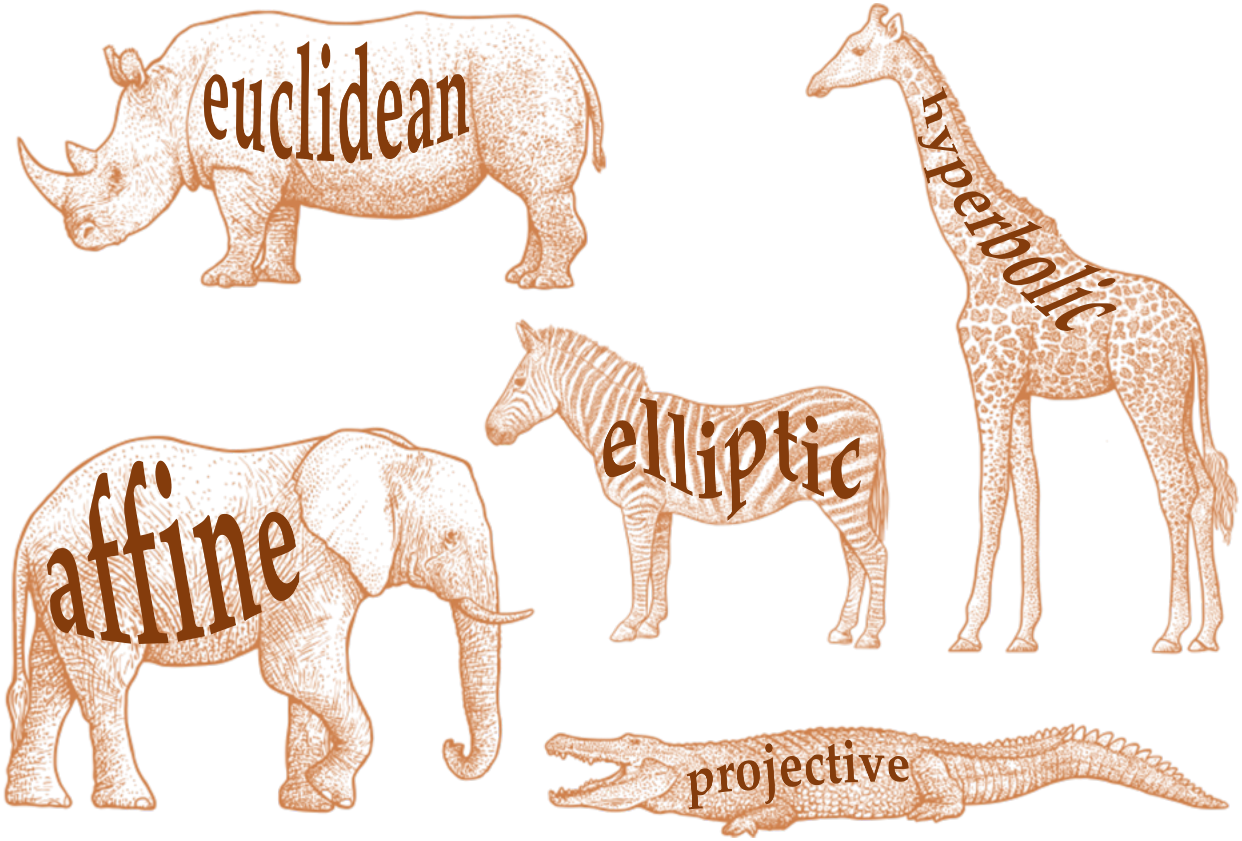
Variable-curvature Riemannian geometry on manifolds (*"Mannigfaltigkeit"*)

B. Riemann

1856

Riemann 1856

19th Century Zoo of Geometries



The Erlangen Programme

"Given a [homogeneous] manifold and a transformation group acting [transitively] on it, to investigate those properties of figures on that manifold which are invariant under transformations of that group"

Vergleichende Betrachtungen

über

neuere geometrische Forschungen

von

Dr. Felix Klein,

o. ö. Professor der Mathematik an der Universität Erlangen.

Programm

zum Eintritt in die philosophische Facultät und den Senat der k. Friedrich-Alexanders-Universität zu Erlangen.

Erlangen.

Verlag von Andreas Deichert.

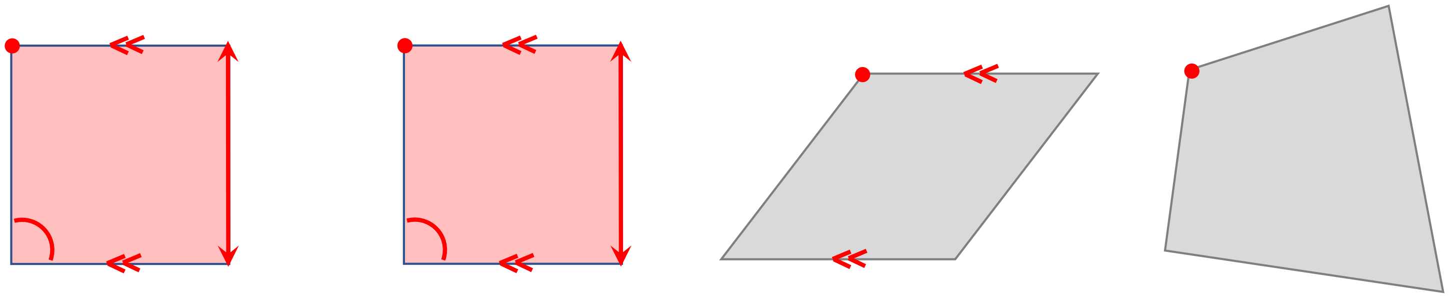
1872.

F. Klein

1872

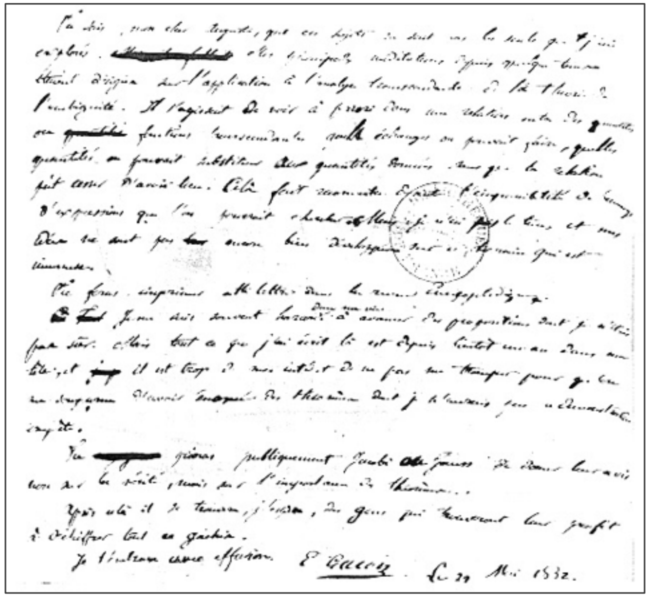
Klein 1872

The Erlangen Programme



	Euclidean	**Affine**	**Projective**
angle	+	—	—
distance	+	—	—
area	+	—	—
parallelism	+	+	—
intersection	+	+	+

Group Theory



Mon cher ami — Galois' last letter written on the night before his duel

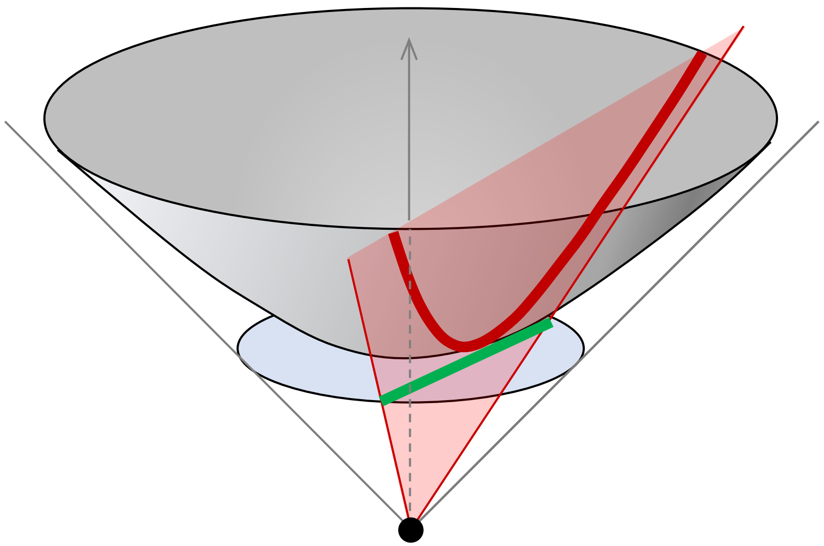
E. Galois

S. Lie

F. Klein

1832

Hyperbolic geometry



Beltrami-Klein projective model of hyperbolic geometry

Beltrami 1868; Klein 1871

E. Beltrami

1868

F. Klein

1871

sogenannte nicht-Euklidische Geometrie

Beyond Erlangen Programme

E. Cartan

=

B. Riemann

+

F. Klein

Category Theory

"…a continuation of the Klein Erlangen Programme, in the sense that a geometrical space with its group of transformations is generalized to a category with its algebra of mappings"

GENERAL THEORY OF NATURAL EQUIVALENCES

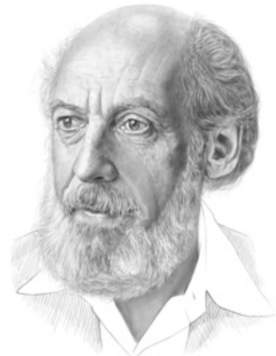
BY

SAMUEL EILENBERG AND SAUNDERS MacLANE

CONTENTS

Introduction. The subject matter of this paper is best explained by an example, such as that of the relation between a vector space L and its "dual"

Presented to the Society, September 8, 1942; received by the editors May 15, 1945.



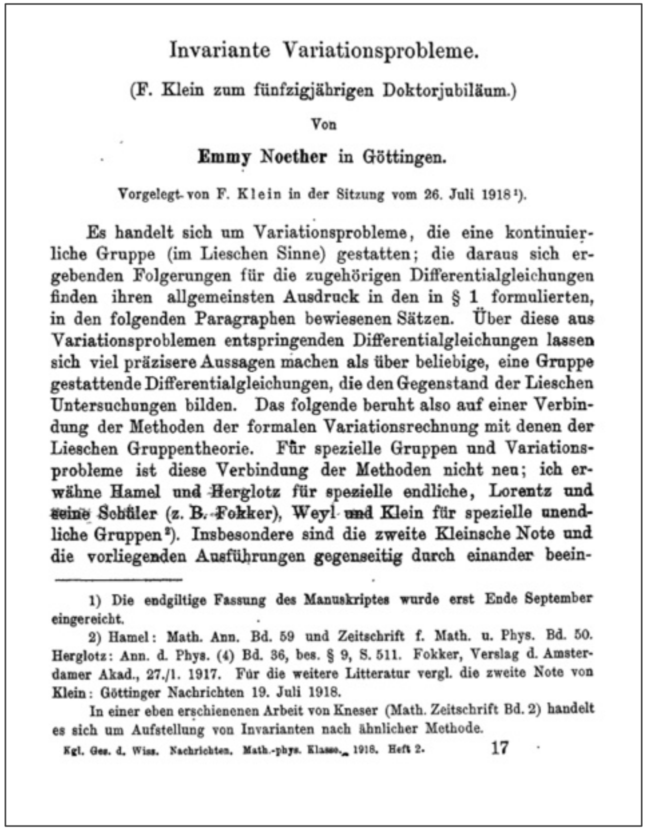
S. Eilenberg

S. Mac Lane

1945

Noether's Theorem

"Every [differentiable] symmetry of the action of a physical system [with conservative forces] has a corresponding conservation law"



Invariante Variationsprobleme.

(F. Klein zum fünfzigjährigen Doktorjubiläum.)

Von

Emmy Noether in Göttingen.

Vorgelegt von F. Klein in der Sitzung vom 26. Juli 1918[1]).

Es handelt sich um Variationsprobleme, die eine kontinuierliche Gruppe (im Lieschen Sinne) gestatten; die daraus sich ergebenden Folgerungen für die zugehörigen Differentialgleichungen finden ihren allgemeinsten Ausdruck in den in § 1 formulierten, in den folgenden Paragraphen bewiesenen Sätzen. Über diese aus Variationsproblemen entspringenden Differentialgleichungen lassen sich viel präzisere Aussagen machen als über beliebige, eine Gruppe gestattende Differentialgleichungen, die den Gegenstand der Lieschen Untersuchungen bilden. Das folgende beruht also auf einer Verbindung der Methoden der formalen Variationsrechnung mit denen der Lieschen Gruppentheorie. Für spezielle Gruppen und Variationsprobleme ist diese Verbindung der Methoden nicht neu; ich erwähne Hamel und Herglotz für spezielle endliche, Lorentz und seine Schüler (z. B. Fokker), Weyl und Klein für spezielle unendliche Gruppen[2]). Insbesondere sind die zweite Kleinsche Note und die vorliegenden Ausführungen gegenseitig durch einander beein-

1) Die endgiltige Fassung des Manuskriptes wurde erst Ende September eingereicht.

2) Hamel: Math. Ann. Bd. 59 und Zeitschrift f. Math. u. Phys. Bd. 50. Herglotz: Ann. d. Phys. (4) Bd. 36, bes. § 9, S. 511. Fokker, Verslag d. Amsterdamer Akad., 27./1. 1917. Für die weitere Litteratur vergl. die zweite Note von Klein: Göttinger Nachrichten 19. Juli 1918.

In einer eben erschienenen Arbeit von Kneser (Math. Zeitschrift Bd. 2) handelt es sich um Aufstellung von Invarianten nach ähnlicher Methode.

Kgl. Ges. d. Wiss. Nachrichten. Math.-phys. Klasse. 1918. Heft 2. 17

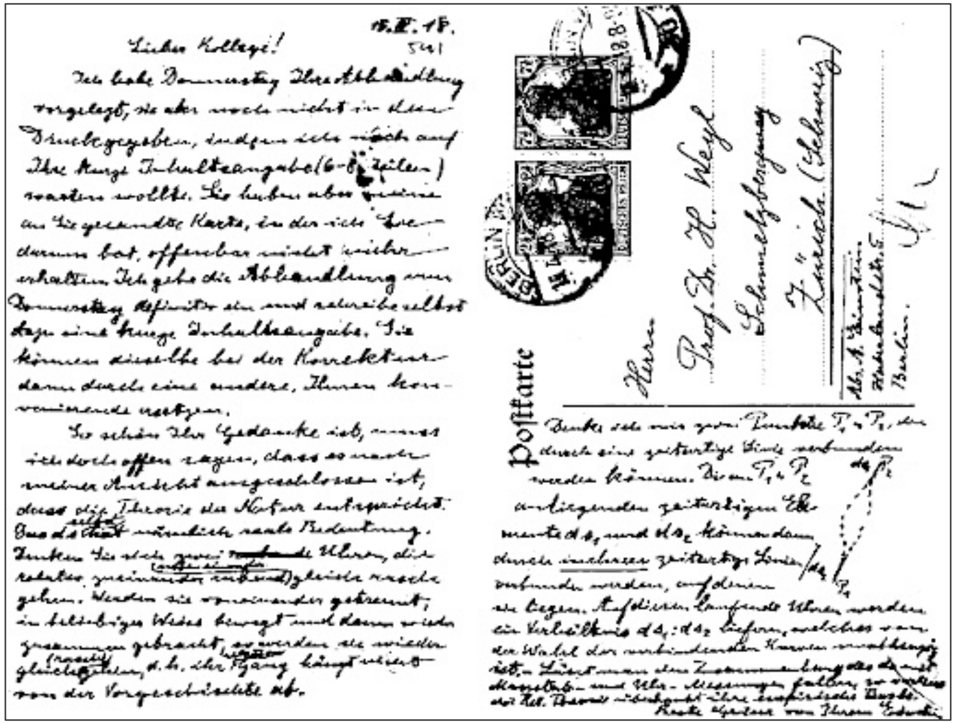
E. Noether

1918

Noether 1918

Gauge invariance

Lieber Kollege! —
Postcard dated 15 April 1918 from Einstein to Weyl arguing with his initially proposed gauge theory

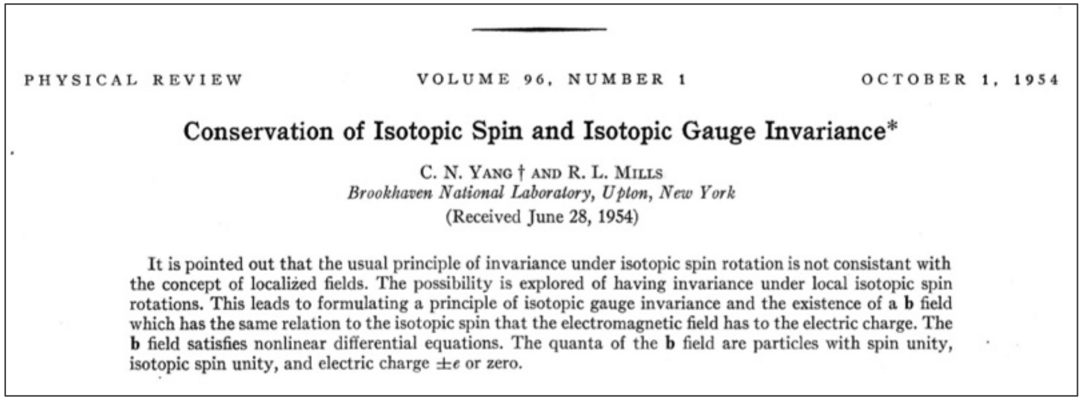


H. Weyl

1929

Weyl 1919; 1929 (see Straumann 1987)

Unification of forces



PHYSICAL REVIEW VOLUME 96, NUMBER 1 OCTOBER 1, 1954

Conservation of Isotopic Spin and Isotopic Gauge Invariance*

C. N. YANG † AND R. L. MILLS
Brookhaven National Laboratory, Upton, New York
(Received June 28, 1954)

It is pointed out that the usual principle of invariance under isotopic spin rotation is not consistant with the concept of localized fields. The possibility is explored of having invariance under local isotopic spin rotations. This leads to formulating a principle of isotopic gauge invariance and the existence of a **b** field which has the same relation to the isotopic spin that the electromagnetic field has to the electric charge. The **b** field satisfies nonlinear differential equations. The quanta of the **b** field are particles with spin unity, isotopic spin unity, and electric charge $\pm e$ or zero.

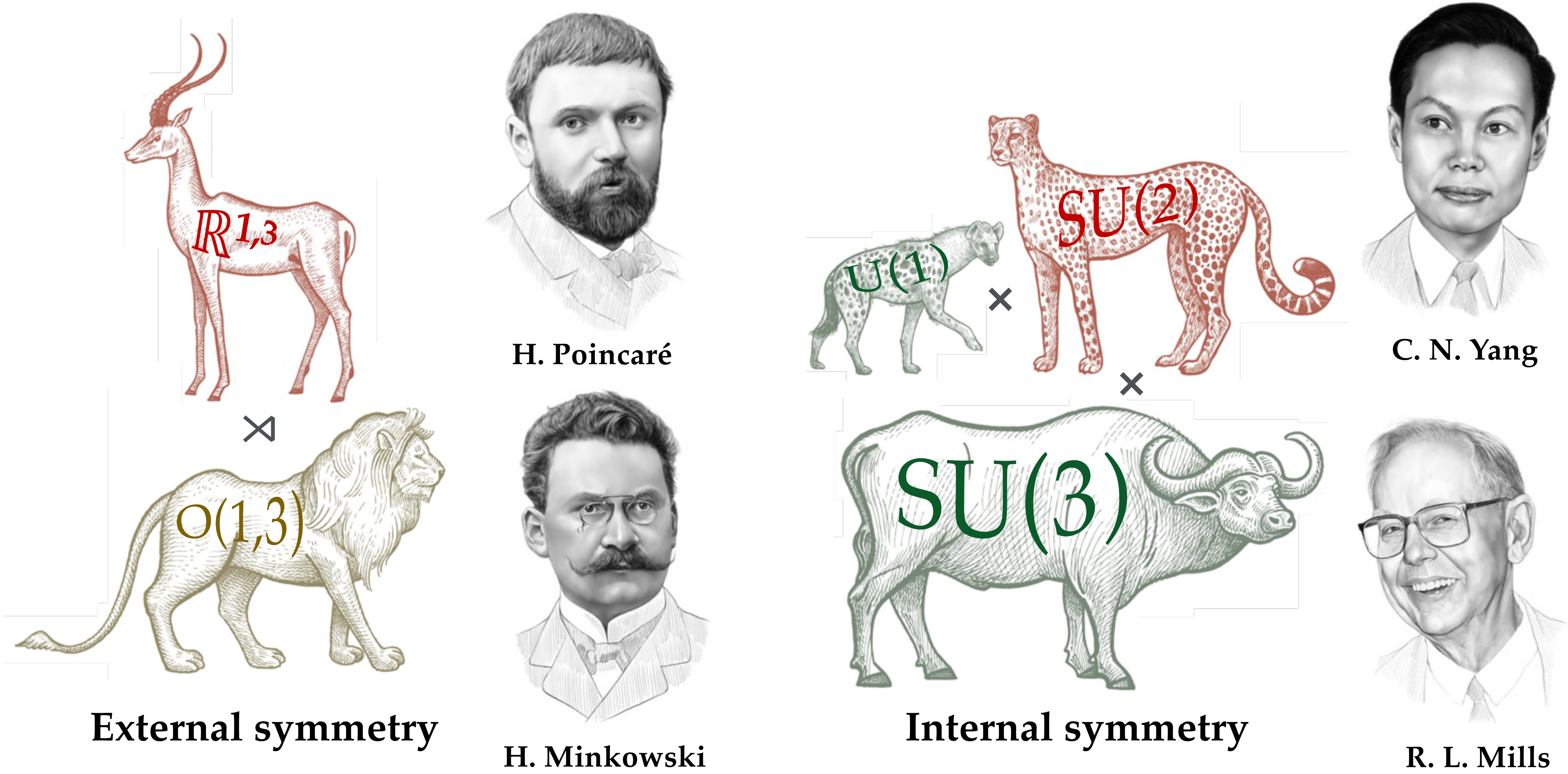
Unification of electromagnetic and weak forces (modelled with the groups U(1) × SU(2)) and the strong force (based on the group SU(3))

C. N. Yang

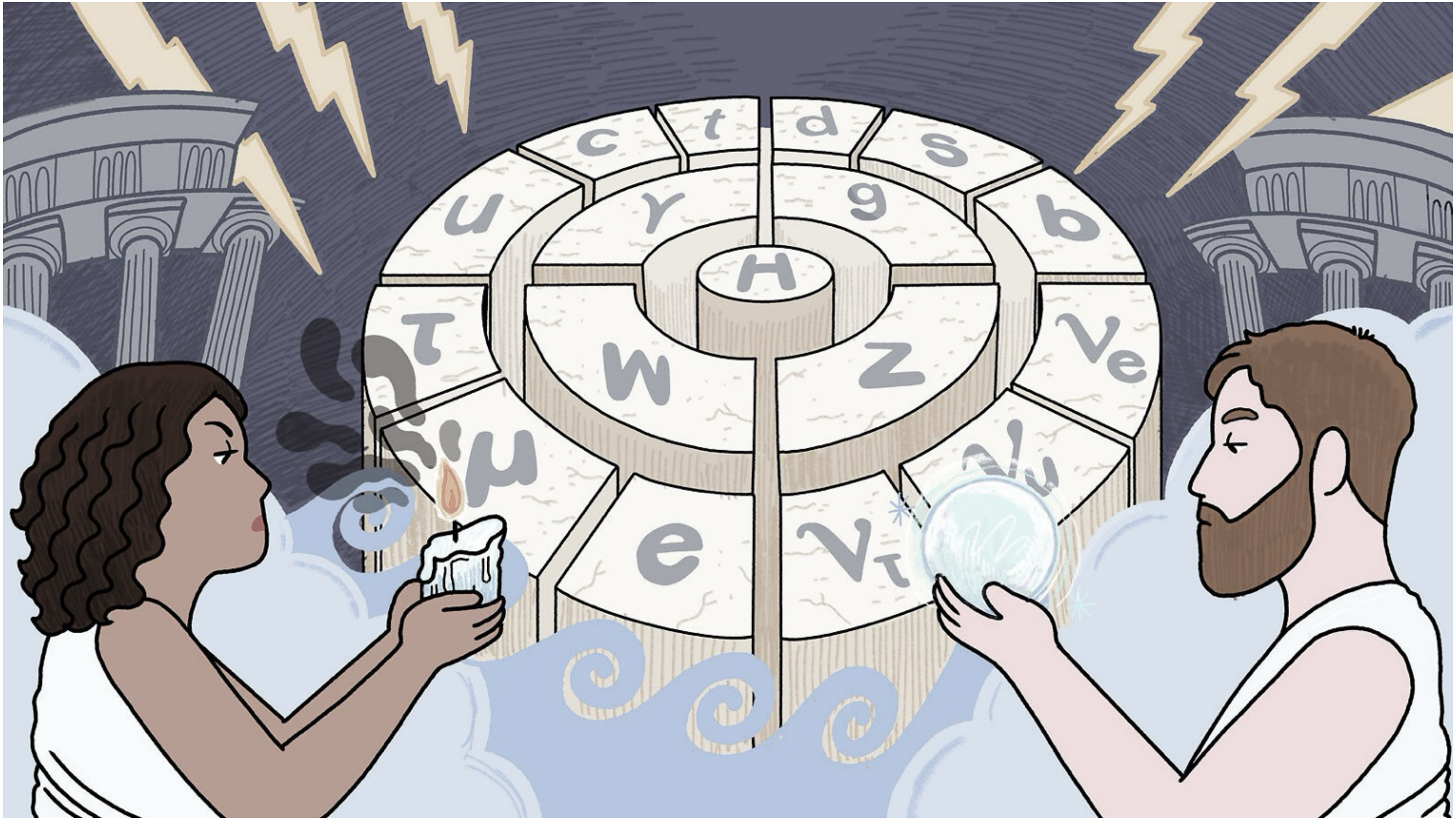
R. L. Mills

1954

Yang, Mills 1954



ℝ1,3
⋊
O(1,3)
H. Poincaré
H. Minkowski
External symmetry
U(1)
×
SU(2)
×
SU(3)
C. N. Yang
R. L. Mills
Internal symmetry


c
t
d
s
u
γ
g
b
H
τ
W
Z
νe
μ
νμ
e
ντ

"It is only slightly overstating the case to say that Physics is the study of symmetry"

— "More is different", Science 1972

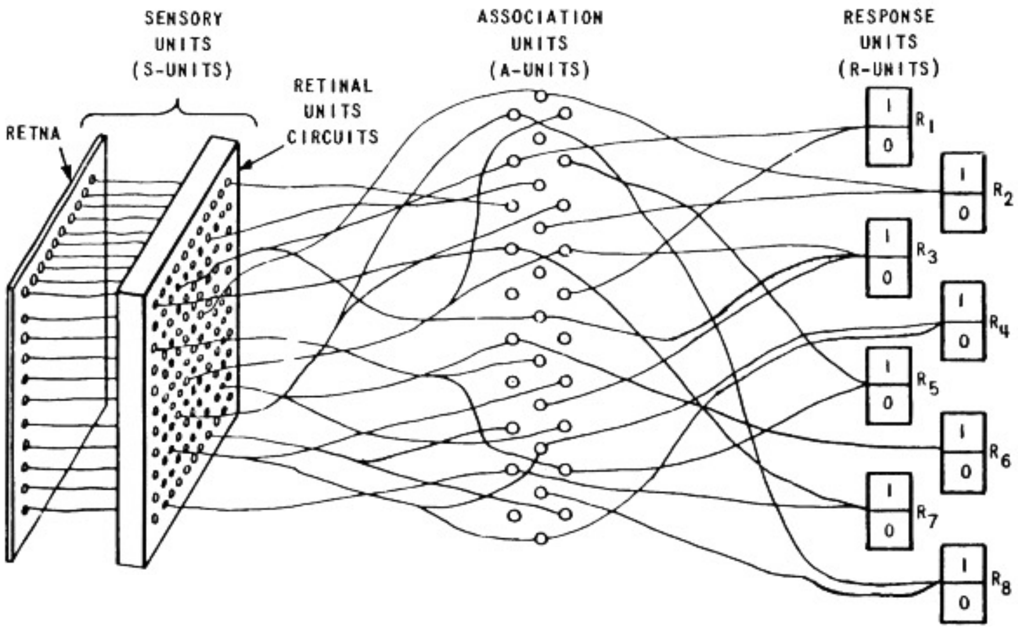
P. Anderson

?

EARLY NEURAL NETWORKS
& THE AI WINTER

Dartmouth AI Conference 1956

Early neural networks



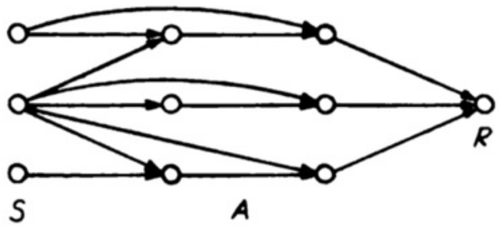
Perceptron, one of the first neural network architectures

F. Rosenblatt

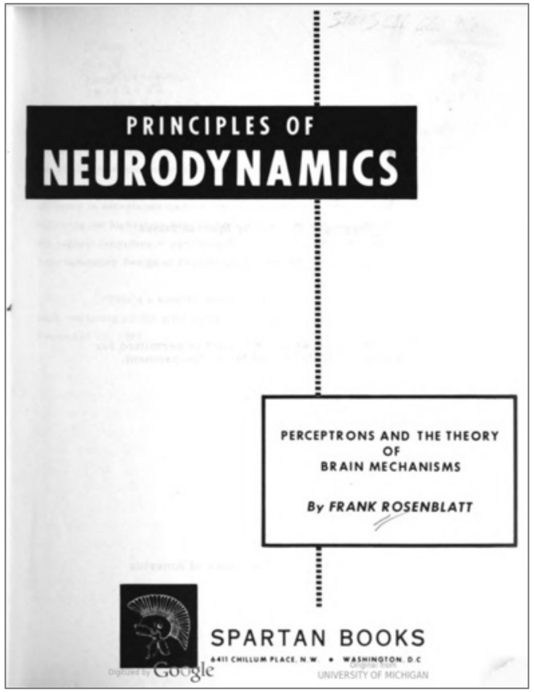
1957

Rosenblatt 1957

Early neural networks



Early skip connections


PRINCIPLES OF
NEURODYNAMICS

PERCEPTRONS AND THE THEORY OF BRAIN MECHANISMS

By FRANK ROSENBLATT

SPARTAN BOOKS
6411 CHILLUM PLACE, N.W. • WASHINGTON, D.C.

F. Rosenblatt

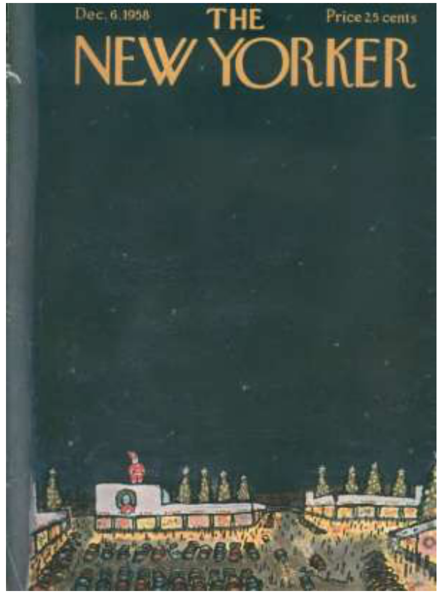
Rosenblatt 1962

Early hype

"First serious rival to the human brain even devised."

"Remarkable machine capable of what amounts to thought"

— The New Yorker



1958

Manson, Stewart, Gill 1958

Early hype

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

PROJECT MAC

Artificial Intelligence Group　　　　July 7, 1966

Vision Memo. No. 100.

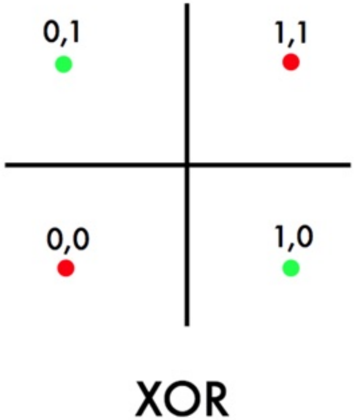
THE SUMMER VISION PROJECT

Seymour Papert

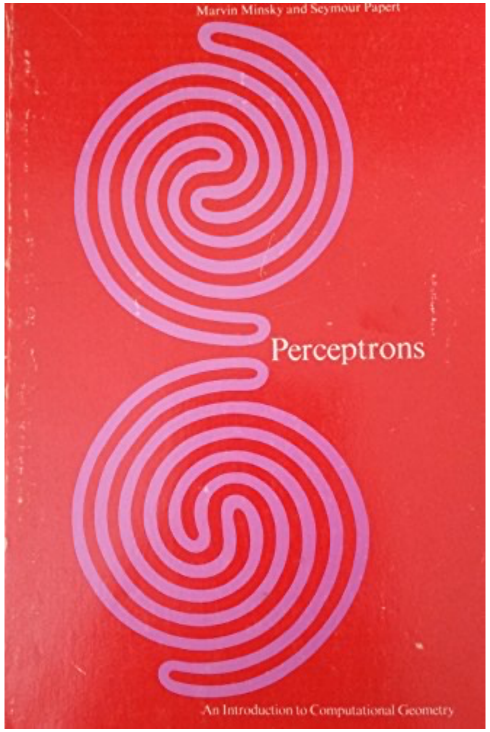
The summer vision project is an attempt to use our summer workers effectively in the construction of a significant part of a visual system. The particular task was chosen partly because it can be segmented into sub-problems which will allow individuals to work independently and yet participate in the construction of a system complex enough to be a real landmark in the development of "pattern recognition".

Papert 1966

The "XOR Affair"



"[simple] perceptron cannot represent even the XOR function"



M. Minsky

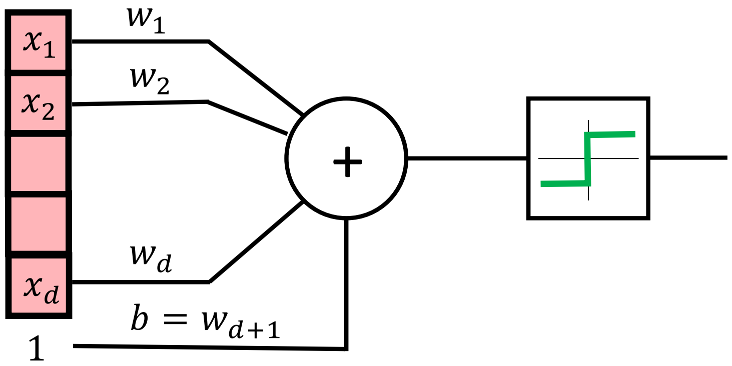
S. Papert

1969

Minsky, Papert 1969


“AI WINTER”

“Simple perceptron”



$$y = \mathrm{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x})$$

First "geometric" machine learning

Group Invariance Theorem: "if a neural network is invariant to a group, then its output can be expressed as functions of the orbits of the group"

M. Minsky

S. Papert

1969

Minsky, Papert 1969

Universal approximation

D. Hilbert

A. Kolmogorov

V. Arnold

G. Cybenko

K. Hornik

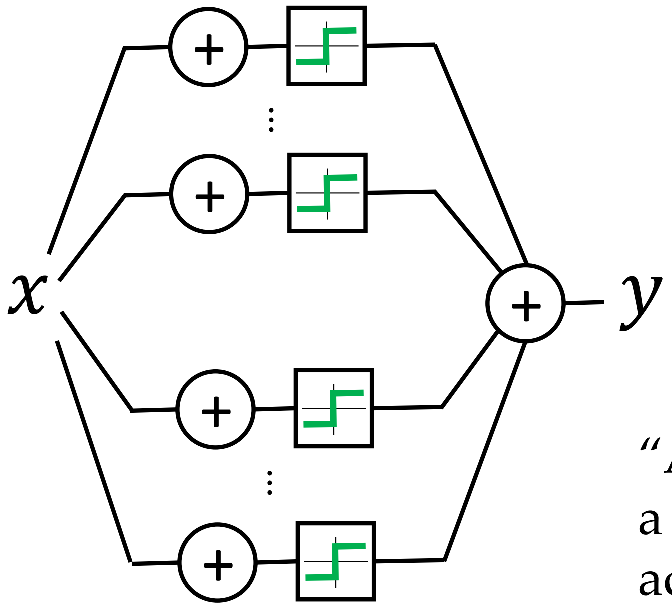
13$^{\text{th}}$ Problem

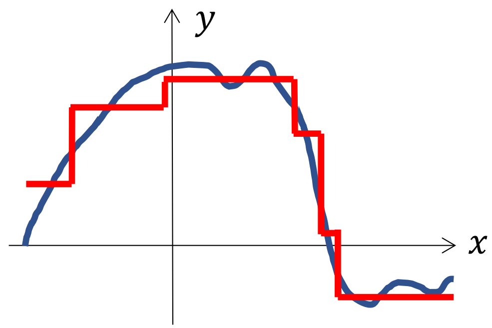
$$f(x_1, \ldots, x_n) = \sum_{q=0}^{2n} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}(x_p) \right)$$

"Modern" results specific to multilayer neural networks

Hilbert 1900; Arnold 1956; Kolmogorov 1957; Cybenko 1989; Hornik et al. 1989

Universal approximation



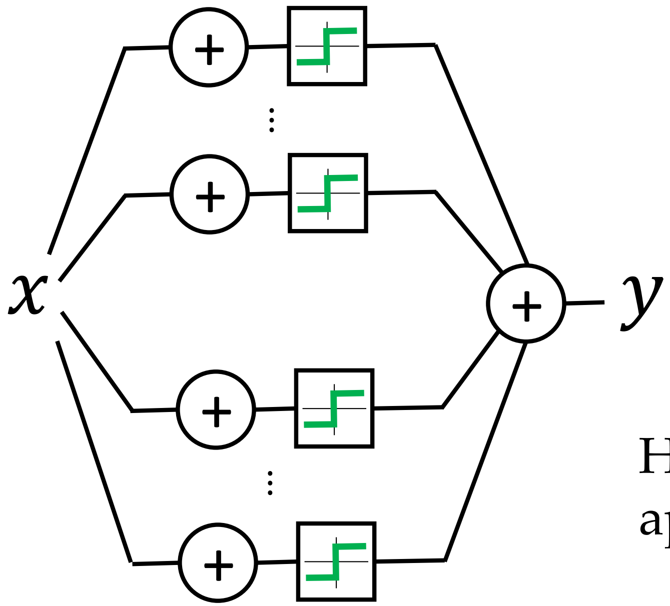


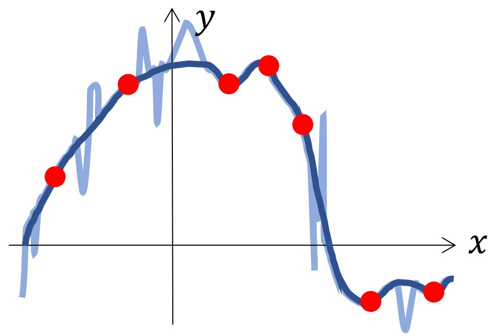
"A 2-layer perceptron can approximate a continuous function to any desired accuracy"

Cybenko 1989; Hornik 1991; Barron 1993; Leshno et al 1993; Maiorov 1999; Pinkus 1999

Deep learning = glorified curve fitting

Universal approximation

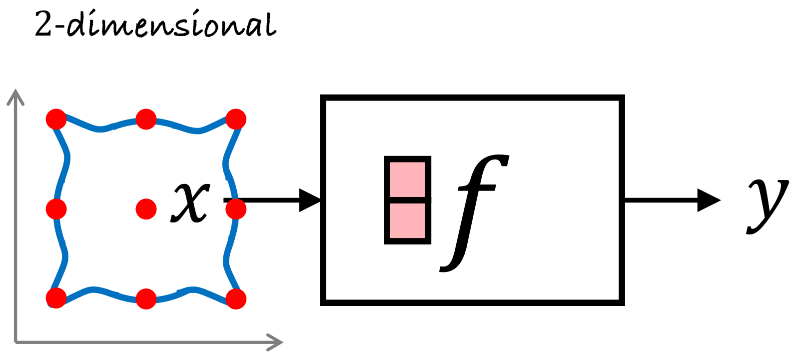




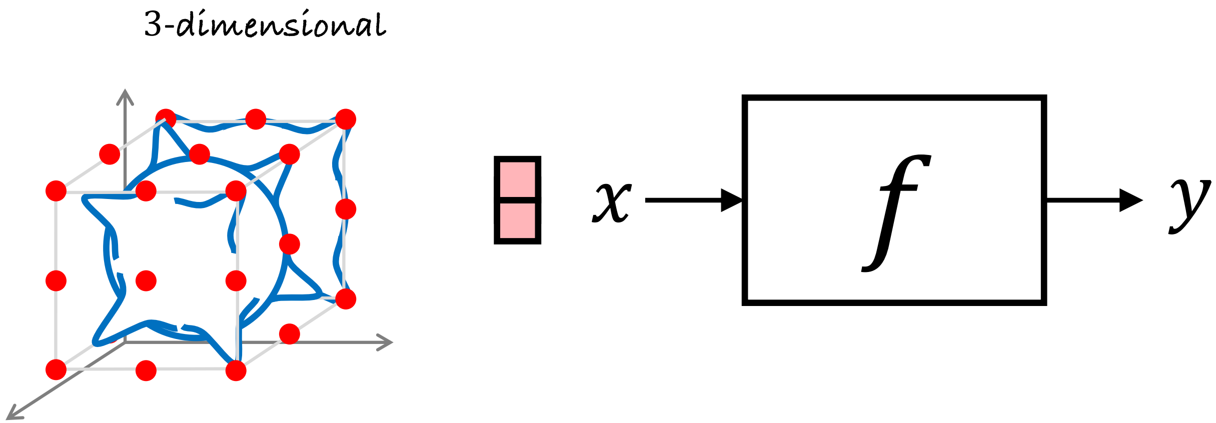
How many samples are needed to approximate to accuracy ε ?

Cybenko 1989; Hornik 1991; Barron 1993; Leshno et al 1993; Maiorov 1999; Pinkus 1999

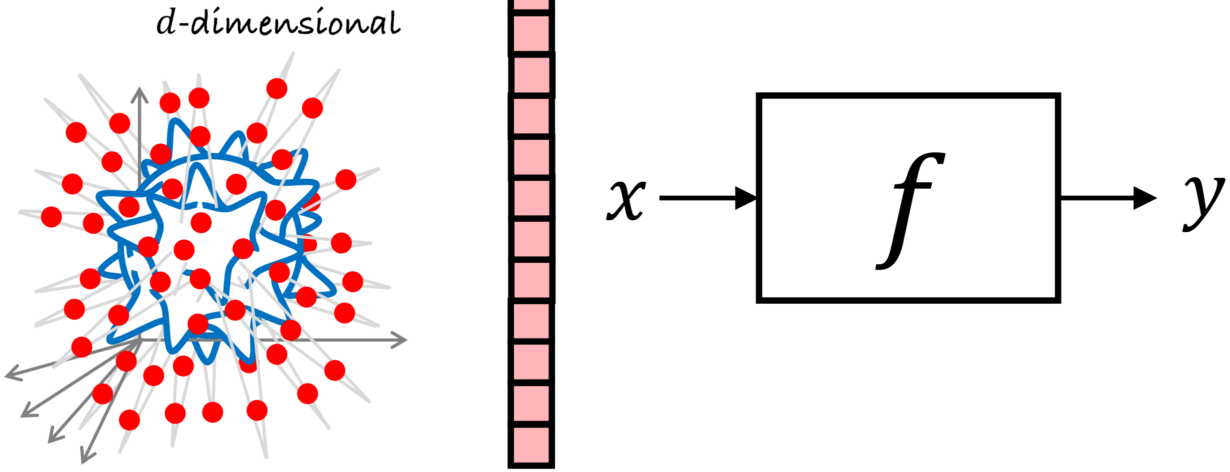
The Curse of Dimensionality



The Curse of Dimensionality



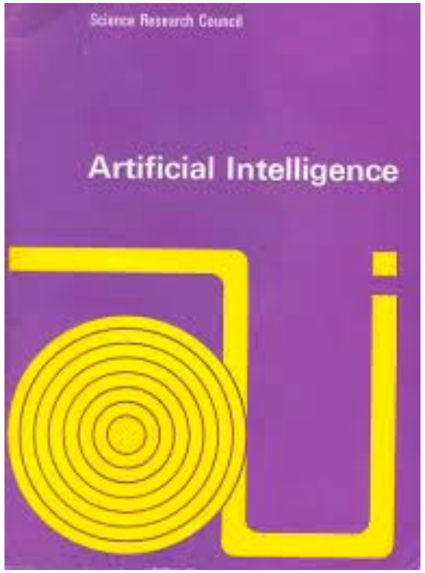
The Curse of Dimensionality



$O(\varepsilon^{-d})$ samples

The Lighthill Report

"Most workers in AI research and in related fields confess to a pronounced feeling of disappointment in what has been achieved in the past twenty-five years. […] In no part of the field have the discoveries made so far produced the major impact that was then promised."



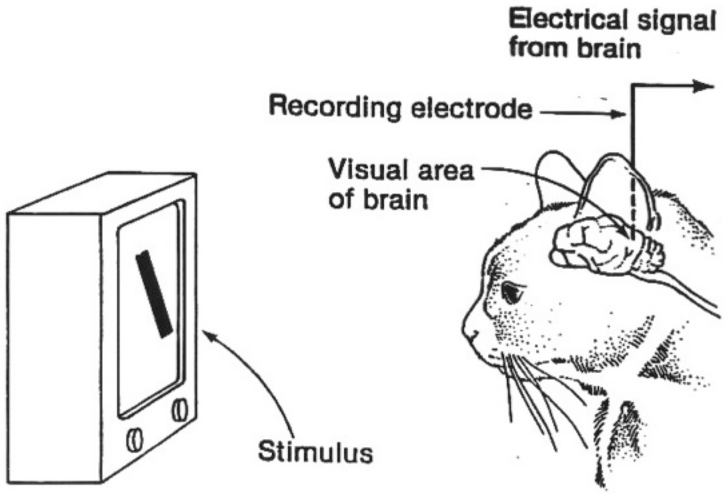
J. Lighthill

1972

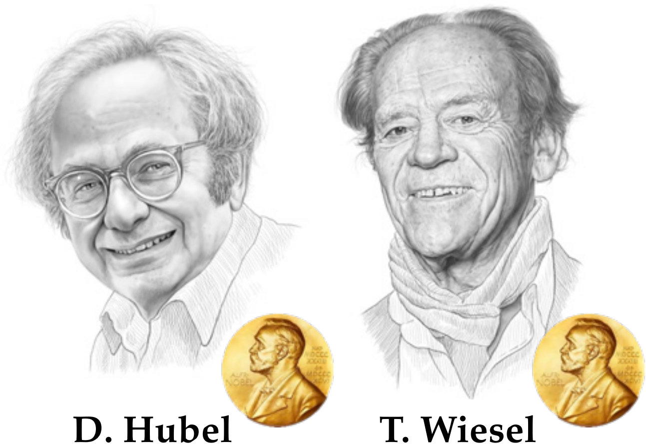
Lighthill 1972

THE EMERGENCE OF GEOMETRIC ARCHITECTURES

Secrets of the visual cortex



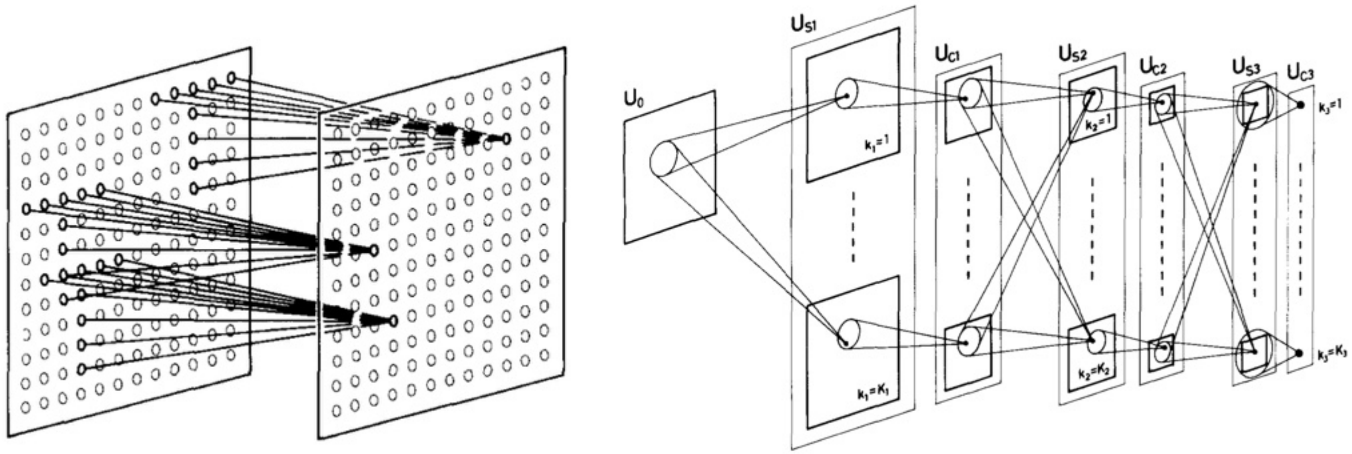
Experiments of Hubel and Wiesel that established the structure of the visual cortex



1959

Hubel, Wiesel 1959; 1962

Neocognitron

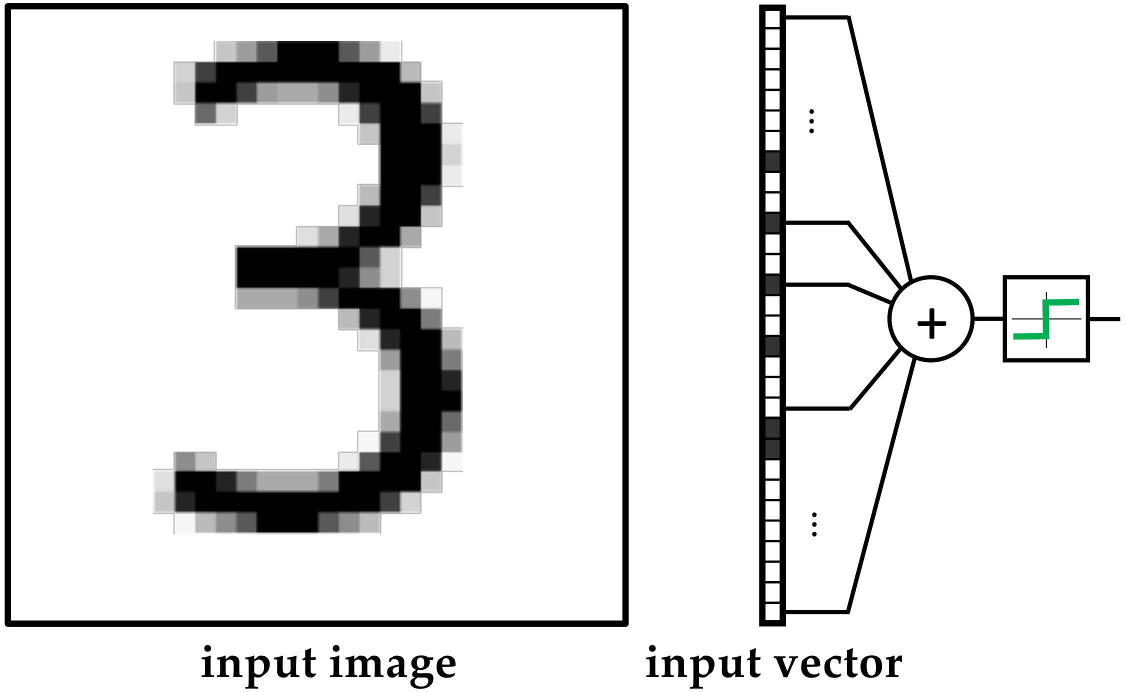


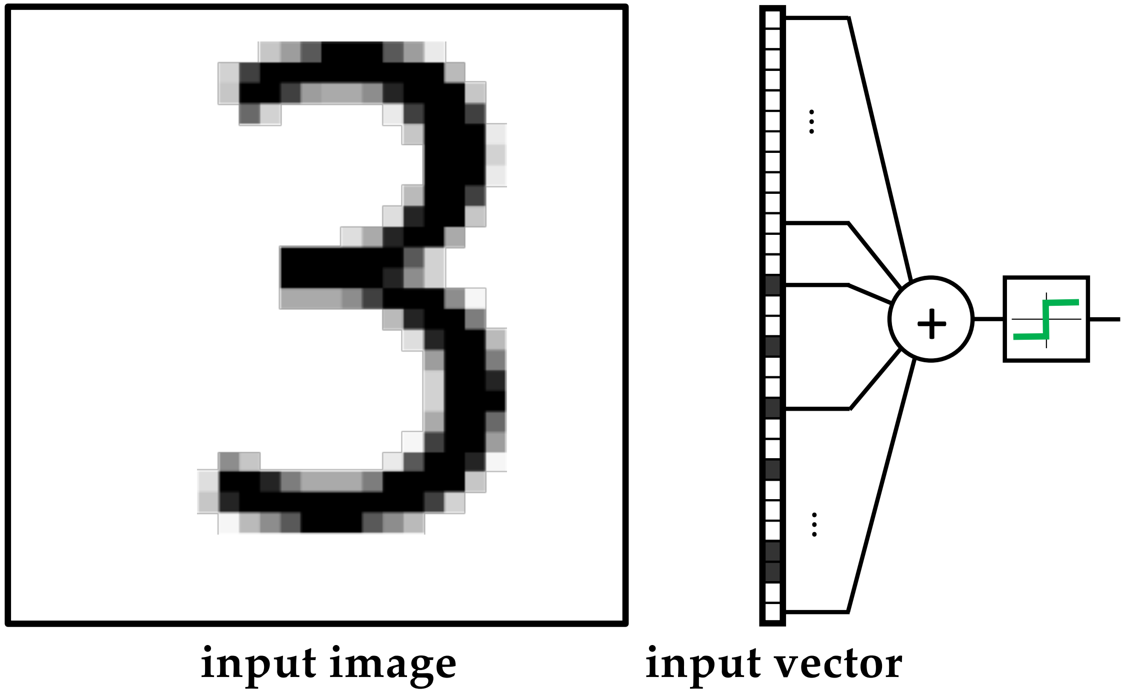
Neocognitron, an early geometric neural network

K. Fukushima

1980

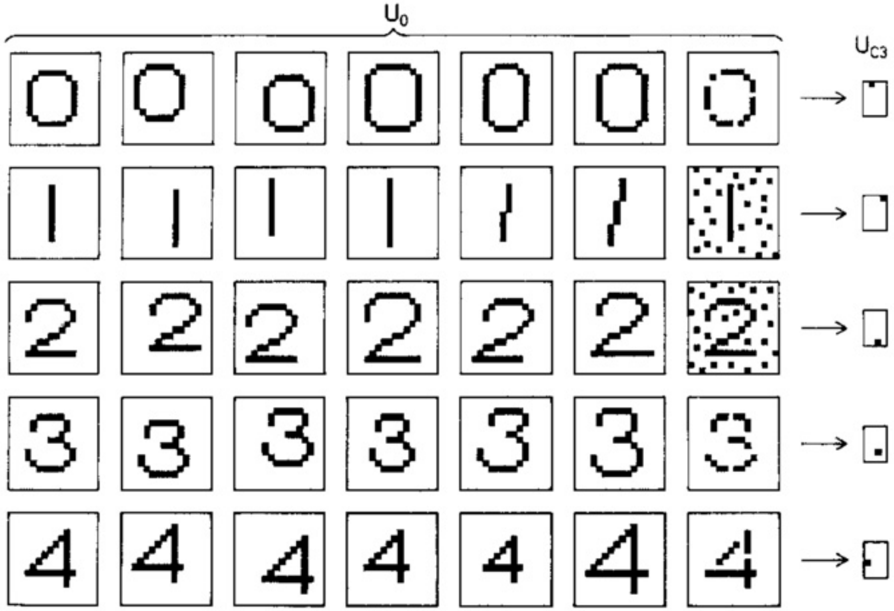
Fukushima 1980


input image
input vector



“The response of [Perceptrons] was severely affected by the shift in position […] of the input patterns. Hence, their ability for pattern recognition was not so high.”— Fukushima

Neocognitron



Experimental evaluation of the Neocognitron

K. Fukushima

1980

Fukushima 1980

Neocognitron

- Deep neural network (7 layers tested)
- Local connectivity (“receptive fields”)
- Nonlinear filters with shared weights (S-layers)
- Average pooling (C-layers)
- ReLU activation function
- ”Self-organised” (unsupervised) **– no backprop yet!**

K. Fukushima

1980

Fukushima 1980

How to train your neural network?

F. Rosenblatt

Perceptron learning rule (1 layer)

A. Ivakhnenko

Group method of data handling

S. Linnainmaa

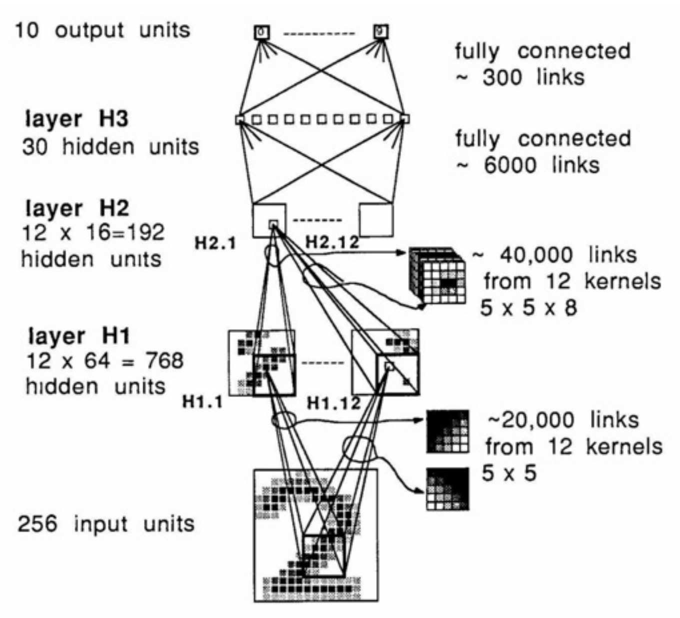
P. Werbos

Backpropagation

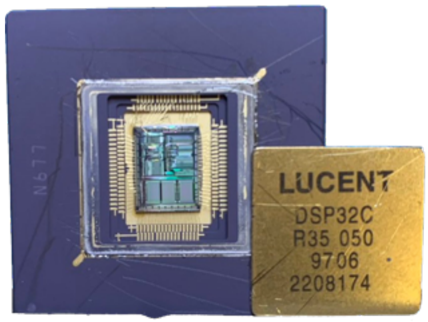
D. Rumelhart

Rosenblatt 1957; Ivakhnenko, Lapa 1966; Linnainmaa 1970; Werbos 1982; Rumelhart et al. 1986

Convolutional neural networks



First version of a CNN

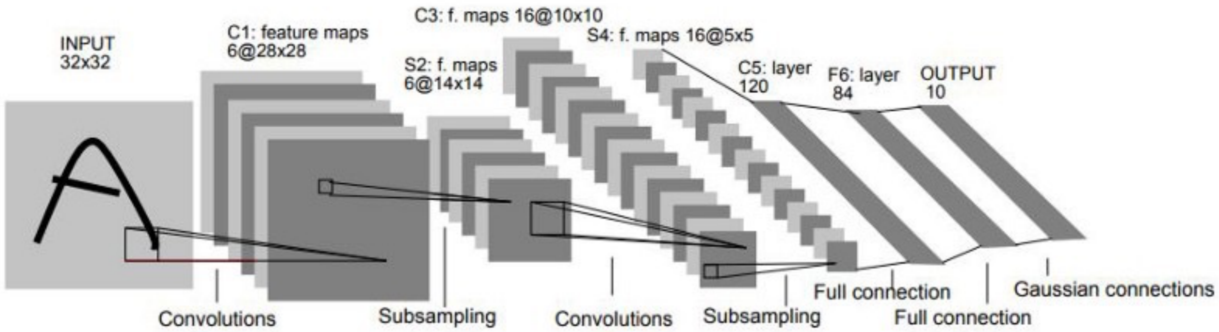


AT&T DSP-32C
capable of 125m floating
point multiply-accumulate
operations/sec

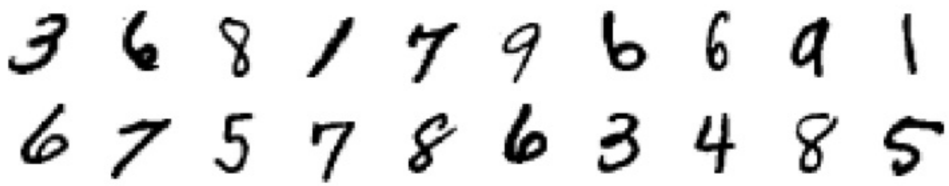
Y. LeCun

LeCun et al. 1989

LeNet-5



LeNet-5 classical CNN architecture

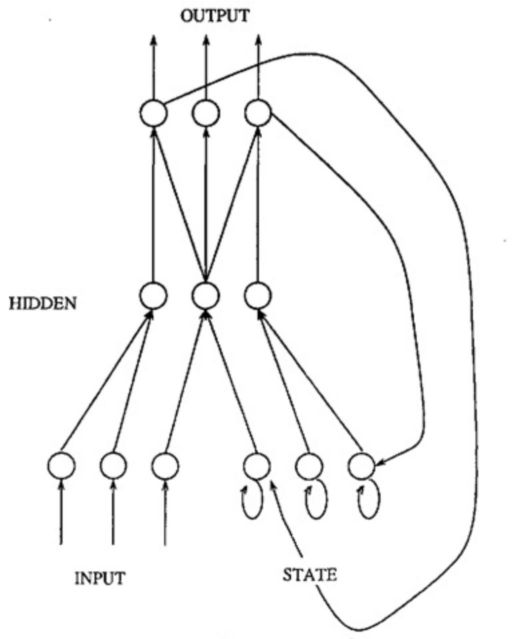


MNIST digits dataset

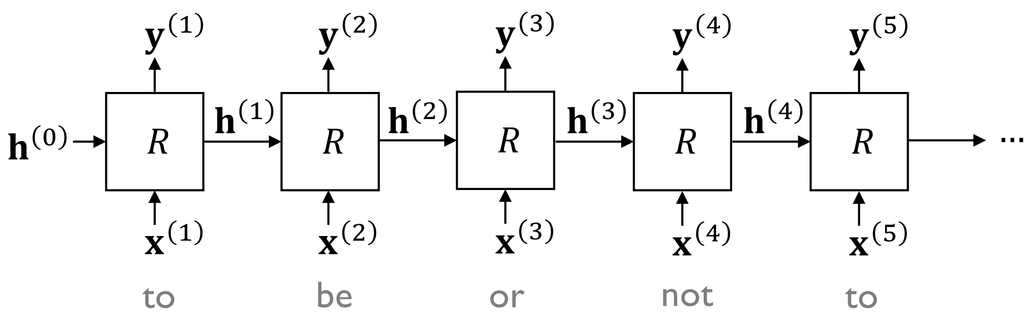
Y. LeCun

LeCun et al. 1998

Recurrent Neural Networks



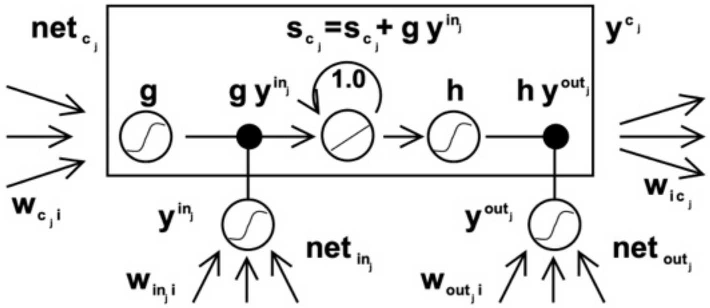
Simple RNN architecture used
by Michael Jordan



Unfolded RNN and the Vanishing Gradient problem

McCulloch, Pitts 1943 ("circular paths"); Minsky 1967 ("networks with cycles"); Rumelhart et al. 1985 (generalisation of gradient-based learning in "recurrent nets")
Jordan 1986; Elman 1990

Long Short Term Memory (LSTM)



S. Hochreiter **J. Schmidhuber**

Hochreiter 1995; Hochreiter, Schmidhuber 1997; Pascanu et al. 2003

Time warping

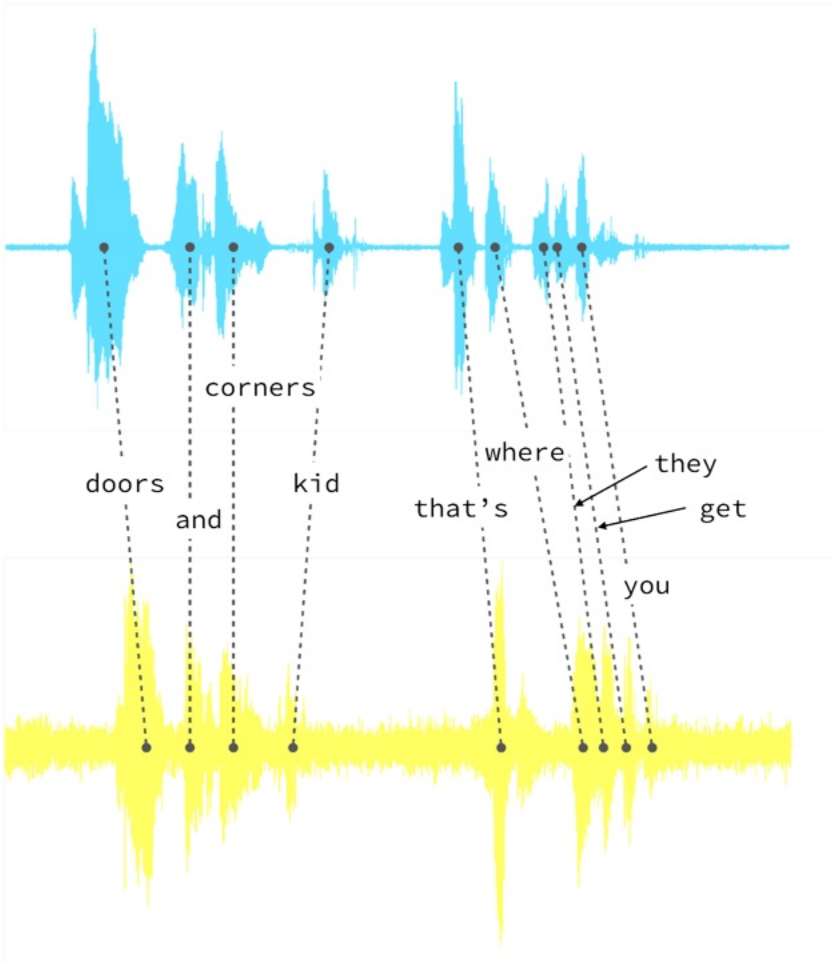
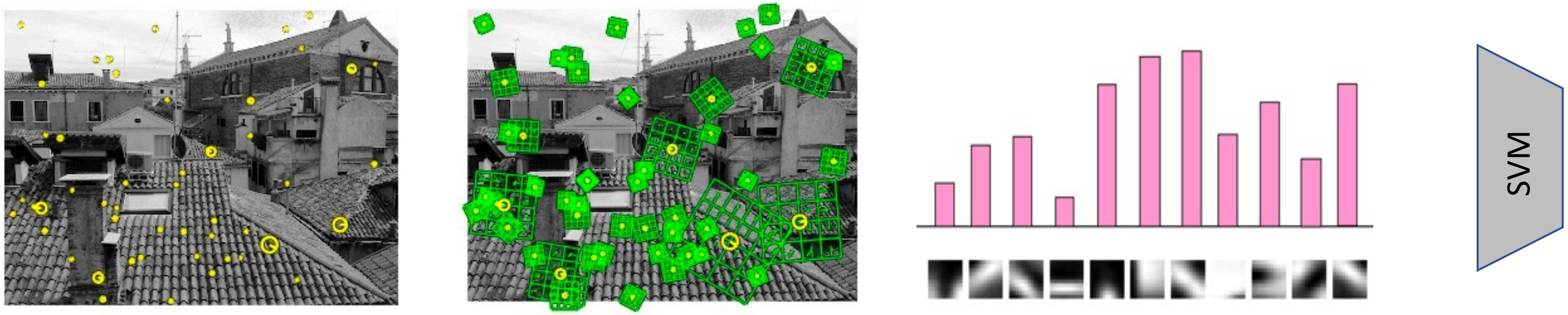


Image: Portilla, Heintz

Computer vision in the 2000s

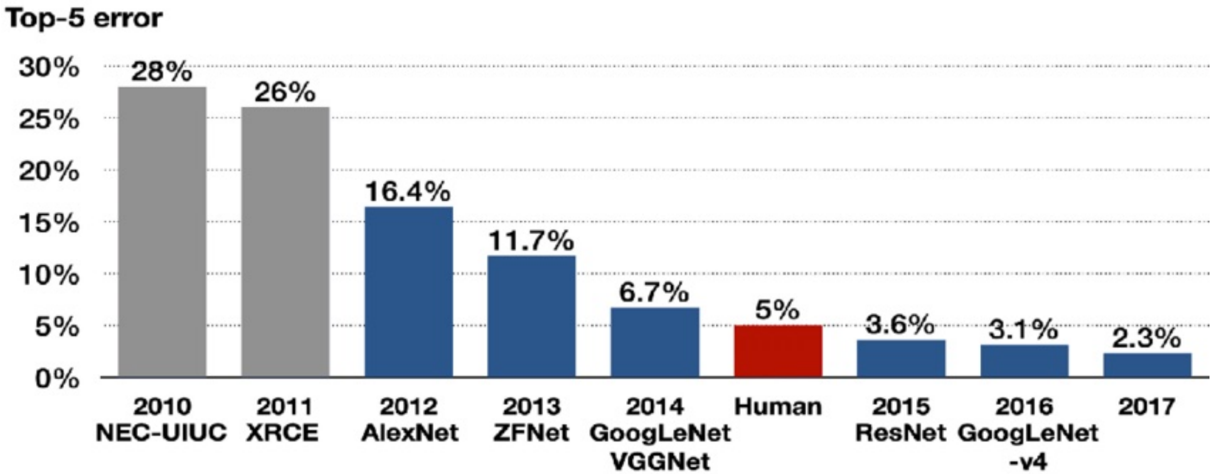


Feature detection **Feature description** **Feature aggregation** **Classification**

A typical image classification pipeline from the 2000s

Sivic, Zisserman 2003

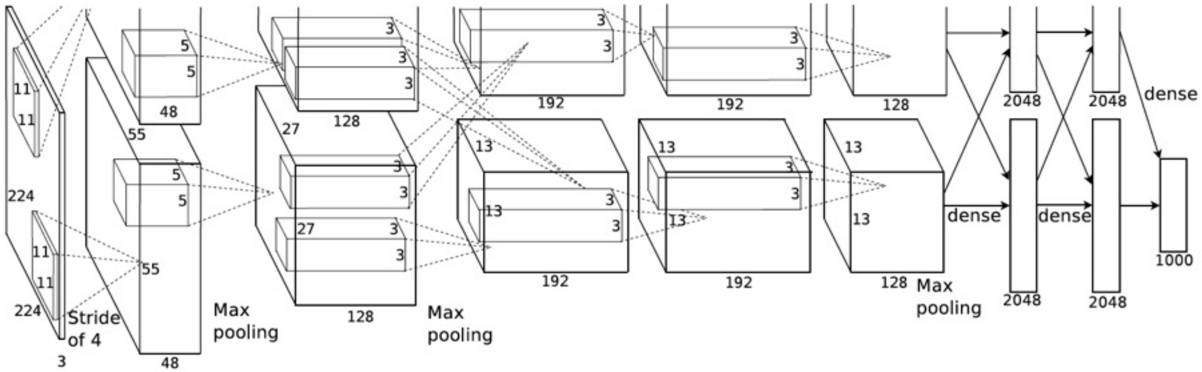
ImageNet



AlexNet beating all "handcrafted" approaches on ImageNet benchmark—the moment of truth for computer vision

L. Fei-Fei

AlexNet

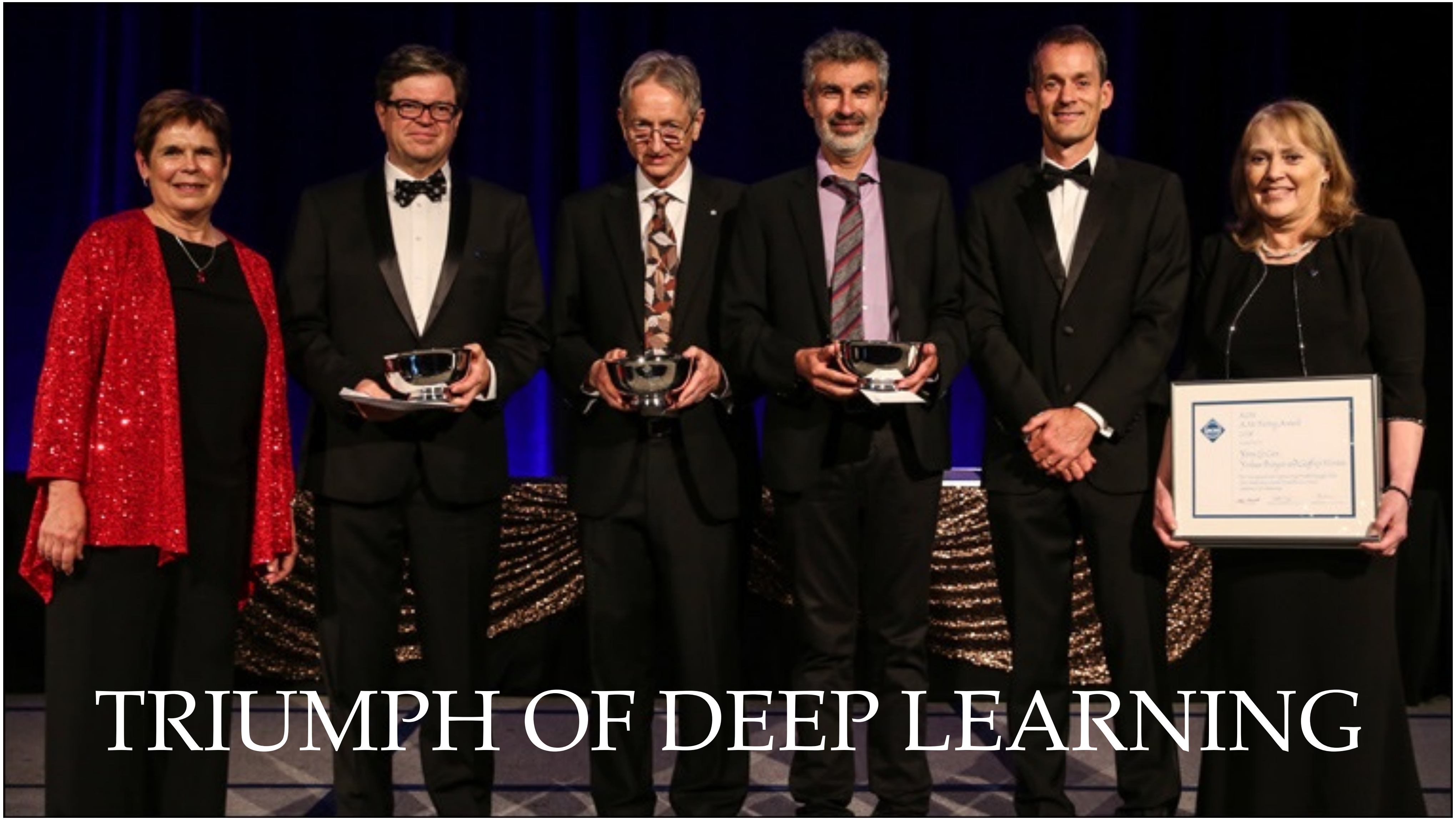


AlexNet architecture

Nvdia GTX 580 GPU capable of
~200G FLOP/sec

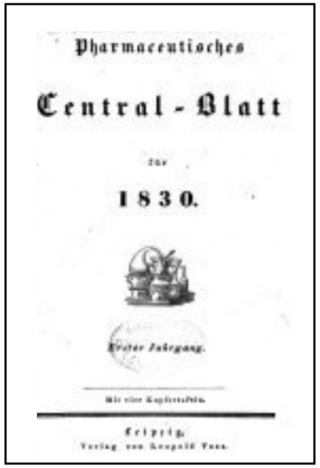
A. Krizhevsky

Krizhevsky et al. 2012

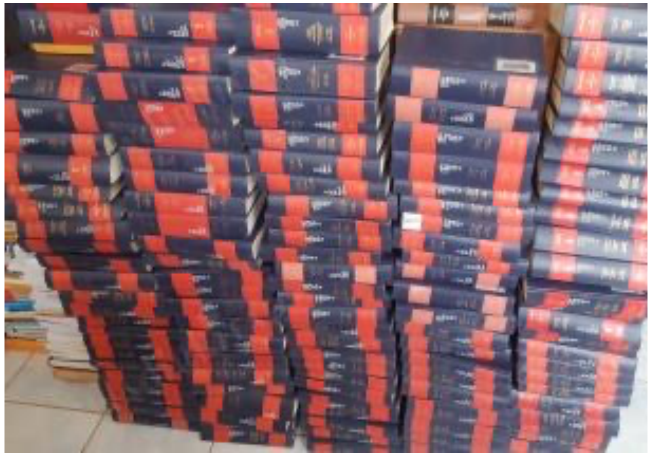

TRIUMPH OF DEEP LEARNING

GRAPH NEURAL NETWORKS & THEIR CHEMICAL PRECURSORS

Early chemoinformatics



First chemical abstracts journal
Chemisches Zentralblatt 1830–1969

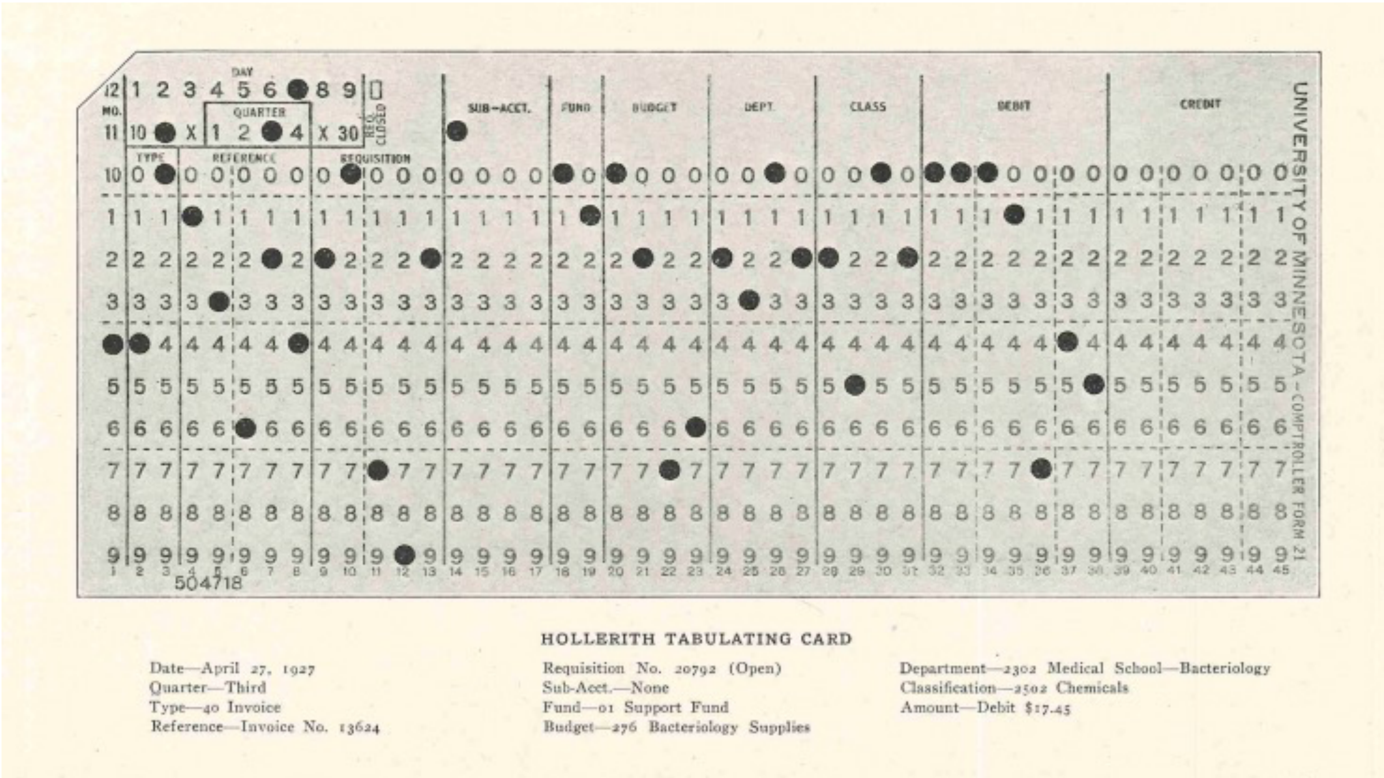


Beilstein Handbusch
~500 volumes, 500k pages

CAS
A division of the
American Chemical Society

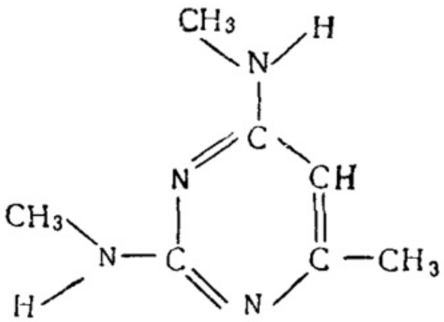
Chemical Abstracts Service
as of today ~200m compounds

Early chemoinformatics



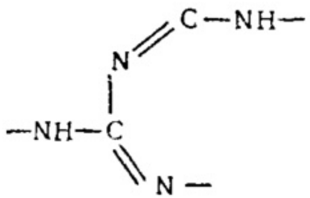
Punch card for early computer

Structural similarity of molecules



II

$H^1N^3J^1C^3NC^3J^1MC^3NX3N^3H^1J^1$



a)

$H^1N^3R^1C^3R^1NC^3NR^1N^3H^1R^1$

Early “chemical ciphers” used for molecule representations
fail to capture structural similarity

G. Vlăduţ

1959

Vlăduţ et al. 1959; Portrait: Ihor Gorskiy (from a photo courtesy of Serge Vlăduţ)

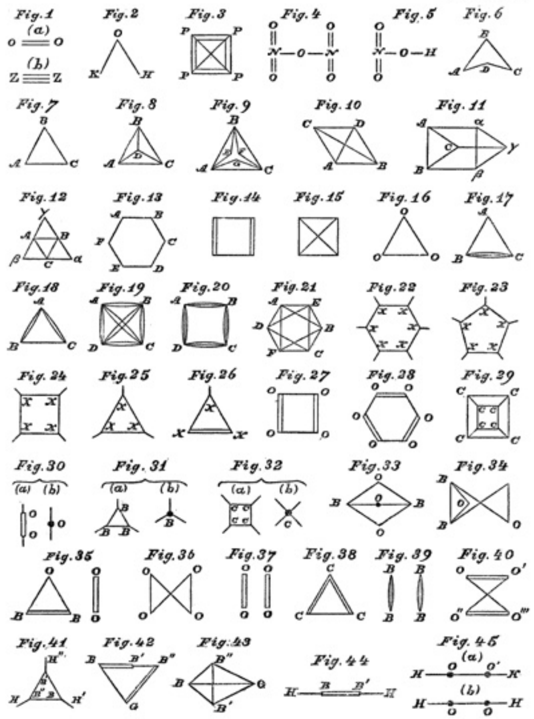
Graph theory & Chemistry

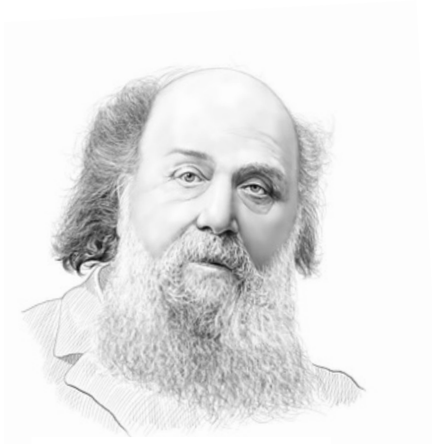
CHEMISTRY AND ALGEBRA

IT may not be wholly without interest to some of the readers of NATURE to be made acquainted with an analogy that has recently forcibly impressed me between branches of human knowledge apparently so dissimilar as modern chemistry and modern algebra.

The weight of an invariant is identical with the number of the bonds in the chemicograph of the analogous chemical substance, and the weight of the leading term (or basic differentiant) of a co-variant is the same as the number of bonds in the chemicograph of the analogous compound radical. Every invariant and covariant thus becomes expressible by a *graph* precisely identical with a Kekuléan diagram or chemicograph.

Baltimore, January 1 **J. J. SYLVESTER**





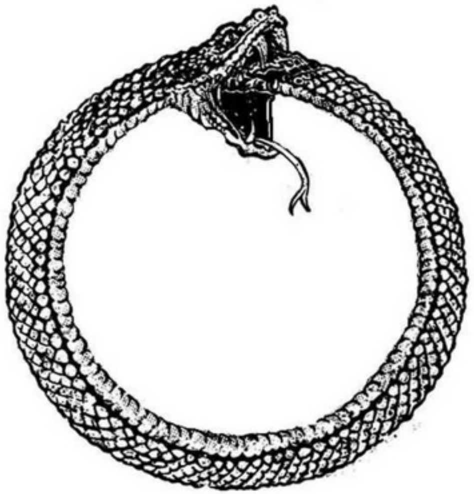
J. Sylvester

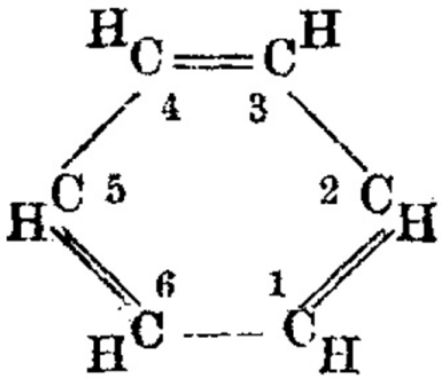
1878

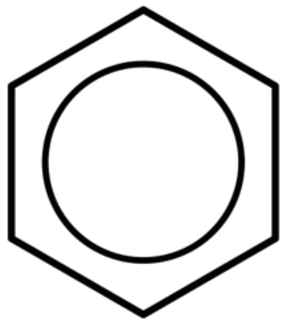
The term "graph" appeared first in the chemical context

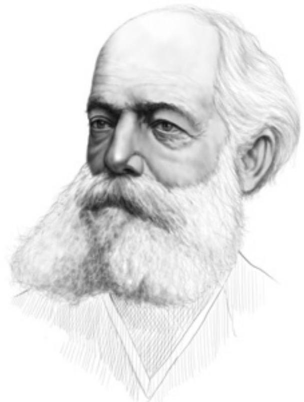
Sylvester 1878

Graph theory & Chemistry









A. Kekulé

Weisfeiler-Lehman test

УДК 519.1

ПРИВЕДЕНИЕ ГРАФА К КАНОНИЧЕСКОМУ ВИДУ И ВОЗНИКАЮЩАЯ ПРИ ЭТОМ АЛГЕБРА

Б. Ю. ВЕЙСФЕЙЛЕР, А. А. ЛЕМАН

Рассматривается алгоритм приведения заданного конечного мультиграфа Г к каноническому виду. В процессе такого приведения возникает новый инвариант графа — алгебра 𝔄 (Г). Изучение свойств алгебры 𝔄 (Г) оказывается полезным при решении некоторых задач теории графов.

Выдвигаются и обсуждаются некоторые предположения относительно связи между свойствами алгебры 𝔄 (Г) и группой автоморфизмов графа Aut (Г). Построен пример неориентированного графа Г, алгебра 𝔄 (Г) которого совпадает с групповой алгеброй некоторой некоммутативной группы.

An algorithm is considered, reducing the specified finite multigraph Г to canonical form. In the course of this reduction, a new invariant of the graph is generated — algebra 𝔄 (Г). Study of the properties of the algebra 𝔄 (Г) proves helpful in solving a number of graph-theoretic problems. Some propositions concerning the relationships between the properties of the algebra 𝔄 (Г) and the graph's automorphism group Aut (Г) are discussed. An example of non—oriented graph Г is constructed whose algebra 𝔄 (Г) coincides with the group algebra of a non—commutative group.

A. Lehman

B. Weisfeiler

1968

Weisfeiler, Lehman 1968; Portraits: Ihor Gorskiy

First Graph Neural Networks

A. Sperduti

C. Goller

A. Küchler

M. Gori

F. Scarselli

A. Micheli

Labeling RAAM

1994

Backprop through structure

1996

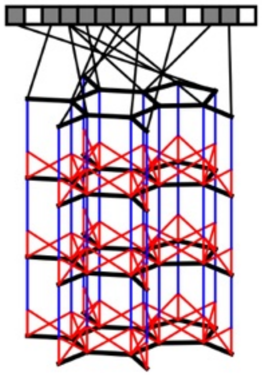
"Graph Neural Networks"

2005, 2008

"NN4G"

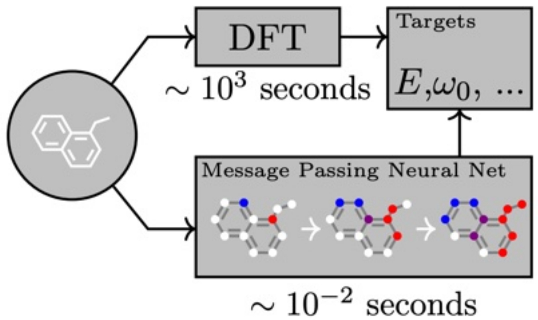
2009

Back to the chemical roots



GNN-based
molecular fingerprints

D. Duvenaud

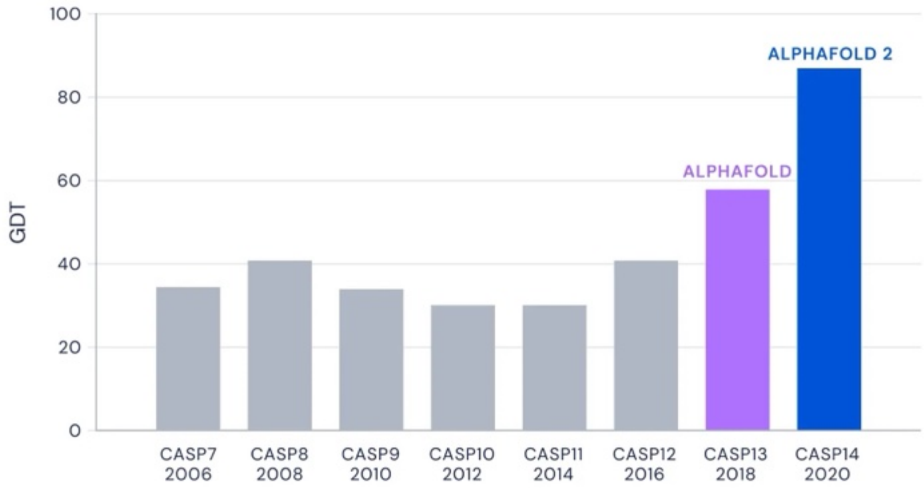


Chemical property prediction
using message passing GNNs

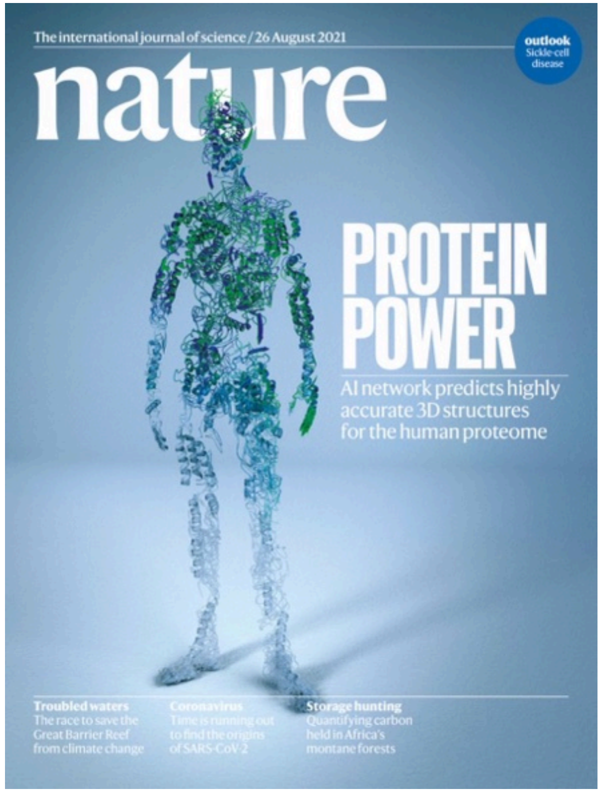
J. Gilmer

Duvenaud et al. 2015; Gilmer et al. 2017

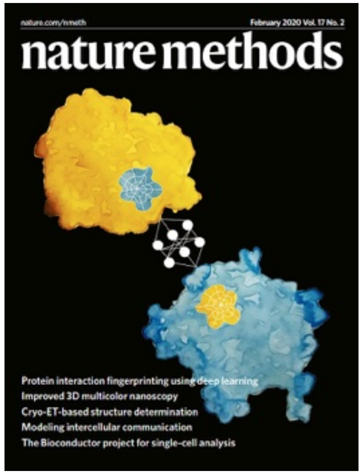
Back to the chemical roots



An "ImageNet" moment of structural biology



Jumper et al. 2021


nature.com/nmeth
February 2020 Vol. 17 No. 2
nature methods
Protein interaction fingerprinting using deep learning
Improved 3D multicolor nanoscopy
Cryo-ET-based structure determination
Modeling intercellular communication
The Bioconductor project for single-cell analysis


Cell
Volume 180
Number 4
February 20, 2020
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nature machine intelligence
Bioactive molecule design with geometric deep learning


SARS-CoV-2 is evolving fast. What will it do next?
Effects on surface water from hydraulic fracturing
Baby bats babble like human babies
Science
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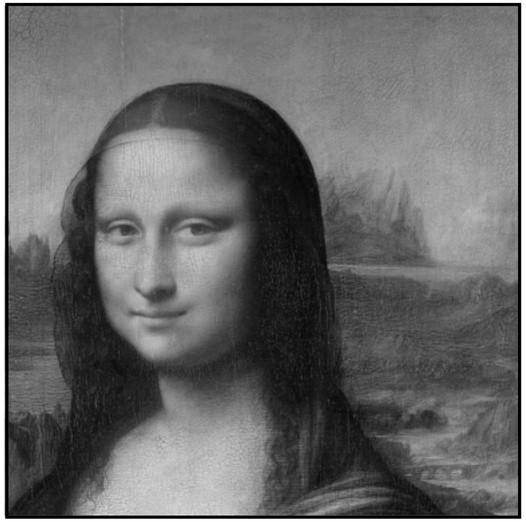
AAAS
PREDICTING
STRUCTURES
Deep learning accurately folds proteins

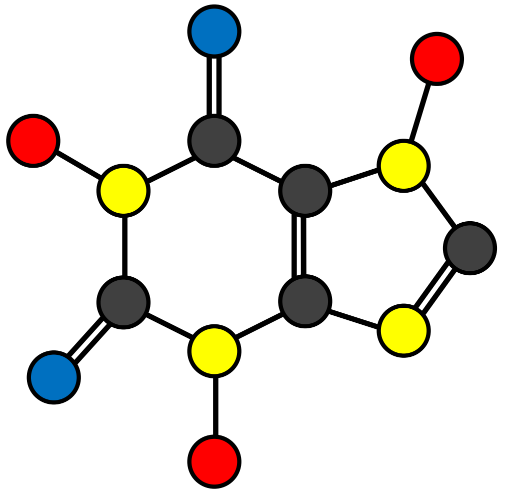

www.nature.com/natcomputsci / July 2021 Vol. 1 No. 7
nature computational science
Efficient protein model refinement with deep learning

THE BLUEPRINT

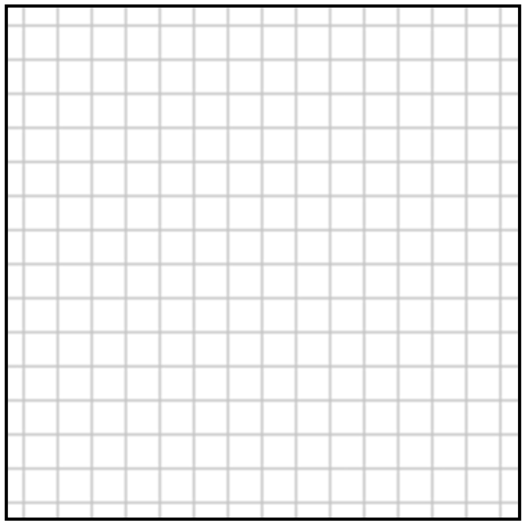
Convolutional Neural Network



Graph Neural Network

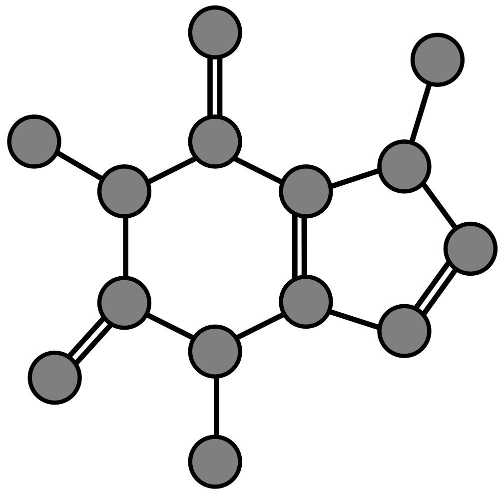


Convolutional Neural Network

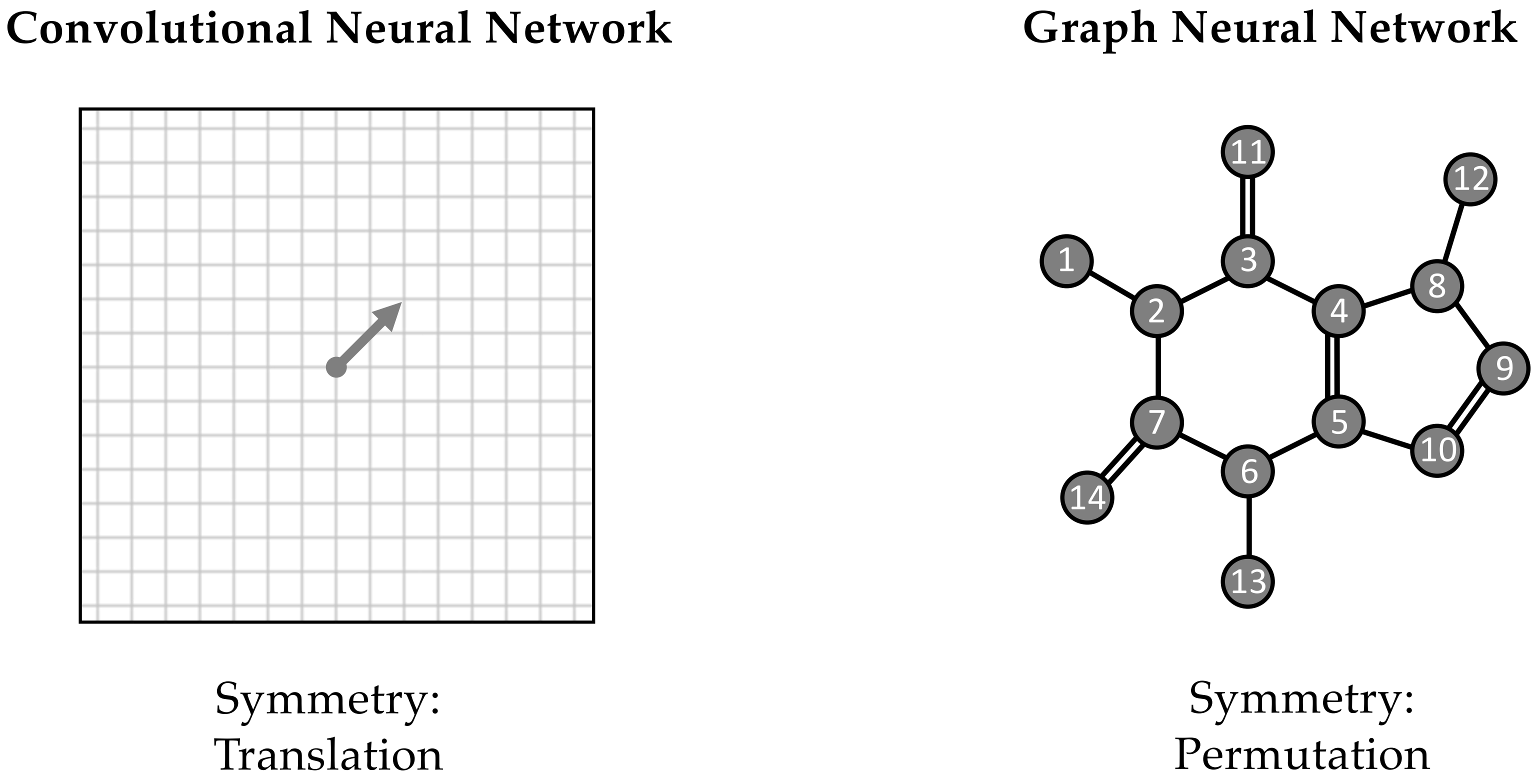


Underlying domain:
grid

Graph Neural Network

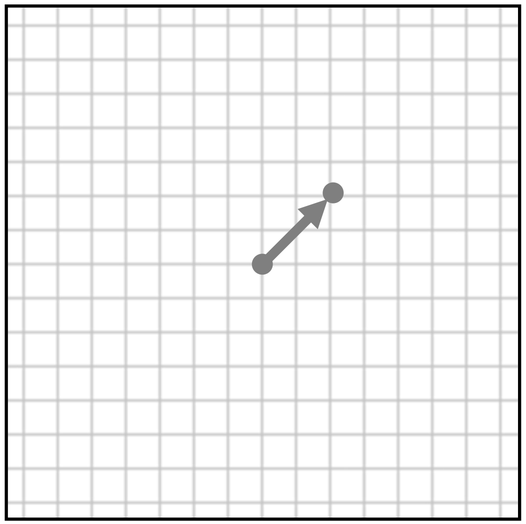


Underlying domain:
graph



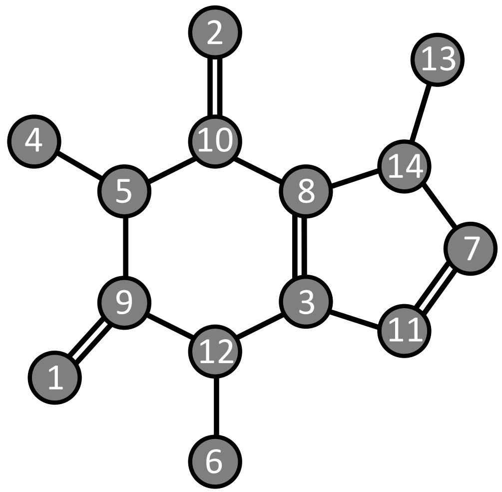
Convolutional Neural Network
Graph Neural Network
1
2
3
4
5
6
7
8
9
10
11
12
13
14
Symmetry:
Translation
Symmetry:
Permutation

Convolutional Neural Network



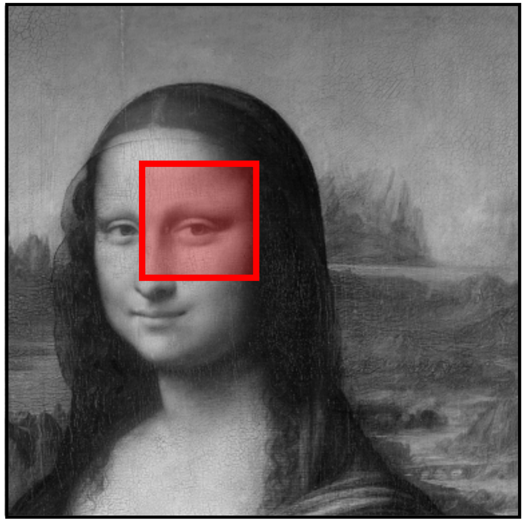
Symmetry:
Translation

Graph Neural Network



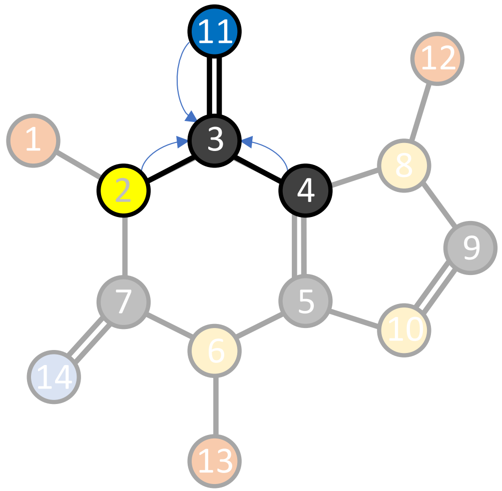
Symmetry:
Permutation

Convolutional Neural Network



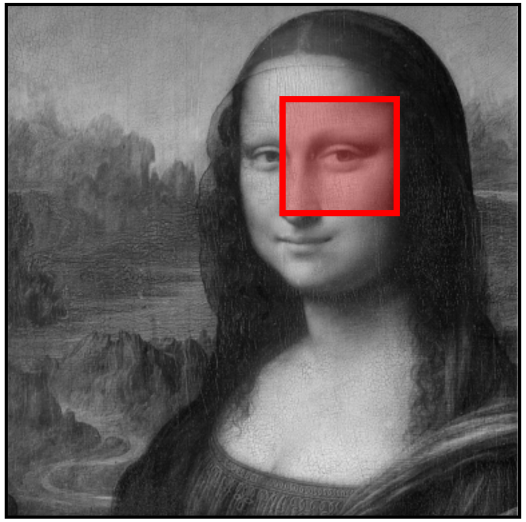
Convolution:
translation equivariant

Graph Neural Network



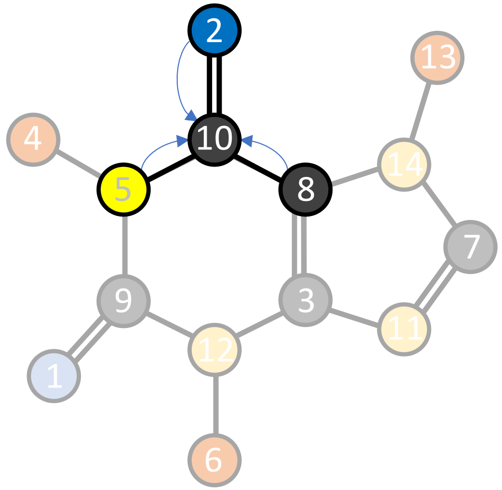
Message passing:
permutation equivariant

Convolutional Neural Network



Convolution:
translation equivariant

Graph Neural Network



Message passing:
permutation equivariant

Michael M. Bronstein, Joan Bruna, Yann LeCun,
Arthur Szlam, and Pierre Vandergheynst

Many scientific fields study data with an underlying structure that is non-Euclidean. Some examples include social networks in computational social sciences, sensor networks in communications, functional networks in brain imaging, regulatory networks in genetics, and meshed surfaces in computer graphics. In many applications, such geometric data are large and complex (in the case of social networks, on the scale of billions) and are natural targets for machine-learning techniques. In particular, we would like to use deep neural networks, which have recently proven to be powerful tools for a broad range of problems from computer vision, natural-language processing, and audio analysis. However, these tools have been most successful on data with an underlying Euclidean or grid-like structure and in cases where the invariances of these structures are built into networks used to model them.

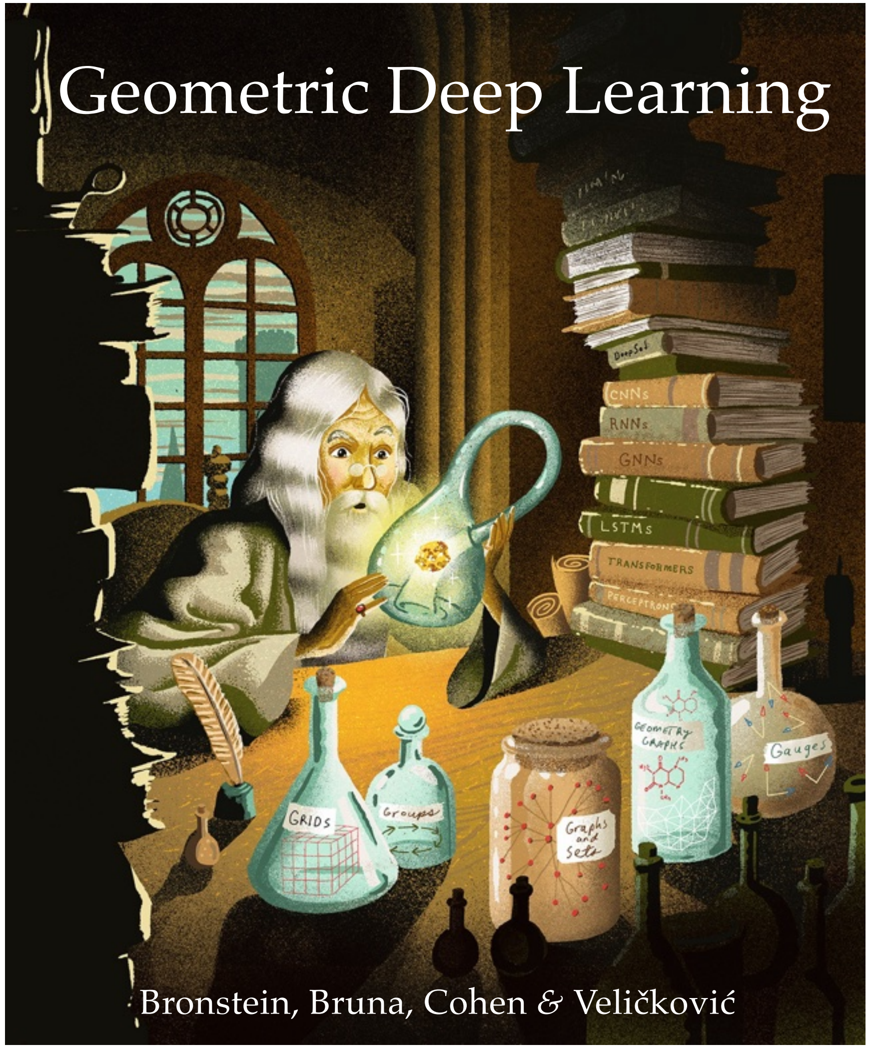
Geometric deep learning is an umbrella term for emerging techniques attempting to generalize (structured) deep neural models to non-Euclidean domains, such as graphs and manifolds. The purpose of this article is to overview different examples of geometric deep-learning problems and present available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

Overview of deep learning

Deep learning refers to learning complicated concepts by building them from simpler ones in a hierarchical or multilayer manner. Artificial neural networks are popular realizations of such deep multilayer hierarchies. In the past few years, the growing computational power of modern graphics processing unit (GPU)-based computers and the availability of large training data sets have allowed successfully training neural networks with many layers and degrees of freedom (DoF) [1]. This has led to qualitative breakthroughs on a wide variety of tasks, from speech recognition [2], [3] and machine translation [4] to image analysis and computer vision [5]–[11] (see [12]

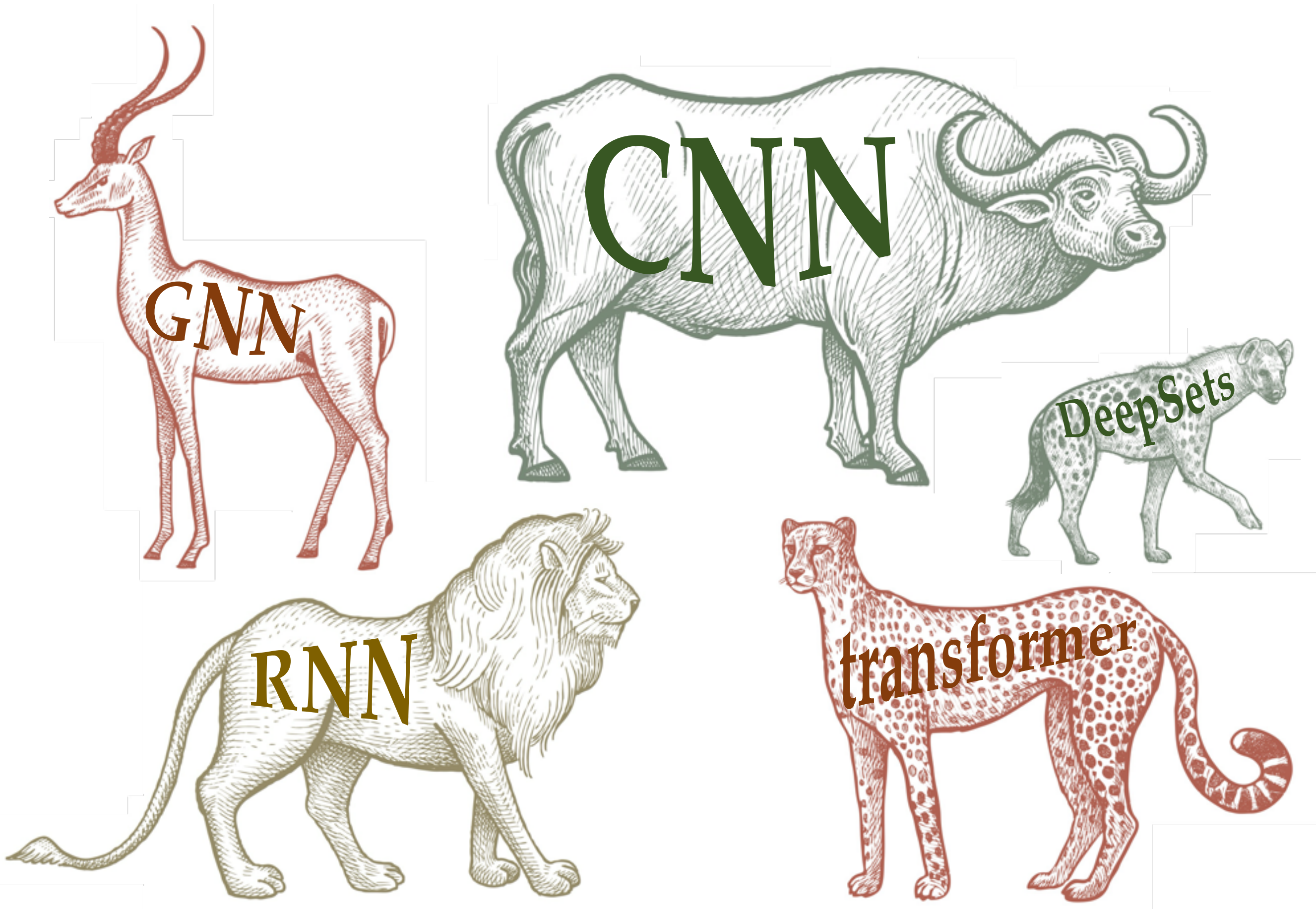
Geometric Deep Learning

Going beyond Euclidean data

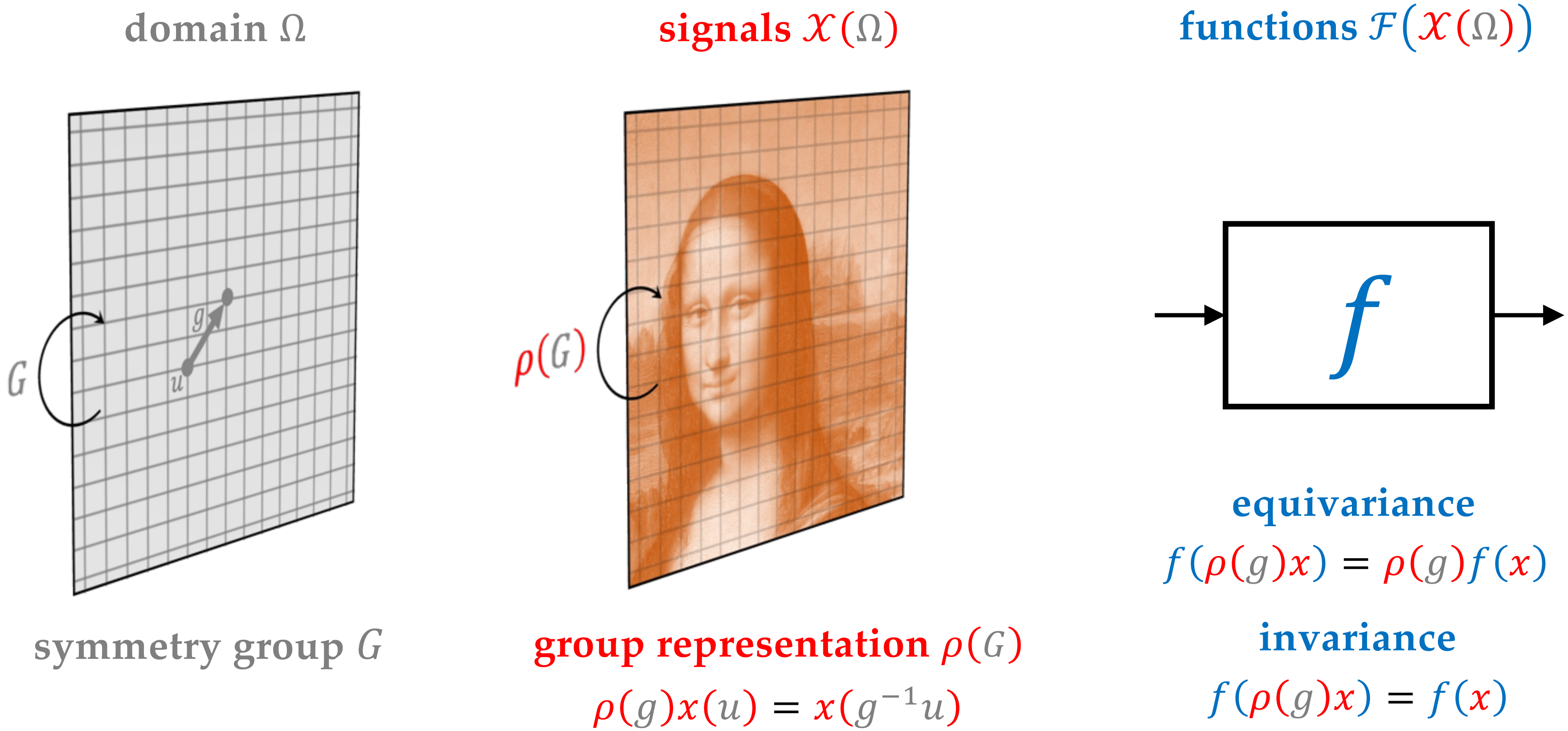


The Erlangen Programme of ML

Geometric Deep Learning

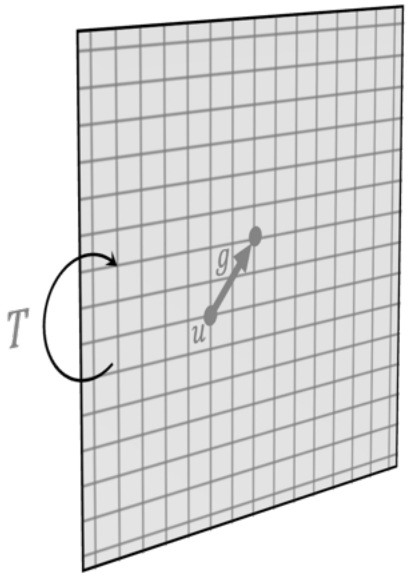

GNN
CNN
DeepSets
RNN
transformer

Geometric Deep Learning Blueprint



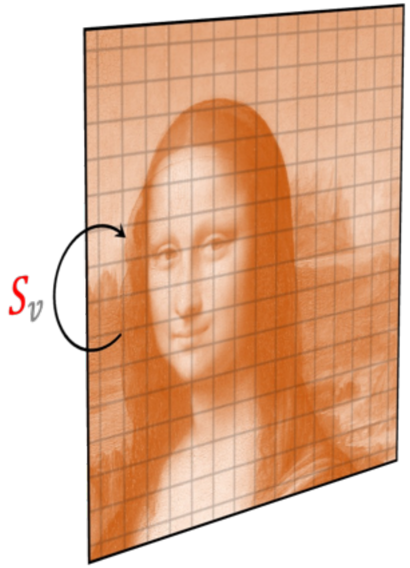
Example: Convolutional Neural Networks

Plane $\mathbb{R}^2$



Translation group $T(2)$

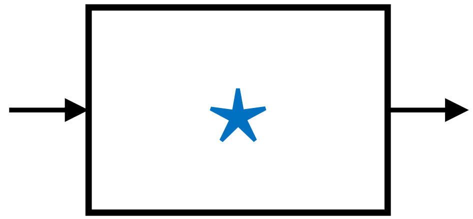
images $\mathcal{X}(\mathbb{R}^2)$



Shift operator S

$S_v x(u) = x(u - v)$

functions $\mathcal{F}(\mathcal{X}(\Omega))$

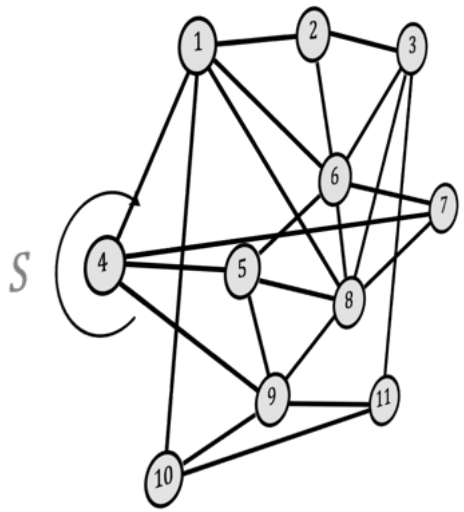


Convolutional layer

$(Sx \star y) = S(x \star y)$

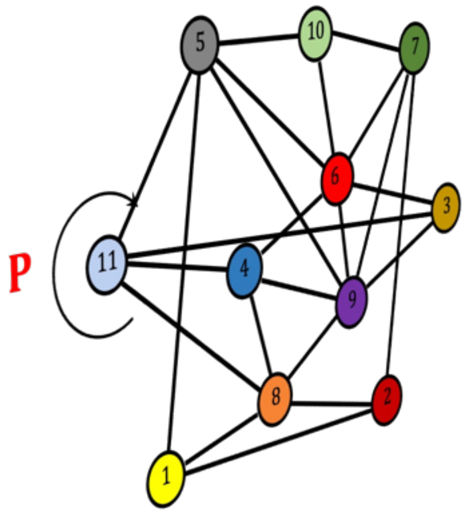
Example: Graph Neural Networks

Graph $G = (V, E)$



Permutation group S_n

Node features $\mathcal{X}(G)$



Permutation matrix P

$$\mathbf{PX} = \left(x_{\pi^{-1}(i),j}\right)$$

functions $\mathcal{F}(\mathcal{X}(\Omega))$

Message passing

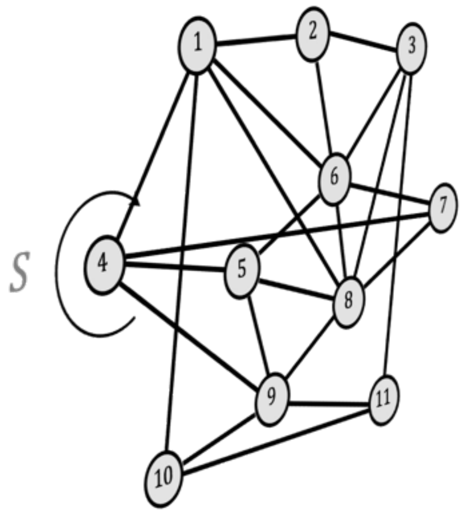
$$\mathbf{F}(\mathbf{PX}, \mathbf{PAP}^\top) = \mathbf{PF}(\mathbf{X}, \mathbf{A})$$

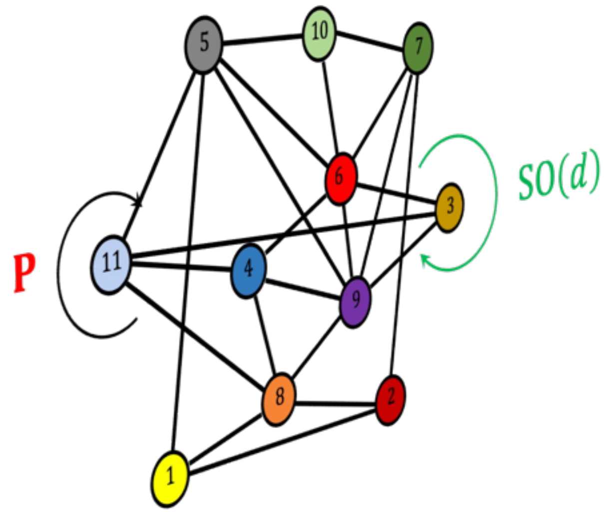
Example: Equivariant Graph Neural Networks

Graph $G = (V, E)$

Node features $\mathcal{X}(G)$

functions $\mathcal{F}(\mathcal{X}(\Omega))$





Permutation group S_n

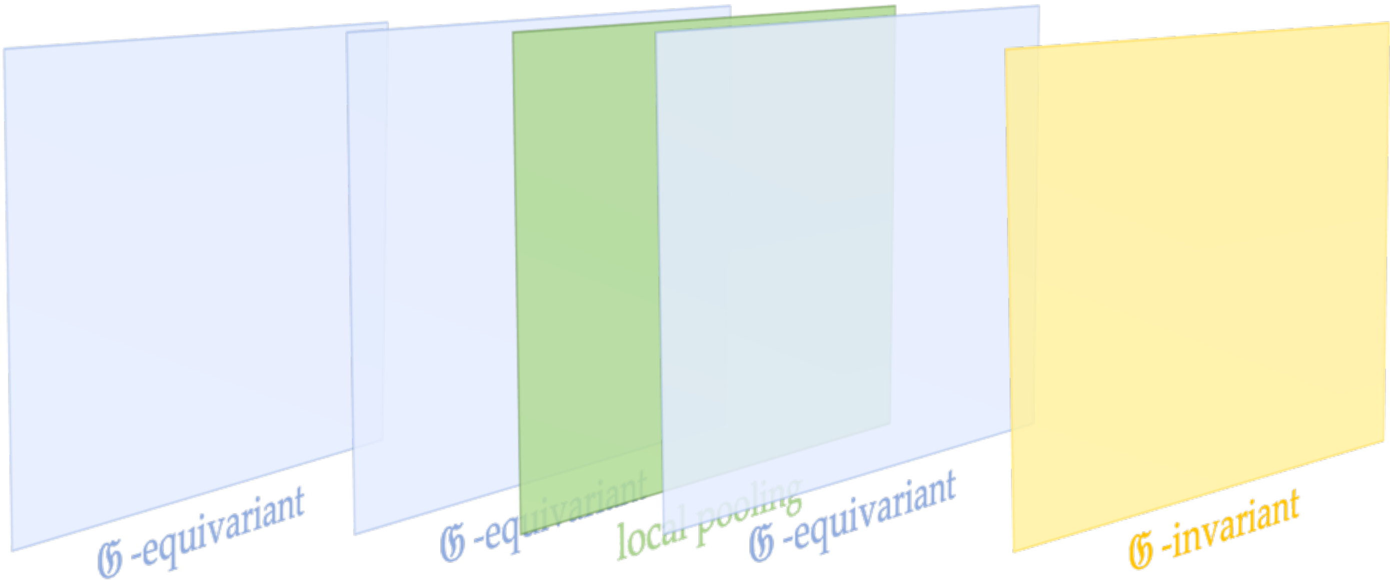
Permutation matrix P

Rotation R

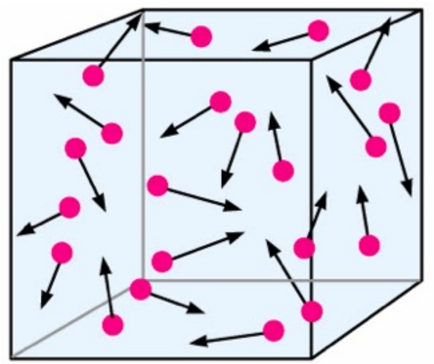
Equivariant message passing

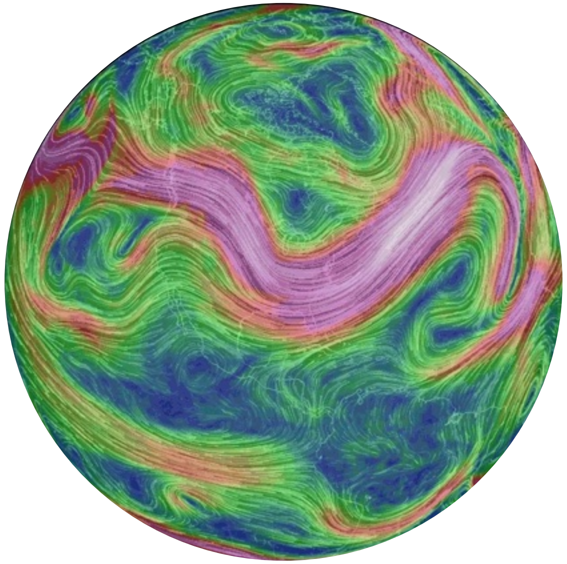
$$\mathbf{F}(\mathbf{PXR}, \mathbf{PAP}^\top) = \mathbf{PF}(\mathbf{X}, \mathbf{A})\mathbf{R}$$

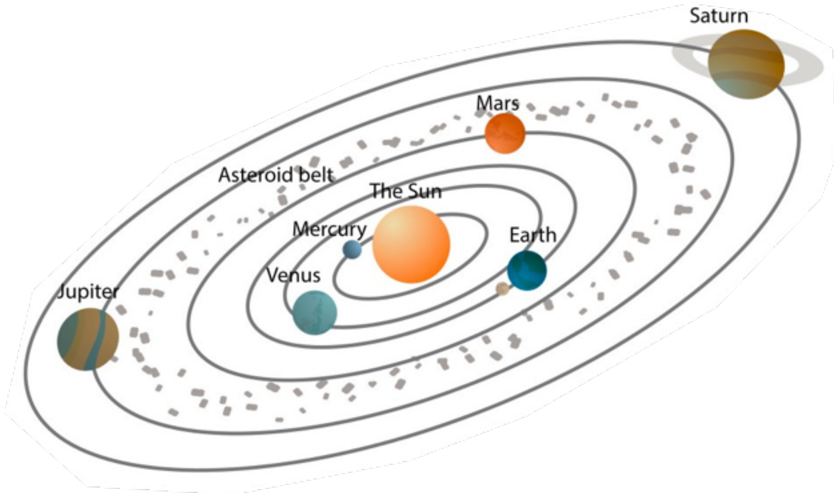
Geometric Deep Learning Blueprint



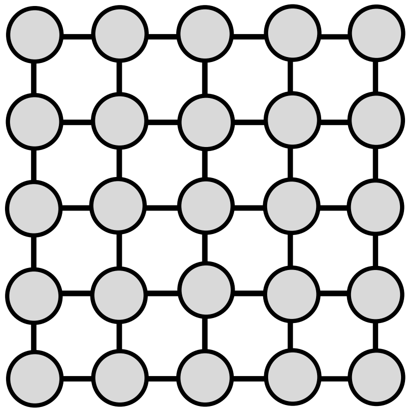
Scale Separation in Physics



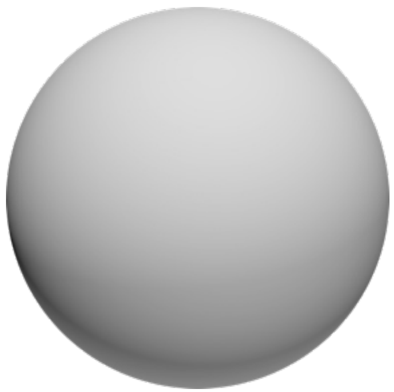




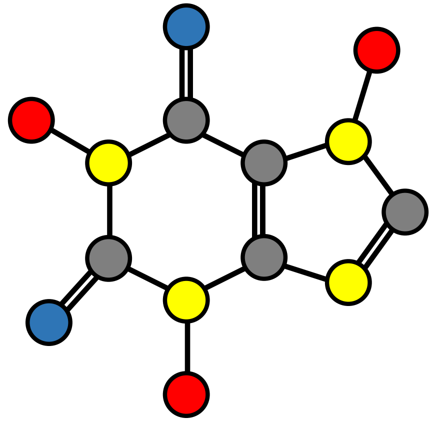
The “5G” of Geometric Deep Learning



Grids



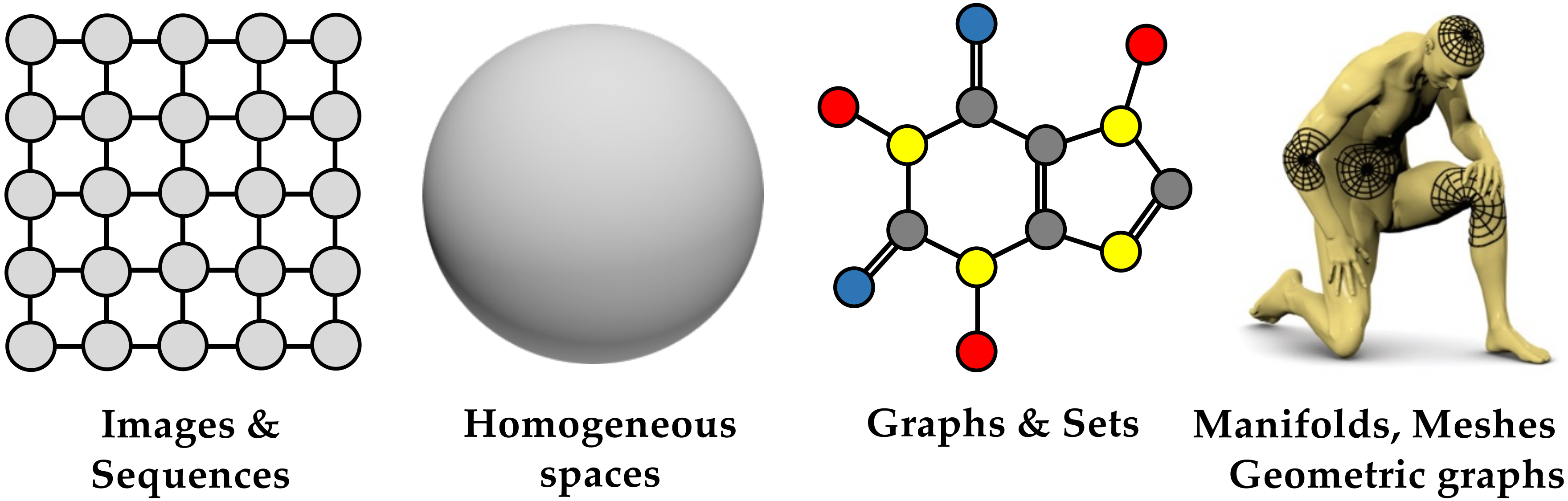
Groups

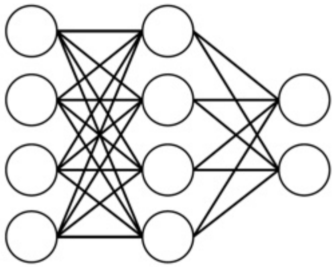


Graphs

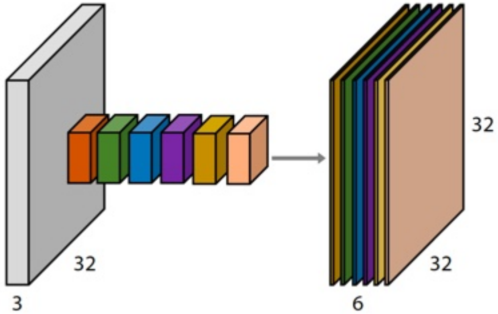
Geometric Graphs & Gauges

The "5G" of Geometric Deep Learning

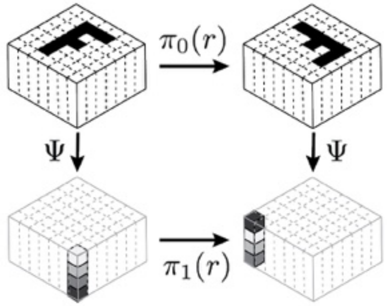




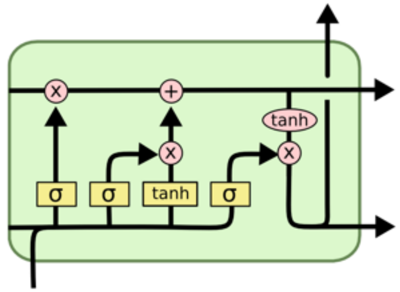
Perceptrons
Function regularity



CNNs
Translation

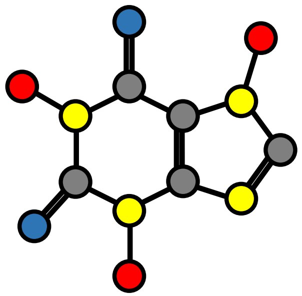


Group-CNNs
Translation+Rotation,
Global groups



LSTMs
Time warping

DeepSets / Transformers
Permutation



GNNs
Permutation

Intrinsic CNNs
Isometry / Gauge choice

nature machine intelligence
Crystal Hamiltonian graph neural networks
nature physics
Glassy learning
nature computational science
Predicting properties of materials using graph networks
nature machine intelligence
Graph learning for resistive memory arrays
nature machine intelligence
Learning causal structures in biological data
nature computational science
Architectural design at the molecular level
Physics
Materials
Chip design
Biology
nature computational science
Advancing transition state structure generation
nature machine intelligence
Predicting chemical reactivity in a digital lab
nature computational science
Opportunities for machine learning in chemical reaction networks
nature machine intelligence
Urban insights from graph-based machine learning
nature
AI-GUIDED INTUITION
Science
AI-POWERED FORECASTING
Chemistry
Urban planning
Pure math
Weather

Generate : Biomedicines
A Flagship Pioneering Company

VANTAI

Isomorphic Laboratories

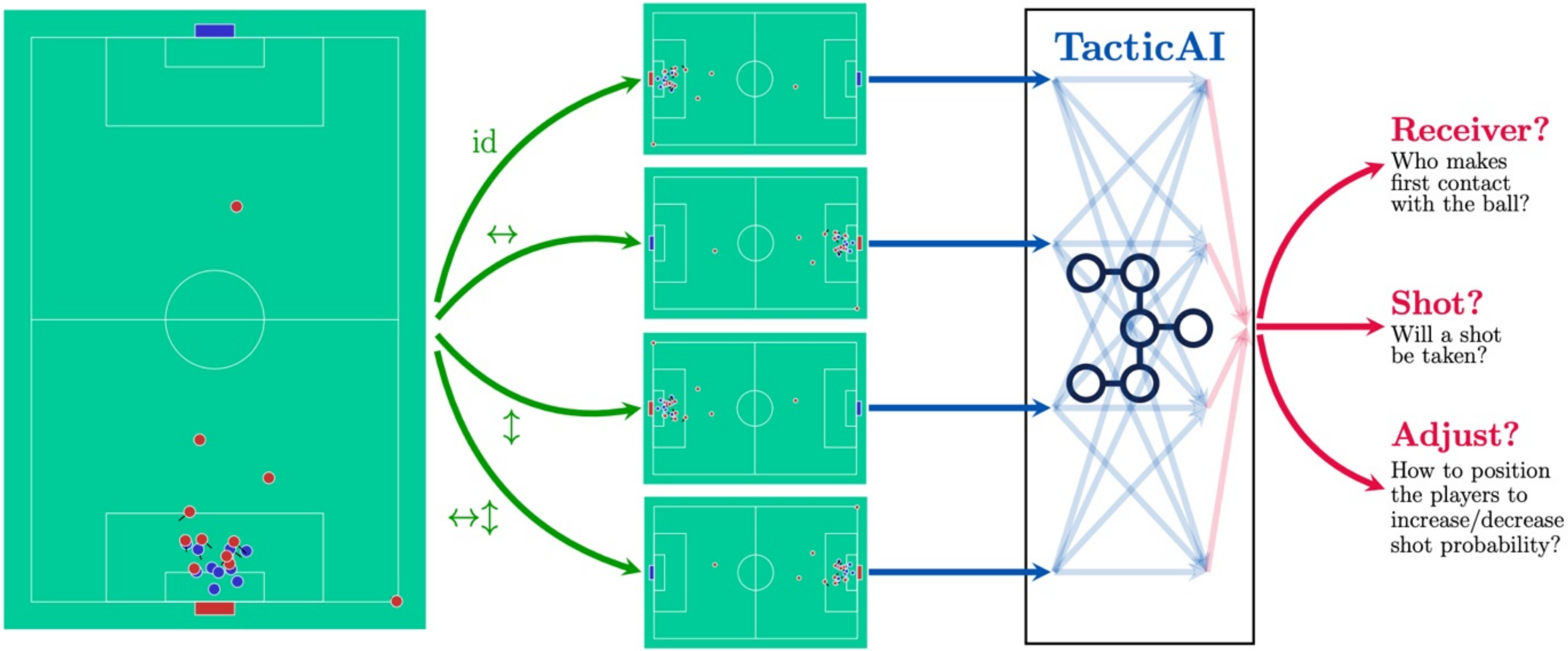
Recursion

Genentech

Monte Rosa
THERAPEUTICS

CHARM
THERAPEUTICS

dreamfold



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Main References

- M. Bronstein et al., Geometric deep learning, *arXiv:2104.13478, 2021*. Section 7 "Historic perspective"
- M. Bronstein, Towards geometric deep learning, *The Gradient, 2022*. Historical overview of the field following this lecture