



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

Are modern ML models like scientific instruments?

Anand D. Sarwate (Rutgers University)
28 July 2025

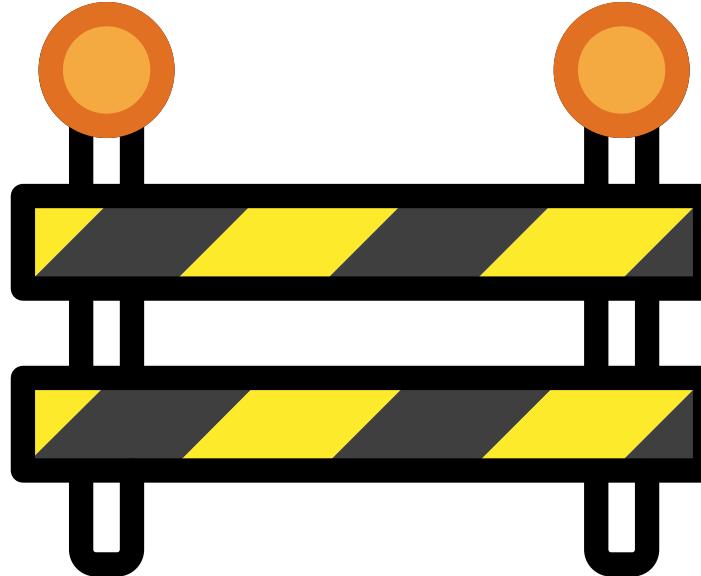
2025 Guangzhou, Hong Kong and Taipei Joint Workshop
on Artificial Intelligence, Communications and Information Theory (AICIT2025)
Sun Yat-sen University (中山大学), Guangzhou, China

Some pre-apologies

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

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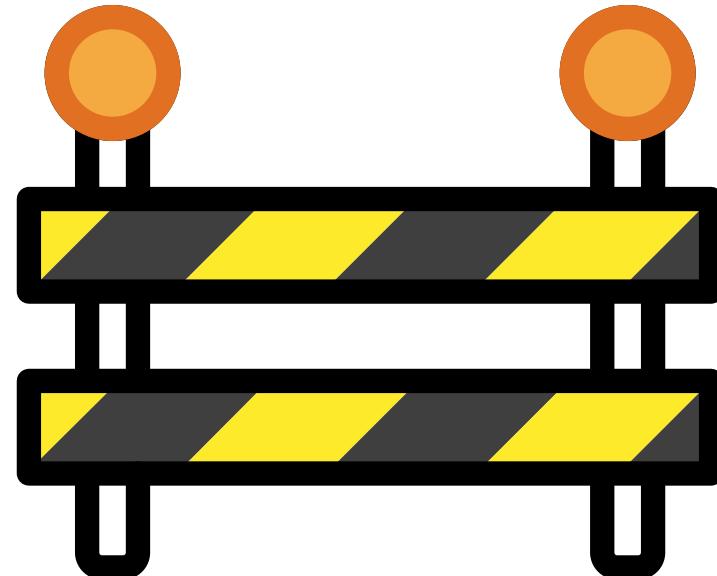
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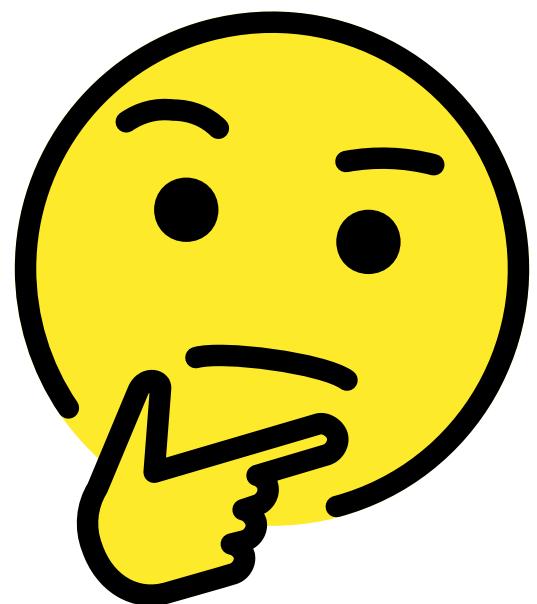
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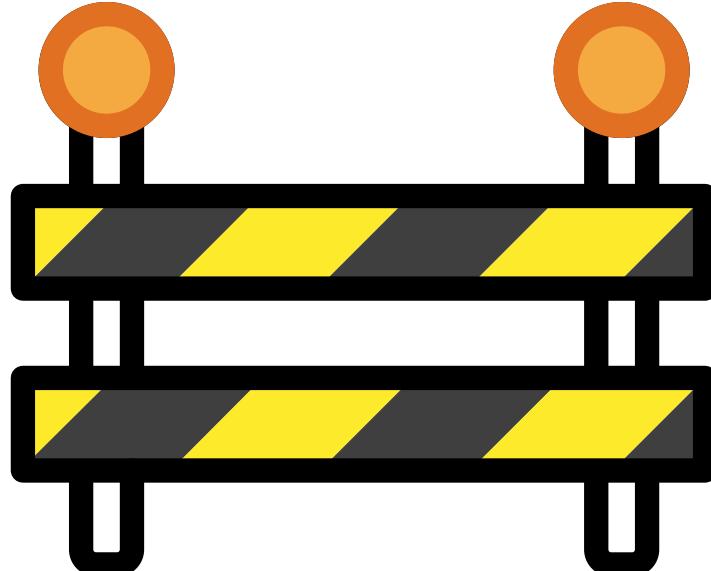
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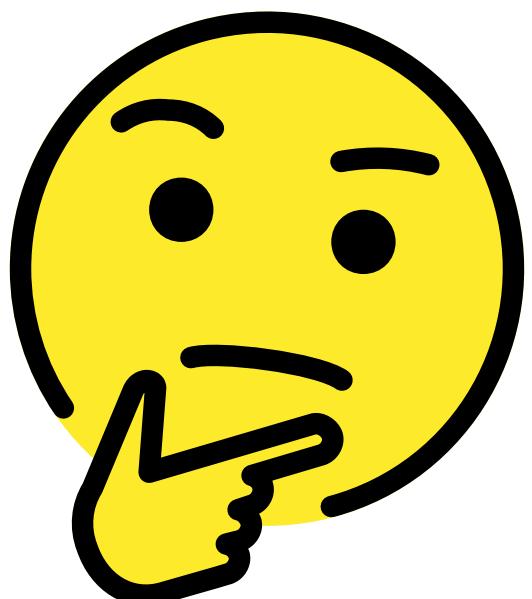
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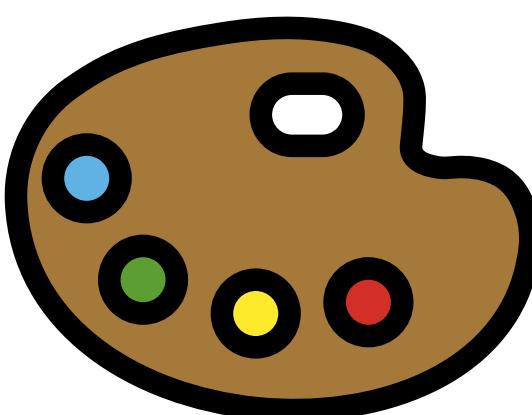
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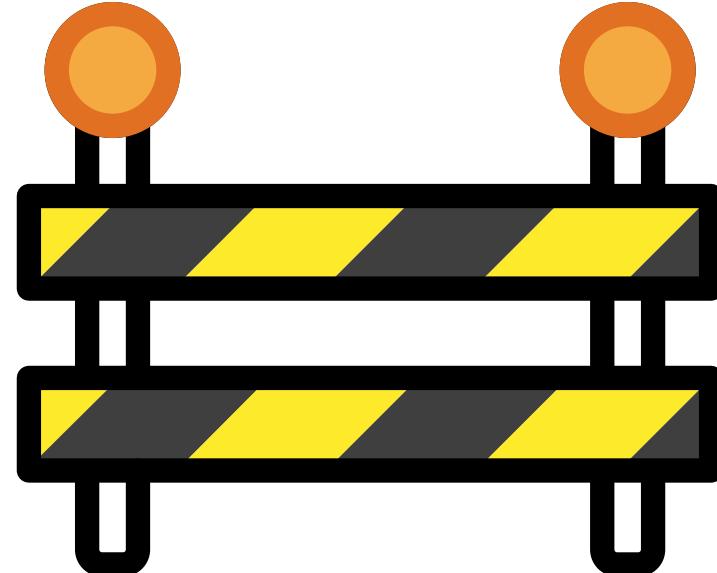
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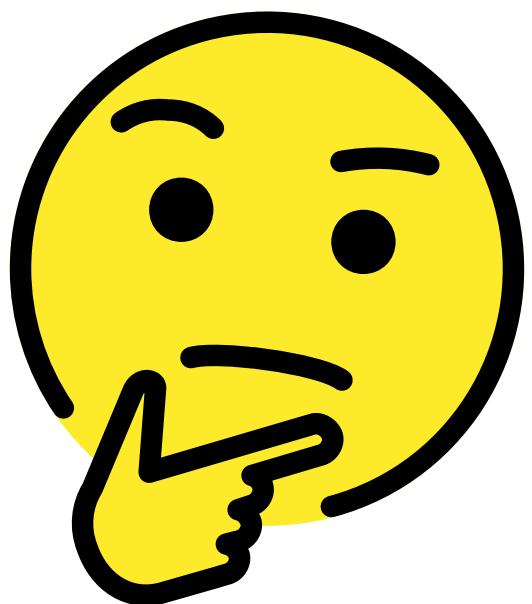
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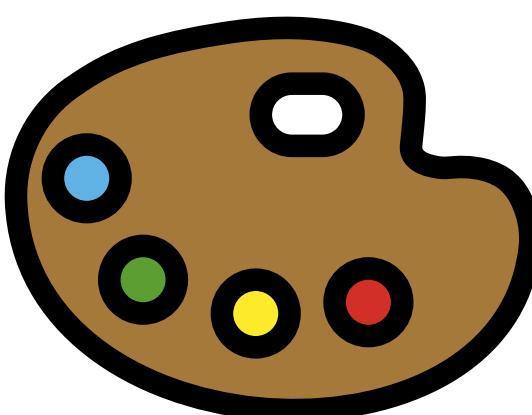
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Real life is a bit messy...

Thanks to my collaborators/coauthors!

Most of this is their work, obviously

Sinjini Banerjee (Rutgers)

Sutenay Choudhury (PNNL)

Xin Li (Rutgers)

Reilly Cannon (PNNL)

Ioana Dumitriu (UC San Diego)

Tim Marrinan (PNNL)

Tony Chiang (ARPA-H)

Andrew Engel (Ohio State)

Max Vargas (PNNL)

Sutenay Choudhury (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=gpqBGyKeKH>

[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?

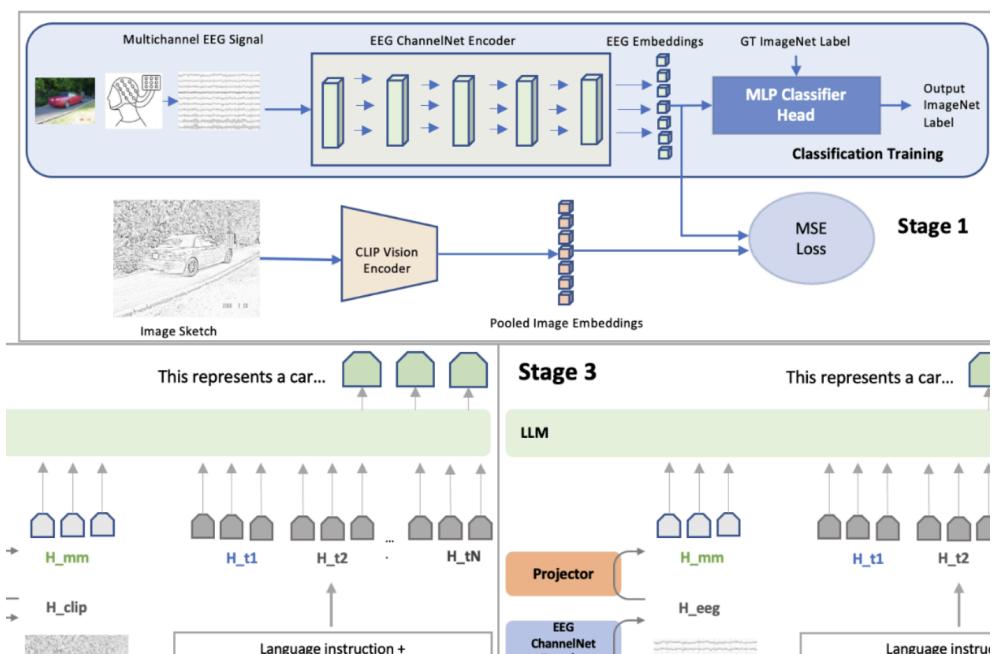
Source: Wikipedia



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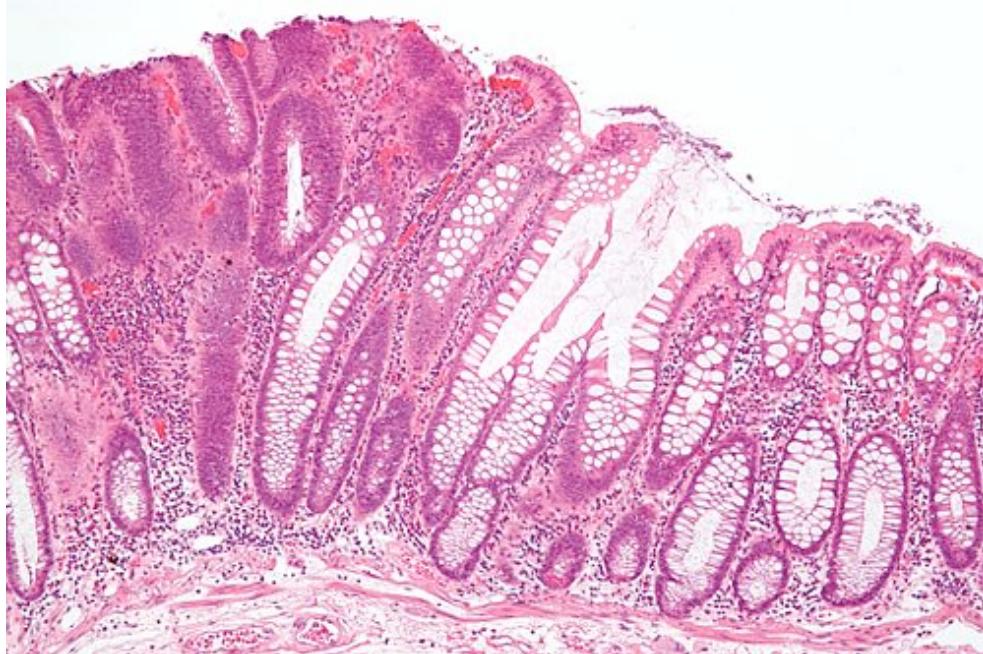
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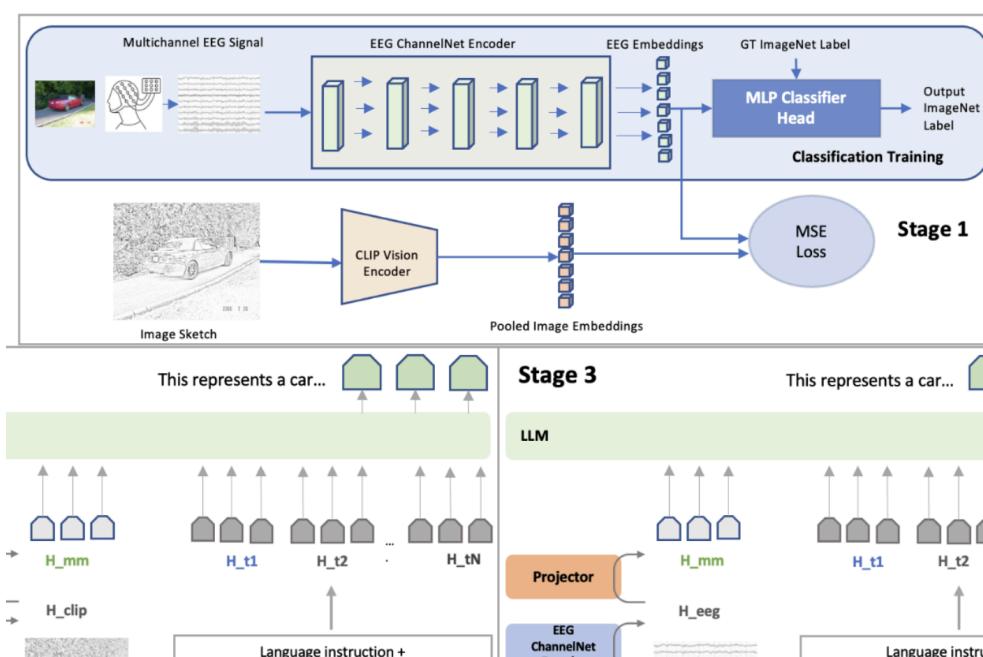
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We often hear a lot about “**AI for Science**” but that can mean a lot of different things! Some examples:

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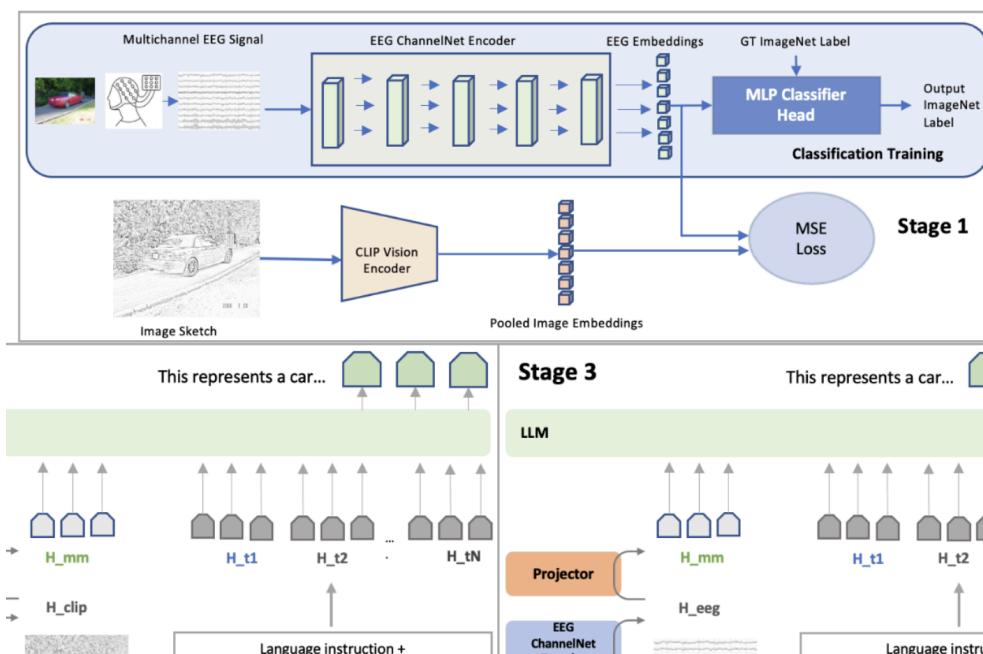
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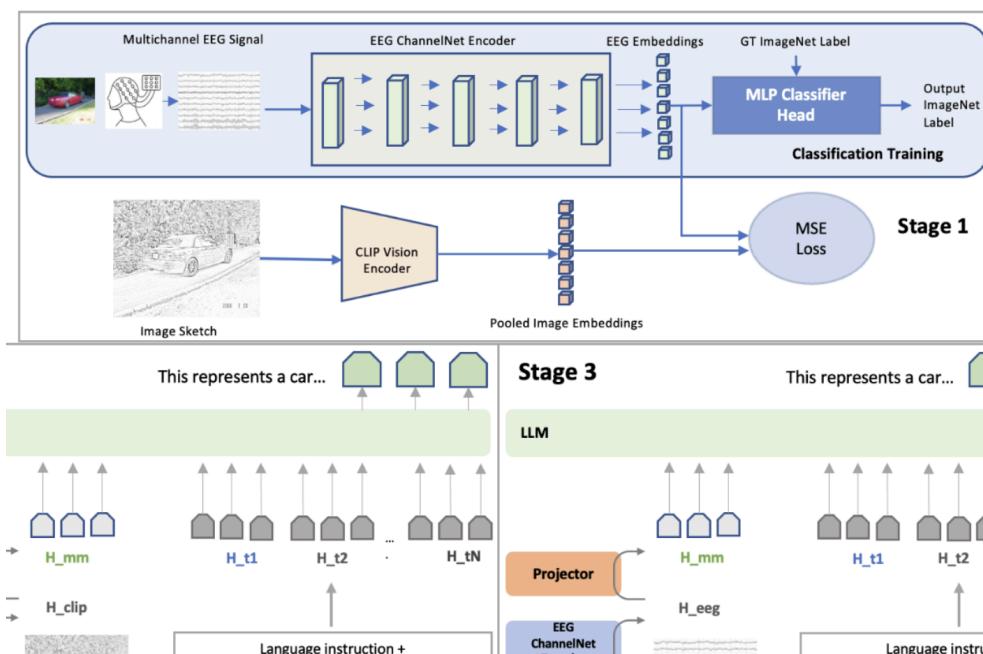
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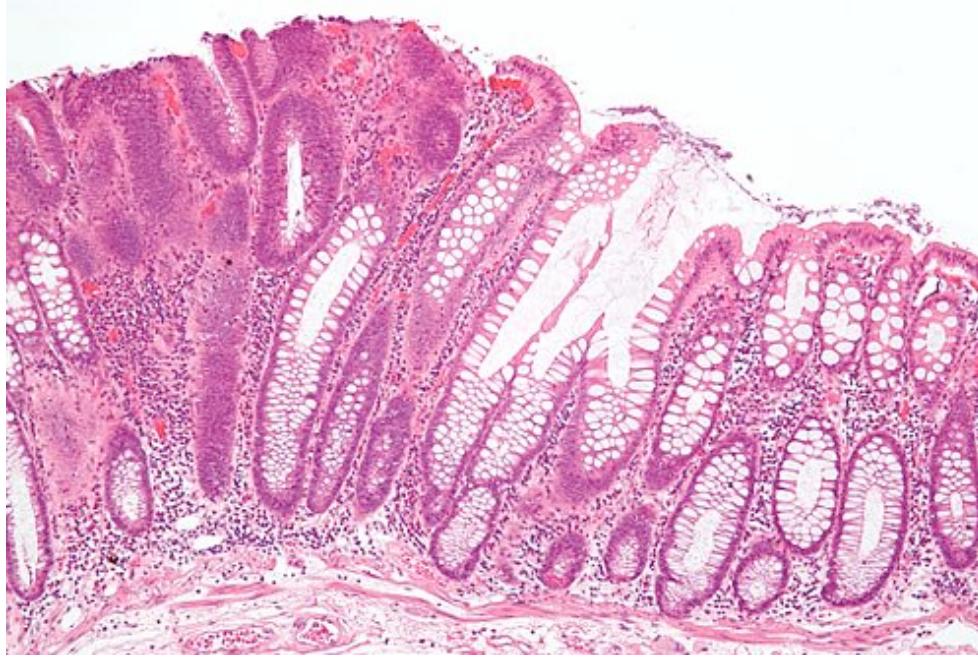
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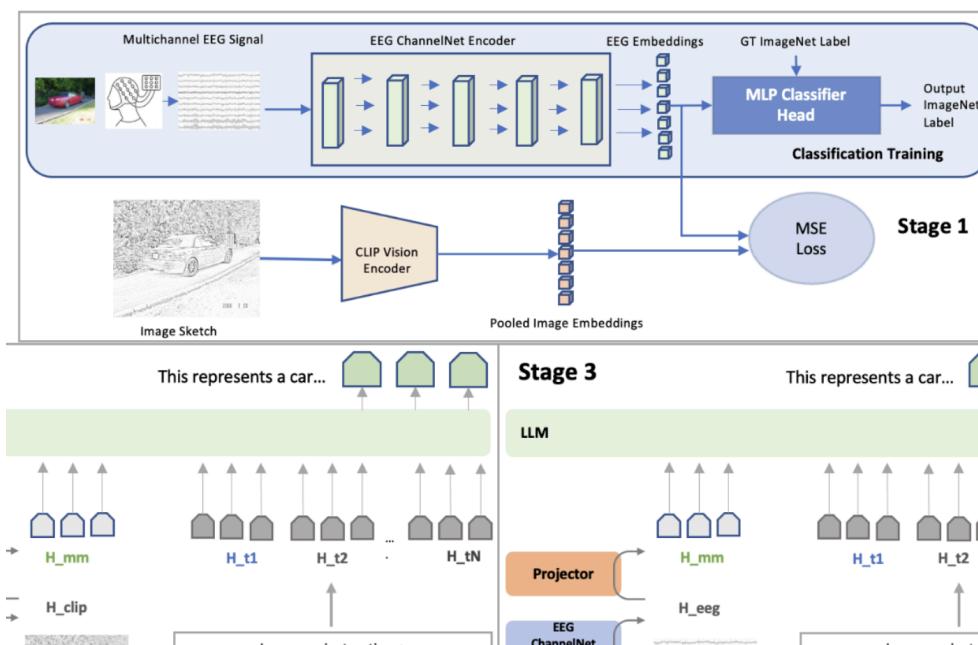
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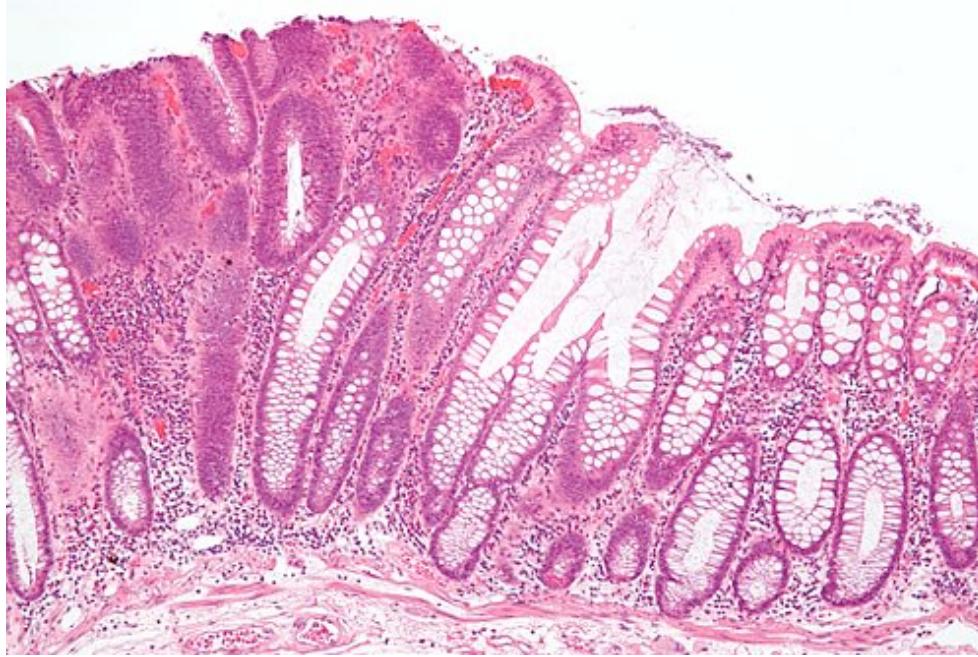
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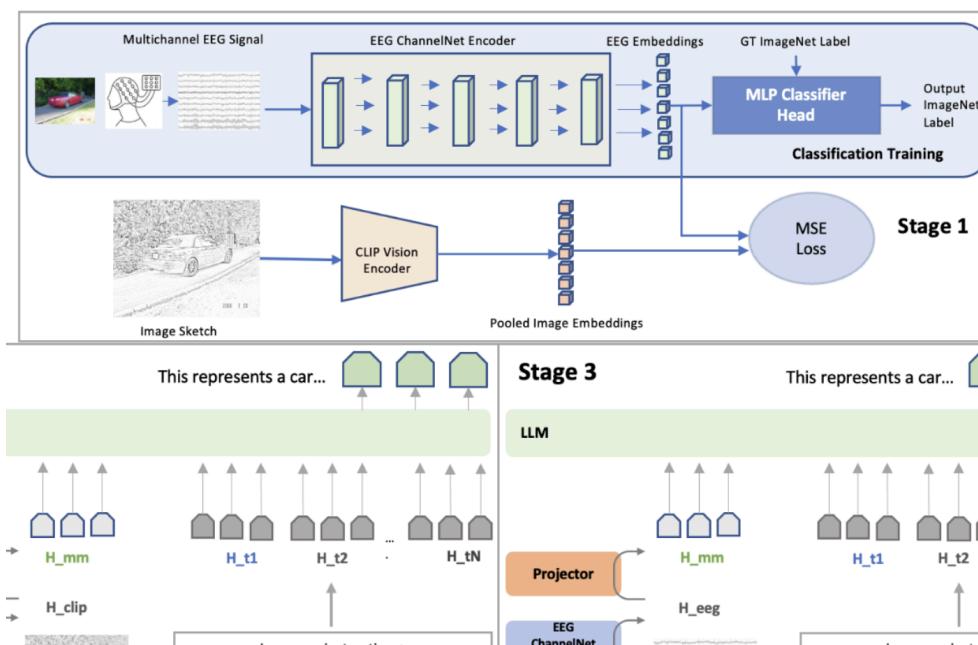
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- Many more...

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

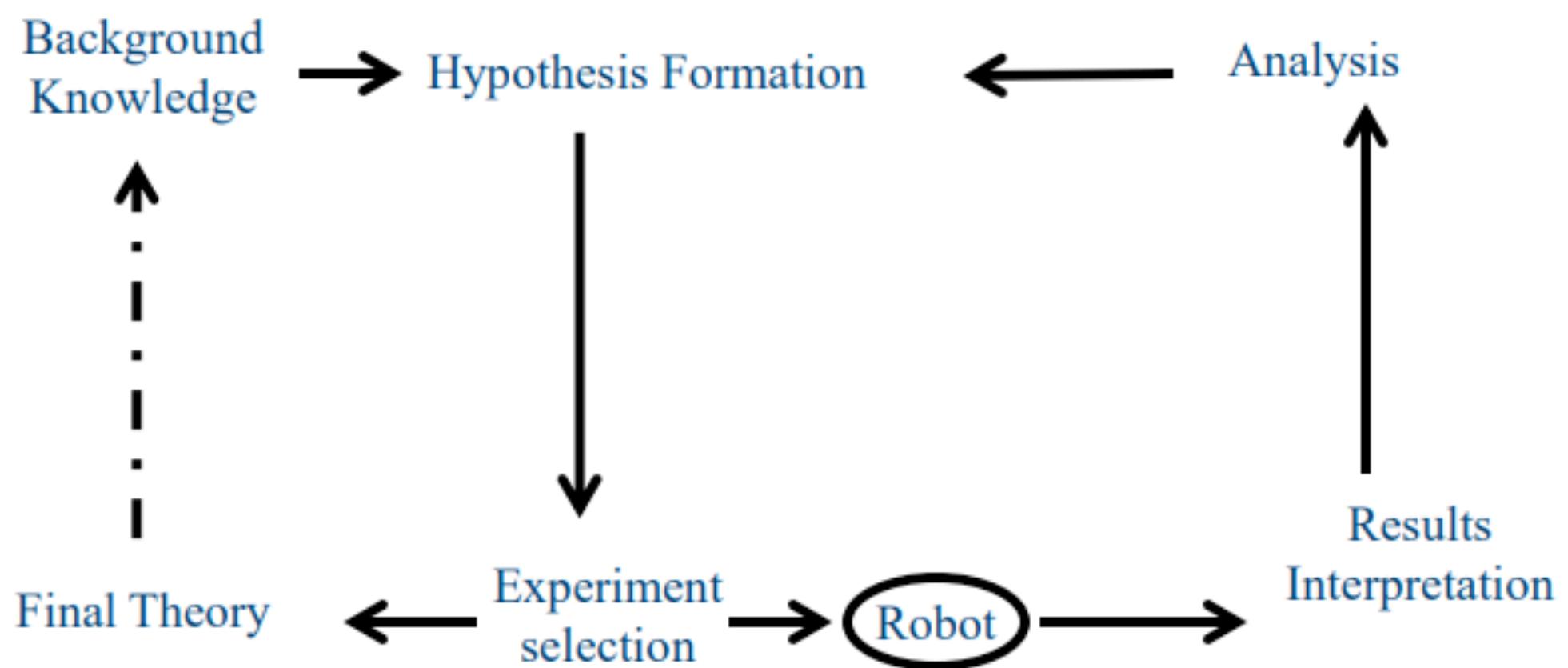
Some gap between hype and reality

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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.



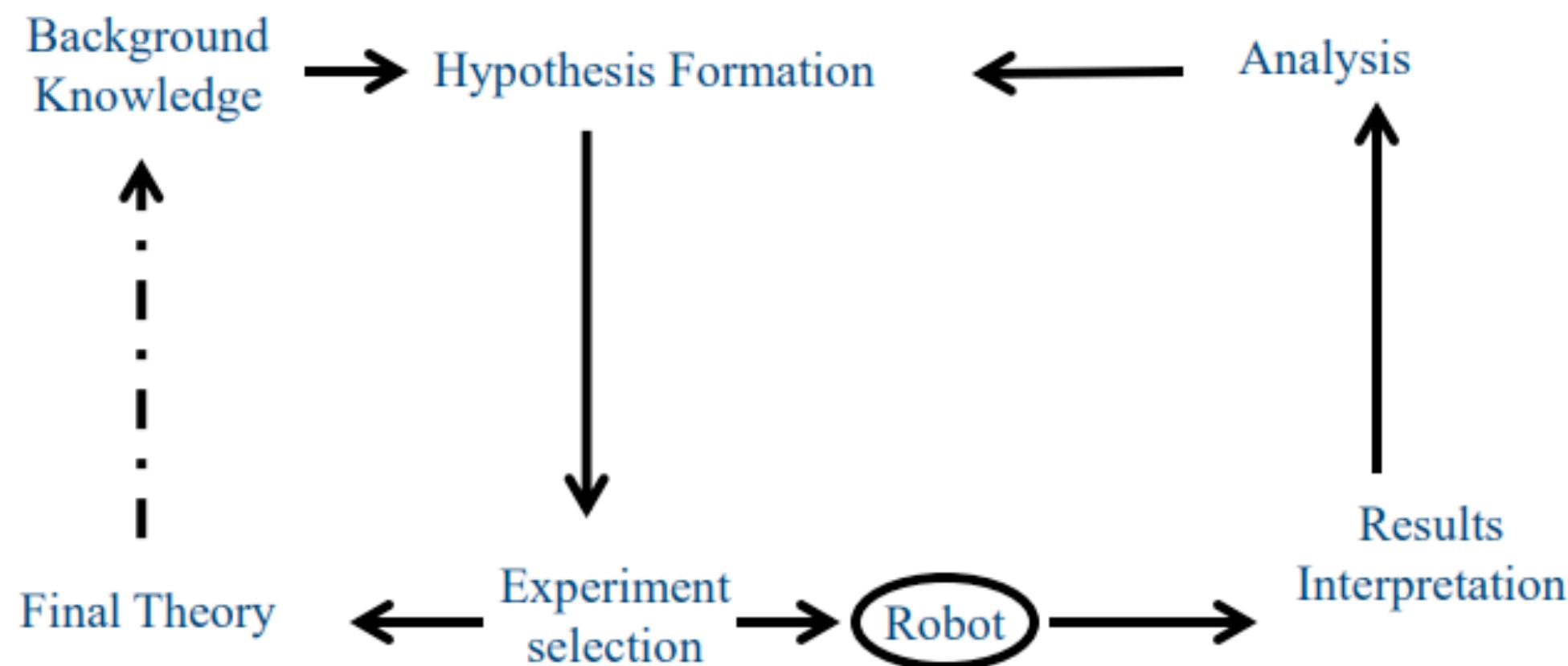
<https://futuretech.mit.edu/news/ai-and-the-future-of-scientific-discovery>

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

NY Times
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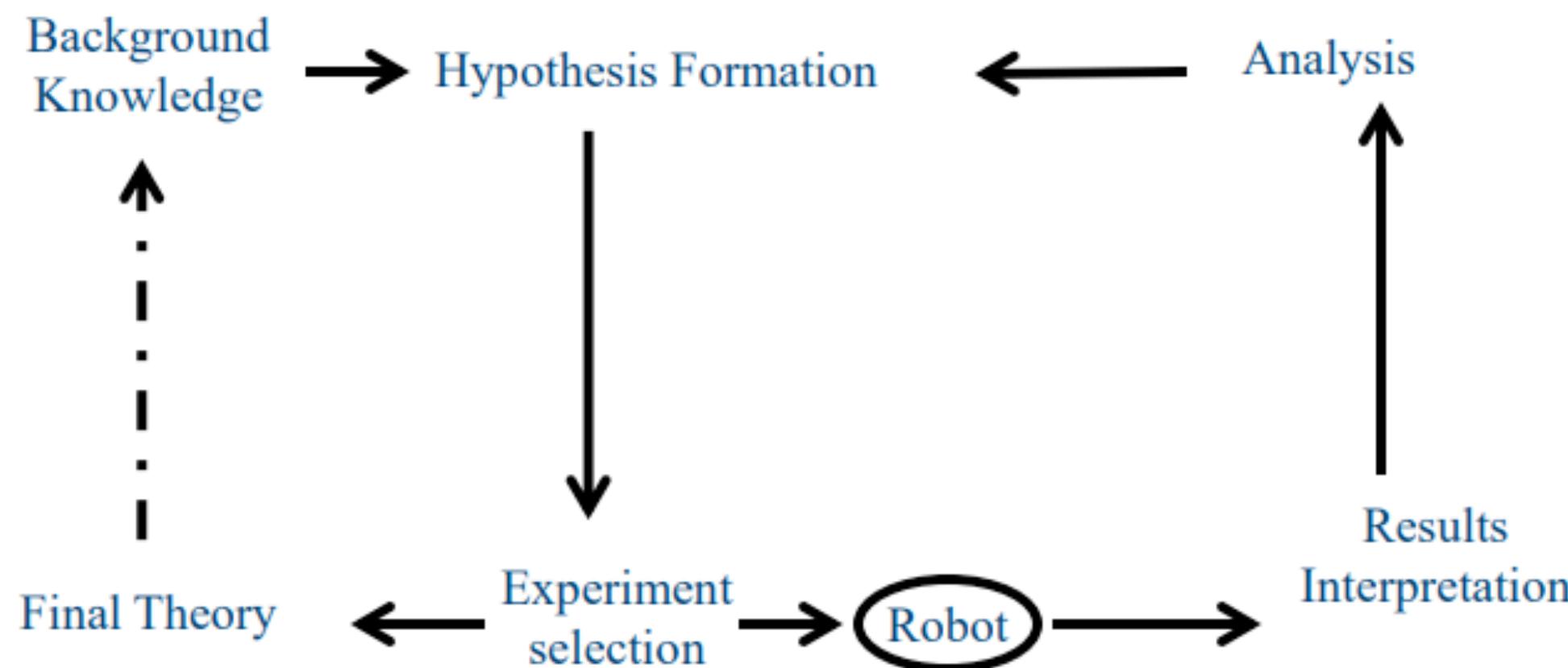
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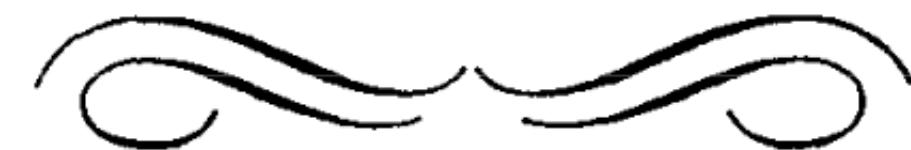
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IRE TRANSACTIONS—INFORMATION THEORY



The Bandwagon

CLAUDE E. SHANNON

Shannon, 1956

What about information/signal processing?

Some perspective from more solid ground

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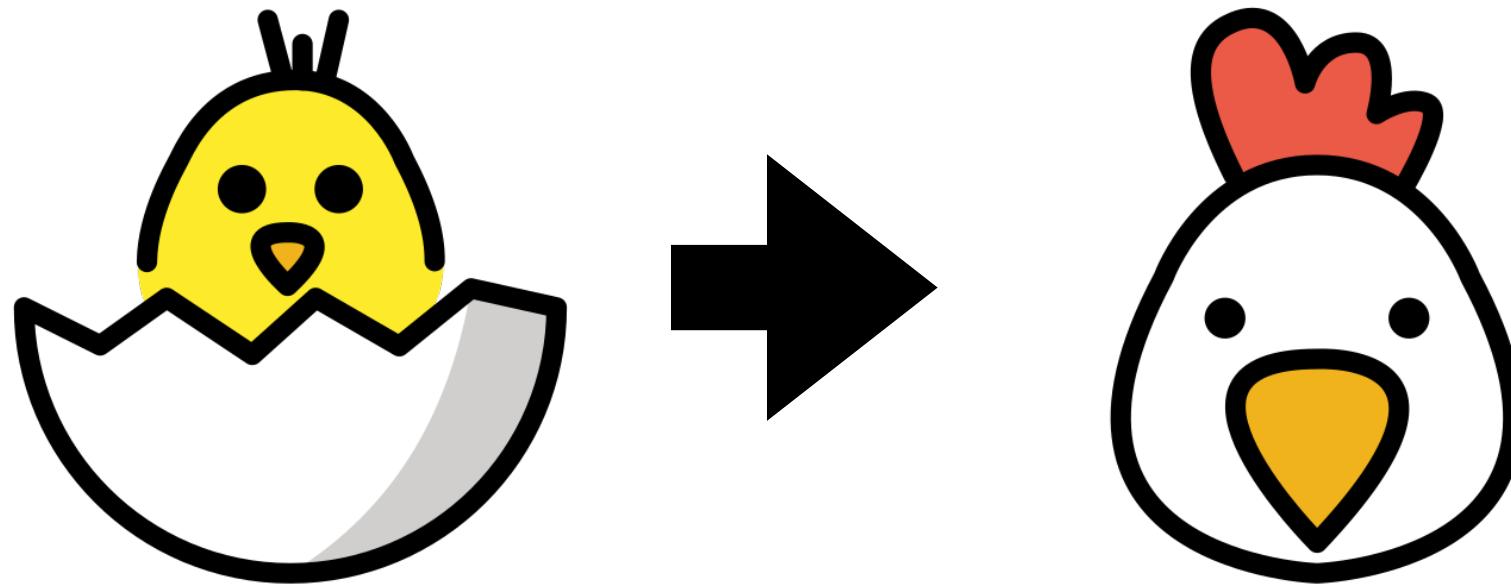
Some perspective from more solid ground

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](#))

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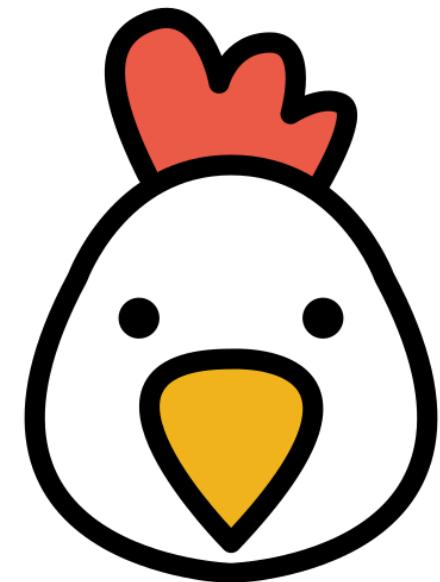
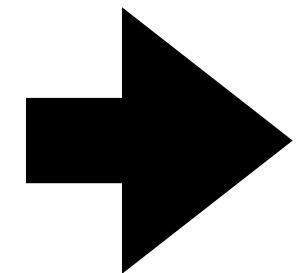
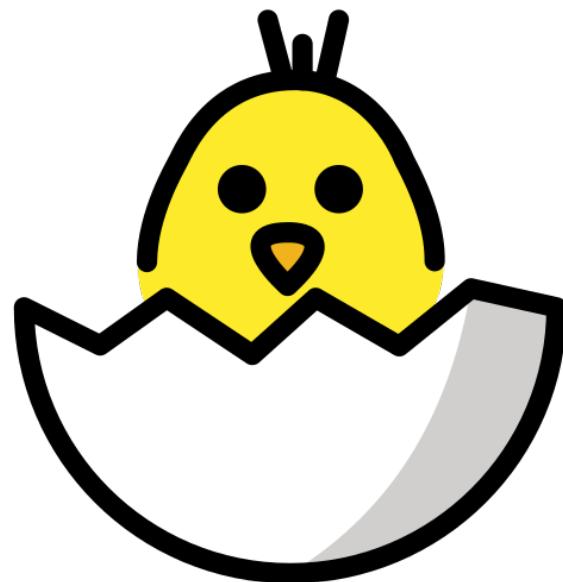
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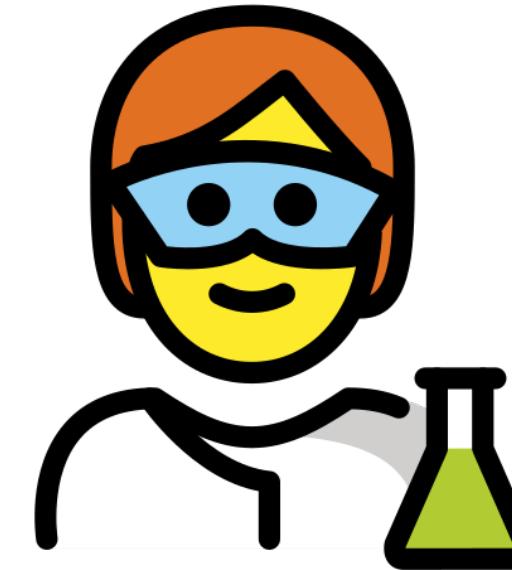
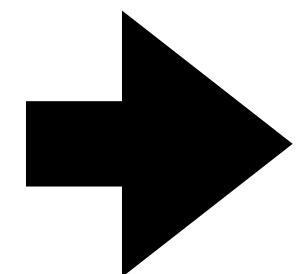
ML/AI frameworks are evolving very quickly.

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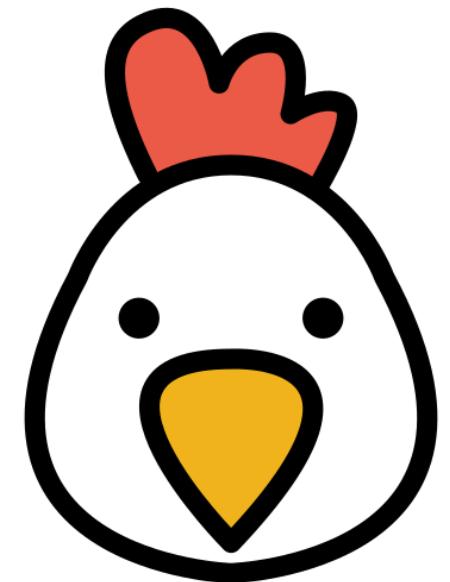
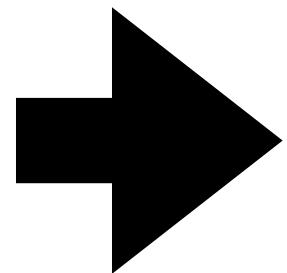
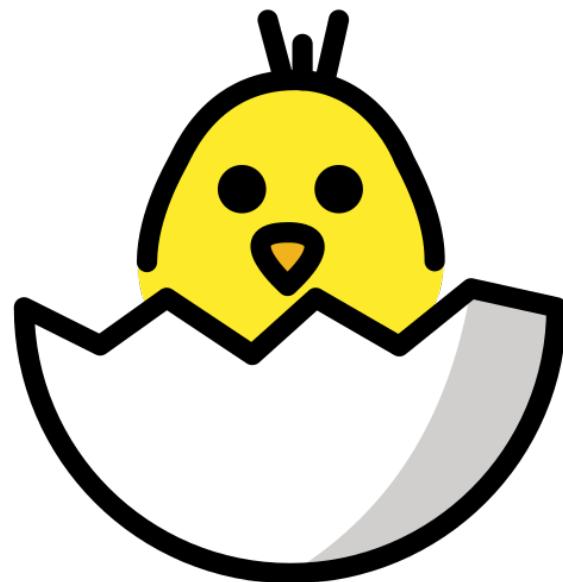


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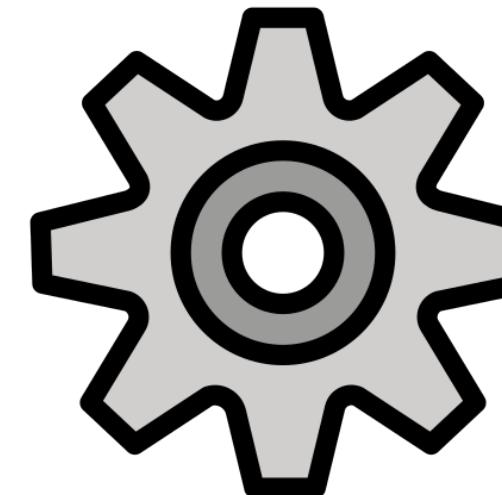
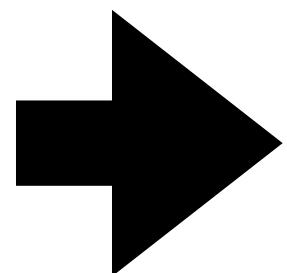
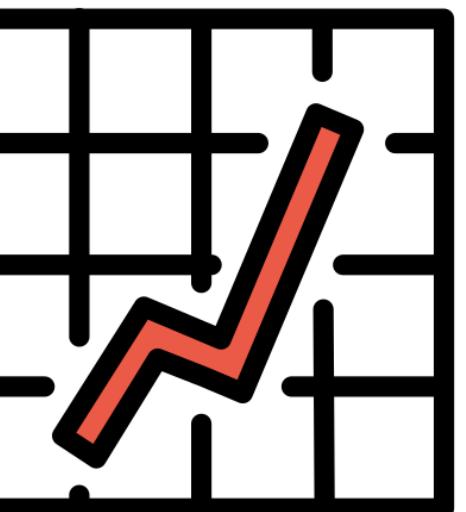
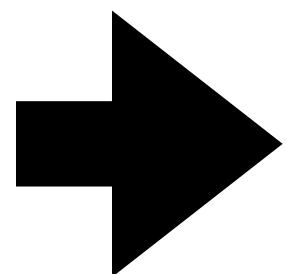
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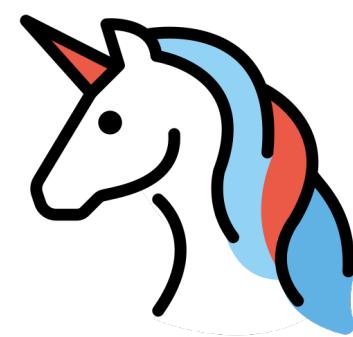
→ IT, SP, control, etc. are still relevant!

A traditional division of labor

The EE/CS divide in some sense

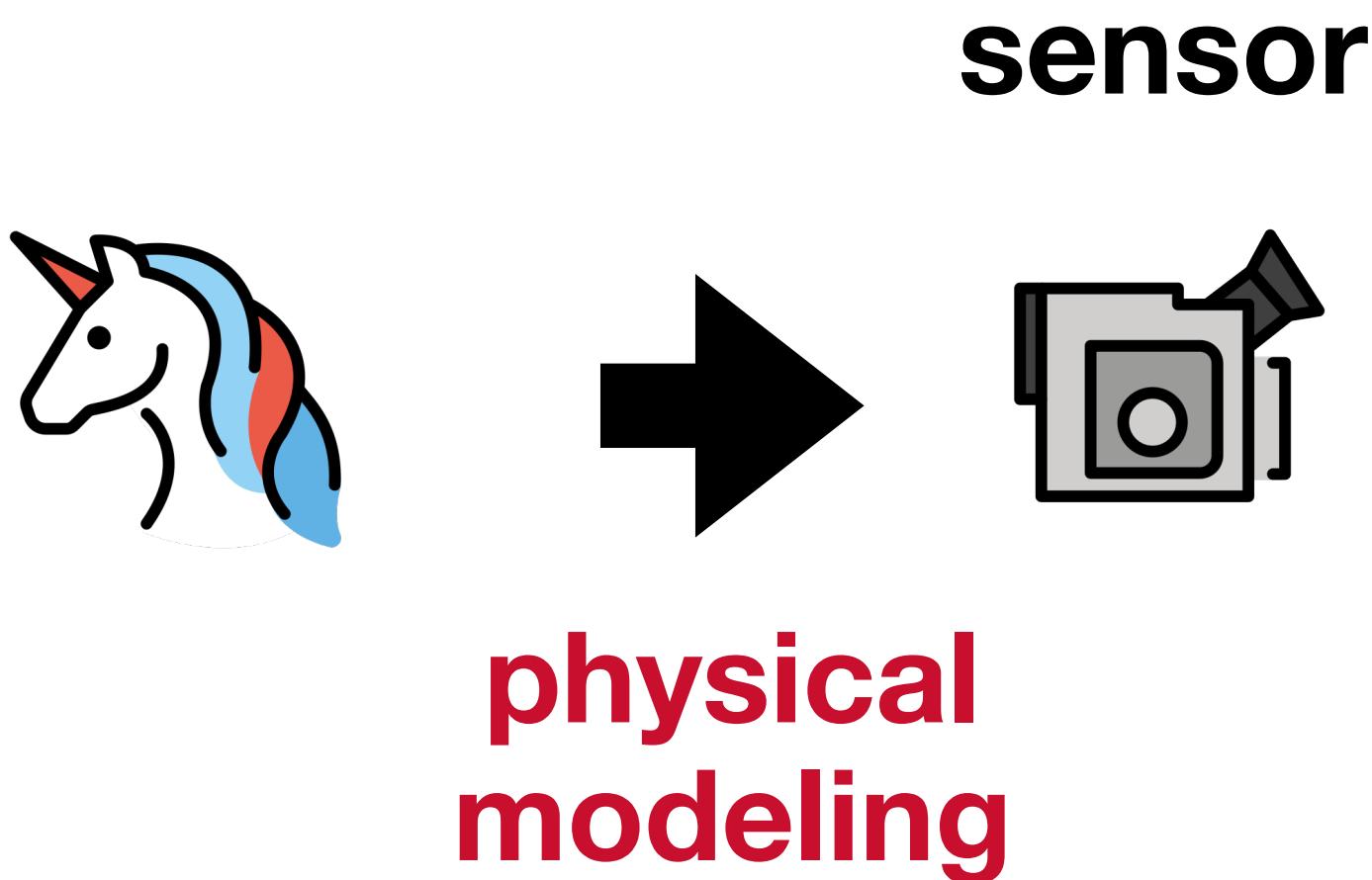
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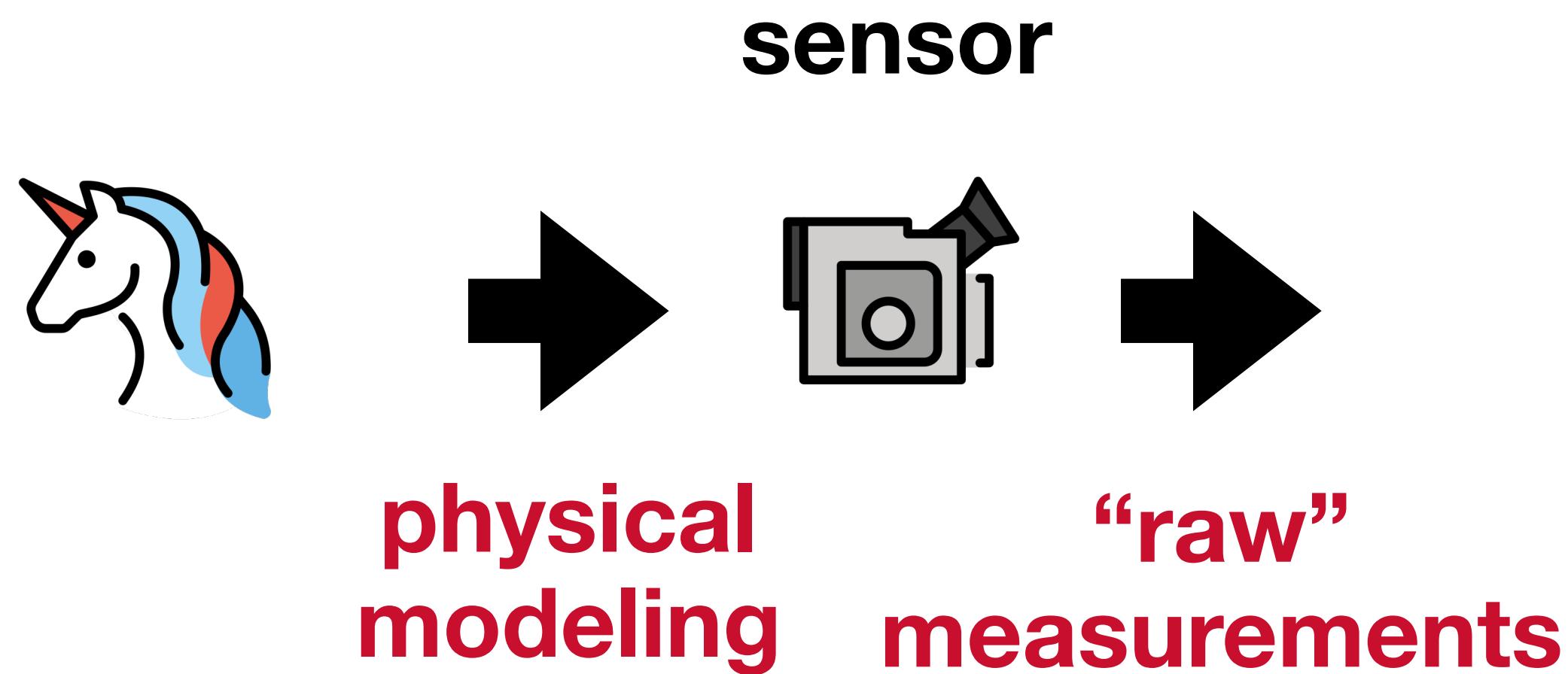
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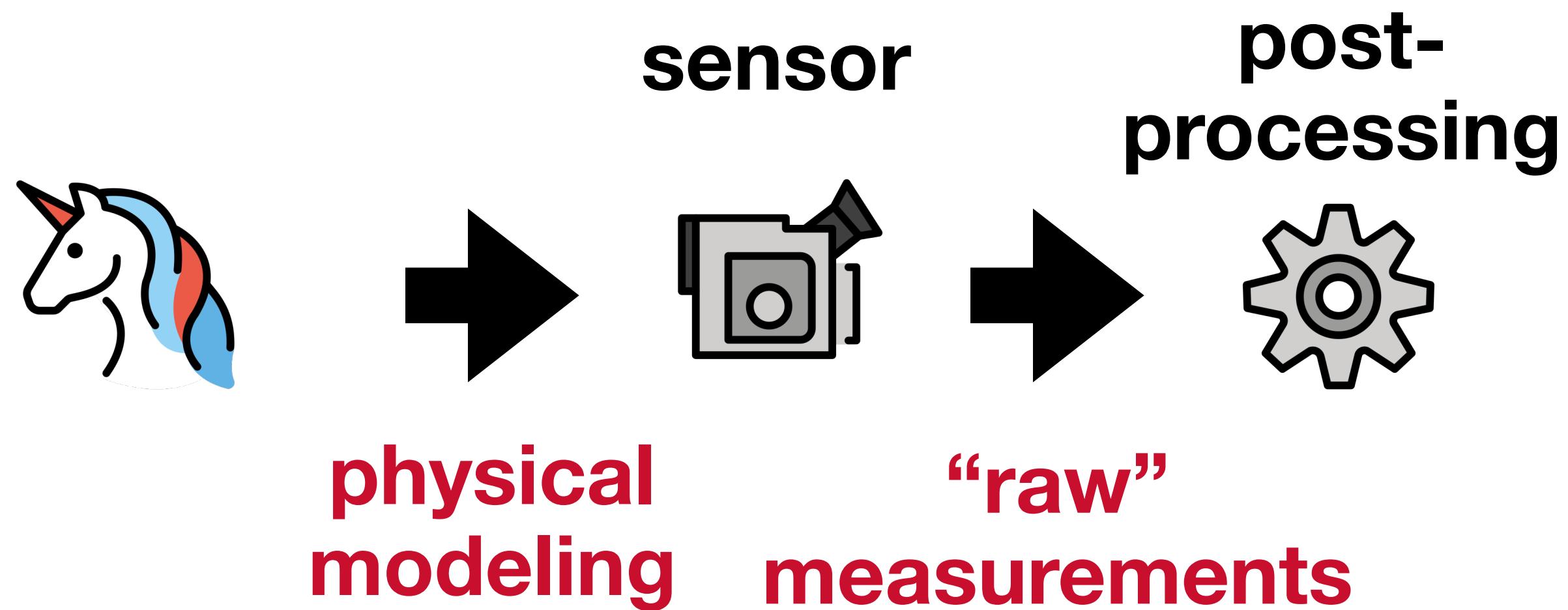
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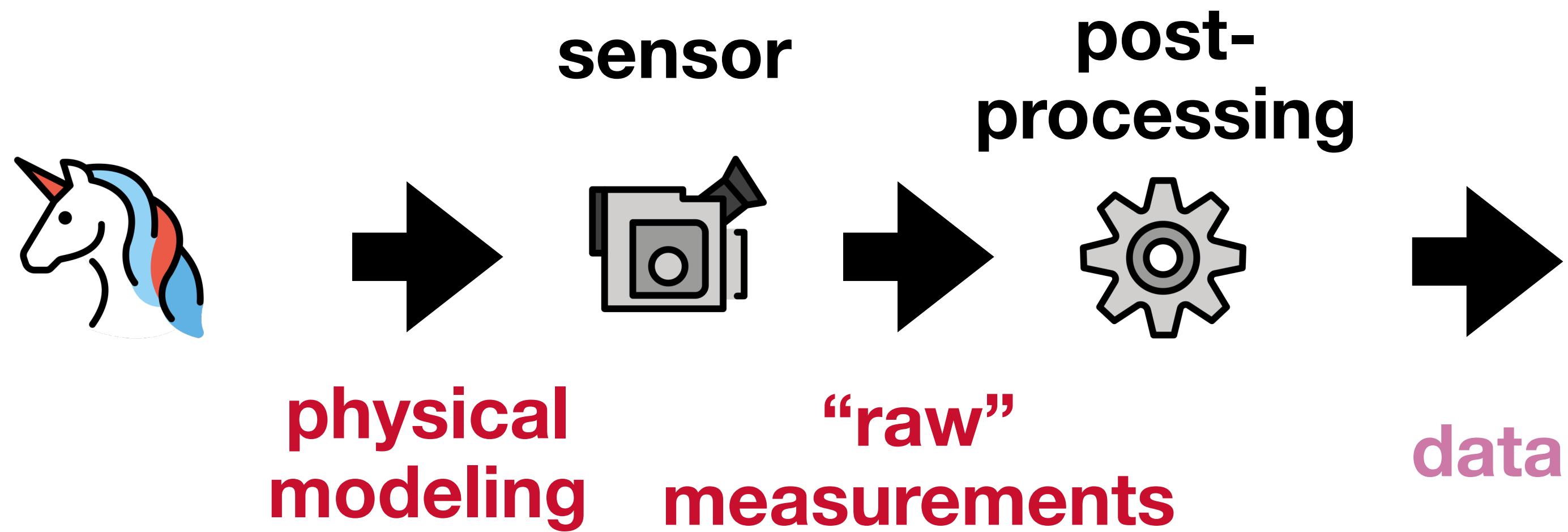
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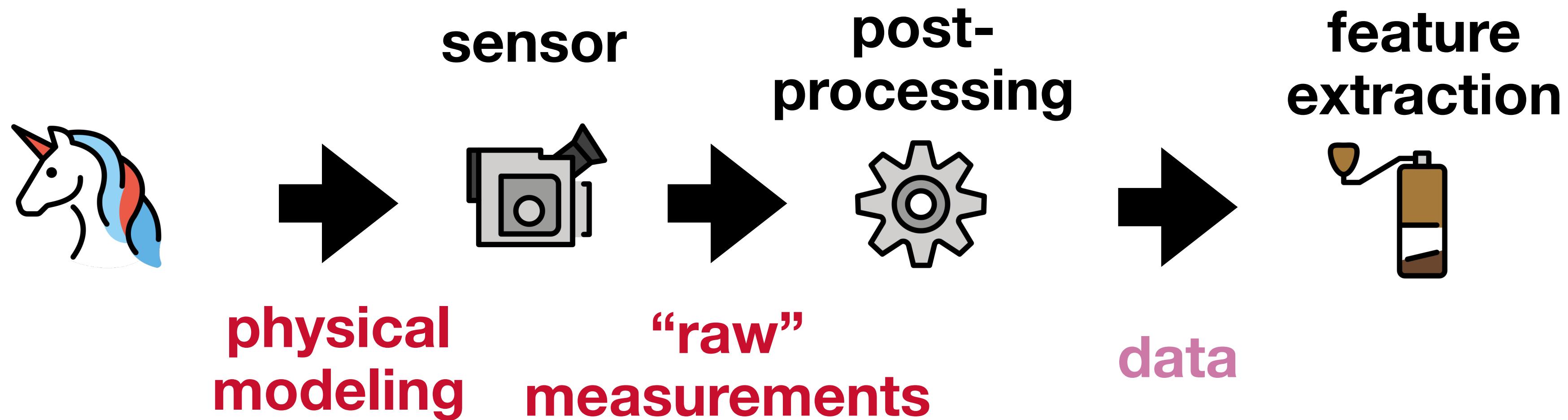
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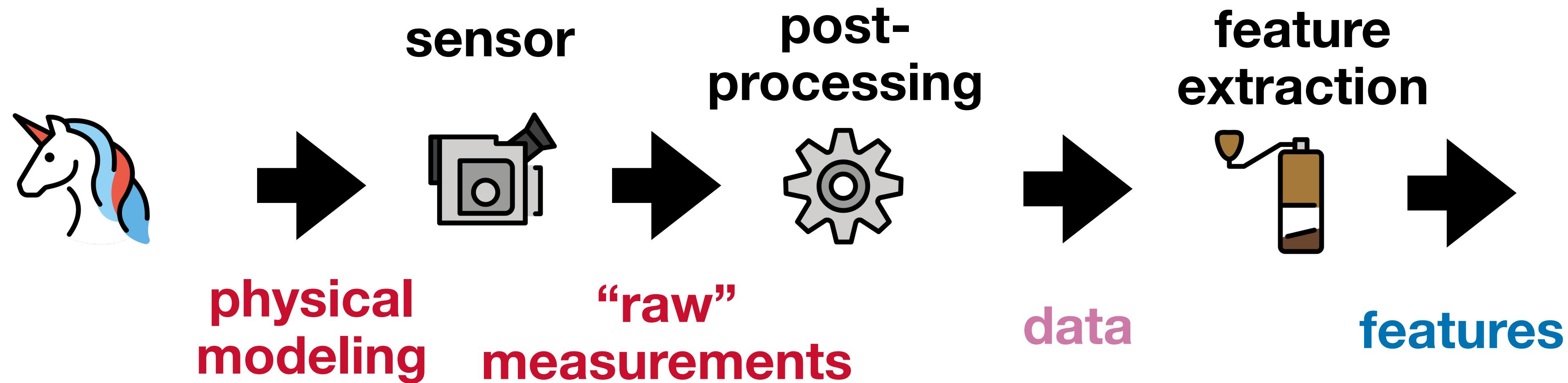
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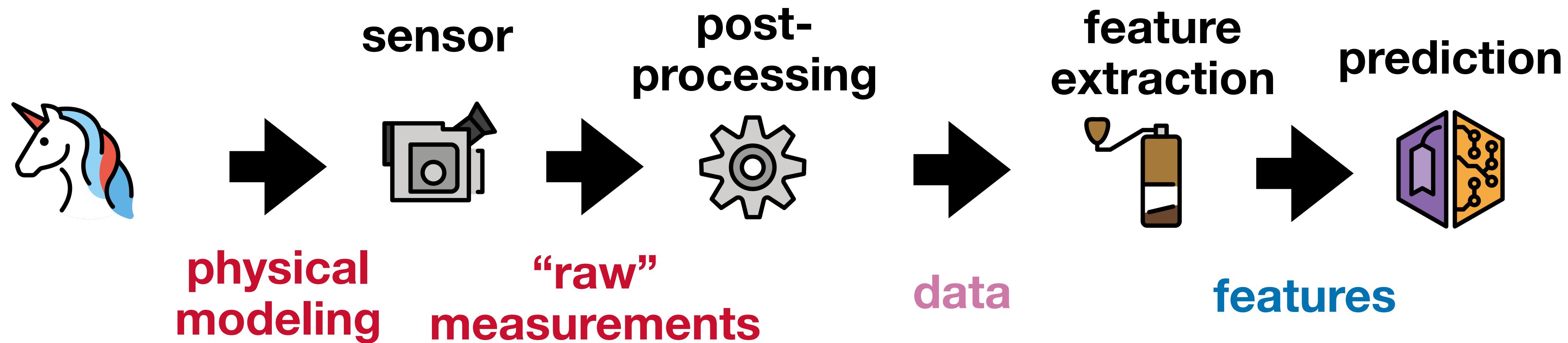
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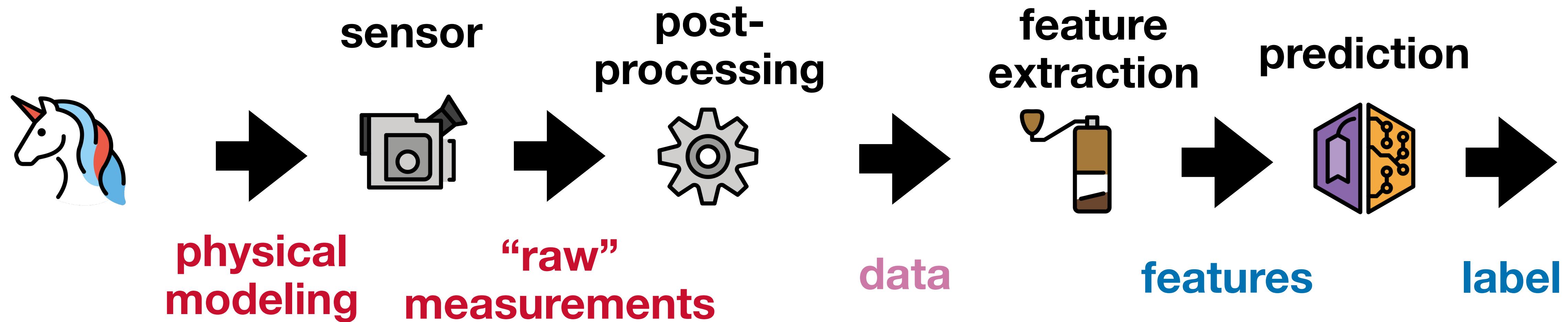
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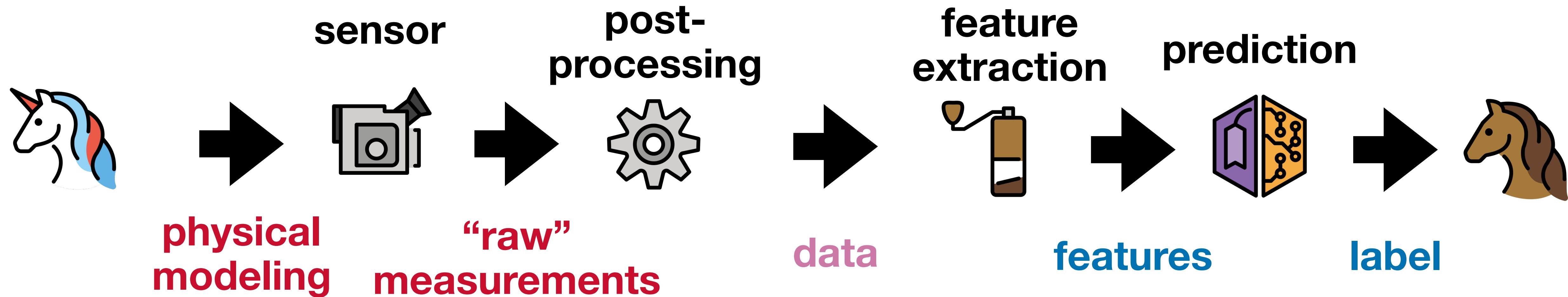
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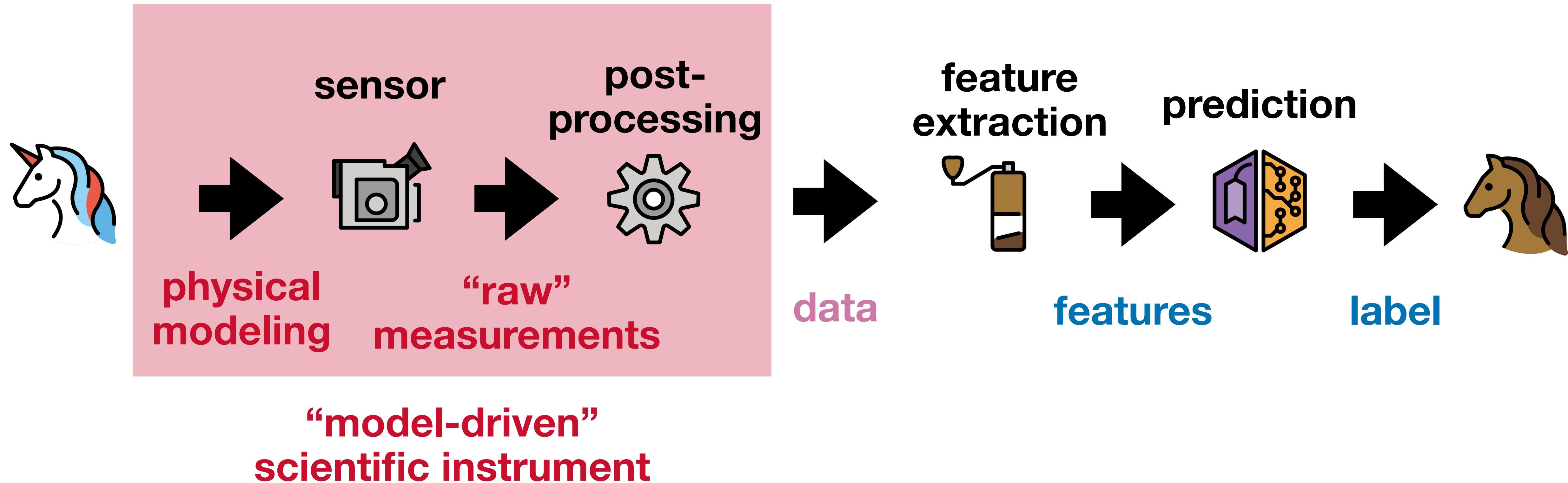
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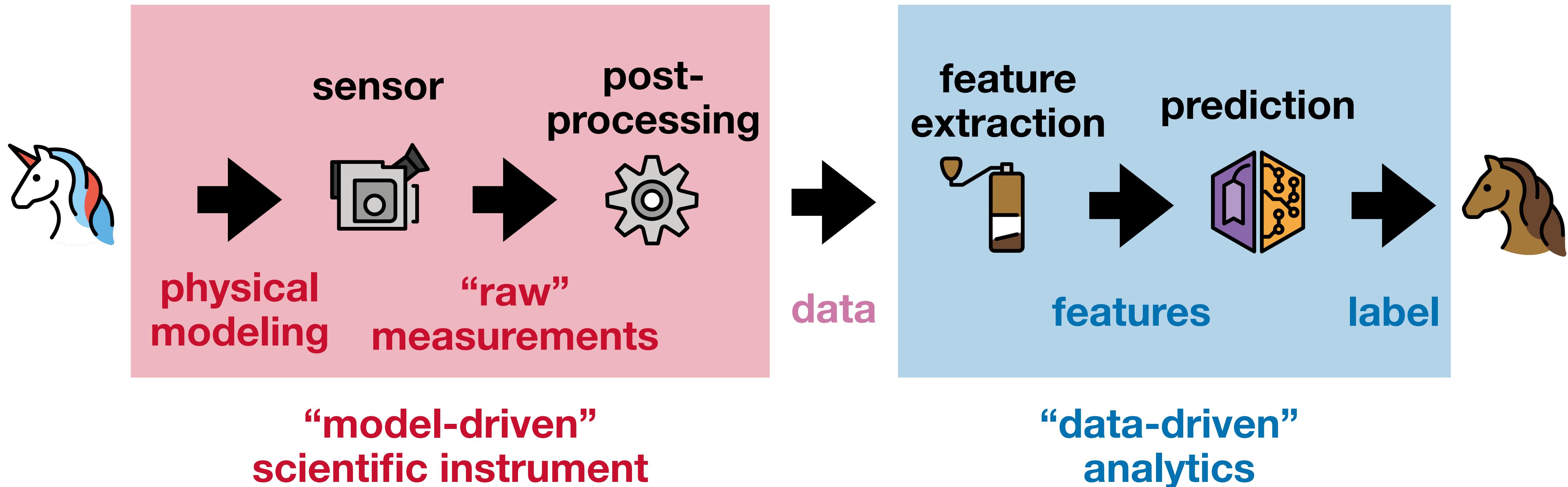
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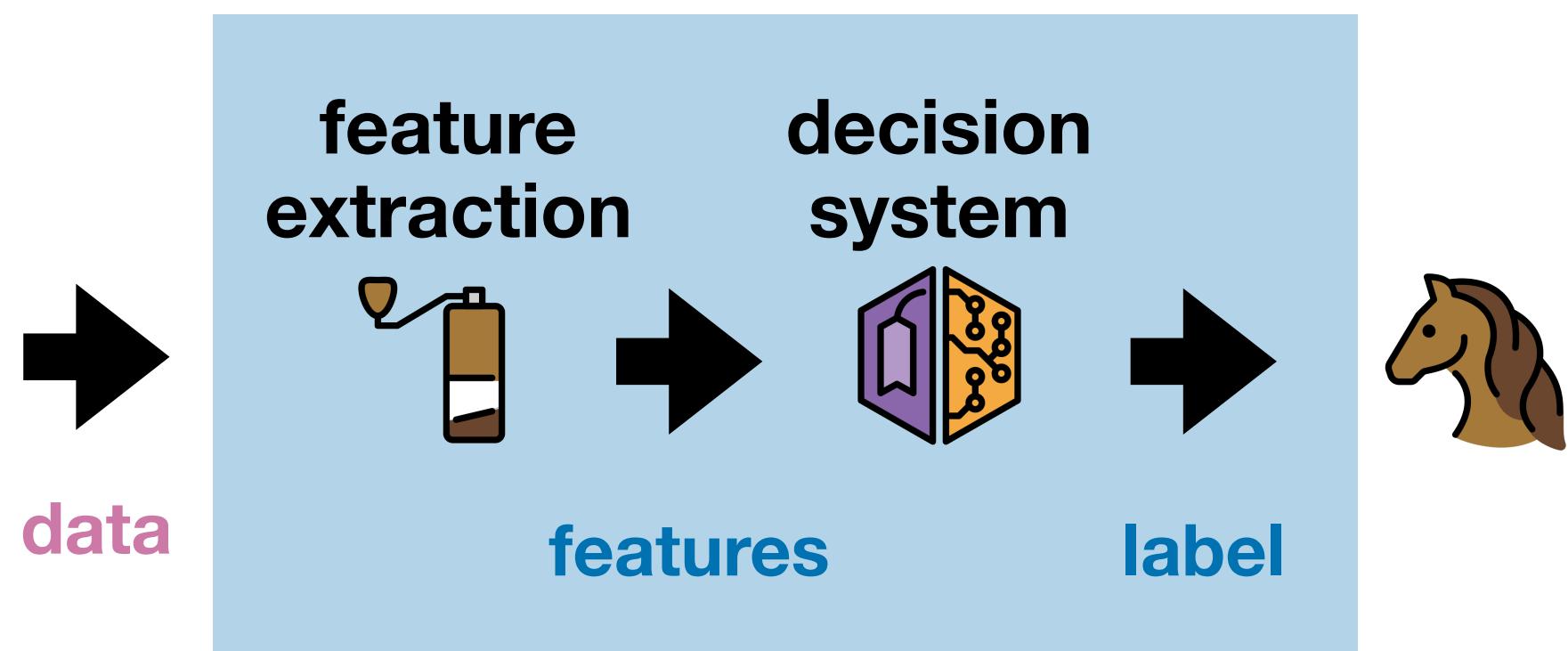
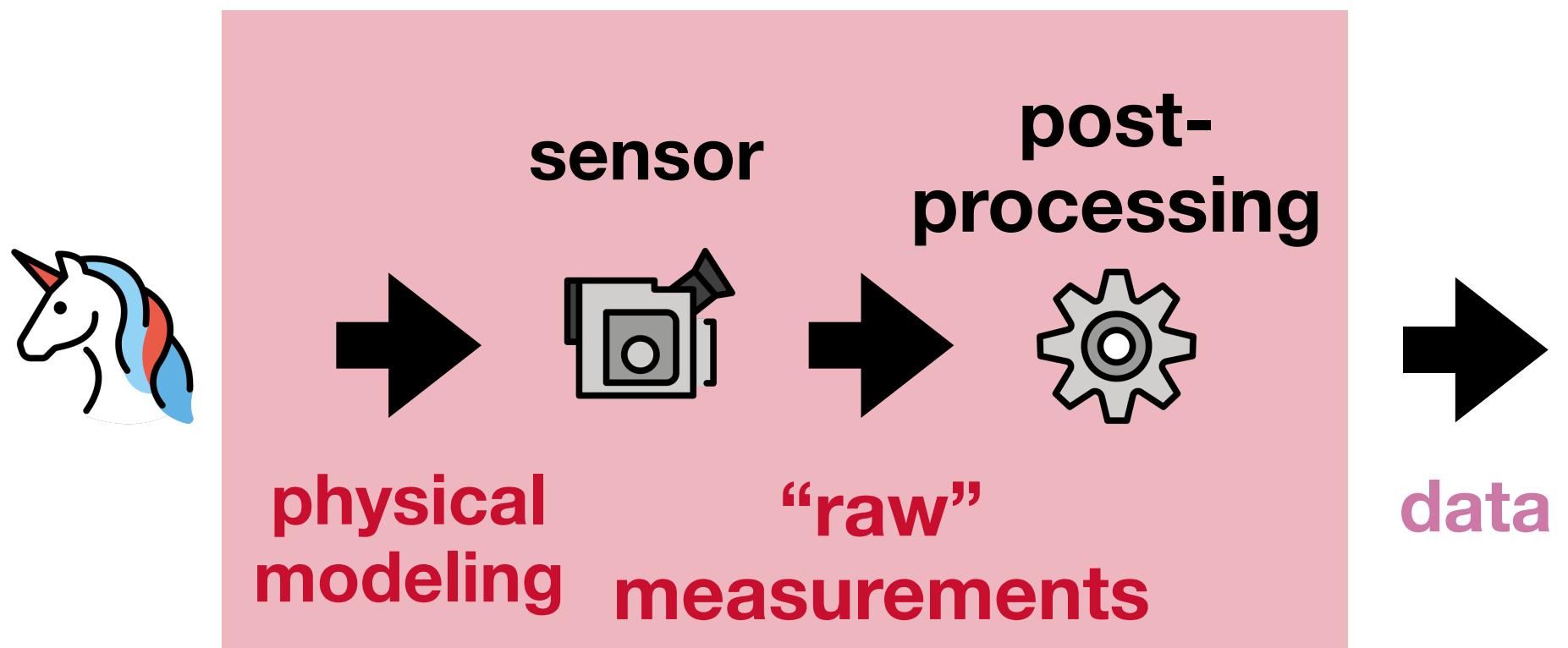
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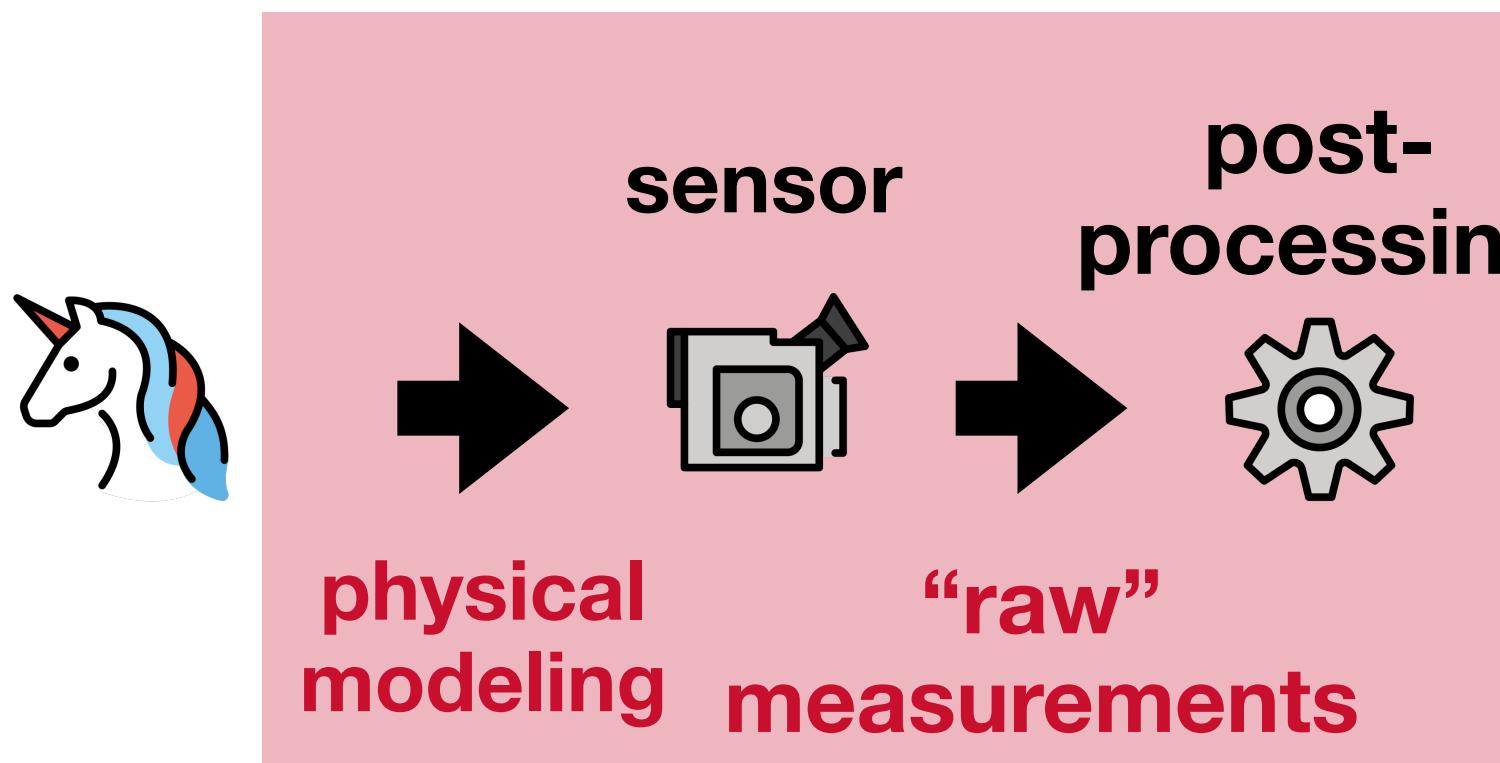
What is “AI as instrumentation”?

Putting neural networks into measurement devices

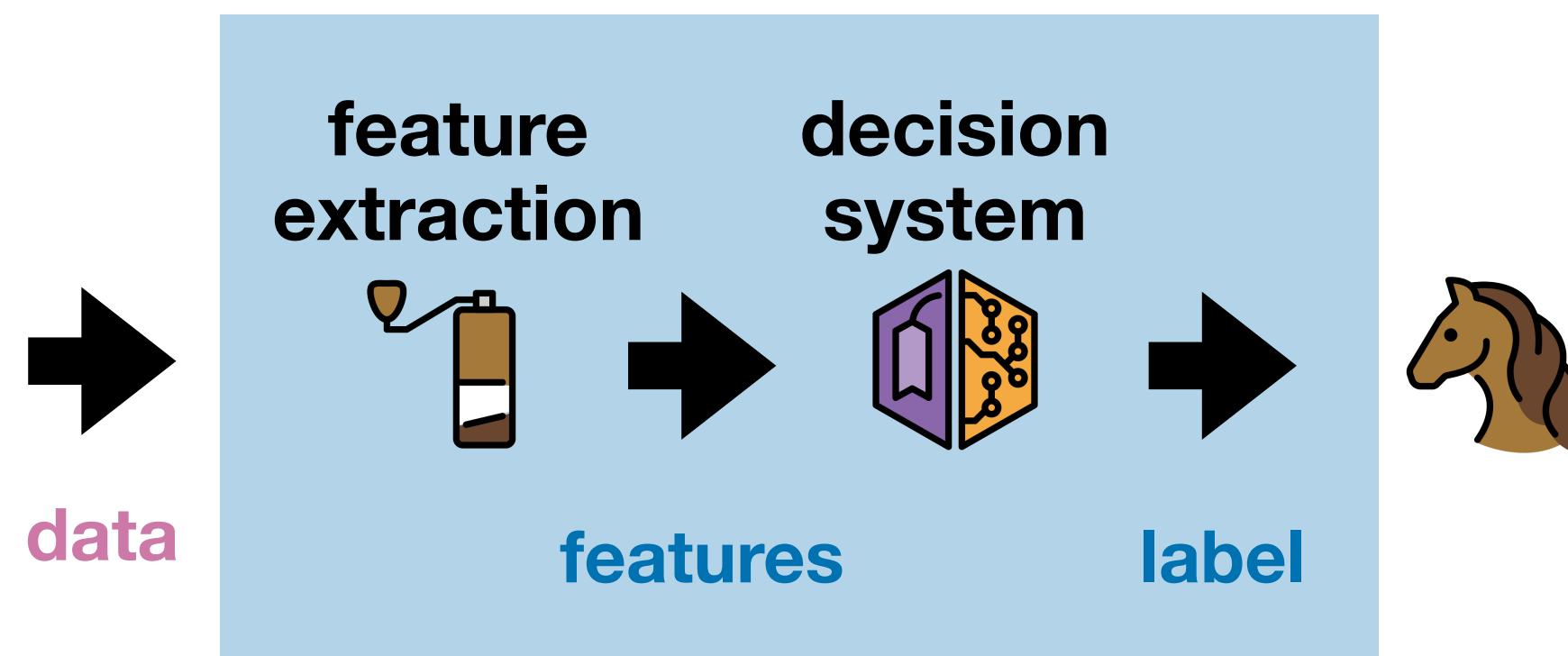


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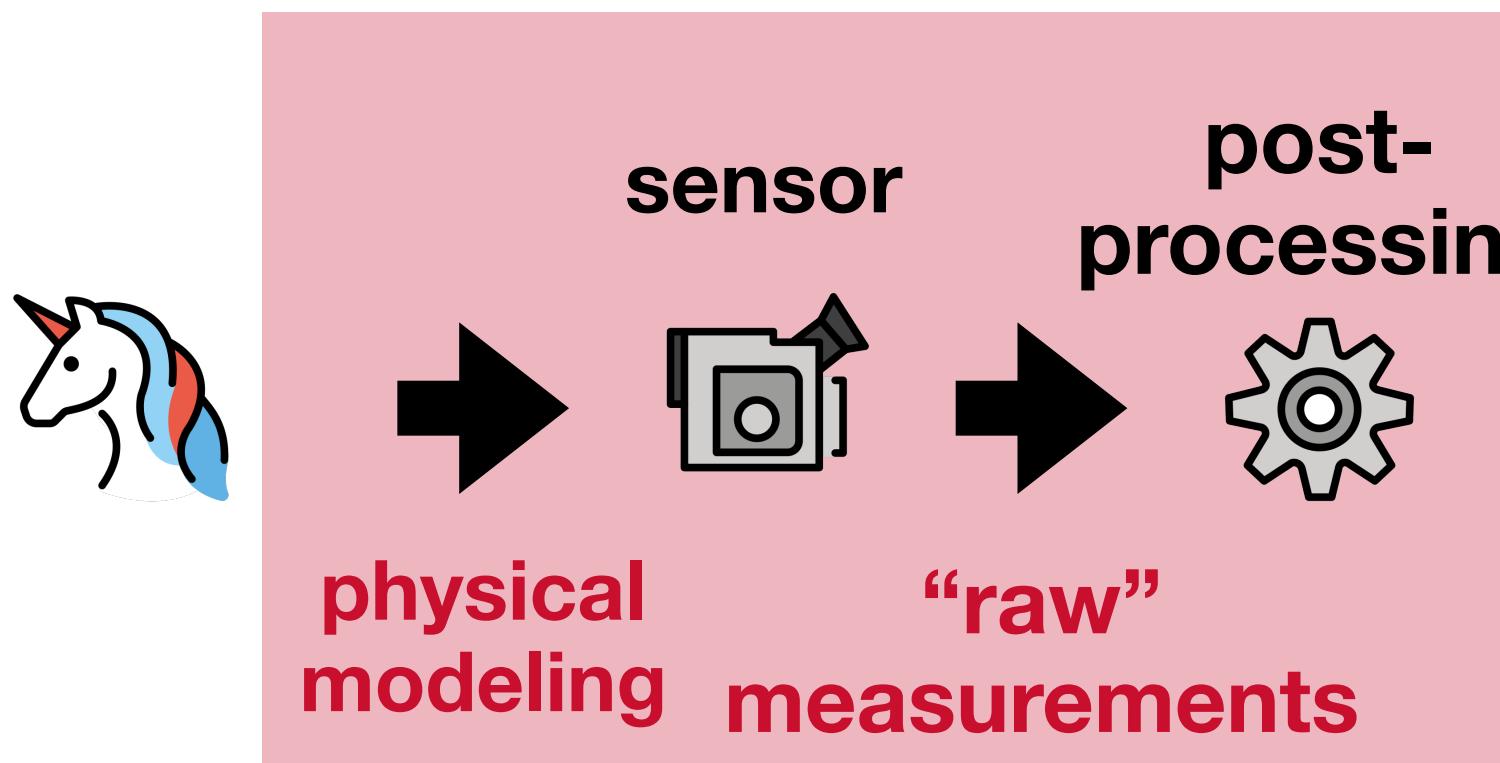


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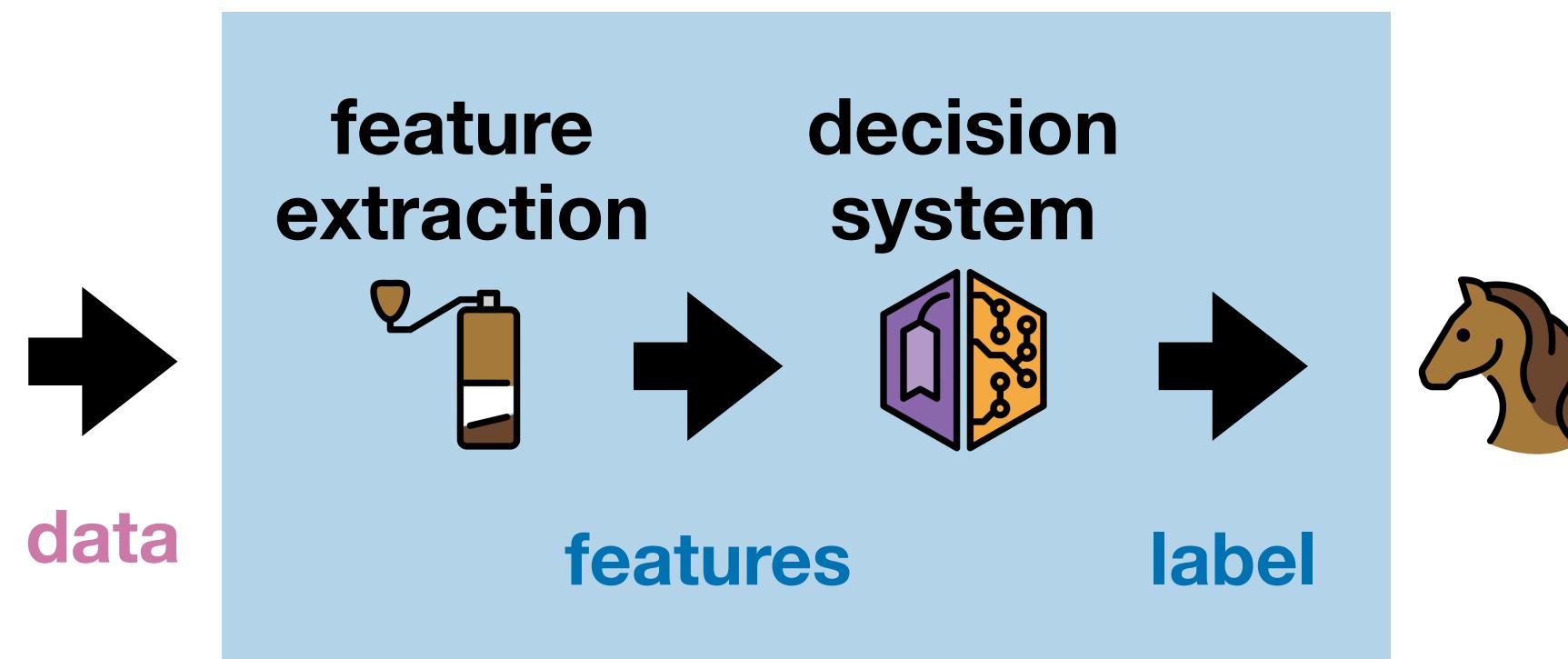
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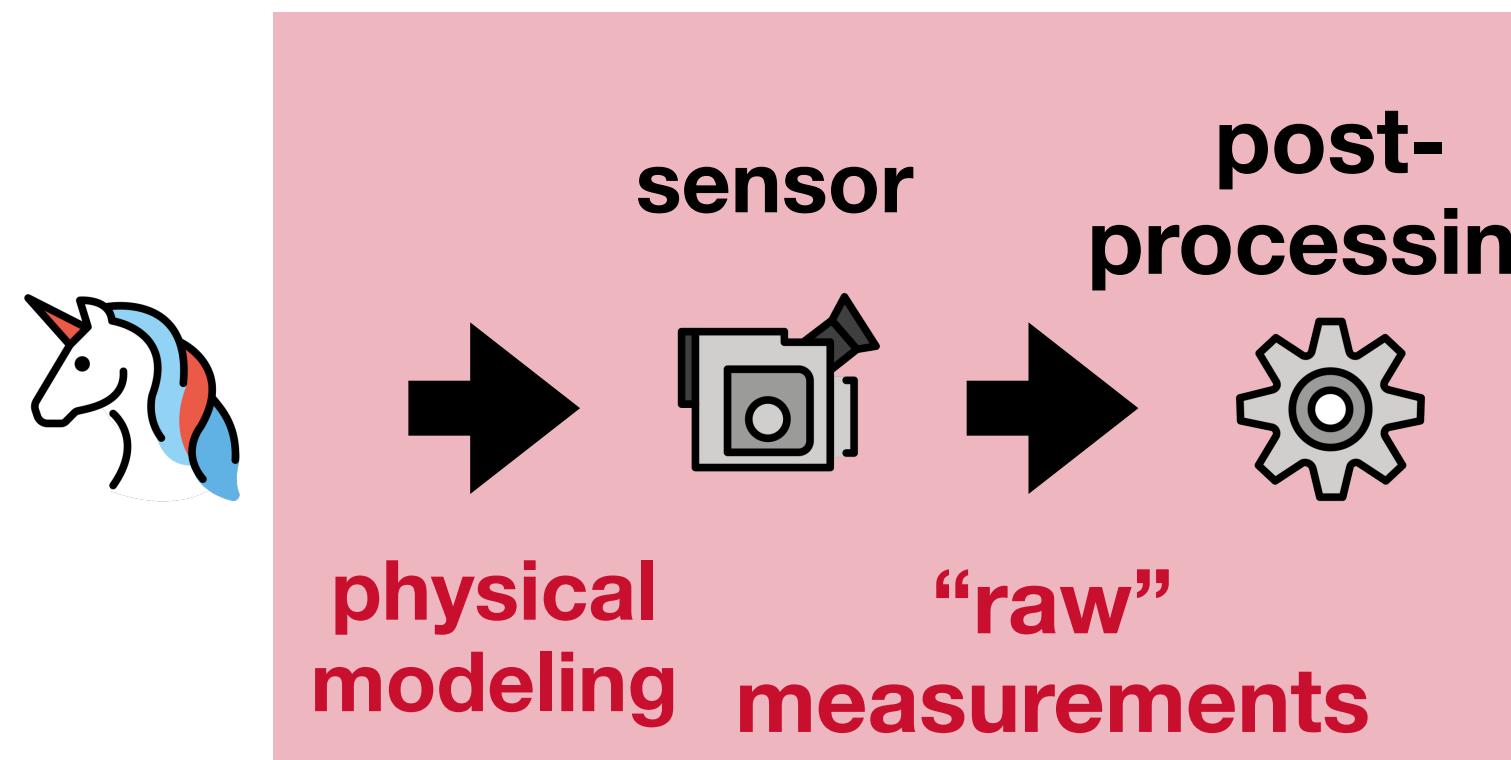
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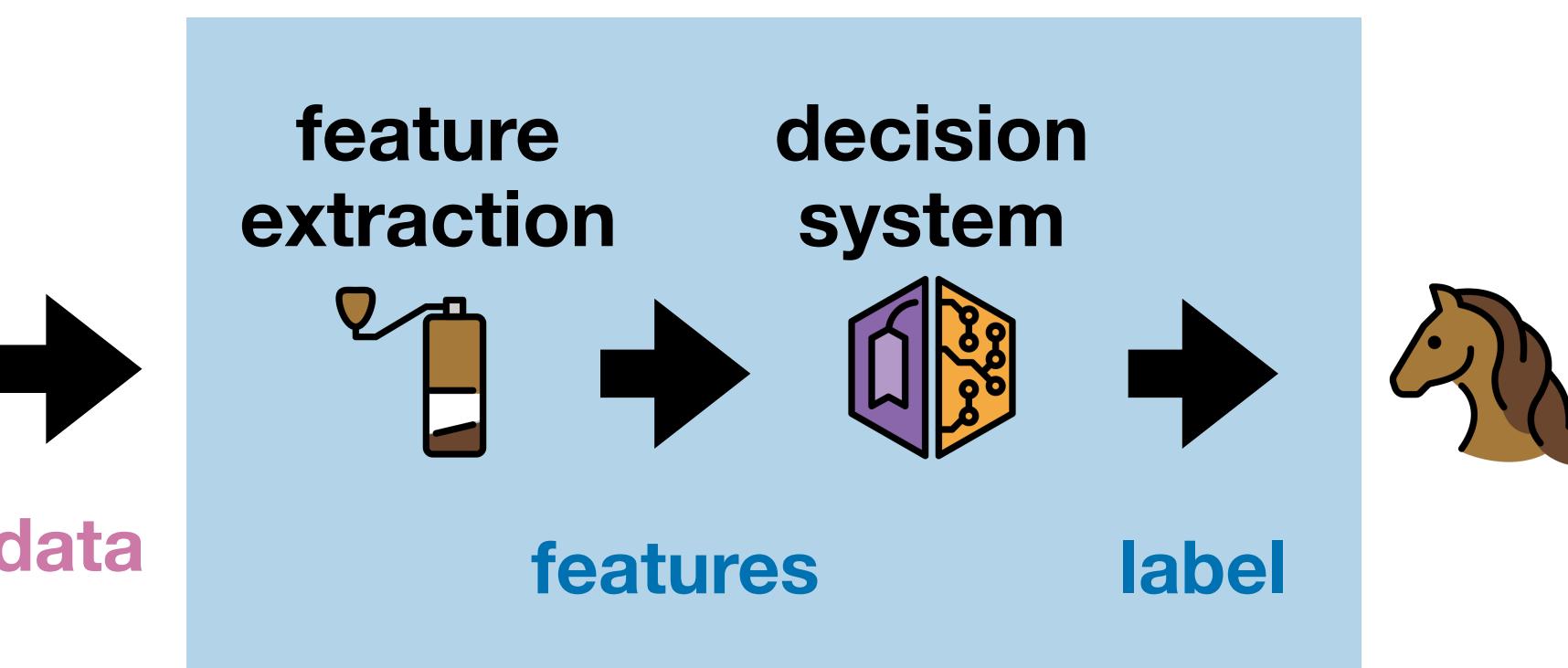
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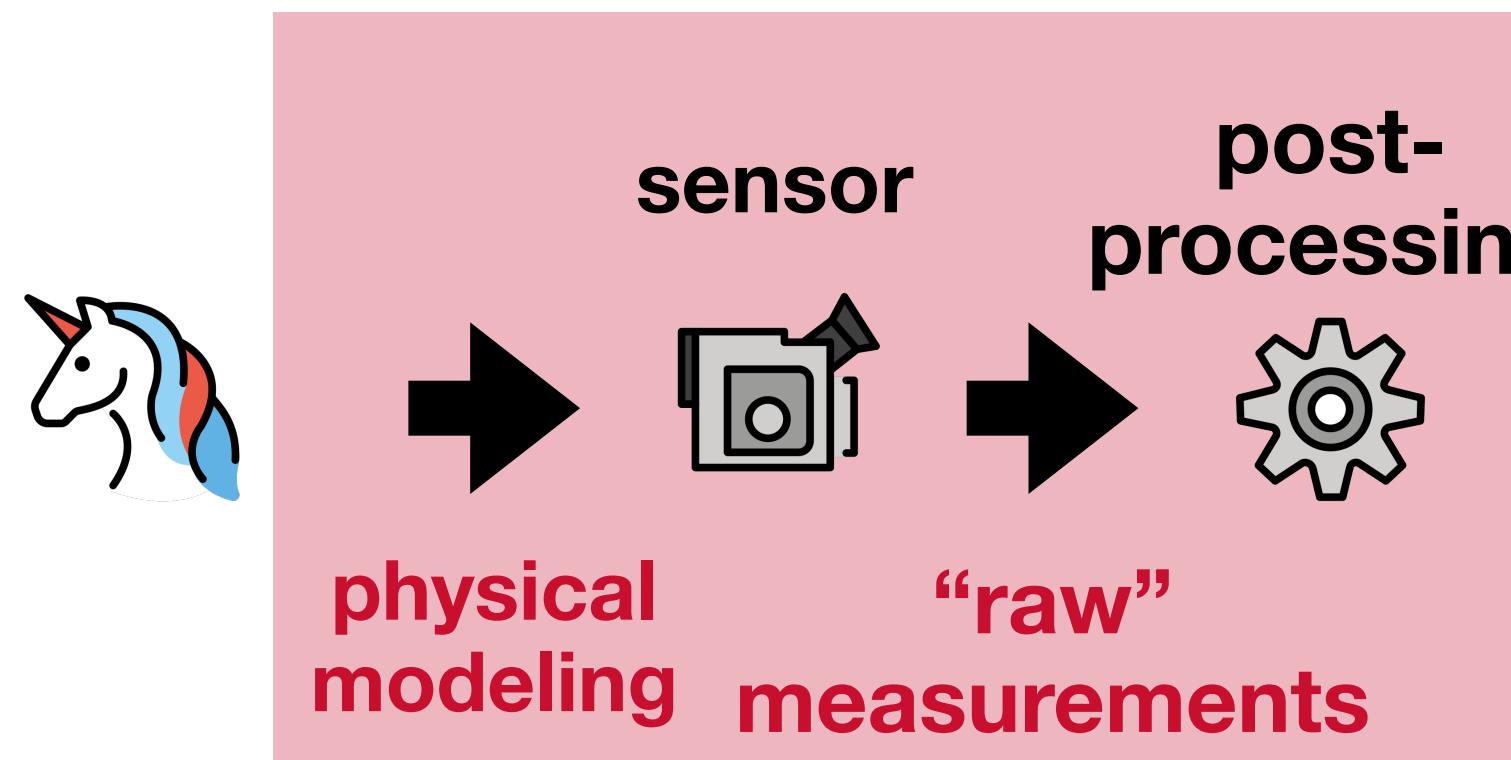


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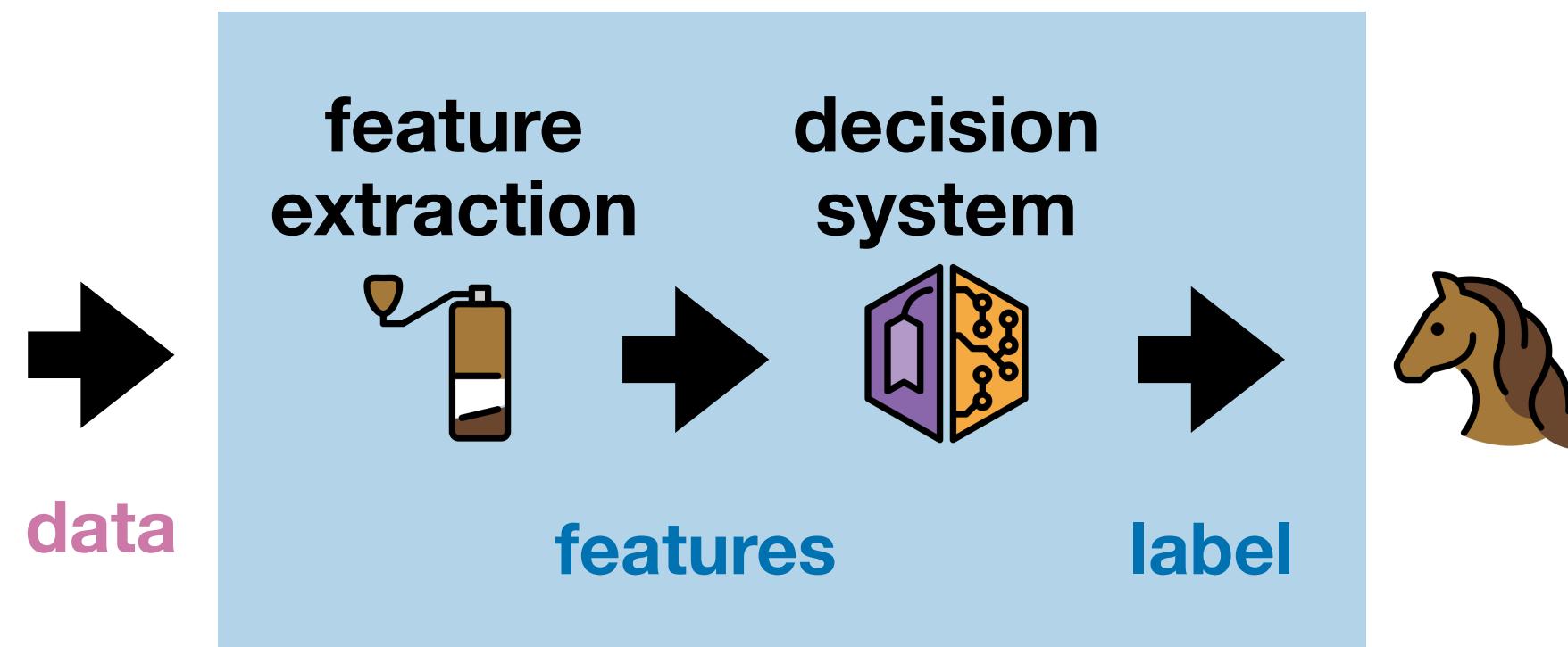


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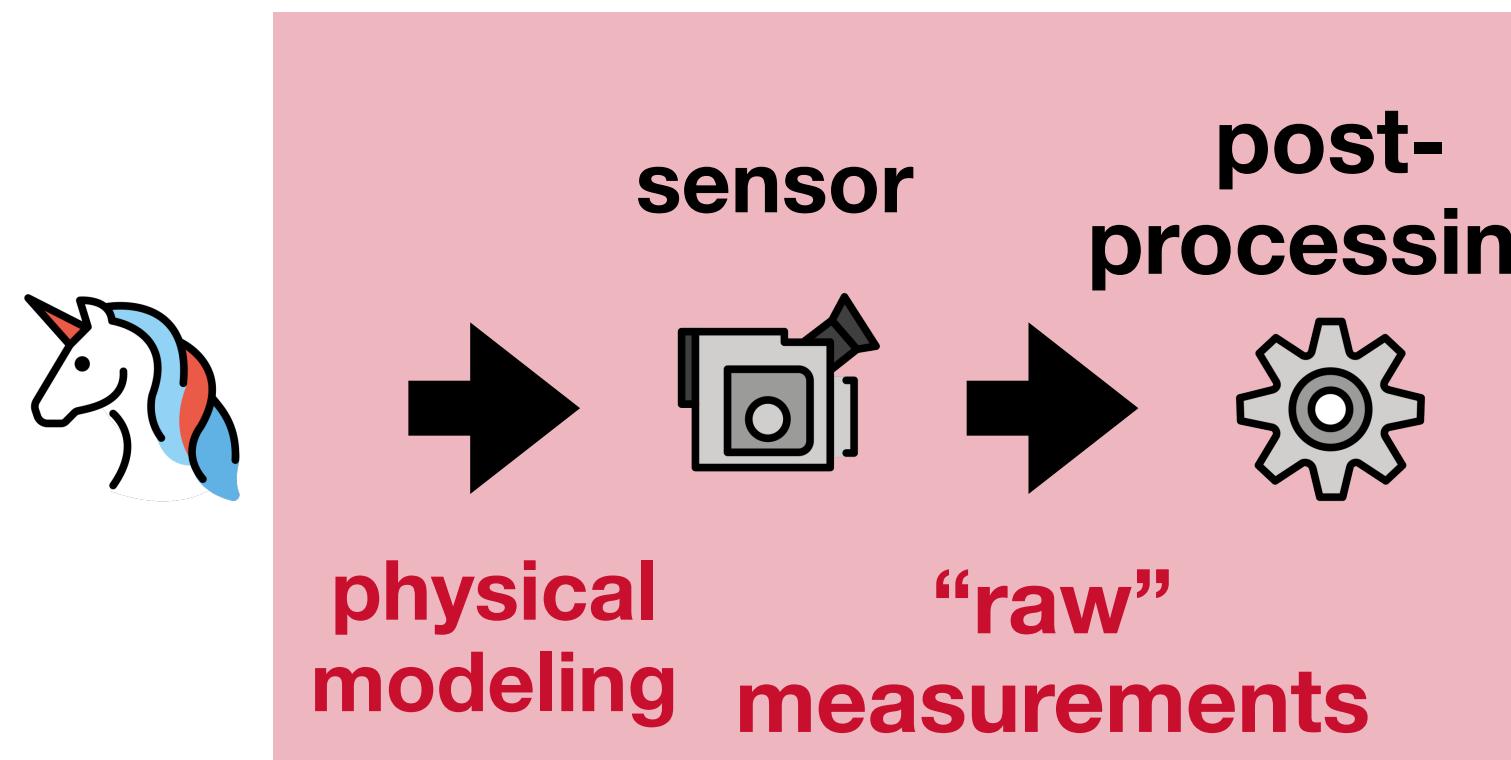
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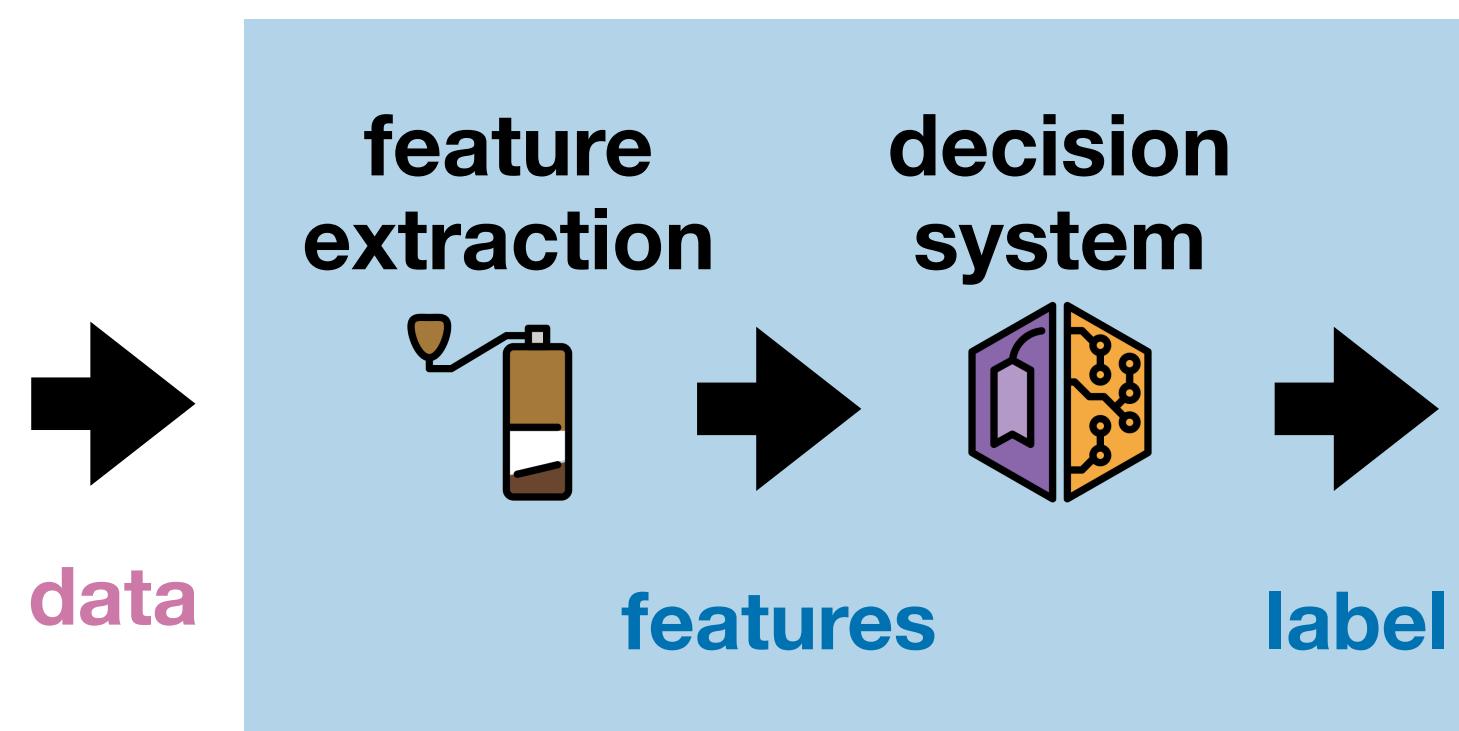
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If we put AI “into the camera” will these be true?

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Assumptions are wrong, but maybe correctable?

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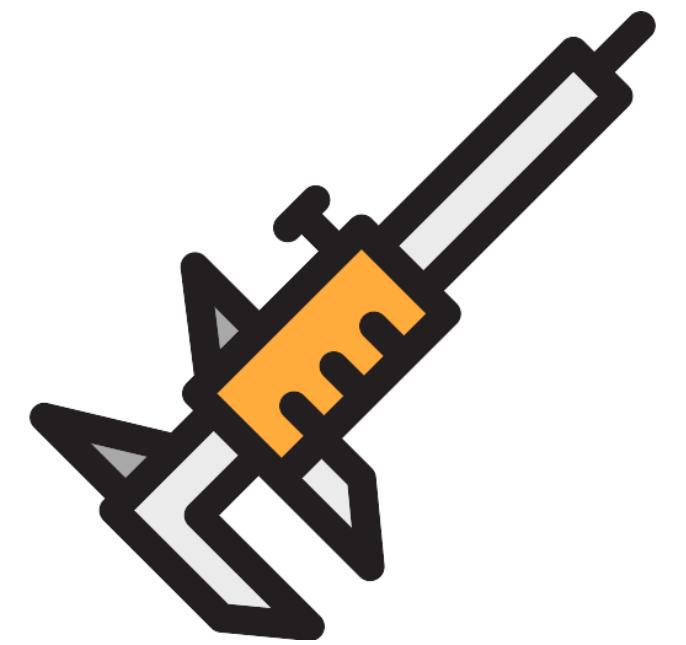
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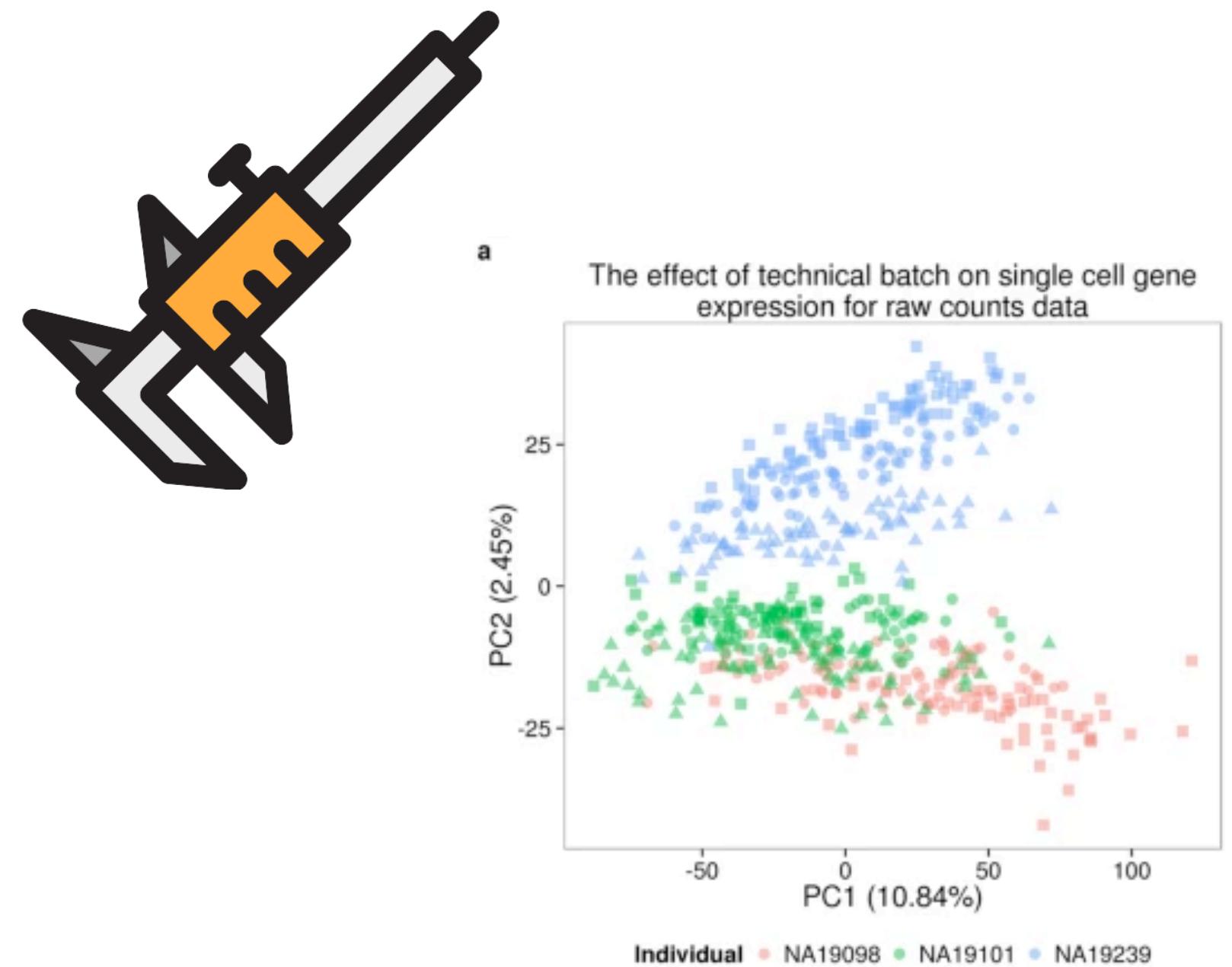


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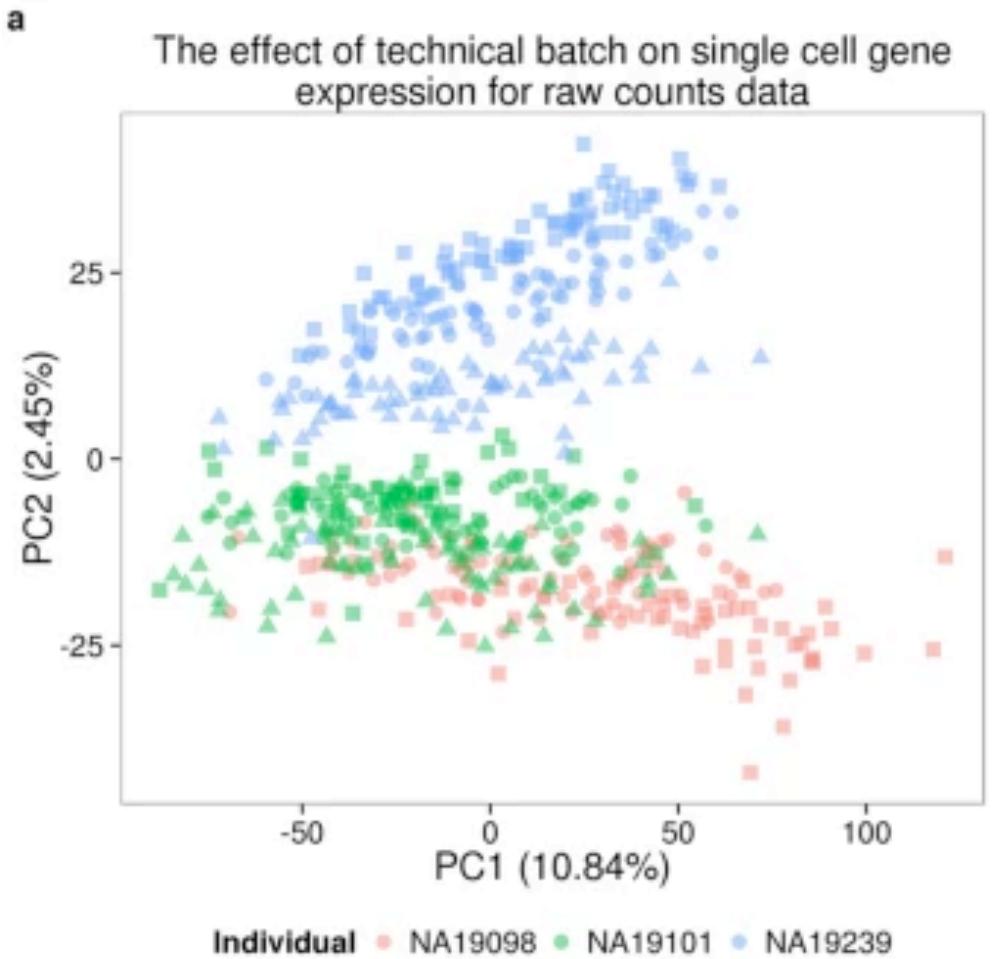


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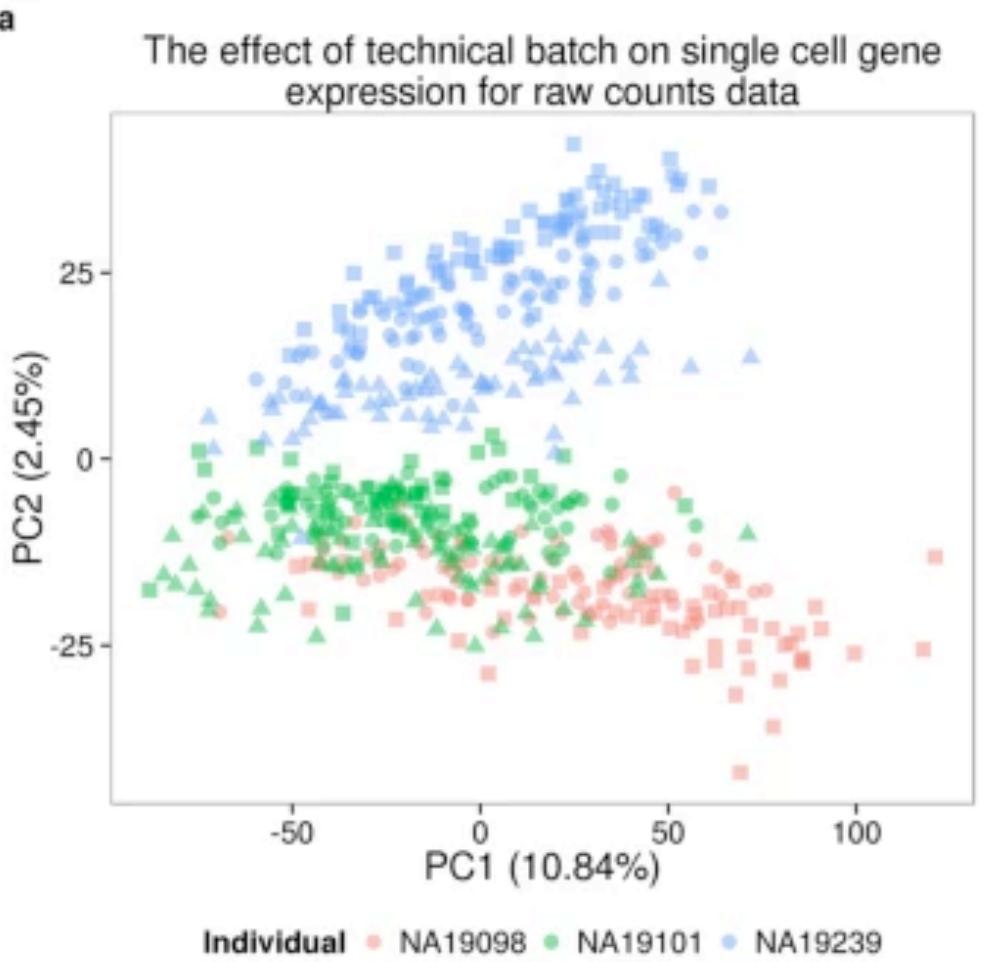


It already is not true in actual practice

Assumptions are wrong, but maybe correctable?

Data are almost never consistent in the ways we assume.

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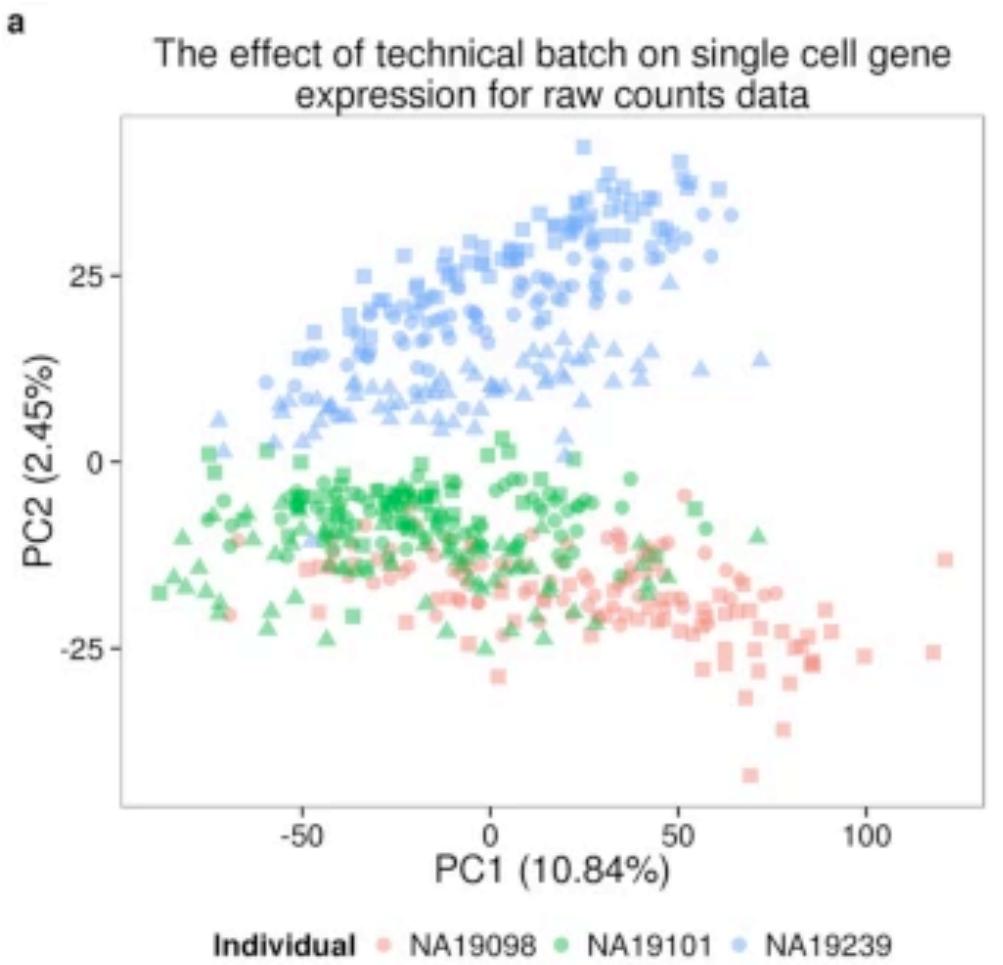


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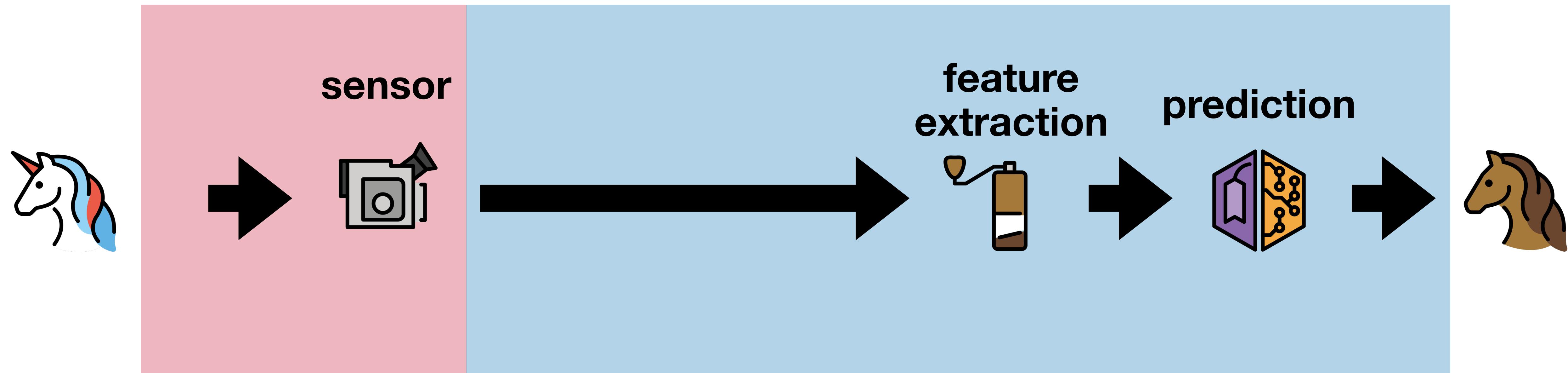
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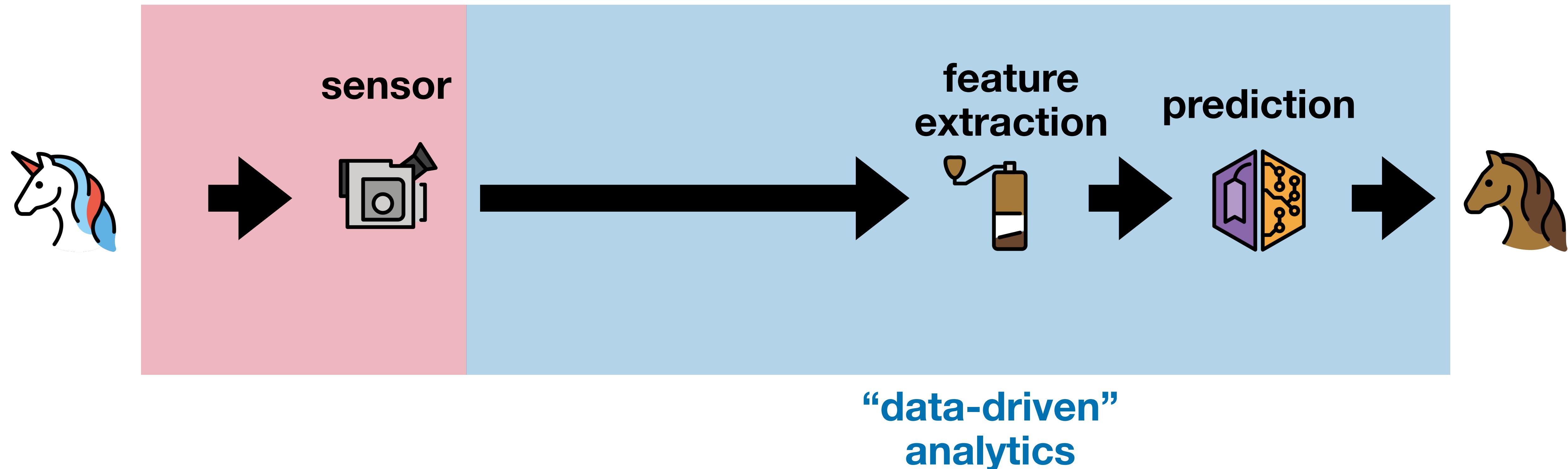
Pushing the kitchen sink backwards

Sensors, instrumentation, and decision support



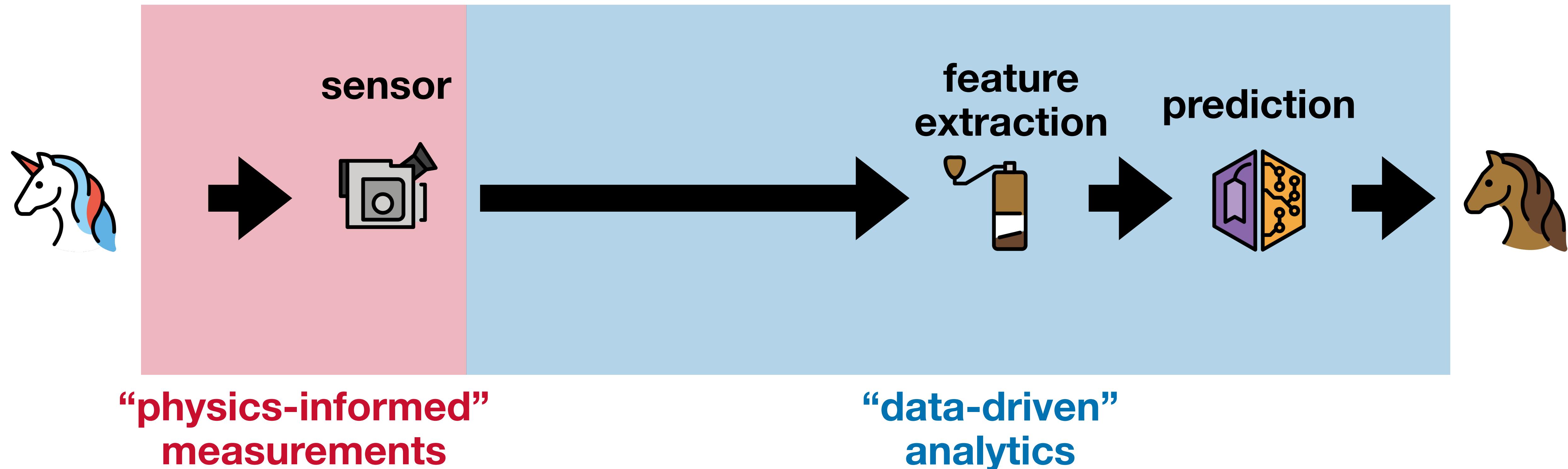
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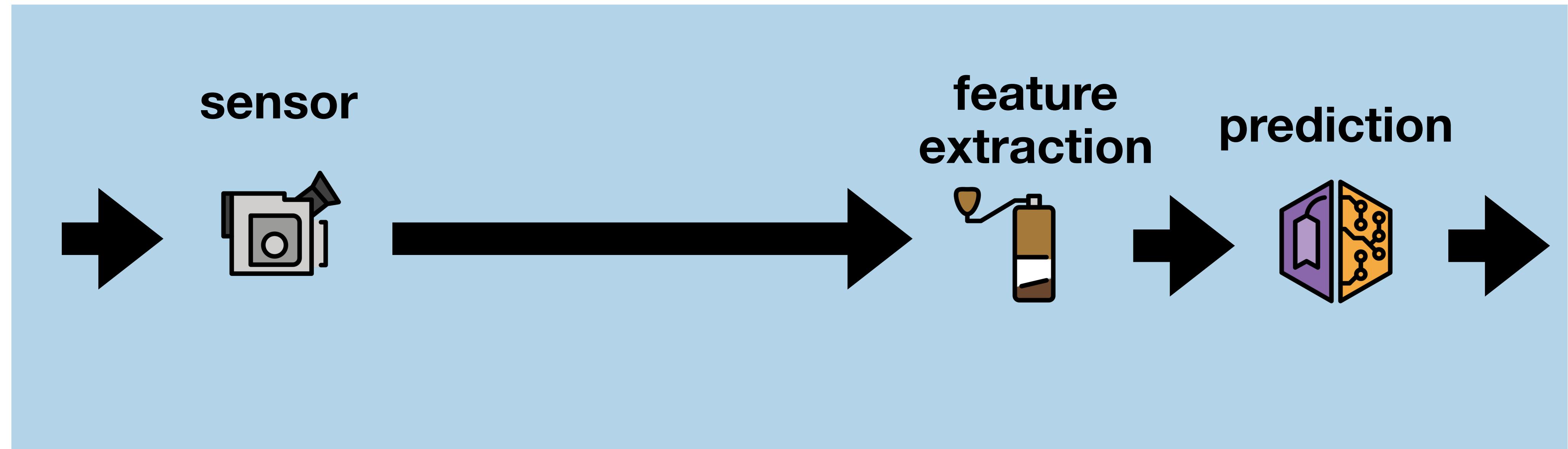
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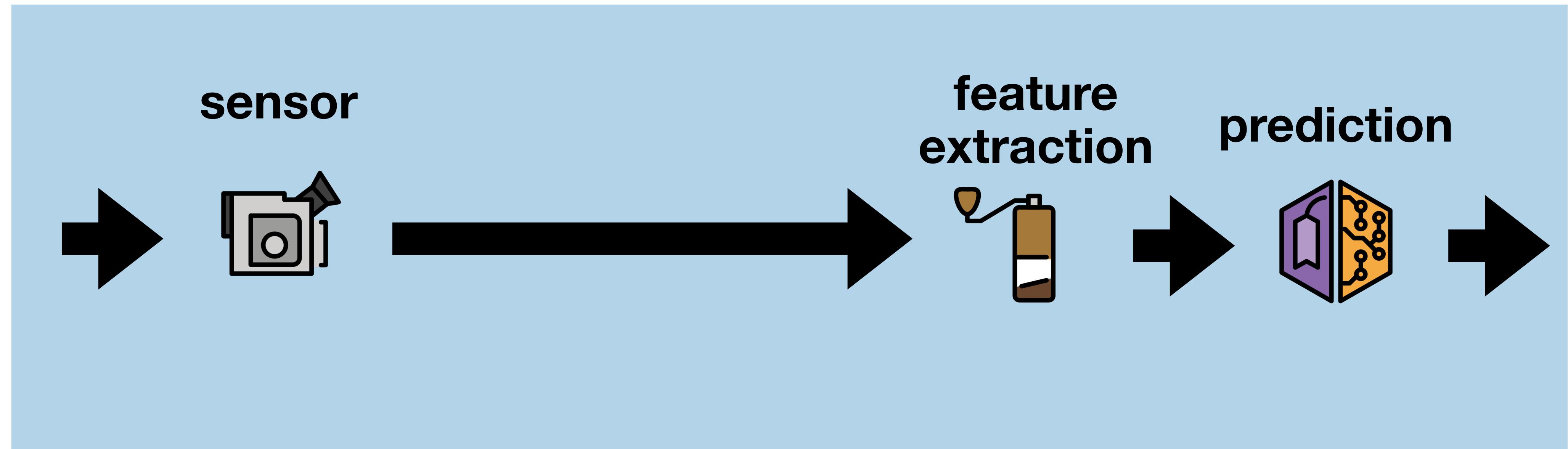
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(Asking for an undergrad friend)



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**“data-driven”
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What about our assumptions?

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



iOS 8.3



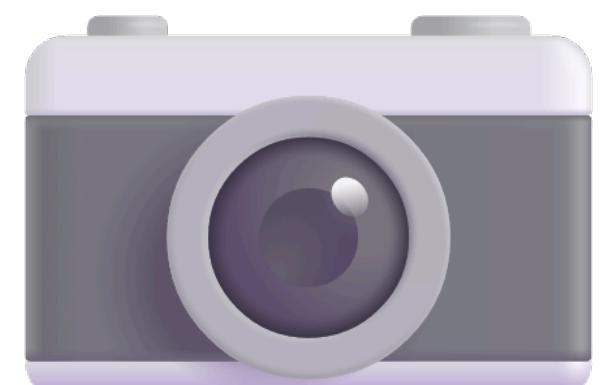
iOS 18.4



HarmonyOS 4.0



Samsung UI 7.0



MS 3D Fluent



SerenityOS

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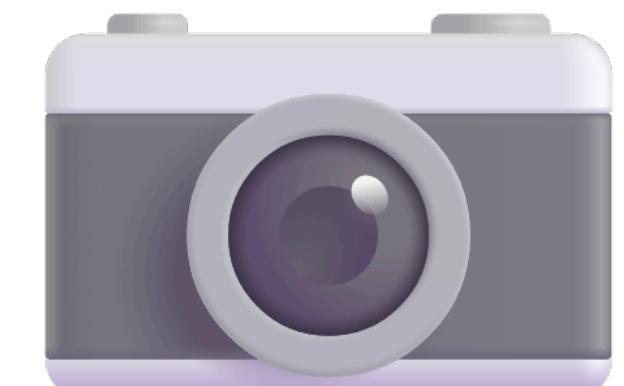
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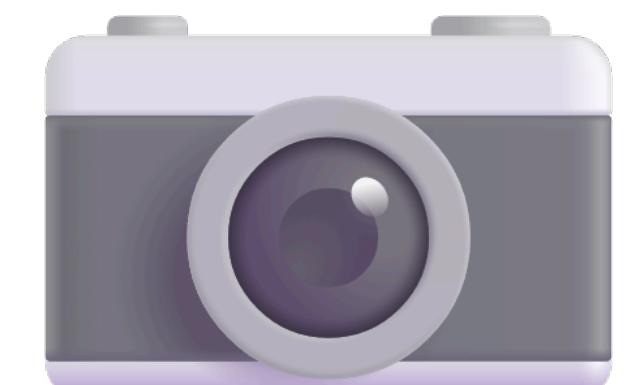
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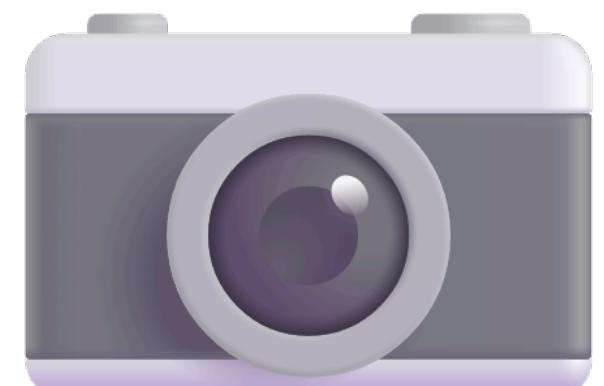
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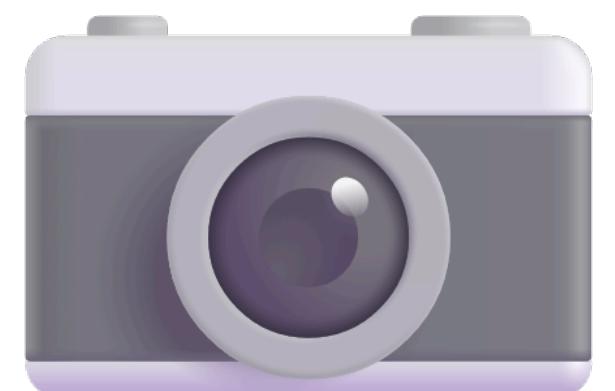
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These questions are not new! We can use “classical” tools to try and understand them.



iOS 8.3



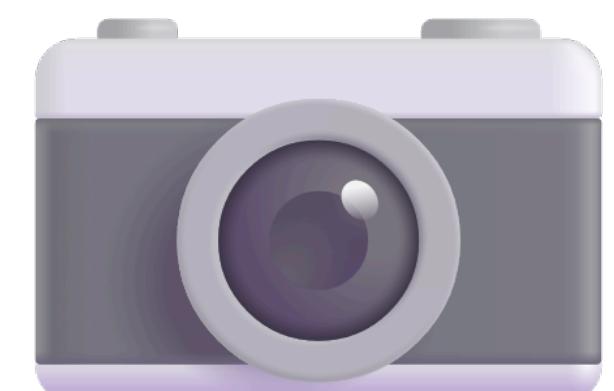
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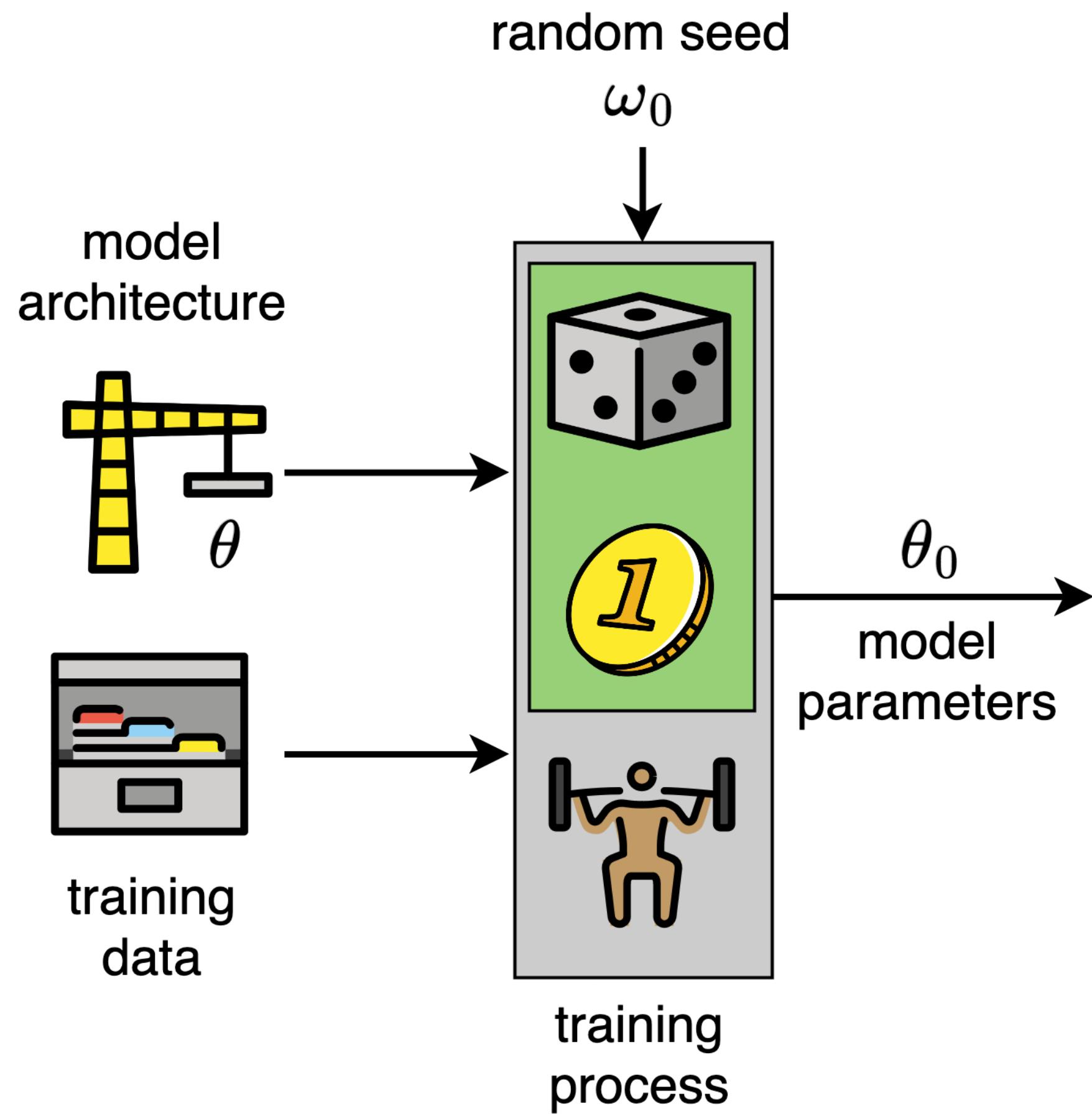
Some preliminaries



Rm Palaniappan, *Alien Planet-A*
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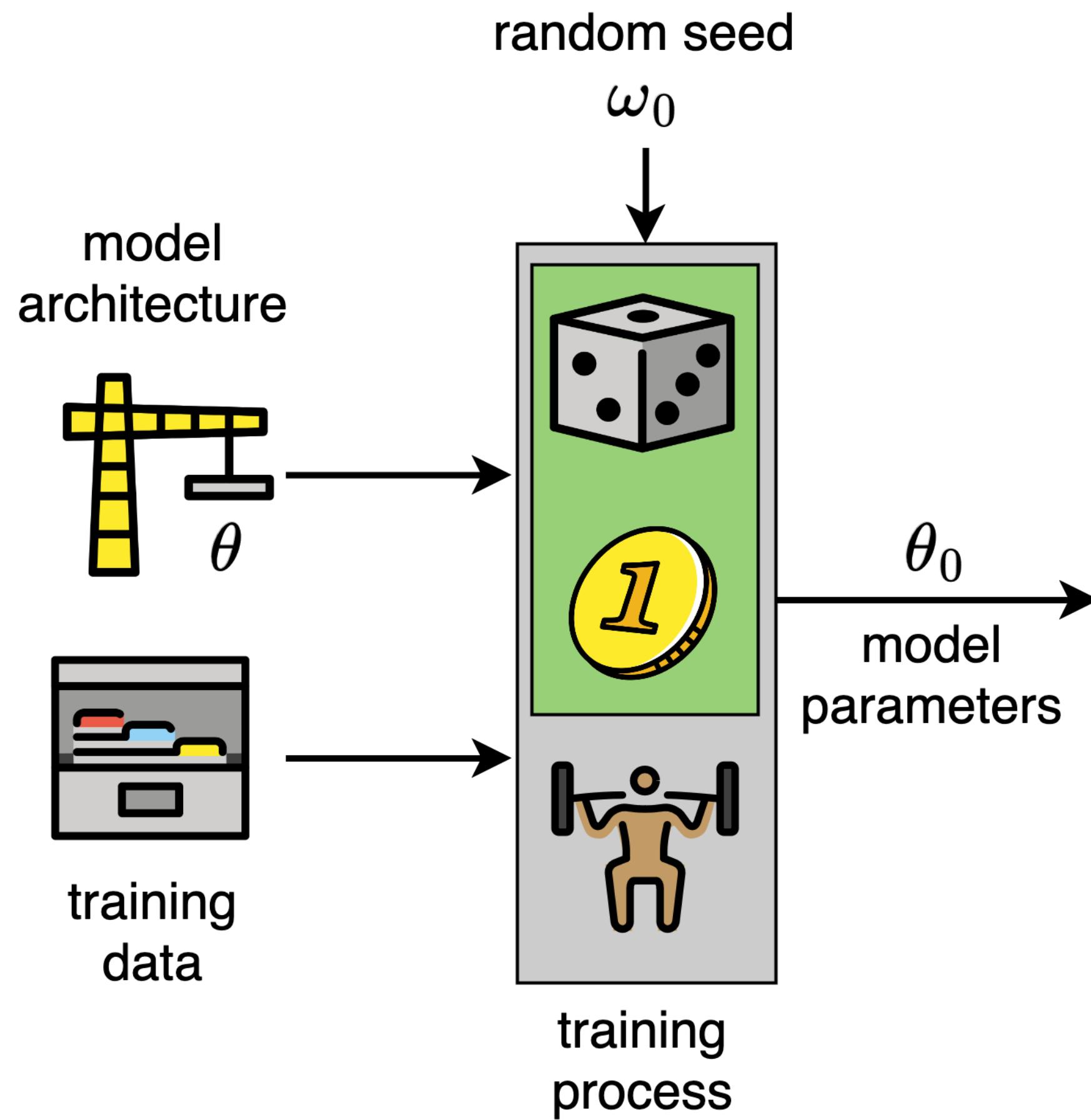
The standard statistical setup for modern ML

Machine learning as function-fitting



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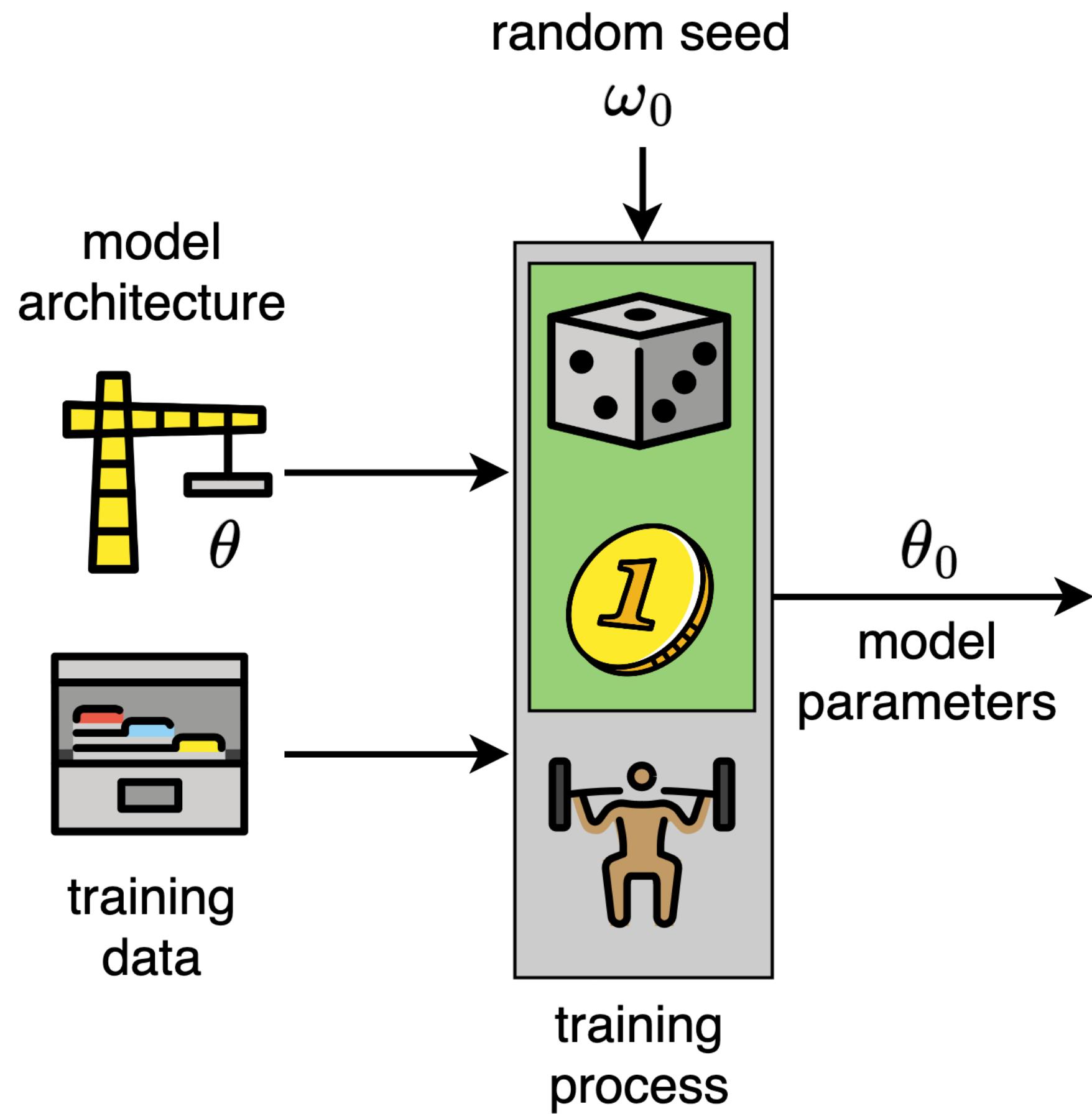
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The traditional setup for estimating parameters in a statistical model (or training a neural network):

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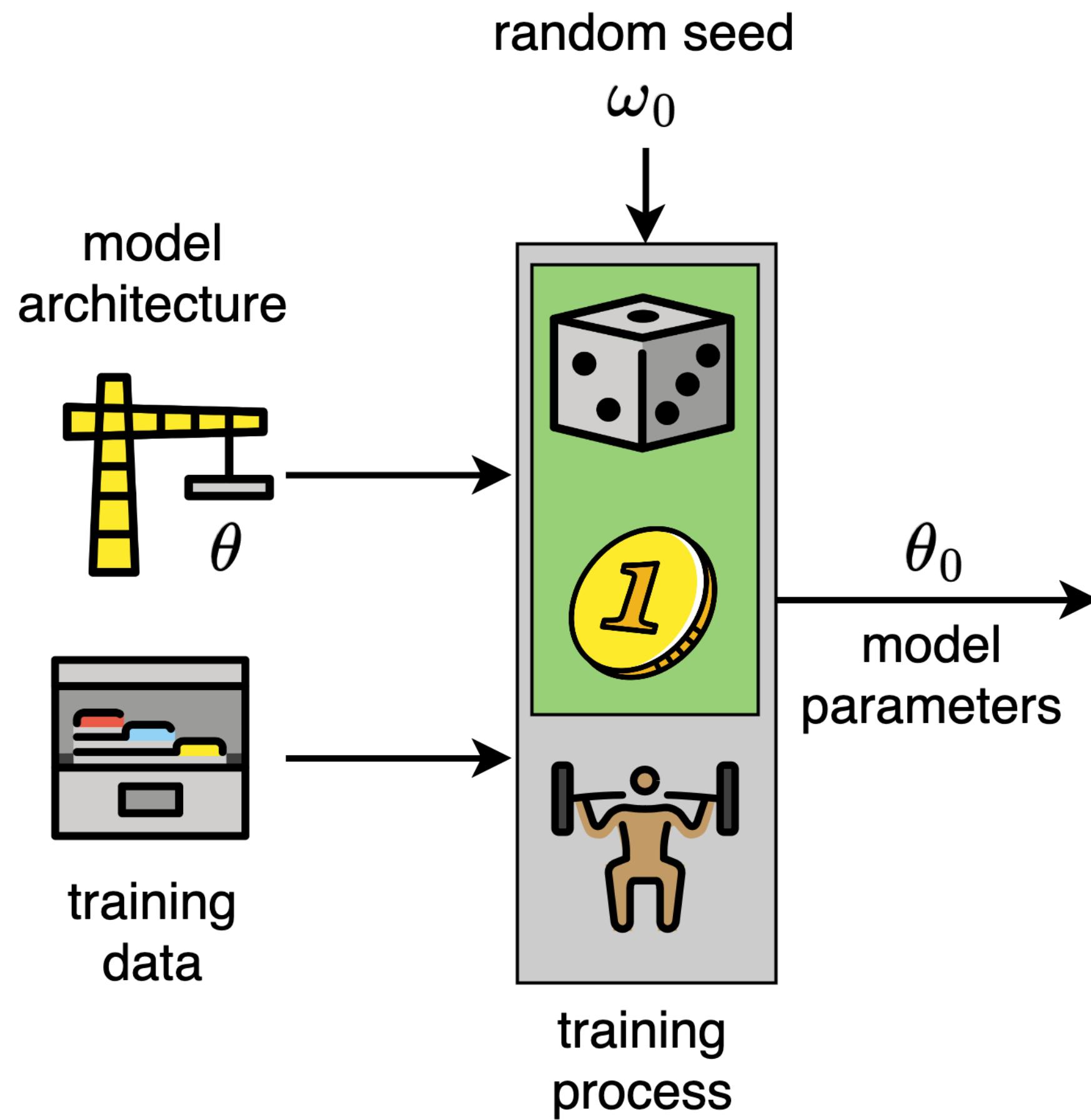


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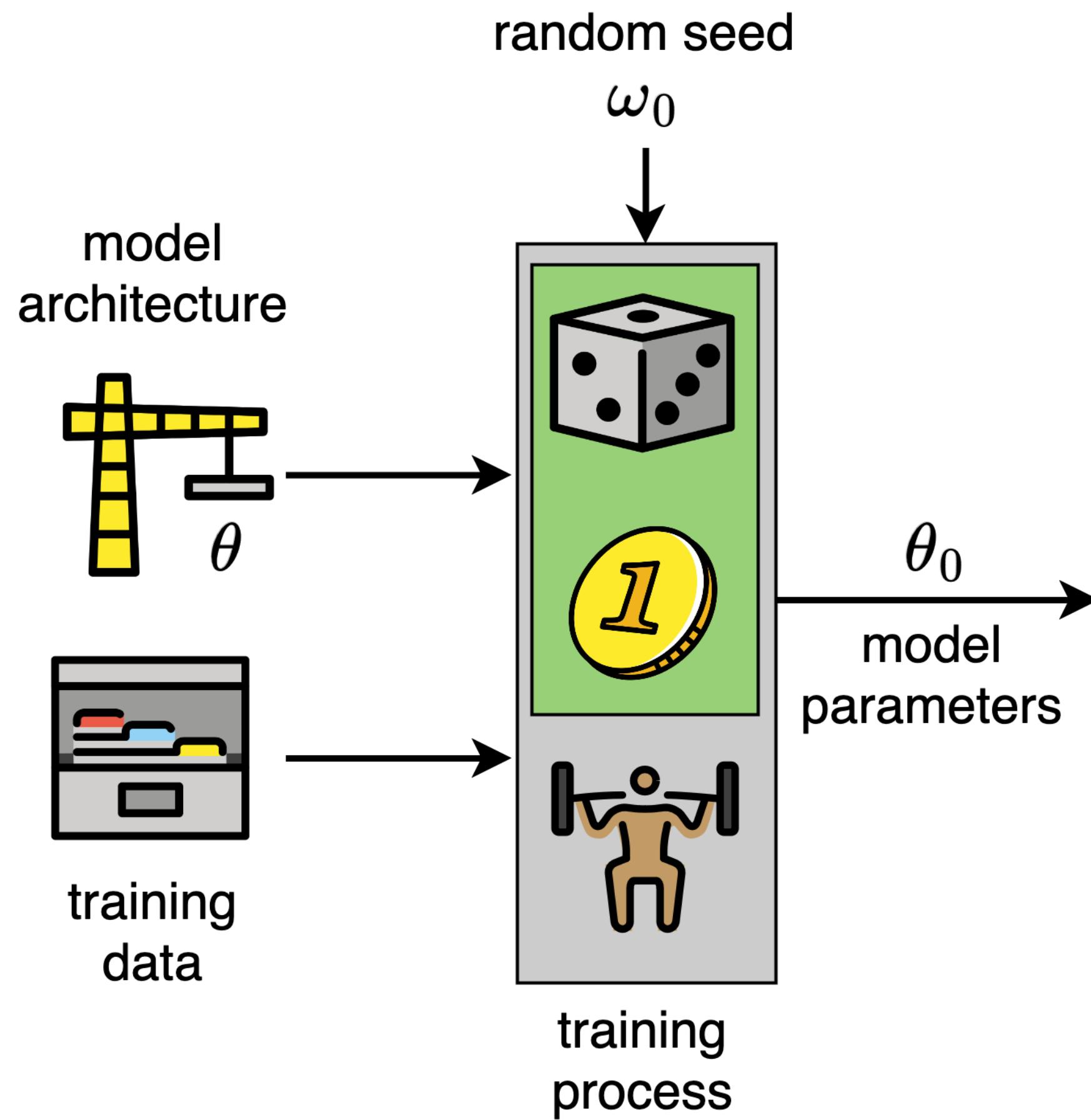


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- Stochastic optimization algorithm that does the actual minimization.

How should we characterize a model?

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- In representation learning, each $f: \mathcal{X} \rightarrow \mathcal{R}$ maps inputs to representations/embeddings.

Some natural questions

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Can we meaningfully compare these models?

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

Variability in the training process

Is training reliable?



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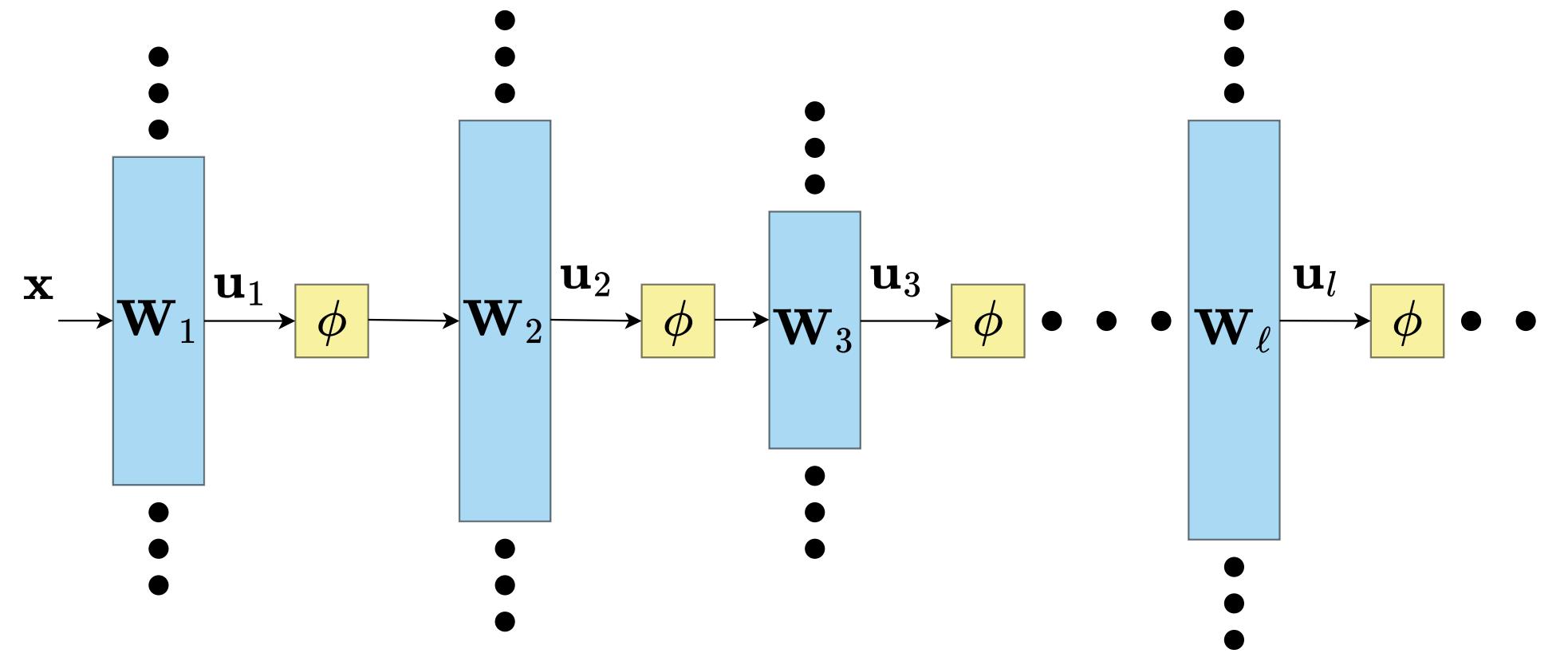
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If we have two different architectures \mathcal{F} and \mathcal{G} with different output spaces, how can we measure their similarity?

- 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.

Approximating the NN with a kernel machine

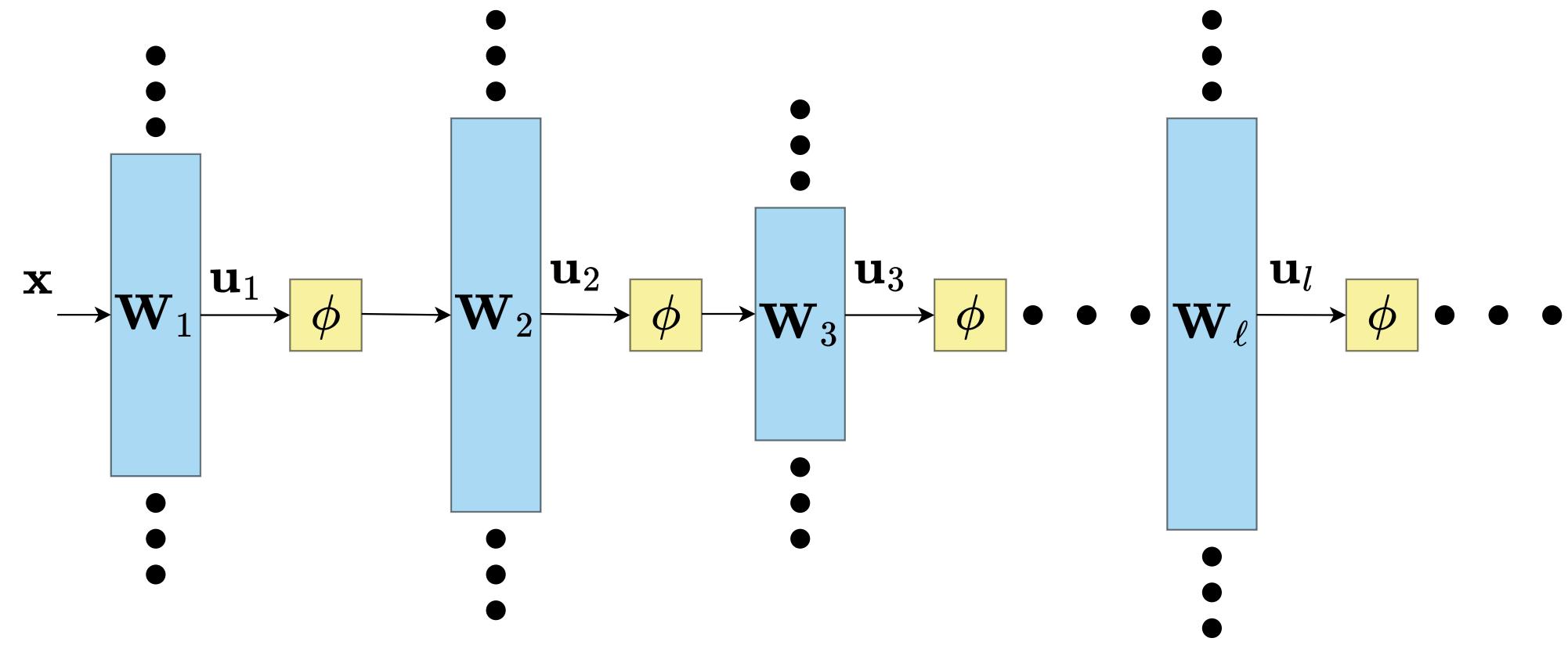
Not practical, but perhaps informative?



\approx
kGLM

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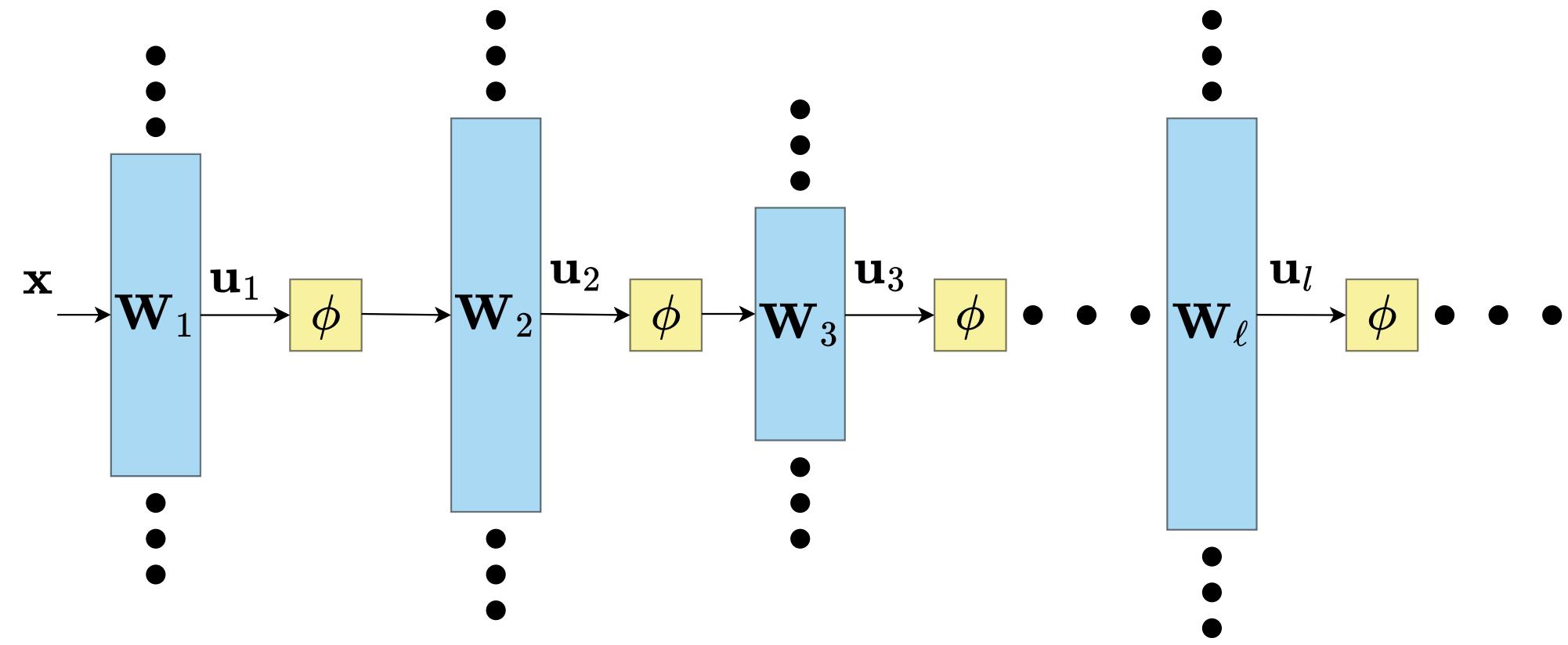
Suppose we compute some kernel function \mathbf{K} associated to the model and fit a **surrogate model** (\mathbf{V}, \mathbf{b}) :

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

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).

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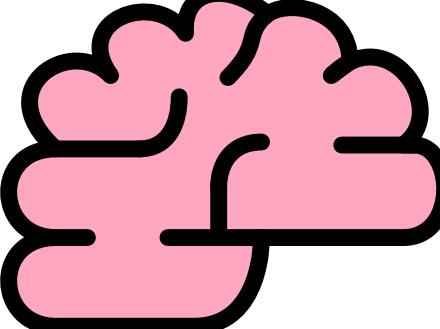
One example: the **neural tangent kernel**.

Neural Networks as Kernel Machines

Approximating an NN with a “simpler” model

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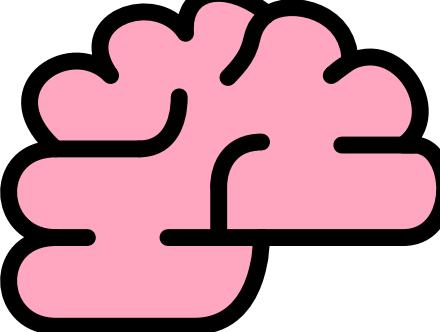
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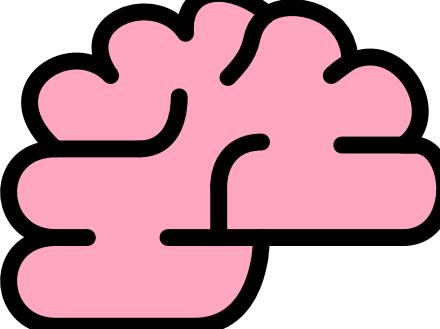


Jacot et al. (2018) showed that **infinitely wide** NNs are equivalent to a kernel machine with the “**neural tangent kernel**” (NTK):

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

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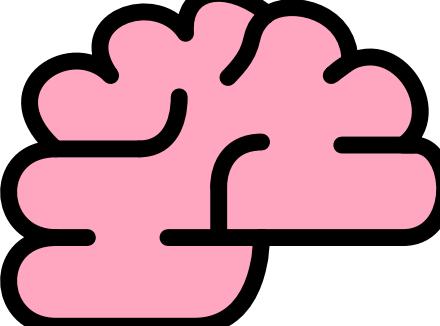
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Finite width networks don’t really behave like infinite width networks... (Chizat et al., 2018; Yang & Hu, 2021; Wang et al., 2022).

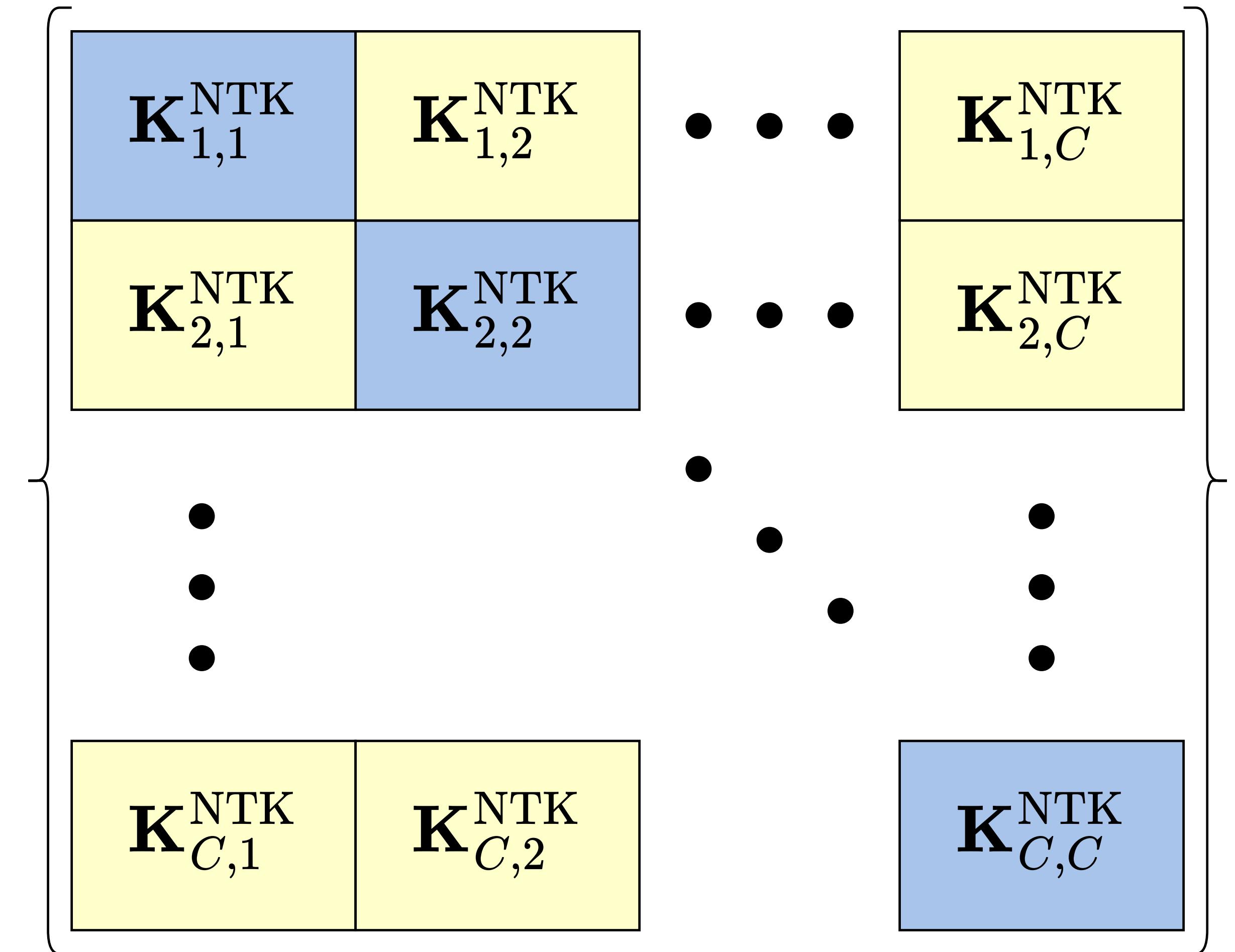
Challenge: NTK is asymptotic (infinite width)

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:

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

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.



Trace NTK: a proxy for the eNTK

Much lower computational overhead needed

We look at a simplification of the NTK:

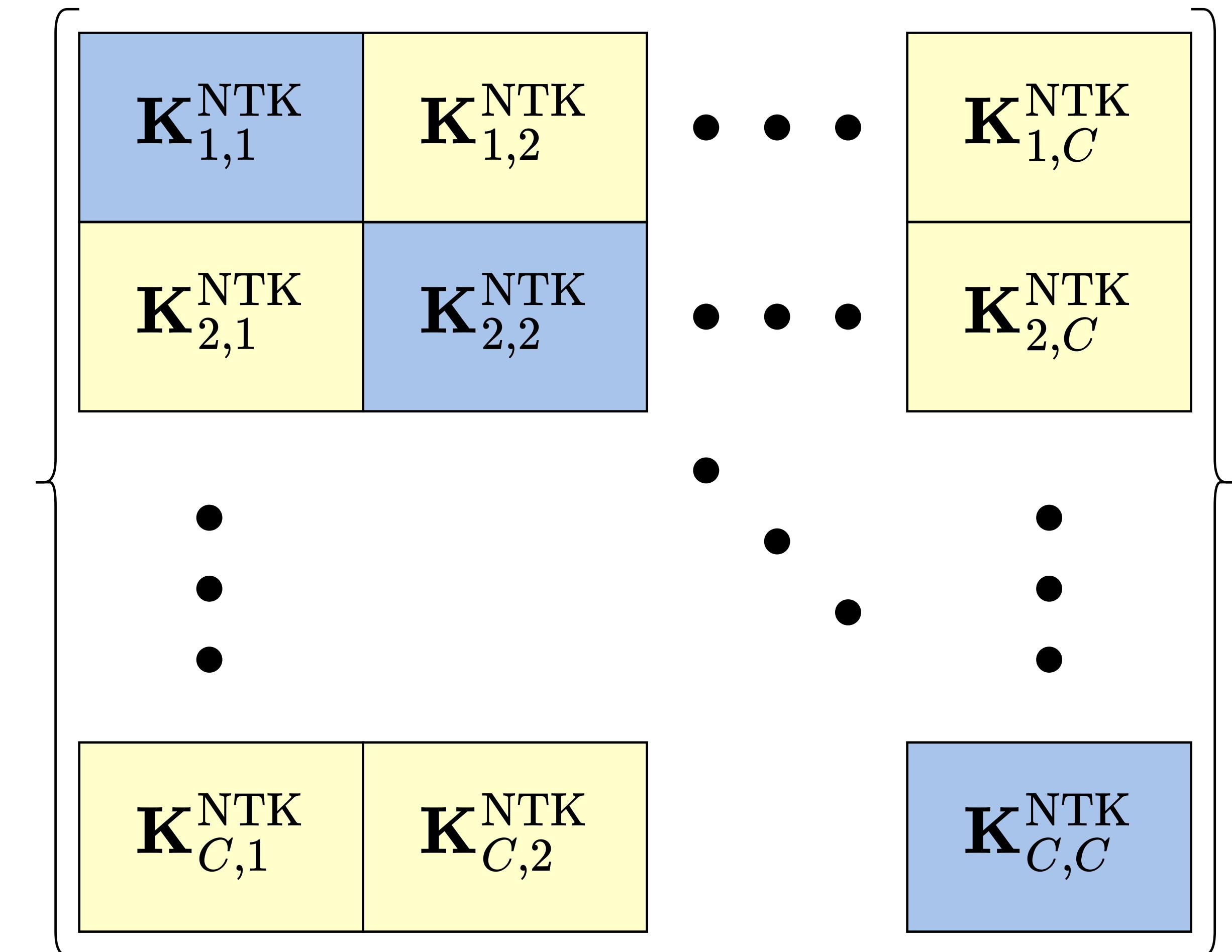
$$K^{\text{trNTK}}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{c=1}^C \left\langle \nabla_{\theta} f^c(\mathbf{x}_i; \theta), \nabla_{\theta} f^c(\mathbf{x}_j; \theta) \right\rangle}{\left(\sum_{c=1}^C \|f^c(\mathbf{x}_i; \theta)\|^2 \right)^{1/2} \left(\sum_{c=1}^C \|f^c(\mathbf{x}_j; \theta)\|^2 \right)^{1/2}}$$

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

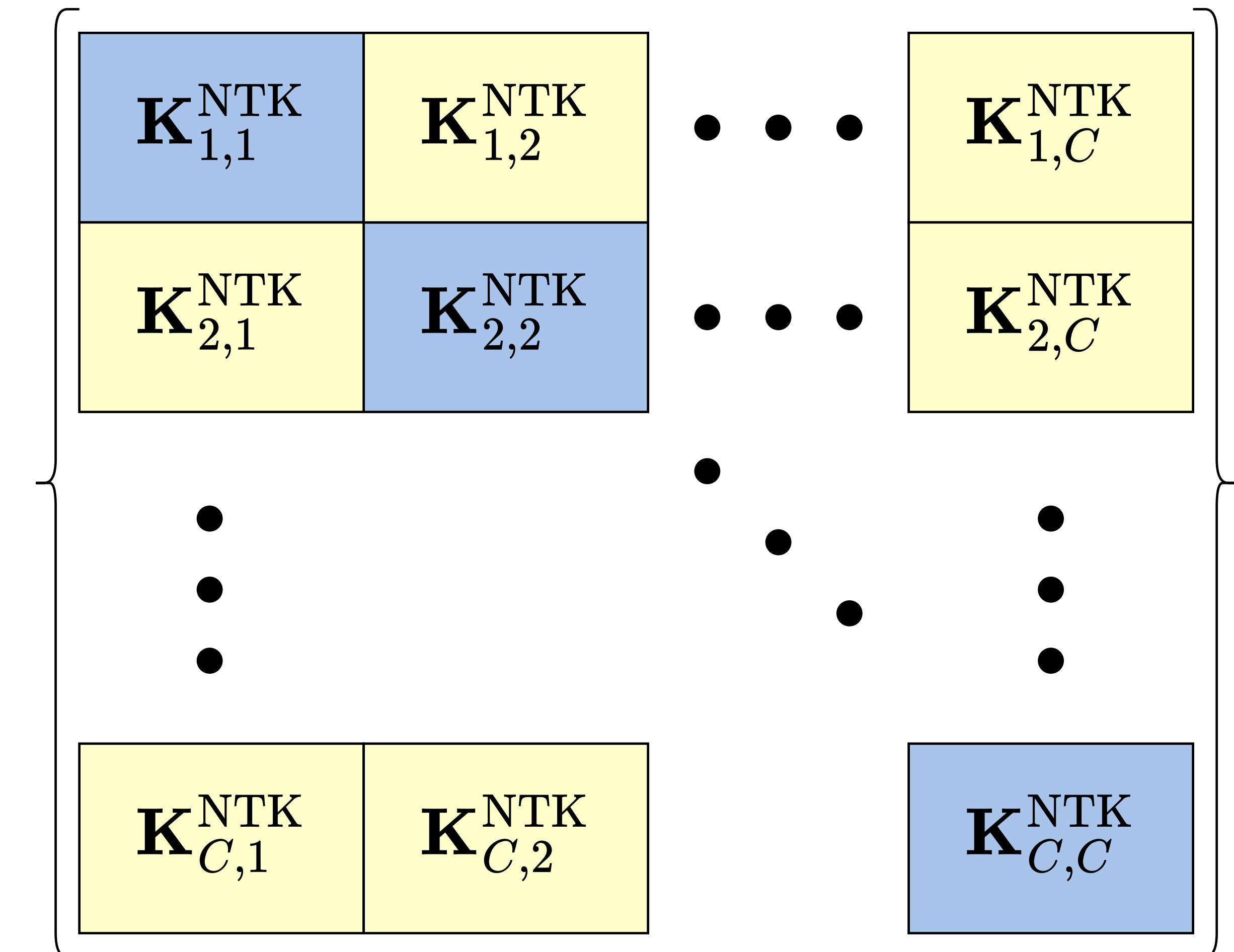
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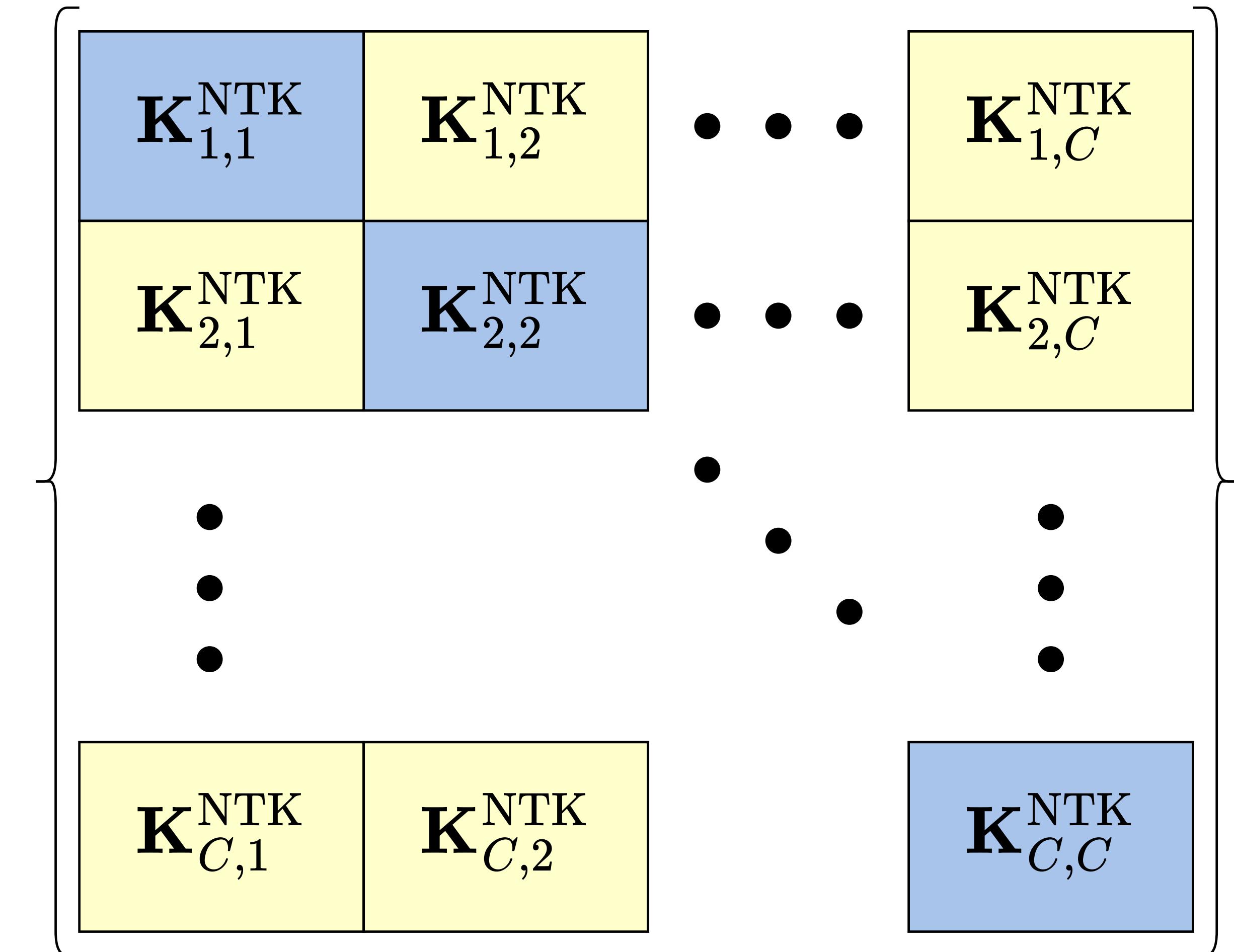


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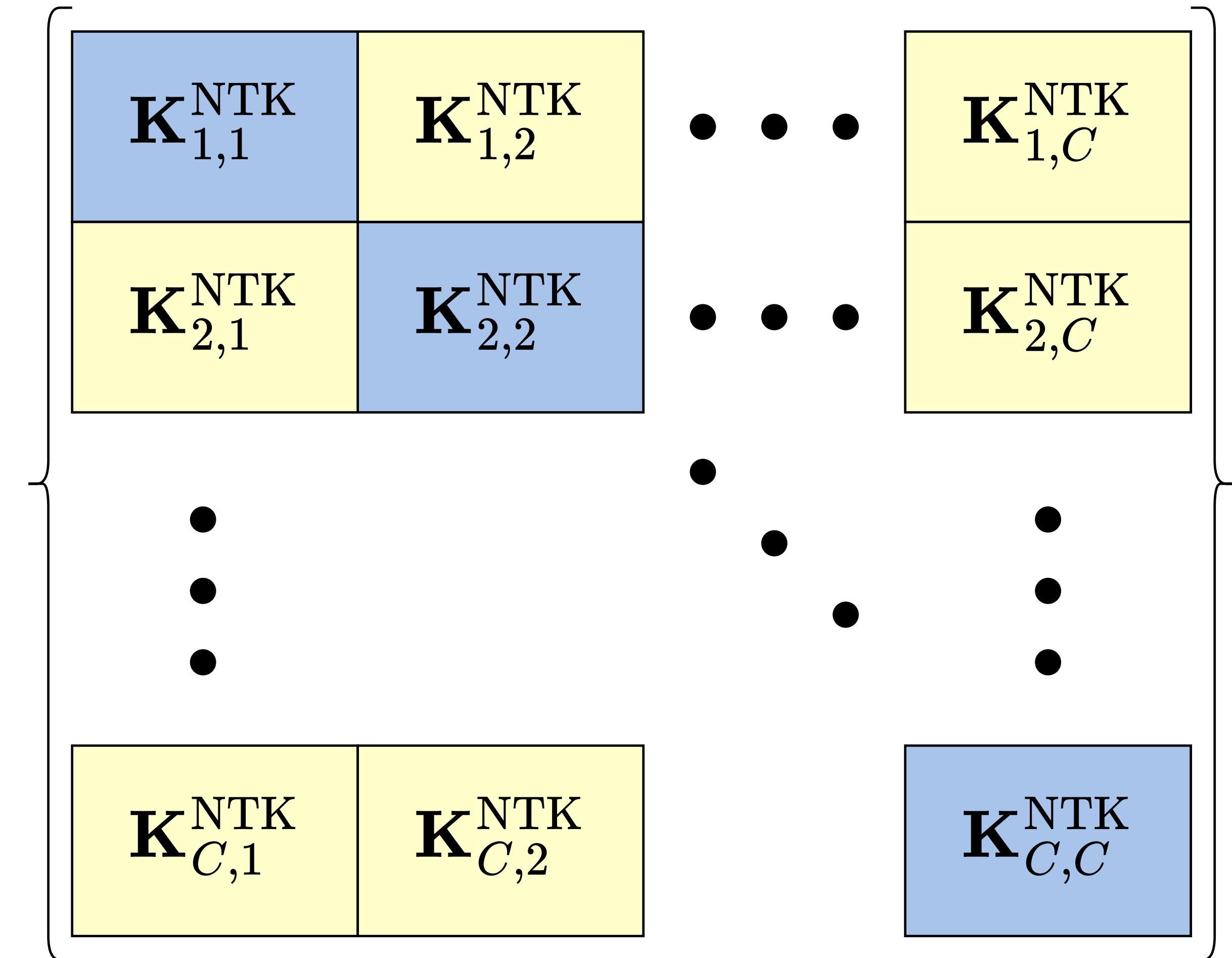


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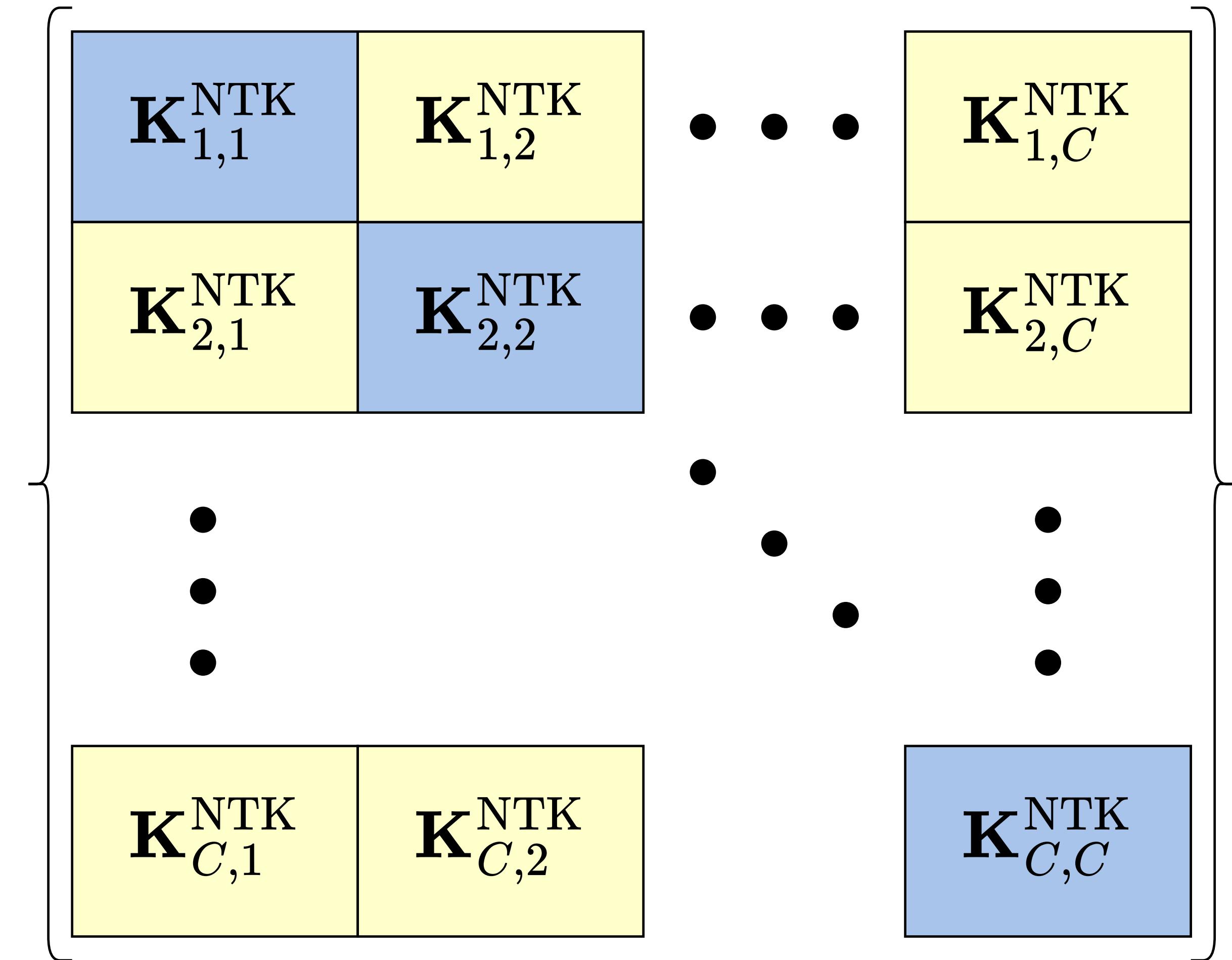


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- Challenging because of invariants.



Embedding spaces and model comparisons



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

A question of interoperability

Challenges in collaborating with AI instruments



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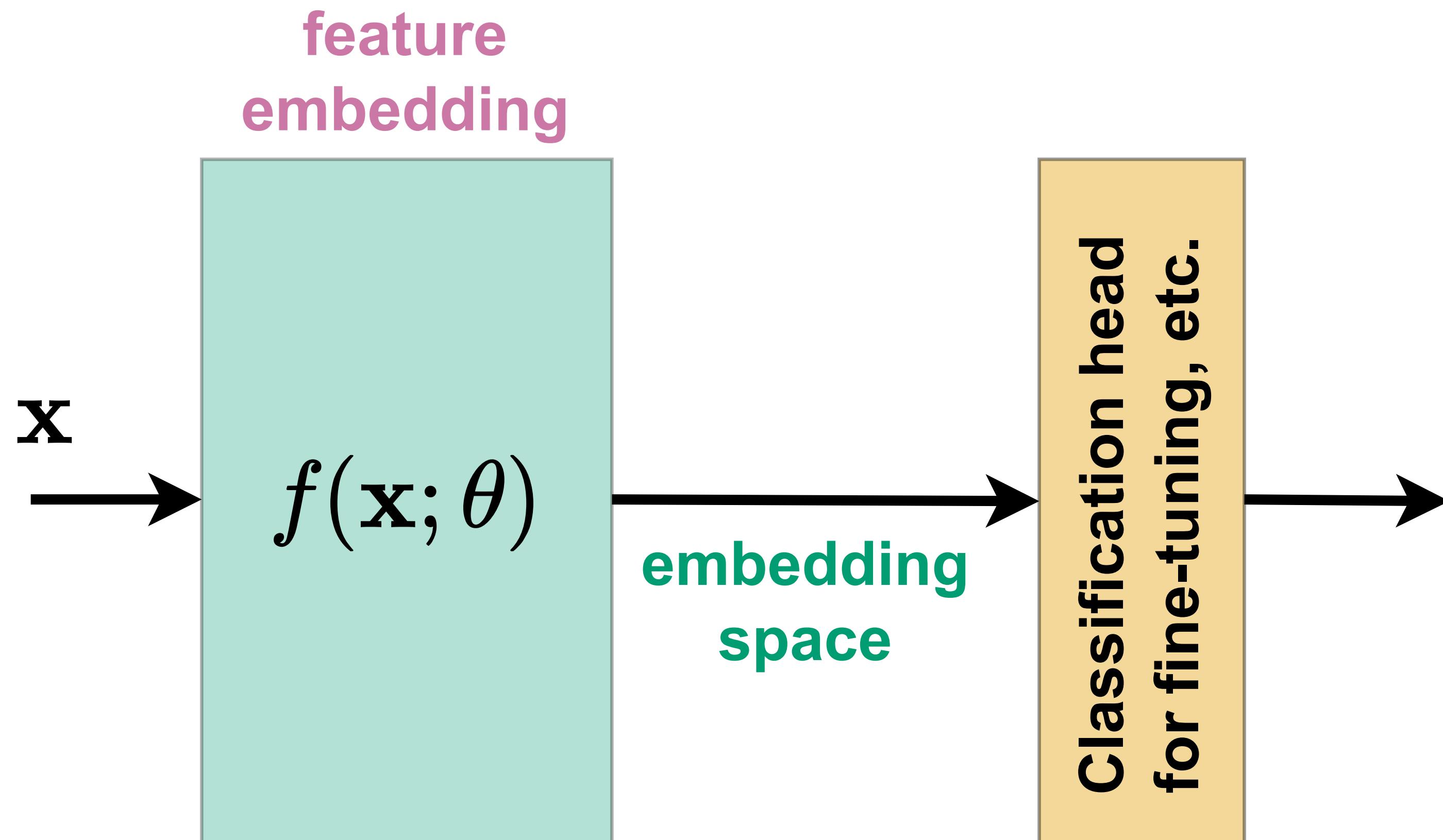
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- To the human eye, they are functionally similar.
- Can we quantitatively see if they are different?

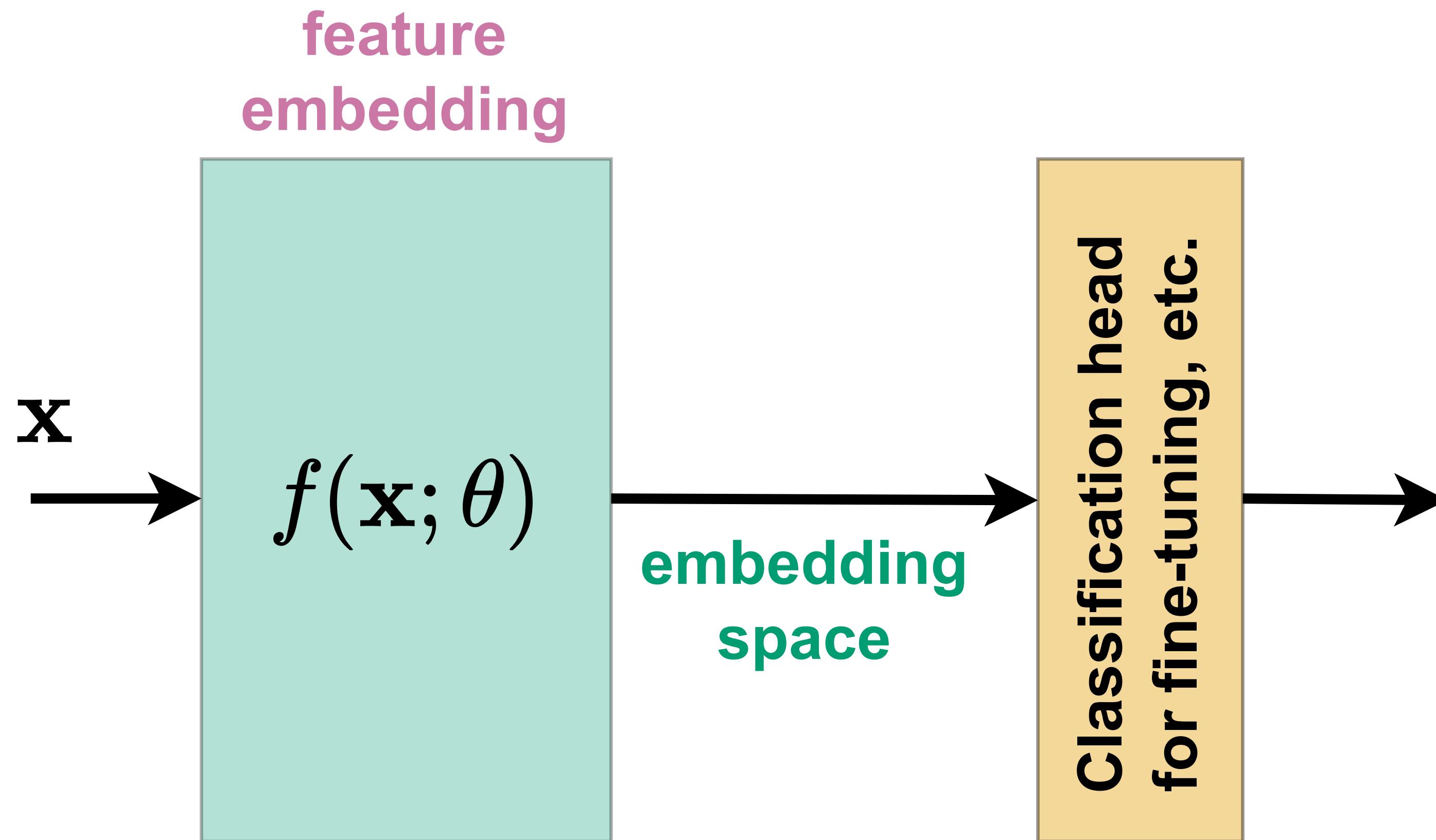
Embedding spaces of large models

Splitting a model into a feature extraction and decision



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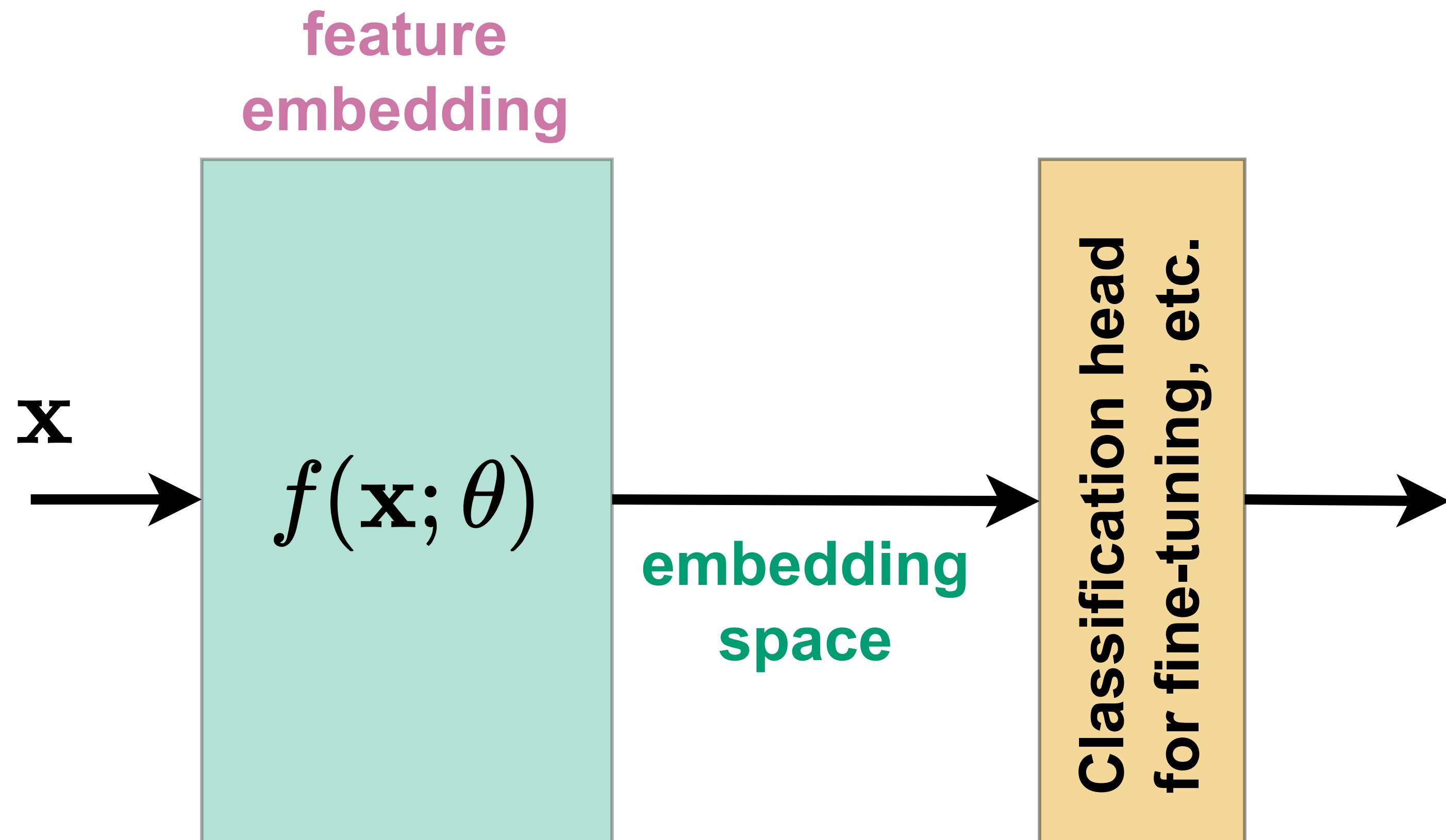
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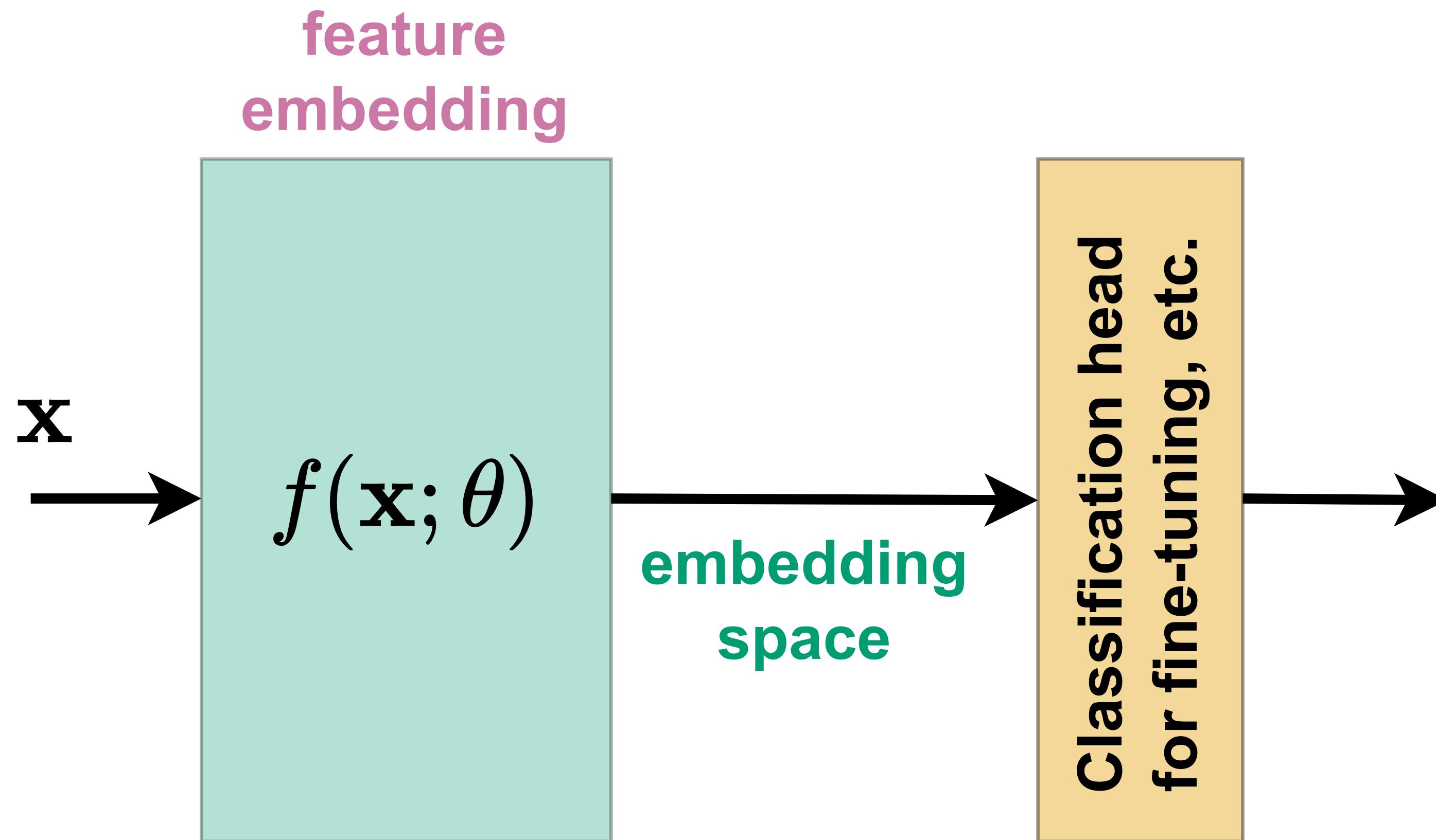


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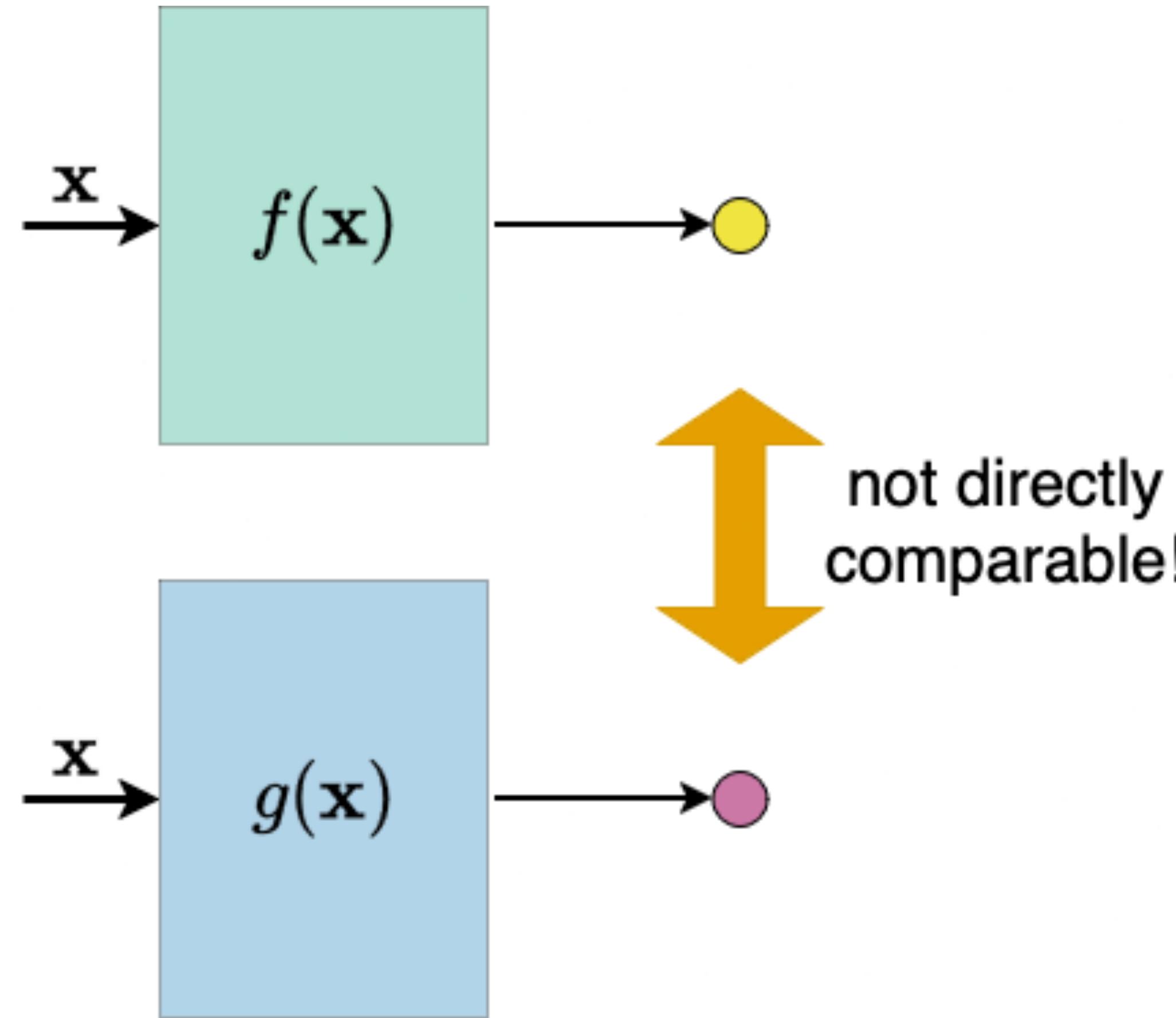
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Idea: can we compare the embedding spaces of models to tell the difference between them?

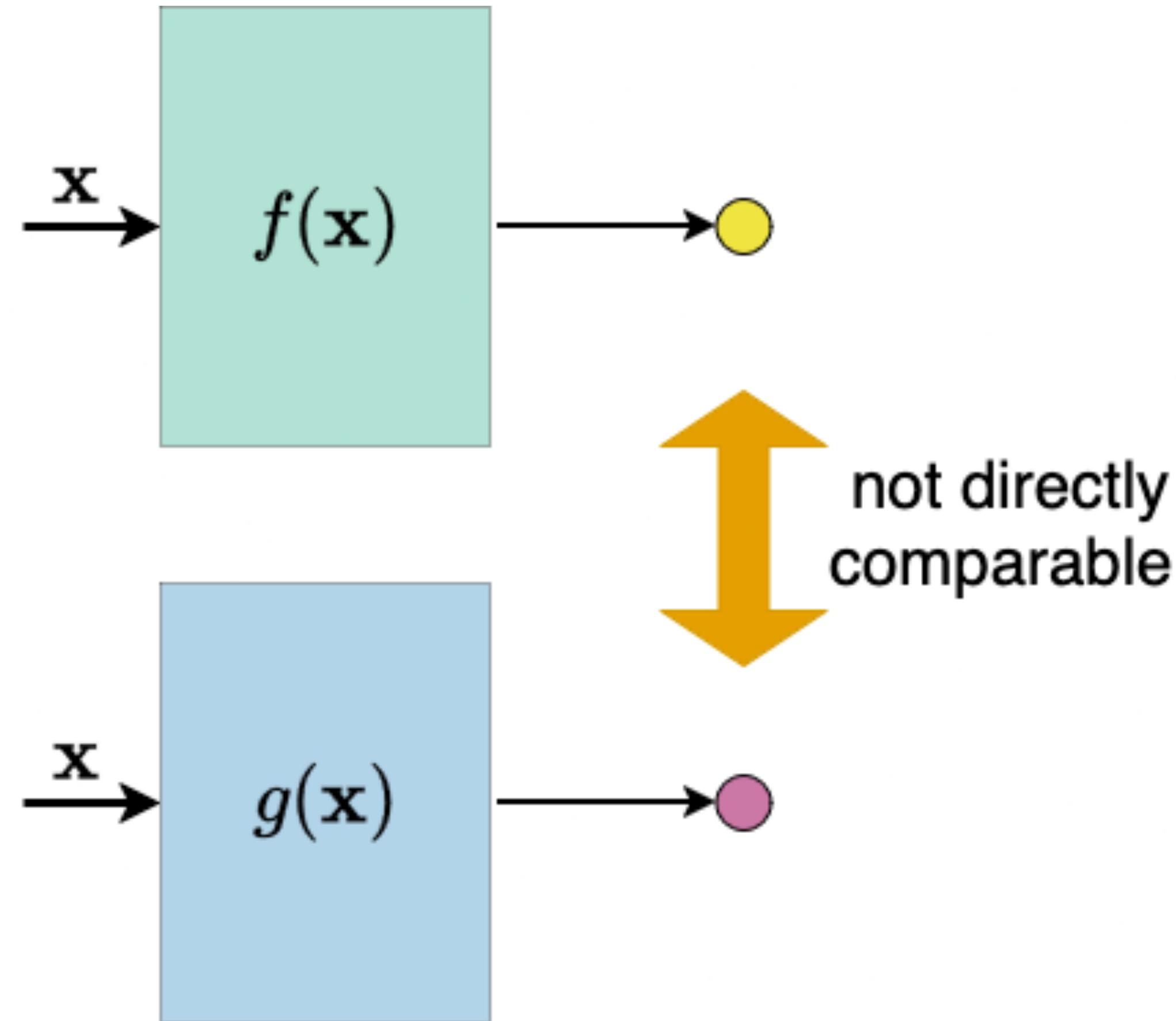
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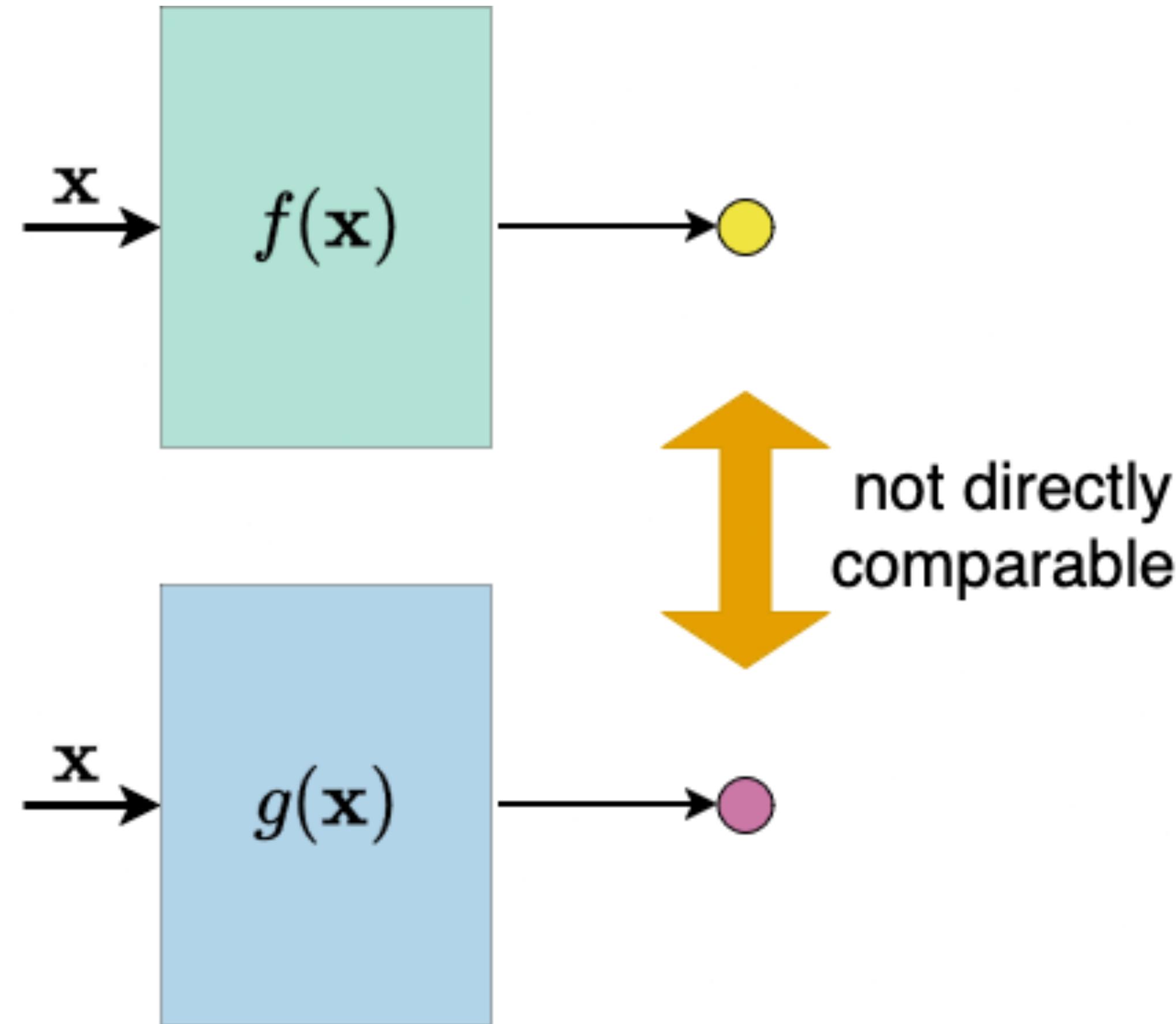
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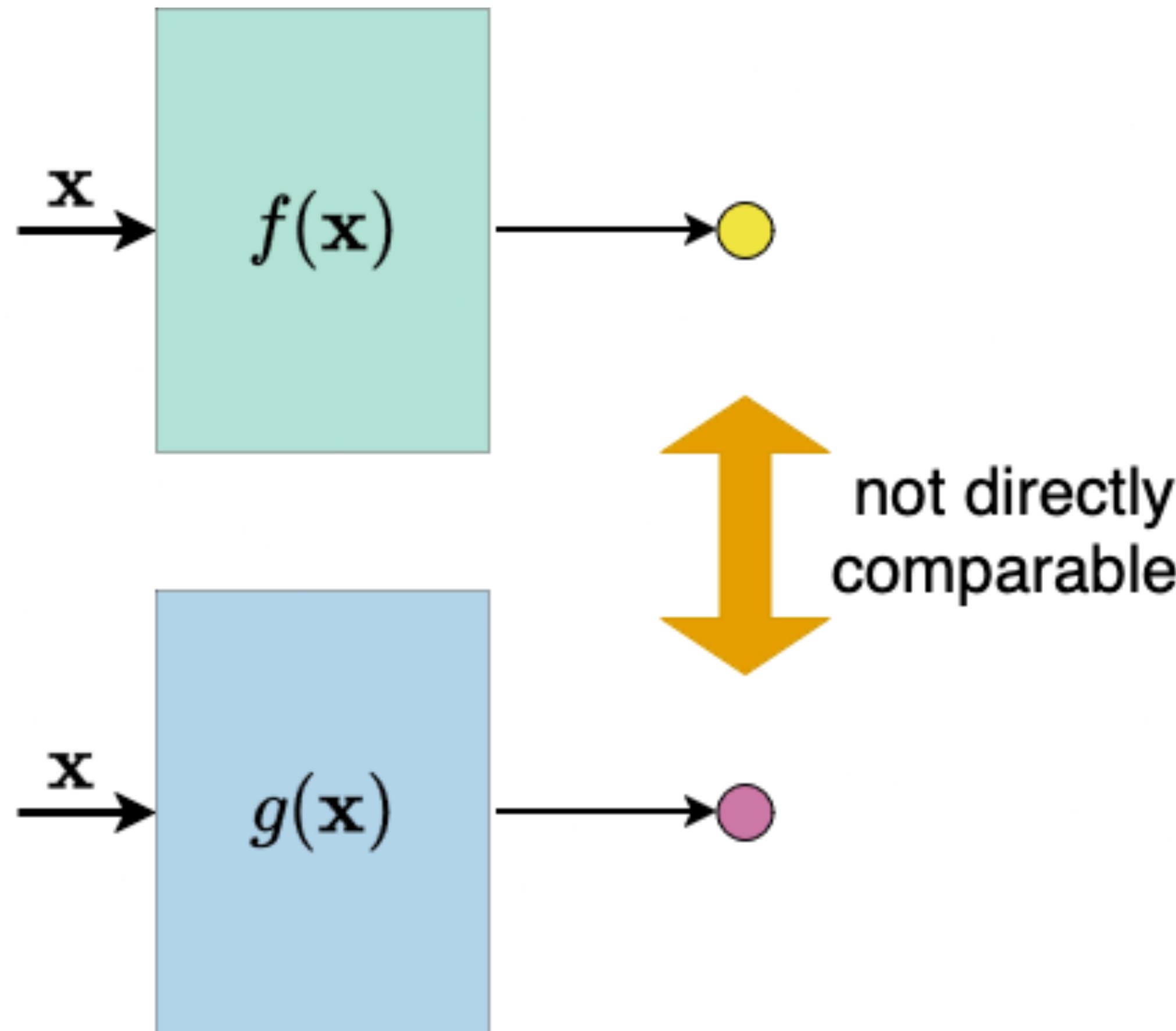


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- Different **dimensions**.

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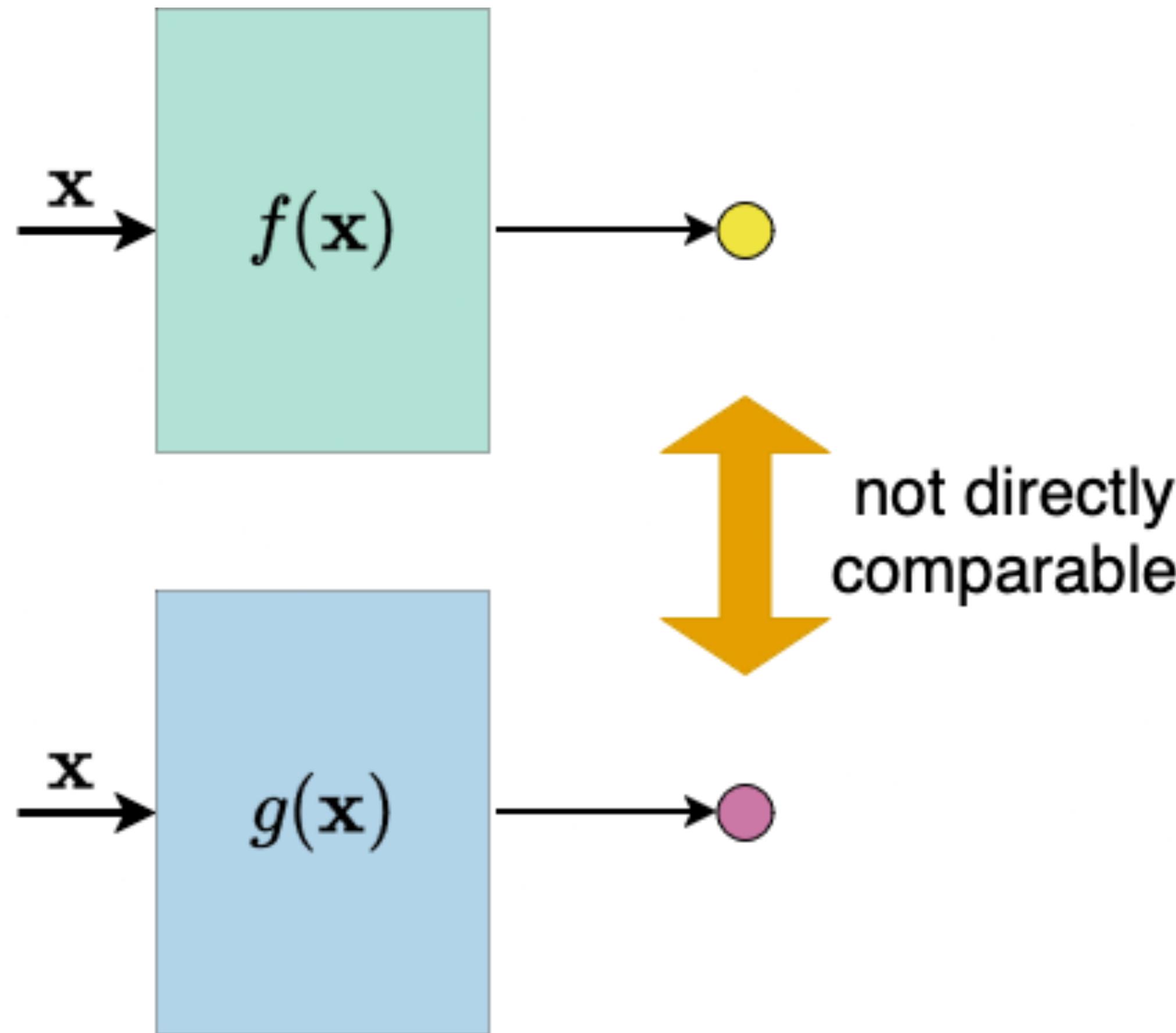


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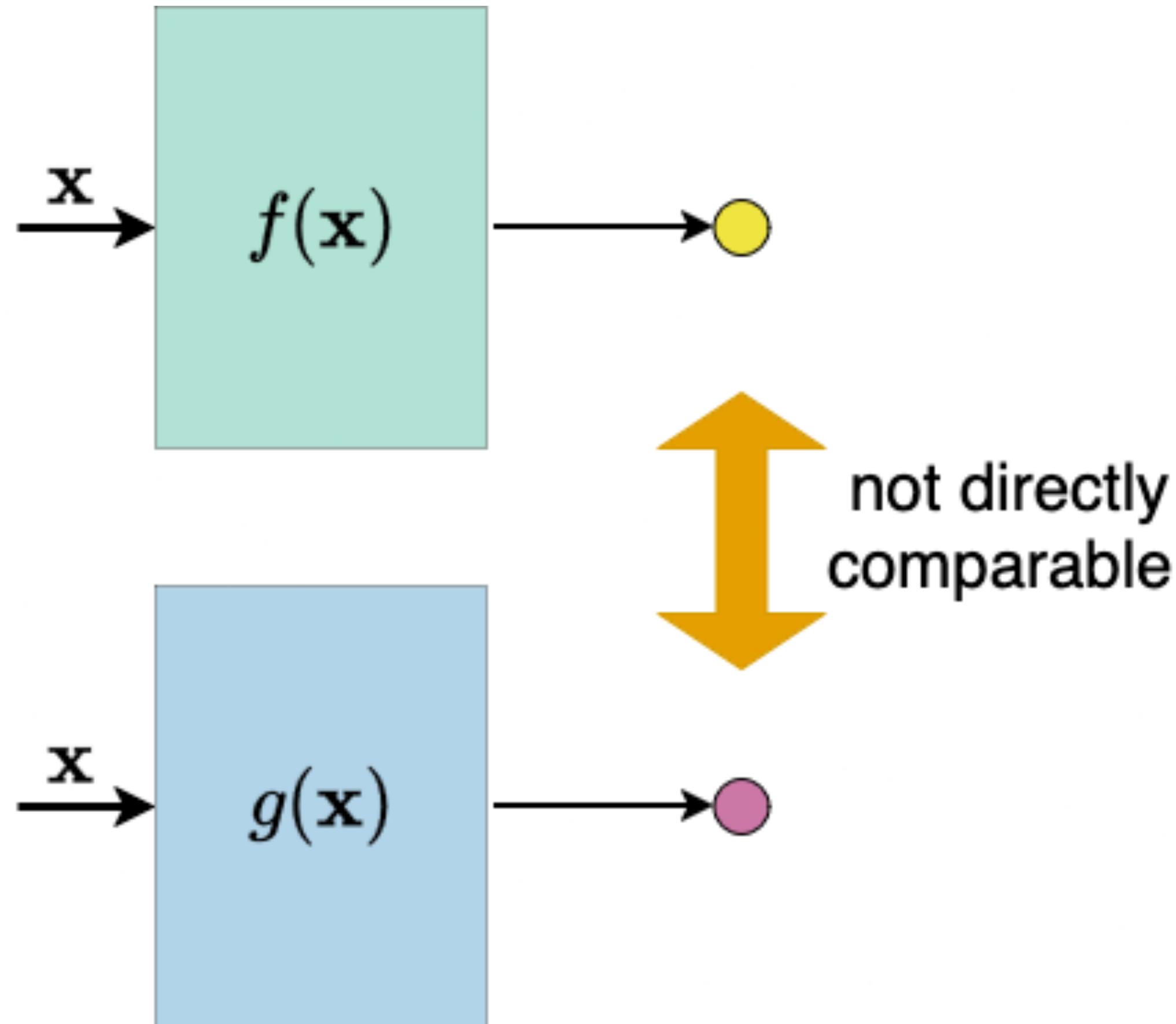


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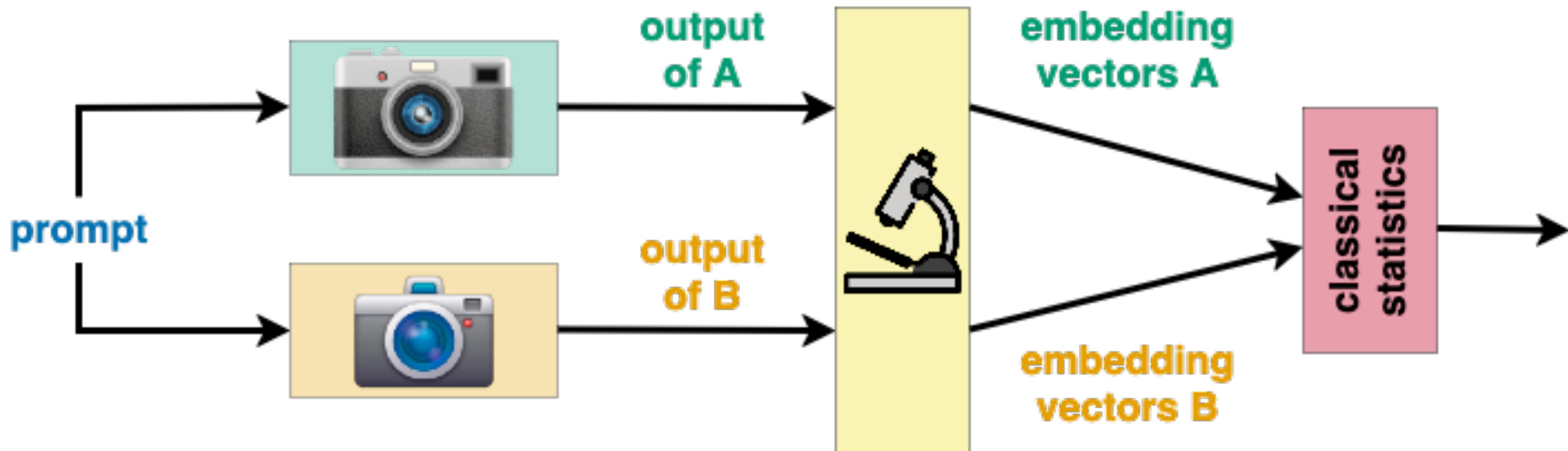
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Unlike with classification, we need to compare the outputs of the generative models.

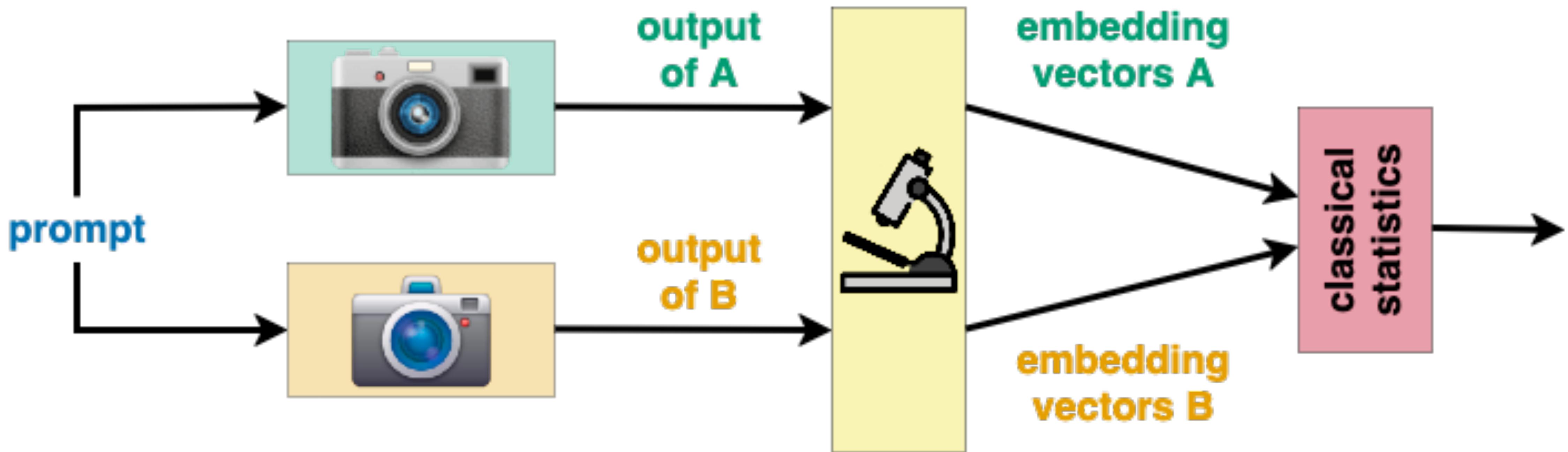
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Use the embedding space to compare outputs of models



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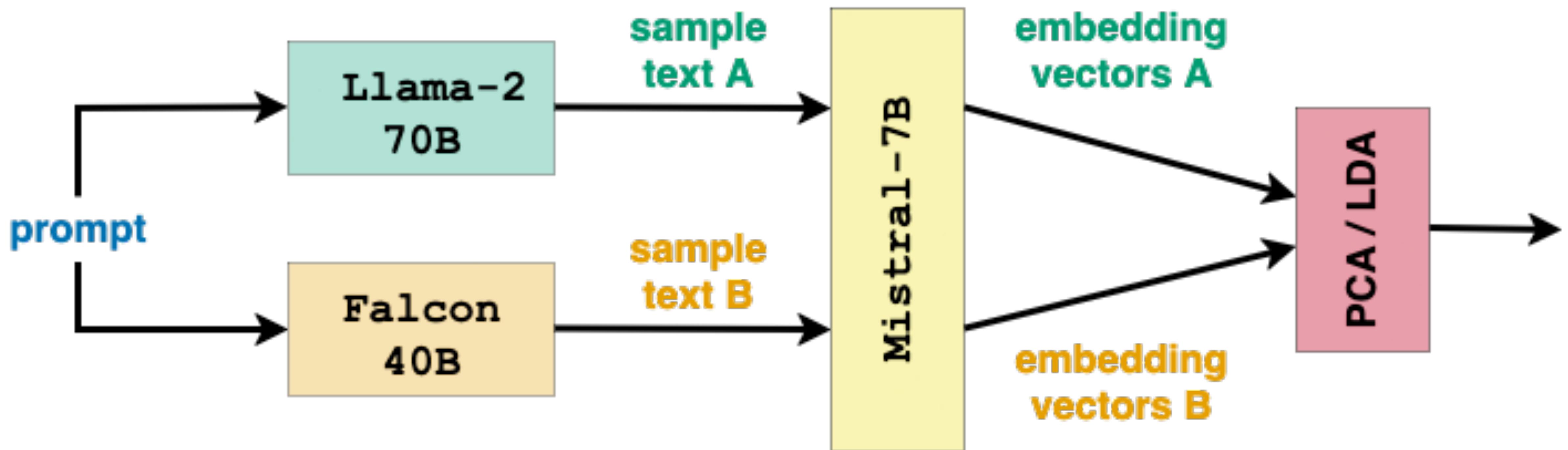
Use the embedding space to compare outputs of models



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

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

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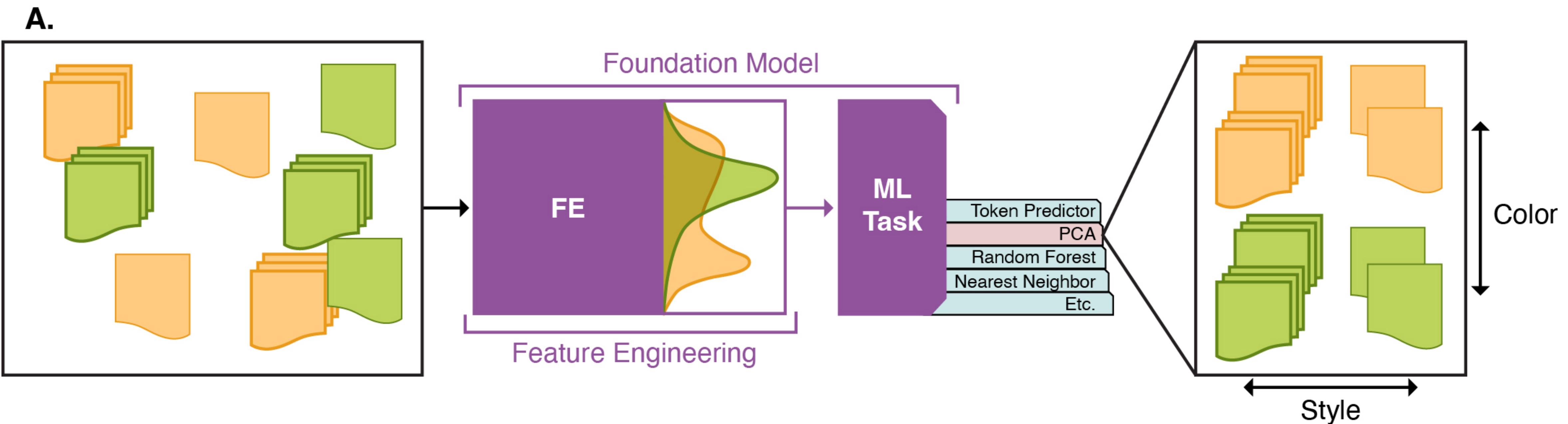
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- **Multilingual-e5-large**: extracts sentence embeddings from text in different languages to 1024-dimensional embedding vectors. 60M parameters, context window of 512 tokens and long text is truncated to fit within this window.
- **Data Filtering 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.

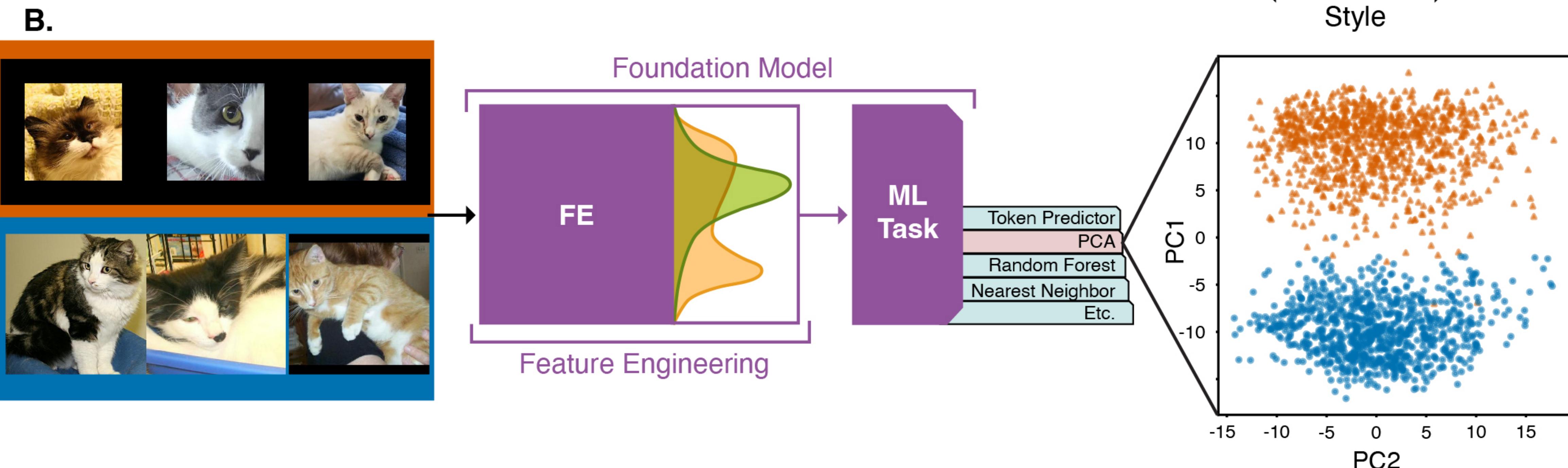
The generic approach in different contexts

The structure is similar, but the models are different



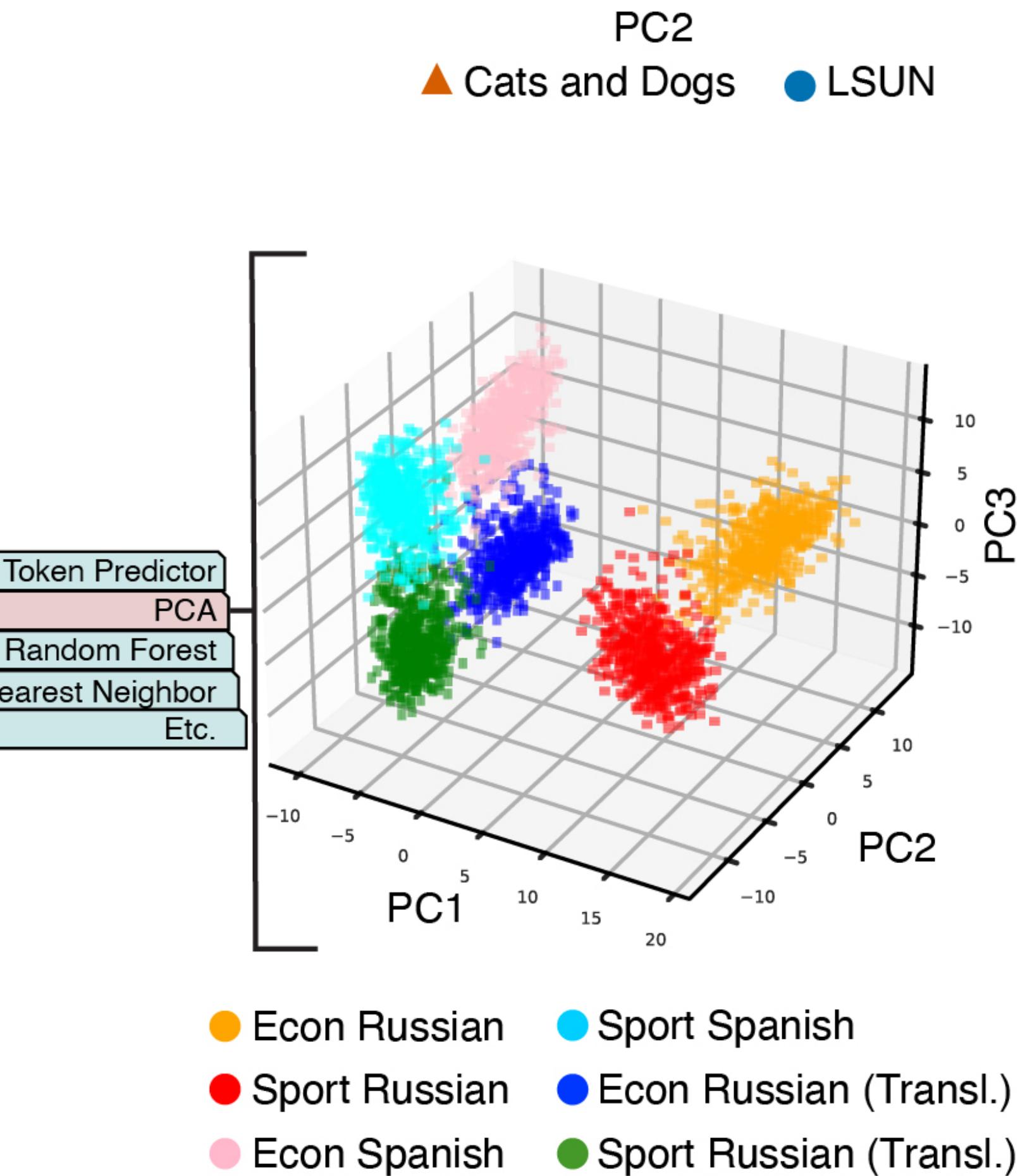
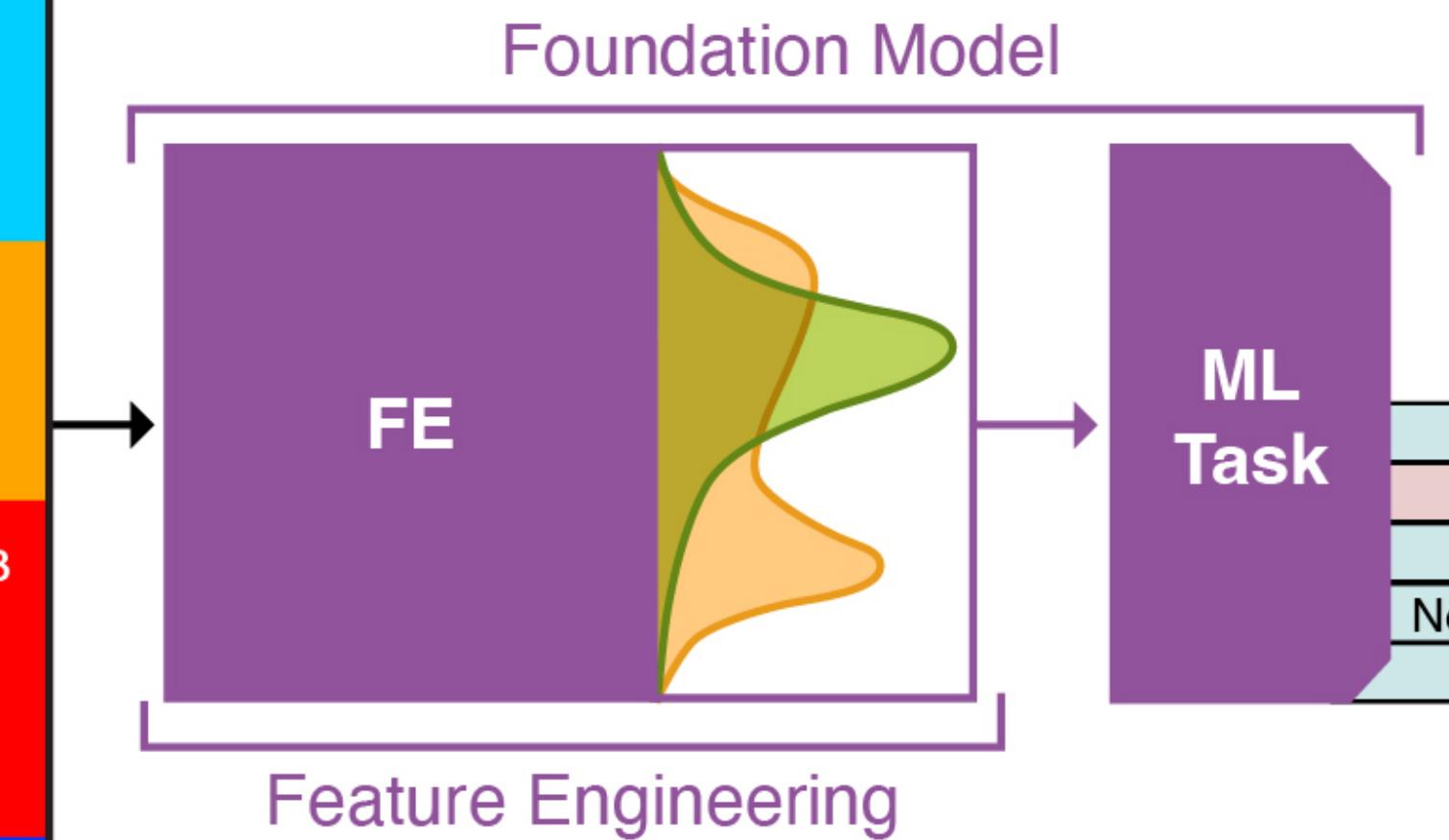
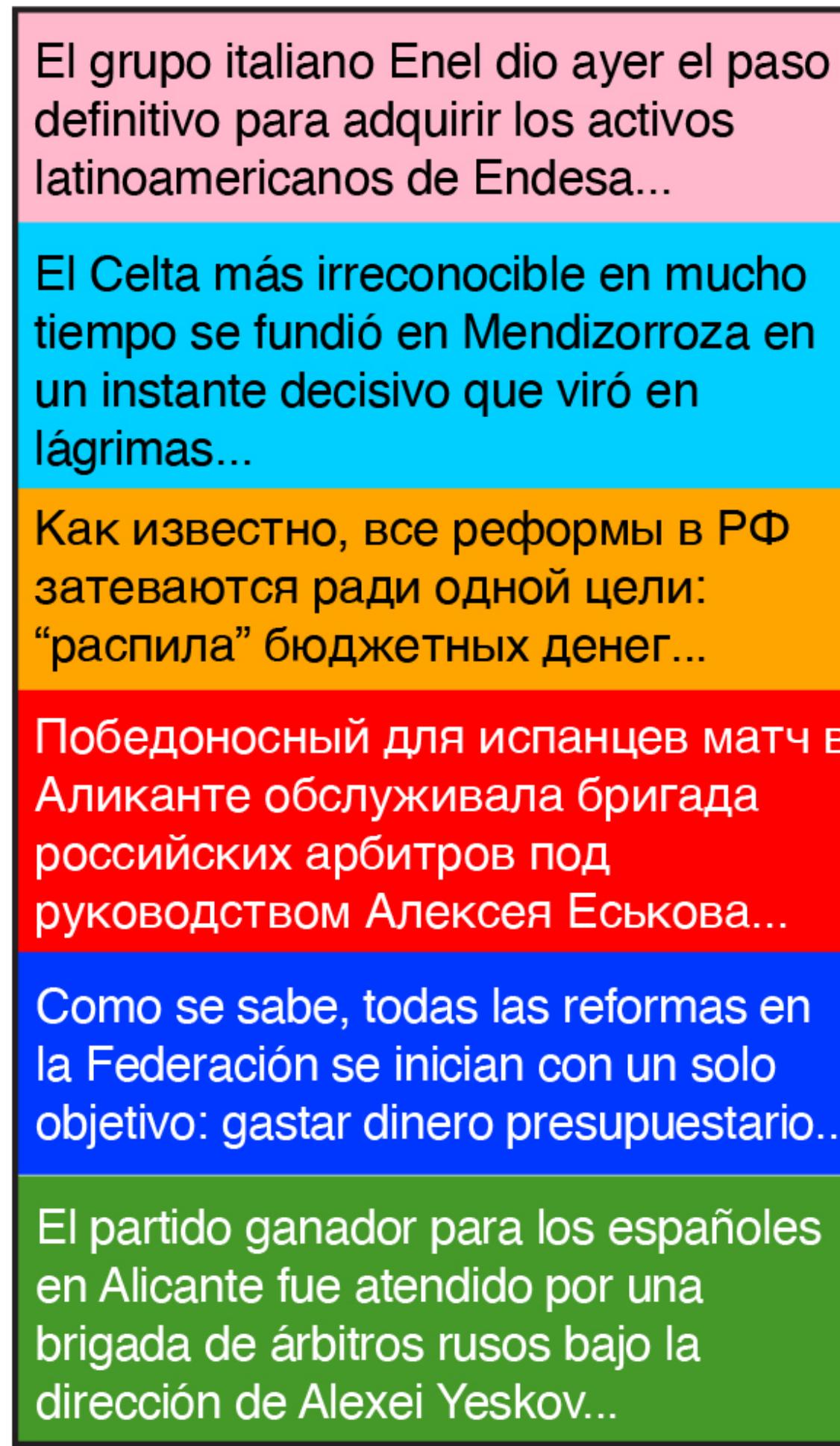
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1. Embed real data and AI-generated data to see if the embedding vectors cluster.
2. Unsupervised clustering of embedded data recreates the labels in the original.
3. Detect the difference between real and machine-translated data.

A.**PCA****Stack exchange**

PC2

PC1

- Real
- Mixtral 8x7B
- Falcon 40B
- Llama-2 70B

LDA

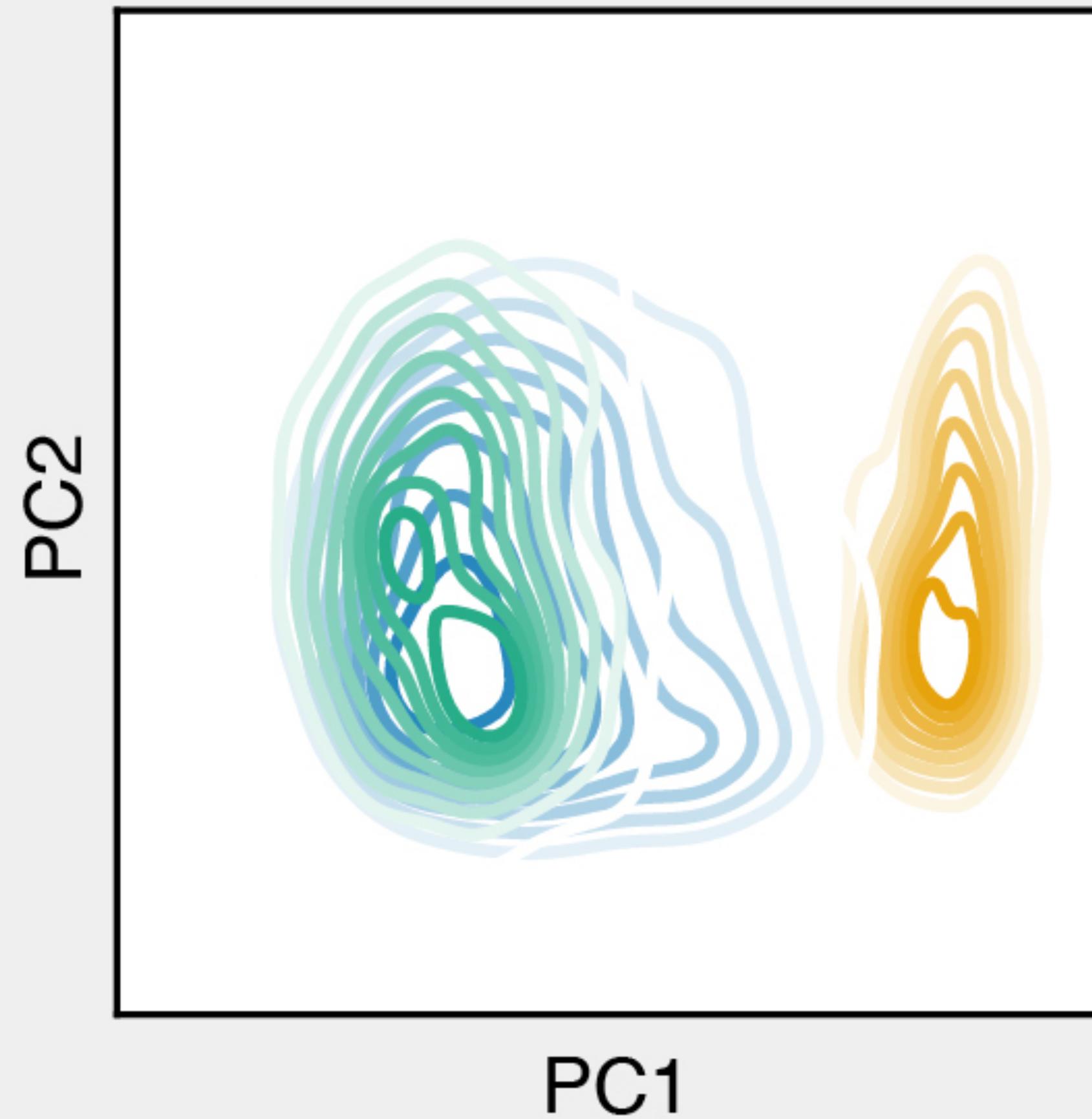
LD1

LD2

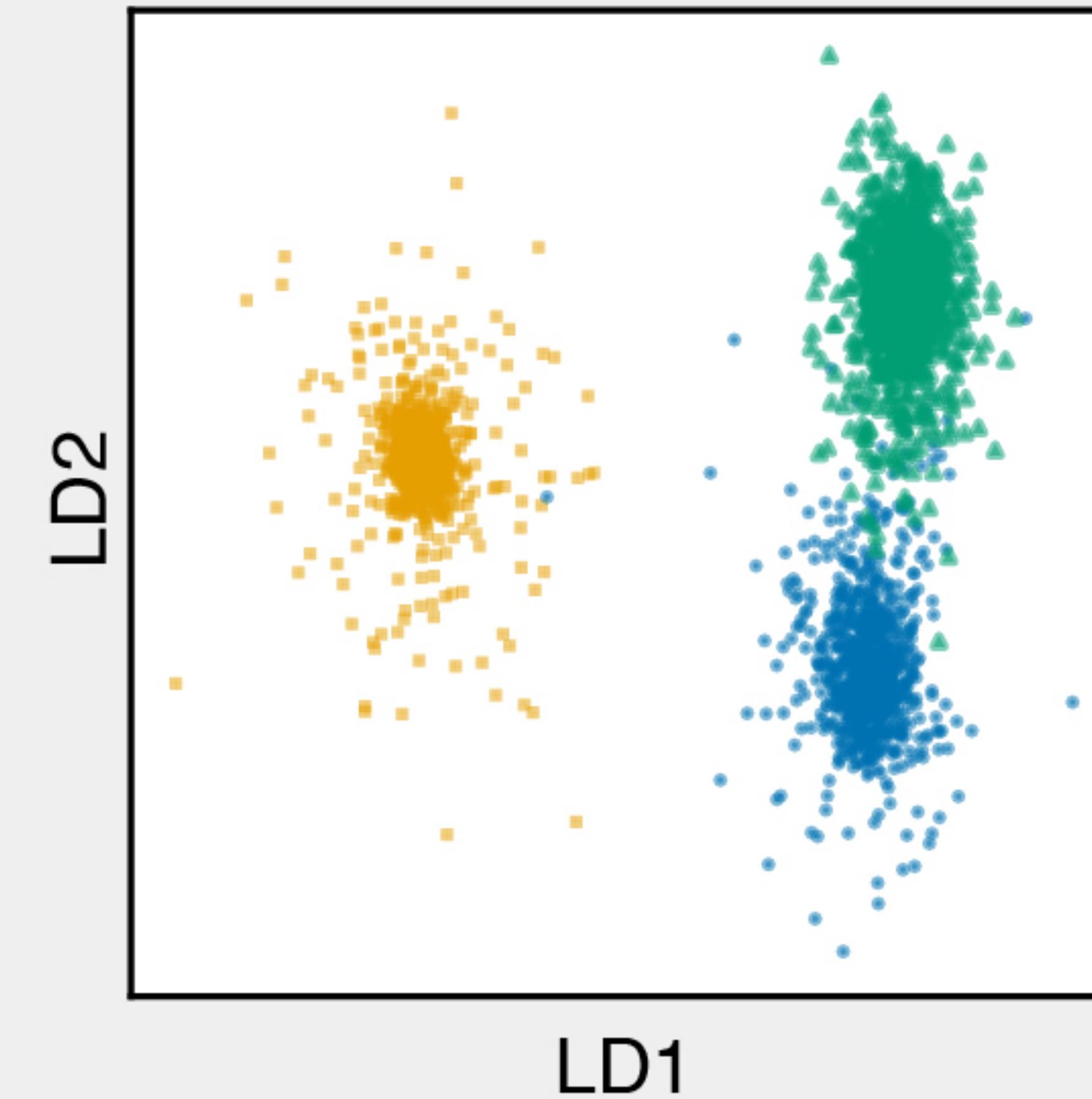
LD3

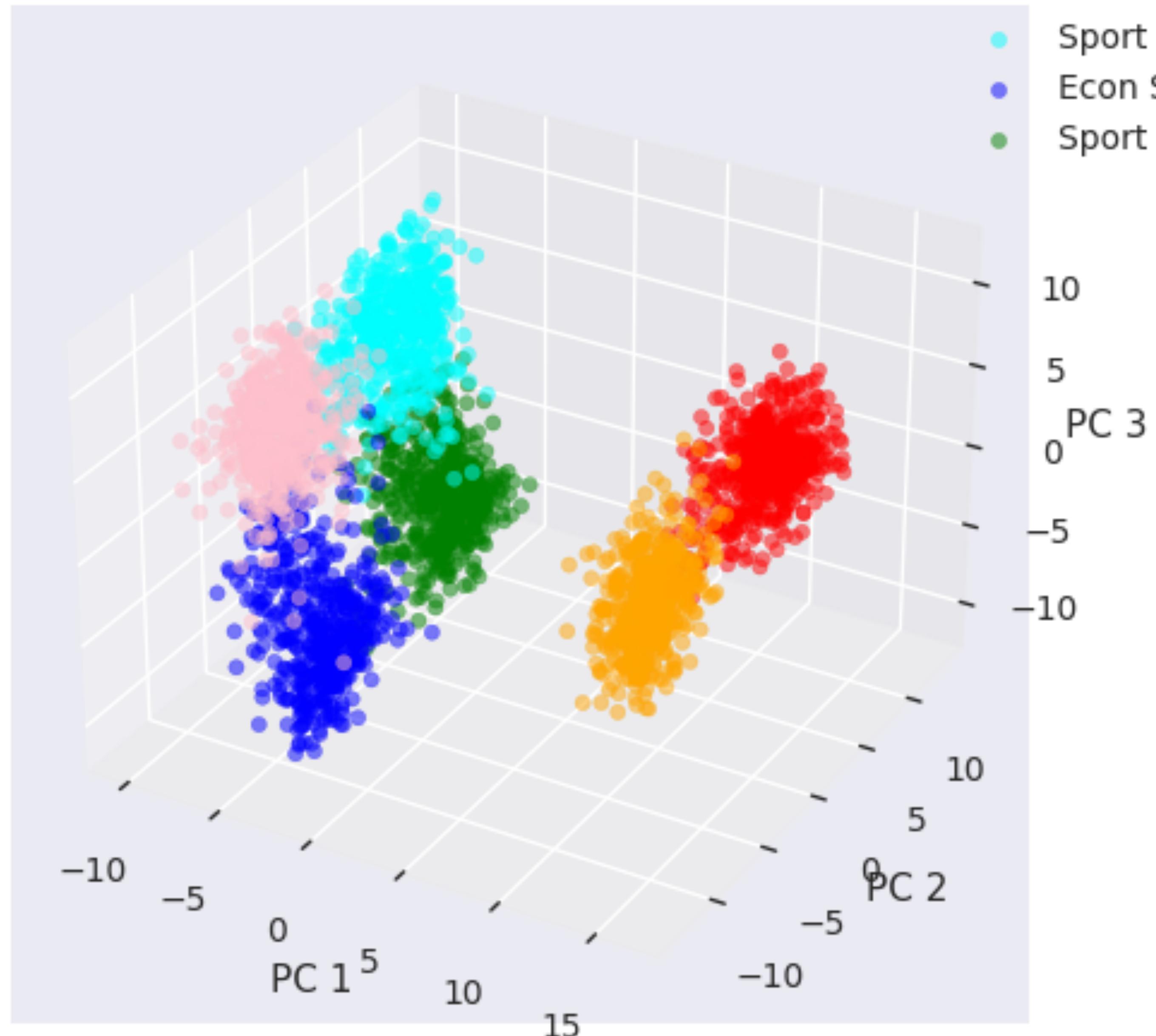
C.

Economics abstracts



● Real ● Prompt 1 ● Prompt 2





- Econ Spanish
- Sport Spanish
- Econ German
- Sport German
- Econ Spanish (Transl.)
- Sport Spanish (Transl.)

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



HarmonyOS 4.0



Samsung UI 7.0

Some takeaways and ongoing work

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HarmonyOS 4.0

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



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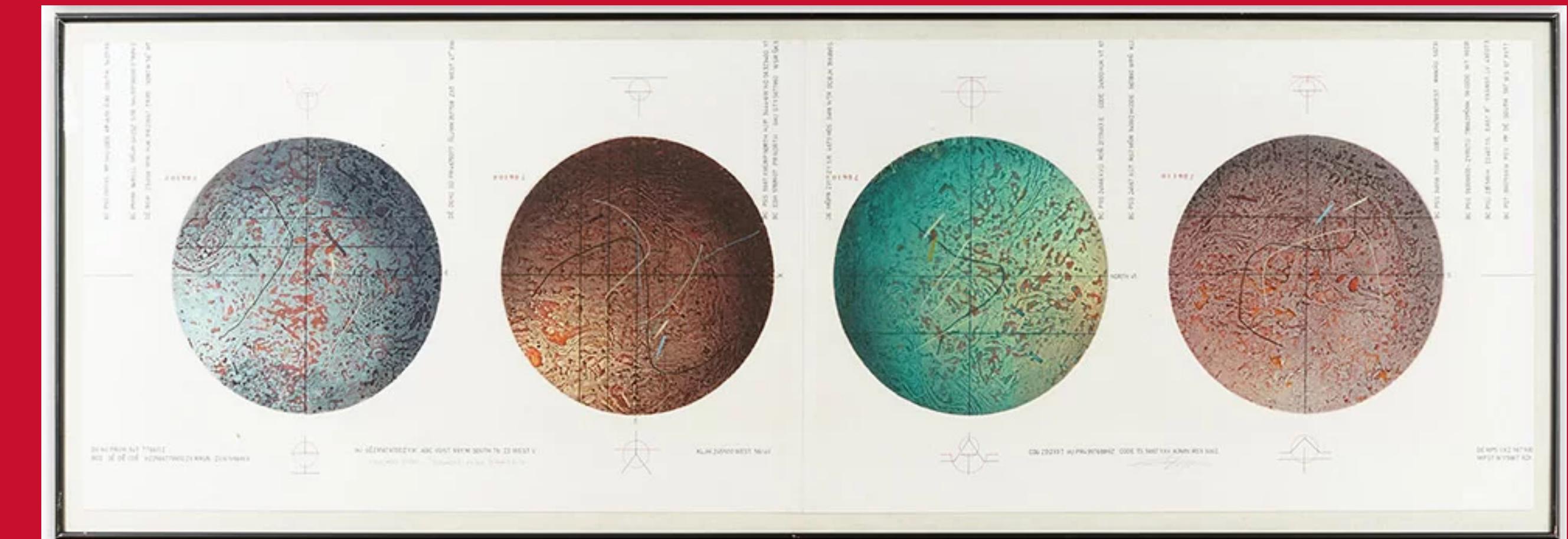
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- Forensics applications: comparing models, detecting deepfakes, etc.
- “Model DNA”: fine-tuned or “lightly modified” models make minor modifications to the embeddings.
- Use post processing to “align” embeddings for calibration, ensembling, federated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



Samsung UI 7.0

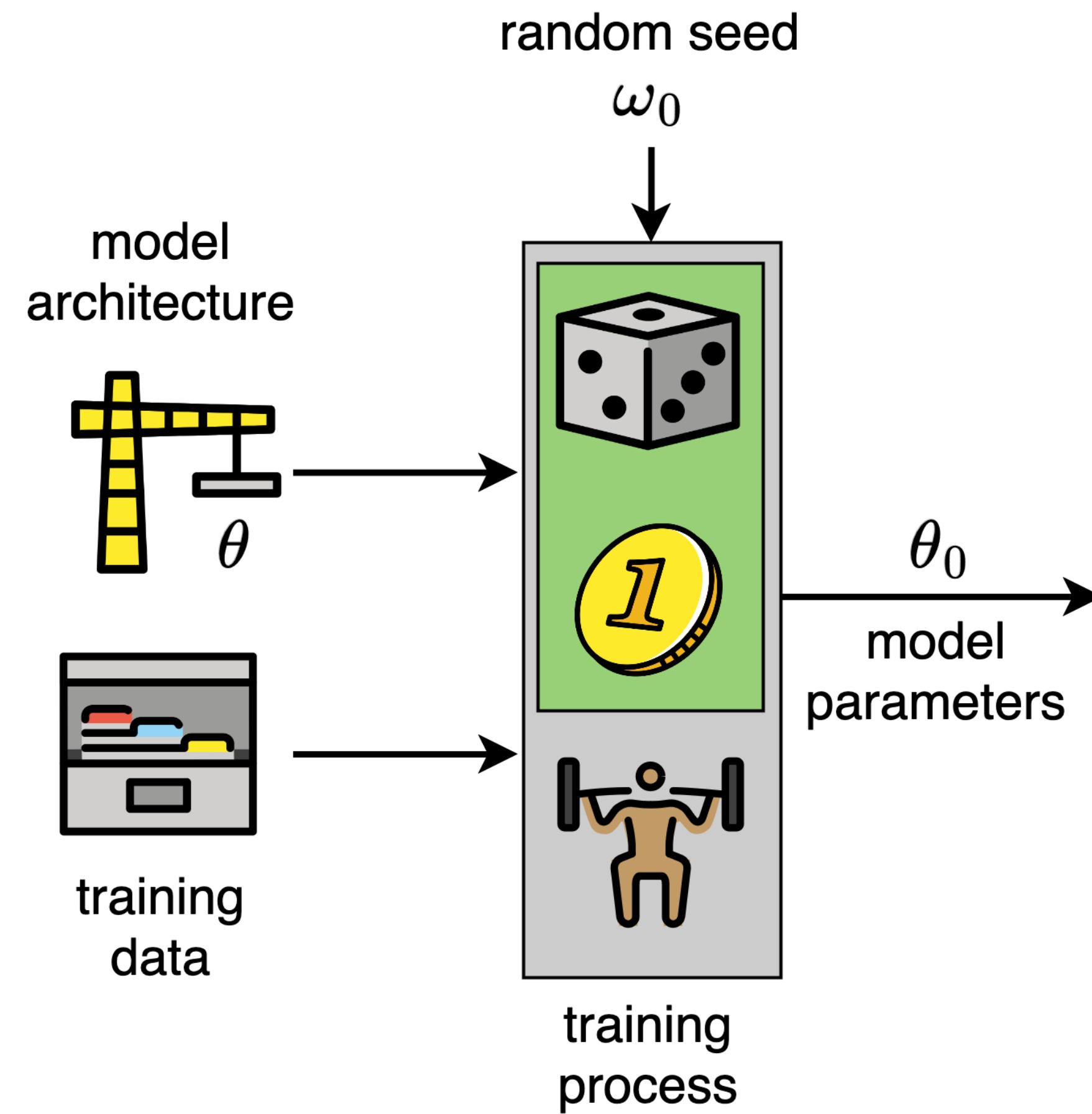
Model comparisons in training



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

Variability in the training process

Is training reliable?



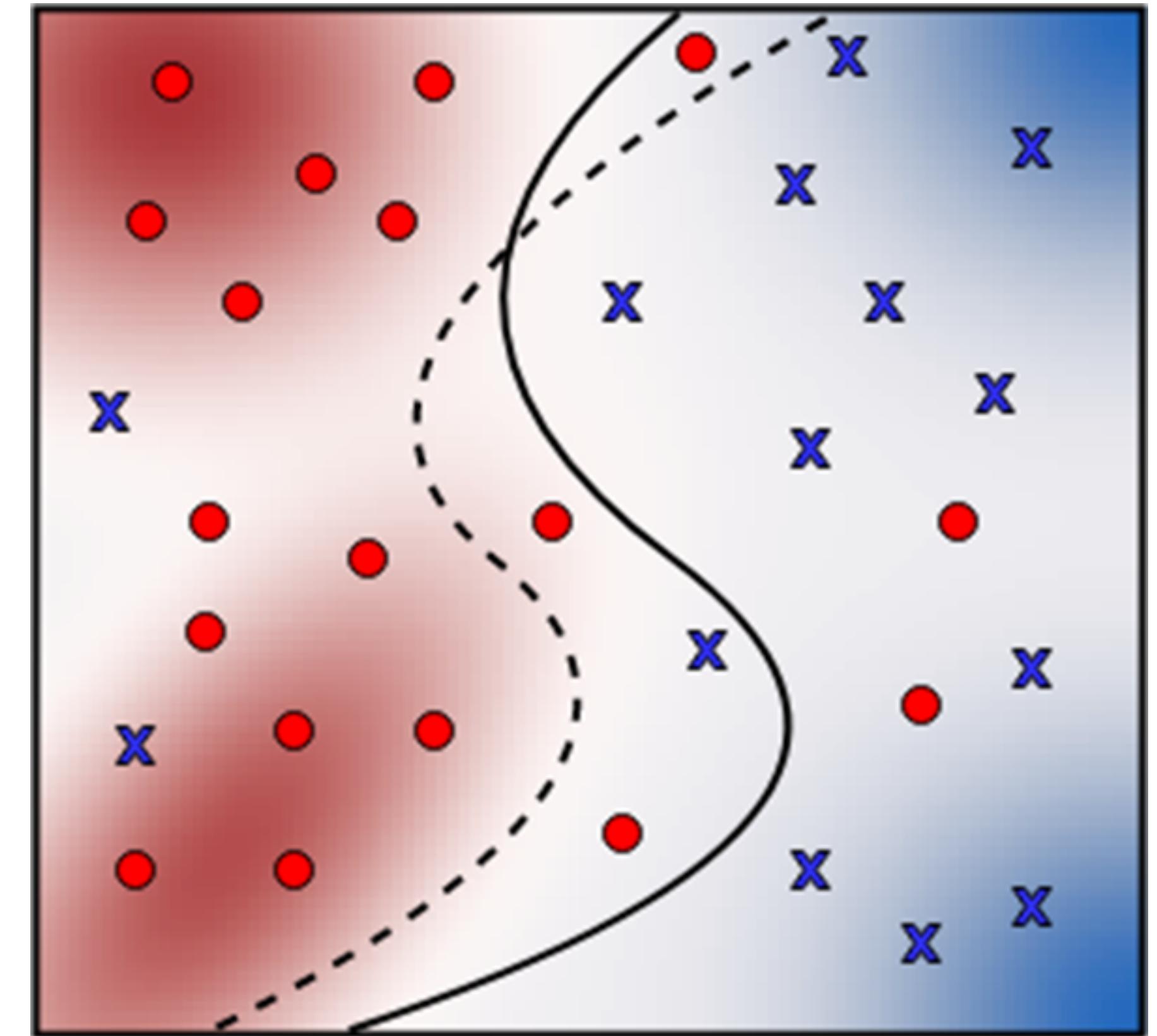
Each time we run the training algorithm on the **same training set, same architecture, same algorithm**, we still use (pseudo-)**independent randomness**.

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

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

Comparing two runs of training

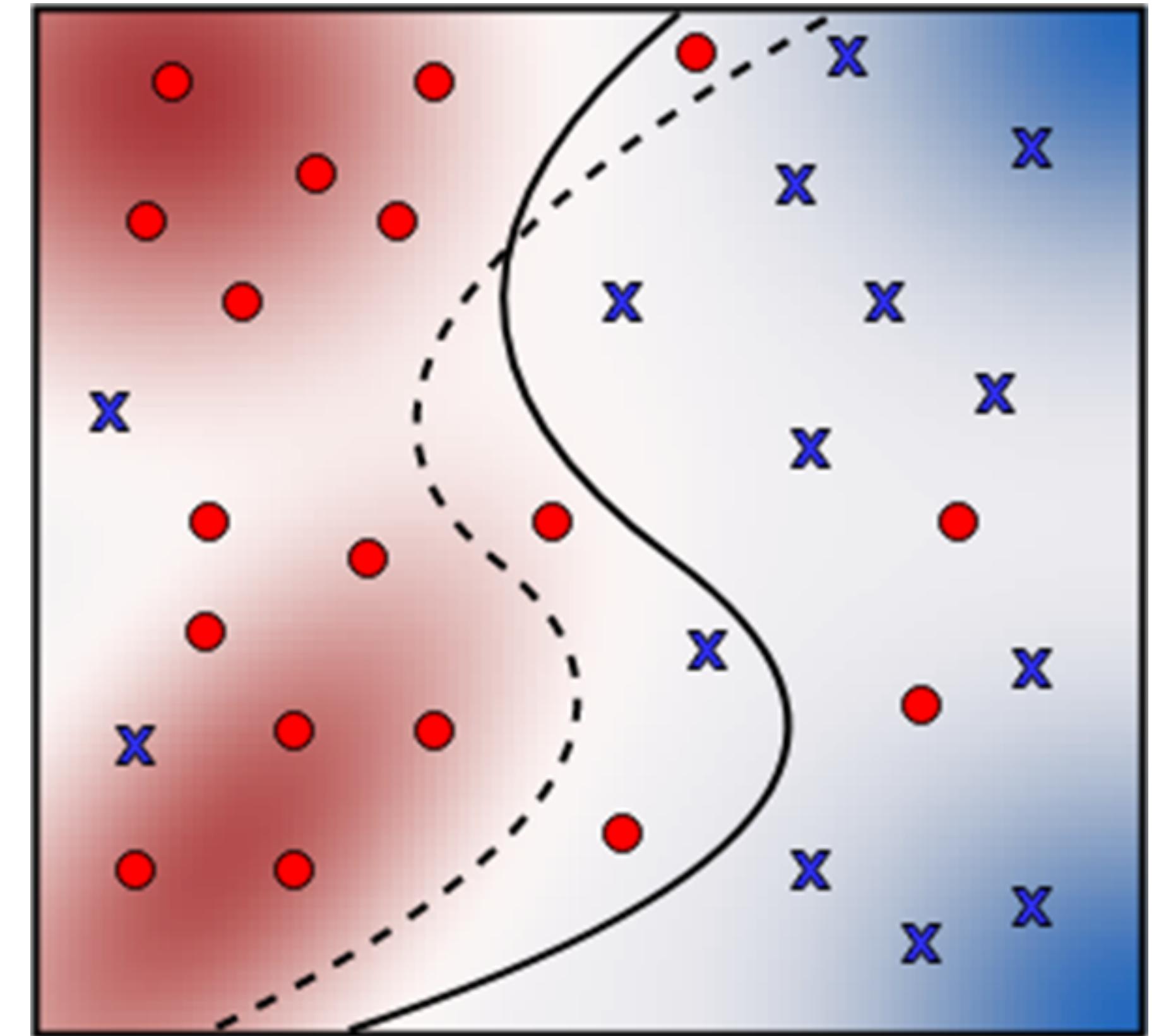
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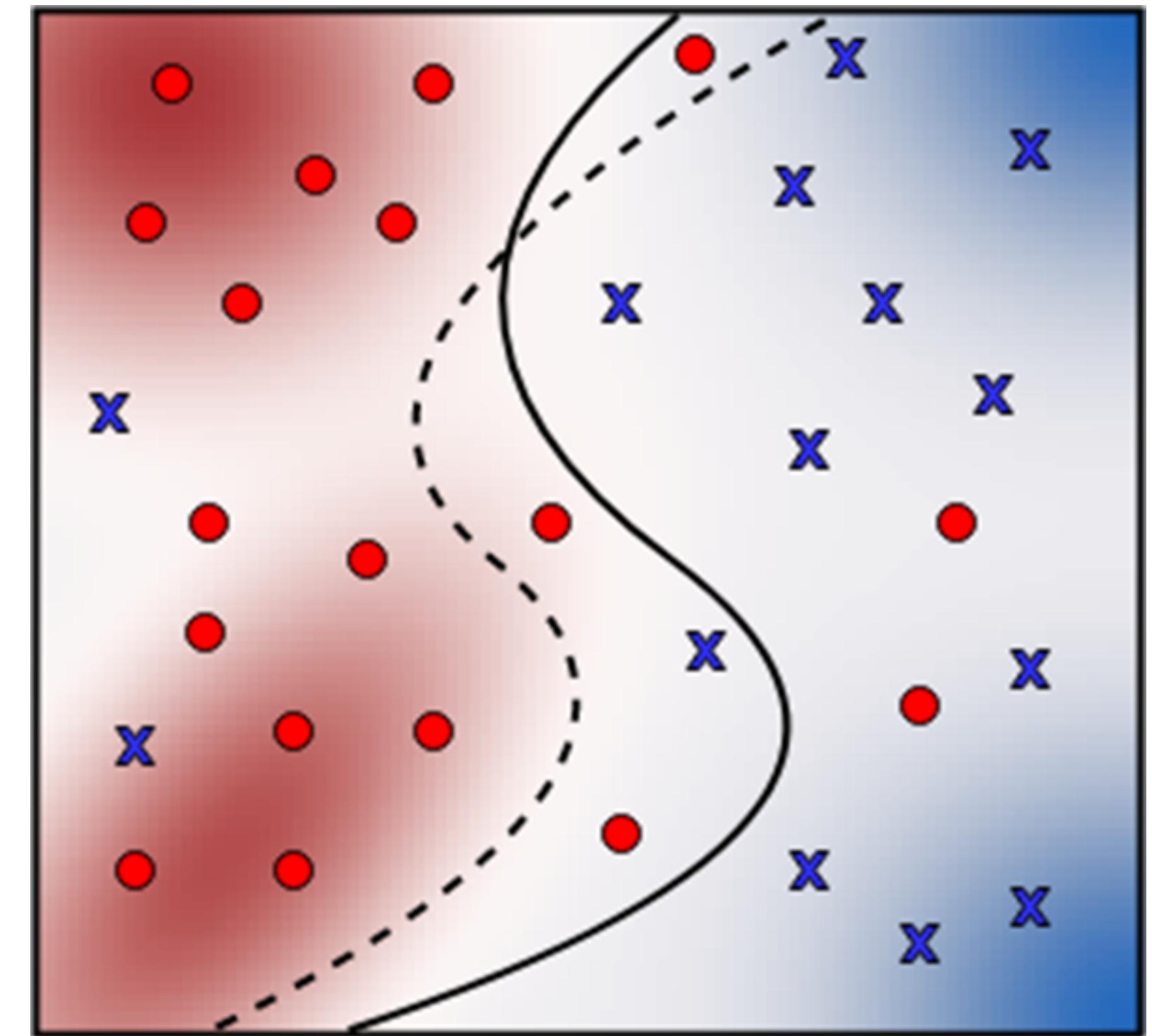
- Determining if one model is "better" than another is **not well-posed**.



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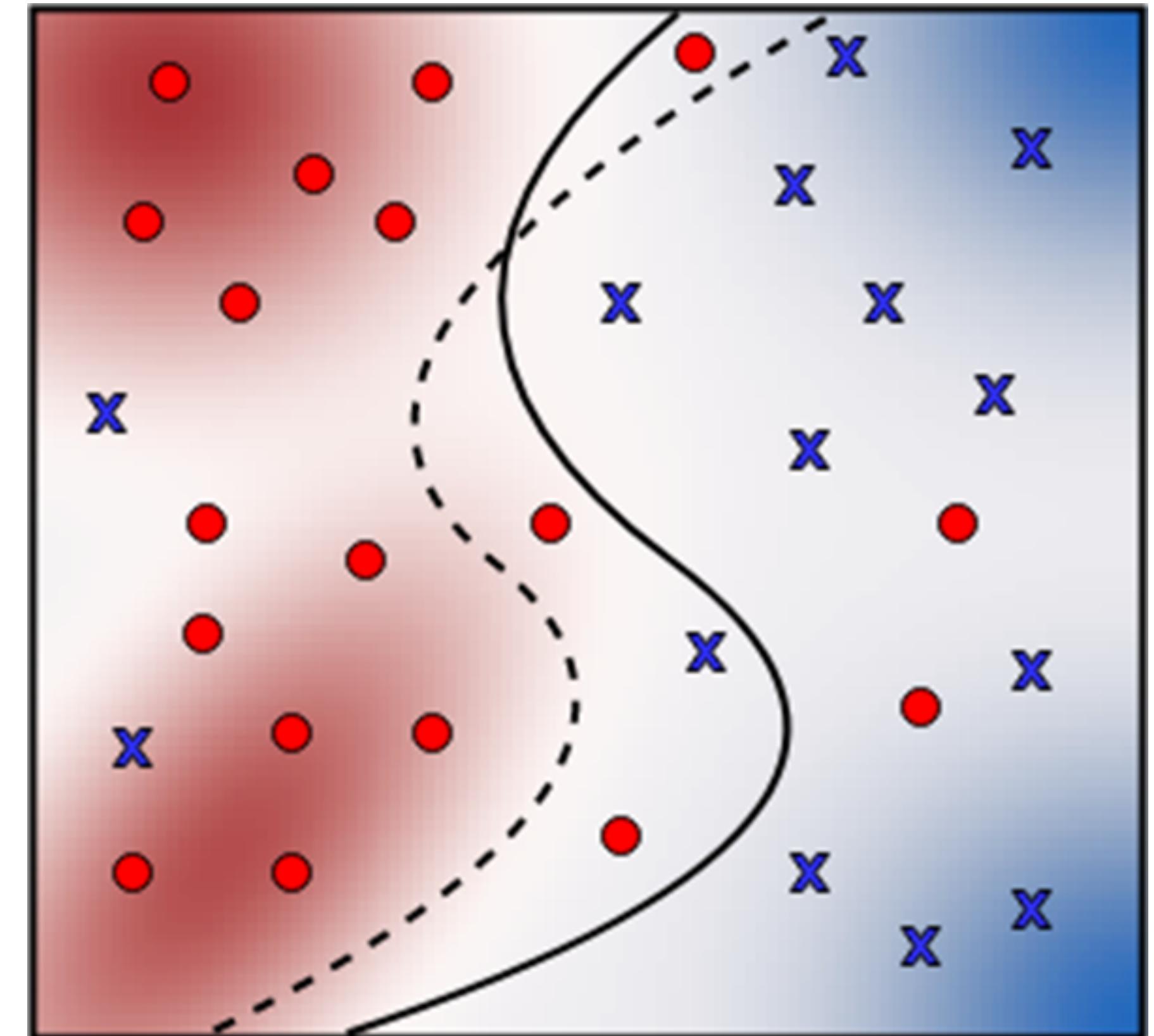


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Terms like the **Rashomon effect**^{[1][2][3]}, **predictive multiplicity**^[4], or **prediction churn**^[5] have been used to describe this phenomena.



[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.

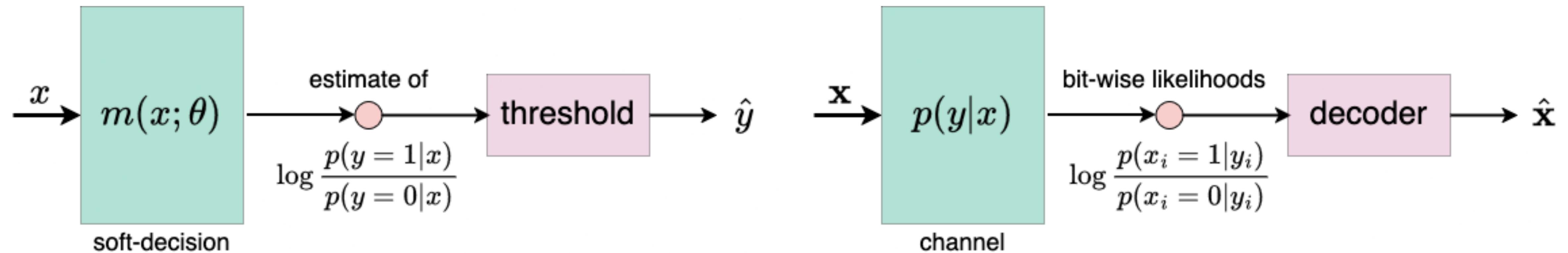
[3] Hsu, H., & Calmon, F. (2022). Rashomon capacity: A metric for predictive multiplicity in classification. *Advances in Neural Information Processing Systems*, 35, 28988-29000.

[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.

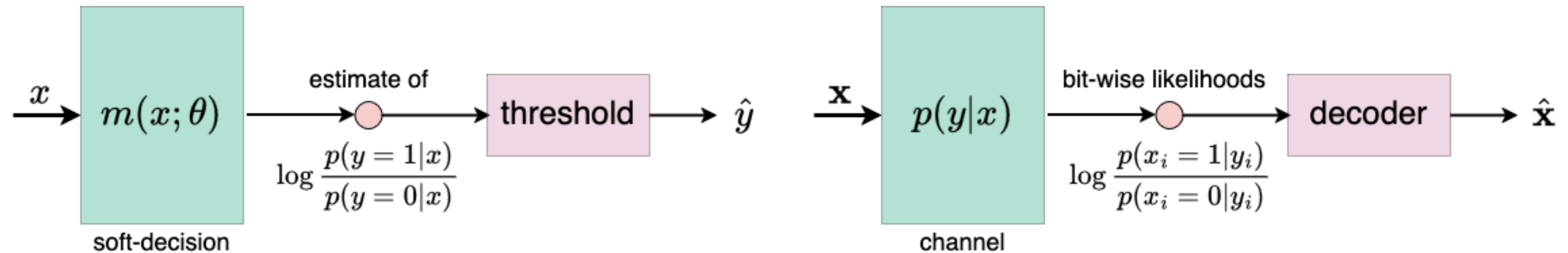
Hard decisions vs. soft decisions

Putting on a communications hat



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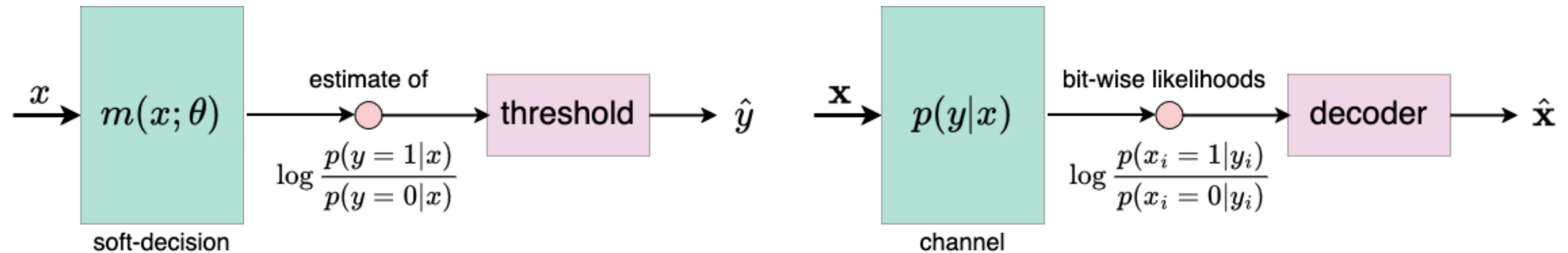
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Test error and **churn** measure differences in “hard decisions” $f: \mathcal{X} \rightarrow [L]$.

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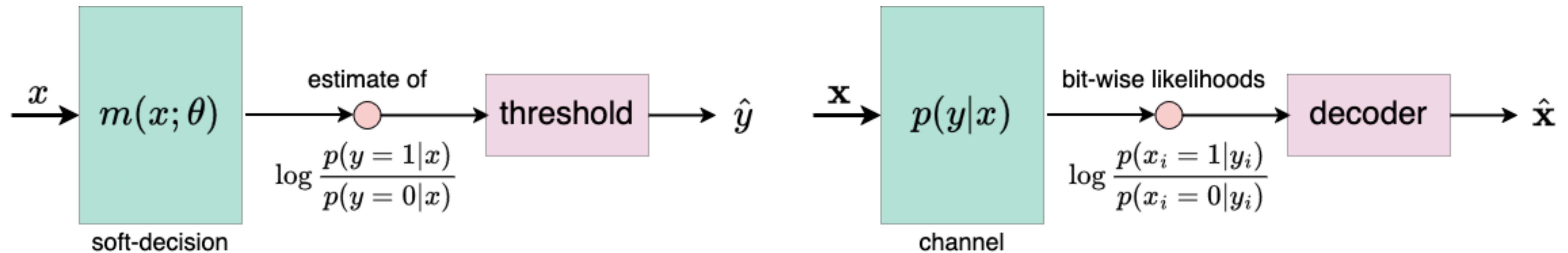


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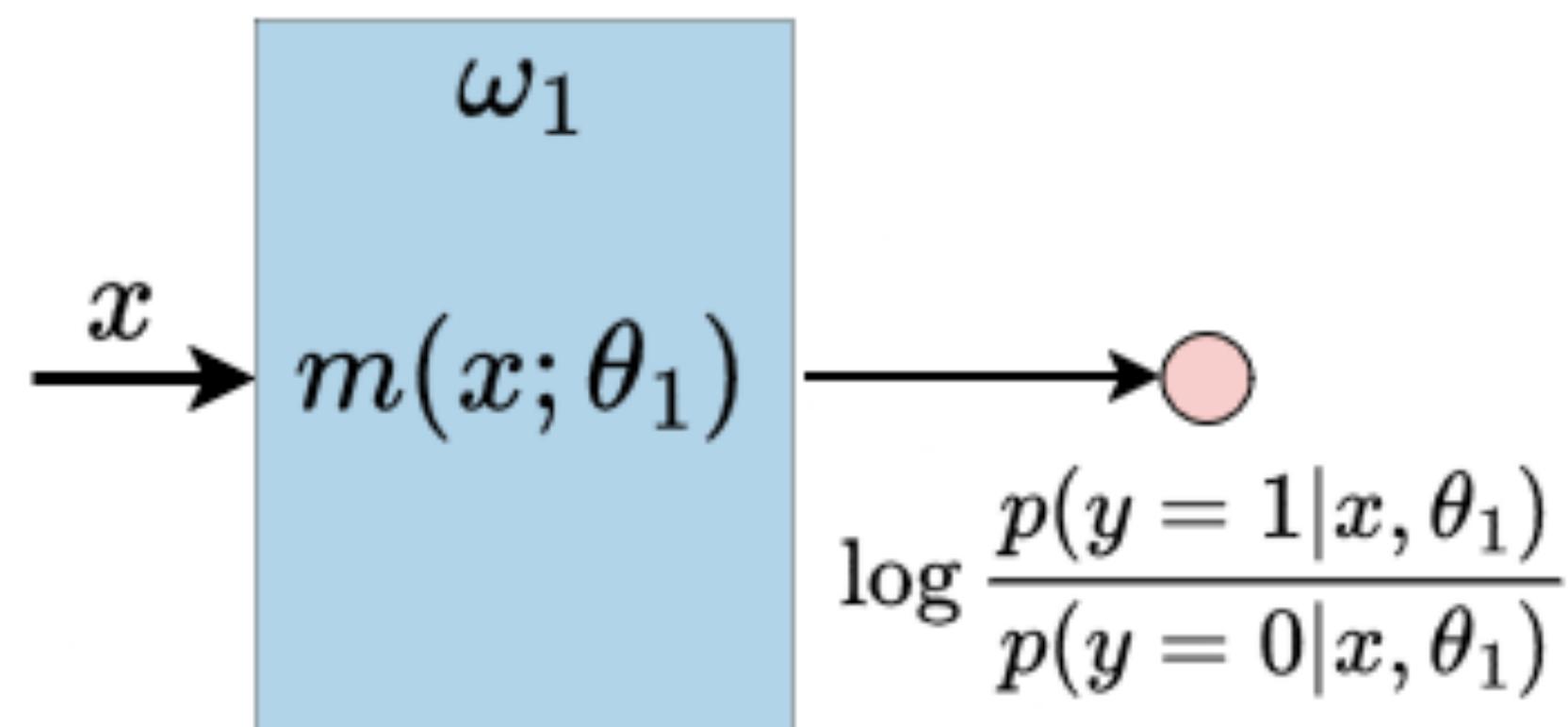
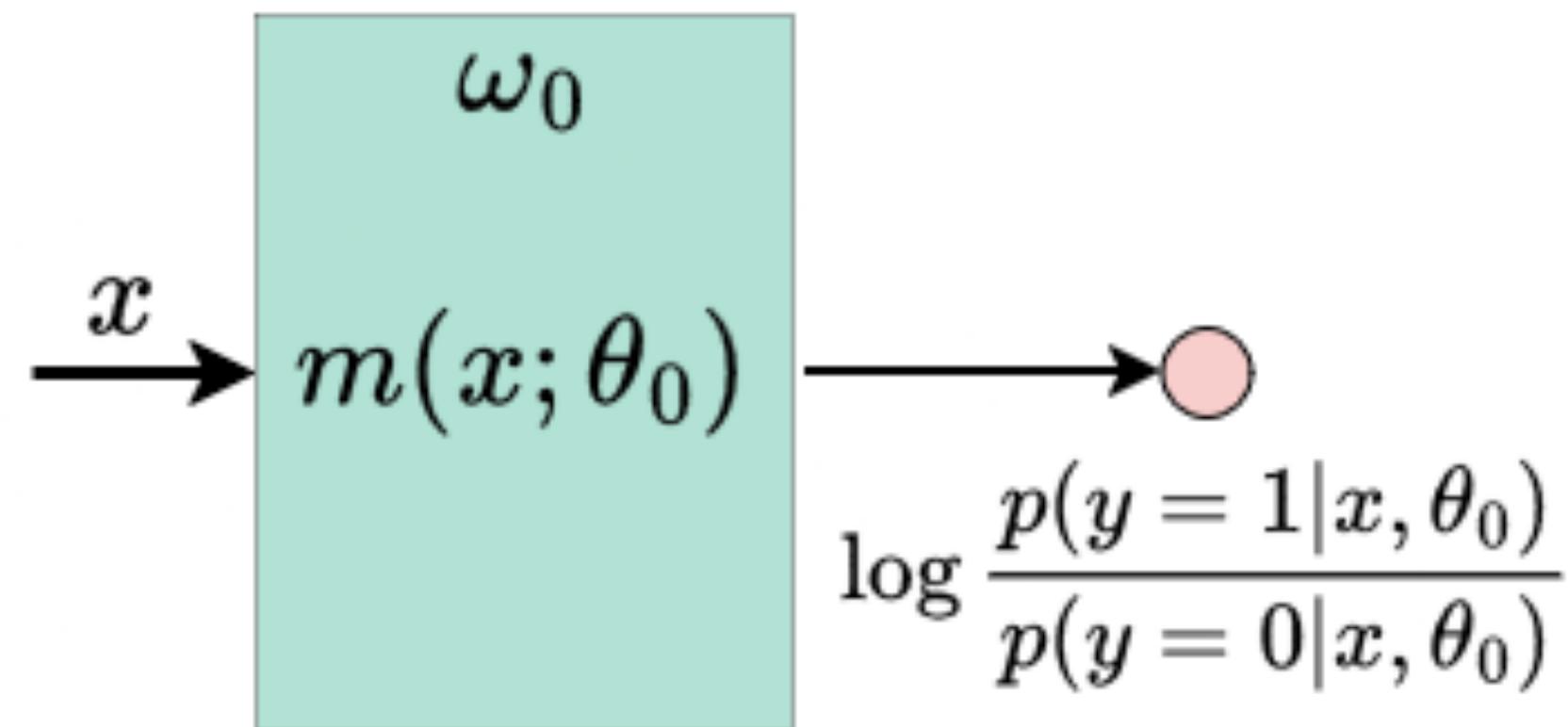


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- These are usually made using (softmax) probability estimates $\hat{p}(y|x, \theta)$.
- Instead look at **pre-threshold “soft decision”** $m(x|\theta)$ for the model.

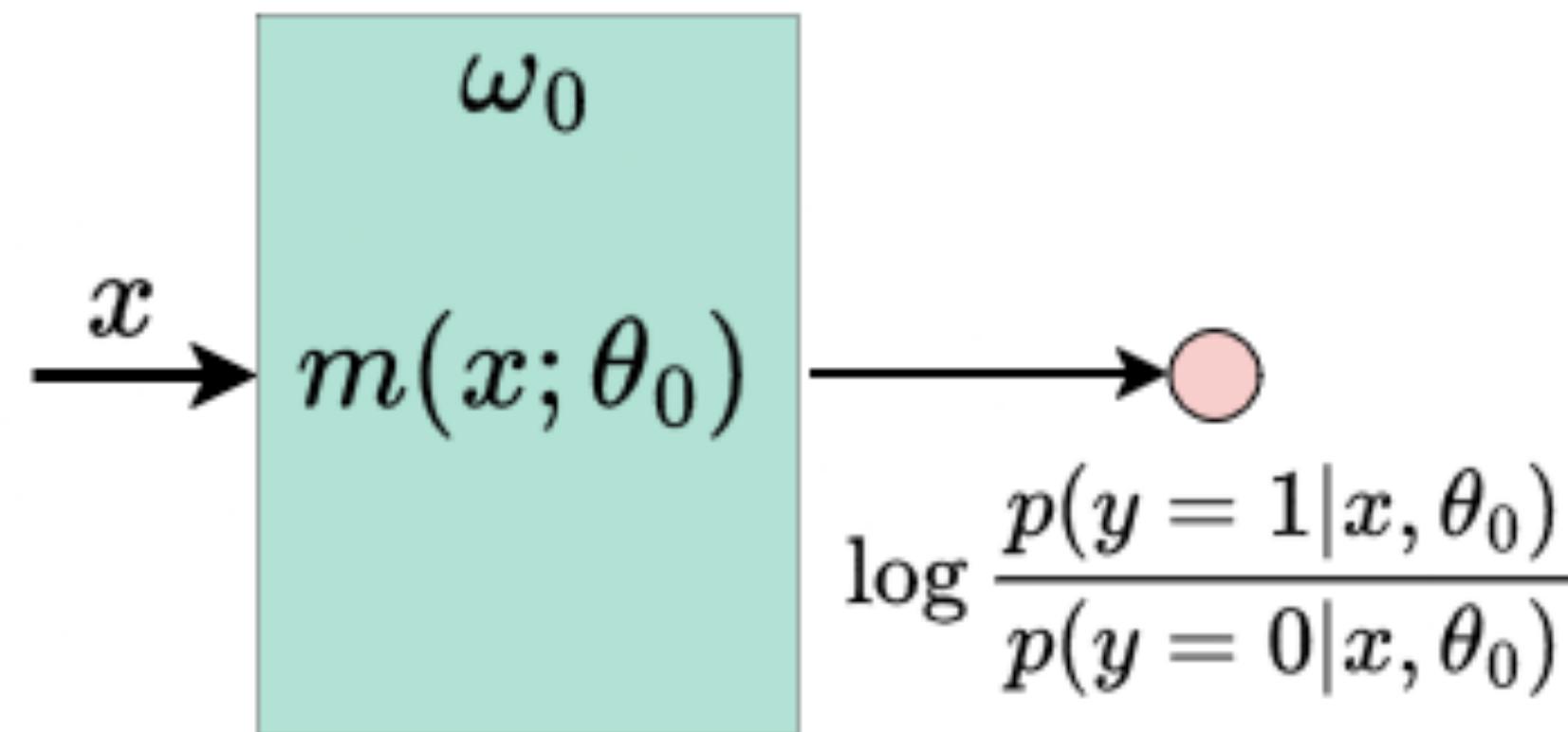
Comparing two binary classifiers

Soft decisions are different even if decisions are the same

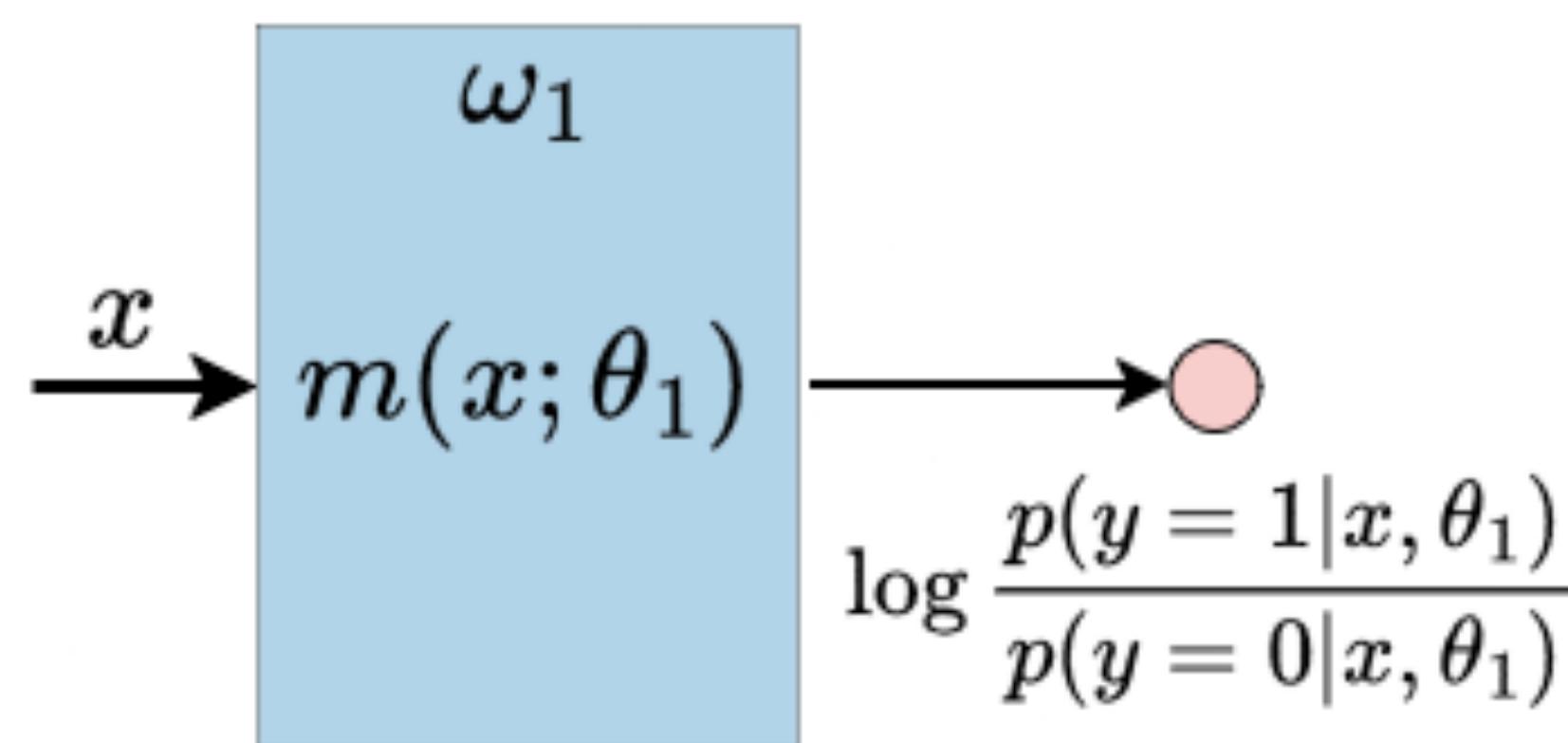


Comparing two binary classifiers

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



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.



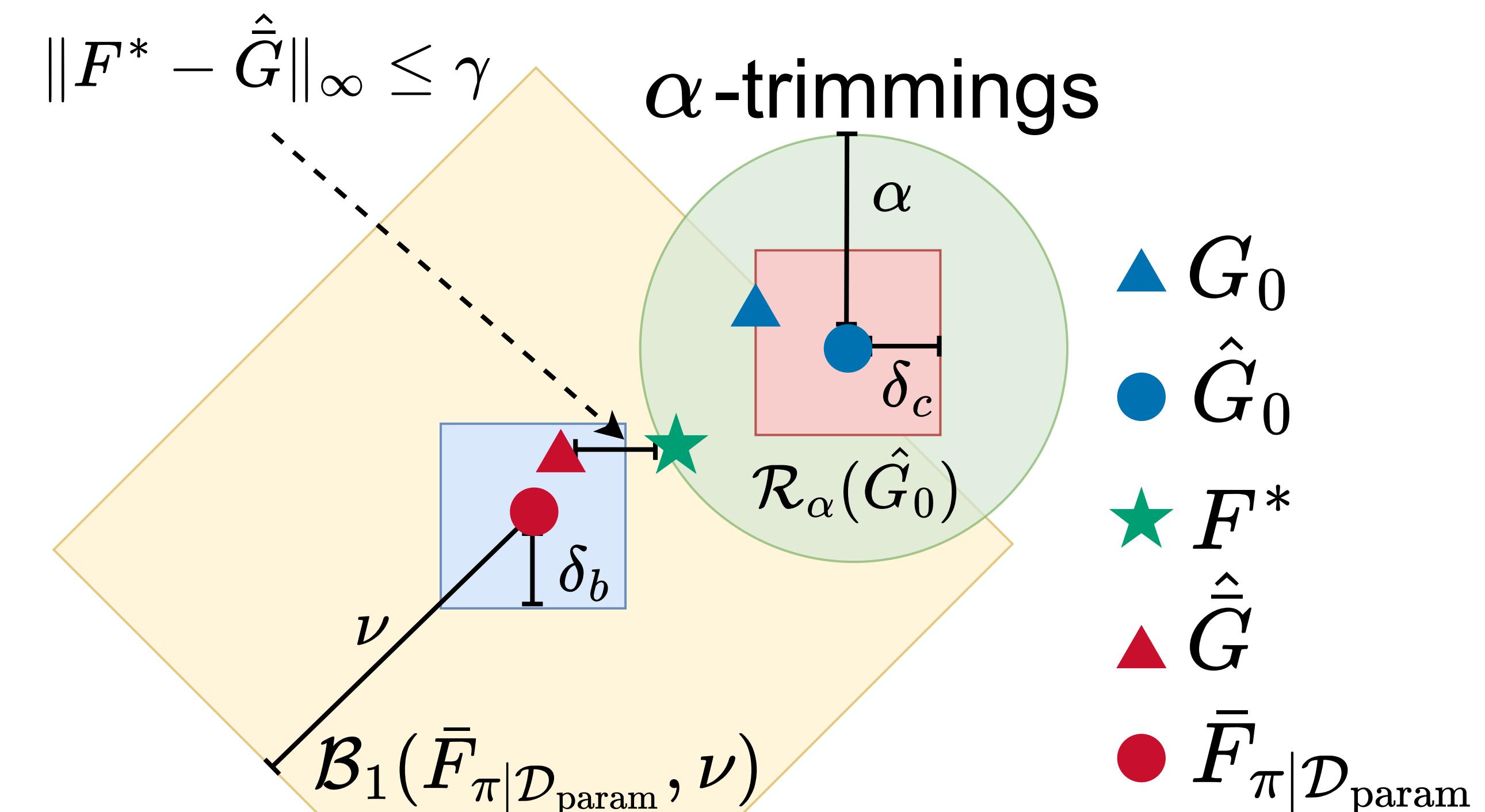
Are the models the same or different? Answer this by testing:

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

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

Hypothesis testing for model comparisons

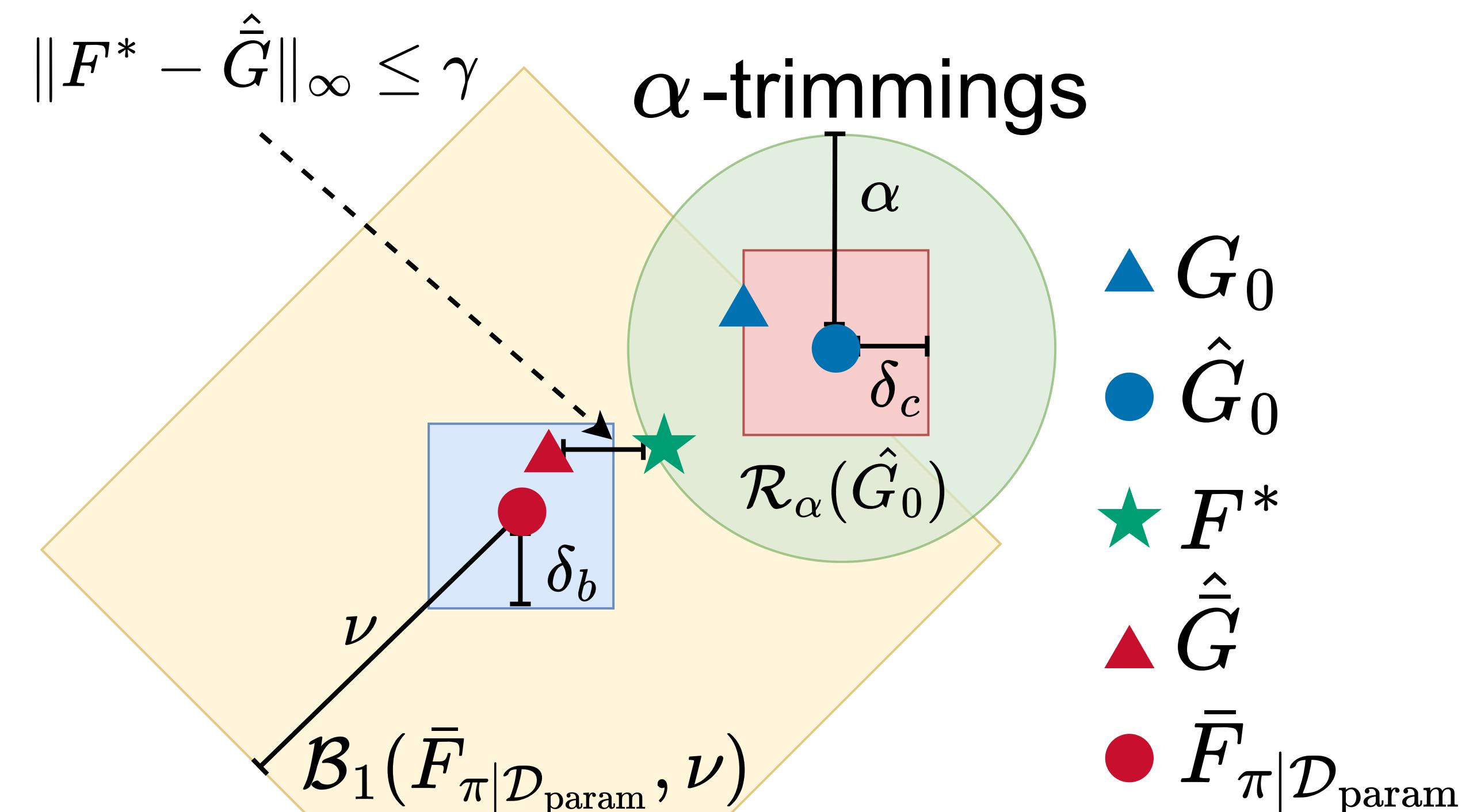
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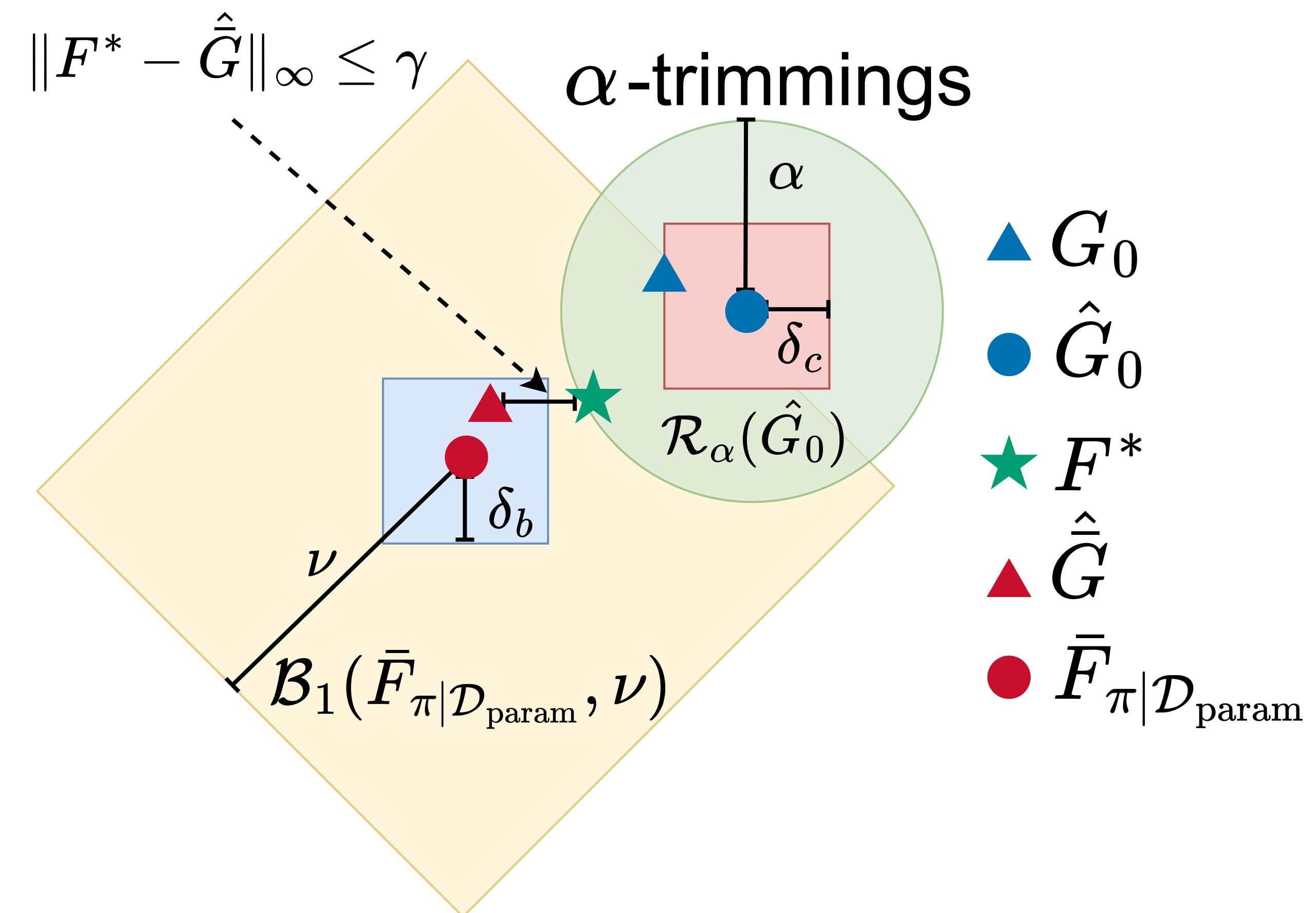


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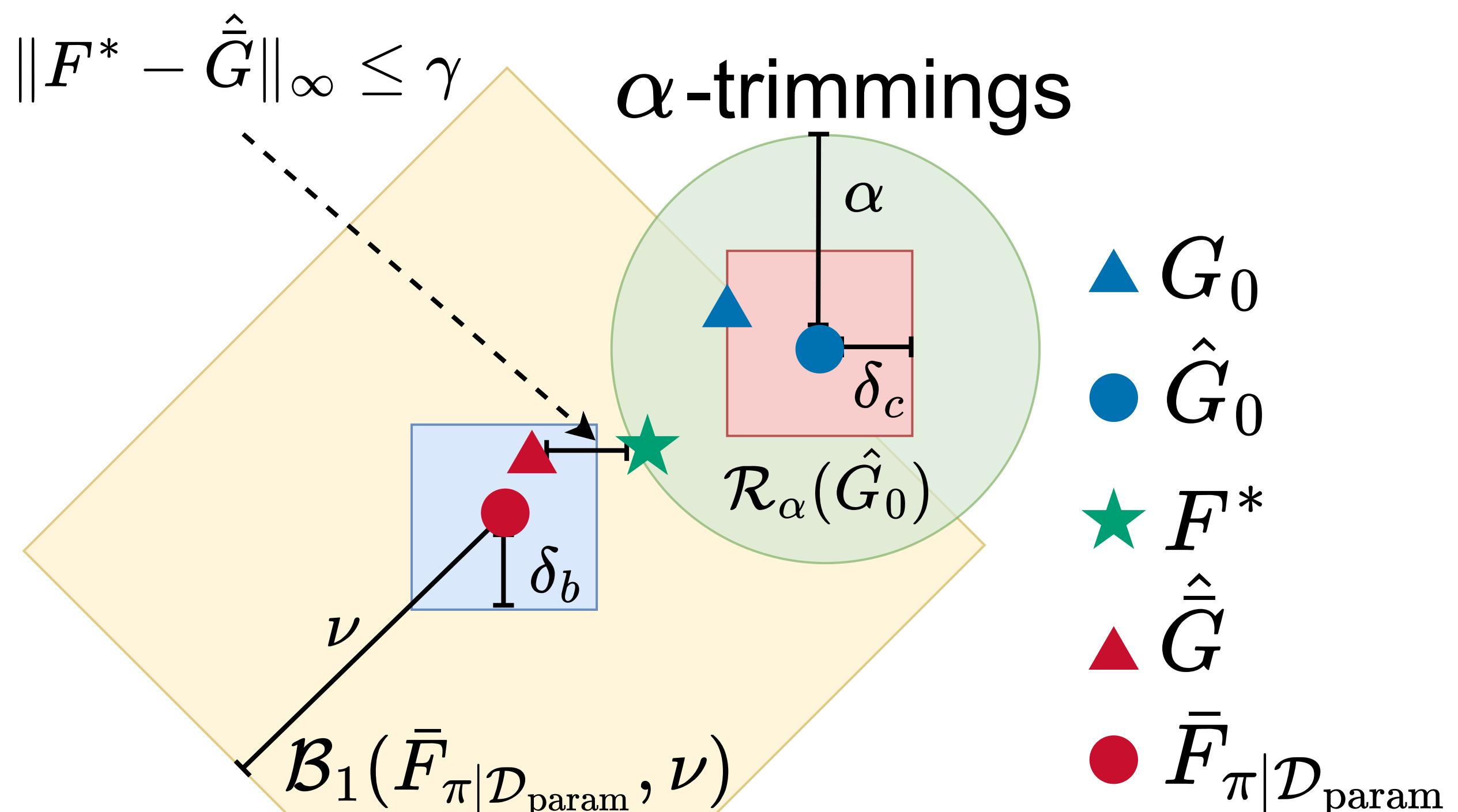
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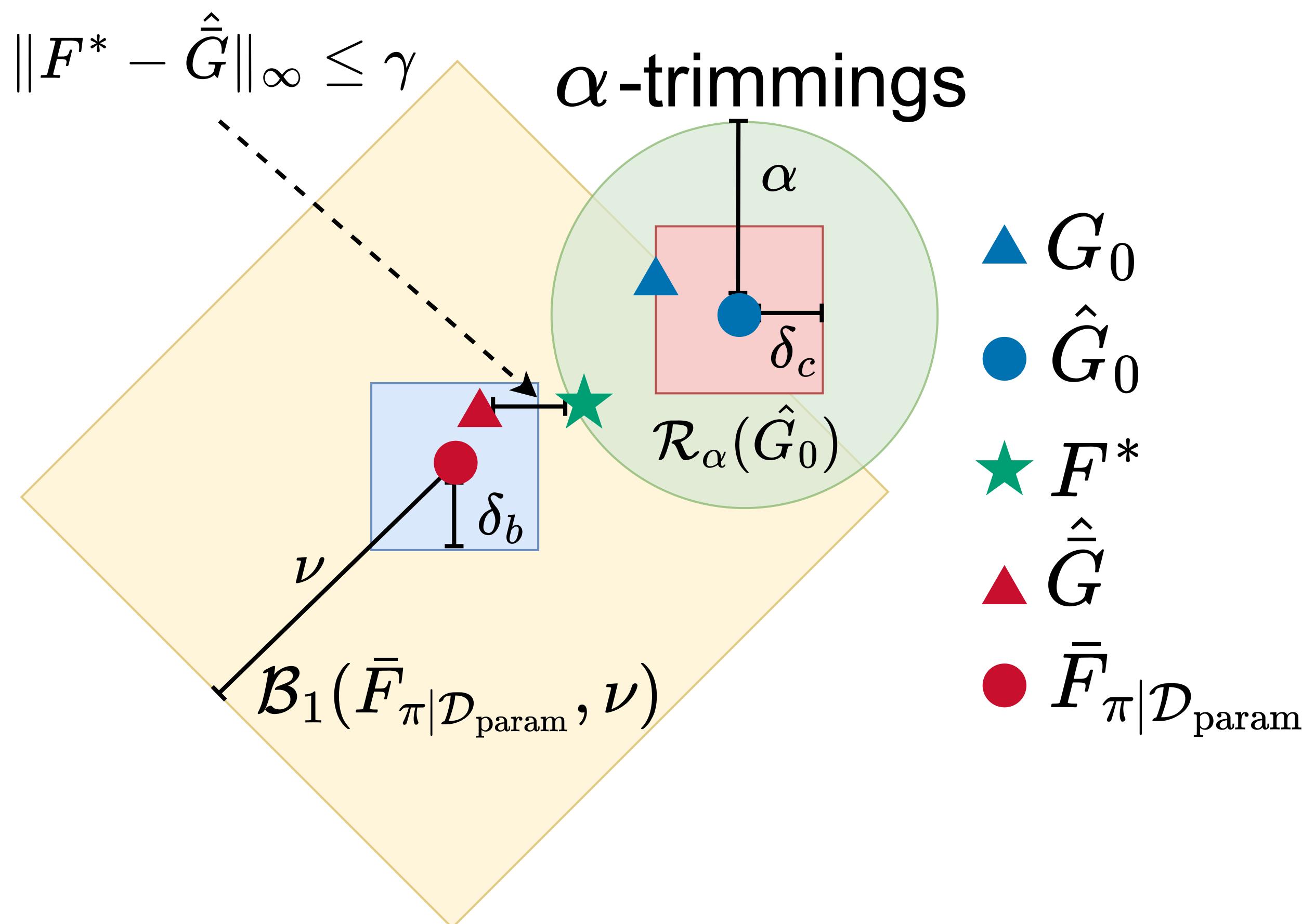
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Define a new discrepancy measure $\hat{\alpha}$ as the minimum level for the test (= radius of the ball) to accept.



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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



iOS 8.3



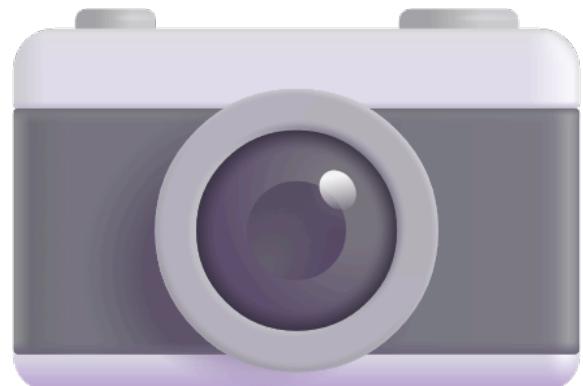
iOS 18.4



HarmonyOS 4.0



Samsung UI 7.0



MS 3D Fluent



SerenityOS

Connecting back to our story

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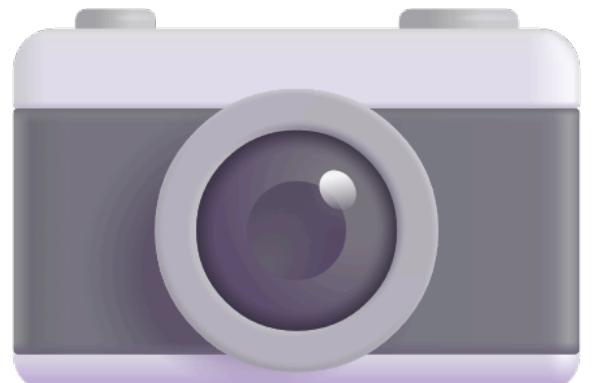
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SerenityOS

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iOS 8.3



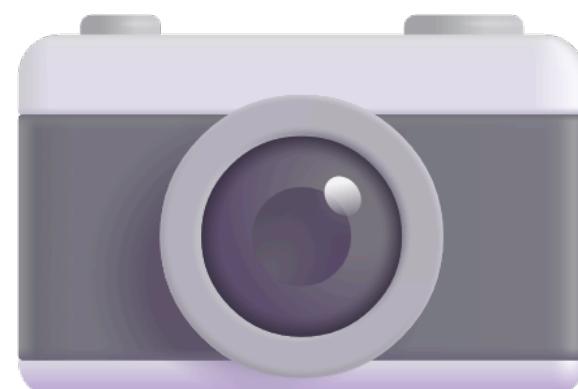
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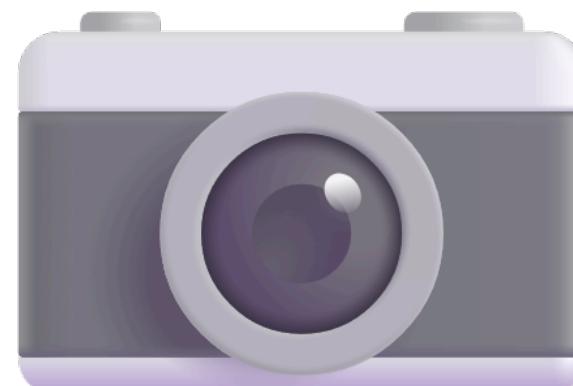
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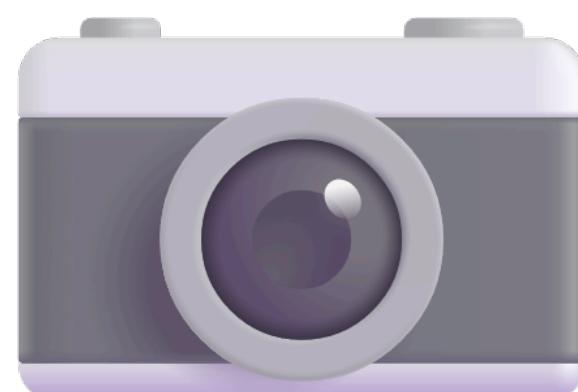
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MS 3D Fluent

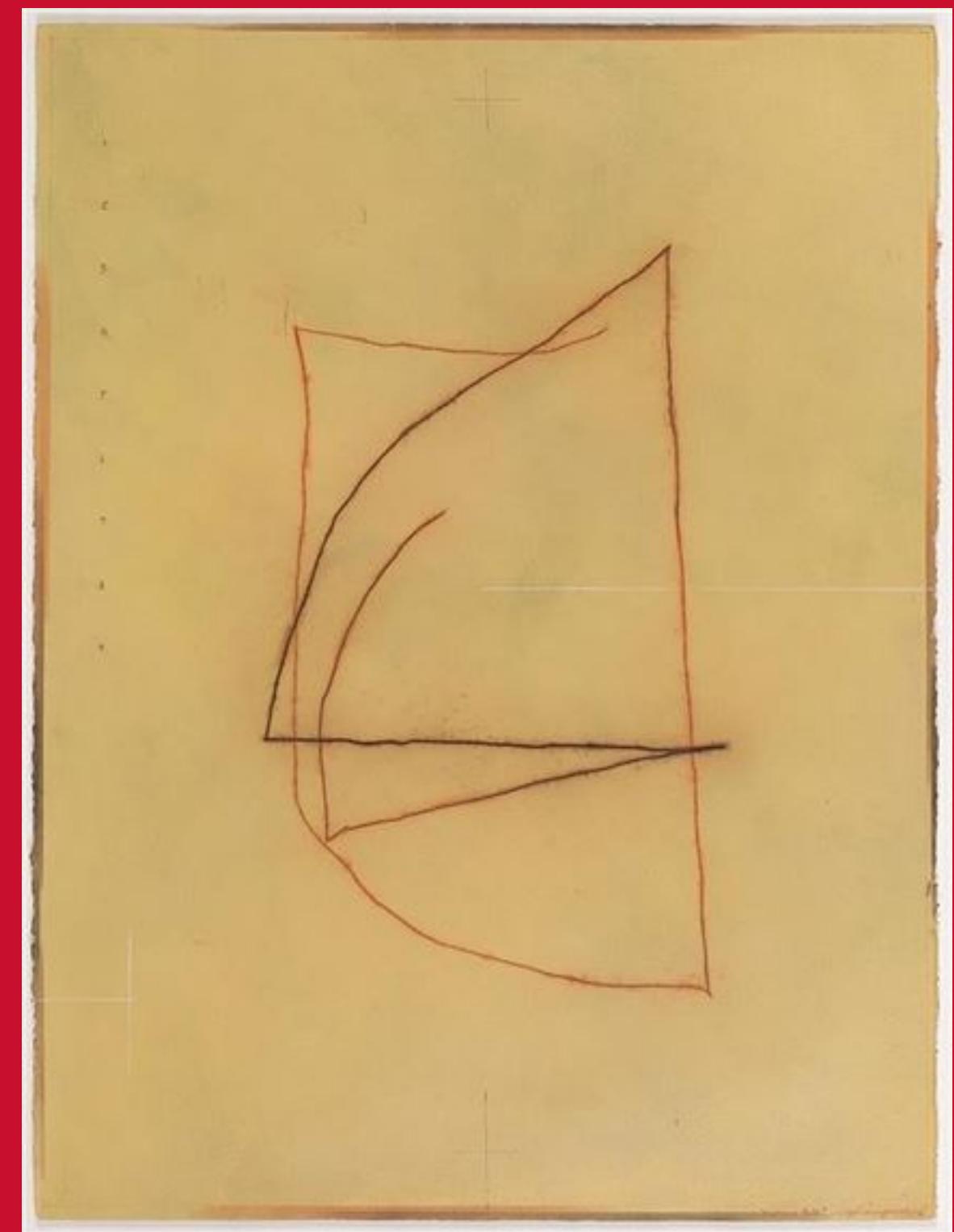


SerenityOS

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- 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.

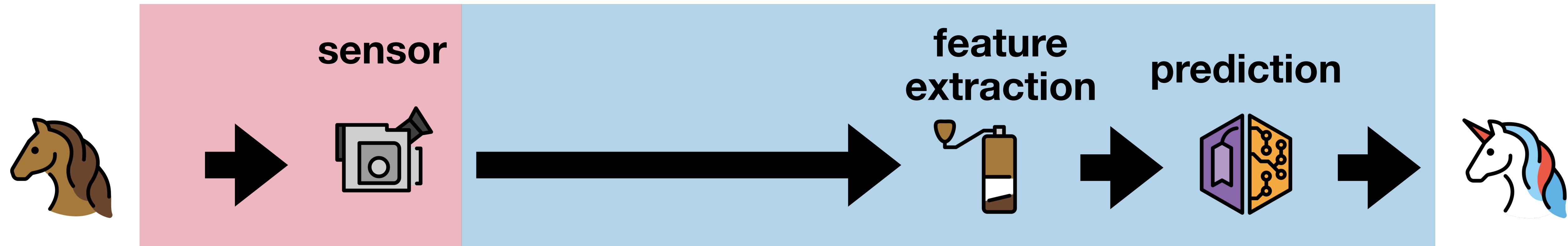
Some final remarks



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

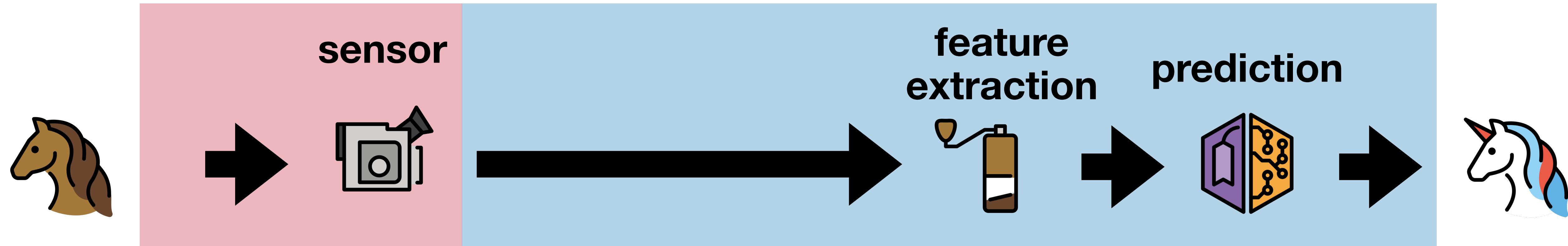
Back to the original question

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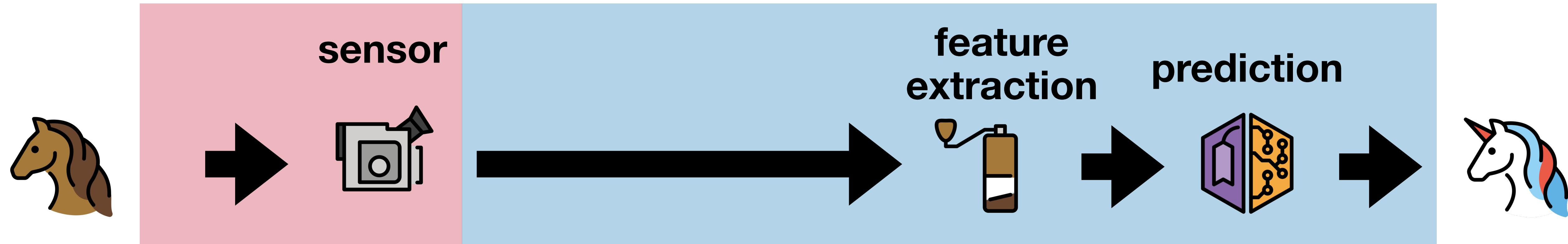
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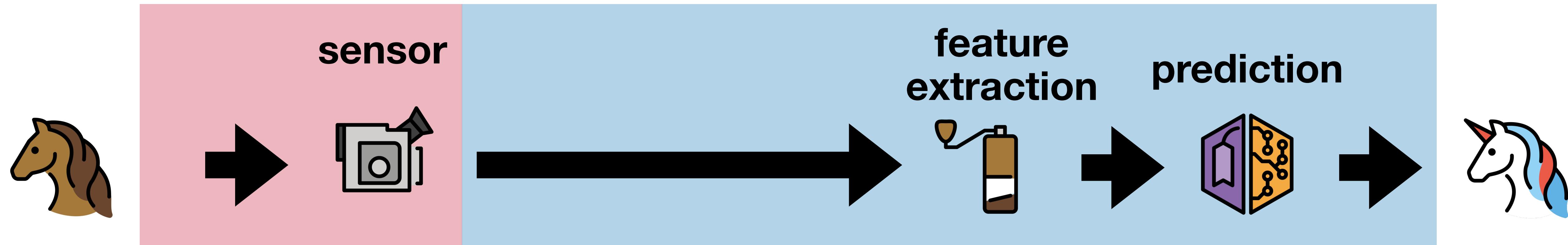


To use large ML/AI models as part of a scientific workflow, we need “interpretability” and “reliability.”

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

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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.”

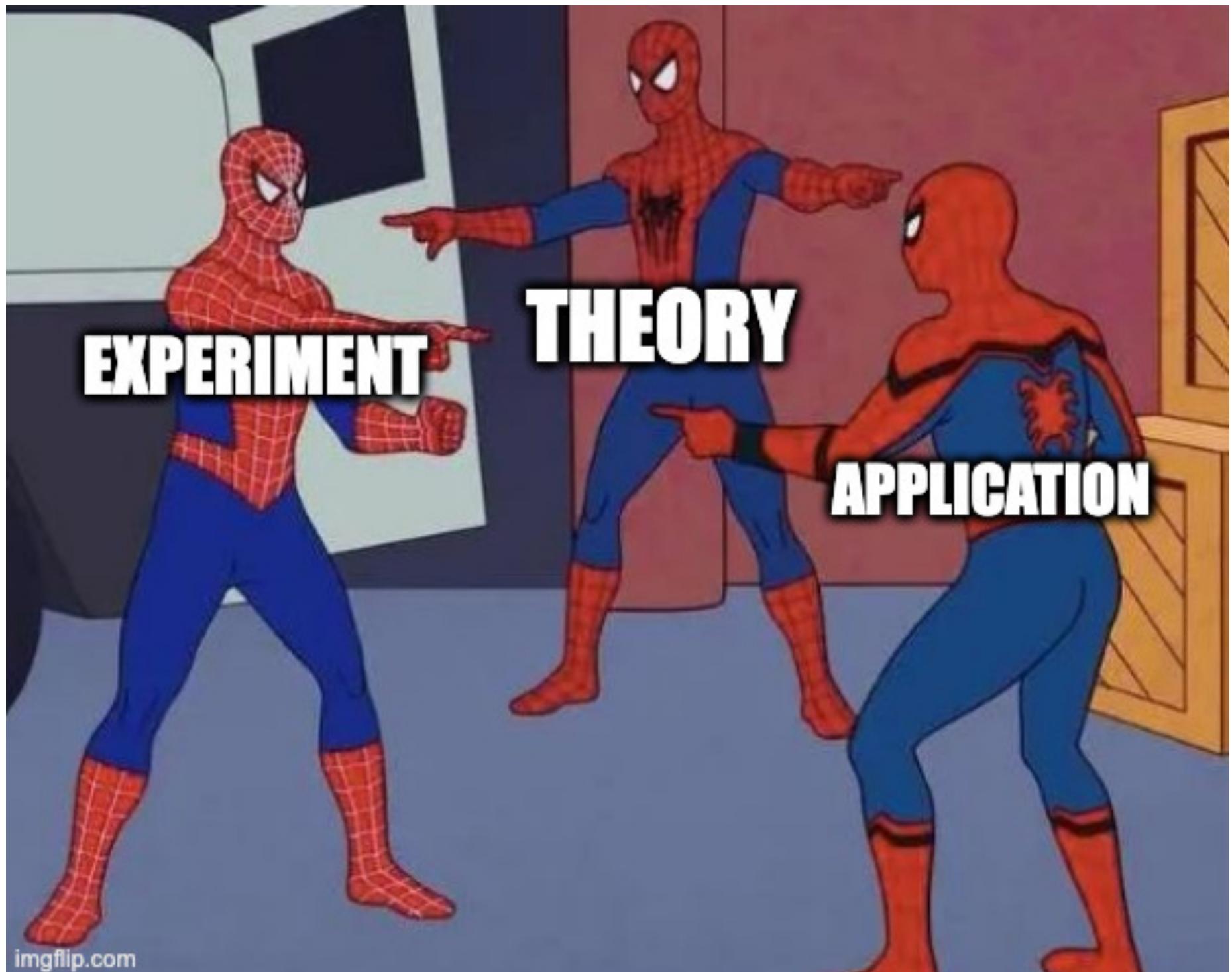
We also need to understand “reliability” for the training/fine-tuning processes.

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

Where is this all going?

Maybe some strange new worlds

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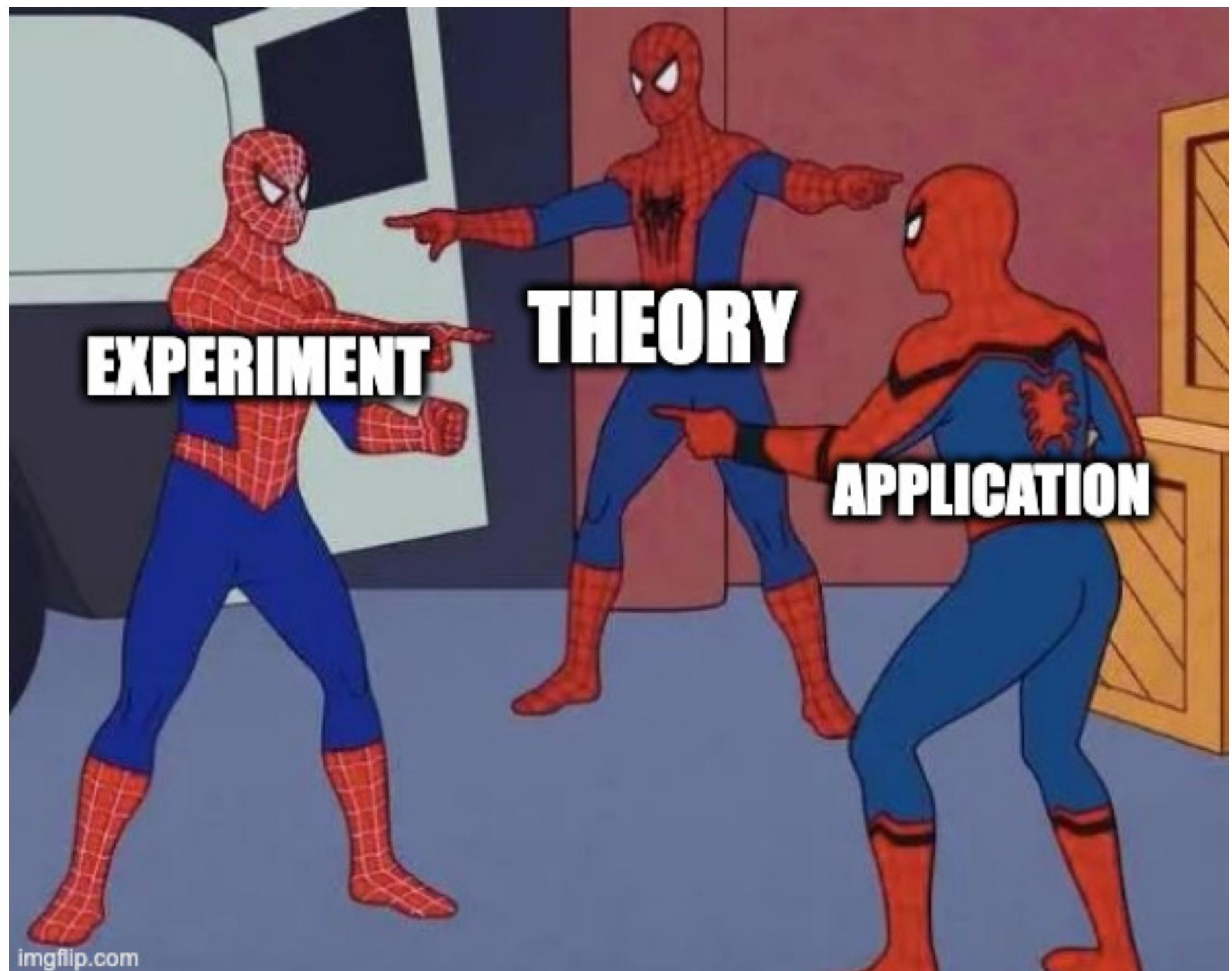


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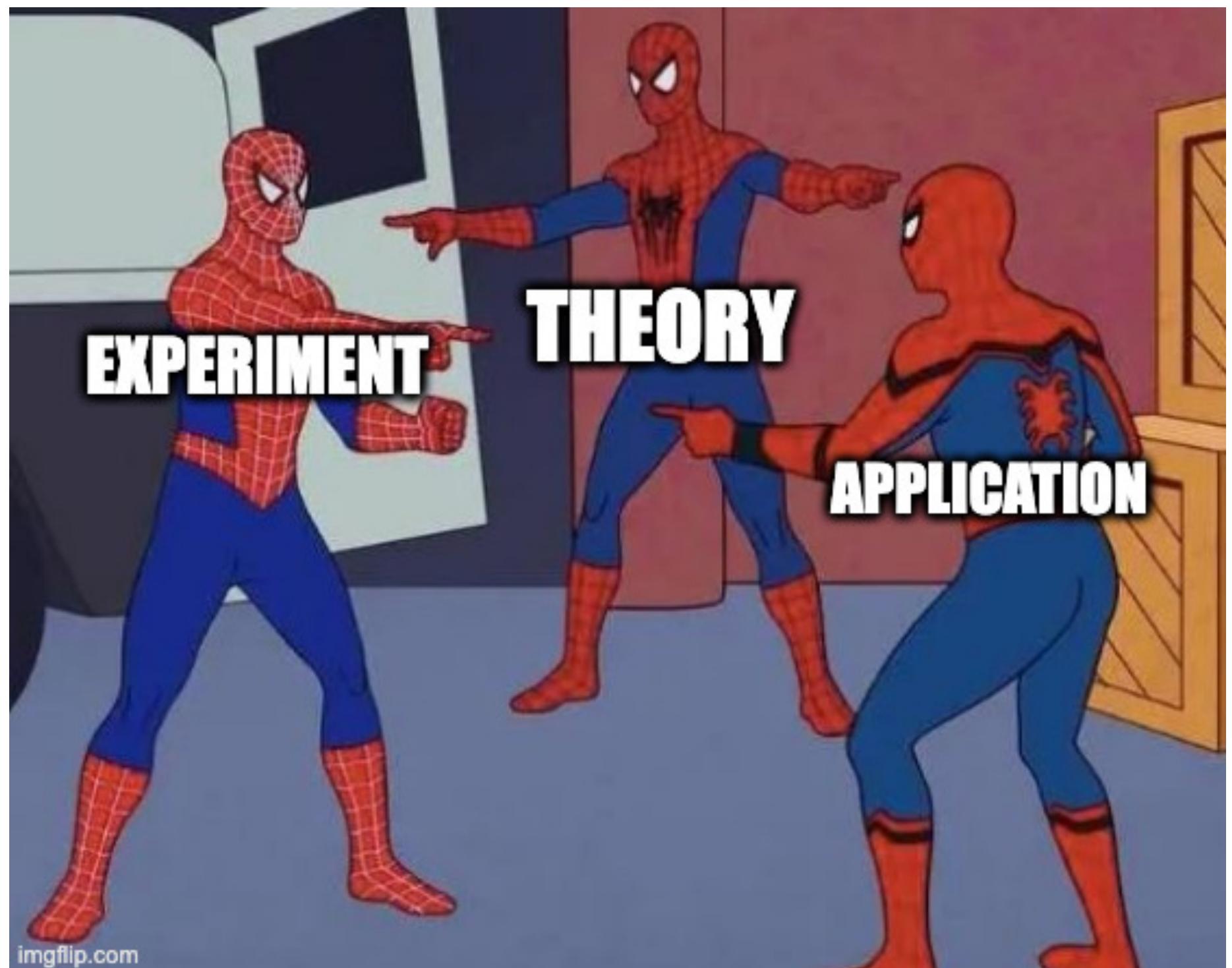


- **Theory:** can we instead compare surrogate models like “faithful” NTK representations (Engel et al. 2024)?
- **Experiment:** can we do these comparisons cheaply (e.g. using academic-level resources)?

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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?

谢谢大家的关注!