GEOMETRIC DEEP LEARNING (**L65**)

Pietro Liò *University of Cambridge*
Petar Veličković *Google DeepMind / University of Cambridge*

Lent Term 2024

CST Part III / MPhil ACS / MPhil MLMI

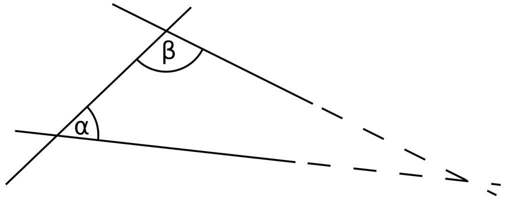
0. COURSE INTRODUCTION

*Why **geometric** deep learning?*

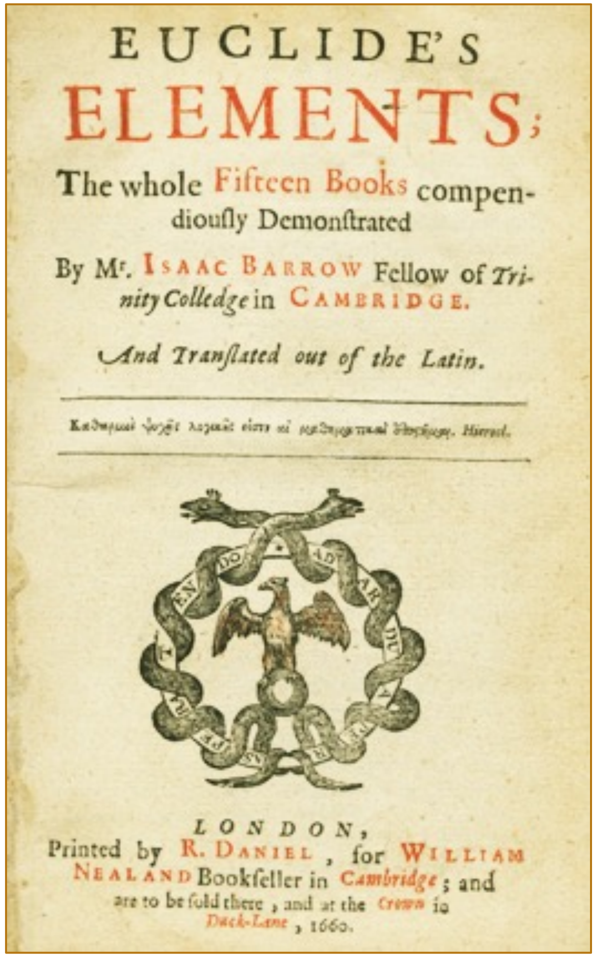
Petar Veličković

Going back in time…

Going back in time…



Euclid
~300 B.C.

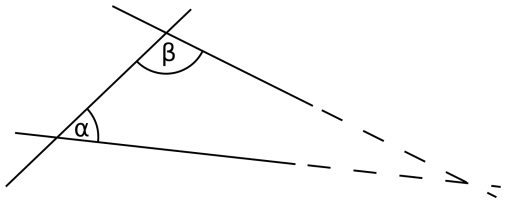


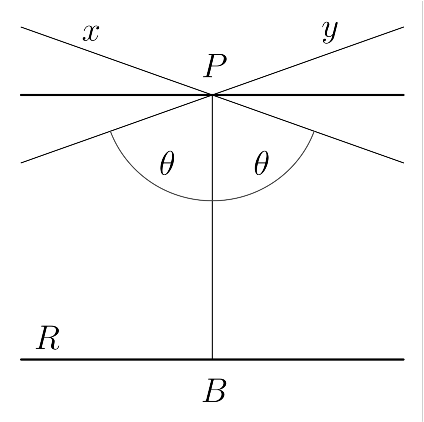
EUCLIDE'S
ELEMENTS;
The whole Fifteen Books compendiouſly Demonſtrated
By Mr. ISAAC BARROW Fellow of *Trinity Colledge* in CAMBRIDGE.
And Tranſlated out of the Latin.

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.

"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"

Going back in time…





"I have discovered such wonderful things that I was amazed…out of nothing I have created a strange new universe."—János Bolyai, to his father

Euclid

~300 B.C.

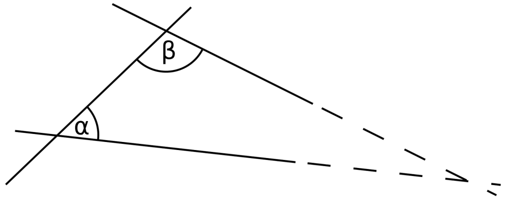
Lobachevsky

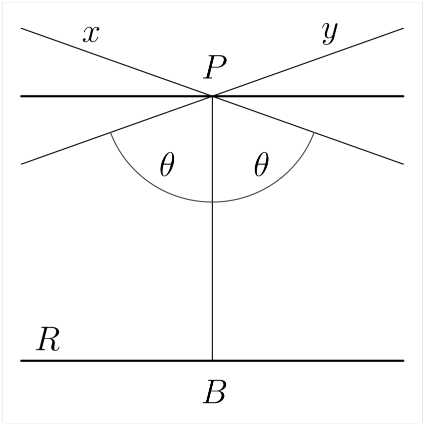
1826

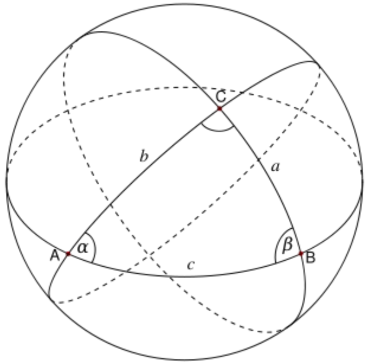
Bolyai

1832

Going back in time…







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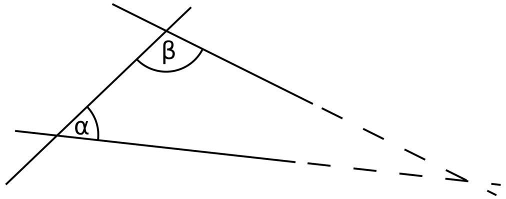
~300 B.C.

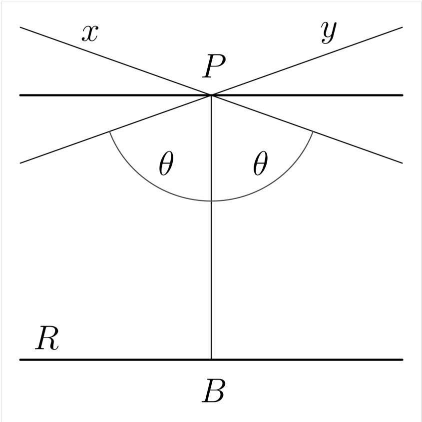
Lobachevsky
1826

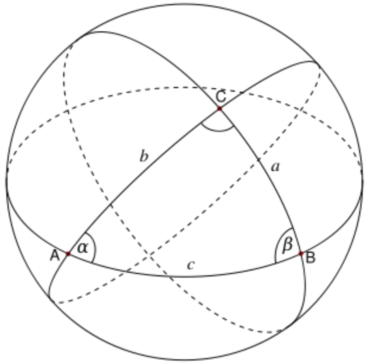
Bolyai
1832

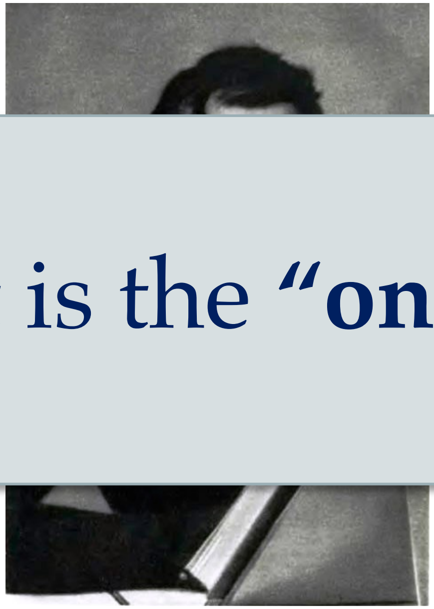
Riemann
1856

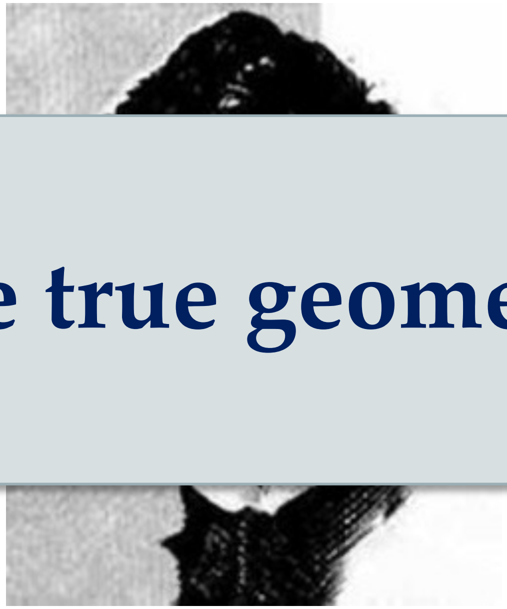
Going back in time…

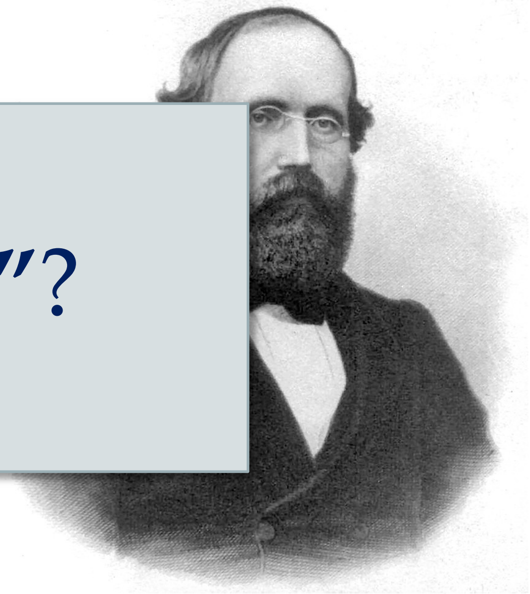












What is the “**one true geometry**”?

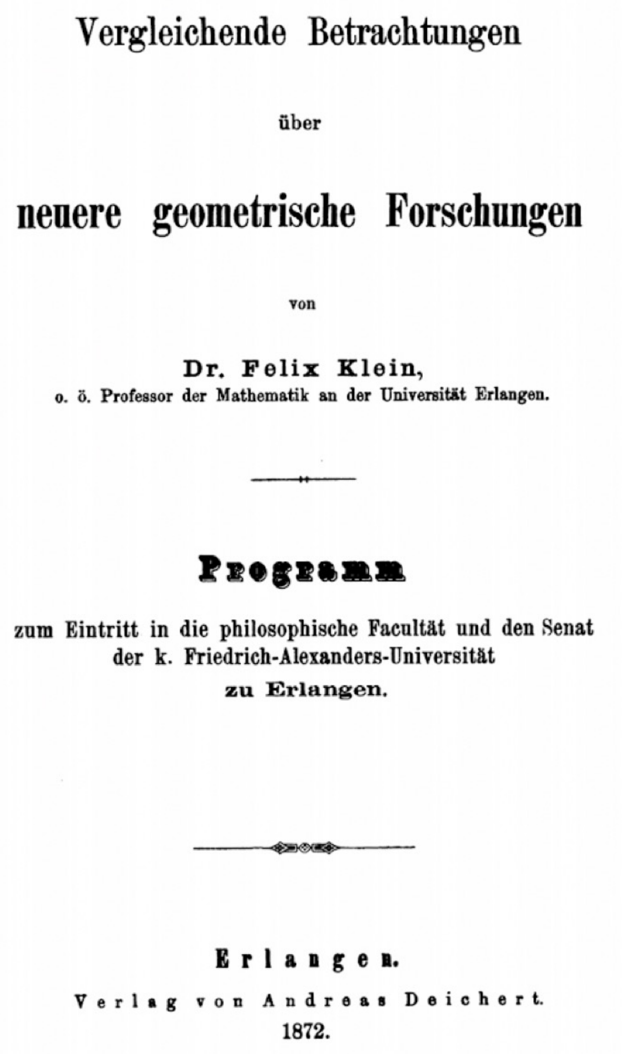
Euclid
~300 B.C.

Lobachevsky
1826

Bolyai
1832

Riemann
1856

Felix Klein and the "Erlangen Program" (1872)



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.

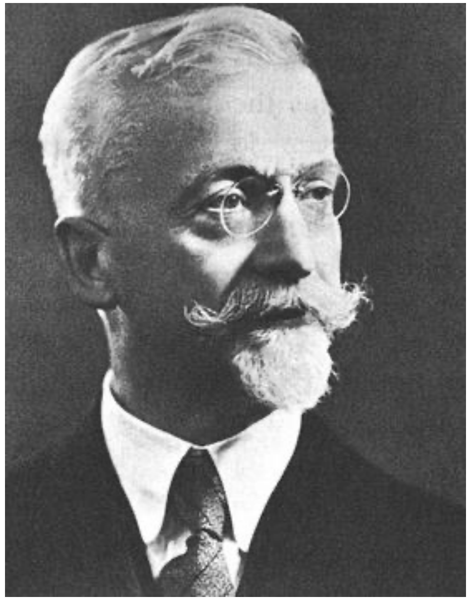
Blueprint for **unifying** geometries

Using **invariance** and **symmetry**

Formalised using **group theory**

The impact of the Erlangen Program is hard to overstate!

Unified all geometries



Cartan

1920s

LES GROUPES D'HOLONOMIE DES ESPACES GÉNÉRALISÉS.

PAR

E. CARTAN

à PARIS.

Introduction.

1. J'ai développé, dans ces dernières années, une théorie générale des espaces englobant la théorie classique des espaces de RIEMANN et celle plus récente des espaces de WEYL[1]. Je me suis rencontré sur certains points avec différents auteurs, particulièrement M. J. A. SCHOUTEN, qui poursuivaient des généralisations analogues, mais mon idée directrice était cependant nettement différente des leurs. Au lieu de généraliser d'une manière plus ou moins naturelle les lois du transport par parallélisme des vecteurs, j'ai cherché à étendre le principe si fécond de KLEIN, d'après lequel toute Géométrie est l'étude des propriétés d'un groupe de transformations G: le *continuum* dans lequel sont localisées les figures dont s'occupe cette Géométrie, et dont les seules propriétés jugées essentielles sont celles qui se conservent par une transformation arbitraire de G, s'appelle un *espace*[2] *à groupe fondamental* G.

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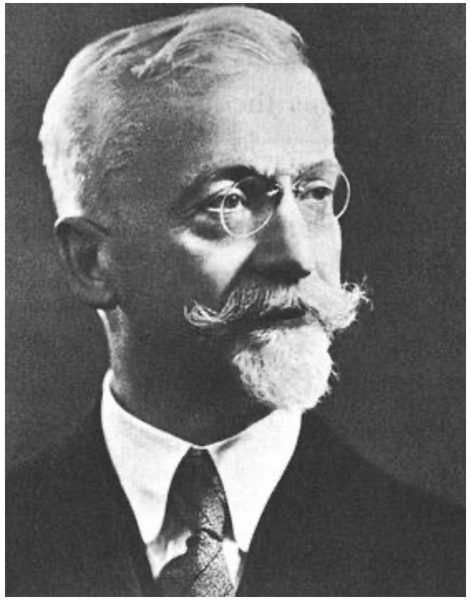
Unified all geometries



Cartan

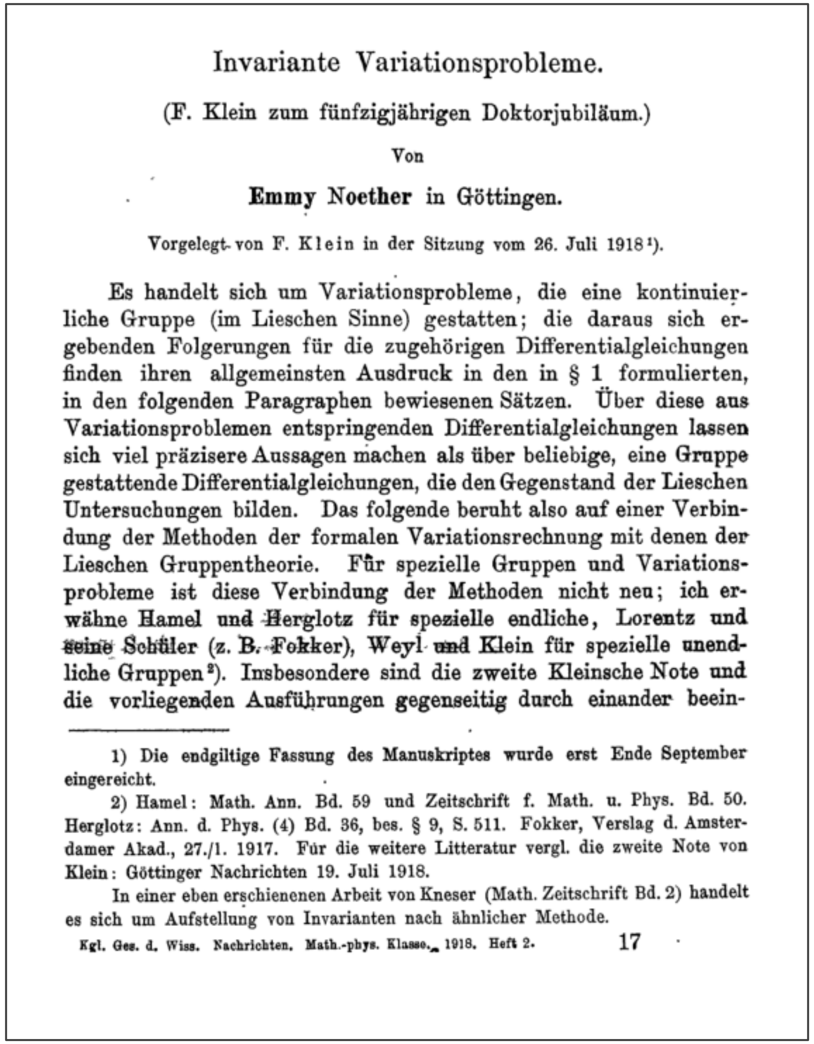
1920s

Conservation laws from symmetry

+ Standard model!

Noether

1918



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.

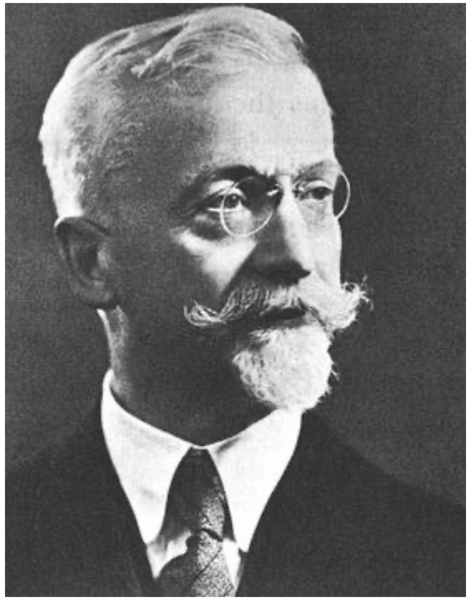
2) Hamel: Math. Ann. Bd. 59 und Zeitschrift f. Math. u. Phys. Bd. 50. Herglotz: Ann. d. Phys. (4) Bd. 36, bes. § 9, S. 511. Fokker, Verslag d. Amsterdamer Akad., 27./1. 1917. Für die weitere Litteratur vergl. die zweite Note von Klein: Göttinger Nachrichten 19. Juli 1918.

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

The impact of the Erlangen Program is hard to overstate!

Unified all geometries



Cartan
1920s

Conservation laws from symmetry

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Noether
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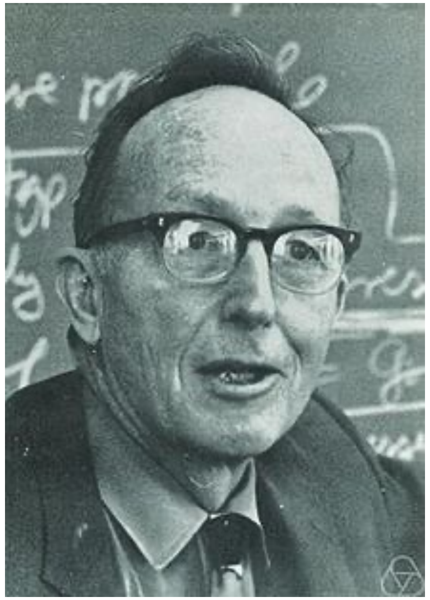
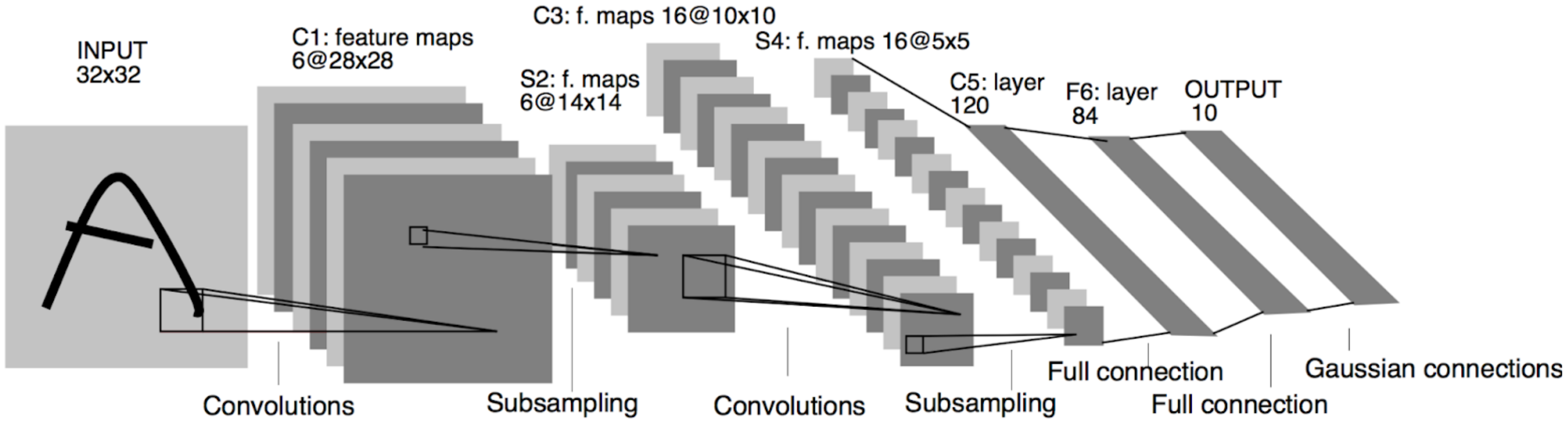
Category Theory

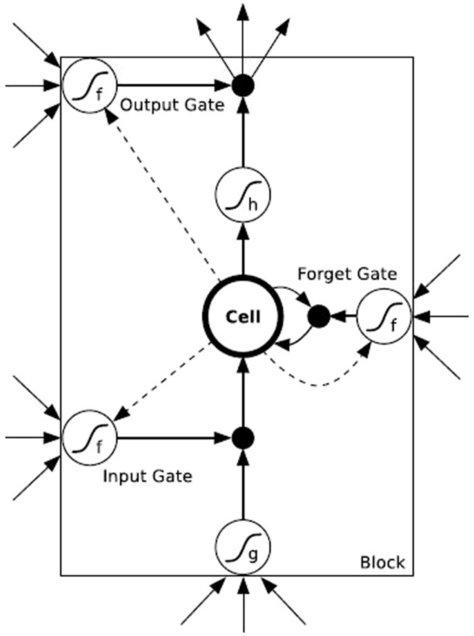


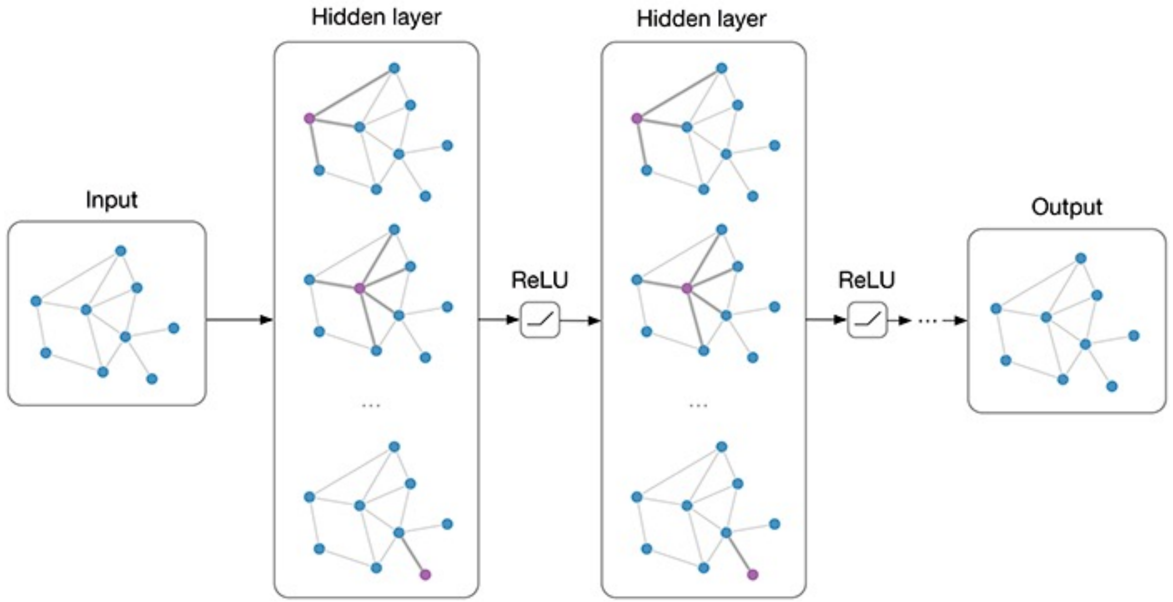
Eilenberg & Mac Lane
1945

?

Deep Learning, circa 2020







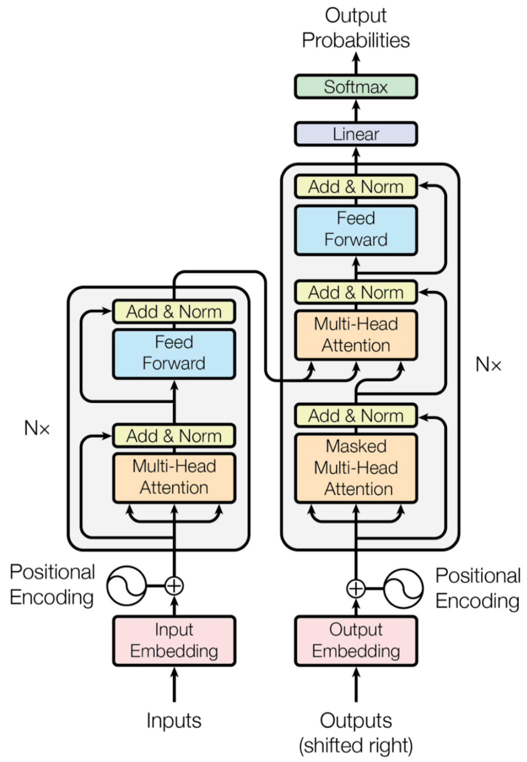
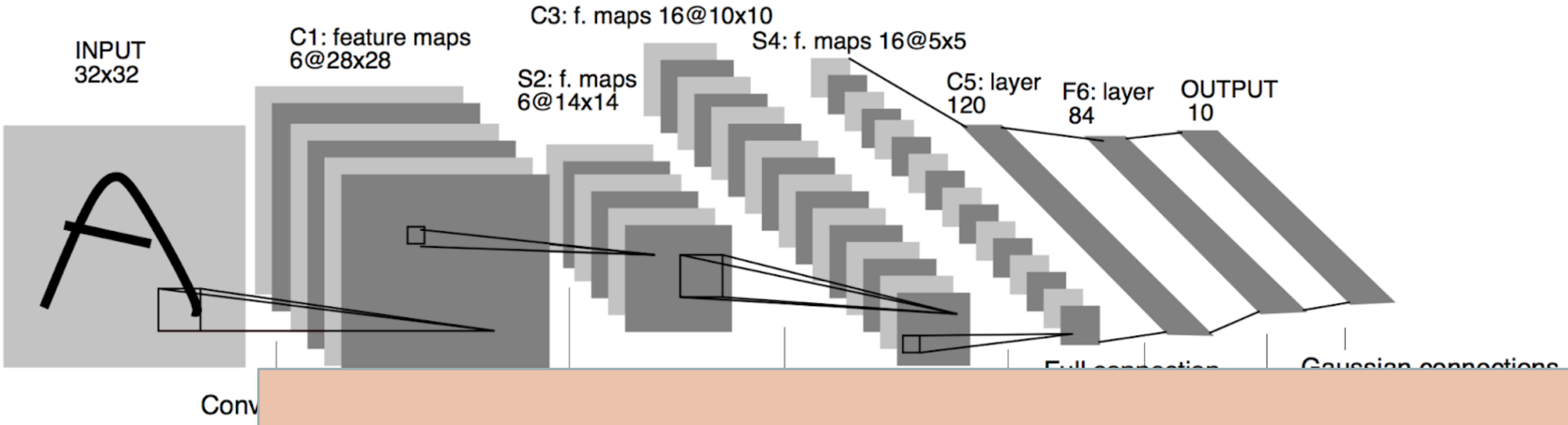
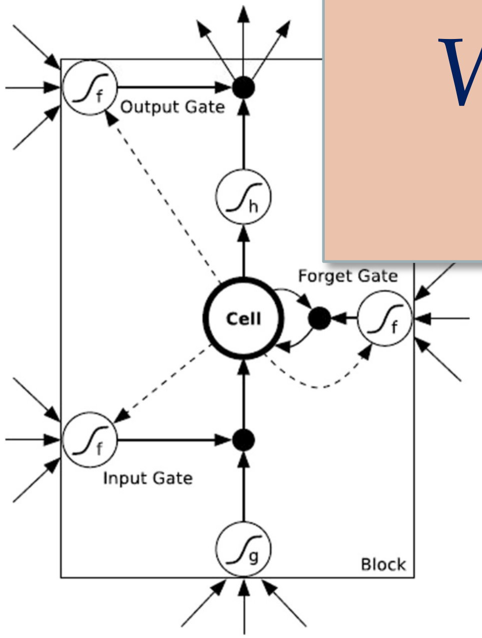


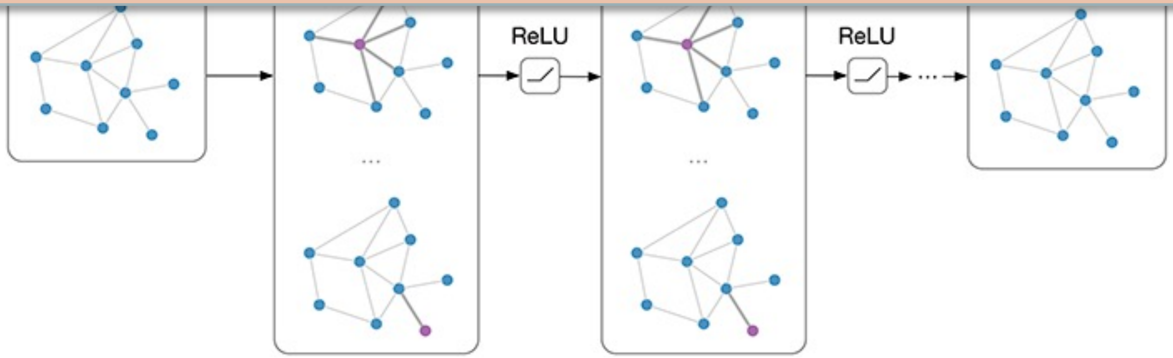
Figure 1: The Transformer - model architecture.

Deep Learning, circa 2020



What is the “**one true architecture**”?





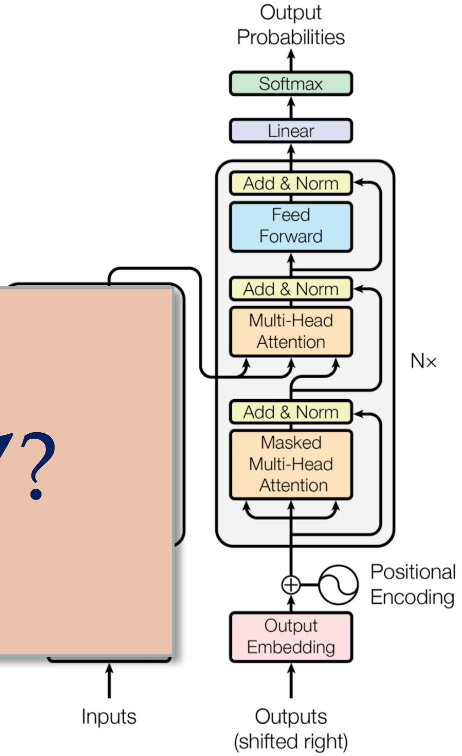
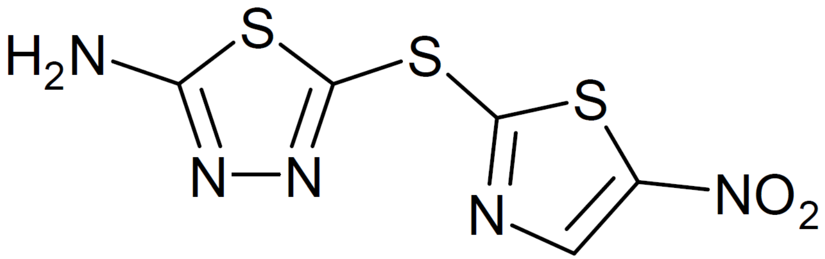
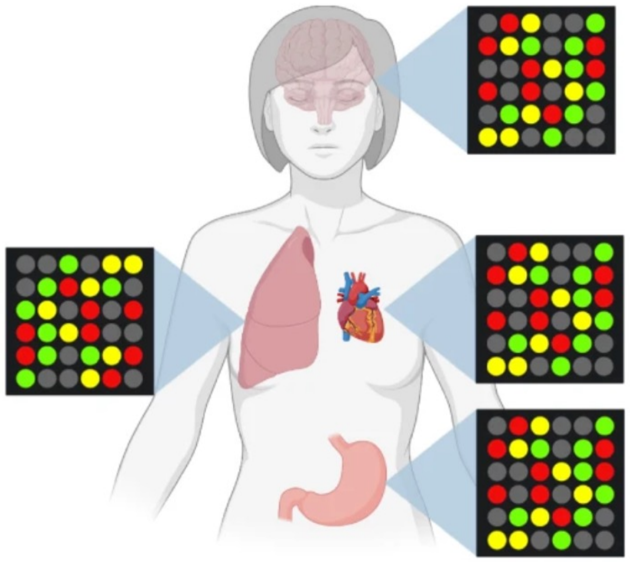


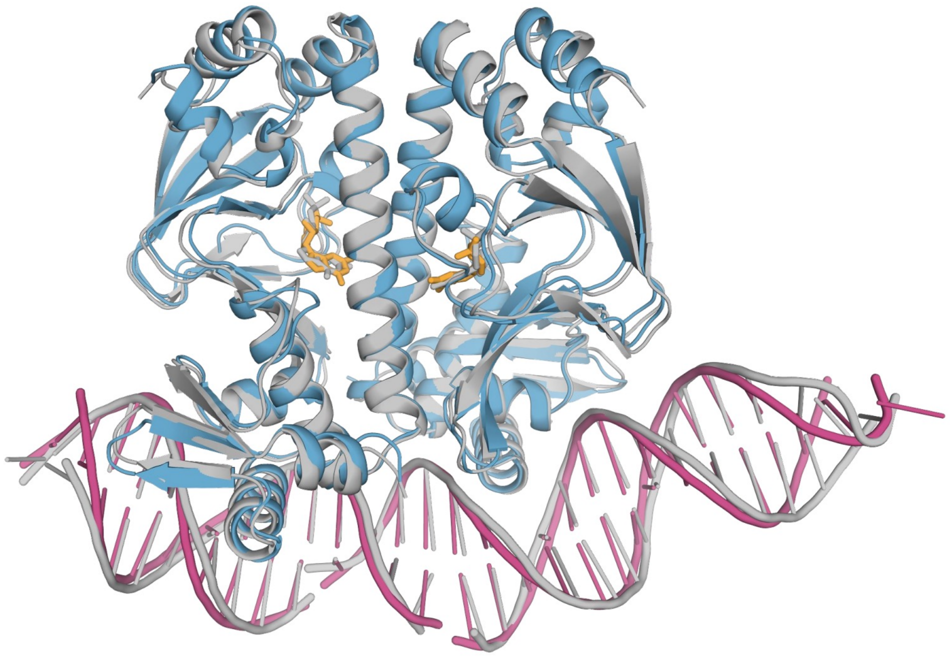
Figure 1: The Transformer - model architecture.

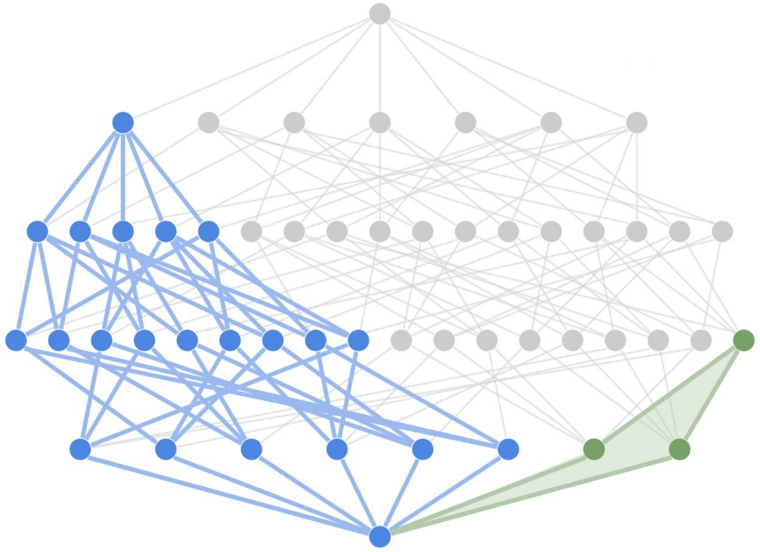
…now it's our turn to study geometry ☺

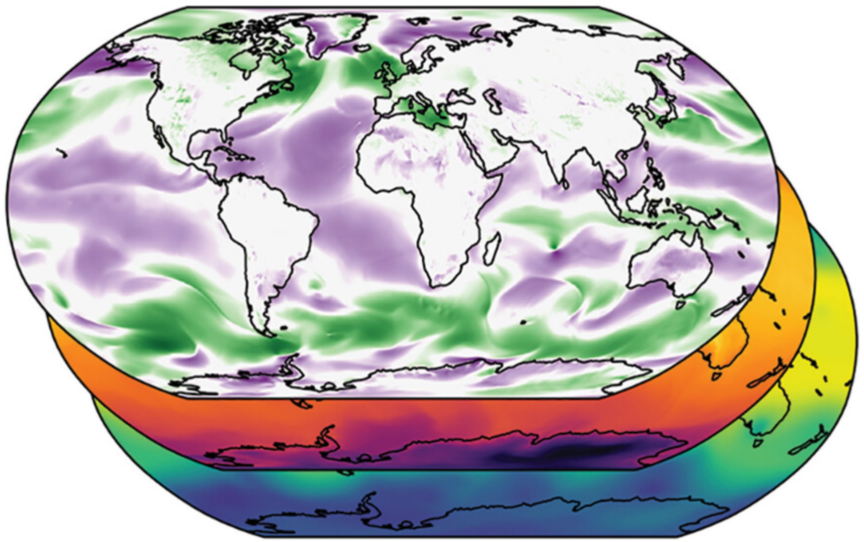
*Data from **nature** is often **geometric***

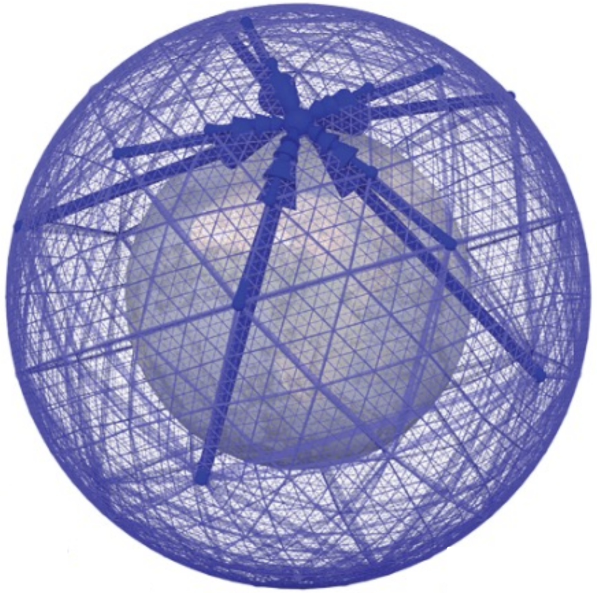




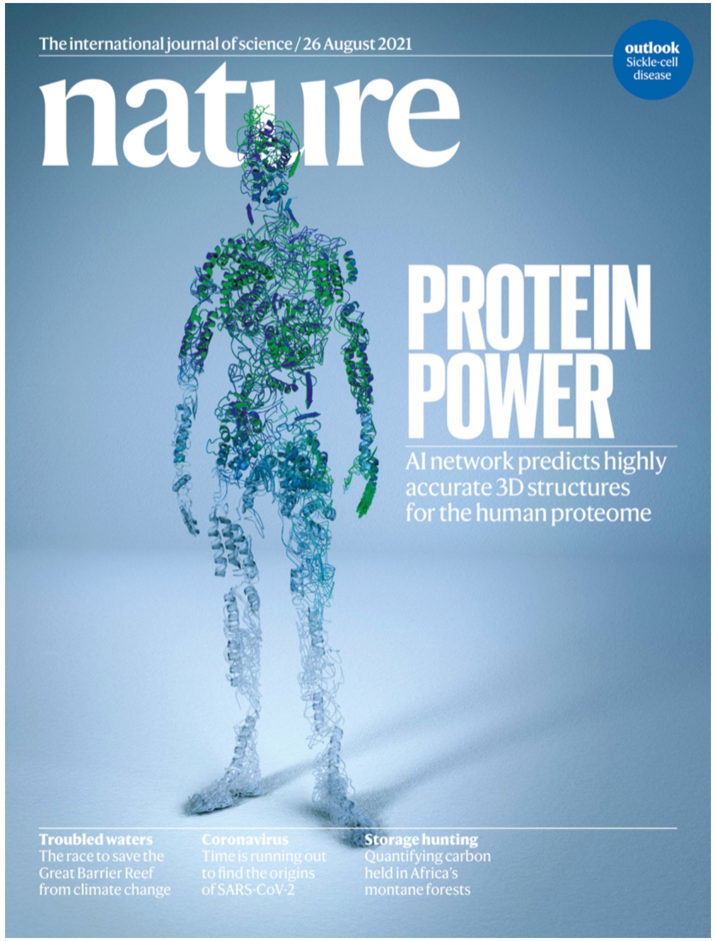


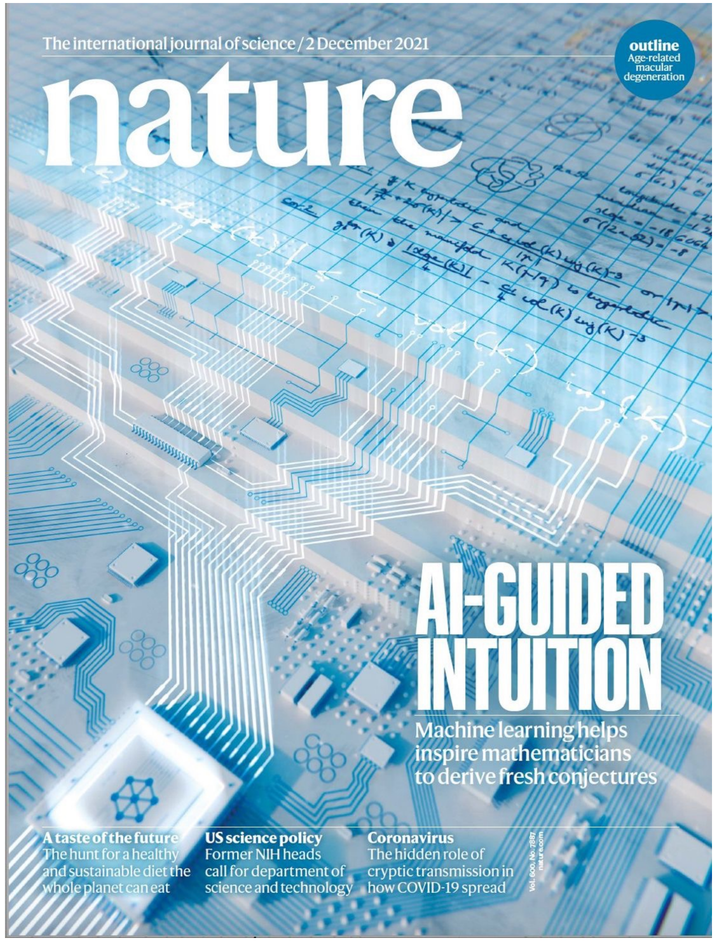






*Models of **nature** are often **geometric***





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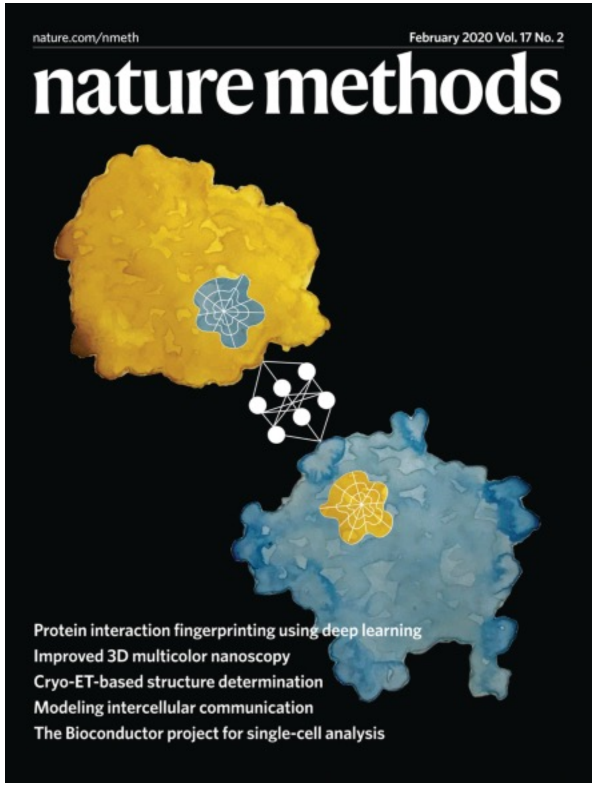
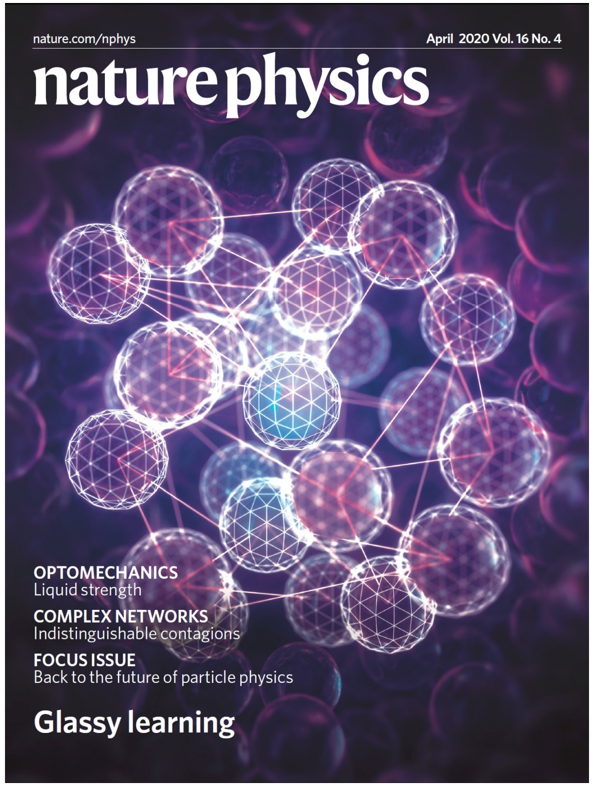
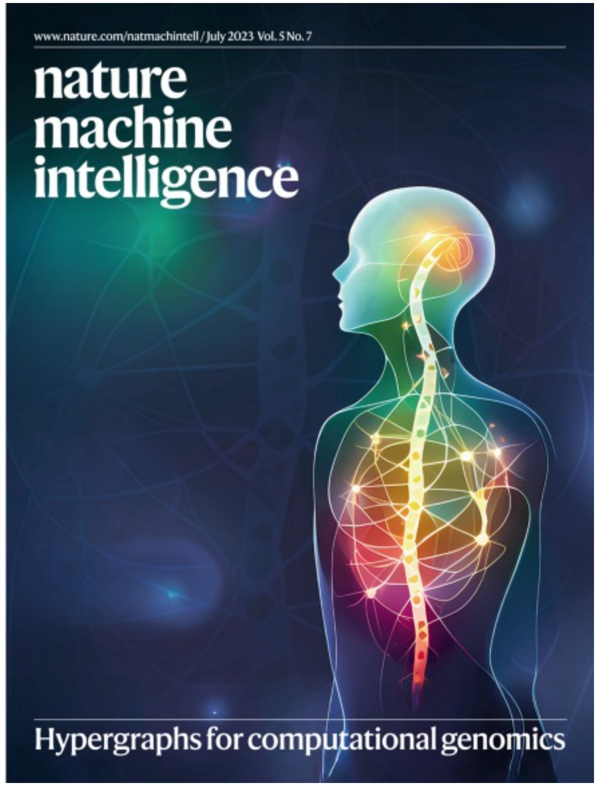
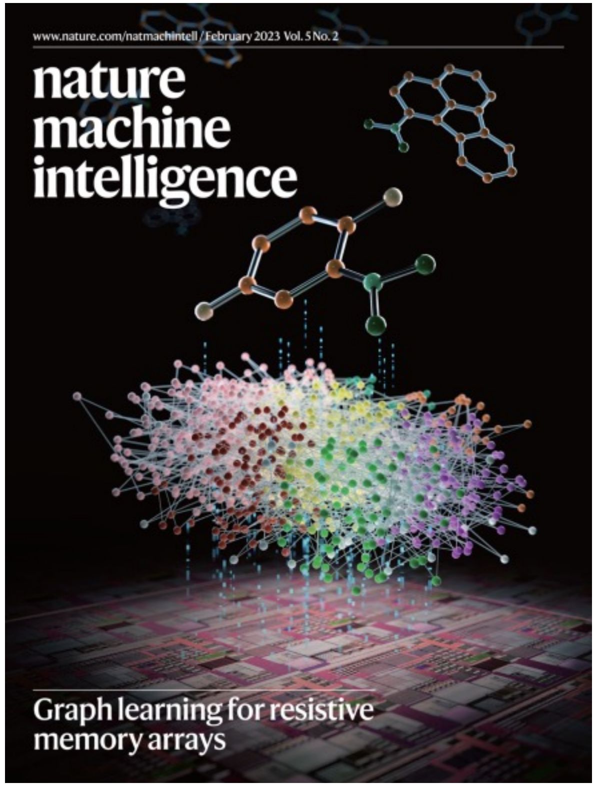


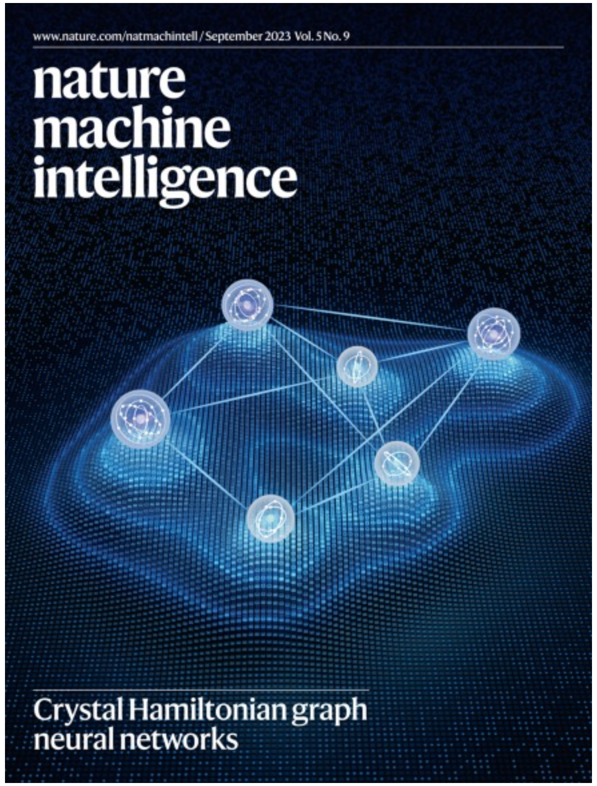


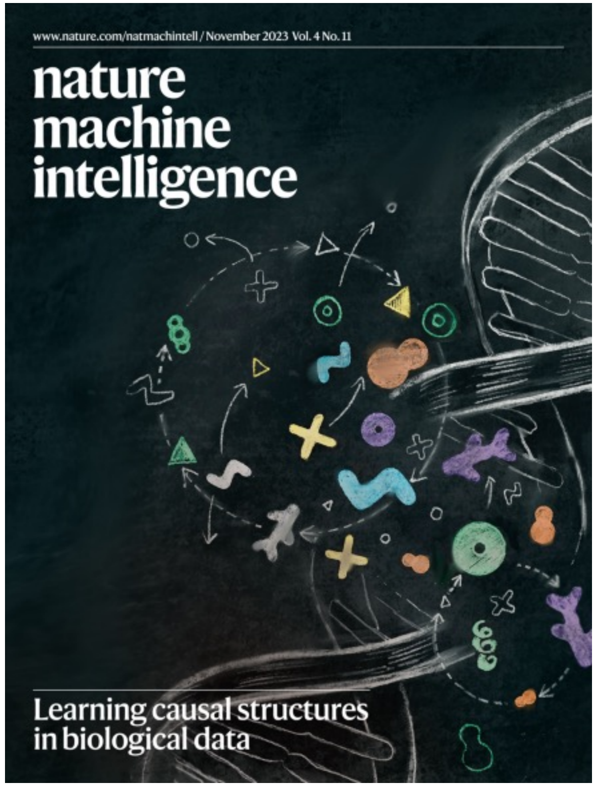


…and these are just the covers!

Models of ***nature*** *are often* ***geometric***







…and these are just the covers!

Even "non-geometric" models secretly have geometric constraints

Those coming from NLP may say *"no such geometry in language"*
But "geometry" is not just about *spatial* arrangement!

Even "non-geometric" models secretly have geometric constraints

Those coming from NLP may say *"no such geometry in language"*
But "geometry" is not just about *spatial* arrangement!

It is about *constraints*: design model to "respect" regularity in data
Models like Transformers touted as "generic", but *significantly constrained*

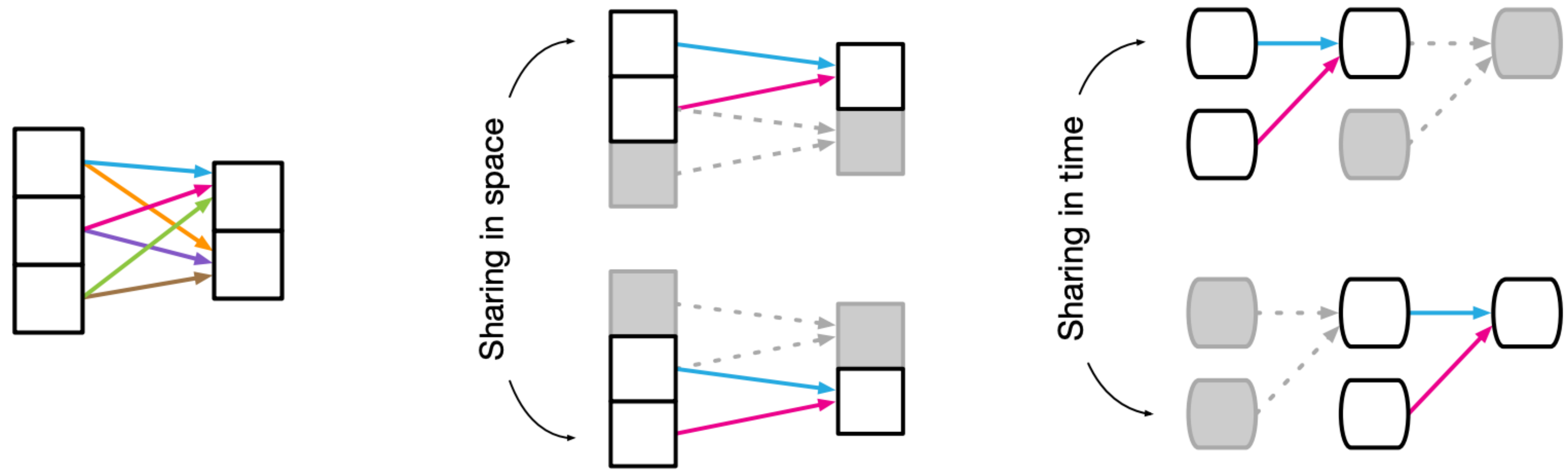
Generally, GDL offers us a *perspective* to categorise existing architectures
Based on which ***data regularity constraints*** they satisfy

This is a *useful perspective* even if you *never* encounter "geometric" data

In the very least, it will allow you to reason about 'frontier models' of the past, present *and* future, in a less handwavy and more principled way

*Could **graphs** be the answer?*

If we squint hard enough,
(m)any NNs can be seen as *passing data* over a *graph*!



(a) Fully connected (b) Convolutional (c) Recurrent

The *graph neural network* (**GNN**) may be the "one true architecture"!
Accordingly, this course's approach to GDL will be very "*graphy*"

*We come into **daily** contact with GNNs*

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Kyle Wiggers @Kyle_L_Wiggers September 3, 2020 7:00 AM

Food Discovery with Uber Eats: Using Graph Learning to Power Recommendations

Ankit Jain, Isaac Liu, Ankur Sarda, and Piero Molino December 4, 2019
0

GOOGLE | TECH | ARTIFICIAL INTELLIGENCE

Google is using AI to design its next generation of AI chips more quickly than humans can

Designs that take humans months can be matched or beaten by AI in six hours

By James Vincent | Jun 10, 2021, 9:13am EDT

GNN applications are still ripe in 2023!

MIT News
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Anne Trafton | MIT News Office
May 25, 2023

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RESEARCH ARTICLE | NEUROSCIENCE

A principal odor map unifies diverse tasks in olfactory perception

BRIAN K. LEE, EMILY J. MAYHEW, BENJAMIN SANCHEZ-LENGELING, JENNIFER N. WEI, WESLEY W. QIAN, KELSIE A. LITTLE, MATTHEW ANDRES, BRITNEY B. NGUYEN, THERESA MOLOY, [...], AND ALEXANDER B. WILTSCHKO +4 authors Authors Info & Affiliations

SCIENCE • 31 Aug 2023 • Vol 381, Issue 6661 • pp. 999-1006

nature reviews physics https://doi.org/10.1038/s42254-023-00569-0

Technical review Check for updates

Graph neural networks at the Large Hadron Collider

Gage DeZoort[1], Peter W. Battaglia[2], Catherine Biscarat[3] & Jean-Roch Vlimant[4]

Millions of new materials discovered with deep learning

29 NOVEMBER 2023

Amil Merchant and Ekin Dogus Cubuk

Google DeepMind *2023-10-18*

TacticAI: an AI assistant for football tactics

Zhe Wang[*,1], Petar Veličković[*,1], Daniel Hennes[*,1], Nenad Tomašev[1], Laurel Prince[1], Michael Kaisers[1], Yoram Bachrach[1], Romuald Elie[1], Li Kevin Wenliang[1], Federico Piccinini[1], William Spearman[2], Ian Graham[4], Jerome Connor[1], Yi Yang[1], Adrià Recasens[1], Mina Khan[1], Nathalie Beauguerlange[1], Pablo Sprechmann[1], Pol Moreno[1], Nicolas Heess[1], Michael Bowling[3], Demis Hassabis[1] and Karl Tuyls[1]

[*]Contributed equally to this work, [1]Google DeepMind, [2]Liverpool FC, [3]University of Alberta, [4]Work completed while at Liverpool FC

GNN applicatio

MIT News
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Using AI, scientists find a c drug-resistant infections

The machine-learning algorithm identifie Acinetobacter baumannii, a bacterium th

Anne Trafton | MIT News Office
May 25, 2023

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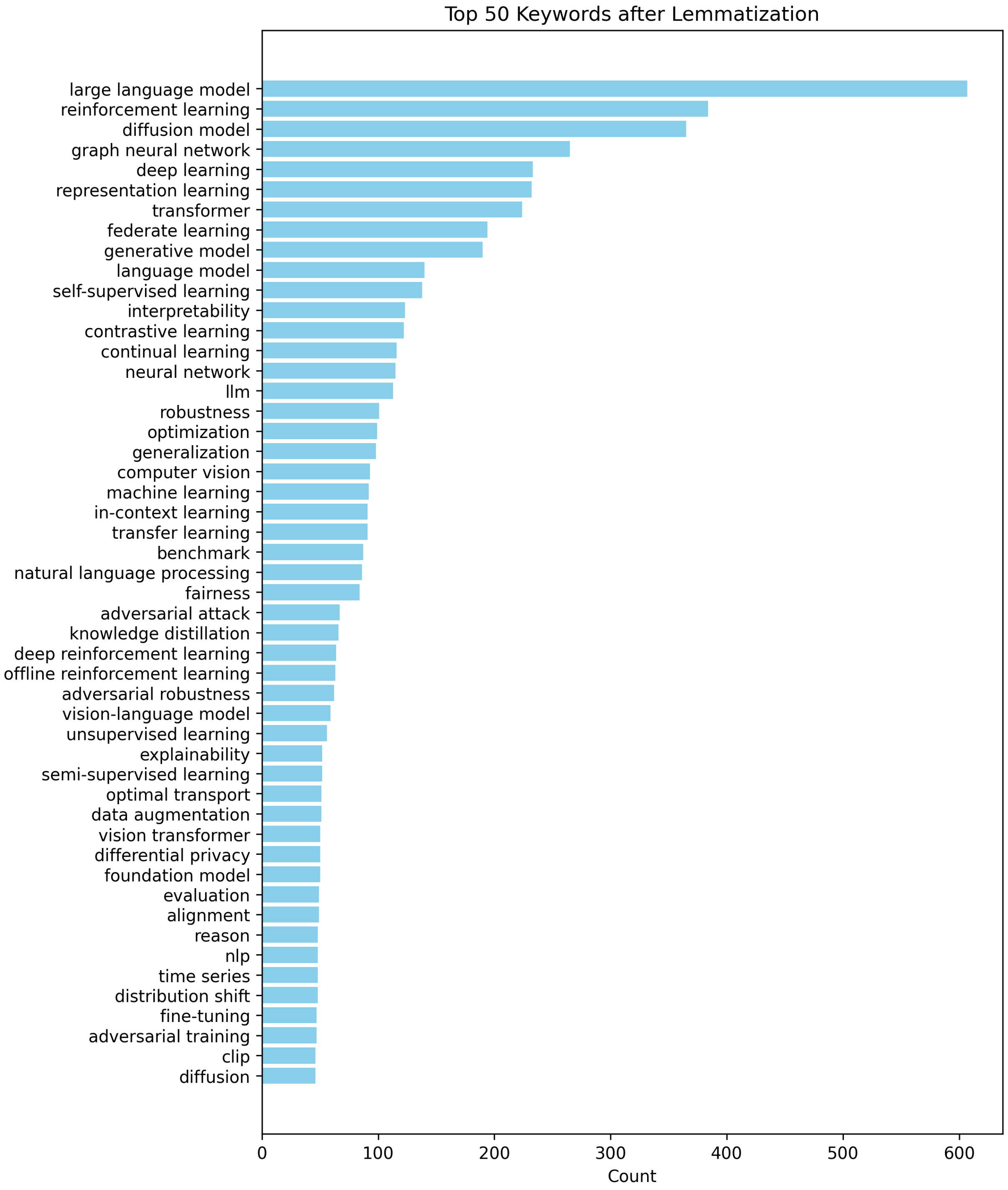
Technical review

Graph neural netwo Large Hadron Collic

Gage DeZoort [1], Peter W. Battaglia[2], Catherine Biscarat [3] & .



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IVERSE TASKS IN OLFACTORY PERCEPTION

; diverse tasks in olfactory

FER N. WEI, WESLEY W. QIAN, KELSIE A. LITTLE, MATTHEW ANDRES,
+4 authors Authors Info & Affiliations

aterials discovered p learning

EMBER 2023
nd Ekin Dogus Cubuk

2023-10-18

or football tactics

mašev[1], Laurel Prince[1], Michael Kaisers[1], Yoram nini[1], William Spearman[2], Ian Graham[4], Jerome eauguerlange[1], Pablo Sprechmann[1], Pol ;[1] and Karl Tuyls[1]
iversity of Alberta, [4]Work completed while at Liverpool FC

Why are we here?

Geometric data --- especially *graphs* --- are *everywhere*!

Geometric deep learning (GDL) is here to stay, especially over *natural* data

Geometric understanding of deep learning is a very useful *perspective*

No matter what field you choose to specialise in, there is a good chance you will come into contact with GDL concepts

We want to make GDL easy to *navigate*, *leverage*, and *contribute to*

In a way that is **uniquely** suited to Cambridge's strongpoints

(Special focus on graphs!)

Lecturers

Prof Pietro Liò

Professor of Computational Biology

University of Cambridge

pietro.lio@cst.cam.ac.uk

@pl219_Cambridge

Dr Petar Veličković

Staff Research Scientist, Google DeepMind

Affiliated Lecturer, University of Cambridge

petarv@google.com

@PetarV_93

Teaching Assistants

Francesco Ceccarelli

fc485

Miruna Crețu

mtc49 / **@MirunaCretu2**

Iulia Duță

id366 / **@DutaIulia**

Dobrik Georgiev

dgg30 / **@DobrikG**

Charlie Harris

cch57 / **@charlieharris01**

Rishabh Jain

rj412

Chaitanya Joshi

ckj24 / **@chaitjo**

Charlotte Magister

lcm67 / **@LC_Magister**

Dr Paul Scherer

pms69 / **@paulmorio**

Key concepts and skills

What do we want you to **take away** from the lectures?

- Why is it a good idea to study the geometry of data?
- Foundational material on groups, representations and graphs
- Theoretical principles of GDL & a way to navigate literature
- Observing GDL through the lens of graph representation learning
- The bigger picture: what lies beyond GDL?

The **assessments** (practical & mini-project) should **ground** these concepts with concrete implementations and **empower** you to derive key results

Recommended reading

Geometric Deep Learning
Grids, Groups, Graphs,
Geodesics, and Gauges

Michael M. Bronstein[1], Joan Bruna[2], Taco Cohen[3], Petar Veličković[4]

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www.geometricdeeplearning.com

GRAPH REPRESENTATION LEARNING

WILLIAM L. HAMILTON
McGill University
2020