What can the working mathematician expect from deep learning?

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Theorem: *There are infinitely many prime numbers.*

Proof:

1) *Assume there are finitely many:* $p_1, p_2, \ldots, p_n$.

2) *Consider* $p_1 p_2 \ldots p_n + 1$.

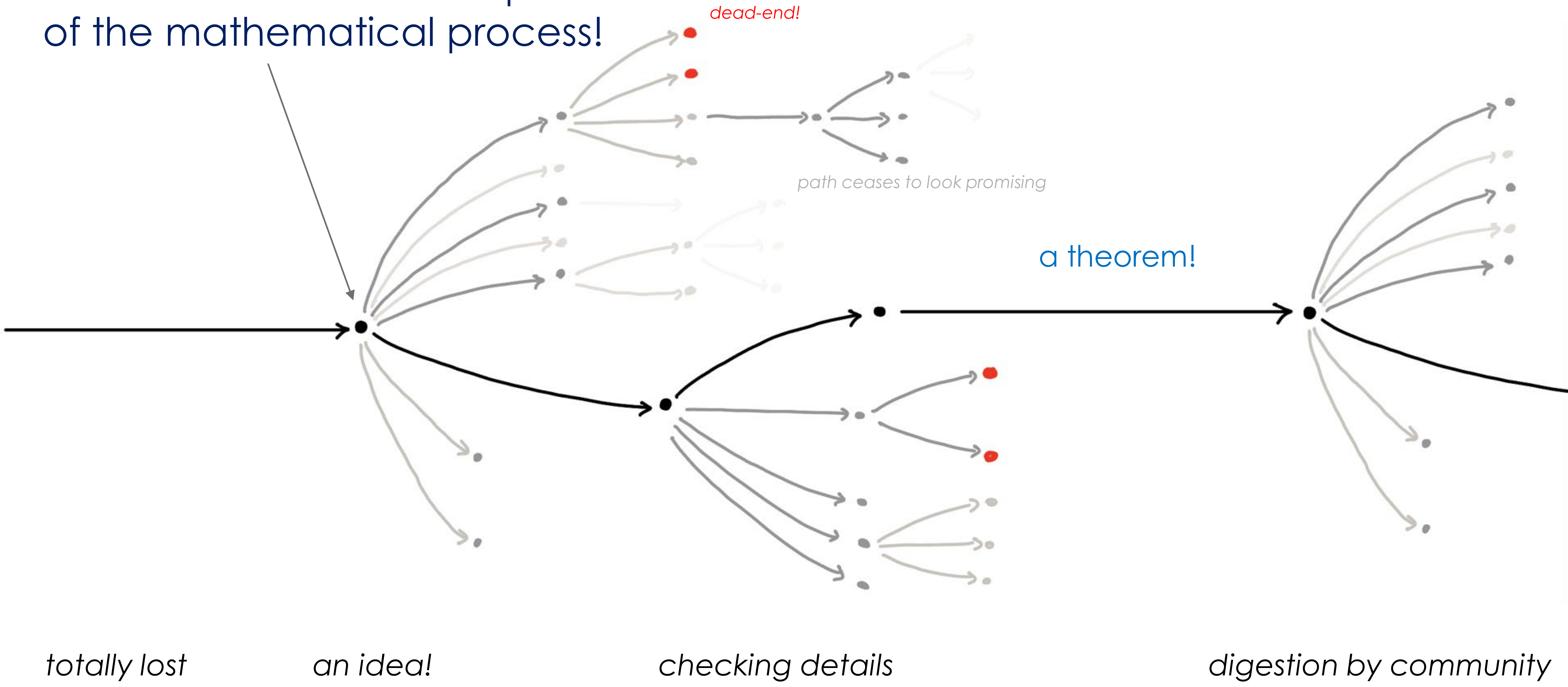
3) *You know the rest…*

"There is the monastic, introverted period, where we are just contemplating the ocean of our ignorance; but then suddenly something happens…the monk becomes busy and excited, in a hurry to look more closely at the details."

—Claire Voisin, *How to make a portrait of a bird.*

The Development of Ideas

We are interested in this part of the mathematical process!



Plan:

1) *Crash course in deep learning*

2) *Simple examples in mathematics*

3) *Myths, advice and scale*

4) *Some examples in (pure) mathematics research.*

Disclaimer:

1) I am a pure mathematician, interested (mostly) in representation theory, algebraic geometry… I won't discuss deep learning in applied math or mathematical questions raised by deep learning.

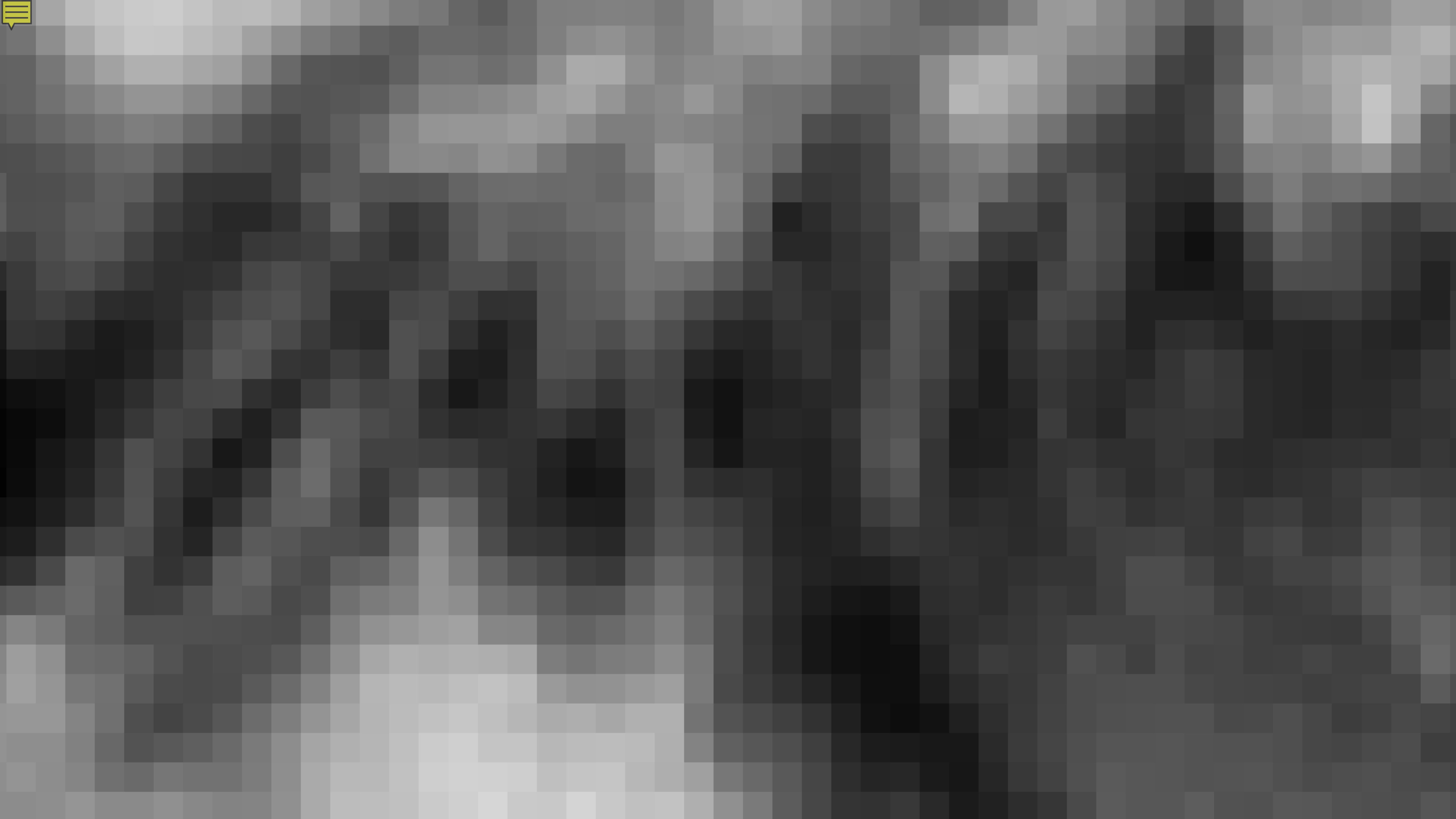
2) I have been working with DeepMind (of AlphaGo fame) tor two years. We are interested in potential interactions of AI and mathematics. This is a two-way bridge.

3) I have spent two years engaging with machine learning. I know the basics but am far from an expert.

4) All opinions are my own.

A crash course in deep learning.

Amélie Rec/Pexels



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079	085	092	103	106	094	078	072	071	063	074	090	112	135	137	134	145	140	121	107	105	125	150	146	123	113	098	060	059	067	098	109	122	129	114	083	071	061	052	049	062	089	127
078	079	085	095	092	070	052	051	051	063	087	090	083	082	085	100	108	109	106	107	102	112	141	148	130	102	066	054	057	067	087	100	116	106	085	069	084	070	051	042	041	075	107
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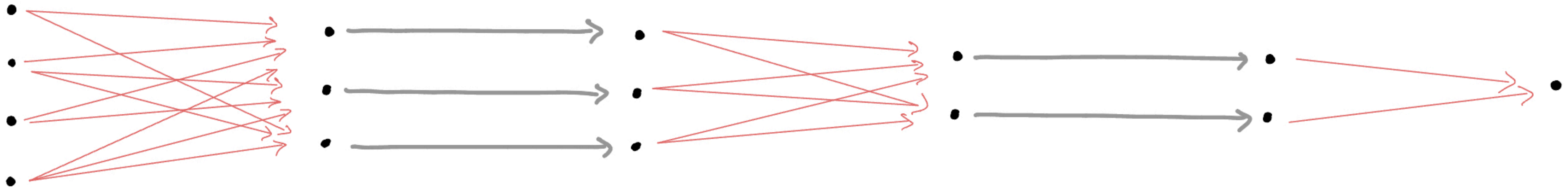
148	141	133	112	106	118	114	114	124	142	170	184	184	193	206	209	208	206	191	196	197	183	174	160	119	105	089	070	046	037	039	027	023	038	056	066	080	090	087	086	083	084	085



$$\phi : \mathbb{R}^{10^4} \xrightarrow[\text{linear}]{} \mathbb{R}^{10^3} \xrightarrow[\text{ReLU}]{} \mathbb{R}^{10^3} \xrightarrow[\text{linear}]{} \mathbb{R}^{10^2} \xrightarrow[\text{ReLU}]{} \mathbb{R}^{10^2} \xrightarrow[\text{linear}]{} \mathbb{R}$$

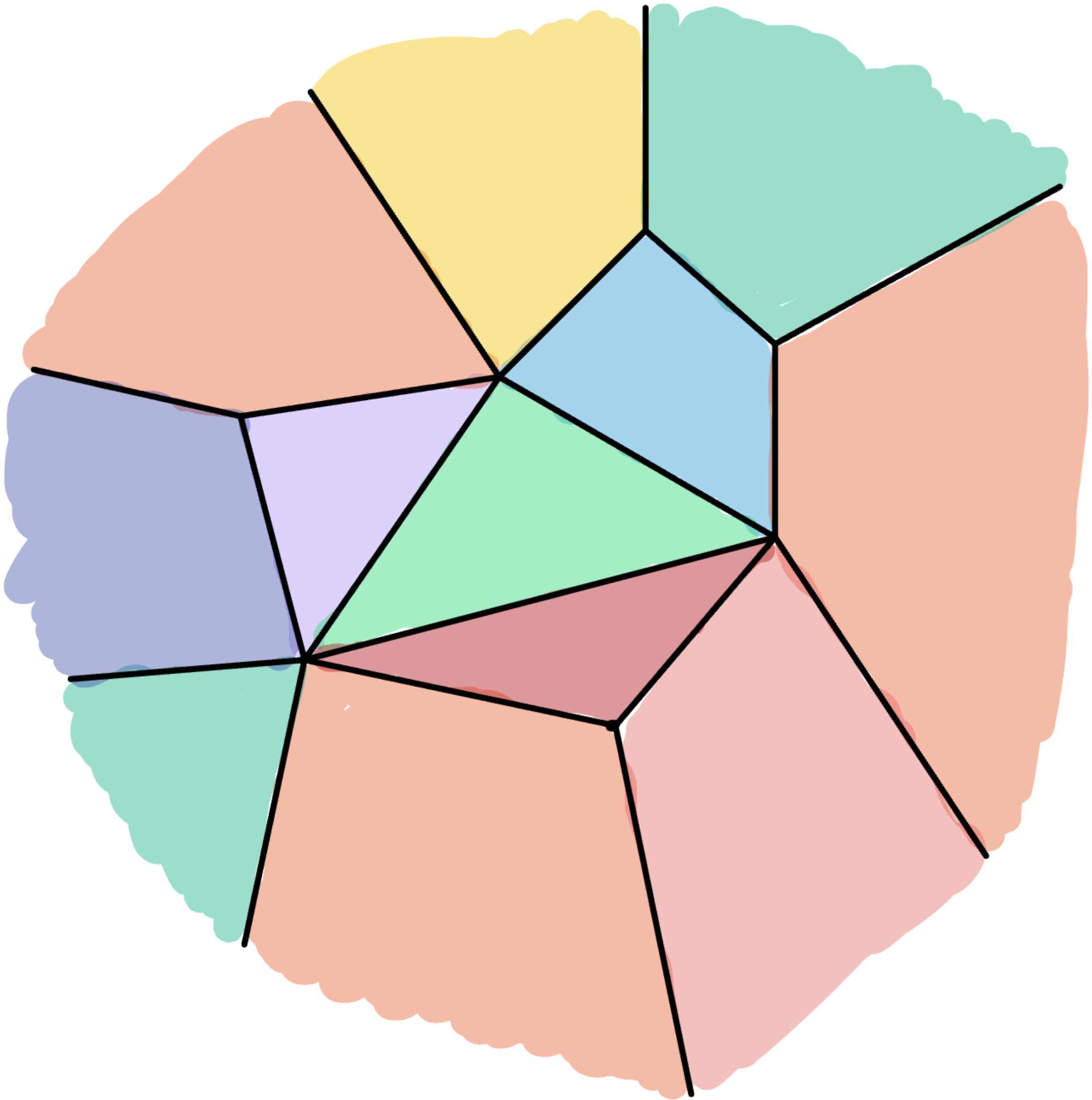
ReLU = coordinatewise max with 0 ("non-linearity")

Trained to approximate a target function $\tilde{\phi}$ via gradient descent on

$$\text{Loss} = \sum \ell(\tilde{\phi}(x), \phi(x)).$$

e.g. mean squared error
or cross entropy

Simple examples in mathematics

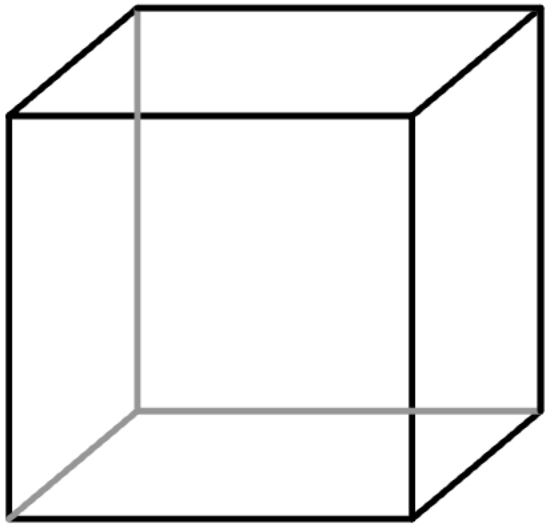


Geometric picture of training

(But try to imagine this happening in 10000 dimensions, rather than 2!)

Deep learning works best when:

1) *Input dimension is high*
2) *Function is on unit cube*
3) *Coordinates have low symbolic content*

$\phi : \mathbb{R}^{10^4} \supset$  $\longrightarrow \mathbb{R}$

In some settings, overcomes "curse of dimensionality".

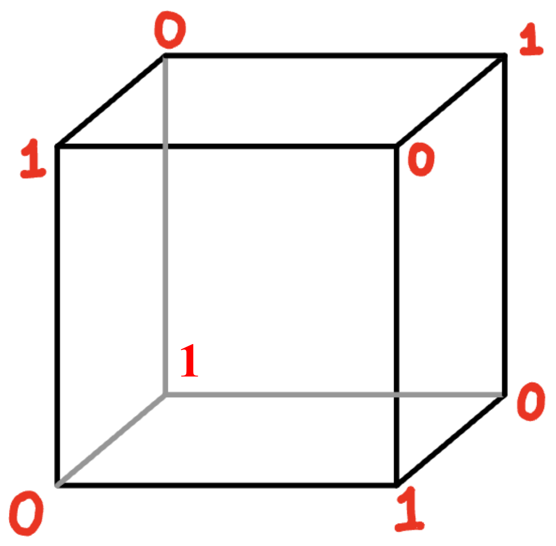
Example: "parity bit" $\{0,1\}^{1000} \longrightarrow \{0,1\}$

$$(x_0, \dots, x_{999}) \longmapsto \sum x_i \mod 2$$

Very noise sensitive.

Difficult to learn!

Many examples in number theory are like this one.



Example: (due to Joel Gibson)

$x = (x_1, \dots, x_n)$ a permutation of n.

$\mathcal{R}(x) = \{ i \mid x_i > x_{i+1} \}$ "right descent set"

$\mathcal{L}(x) = \{ i \mid i \text{ occurs to the right of } i+1 \text{ in } (x_1, \dots, x_n) \}$

"left descent set"

$\mathcal{R}(x) = \mathcal{L}(x^{-1}) \Rightarrow$ symmetrical concepts.

$x = (x_1, \dots, x_n)$ a permutation of n.

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"left descent set"

Input vector x ($n = 50$):

```
Right descent set:
Epoch  299: Train loss 0.01, Test loss 0.01,  4907 out of  5000 correct (98.14%).
Left descent set:
Epoch  299: Train loss 0.68, Test loss 0.70,     0 out of  5000 correct (0%).
```

Input permutation matrices ($n=20$):

```
Right descent set:
Epoch 64: Train loss 0.00, Test loss 0.01, 4975 out of 5000 correct (99.50%).
Left descent set:
Epoch 64: Train loss 0.00, Test loss 0.01, 4977 out of 5000 correct (99.54%).
```

How input sits in space (the "representation") really matters.

Myths, advice and scale

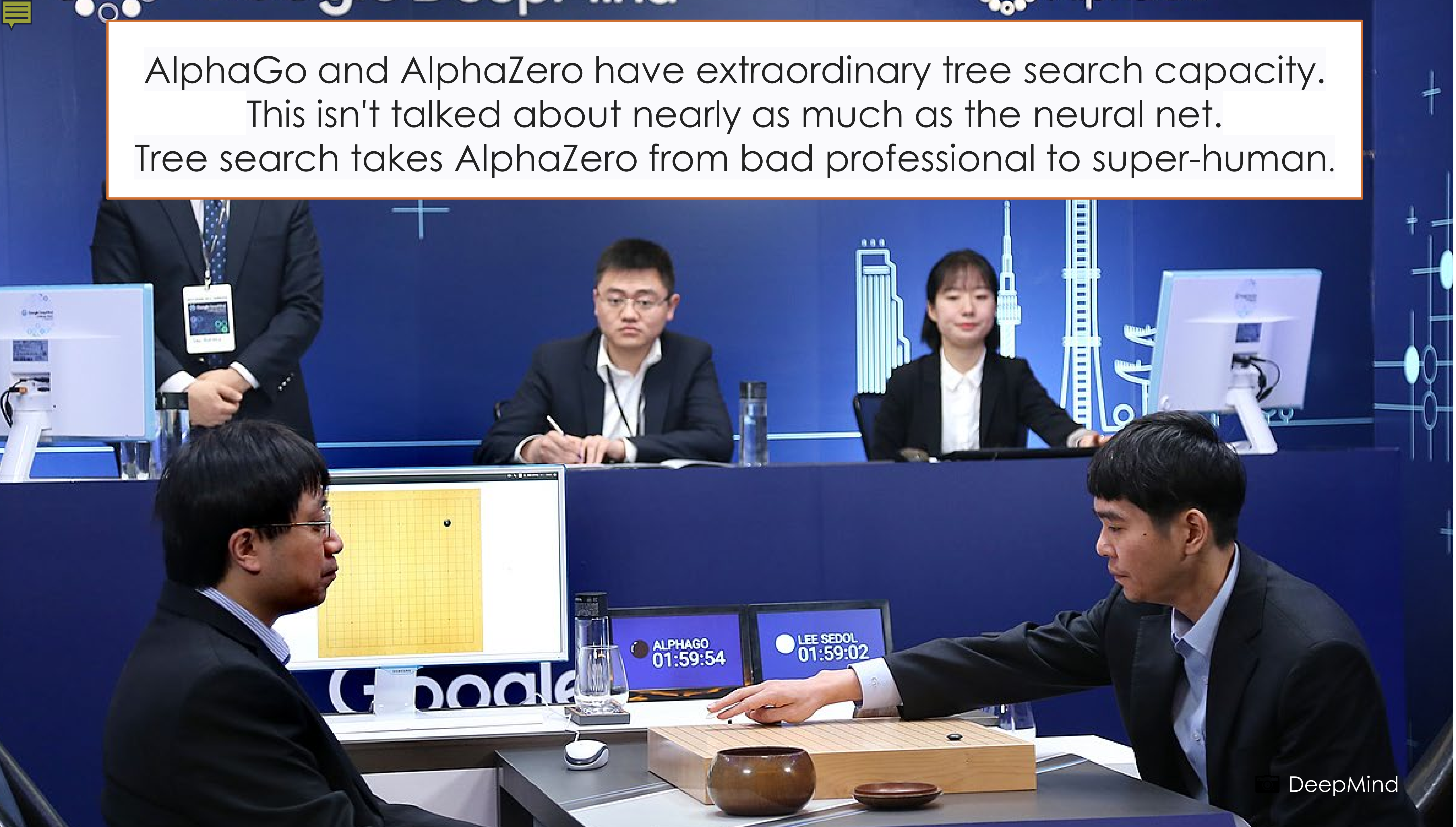
TheDigitalArtist

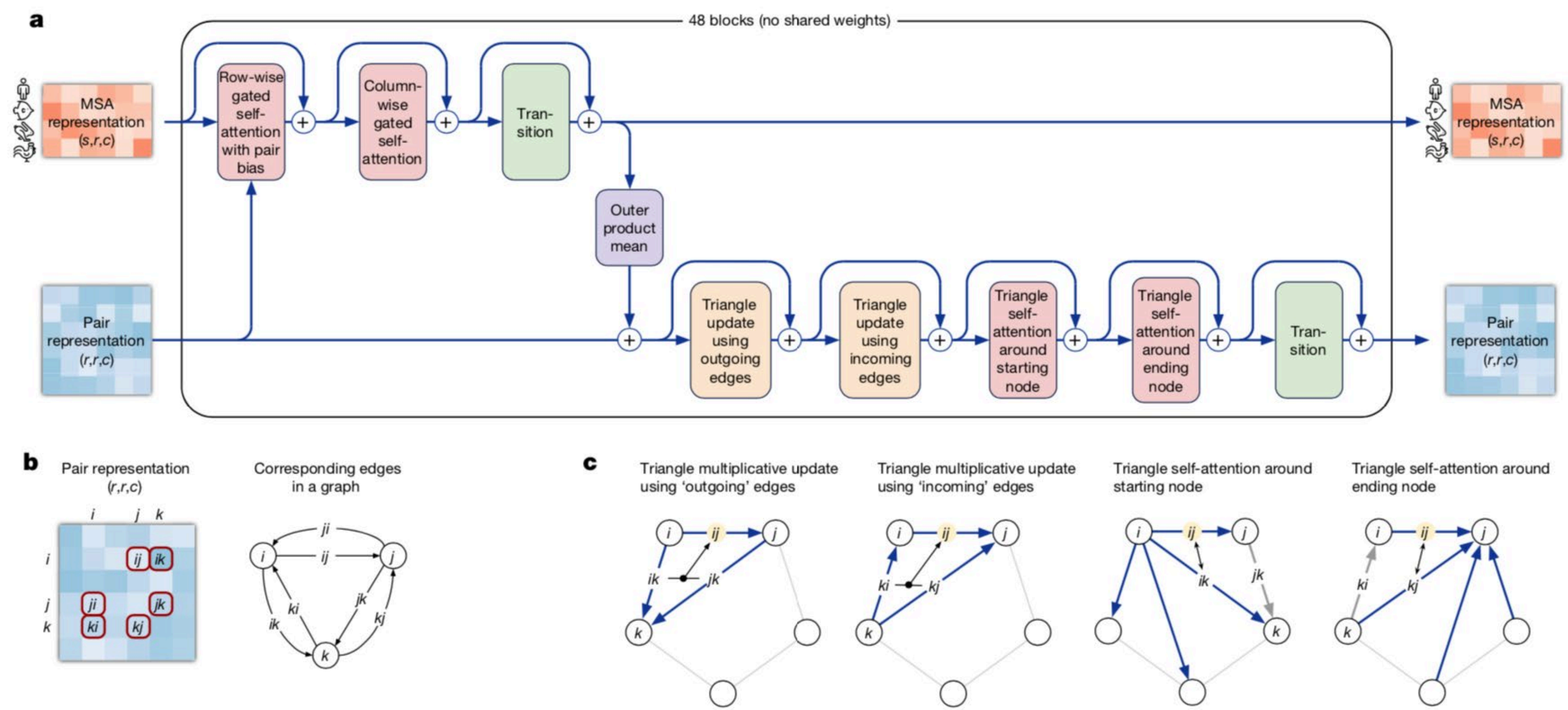
Hype: There is one "vanilla" structure (a "fully connected deep neural net") which is versatile on many problems.

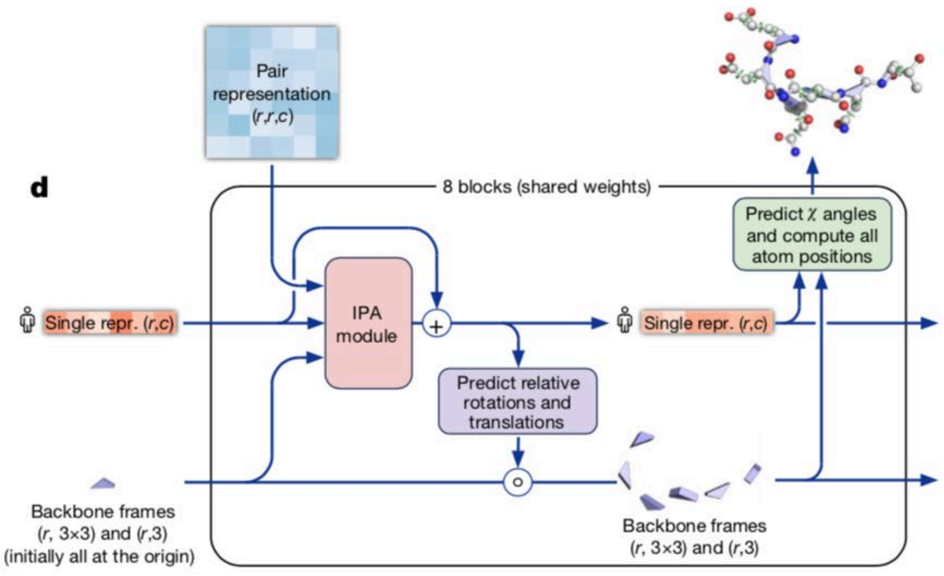
Reality: Vanilla architectures usually only work out of the box on simple problems.

Architecture matters.
Deep learning is often a *piece* of the puzzle.

AlphaGo and AlphaZero have extraordinary tree search capacity.
This isn't talked about nearly as much as the neural net.
Tree search takes AlphaZero from bad professional to super-human.







AlphaFold is often referred to as a "neural net".
This is not accurate.
It is a remarkable piece of software which incorporates neural nets in an essential way. It also incorporates several other components distilled from human understanding of the key features of an extremely difficult problem.

Advice for the interested mathematician:

1) Expect to spend considerable time experimenting with details like learning rate, model selection etc.

2) Try to work with someone who has background in machine learning.

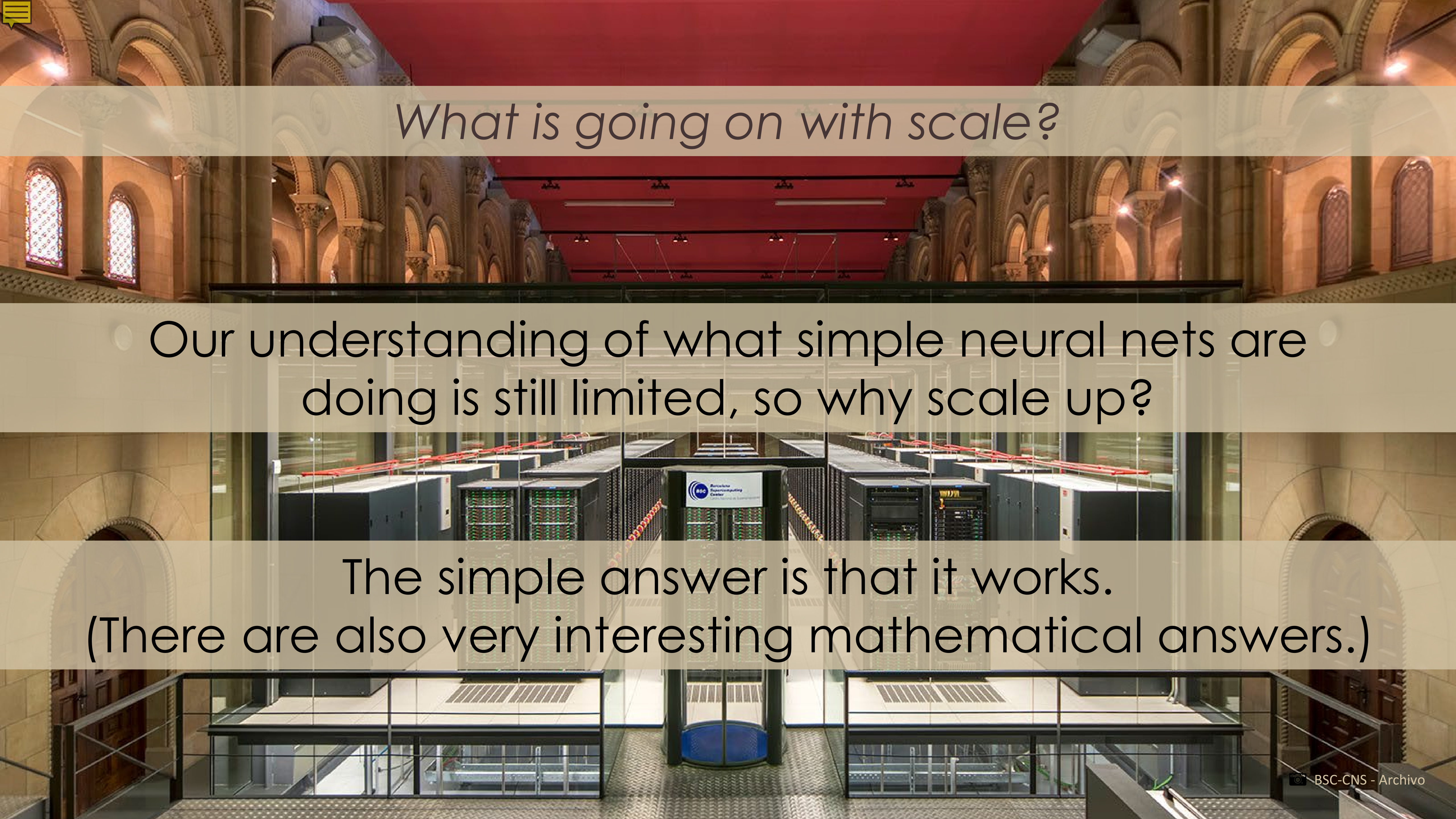
3) Try to push *either* mathematics or machine learning, but not both! (Remember that AlphaGo began as a supervised learning task.)

4) Have a precise idea of what you want machine learning to achieve. (We are not yet at the stage where we can "throw AlphaZero at the problem".)

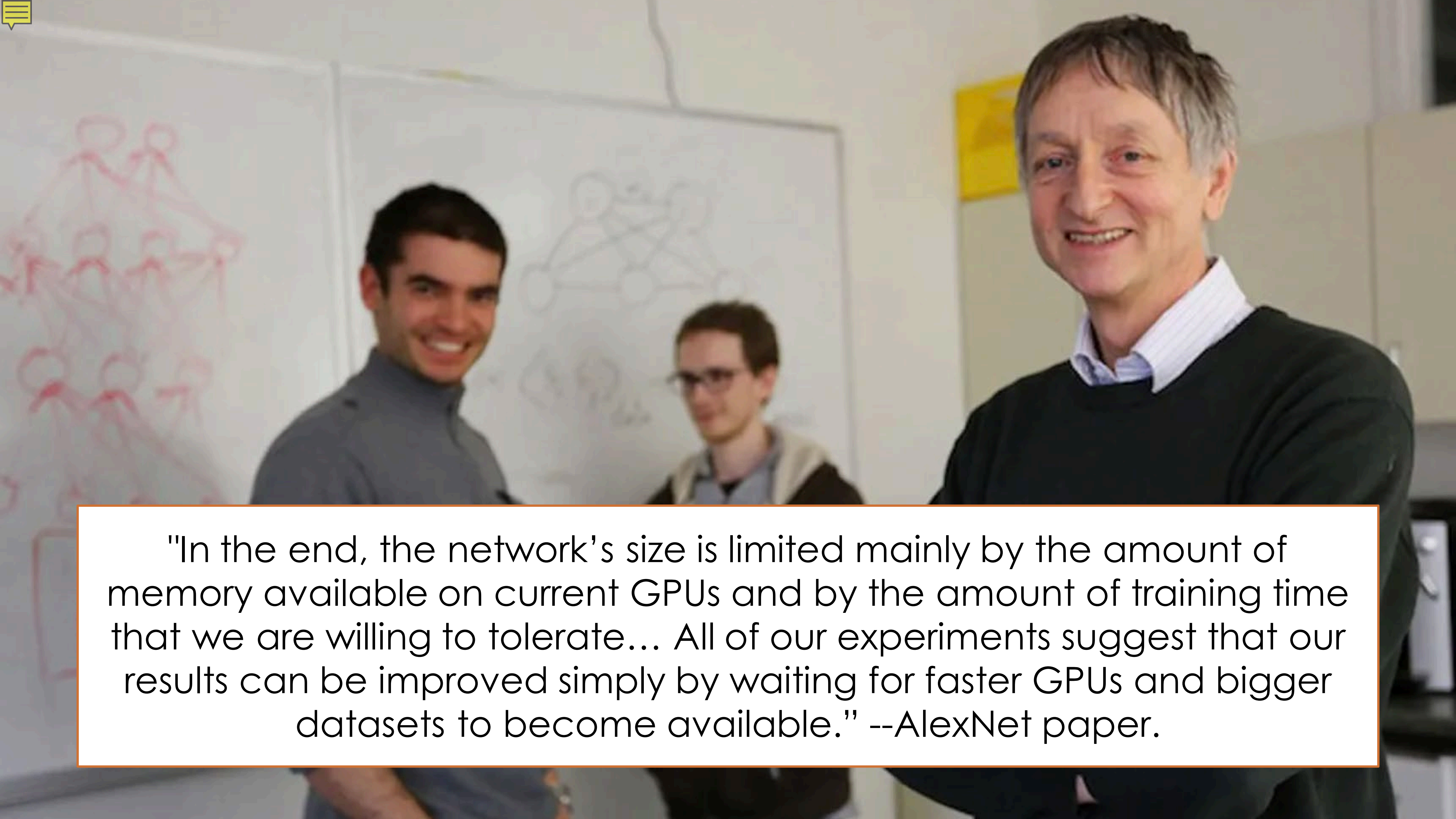
What is going on with scale?

Our understanding of what simple neural nets are doing is still limited, so why scale up?

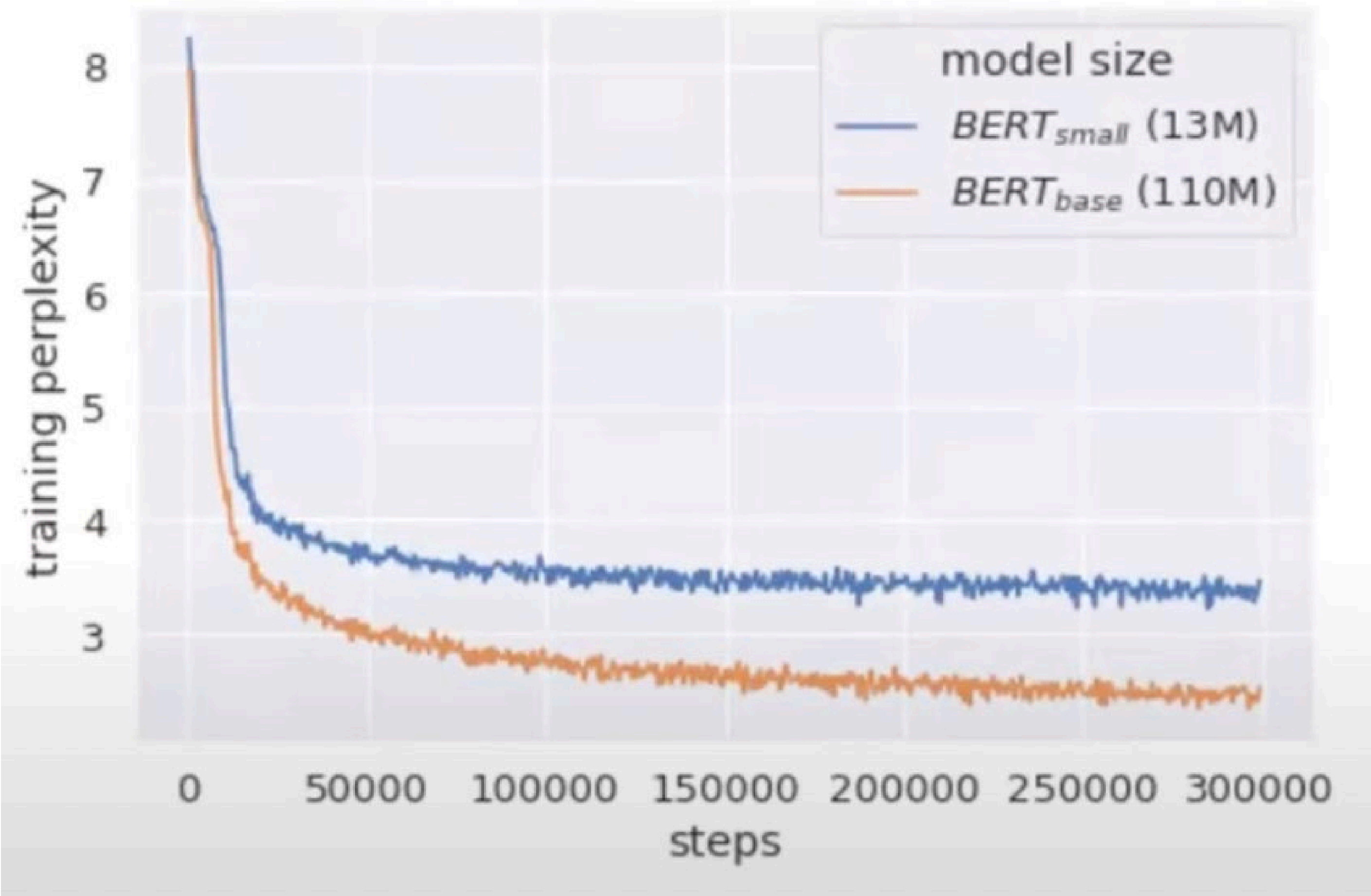
The simple answer is that it works.
(There are also very interesting mathematical answers.)



BSC-CNS - Archivo



"In the end, the network's size is limited mainly by the amount of memory available on current GPUs and by the amount of training time that we are willing to tolerate… All of our experiments suggest that our results can be improved simply by waiting for faster GPUs and bigger datasets to become available." --AlexNet paper.



Greg Yang, https://www.youtube.com/watch?v=XpU3mDKJOak&ab_channel=AutoMLSeminars

Increasing network size appears to monotonically increase performance. (After getting numerous details right!)

Created with DALL·E, an AI system by OpenAI

“An epic fight between a laptop, a lone tiger and a compass, oil painting ”

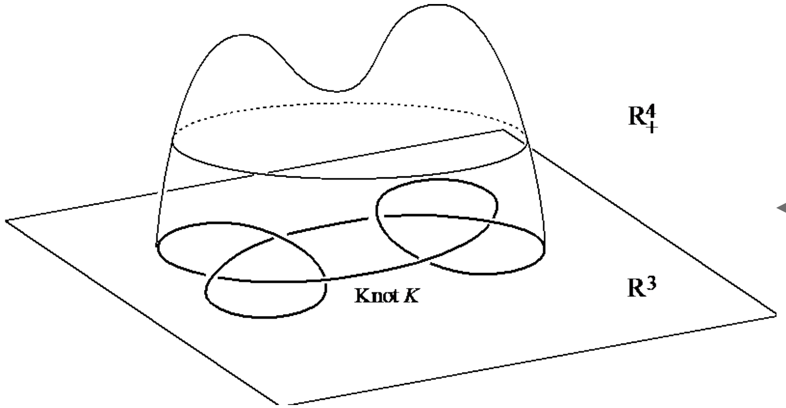
Three Examples

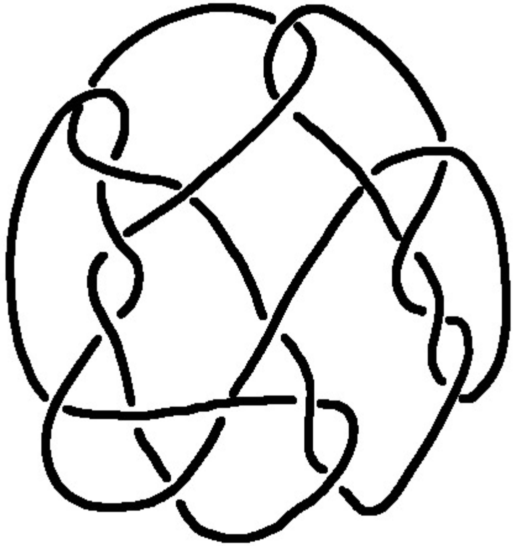
Machine learning in use in knot theory, representation theory and graph theory

Knot theory

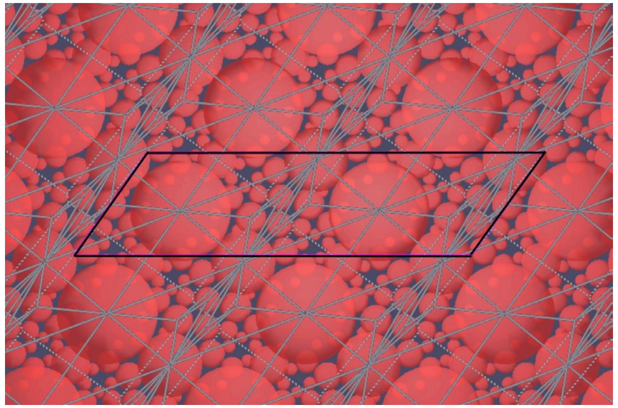
Knot Theory

3d and 4d topology





hyperbolic geometry



quantum topology, mathematical physics, …

Knot Theory

Signature: 2

Alexander polynomial: $t^3 - 5t^2 + 12t - 15 + 12t^{-1} - 5t^{-2} + t^{-3}$

Hyperbolic volume: 13.29

Jones: $-2q^6 - 5q^5 - 7q^4 + 9q^3 - 9q^2 + 8q - 6 + 4q^{-1} - q^{-2}$

HOMFLY-PT: $z^6a^{-2} + 3z^4a^{-4} - z^4a^{-4} - z^4 + 2z^2a^{-2} - z^2 - a^{-2} + 2a^{-4} - a^{-6} + 1$

A2: $-q^6 + 2q^4 + 1 + 2q^{-2} - 3q^{-4} + q^{-6} - 2q^{-8} + 2q^{-10} + 2q^{-12} + 2q^{-16} - 2q^{-18} - q^{-20}$

3-genus: 3

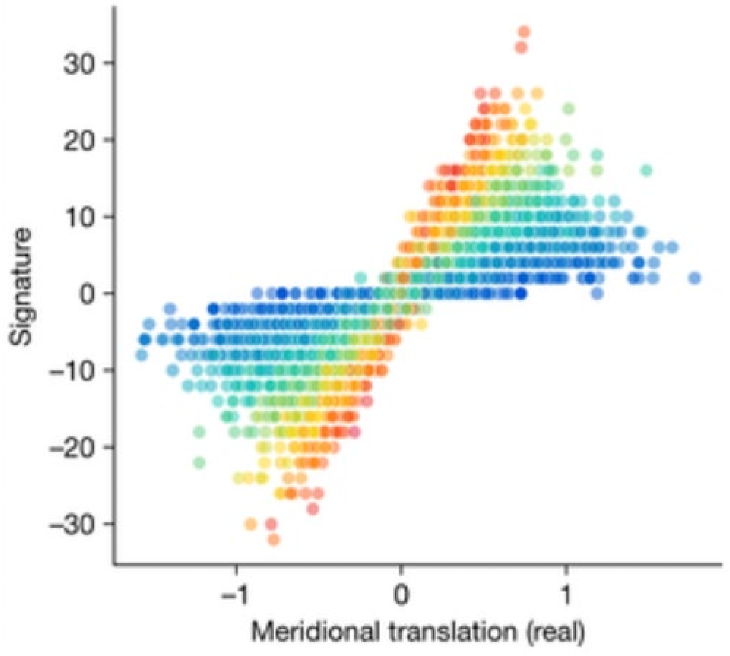
Topological 4-genus: 1

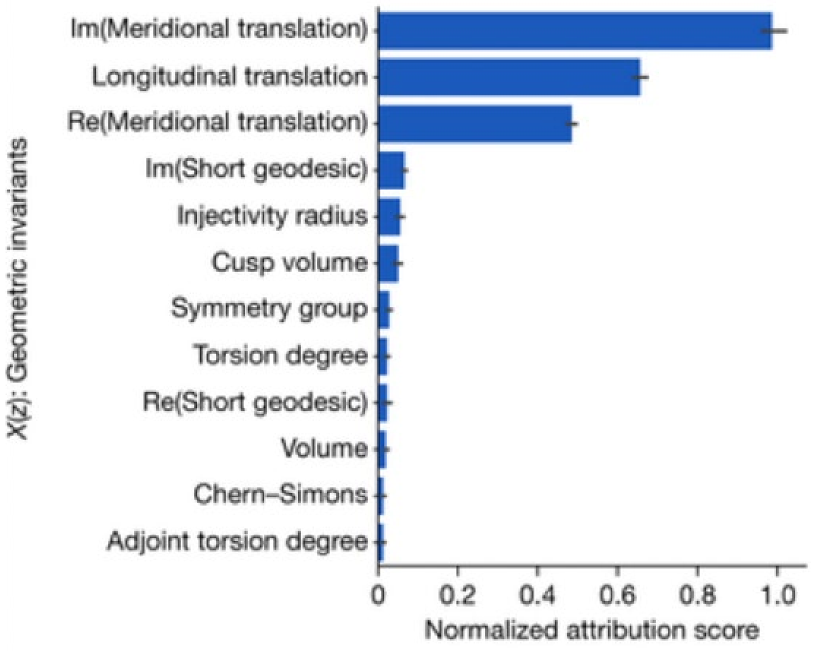
Do there exist unexpected relations between these invariants?

Smooth 4-genus: 1

Determinant: 51

Knot Theory





Davies, Juhász, Lackenby and Tomasev prove:

Theorem 1.1. *There exists a constant c_1 such that, for any hyperbolic knot K,*

$$|2\sigma(K) - \mathrm{slope}(K)| \leq c_1 \,\mathrm{vol}(K)\,\mathrm{inj}(K)^{-3}.$$

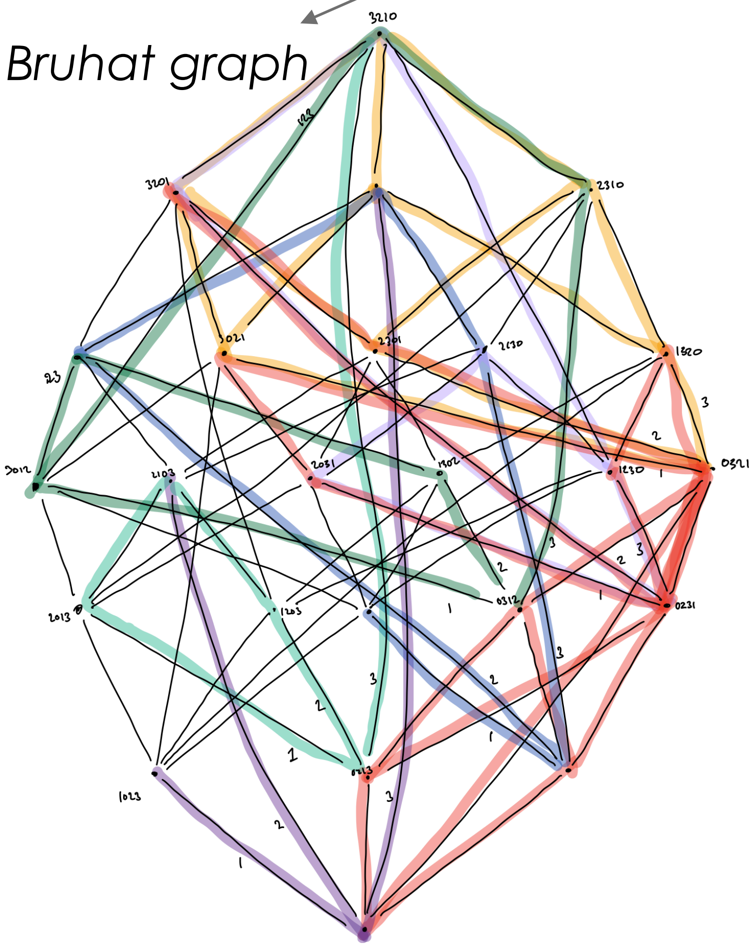
Representation theory

Representation Theory

Combinatorial invariance conjecture (Dyer, Lusztig 1980s)

x, y (pair of permutations)

Bruhat graph



Kazhdan-Lusztig polynomial

$$1+3q+q^2$$

Representation Theory

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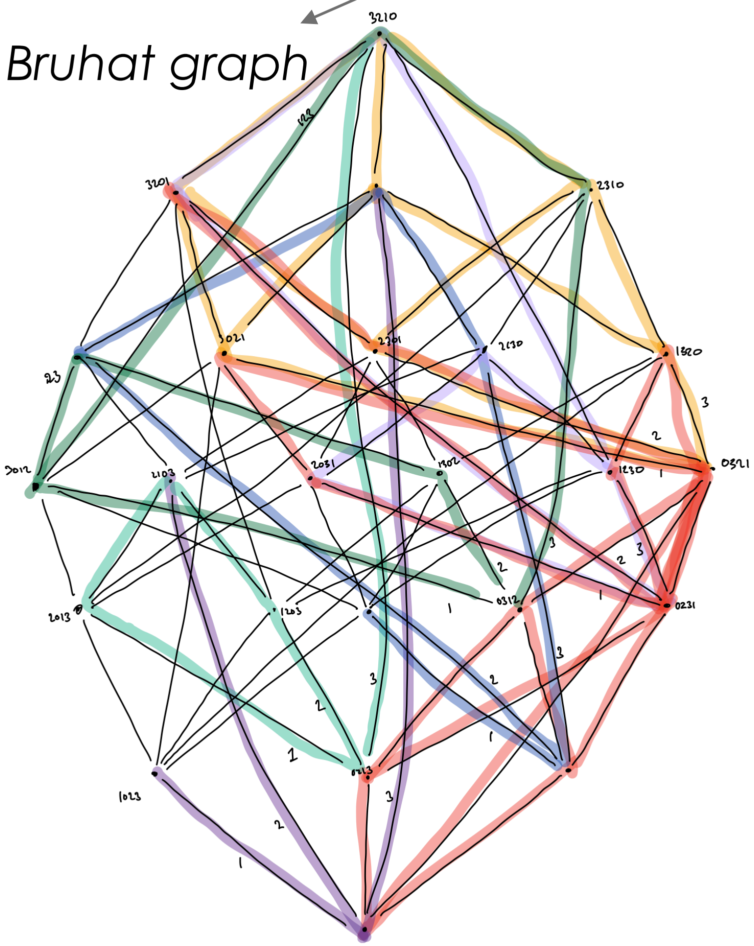


Kazhdan-Lusztig polynomial

conjecture

$$1+3q+q^2$$


3210
4
3201
2310
2
3021
2301
2130
1320
1
3012
3
2103
2031
1302
1230
0321
2013
1203
0312
0231
1023
0213
0

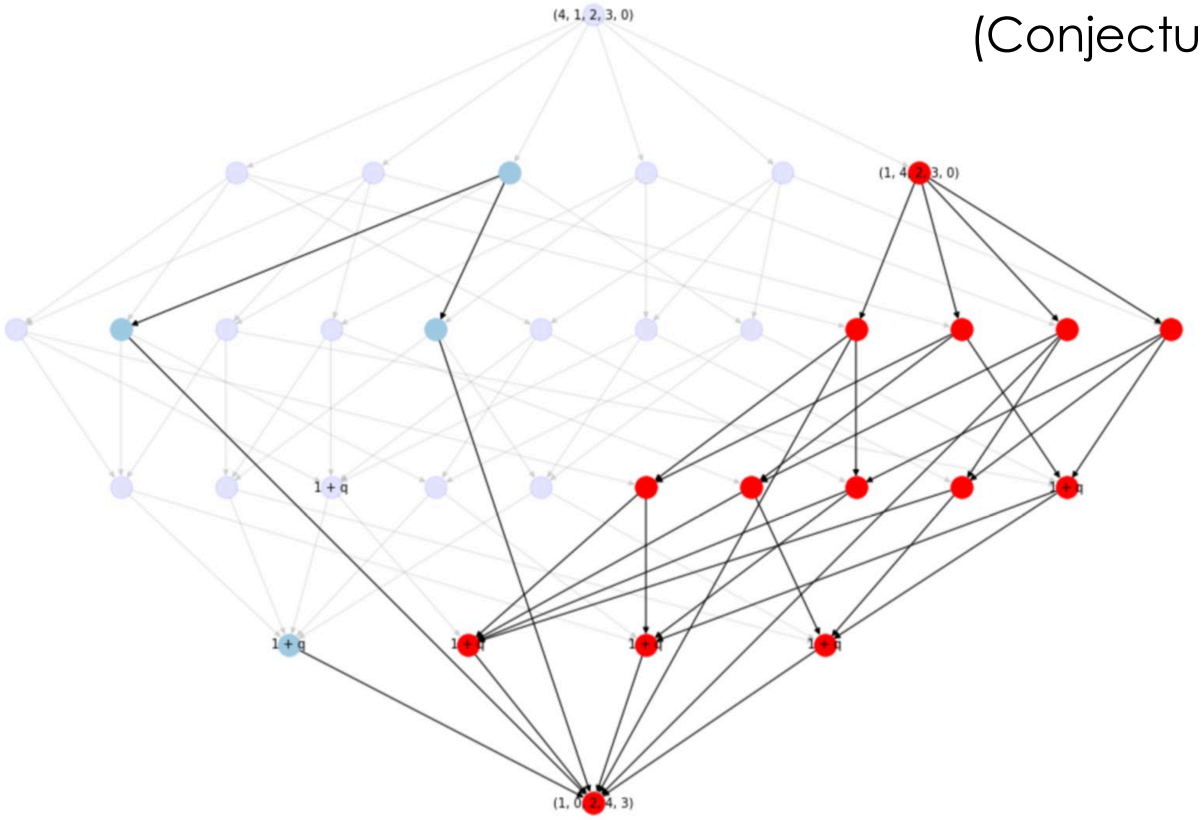
Representation Theory

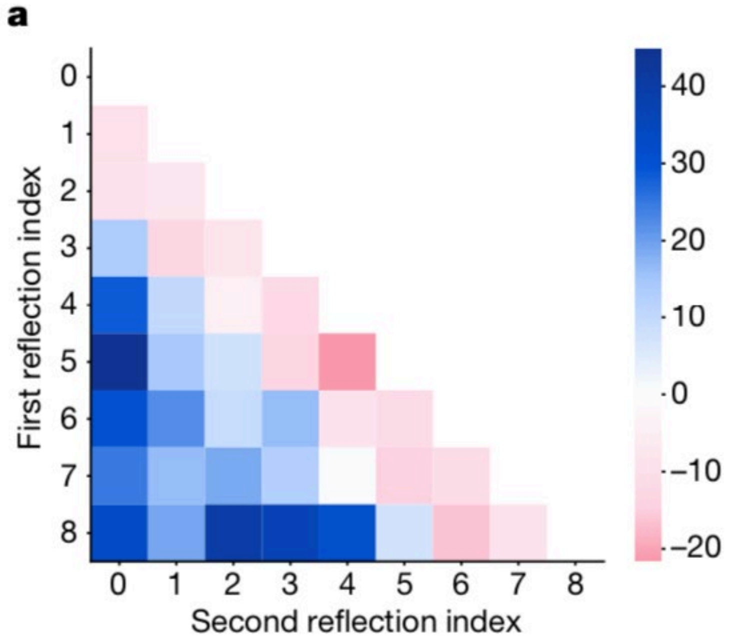
Blundell, Buesing, Davies, Veličković, Williamson:

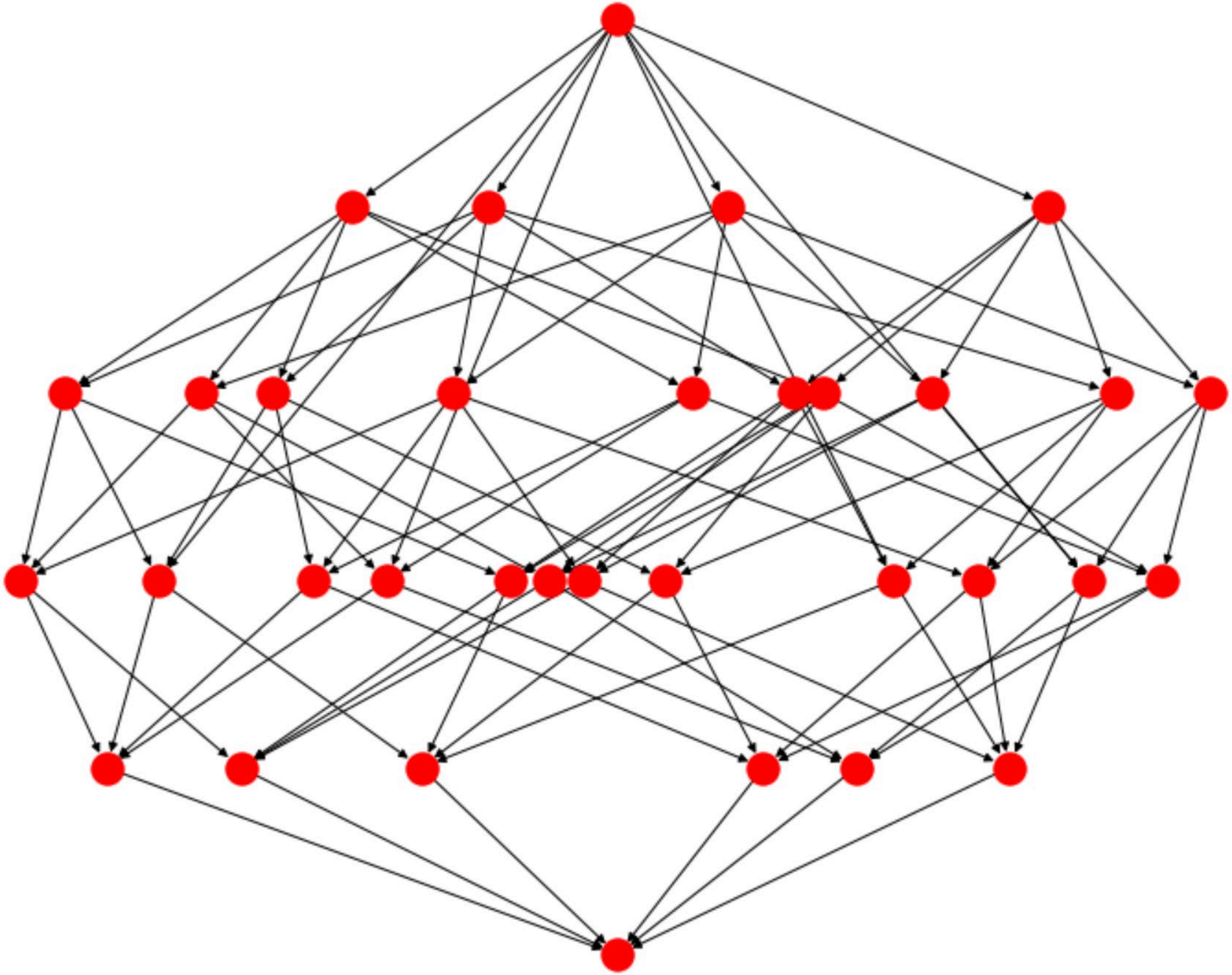
Conjecture 3.1. *For any hypercube decomposition we have*

$$P^{\partial}_{x,y} = q^{\ell(y)-\ell(x)-1} \sum_{\varnothing \neq I \subset E} (q^{-1}-1)^{|I|-1} P_{\theta(I),y}(q^{-1}) + \sum_{x \neq v \in J} \gamma_v \cdot P^{\partial}_{x,v}$$

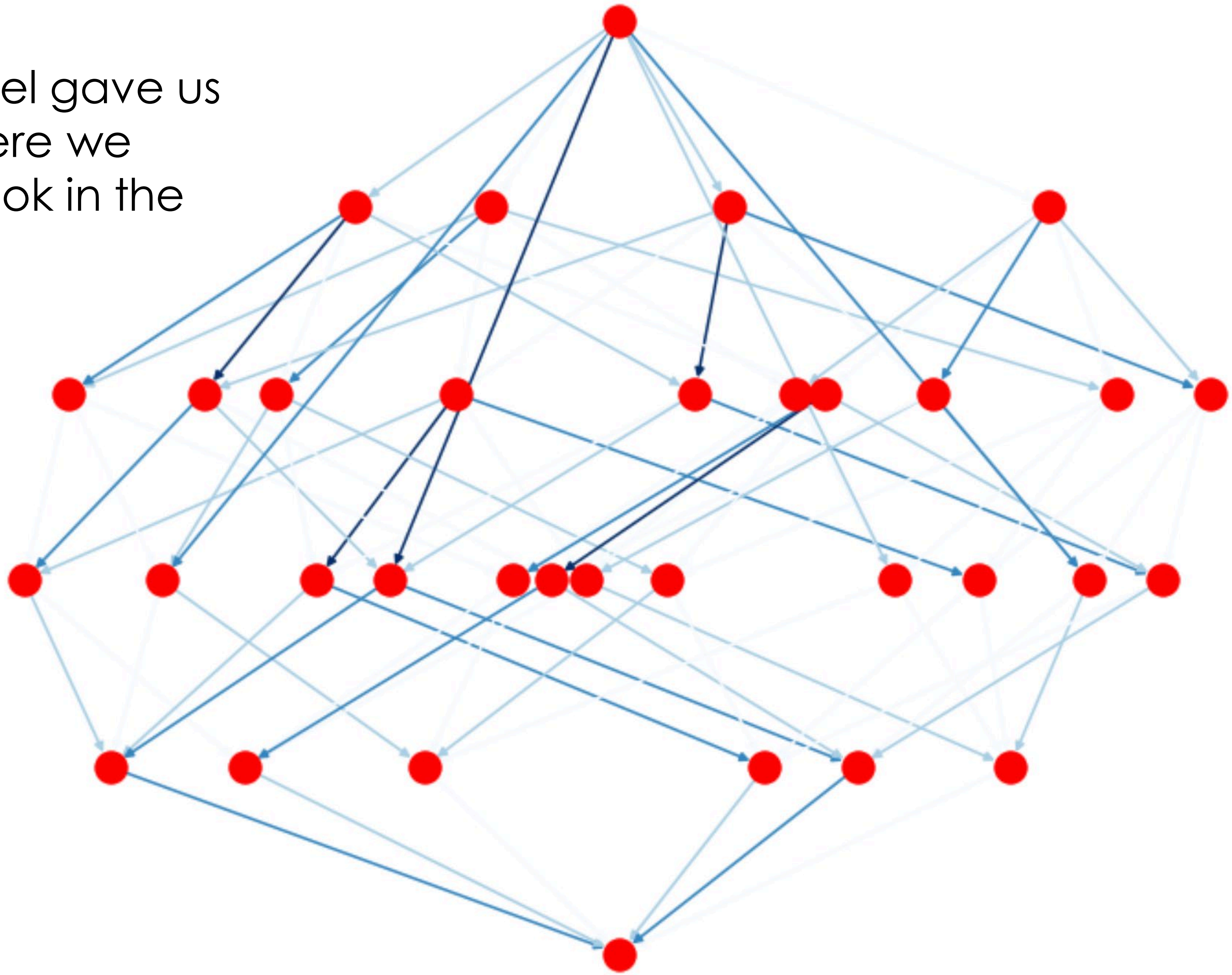
(Conjecture is proved in an important special case.)





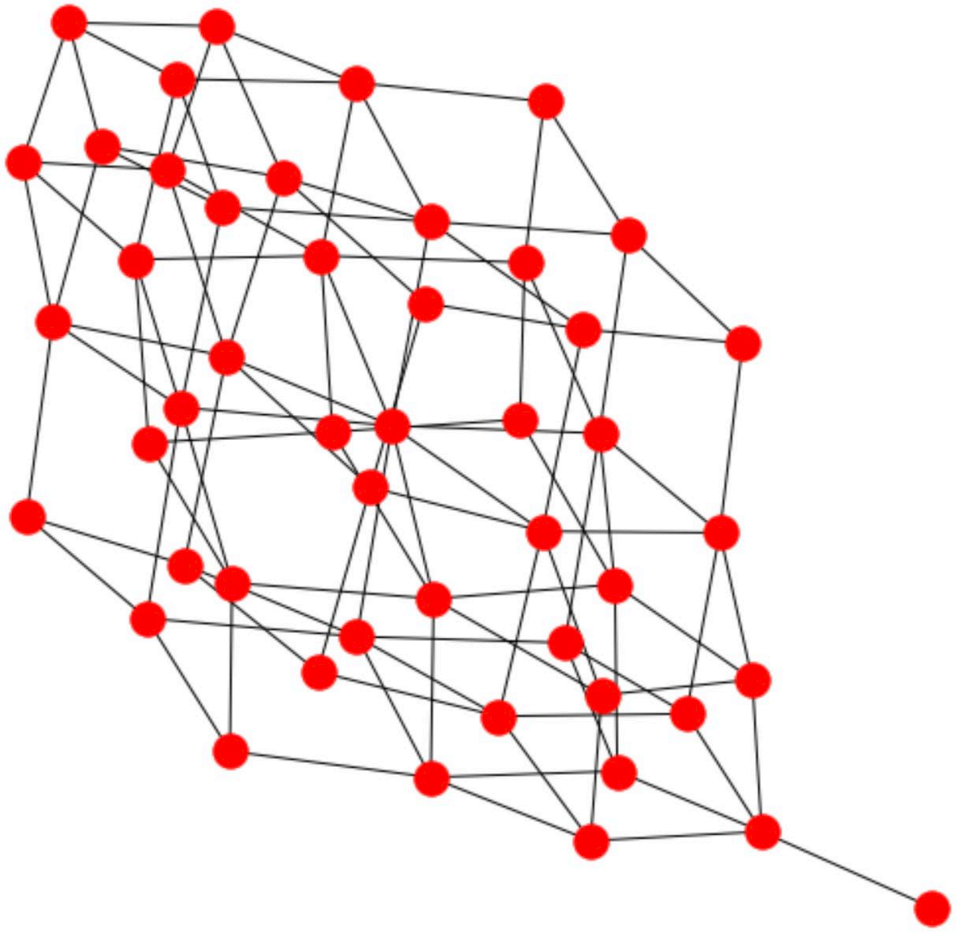


The model gave us hints where we should look in the graph.



Graph Theory

Graph Theory



Graph theory contains many conjectures.
Some are true. Some are simply false.

However, finding counter-examples is difficult!

Wagner: Finding a counter-example can be posed as a game, and computers can be trained to play the game via reinforcement learning.

Thus, the computer generates hundreds of examples at random, by accepting or rejecting an edge. Over multiple training rounds it learns patterns that result in graphs which are close to being counter-examples.

Conjecture 2.1 ([4]). *Let G be a connected graph on $n \geq 3$ vertices, with largest eigenvalue λ_1 and matching number μ. Then*

$$\lambda_1 + \mu \geq \sqrt{n-1} + 1.$$

Conjecture 2.3 (Auchiche–Hansen [6]). *Let G be a connected graph on $n \geq 4$ vertices with diameter D, proximity π and distance spectrum $\partial_1 \geq \ldots \geq \partial_n$. Then*

$$\pi + \partial_{\lfloor \frac{2D}{3} \rfloor} > 0.$$

Summary

Neural nets perform some tasks remarkably well. They are strongest on tasks like speech recognition and image classification that is simple and intuitive for us.

The functions that neural nets like to learn are rather different from the functions I usually think about.

Architecture matters, and most applications of neural nets to “difficult” problems incorporate them into more complicated architectures.

Neural nets can provide useful tools for conjecture generation and refutation.

I suspect that the next few years will see many more applications in pure mathematics, particularly organising calculation and guiding search.

I don’t yet see convincing evidence that neural nets are capable of replicating the “system 2” parts of the mathematical process.

“We can predict everything, except the future.”
-- A Sydney fortune cookie.

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www.sydney.edu.au/research/centres/mathematical-research-institute.html

Photography & artwork

DeepMind
Mare Nostrum/BSC-CNS
Christian Haugen/Flickr
Marc Chagall: Sandi Hemmerlein/avoidingregret.com

Simulation & knot measurements

A Neural Network Playground: TensorFlow on GitHub
bit.ly/network-playground

Benjamin Burton (Regina), Jessica Purcell

Papers

Davies et al., *Advancing mathematics by guiding human intuition with AI*: nature.com/articles/s41586-021-04086-x

Davies, Juhász, Lackenby, Tomasev, *The signature and cusp geometry of hyperbolic knots*: arXiv:2111.15323

Blundell, Buesing, Davies, Veličković, Williamson, *Towards combinatorial invariance for Kazhdan-Lusztig polynomials*: arXiv:2111.15161

Wagner, *Constructions in combinatorics via neural networks*: arXiv:2104.14516v1