Rm Palaniappan, *Alien Planet-X-9*
Viscosity, pencil colour and ink on handmade paper

Are modern ML models like scientific instruments?

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Some pre-apologies

I am still trying to figure out how to talk about this work

This is (mostly) based on pretty empirical work: not sure if it counts as information ***theory***.

I think there are lots of **interesting questions for theory** which this brings up!

There are a lot of metaphors and analogies (some science-fictional) which are **not always precise**.

Real life is a bit messy…

Thanks to my collaborators/coauthors!

Most of this is their work, obviously

Sinjini Banerjee (Rutgers)

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Andrew Engel (Ohio State)

Xin Li (Rutgers)

Tim Marrinan (PNNL)

Max Vargas (PNNL)

Zhichao Wang (UC Berkeley)

Papers:

[JSTSP] Banerjee et al. https://doi.org/10.1109/JSTSP.2025.3583140
[NeurIPS 2023] Wang et al. https://openreview.net/forum?id=qpqBGyKeKH
[ICLR 2024] Engel et al. https://openreview.net/forum?id=yKksu38BpM
[ArXiV] Vargas et al. https://arxiv.org/abs/2408.10437

What does the title mean?

What do ML models have to do with science?

Source: Wikipedia

Source: IBM

Source: Mishra et al.

We often hear a lot about "**AI for Science**" but that can mean a lot of different things! Some examples:

- Using computer vision to do automated analysis of medical images.
- Use generative AI to build a "digital twin" of energy/utility networks for simulation/design
- Use LLM architectures to decode brain activity for assistive technology.
- Many more…

Is “AI for science” the new “Bandwagon”?

Some gap between hype and reality

The Concept of a Robot Scientist

Computer system capable of originating its own experiments, physically executing them, interpreting the results, and then repeating the cycle.

https://futuretech.mit.edu/news/ai-and-the-future-of-scientific-discovery

NY Times
14 May 2025

Your A.I. Radiologist Will Not Be With You Soon

Experts predicted that artificial intelligence would steal radiology jobs. But at the Mayo Clinic, the technology has been more friend than foe.

IRE TRANSACTIONS—INFORMATION THEORY

The Bandwagon

CLAUDE E. SHANNON

Shannon, 1956

What about information/signal processing?

Some perspective from more solid ground

At the end of the day "artificial neural nets" are just a bunch of computational signal processing primitives chained together and jointly optimized with stochastic gradient methods.

- Ben Recht (on argmin.net)

ML/AI frameworks are evolving very quickly.

➜ Theory often lags behind practice.

➜ IT, SP, control, etc. are still relevant!

A traditional division of labor

The EE/CS divide in some sense

"model-driven" scientific instrument

"data-driven" analytics

What is “AI as instrumentation”?

Putting neural networks into measurement devices

The **data** (images, time series, etc.) produced by a **scientific instrument** (camera/microscope/scanner) can be described in terms of the **science** (physics, chemistry, biology).

We use the data in **analytics pipelines** for more complex tasks. This relies on assumptions:

- Data from the **same camera** is “consistent”.
- Data from **different cameras** are “consistent”.

If we put AI “into the camera” will these be true?

It already is not true in actual practice

Assumptions are wrong, but maybe correctable?

Data are almost never consistent in the ways we assume.

- Calibration issues
- “Batch effects” (c.f. DNA/RNA sequencing)
- Information forensics
- Sampling bias
- Etc…

Images: pngrepo.com, Tung et al. (2017), OpenMoji.org

Pushing the kitchen sink backwards

Sensors, instrumentation, and decision support

“physics-informed” measurements

“data-driven” analytics

Do we even need to understand physics?

(Asking for an undergrad friend)

“data-driven” scientific instrumentation

What about our assumptions?

What would it mean of them to hold (if they do)?

A futuristic thought experiment: **every camera has a AI model** that produces the actual image or a decision based on the image.

- If we build the camera twice, **will it be the same**?
- If we use two different cameras **will they give similar results**?
- **How do we compare** two models?

<u>These questions are not new!</u> We can use “classical” tools to try and understand them.

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Samsung UI 7.0

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Some preliminaries

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The standard statistical setup for modern ML

Machine learning as function-fitting

The traditional setup for estimating parameters in a statistical model (or training a neural network:

- Parameterized set of functions/models $\mathscr{F} = \{f(x \mid \theta) : \theta \in \Theta\}$.
- Training data used to estimate the parameters by minimizing some objective function.
- Stochastic optimization algorithm that does the actual minimization.

Variability in the training process

Is training reliable?

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If we have two different architectures $\mathscr{F}$ and $\mathscr{G}$, how can we measure their similarity?

- Focus on **performance**: two models with the same error are “effectively the same”.
- Focus on **features**: come up with a mapping from one model to the other to show they are the same.
- Focus on **approximations**: use proxies for each model which are more comparable.

How should we characterize a model?

Drawing samples from the function space

For a **fixed training set**, **architecture**, and **training algorithm**, we can think of an ML/AI model as a sample from a function space:

$$\mathscr{F} = \{f : f \text{ representable by the NN}\}$$

Examples:

- In classification, each $f : \mathscr{X} \to [L]$ labels input data points.
- In representation learning, each $f : \mathscr{X} \to \mathscr{R}$ maps inputs to representations/embeddings.

Some natural questions

Comparing models is not clear

If we have two different models we might have

$$\mathscr{F} = \{f : f \text{ representable by NN A}\}$$
$$\mathscr{G} = \{g : g \text{ representable by NN B}\}$$

Can we meaningfully compare these models?

- If $\mathscr{F} = \mathscr{G}$ we can use their outputs to do a comparison.
- If $\mathscr{F} \neq \mathscr{G}$ we need some way to do a comparison.

Approximating the NN with a kernel machine

Not practical, but perhaps informative?

$$\approx$$

$$\text{kGLM}$$

Suppose we compute some kernel function $\mathbf{K}$ associated to the model and fit a **surrogate model** $(\mathbf{V}, \mathbf{b})$:

$$\mathbf{y}_i = \mathbf{V}\mathbf{K}(\mathbf{x}_i, \mathbf{X}) + \mathbf{b}$$

where $\mathbf{y}_i, \mathbf{b} \in \mathbb{R}^C$ and $\mathbf{V} \in \mathbb{R}^{C \times N}$. Fitting is done with the same training data (double dipping).

One example: the **neural tangent kernel**.

Neural Networks as Kernel Machines

Approximating an NN with a “simpler” model

NTK $\neq$

Jacot et al. (2018) showed that **infinitely wide** NNs are equivalent to a kernel machine with with the “**neural tangent kernel**” (NTK):

$$K(\mathbf{x}, \mathbf{x}') = \left\langle \nabla_\theta f(\mathbf{x}; \theta), \nabla_\theta f(\mathbf{x}'; \theta) \right\rangle$$

Measures the **(cosine) similarity between tangent hyperplanes** for $\mathbf{x}$ and $\mathbf{x}'$ at θ.

Finite width networks don’t really behave like infinite width networks… (Chizat et al., 2018; Yang & Hu, 2021; Wang et al., 2022).

Challenge: NTK is asymptotic (infinite width)

Writing an empirical version of the NTK

We would like to handle multi-class problems and large data sets. In the setting **the empirical NTK becomes huge**. For classes i and j define:

$$\mathbf{K}^{\mathrm{NTK}}_{(c,c')}(\mathbf{x}_i, \mathbf{x}_j) = \left\langle \nabla_\theta f^c(\mathbf{x}_i; \theta), \nabla_\theta f^{c'}(\mathbf{x}_j; \theta) \right\rangle$$

Then the NTK has a block structure, where each diagonal block has the "regular" NTK for each class and the off-diagonal blocks are cross terms.

$$\left\{ \begin{array}{cccc} \mathbf{K}^{\mathrm{NTK}}_{1,1} & \mathbf{K}^{\mathrm{NTK}}_{1,2} & \cdots & \mathbf{K}^{\mathrm{NTK}}_{1,C} \\ \mathbf{K}^{\mathrm{NTK}}_{2,1} & \mathbf{K}^{\mathrm{NTK}}_{2,2} & \cdots & \mathbf{K}^{\mathrm{NTK}}_{2,C} \\ \vdots & & \ddots & \vdots \\ \mathbf{K}^{\mathrm{NTK}}_{C,1} & \mathbf{K}^{\mathrm{NTK}}_{C,2} & & \mathbf{K}^{\mathrm{NTK}}_{C,C} \end{array} \right\}$$

Trace NTK: a proxy for the eNTK

Much lower computational overhead needed

We look at a simplification of the NTK:

$$\mathbf{K}^{\mathrm{trNTK}}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{c=1}^{C} \left\langle \nabla_\theta f^c(\mathbf{x}_i; \theta), \nabla_\theta f^c(\mathbf{x}_j; \theta) \right\rangle}{\left(\sum_{c=1}^{C} \left\| f^c(\mathbf{x}_i; \theta) \right\|^2 \right)^{1/2} \left(\sum_{c=1}^{C} \left\| f^c(\mathbf{x}_j; \theta) \right\|^2 \right)^{1/2}}$$

This is **different from other surrogate kernels:** the pseudo NTK (pNTK) (Mohamadi & Sutherland, 2022), things based on the CK (Fan & Wang, 2020; Yeh et al., 2018), the un-normalized trNTK, and the embedding kernel (Akyürek et al., 2023).

Fast to compute, also with random projections (Novak et al., 2022, Park et al., 2023))

Some takeaways from the setup

Formalization shows how under-specified model comparison is

Understanding a model by its NTK sounds OK but can we really compare two models by their NTKs? Maybe!

- Computing even the trNTK is expensive, especially for large models.
- Much easier if you have access to the training corpora.
- Challenging because of invariants.

Embedding spaces and model comparisons

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A question of interoperability

Challenges in collaborating with AI instruments

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Samsung UI 7.0

Suppose we have two manufacturers of these **AI scientific instruments** based on generative AI.

You wan to collaborate with a lab which has a **different model than you do**.

Are these models producing outputs that **“look the same?”**

Challenges:

- To the human eye, they are functionally similar.
- Can we quantitatively see if they are different?

Embedding spaces of large models

Splitting a model into a feature extraction and decision

We can think of many models as having "feature embedding" stage followed by "downstream tasks."

Fine-tuning works because these embeddings carry a lot of information.

Idea: can we compare the embedding spaces of models to tell the difference between them?

Comparing embedding spaces directly?

Generally this is a non-starter

Given two models with different architectures, we cannot compare the embedding spaces directly.

- Different **dimensions**.
- Different **compression strategies**
- Different **"semantics"**

Unlike with classification, we need to compare the outputs of the generative models.

Using a pre-trained model to distinguish

Use the embedding space to compare outputs of models

New idea: use the embedding space of a **third AI model** as a “microscope” to compare the outputs of two AI models.s

A specific example for GenAI

Compare the outputs using a 3rd model for embedding

Using a large model as an instrument

It takes one to know one

Idea: Use a large model to embed the outputs of the models we want to compare.

- **`Mistral-7B`**: LLM, transformer-based, 32 layers, 13b parameters per token and 32 token vocabulary. Embeddings from the final hidden layer of dimension 4,096.
- **`Multilingual-e5-large`**: extracts sentence embeddings from text in different languages to 1024-dimensional embedding vectors. 60M parameters, context window of 512 tokens and long text is truncated to fit within this window.
- **`Data Filtering Network`**: a CLIP model trained on 5B images that were filtered from an uncurated dataset of image-text pairs. It has 1B parameters and can be used to encode both text and images.

The generic approach in different contexts

The structure is similar, but the models are different

The generic approach in different contexts

The structure is similar, but the models are different

The generic approach in different contexts

The structure is similar, but the models are different

A pre-trained model is a kind of instrument

But used to distinguish between other models

Simple tools (PCA, LDA) applied to the embedding vectors reveal differences between samples generated by other models. Some applications:

1. Embed real data and AI-generated data to see if the embedding vectors cluster.

2. Unsupervised clustering of embedded data recreates the labels in the original.

3. Detect the difference between real and machine-translated data.

A.
PCA
LDA
Stack exchange
PC2
PC1
LD1
LD2
LD3
Real
Mixtral 8x7B
Falcon 40B
Llama-2 70B

C.
Economics abstracts
PC2
PC1
LD2
LD1
Real
Prompt 1
Prompt 2

Claim: PCs reflect interpretable features/known hidden labels.

Took news articles in Spanish and German in two topics, economics and sports.

Used a ML translator to translate German to Spanish.

Translating news articles helps reduce the variation in one dimension (language).

Some takeaways and ongoing work

Model forensics and model evolution

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Preliminary experiments show that the embedding spaces of large “foundation models” can separate data generated from different sources.

- Forensics applications: comparing models, detecting deepfakes, etc.
- “Model DNA”: fine-tuned or “lightly modified” models make minor modifications to the embeddings.
- Use post processing to “align” embeddings for calibration, ensembling, federated learning, etc.

Model comparisons in training

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Variability in the training process

Is training reliable?

Each time we run the training algorithm on the **same training set**, **same architecture**, **same algorithm**, we still use (pseudo-)**independent randomness**.

- Each training run is a **sample** from $\mathscr{F}$.
- Given samples $f_1, f_2, \ldots, f_M$ are they similar to each other or different?

This is related to how **reproducible** a model is.

Comparing two runs of training

Model comparisons are ad hoc and waste energy

- Determining if one model is "better" than another is **not well-posed**.
- In practice, end up running the training process many times. Wasted computation, time, energy, etc.

Terms like the **Rashomon effect**[1][2][3], **predictive multiplicity**[4], or **prediction churn**[5] have been used to describe this phenomena.

[1] Breiman, L. (2001). Statistical modeling: The two cultures (with comments and a rejoinder by the author). *Statistical science*, *16*(3), 199-231
[2] Fisher, A., Rudin, C., & Dominici, F. (2019). All models are wrong, but many are useful: Learning a variable's importance by studying an entire class of prediction models simultaneously. *Journal of Machine Learning Research*, *20*(177), 1-81.
[3] Hsu, H., & Calmon, F. (2022). Rashomon capacity: A metric for predictive multiplicity in classification. *Advances in Neural Information Processing Systems*, *35*, 28988-29000.
[4] Milani Fard, M., Cormier, Q., Canini, K., & Gupta, M. (2016). Launch and iterate: Reducing prediction churn. *Advances in Neural Information Processing Systems*, *29*.
[5] Marx, C., Calmon, F., & Ustun, B. (2020, November). Predictive multiplicity in classification. In *International Conference on Machine Learning* (pp. 6765-6774). PMLR.

Hard decisions vs. soft decisions

Putting on a communications hat

Test error and **churn** measure differences in "hard decisions" $f : \mathcal{X} \to [L]$.

- These are usually made using (softmax) probability estimates $\hat{p}(y \mid x, \theta)$.
- Instead look at **pre-threshold "soft decision"** $m(x \mid \theta)$ for the model.

Comparing two binary classifiers

Soft decisions are different even if decisions are the same

Measure the difference between the **soft decisions/LLRs**.

The LLR $m(x\,|\,\theta)$ of a model is a random variable that depends on x.

Assume the test set is made of i.i.d. draws from the input distribution.

Turn this into a **hypothesis testing problem**!

Two-sample tests for model similarity

Back to simple tools: hypothesis testing

VS.

Are the models the same are different? Answer this by testing:

$$\mathscr{H}_0 : m(x; \theta_0) = m(x; \theta_1)$$

$$\mathscr{H}_1 : m(x; \theta_0) \neq m(x; \theta_1)$$

Hypothesis testing for model comparisons

Use the test's threshold as a measure of difference

Need to use empirical CDFs $\hat{G}_0$ (candidate) and $\widehat{\overline{G}}$ (null).

Optimize to find the *closest model to* $\widehat{\overline{G}}$ *in a ball around* $\hat{G}_0$.

This is a search over "α-trimmings" which can be done efficiently (del Barrio el 2020, Álvarez-Esteban et al. 2011).

Define a new discrepancy measure $\hat{\alpha}$ as the minimum level for the test (= radius of the ball) to accept.

Advantages over other measures

Other measures are pairwise or less information about the models

1. **Test/validation accuracy**: if two models have similar test performance, "one is as good as the other."

2. **Churn**: the two models do not disagree on the test set.

3. **Expected Calibration Error** (ECE) (Naeini et al. 2015): measures the difference between accuracy and expected "confidence" (the LLR).

For our new $\hat{\alpha}$ measure:

- When $\hat{\alpha}$ is large, at least one of the other metrics is also large.

- Models with small $\hat{\alpha}$ are generally low on all the other metrics as well.

Connecting back to our story

“Reliable” training algorithm should produce “typical” models

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Measures like $\hat{\alpha}$ (using ℓ_1 balls, Wasserstein balls, etc.) can let us **measure “atypicality.”**

- Use this to design **new methods for model ensembling**.
- Apply it to **other features of trained models** (e.g. NTK spectra) to find model differences.
- Connect it to **process engineering** and other industrial production ideas.

Some final remarks

Rm Palaniappan, *Intense Talk*
Mixed media on paper pasted on mount board

Back to the original question

What does any of this mean for “AI for Science”?

To use large ML/AI models as part of a scientific workflow, we need “interpretability” and “reliability.”

We also need to understand “reliability” for the training/fine-tuning processes.

It’s more important to **compare models directly** and not just their **performance**.

Where is this all going?

Maybe some strange new worlds

Developing a good set of techniques for model comparisons requires thinking from several different directions:

- **Theory:** can we instead compare surrogate models like “faithful” NTK representations (Engel et al. 2024)?
- **Experiment:** can we do these comparisons cheaply (e.g. using academic-level resources)?
- **Application:** how do we use model comparisons in forensics, process engineering, ensembling, and beyond?

Thank you!