AI for healthcare

Lecture 4/4 – Geometric deep learning

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Thursday, 2pm–5pm – 4 lectures

Epita, rooms KB404 + SM15

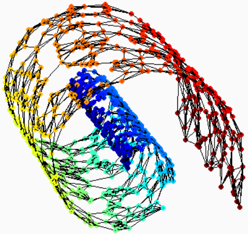
Validation: team project + quizz

Recap of the previous lecture

Lecture 3 – **Graphs**:

- **Curse of dimensionality** $\implies$ Statistics on **white noise** is hopeless.
- We must understand the **intrinsic** structure of our data,
  even when it is **embedded** in a high-dimensional space of features.
- We may need to **unwrap** the manifold of plausible data samples.

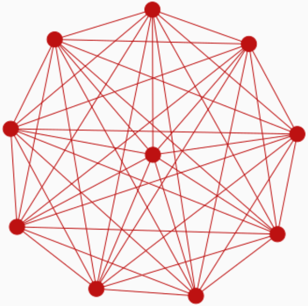
Graphs = local neighborhood structures

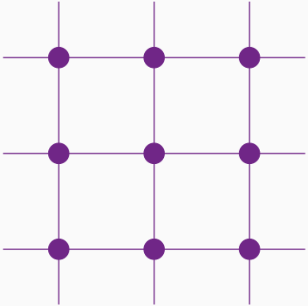


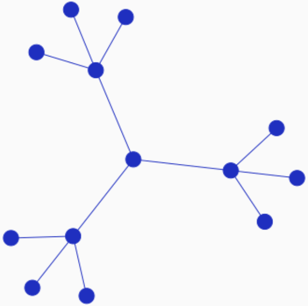
The K-NN graph describes
the **local** structure of a dataset.

Untangling a soup of edges to produce
a **global** understanding is hard.

Simple archetypes [TDGC+21]





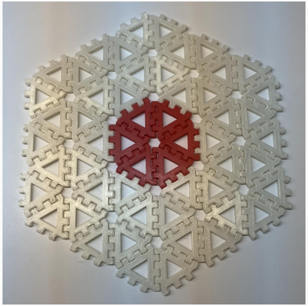


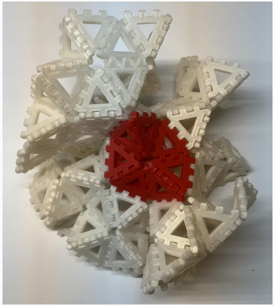
Cliques are like balls with positive curvature.

Grids are like planes with flat curvature.

Trees are like saddles with negative curvature.

Simple archetypes





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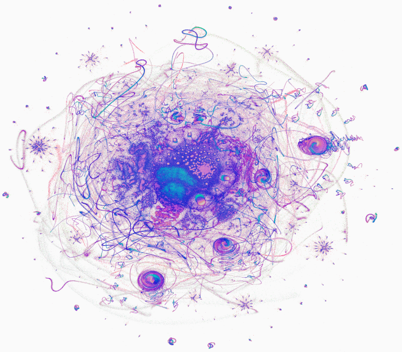
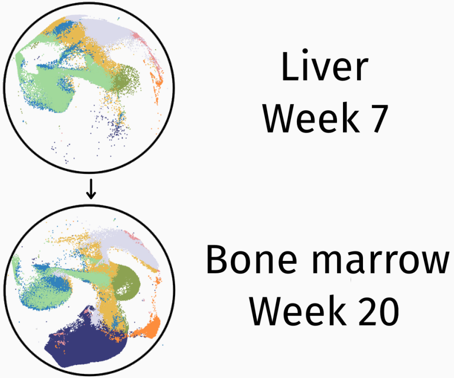
Embedding methods such as UMAP are excellent diagnostic tools [Wil]

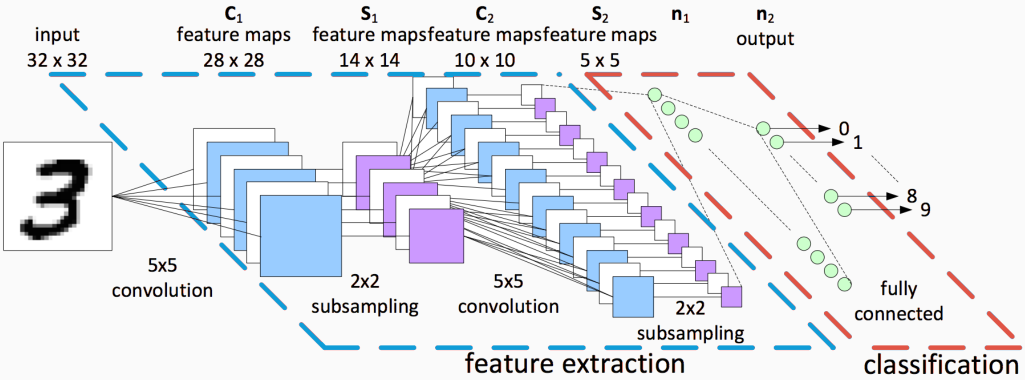


Visualizing the set of **integer numbers** 1, 2, 3, ..., 8,000,000.



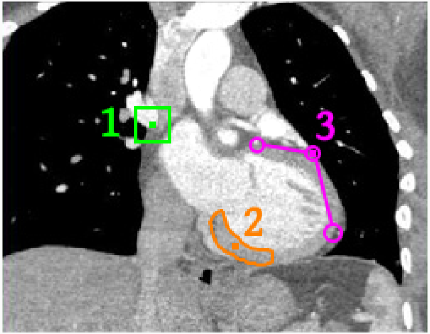
Visualizing the differentiation of Hematopoietic **stem cells**.

Since 2012, we have grown used to convolutional neural networks [PMC11]



Can we apply this methodology to higher-level descriptions? [EPW11, Man11]

1. Pixels 2. Anatomy 3. Function



Simplifying a bit, each level of analysis corresponds to a way of **grouping pixels** with their neighbors.

Today’s lecture – an active research topic

1. **Geometric deep learning is *not* a mature field:**
    - Convolutions on graphs and point clouds.
    - A stimulating environment.
    - Questionable benchmarks.
2. **Personal experience feedback:**
    - Protein docking.
    - Lung registration.
3. **Trying to learn a graph structure:**
    - Dynamic graphs, auto-encoders and transformers.
    - A continuous spectrum of models and jobs.

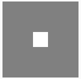
Geometric deep learning is *not* a mature field

What is a convolution?

Convolution (i.e. weighted average of the neighboring pixels) :

Cheap generalization of the **product** “a · x”,

parameterized by the coefficients of a **small filter** φ.



$\star$

$=$

φ x $\varphi \star x$

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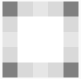 $\star$  $=$ 

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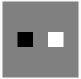

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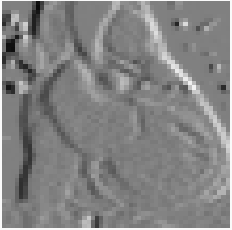

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Convolution (i.e. weighted average of the neighboring pixels) :

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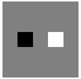

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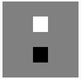

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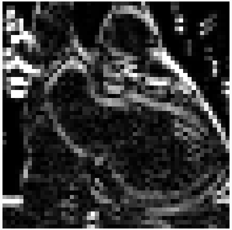

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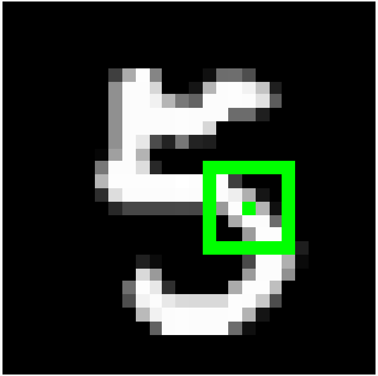
φ $\quad$ x $\quad$ $|\varphi \star x|$

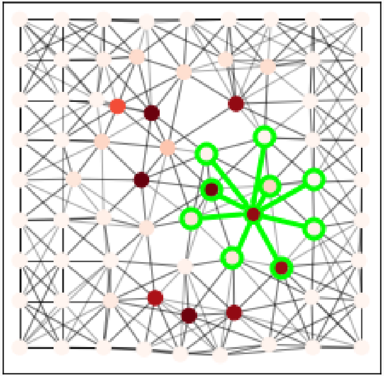
What is a convolution?

Convolutions on **grids**:

- Are **cheap**.
- Enable **pattern** detection and **texture** analysis.
- **Proven track record** since the 1960's:
  Gaussian blur, edge detectors, Laplacian pyramids,
  wavelets, JPEG2000, convolutional neural networks…

Message-passing on graphs [DJL+20]

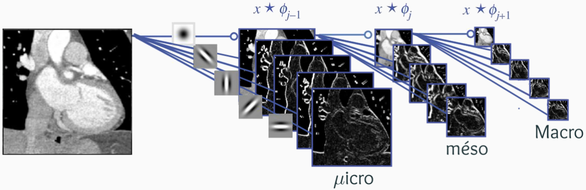


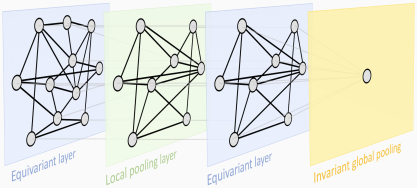


$$x[i,j] \leftarrow \sum_{k,l} \varphi[k,l] \cdot x[i-k, j-l]$$

$$x[i] \leftarrow \sum_{i \leftrightarrow k} \varphi(x[i], x[k], \mathrm{edge}[i,k])$$

Multiscale architectures on graphs [Mal16, BBCV21]





Grid convolutions
+ downsamplings.

Graph convolutions
+ downsamplings.

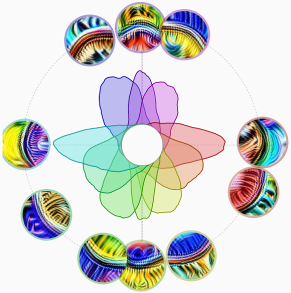
The promises of geometric deep learning

We intend to leverage the **intrinsic structure** of:

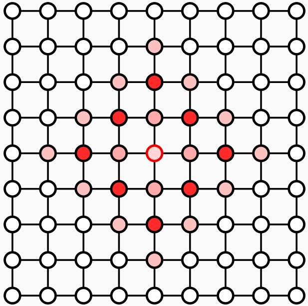
- **Point** clouds.
- Surface and volume **meshes**.
- **Molecular** graphs, proteins.
- Social and communication **networks**.

Unfortunately, things are **not that simple**.

Problem 1: How do we deal with the lack of orientation? [CGC+20, NoJ07]



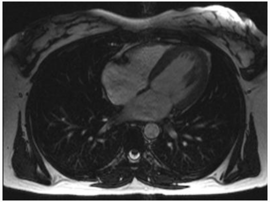
CNNs learn **oriented** curve detectors.



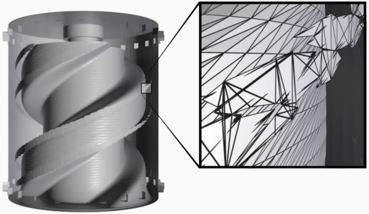
Vanilla graph convolutions define **isotropic** filters.

Hairy ball theorem: no globally consistent 2D coordinates on a sphere.

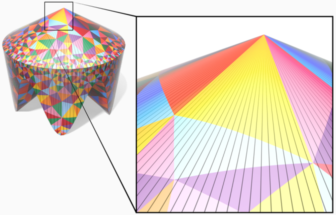
Problem 2: How do we deal with varying sampling densities? [SSC19]



MRI slice:
voxel size = 1 mm^3.

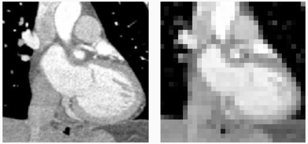


“**Hell** is other people’s meshes”
– Jean-Paul Sartre

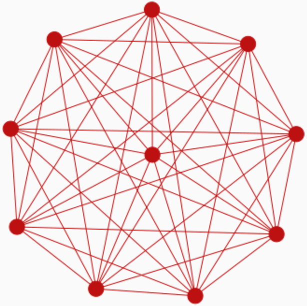


Intrinsic triangulations.
Can we use them for ML?

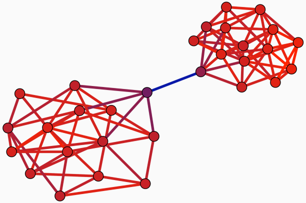
Problem 3: How do we deal with highly non-Euclidean graphs? [TDGC+21]



Downsampling a **grid** is easy.

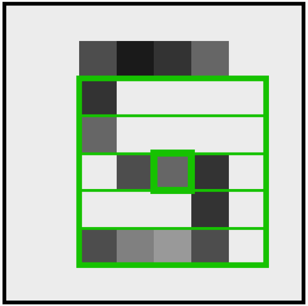


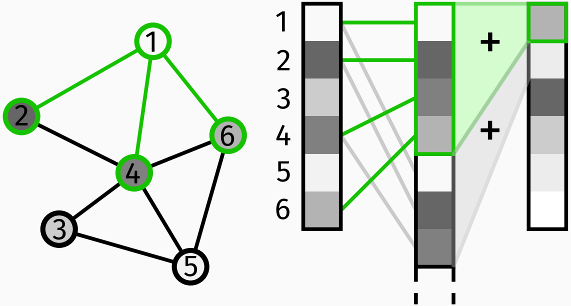
How do we downsample a **clique**?



How do we handle **bottlenecks**?

Problem 4: GPUs are not optimized for graphs





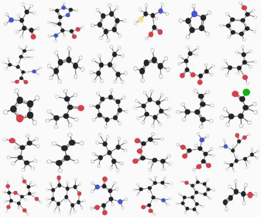
Fixed + **contiguous** neighborhoods

$\Longrightarrow$ Optimal compilation.

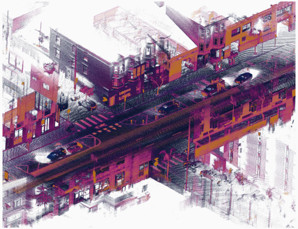
Varying sizes + **random** memory accesses

$\Longrightarrow$ x100 slow-down.

Problem 5: The range of target applications is too wide. [Dil15, Lu19, Gra19]



Molecules.



Lidar scans.

Social networks.

A fast-growing community

In 2017, geometric deep learning was **a solution in search of a problem**.

With an appealing pitch, it attracted:

- **Computer scientists**, looking for new ways of combining features.
- **Mathematicians**, looking for new applications of their insights.
- **Domain experts**, looking for a breakthrough on their data.

A blooming corpus of methods

The literature since 2017:

- Dozens of different **convolution** operators.
- Renewed interest in **theoretical graph ML**.
- Useful **extensions** for PyTorch: PyG, DGL, KeOps...
- **Cross-pollination** between different fields:
  computer graphics, signal processing, chemistry...

A field without consensus

Unfortunately, it is hard to recommend some methods over the others:

- Applications are **wildly different** from each other.
- Most theoretical and experimental works are **proof-of-concepts**.
- Benchmarks are **highly unreliable**.

We like to think that science is done in a vacuum

Archimedes – “Don’t disturb my circles”.

Louis Pasteur, alone in the lab.

Scientific literatures are shaped by structural incentives

French mathematicians – top 3 deepest ideas over a career:

- Promotes **long-term**, original thought.
- No incentives for outreach and interdisciplinary research.

INRIA researchers – 1 meaningful contribution every 5 years:

- A theorem, a piece of software, a patent, a societal breakthrough…
- Outstanding place for **applied** research.

French medical doctors/teachers/researchers – PubMed index:

- MERRI funds compensate hospitals for research activities.
- Fall behind the profitability threshold $\Longrightarrow$ shut down the lab, focus on care.
- **Inflation** of low-quality papers.

Structural incentives in US/UK CS teams

Universities – climb up the Shanghai ranking:

- 1 (foreign) student = \$30k-\$70k per year.
- Maximize the **number** of papers to impress prospective students.

Professors – maximize the hype:

- Unstable "tenure track" contract, commited to a grant, startup to grow…
- Allowed to take risks, but **not allowed to fail**.

Students – target a job in the tech companies:

- Significant debt to pay back.
- Safest route: **incremental** research, claim SOTA every 6 months.

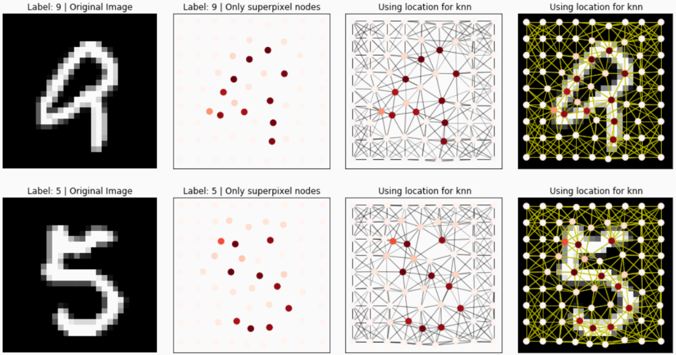
Peer-reviewed $\neq$ Scientific truth

In the current ML community, relatively **few actors are incentivized** to:

- Review papers carefully.
- Document **baselines** thoroughly.
- Admit that an idea **doesn't work**.
- Take the **massive** amount of time that is needed to make their experiments **truly** reproducible.
- Keep the codebase up to date with a software stack that breaks every 6 months.

$\Longrightarrow$ Unfortunately, the NeurIPS/ICML/... stamp means little.
We cannot **trust** the conclusions of a paper
without **reproducing** the experiments
or **checking** the proofs carefully.

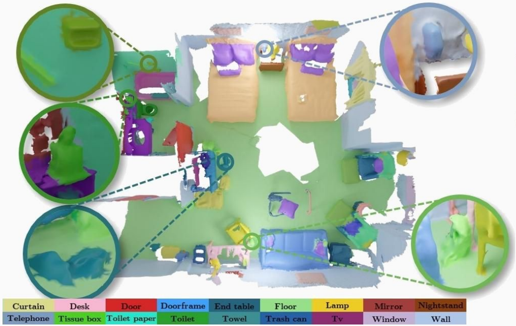
Some common benchmarks are nothing but sanity checks [LCCB98, DJL+20]

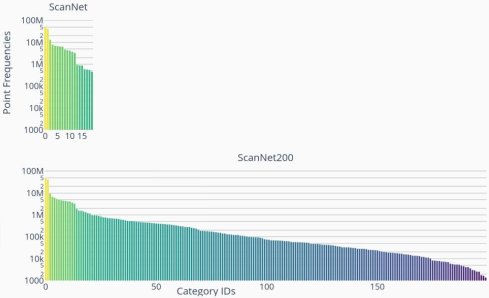


Model	L	MNIST #Param	MNIST Test Acc.±s.d.
MLP	4	104044	95.340±0.138
vanilla GCN	4	101365	90.705±0.218
GraphSage	4	104337	**97.312±0.097**
GCN	4	101365	90.120±0.145
MoNet	4	104049	90.805±0.032
GAT	4	110400	95.535±0.205
GatedGCN	4	104217	**97.340±0.143**
GIN	4	105434	96.485±0.252
RingGNN	2	105398	11.350±0.000
	2	505182	91.860±0.449
	8	506357	Diverged
3WLGNN	3	108024	95.075±0.961
	3	501690	95.002±0.419
	8	500816	Diverged

Results on **Graph-MNIST** look promising… Until you remember that test accuracy for **basic K-NN classifiers** on MNIST is 95%-99%.

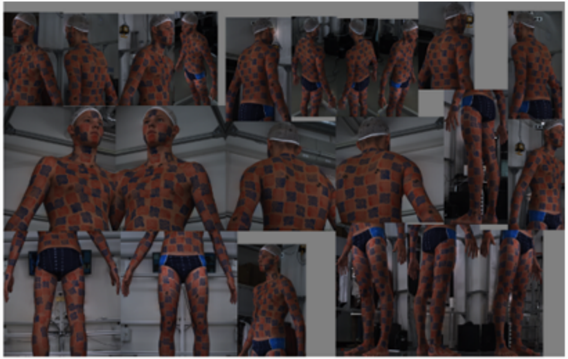
Some common benchmarks have been saturated for years [RLD22]

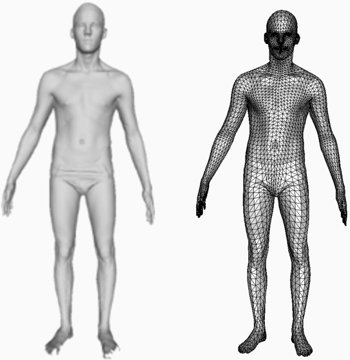




Challenging large-scale benchmarks are published every year…
But the review system pushes authors towards **overfitting on "classic" datasets**.

Some benchmarks have been taken out of context [BRLB14]





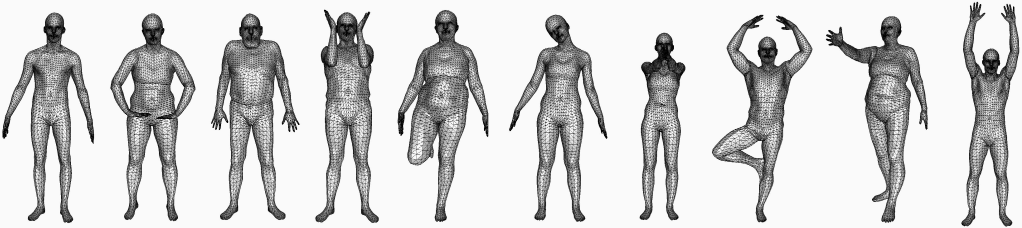
The MPI FAUST dataset contains 300 real-life scans of 10 subjects – 30 poses each.

Problem: fit a reference mesh to the **noisy 3D point clouds**.

Challenges: different topologies, missing data, self contacts.

Dense ground truth correspondence for training = 10x10 meshes with identical topology.

Some benchmarks have been taken out of context [BRLB14]



The PyG library and many papers on graph neural networks
discard the original point clouds to focus entirely on the 100 pre-aligned meshes.
New problem: use (x, y, z) coordinates as input features for each node
$\Longrightarrow$ predict node indices in $[1, 6890]$ as output signal.
Train on 80 surfaces, test on the remaining 20.

Irrelevant to shape registration: we learn to **overfit on the reference triangulation**.

How can we judge?

Keep track of both **classical** and **learning-based** baselines, in each application domain.

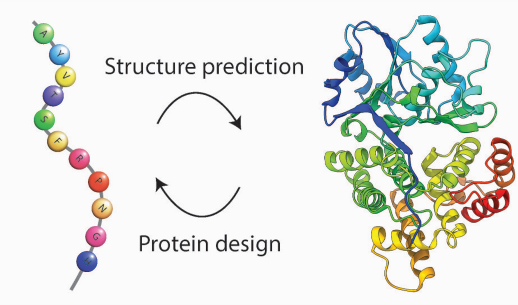
This is time-consuming – **focus on 2-3 subjects at most.**

It is likely that the wave of papers on geometric deep learning will **fade** in most applications settings, and **stick** in some productive niches: Shape analysis? Chemistry? Social sciences?

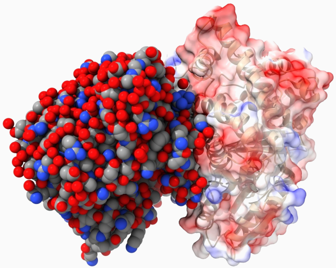
This is how scientific progress takes place. The hype cycle is a **normal** and well-documented phenomenon.

Some personal experience

Two problems in structural biology [SFCB20]

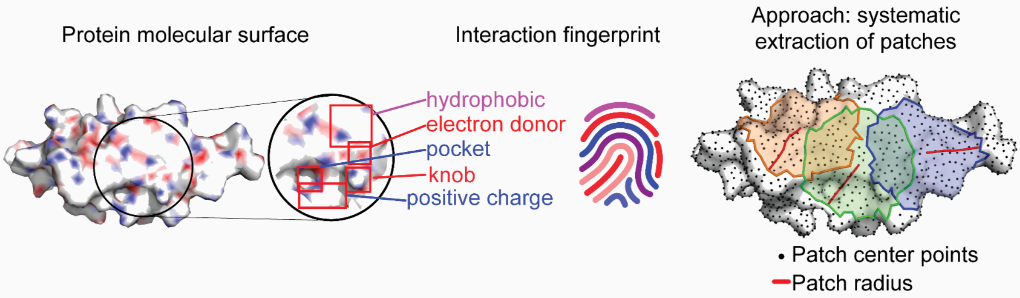


Folding and design.



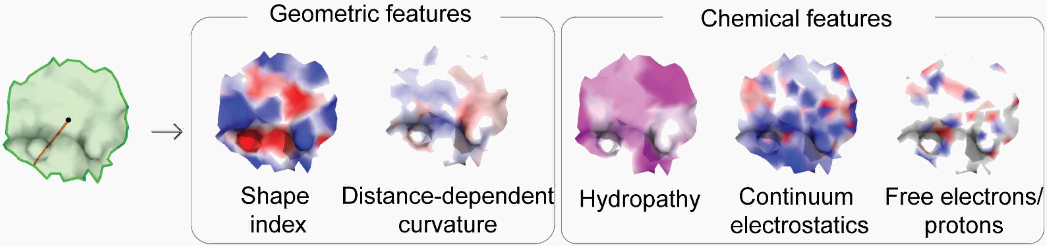
Docking – interacting surfaces.

Docking is a function of the protein surfaces [GSM+20]



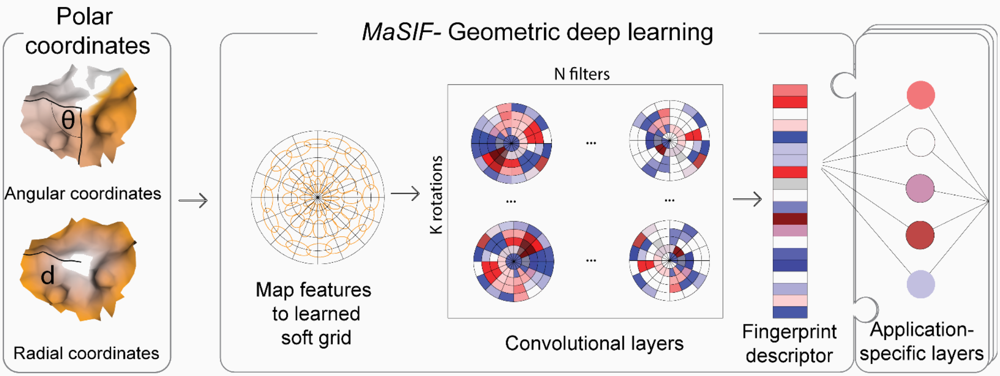
Physical prior: no need to deal with the full volumes, we are looking for **surface fingerprints**.

Docking is a function of the protein surfaces [GSM+20]



We can compute **geometric** and **chemical** **input features**
on local patches with $\simeq 1\,\mathrm{nm}$ radius.

Docking is a function of the protein surfaces [GSM+20]

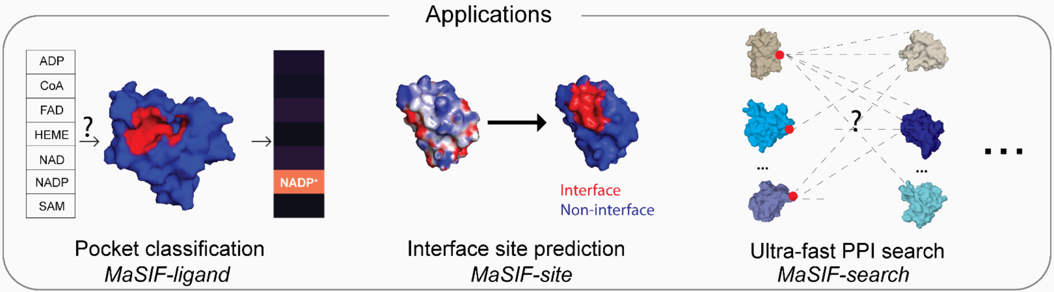


And perform all classification tasks on **geodesic patches**.

Built-in **invariance** to 3D rotations, translations and the inner content of the protein.

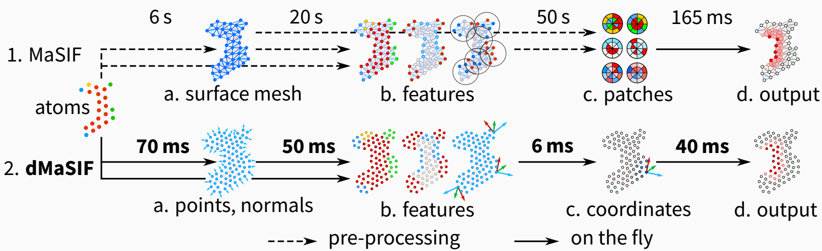
Enforces a **locality** prior: won't overfit on scattered patterns.

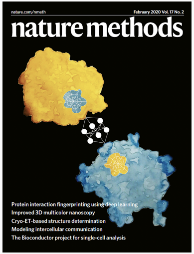
Docking is a function of the protein surfaces [GSM+20]



After training on the Protein Data Bank (with **careful** train-test split), this enables three tasks of interest.

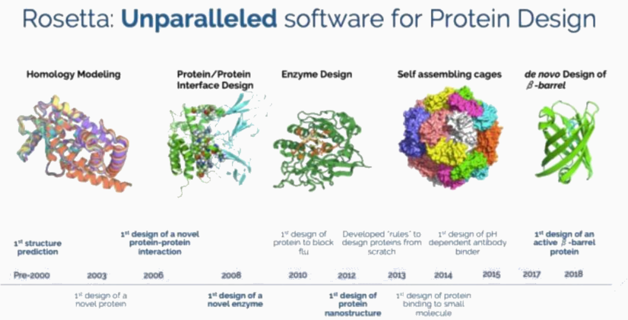
A proof-of-concept that has been received well [GSM+20, SFCB20, SFS+22]

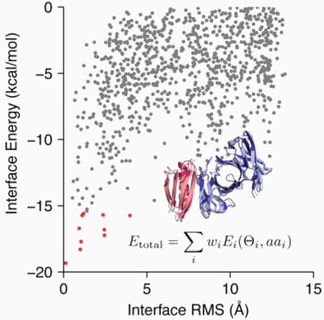




$\longrightarrow$ $\times$100 - $\times$1,000 faster, lighter and fully differentiable.

Is deep learning truly a revolution? [ALFJ+17]





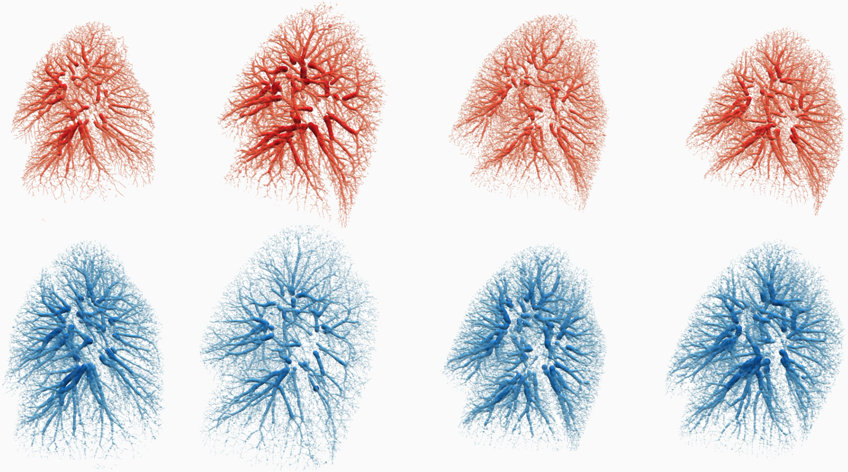
After 20 years of work, the developers of the Rosetta software have *de facto* developed a **hybrid "point neural network"** that combines **physical** potentials with **data-driven** residuals.

Recap on the MaSIF-dMaSIF project

Personal feedback:

- Inspiring **prototype** that shows how far we can go if we
  drop complex physical terms but **preserve** the symmetries of the problem.
- With clever geometry and code, we can do interesting science on a **single GPU**.
- Nowhere near close to a finished product: **maintaining** software is a full-time job.
- **Well-funded** and **mature** fields already showcase formidable baselines.
  As outsiders, we can propose **stimulating** ideas and tools.
  Always **stay humble** – understanding the full context takes years.

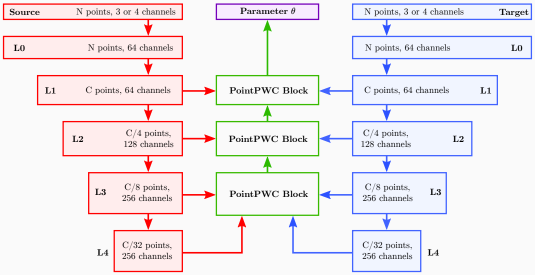
Lung registration “Exhale – Inhale” [SFL+21]



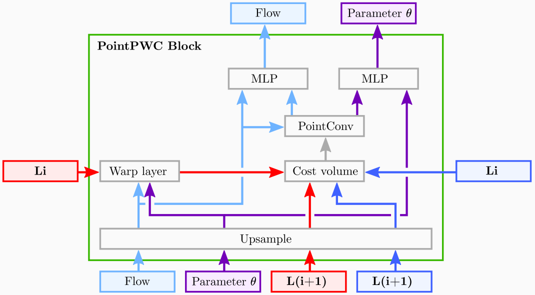
Complex deformations, high **resolution** (50k–300k points), high **accuracy** (< 1mm).

Point clouds are more challenging than volumes, but **robust** to acquisition parameters.

Point neural networks [WWL+20, SFL+21]

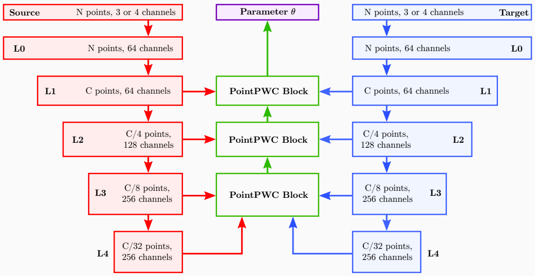


Multi-scale convolutional point neural network.



Architecture of a PointPWC **block**.

Point neural networks – strengths and limitations [SFL+21]



Multi-scale convolutional point neural network.

Point neural nets, **in practice**:

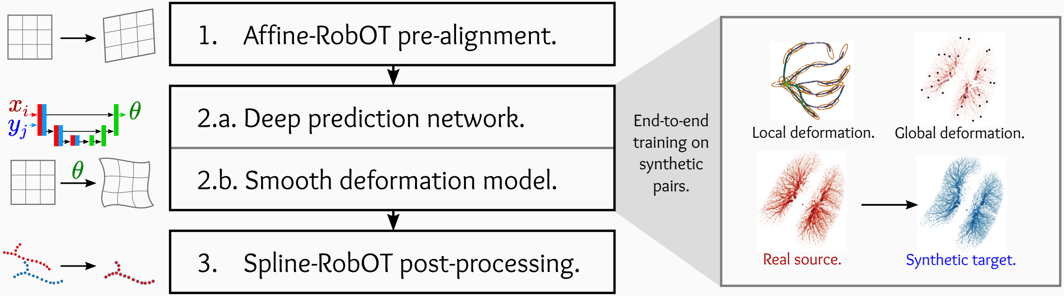
- Compute **descriptors** at all scales.
- **Match** them using geometric layers.
- Train on **synthetic** deformations.

Strengths and weaknesses:

- Good at **pairing** branches.
- Hard to train to high **accuracy**.

$\Longrightarrow$ **Complementary** to geometric methods such as optimal transport.

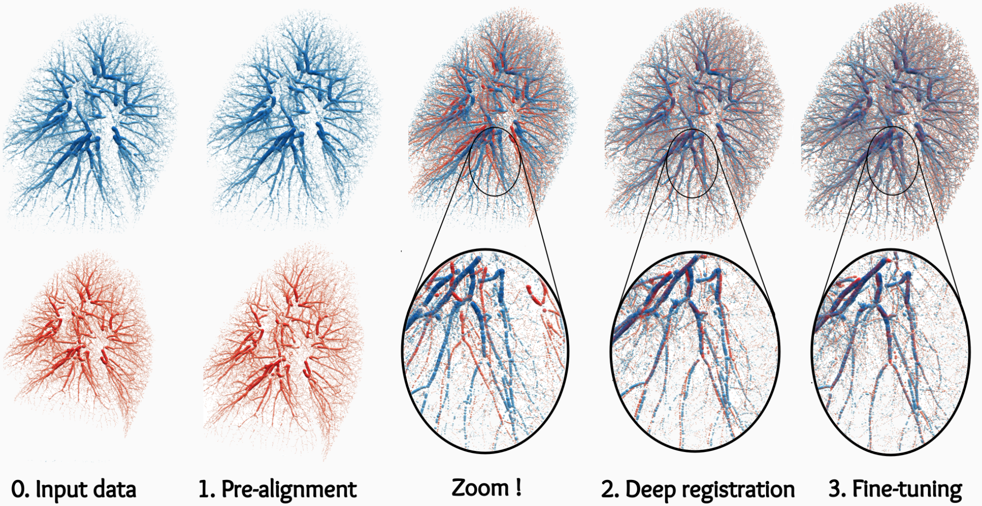
Three-steps registration [SFL+21]



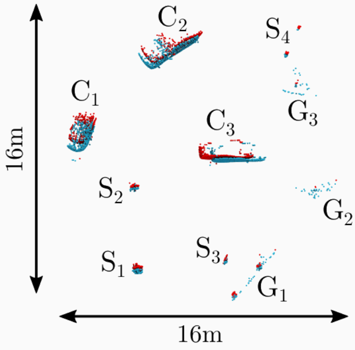
This **pragmatic** method:

- Is **easy to train** on synthetic data.
- Scales up to high-resolution: 100k points in 1s.
- Excellent results: **KITTI** (outdoors scans) and **DirLab** (lungs).

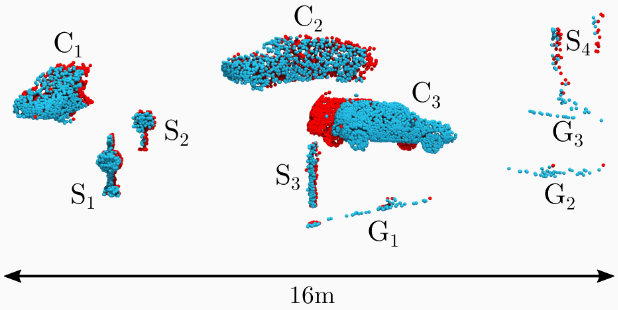
Three-steps registration



Evaluation on the 3D Kitti dataset [MG15, MHG15, SFV+19]



(a) View from above.



(b) Front view.

3D scene flow estimation task, derived from a **2D + depth** dataset.

This is a standard (but maybe questionable) benchmark.

Evaluation on the 3D Kitti dataset [SFL+21]

	Method	Points	Time ms ↓	Memory Mb ↓	EPE3D cm ↓	Acc3DS % ↑	Acc3DR % ↑	Outliers3D % ↓	EPE2D px ↓	Acc2D % ↑
Unsupervised	ICP (rigid) [7]	8k	224	**2**	51.81	6.69	16.67	87.12	27.6752	10.56
	FGR (rigid) [134]	8k	—	30	48.35	13.31	28.51	77.61	18.7464	28.76
	CPD (non-rigid) [81]	8k	34,880	798	41.44	20.58	40.01	71.46	27.0583	19.80
	PWC (self) [126]	8k	237	1,016	25.49	23.79	49.57	68.63	8.9439	32.99
	RobOT (raw)	8k	170	3	**9.12**	**60.43**	**79.39**	**33.65**	**4.9920**	**56.23**
	RobOT (raw)	30k	**166**	**89**	**4.67**	**80.43**	**91.05**	**20.21**	**1.7026**	**85.71**
Supervised training on FlyingThings3D	FlowNet3D [69]	8k	—	690	17.67	37.38	66.77	52.71	7.2141	50.92
	SPLATFlowNet [111]	8k	—	—	19.88	21.74	53.91	65.75	8.2306	41.89
	original BCL [49]	8k	—	—	17.29	25.16	60.11	62.15	7.3476	44.11
	HPLFlowNet [49]	8k	—	—	11.69	47.83	77.76	41.03	4.8055	59.38
	FLOT [49]	8k	324	2,826	5.51	75.79	90.98	23.95	3.3152	75.10
	PWC [126]	8k	**237**	1,016	5.28	85.83	94.08	18.85	3.0074	81.48
	PWC	30k	1,138	10,691	7.63	67.54	92.30	26.09	3.5212	70.74
	Pre + FLOT + Post	8k	487	2,826	5.33	76.84	91.65	23.56	3.2786	75.31
	Pre + PWC + Post	8k	279	1,034	3.35	90.10	97.32	**16.20**	**1.4301**	**93.85**
	Pre + PWC + Post	30k	1,207	10,691	3.50	90.04	96.71	17.28	1.5917	90.37
	D-RobOT (spline)	8k	268	**396**	**3.15**	**90.51**	**97.42**	16.26	1.4532	93.76
	D-RobOT (spline)	30k	**547**	**610**	**2.23**	**95.88**	**99.19**	**12.89**	**1.0336**	**96.75**

Surprise: a **baseline** optimal transport solver with smoothing (RobOT) outperforms many **deep learning** methods on all metrics.

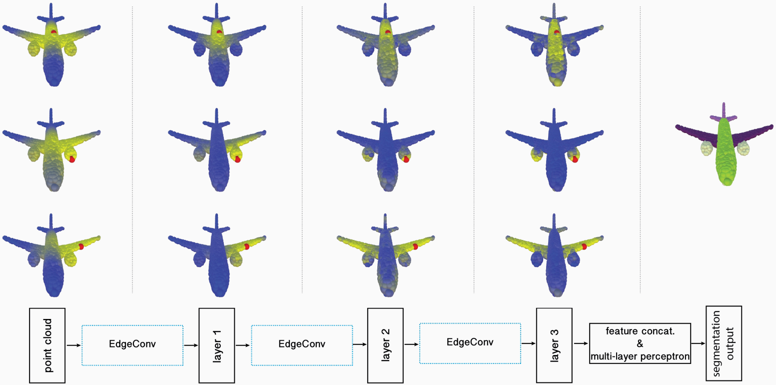
Recap on the registration project [CCF+13]

Personal feedback:

- Pragmatic approach: get the **best of both** **data-driven** and **deterministic** methods.
- **Tables** of numbers look impressive – but can **hide** critical information.
- **Code** base is not clean – top priority going forward.
- Evaluation on 3D scene flow is **questionable**.
  Shouldn't we work with the original 2D data?
- Evaluation on **medical data** is hard:
  - We release a new dataset of **1,000 pairs for training** – without annotations.
  - We only have access to **10 pairs** with dense annotations **for evaluation**.

Should we learn our graphs?

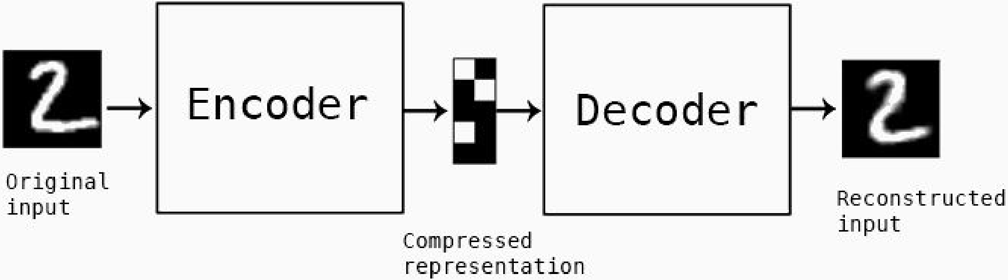
Dynamic graph CNNs [WSL+19]



At every layer, use the **K-NN graph** of the **feature vectors**.

This may promote **semantic** neighborhoods.

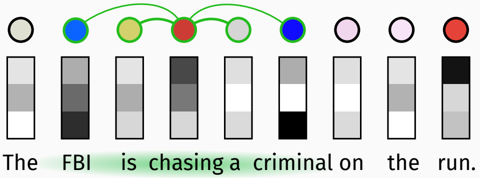
Embeddings and autoencoders [Cho16]



Use the **K-NN graph** of a **low-dimensional** representation:

UMAP, an encoder-decoder architecture…

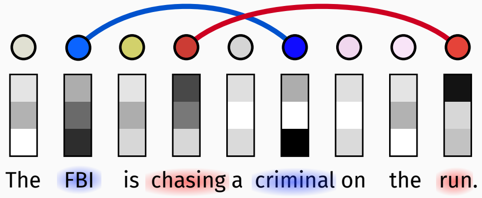
Attention layers and transformers [CDL16, VSP+17]

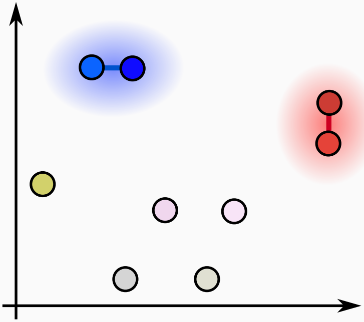


We would like to define convolutional architectures on **sentences**.

But the **1D structure** of the text is not always relevant.

Attention layers and transformers [CDL16, VSP+17]





Instead, we **embed feature vectors** in a semantic space.

Attention $=$ data-driven embedding + convolution.

Transformer $=$ stack of attention layers.

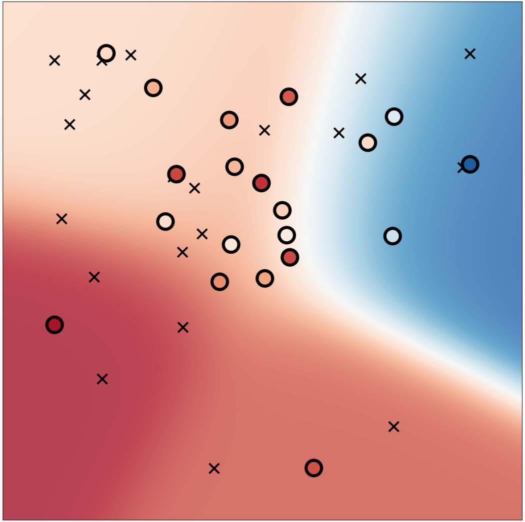
Attention layers and transformers [CDL16, VSP+17]

Cheap and expressive convolution on the feature vectors x_i:

- Query vectors $q_i \leftarrow \text{MLP}_q(x_i)$.
- Key vectors $k_i \leftarrow \text{MLP}_k(x_i)$.
- Value vectors $v_i \leftarrow \text{MLP}_v(x_i)$.
- **Nadaraya–Watson interpolation** with a kernel $k(x, y) = \exp(x \cdot y)$:

$$x_i \leftarrow \frac{\sum_j \exp(q_i \cdot k_j)\, v_j}{\sum_j \exp(q_i \cdot k_j)}$$

This architecture trains remarkably well on **web-scale** corpuses.



Problem 1: In most important settings, data is expensive and fragmented [Ora17]

The Web and the Amazon Mechanical Turk are **the exceptions**, not the rule:

- **1** protein structure in 3D
  $=$ **months** of work for a biologist.
- **50** fully documented patients
  $=$ a great **thesis** for a radiologist.
- **1** patient in a clinical trial
  $\simeq$ **\$40k**, up to \$1M for surgery!

- Getting **legal** access to large datasets *and* computers is extremely difficult in any field that has a signficant **societal impact**.

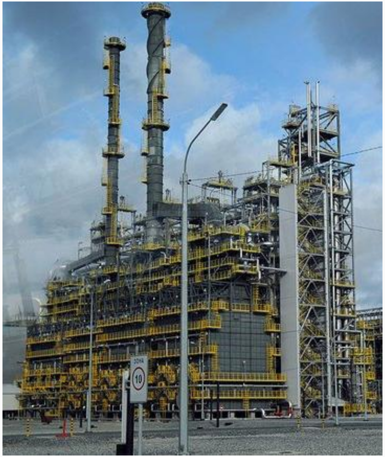
Problem 2: Bigger models are slower, heavier and cumbersome [otRF98]

We must **strike a balance** between:

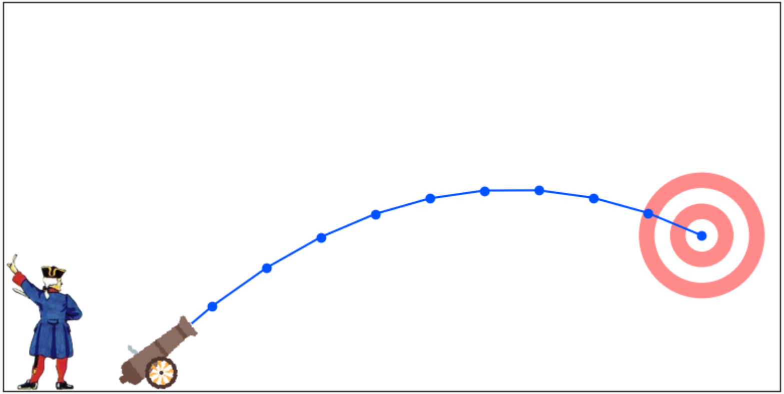
- Speed.
- Accuracy.
- **Hardware** and **development** costs.
- **Energy** consumption $=$ battery life.
- **Interpretability** $=$ easy to debug
  $=$ easy to **maintain**.

Tons of equations $\simeq$ Tons of parameters.

Only worth the **trouble** if there is no other option.



Problem 3: In mature fields, structure is key to generalize

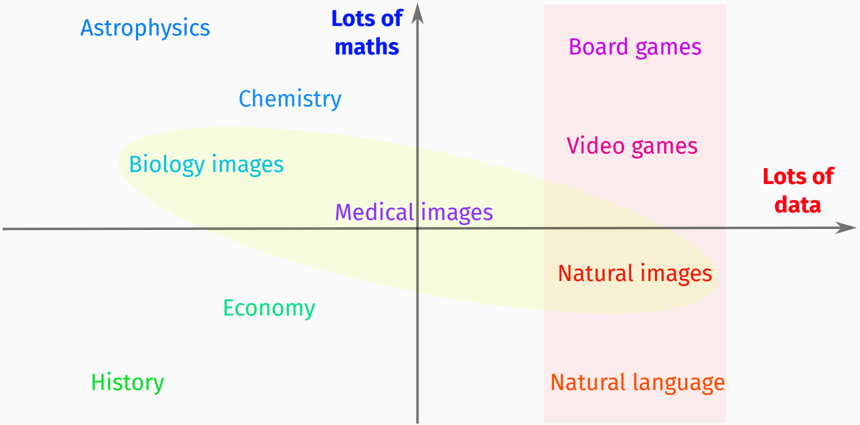


This is especially true in fields that are close to physics, robotics…

Fitting piecewise **linear** functions to **parabolas** or **exponentials**

is fine for **interpolation**, but very limiting for **extrapolation**.

A continuous spectrum of scientific fields



"The **unreasonable effectiveness** of mathematics in the natural sciences" and "the **bitter lesson** of AI" apply to **different ends** of this spectrum.

Monopolies claim that “bigger is better”

Electric bikes travel
at **30 km/h**.

Private jets travel
at **800 km/h**.

Rockets travel
at **30,000 km/h**.

Raw performance metrics **do not tell the whole story.**

Choose your own path

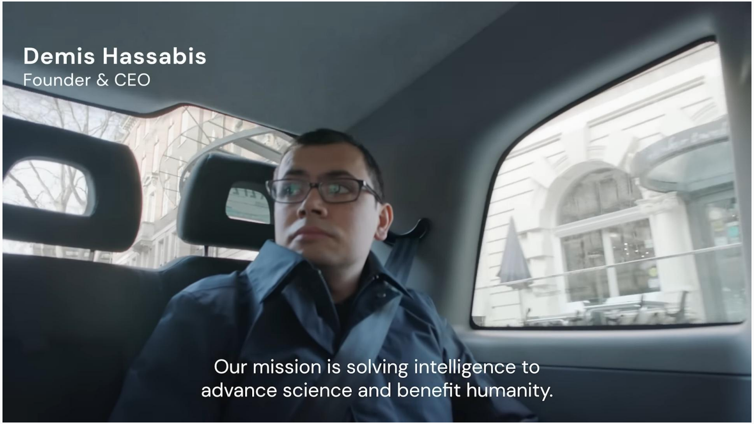
Tech companies target your "fear of missing out"

"We should **stop** training radiologists **now**.

It's just **completely obvious** that within **five years**, deep learning is going to do **better** than radiologists."

– Geoffrey Hinton, Google Brain and UToronto, **in 2016**.

Tech companies want you to forget that targeting ads $\neq$ solving cancer



"Welcome to **DeepMind**: Embarking on **one of the greatest adventures** in scientific history", available on YouTube since September 29, 2022.

2020-2050: tough times ahead. Which problem are you going to solve?

Quantum computers

Chess engine++

Killer drones

Efficient batteries

Autonomous cars

Automated MRI screening

Nuclear fusion

Targeted ads

Drug safety

Protein design

Efficient rail network

Machine translation

The French education system is giving you **genuine freedom** of choice.

Use it **wisely**.

Find your own balance

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