Are modern ML models like scientific instruments?

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

Anand D. Sarwate (Rutgers University)

28 July 2025

IEEE ITSOC Distinguished Lecture

2025 Guangzhou, Hong Kong and Taipei Joint Workshop on Artificial Intelligence, Communications and Information Theory (AICIT 2025)

Guangzhou, China

Some pre-apologies

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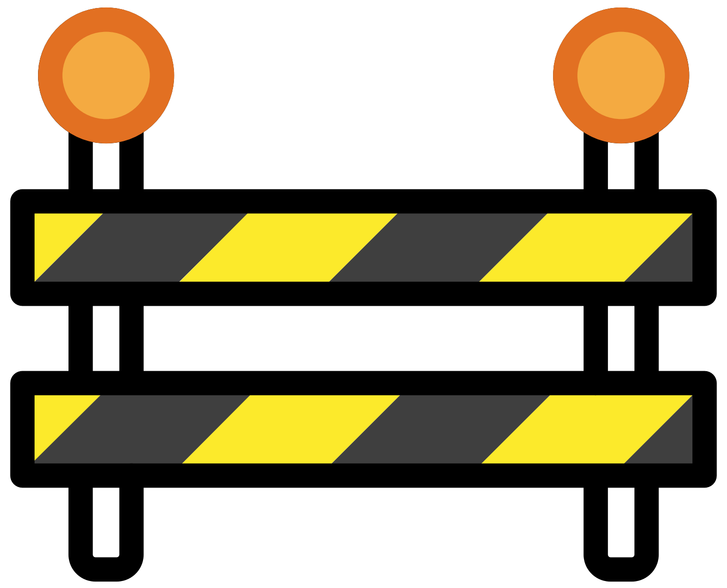

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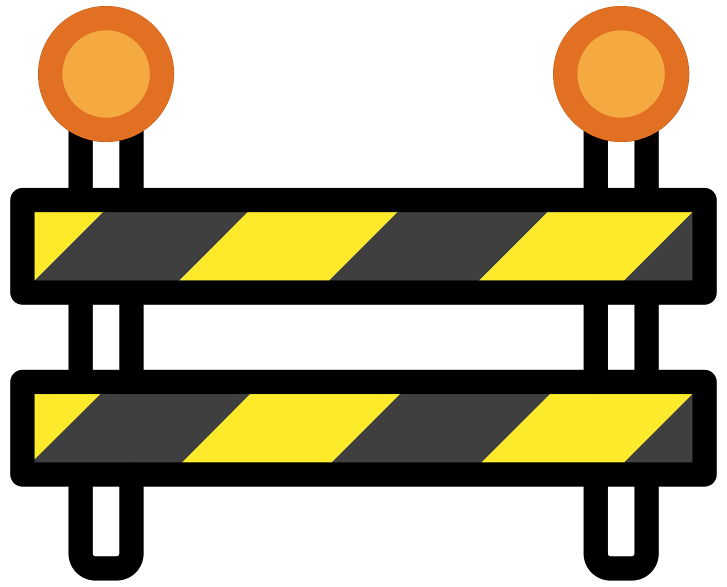

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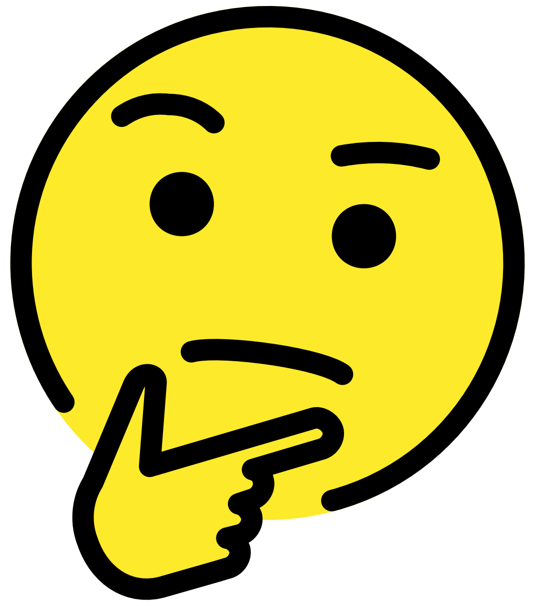

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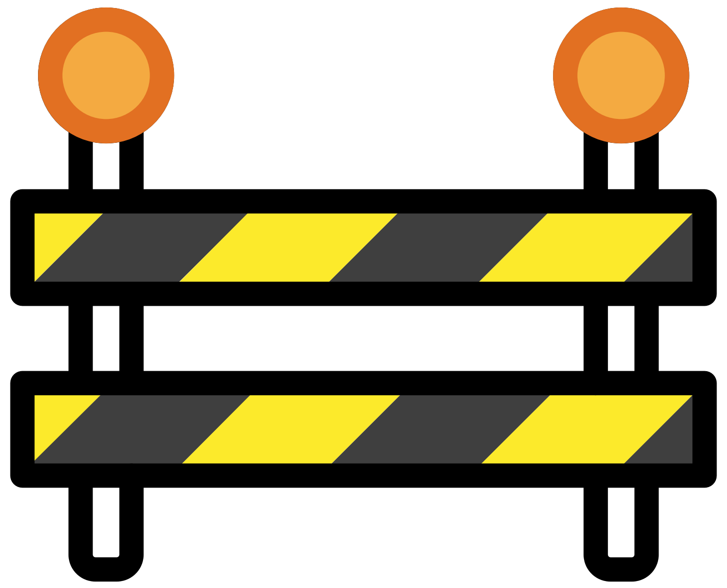

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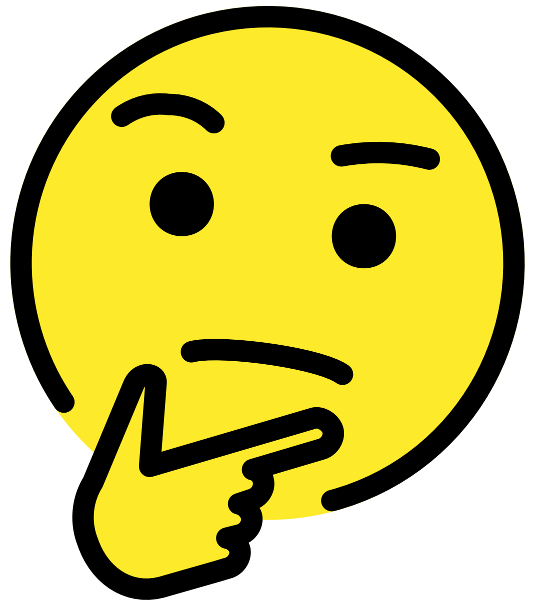

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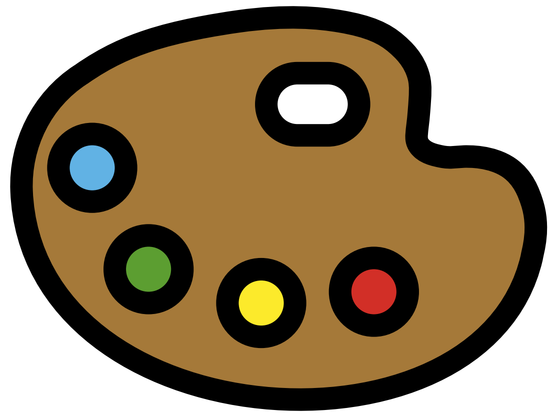

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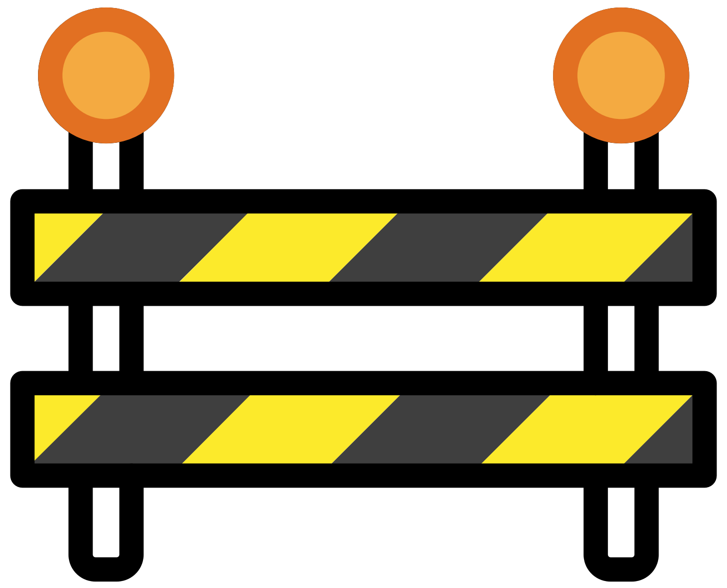

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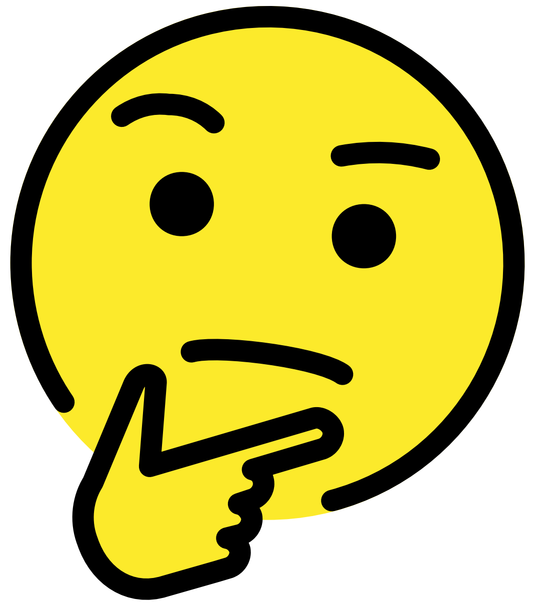

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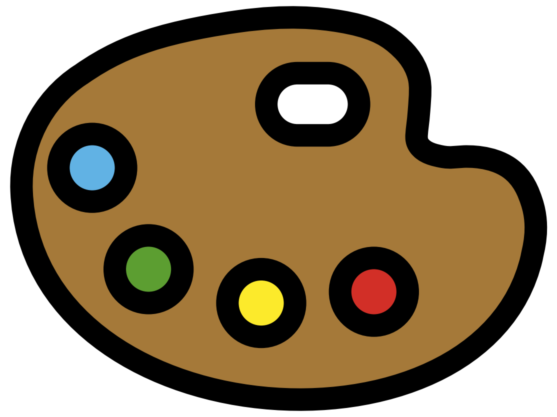

Real life is a bit messy…

Thanks to my collaborators/coauthors!

Most of this is their work, obviously

Sinjini Banerjee (Rutgers)
Reilly Cannon (PNNL)
Tony Chiang (ARPA-H)
Sutenay Choudhury (PNNL)

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Ioana Dumitriu (UC San Diego)
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=gpqBGyKeKH
[ICLR 2024] **Engel et al.** https://openreview.net/forum?id=yKksu38BpM
[ArXiV] **Vargas et al.** https://arxiv.org/abs/2408.10437

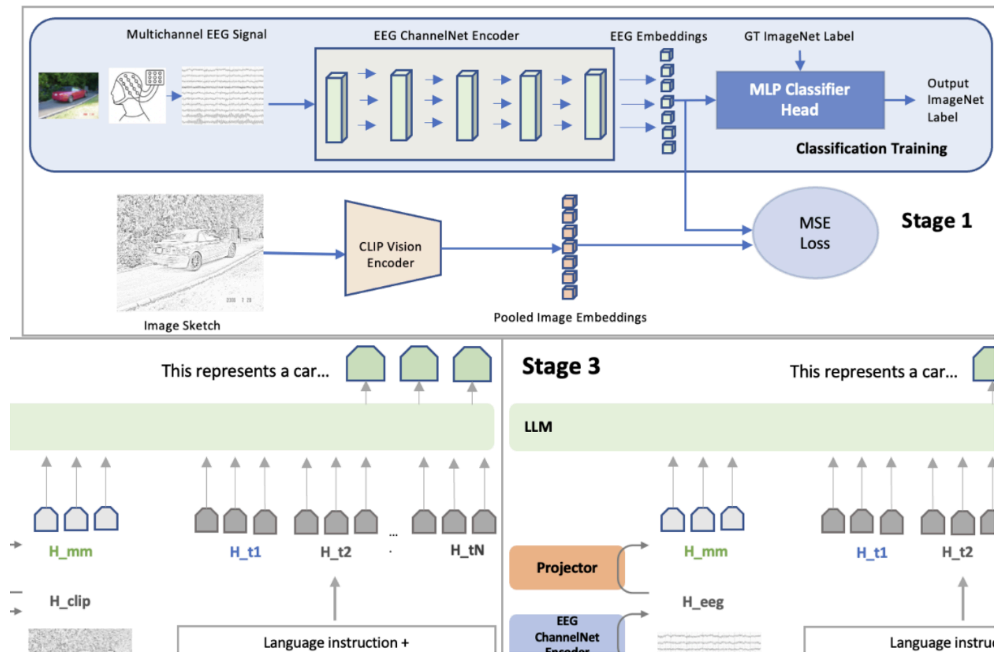
What does the title mean?

What do ML models have to do with science?

Source: Wikipedia

Source: IBM

Source: Mishra et al.



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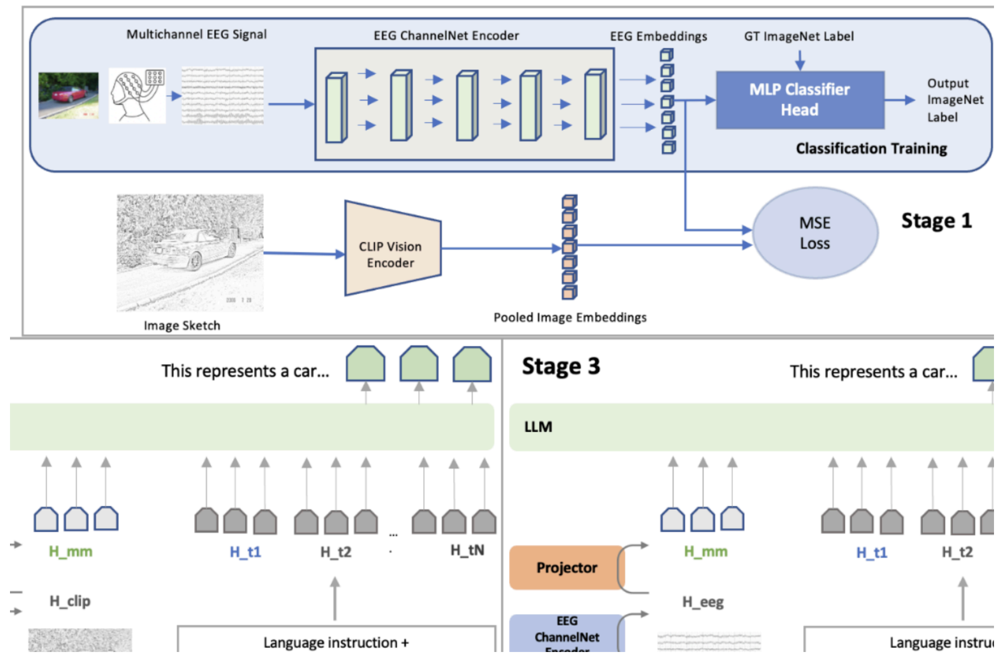

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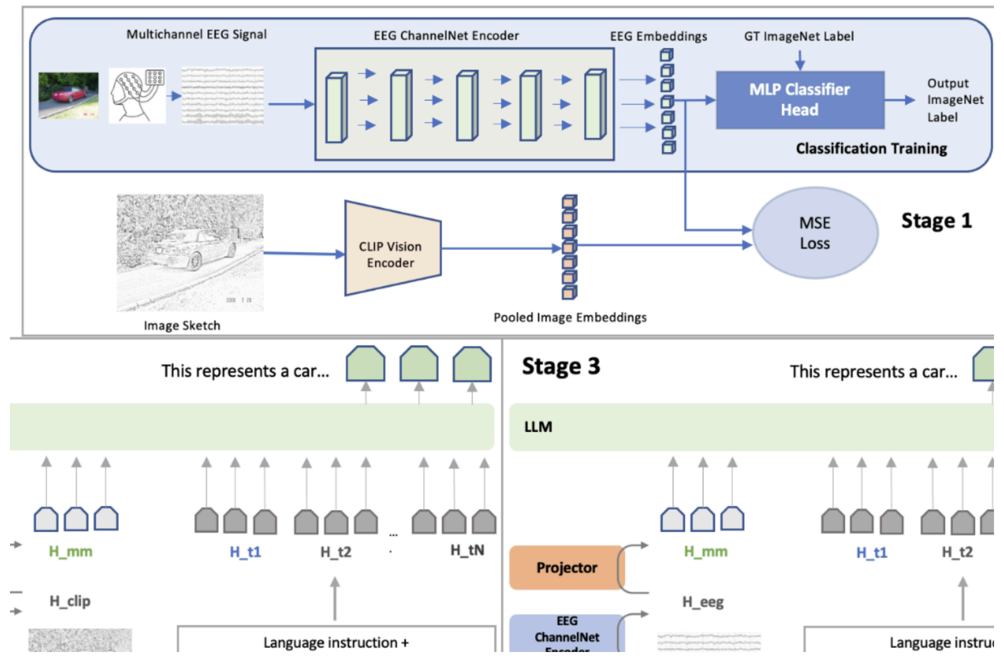

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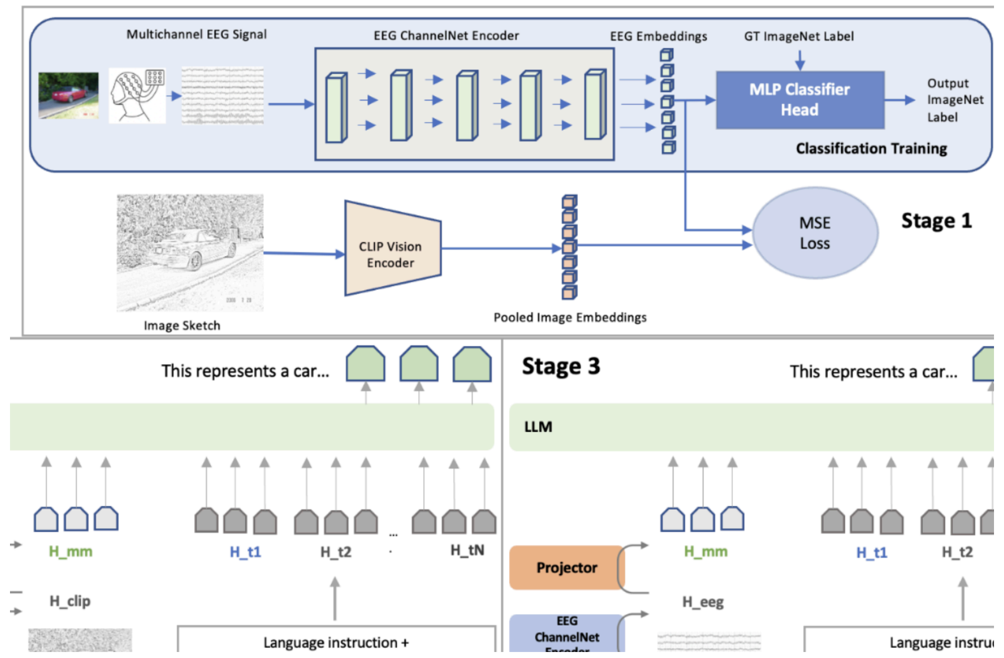

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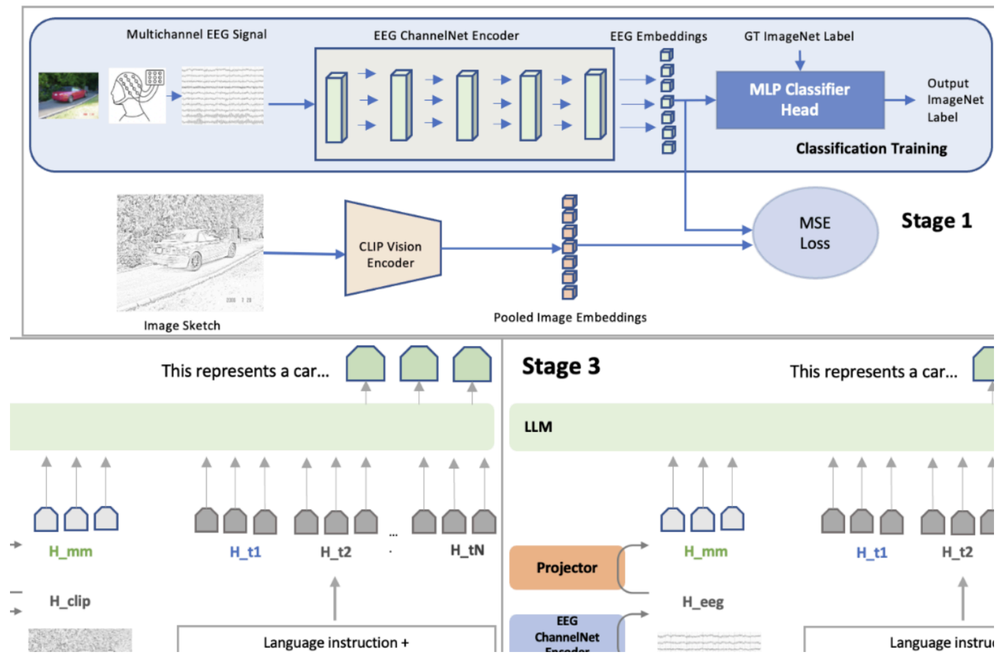

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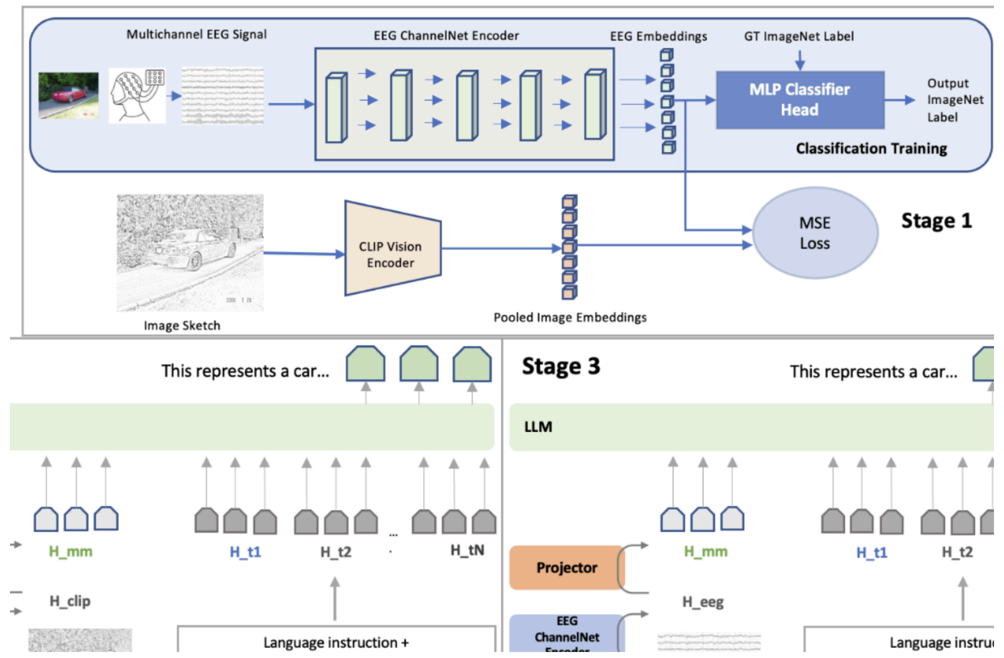

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- Many more…

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Some gap between hype and reality

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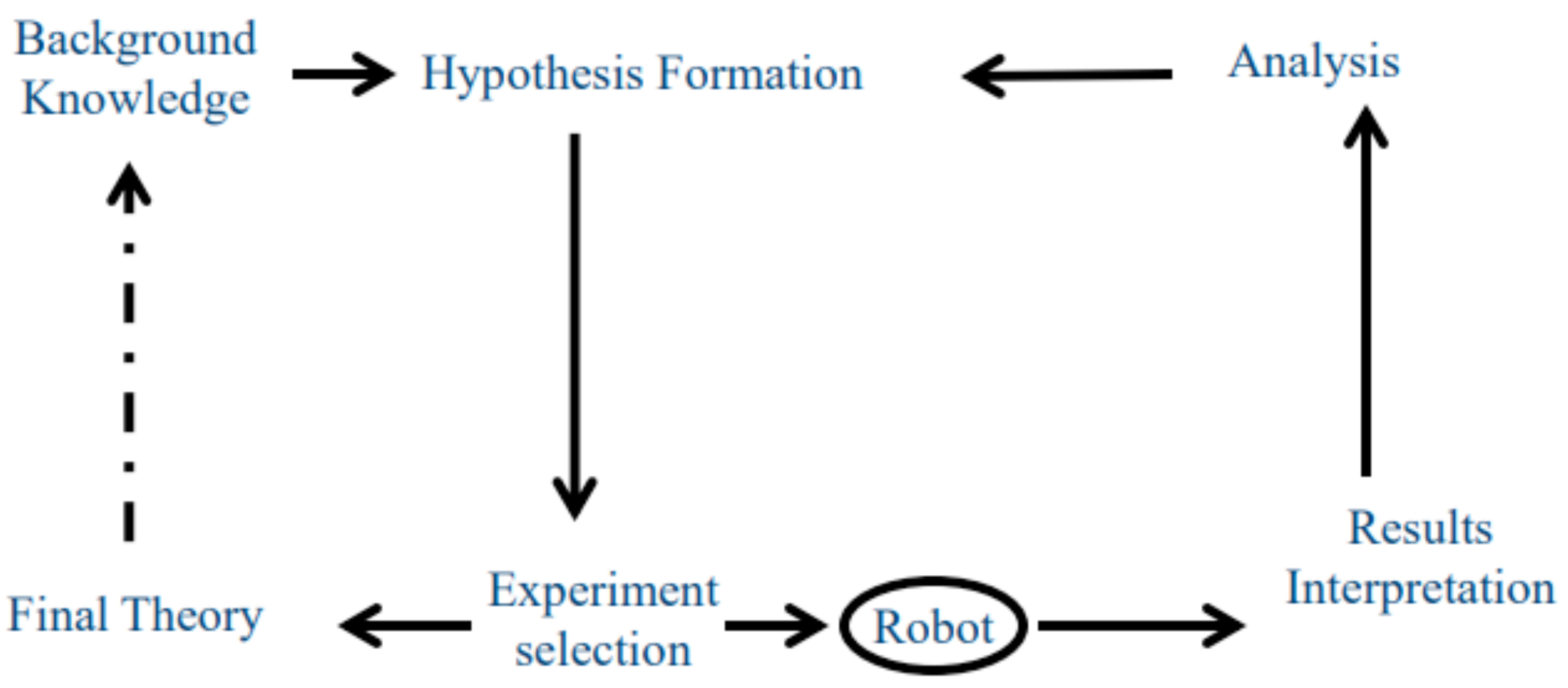
Computer system capable of originating its own experiments, physically executing them, interpreting the results, and then repeating the cycle.



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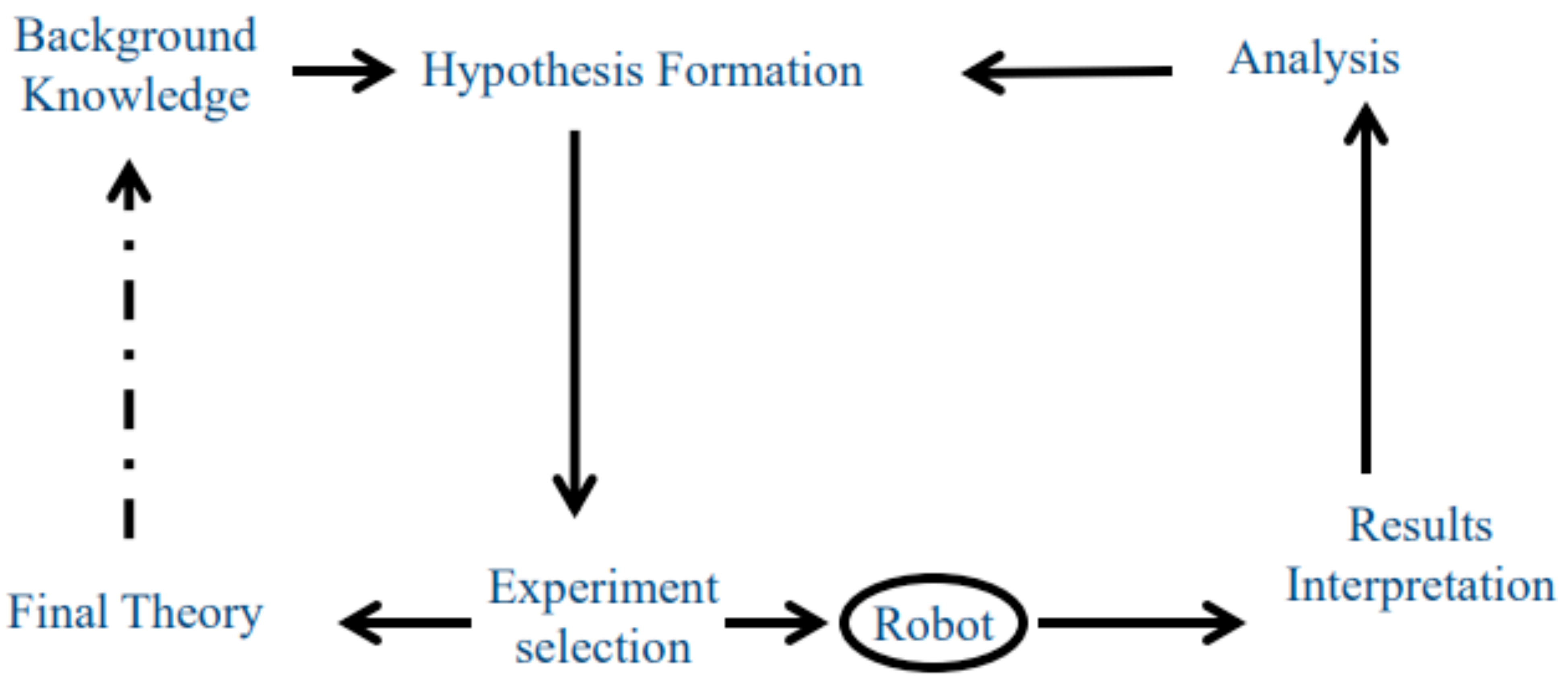

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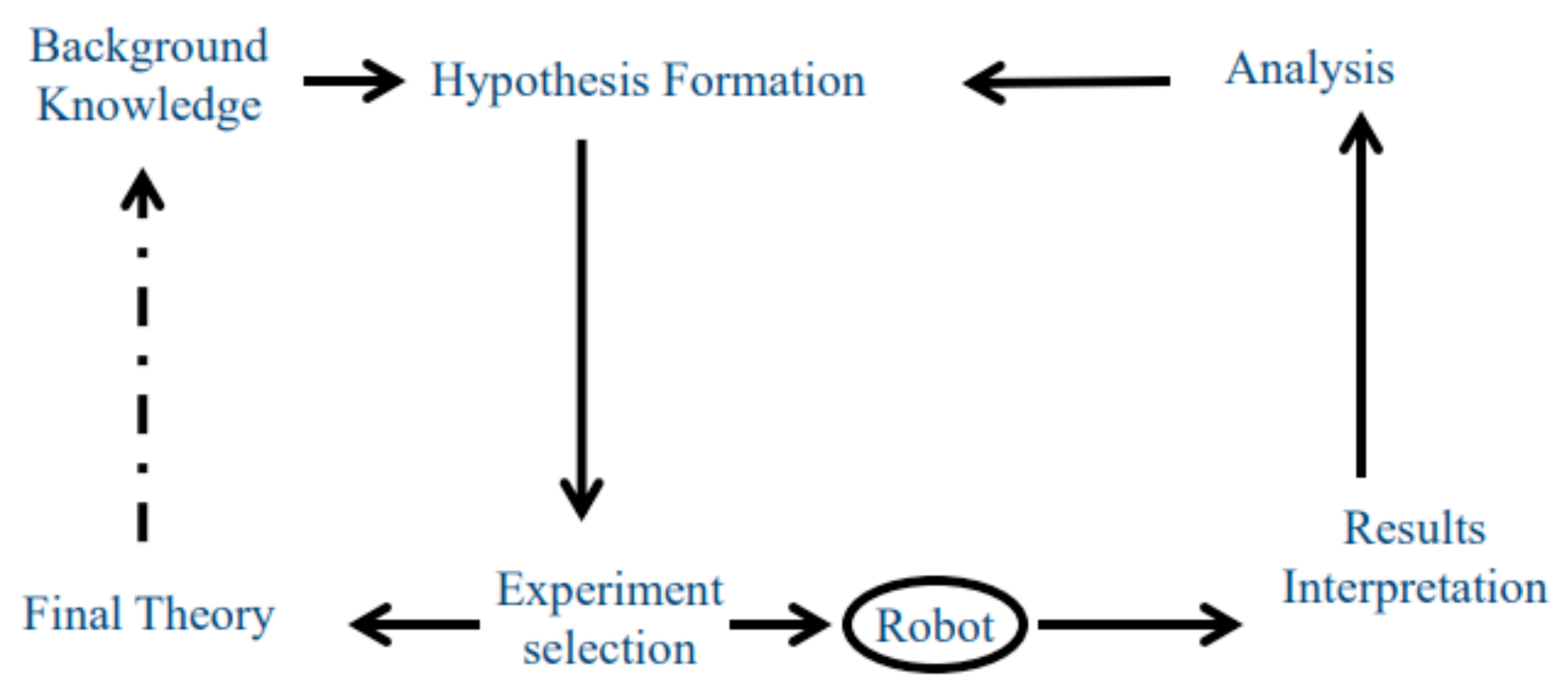

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IRE TRANSACTIONS—INFORMATION THEORY

The Bandwagon

CLAUDE E. SHANNON

Shannon, 1956

What about information/signal processing?

Some perspective from more solid ground

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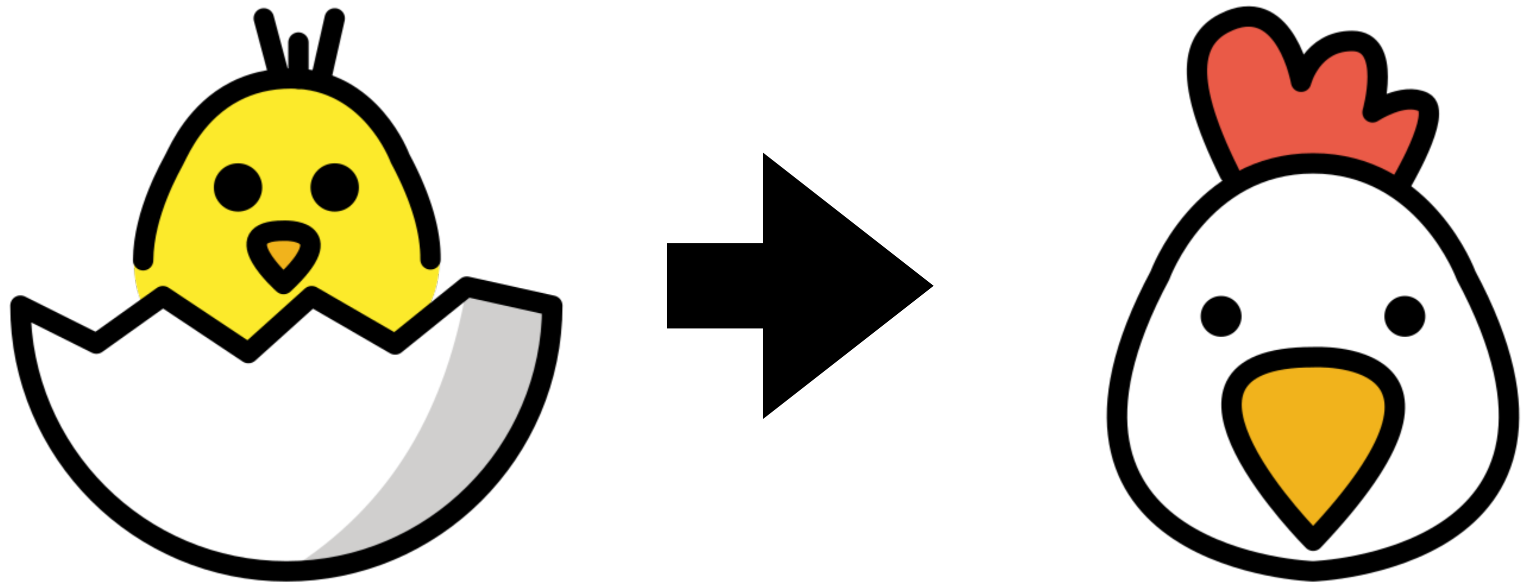

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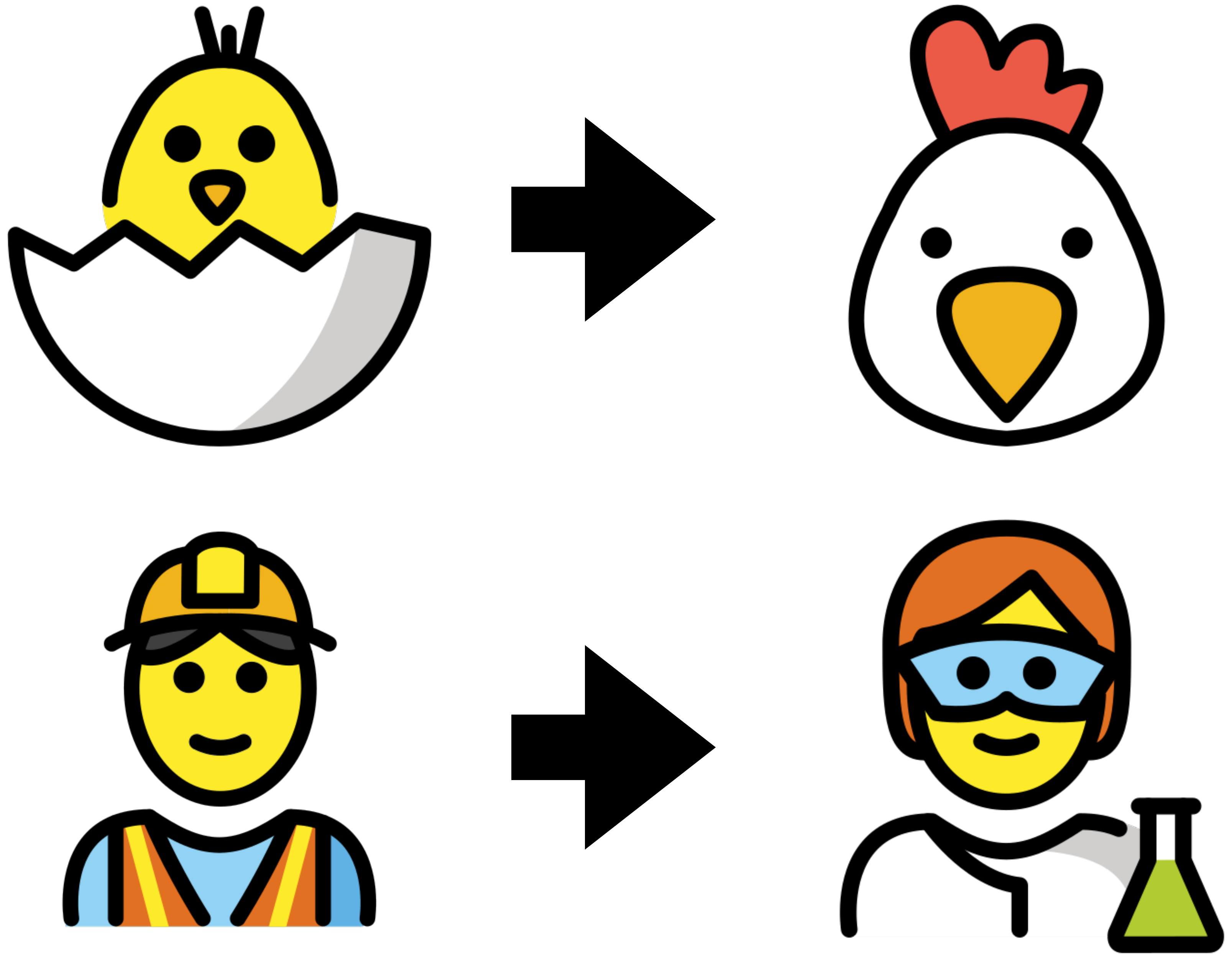

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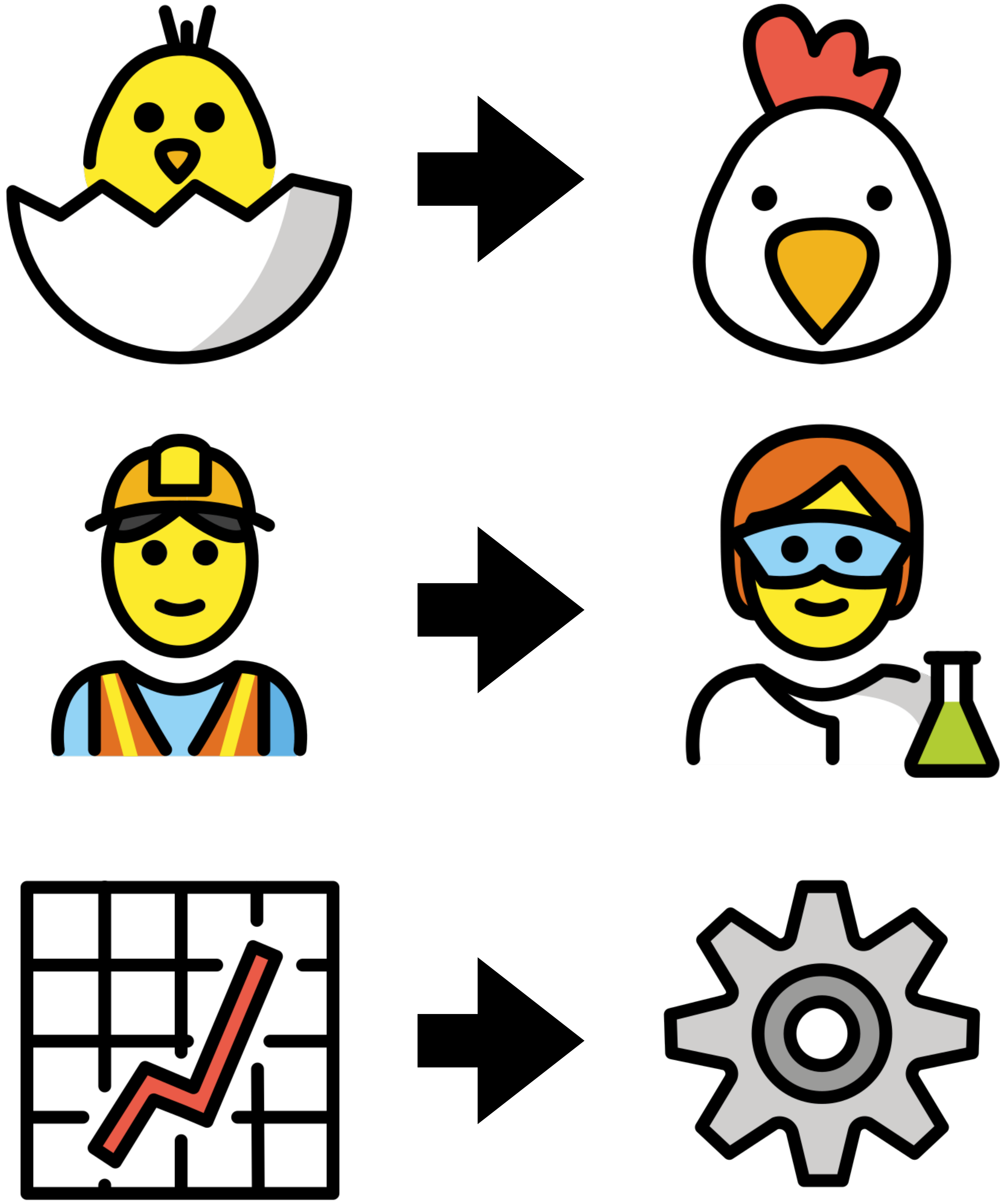

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➜ Theory often lags behind practice.

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

A traditional division of labor

The EE/CS divide in some sense

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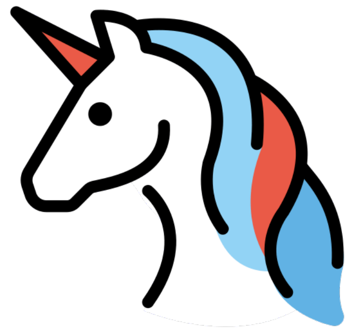

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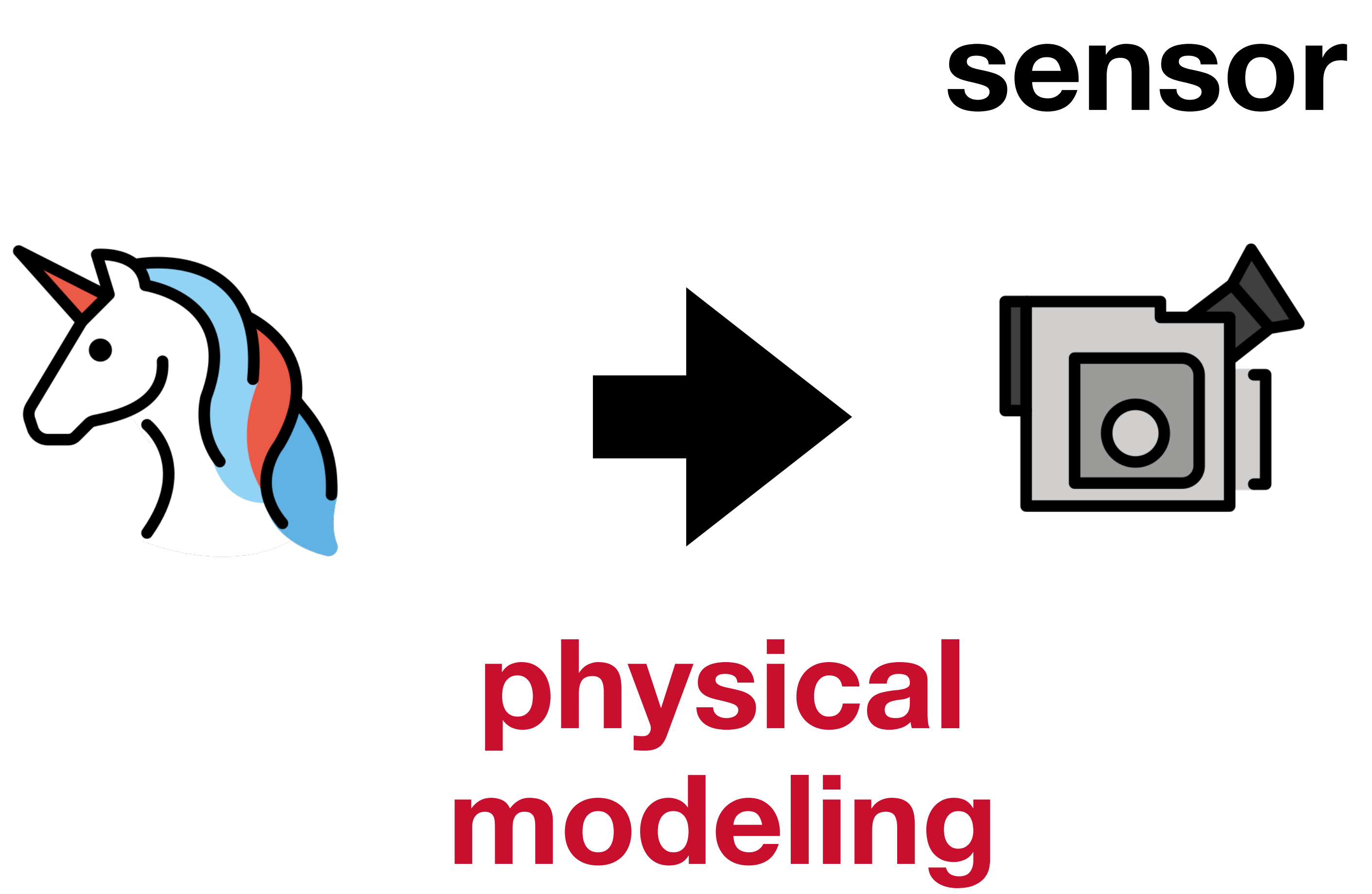

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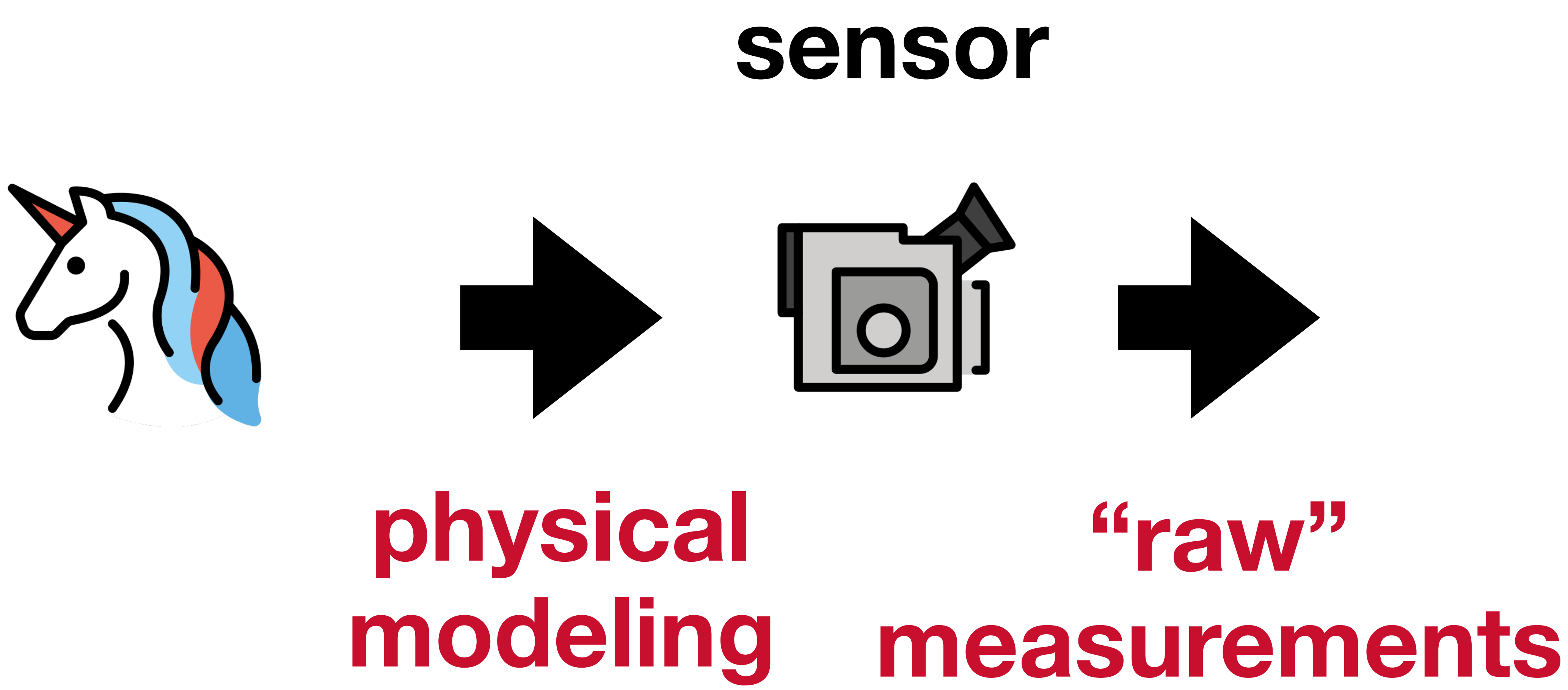

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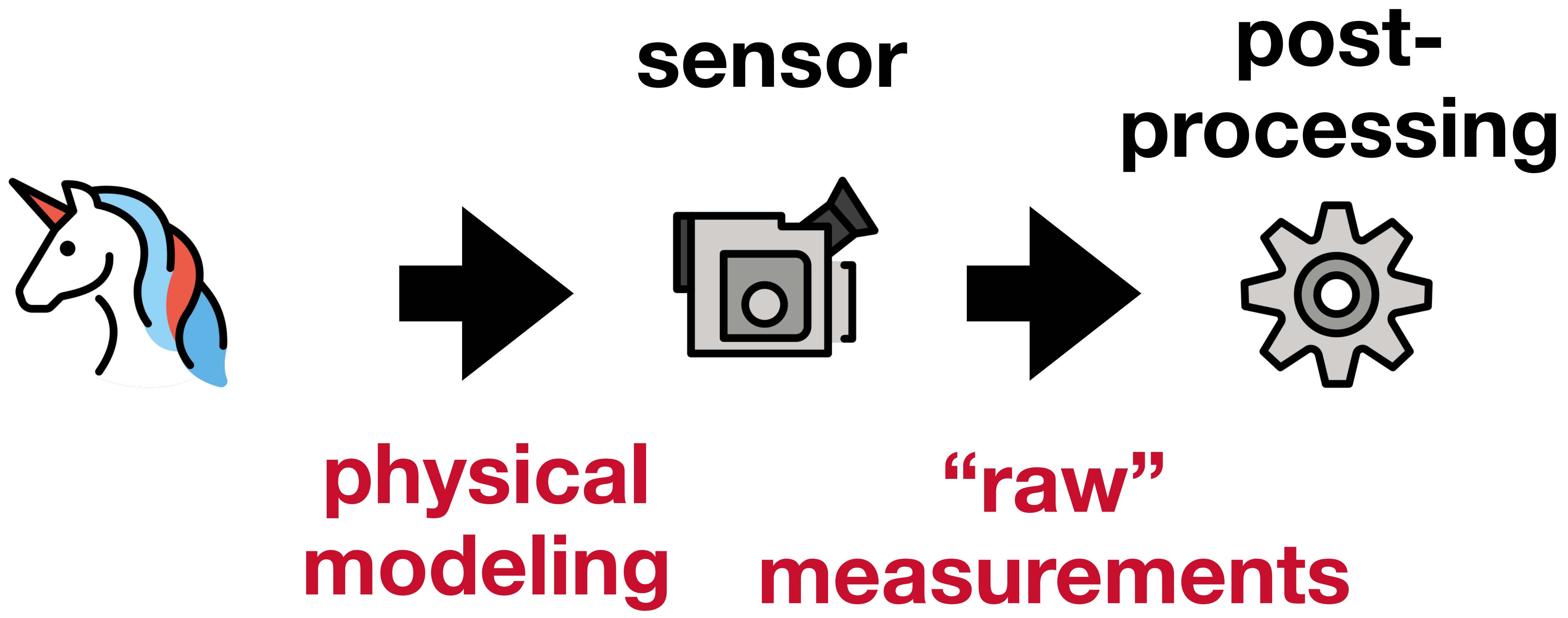

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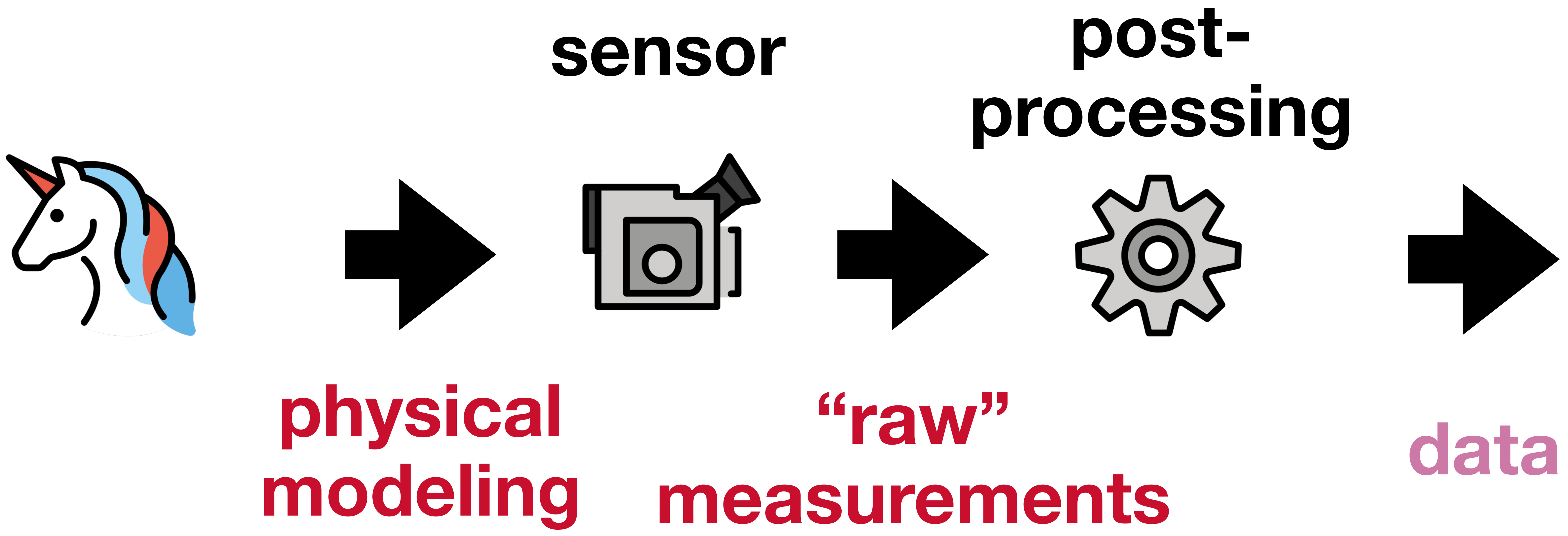

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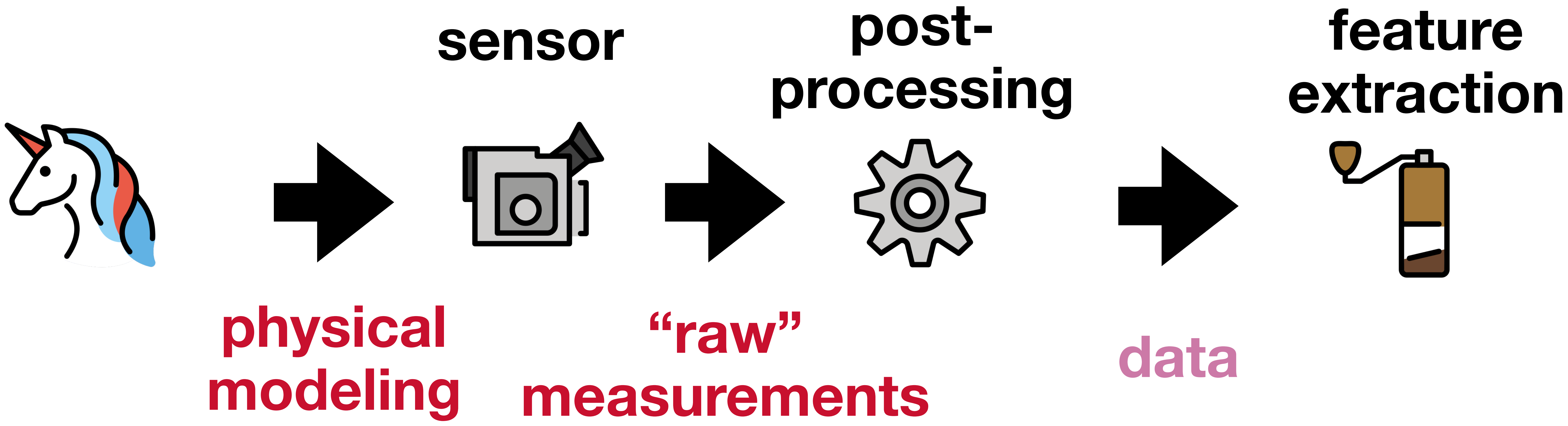

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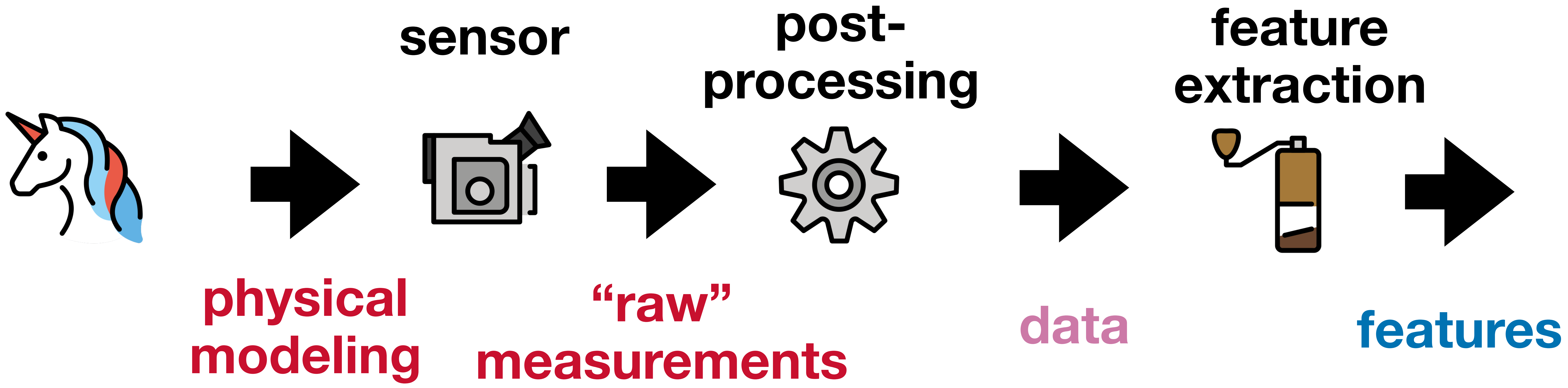

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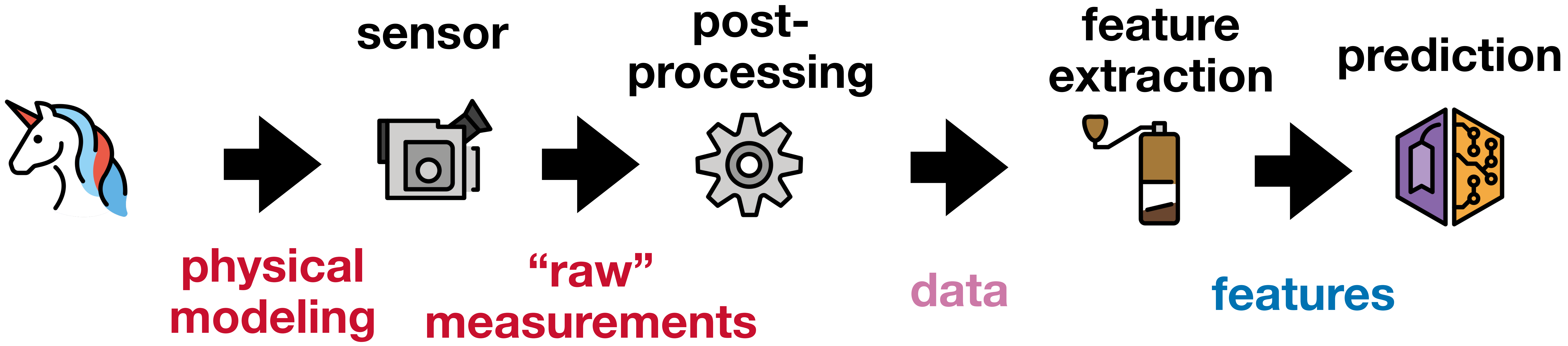

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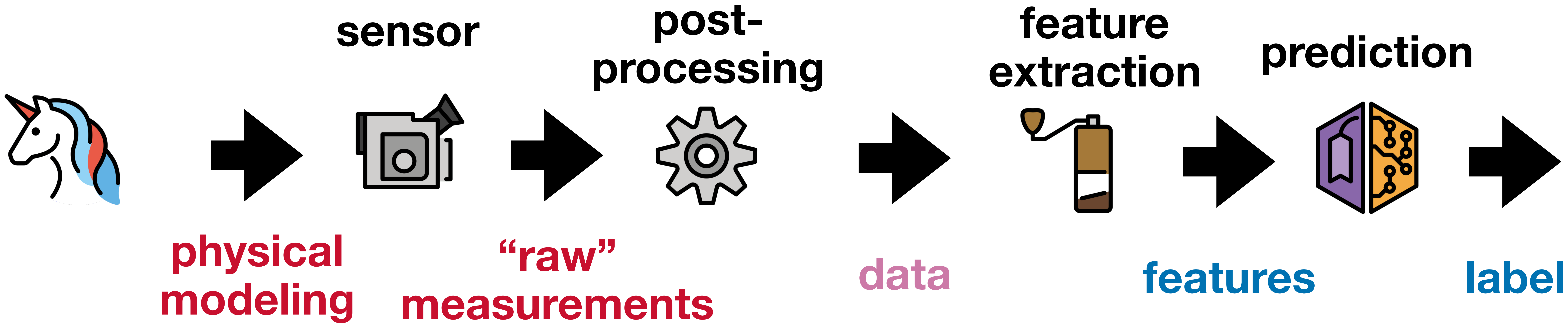

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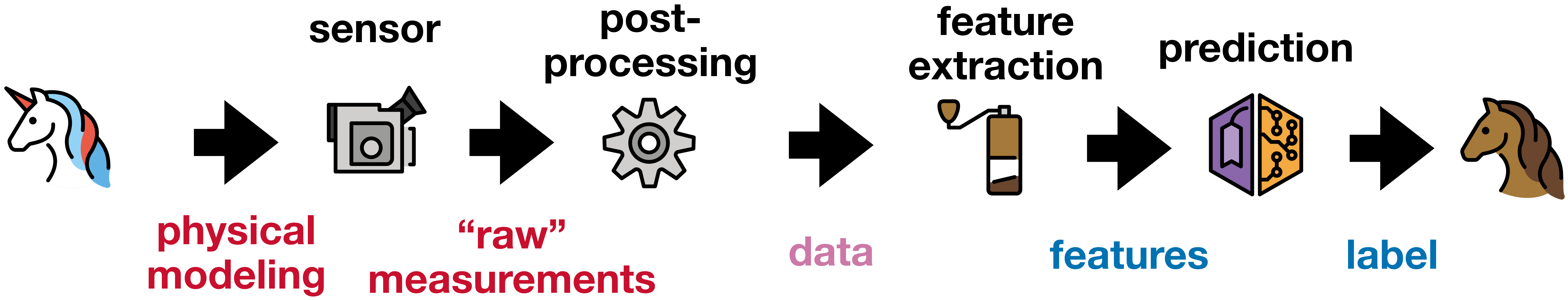

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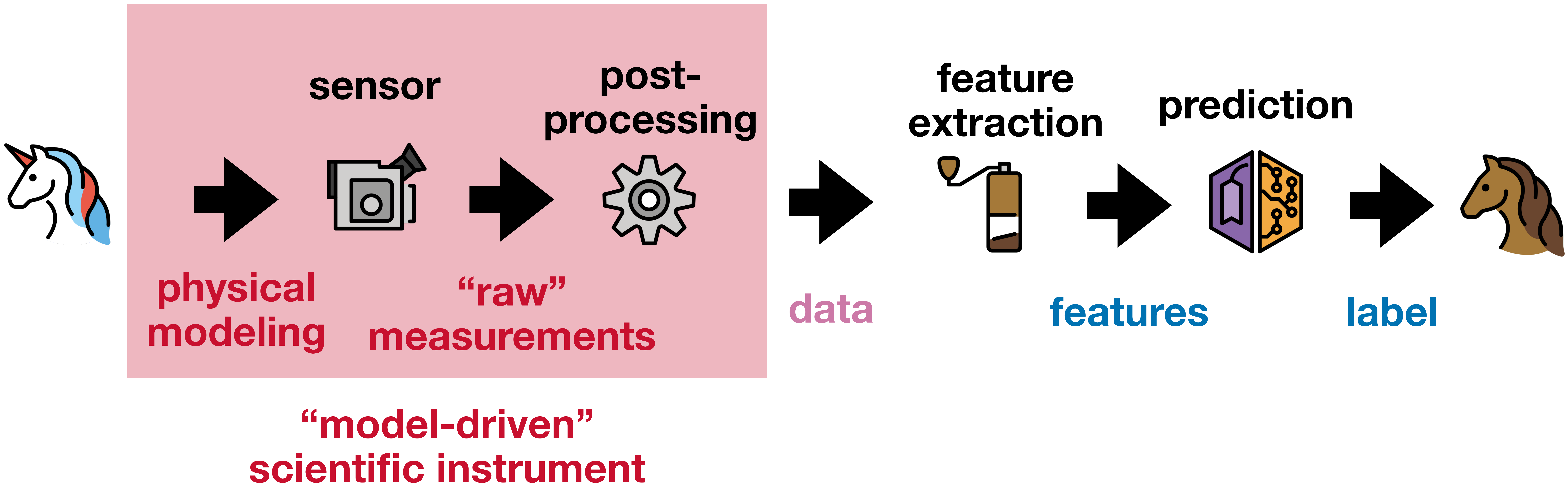

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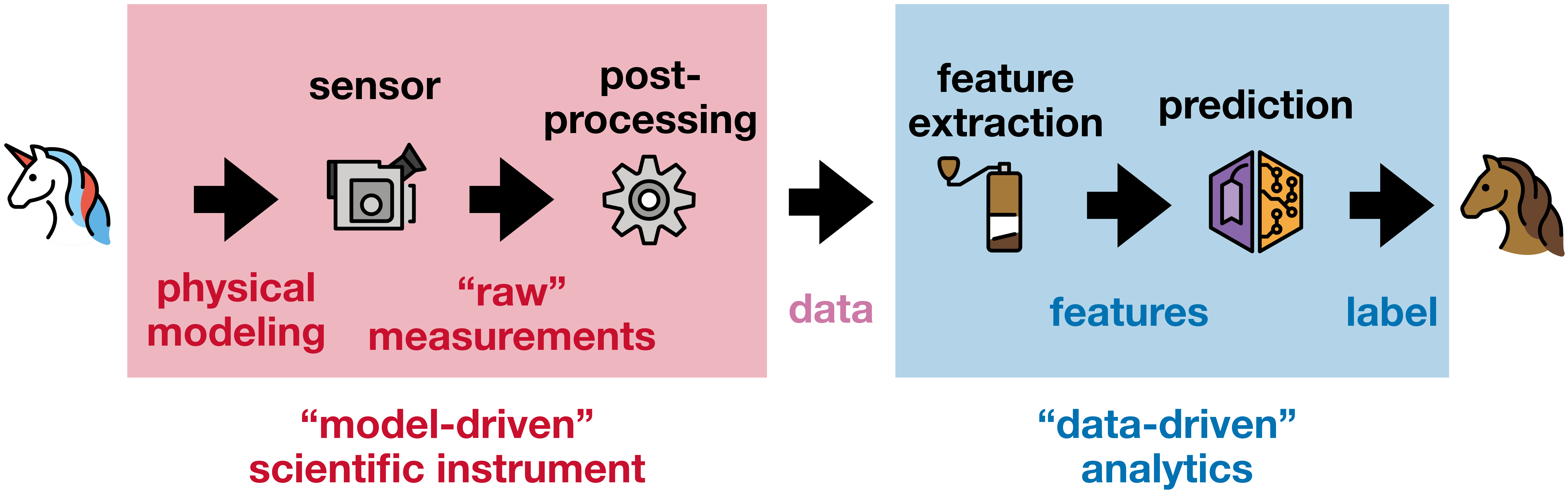
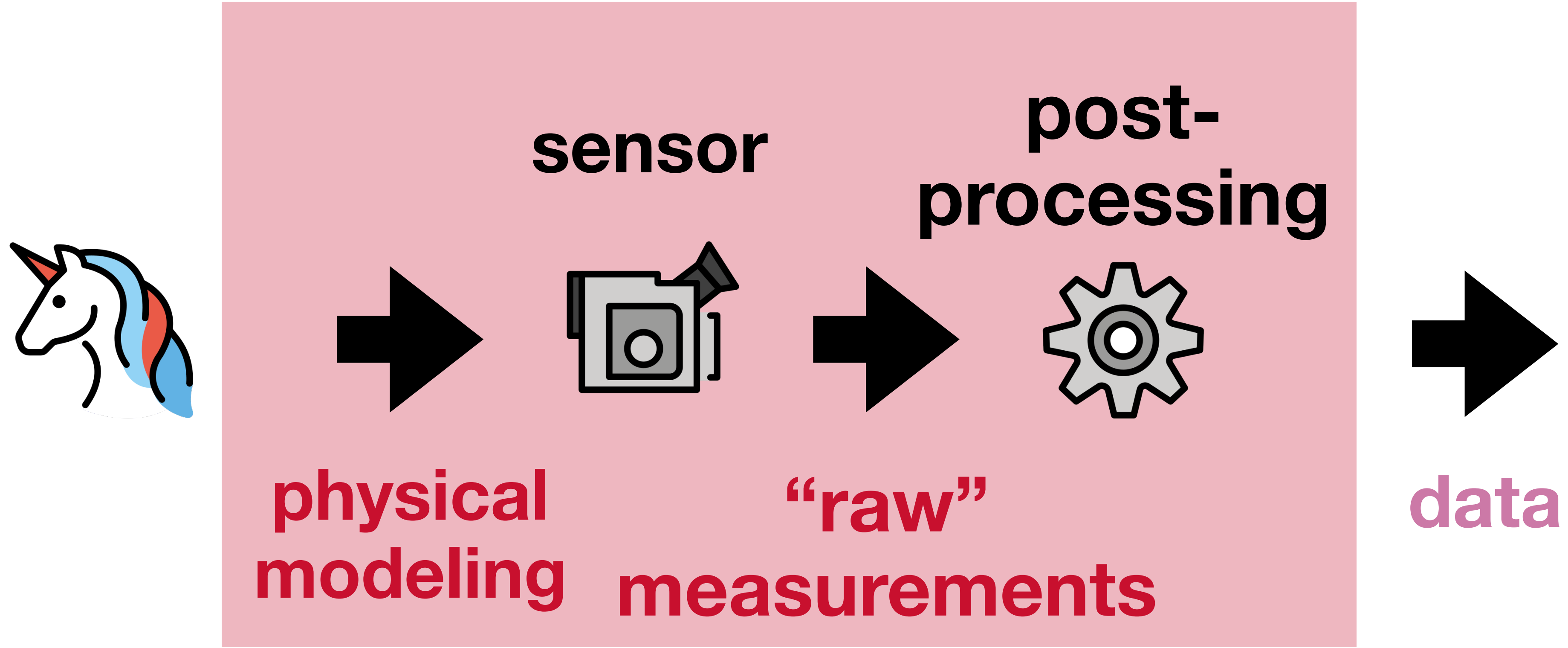
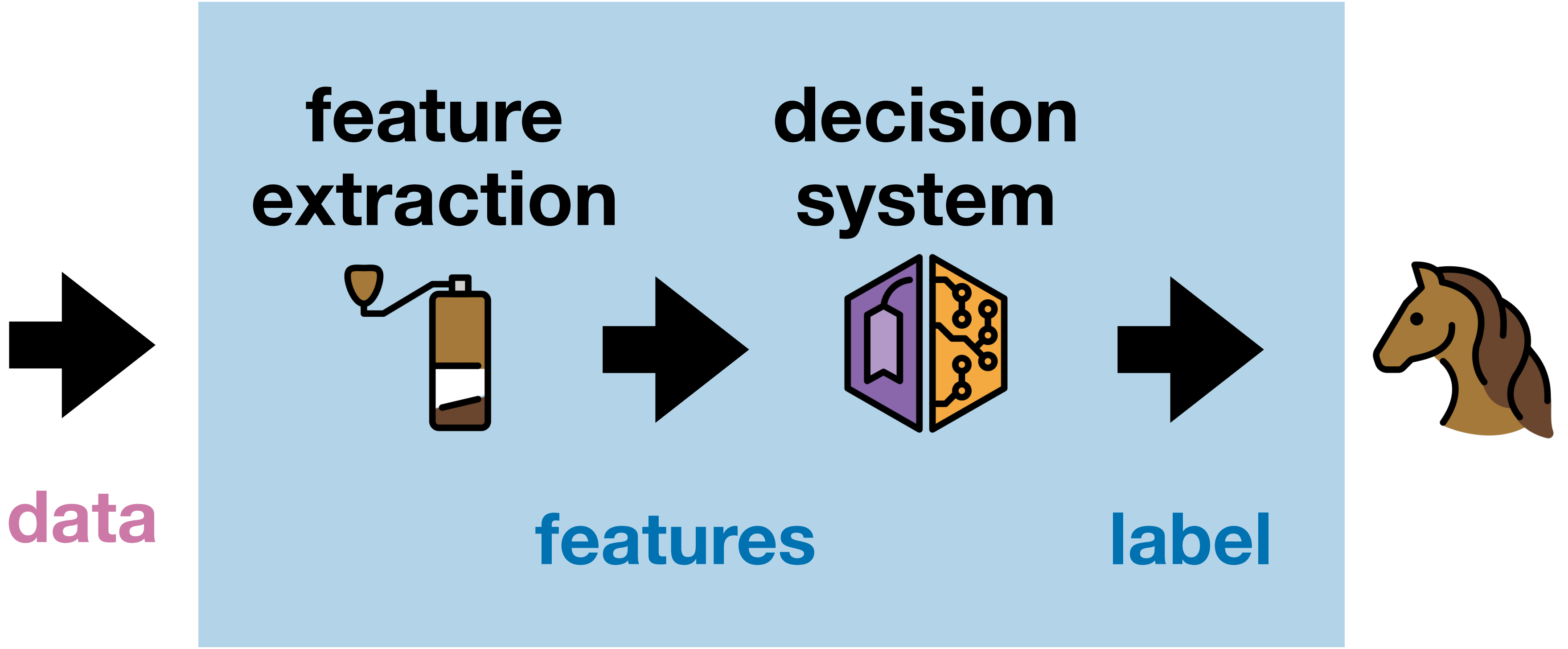


What is “AI as instrumentation”?

Putting neural networks into measurement devices





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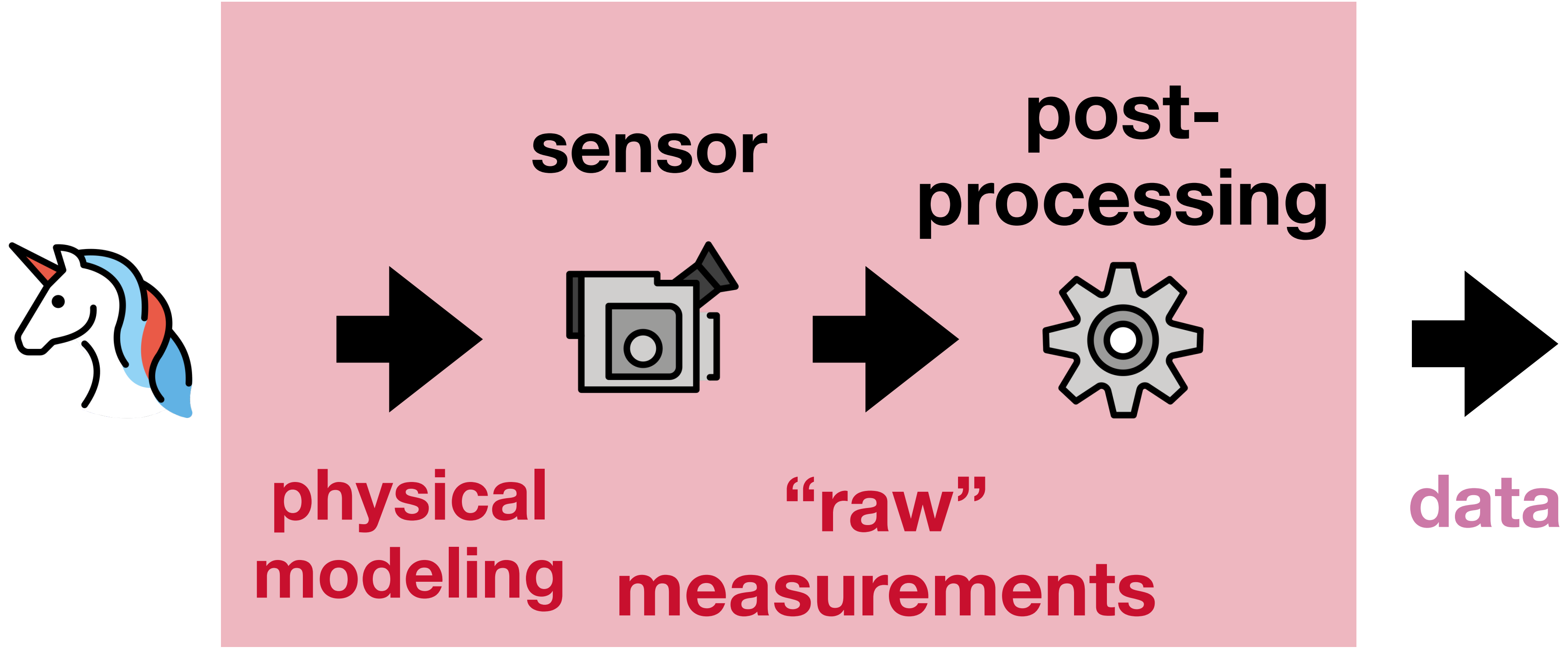

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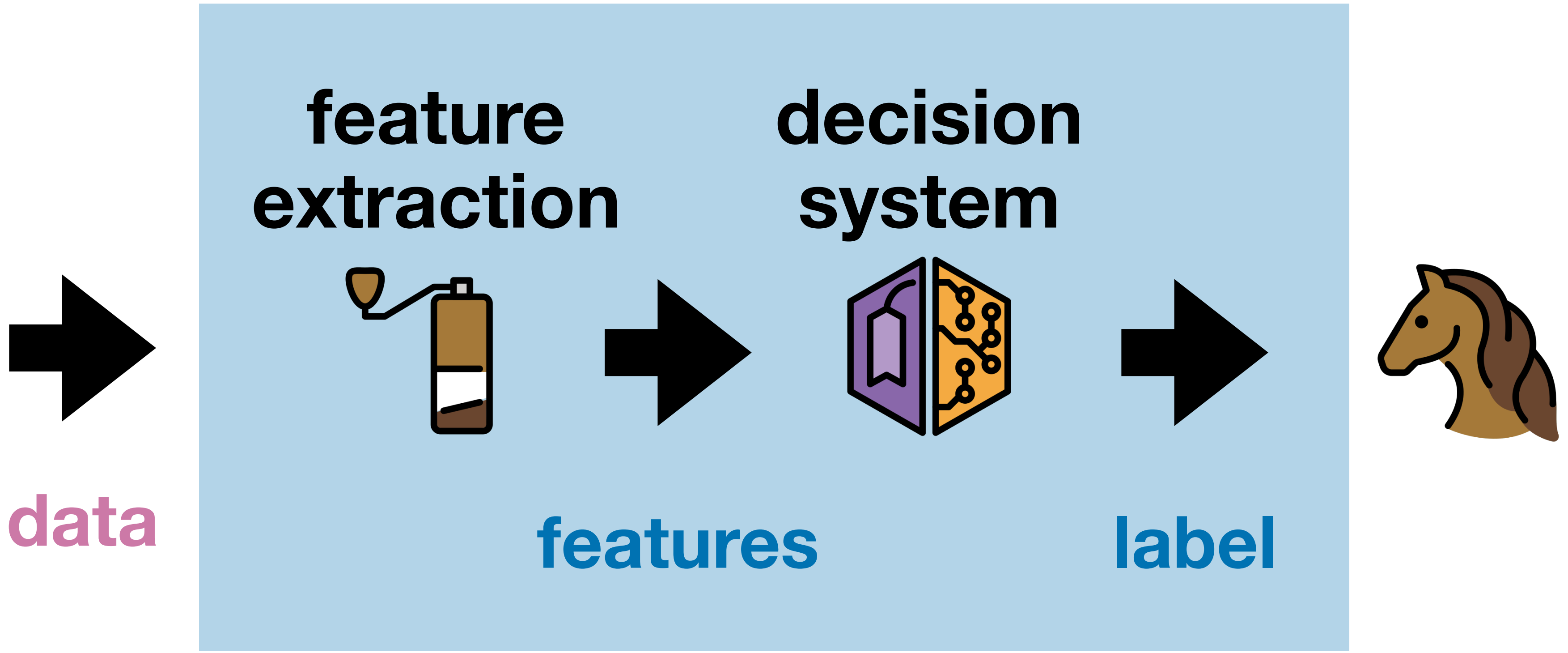

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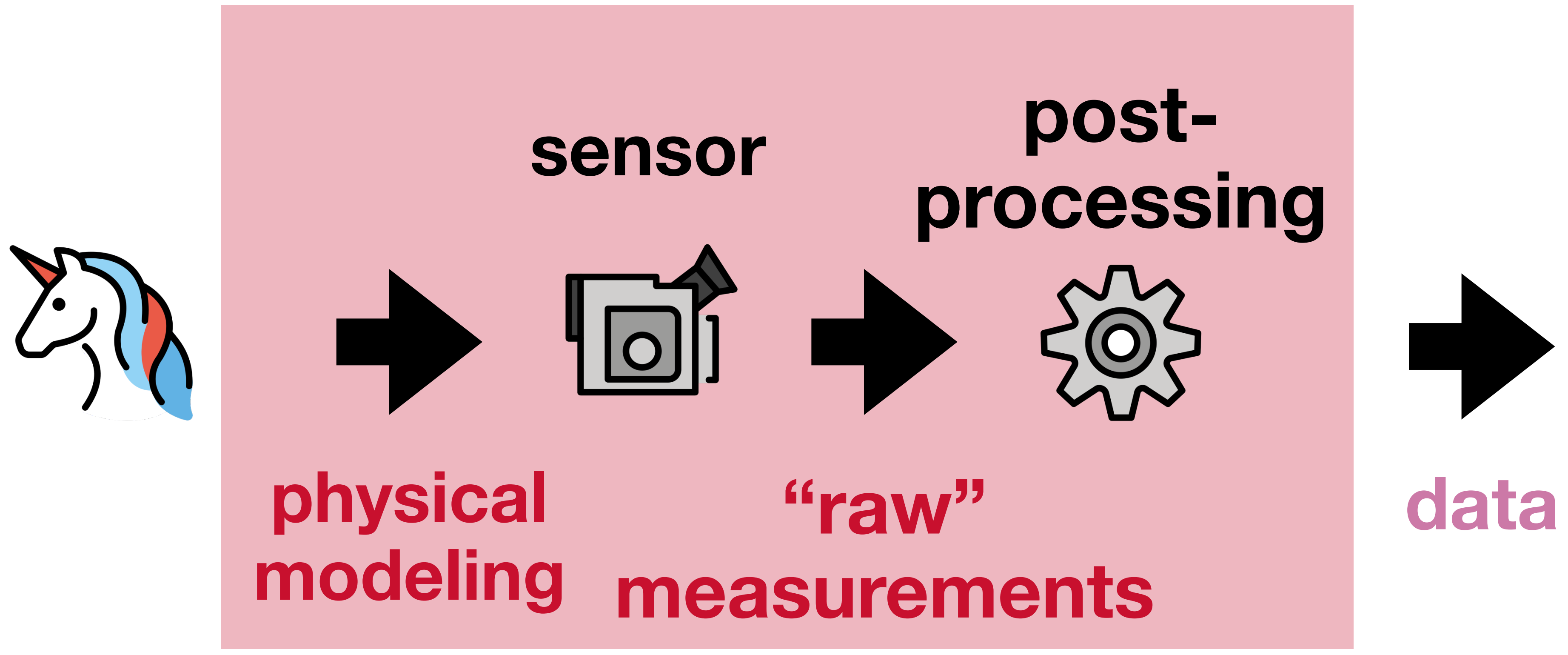

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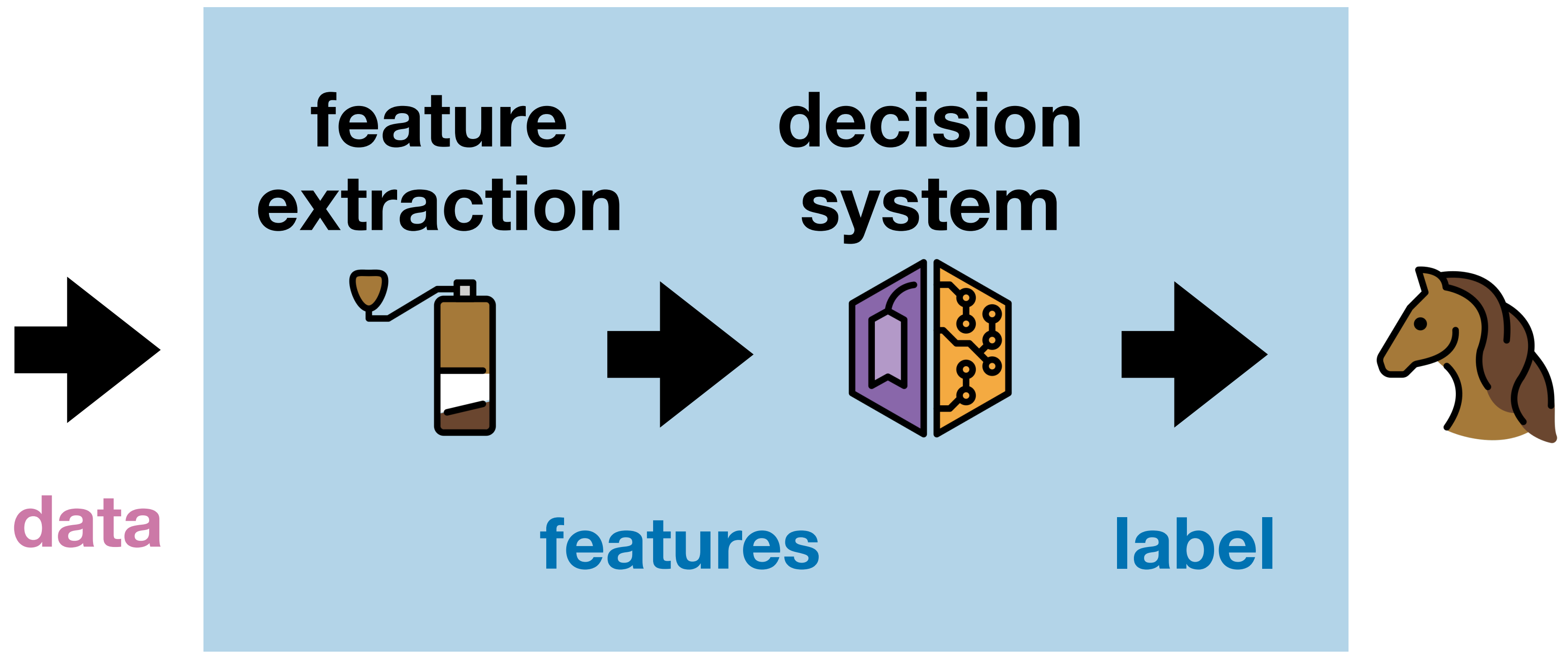

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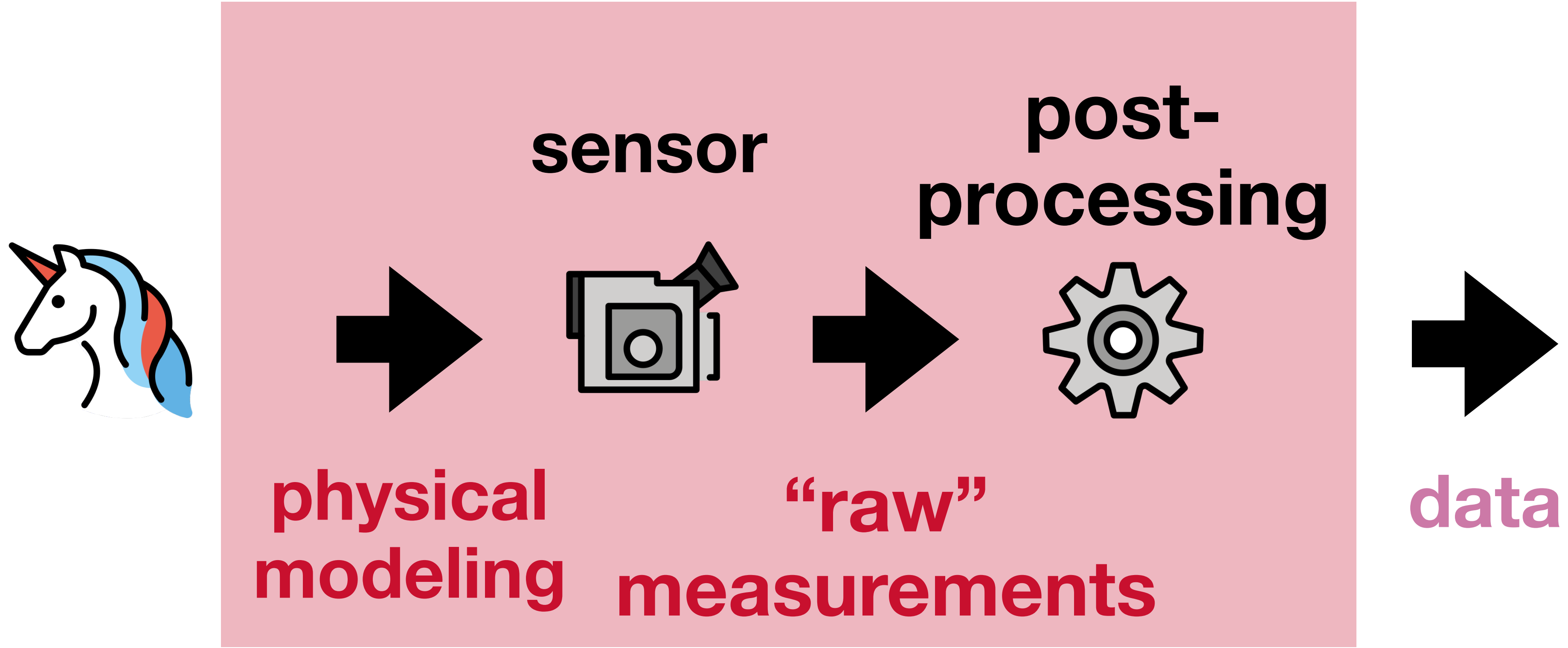

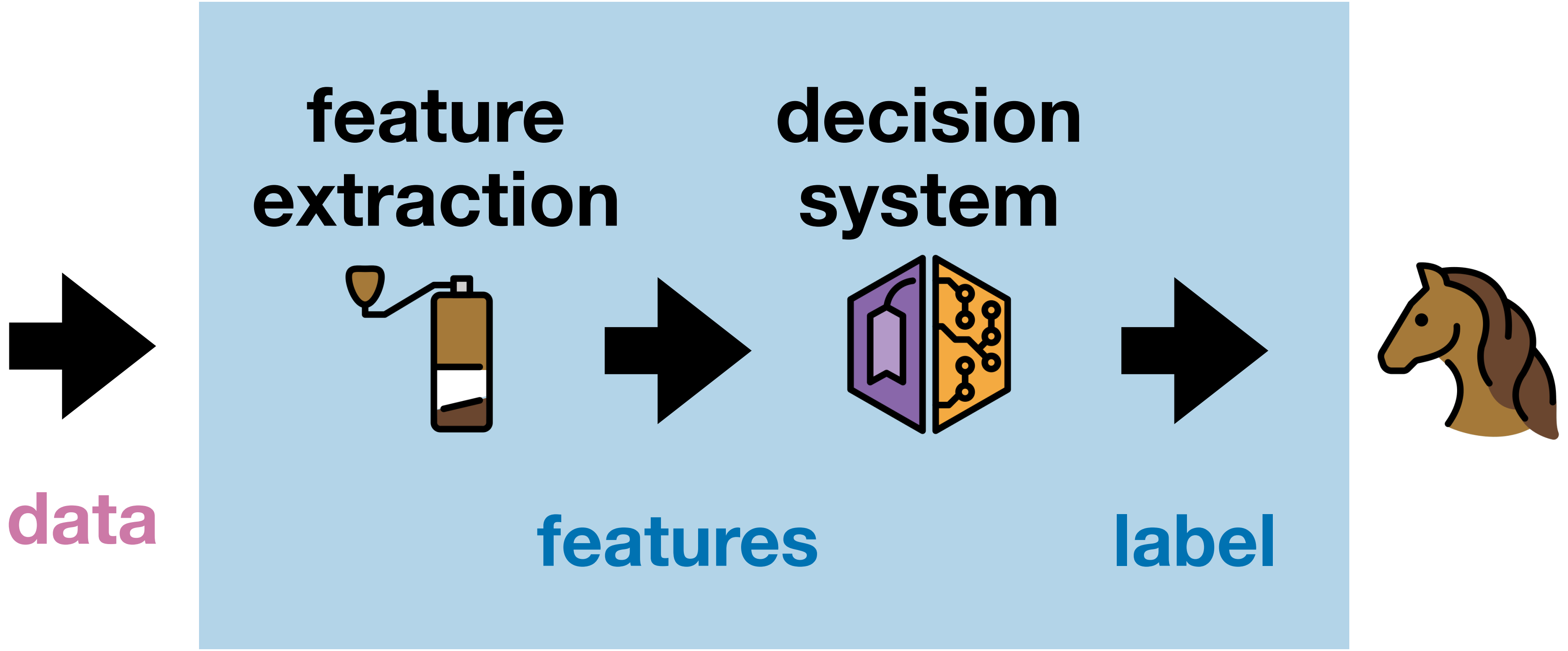

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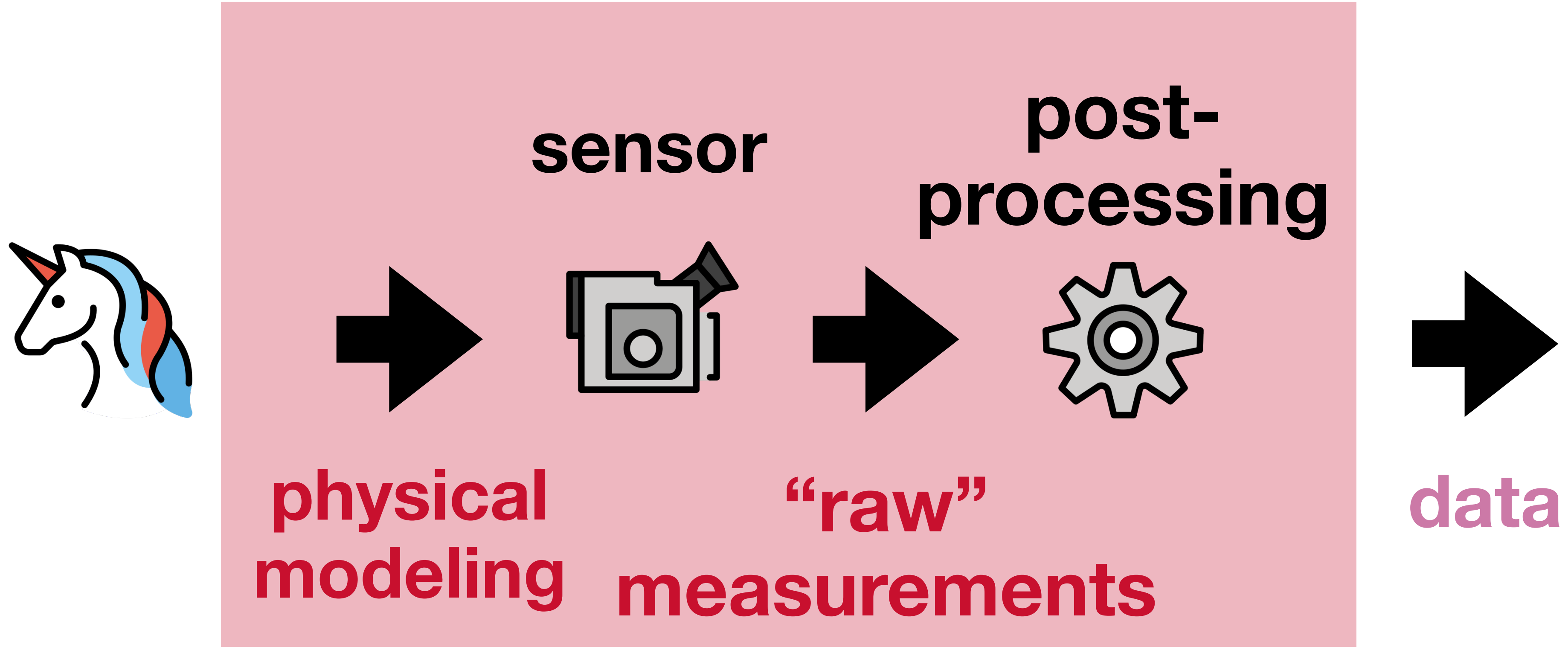

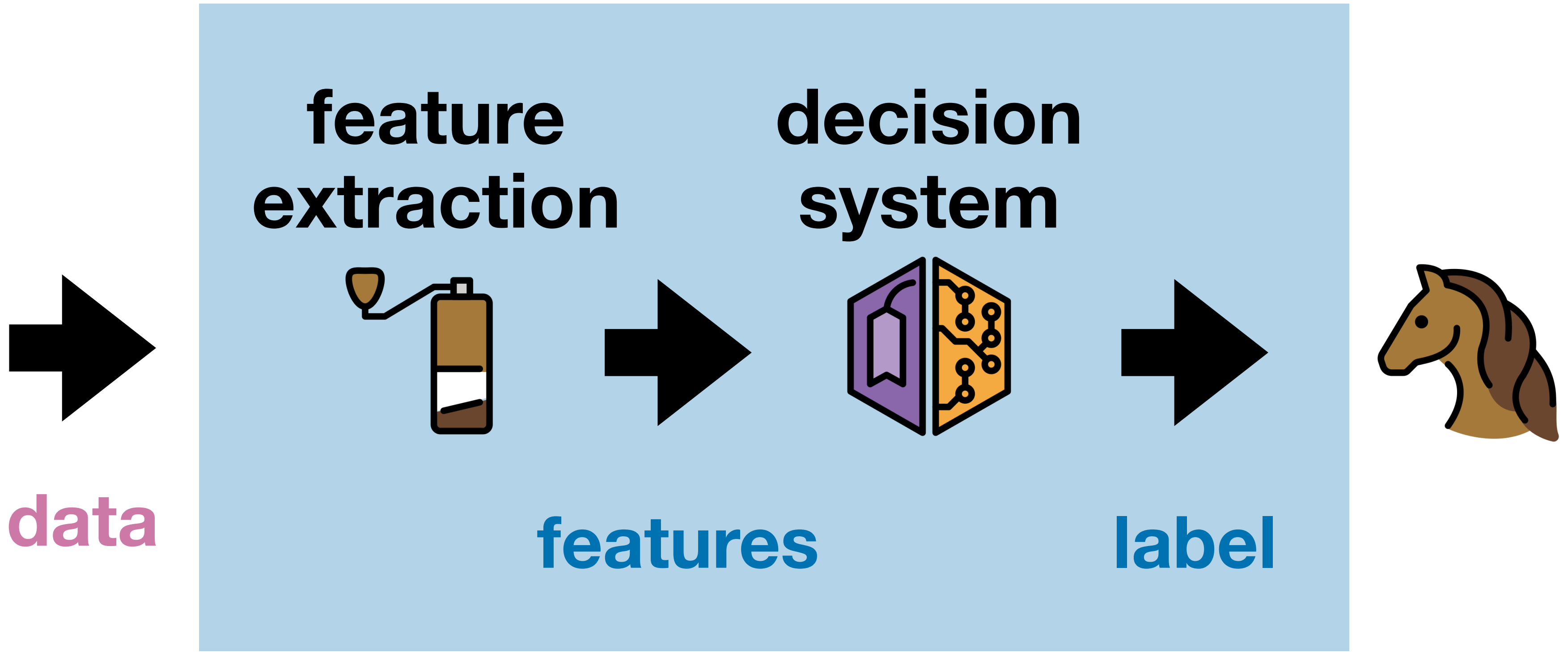

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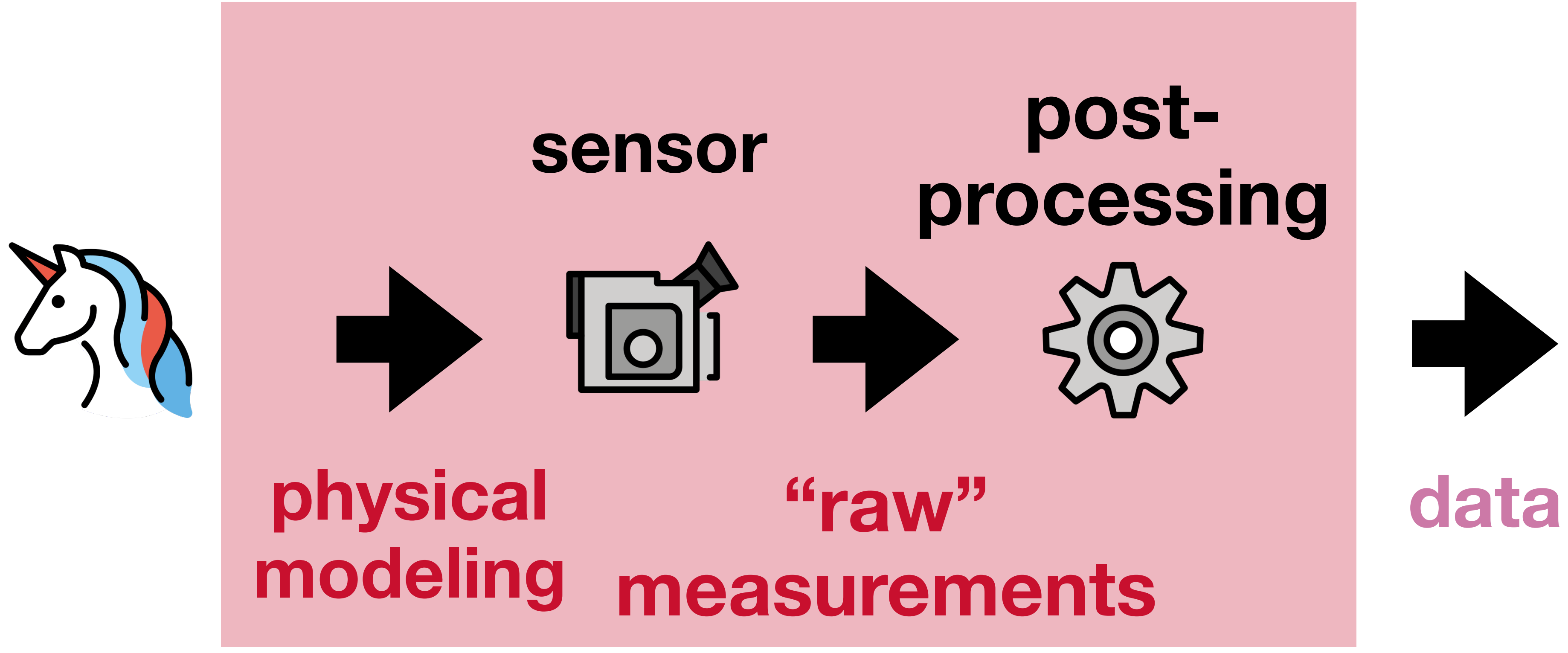

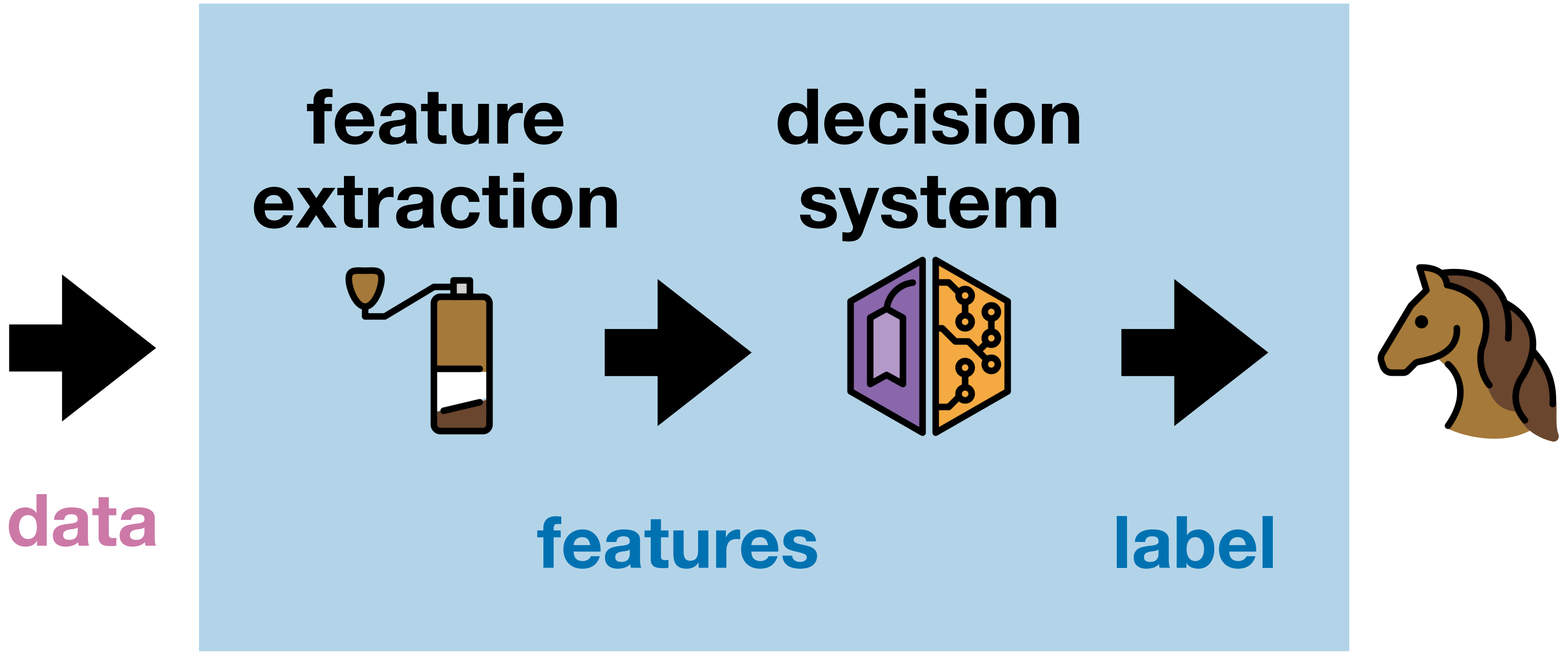

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If we put AI “into the camera” will these be true?

It already is not true in actual practice

Assumptions are wrong, but maybe correctable?

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

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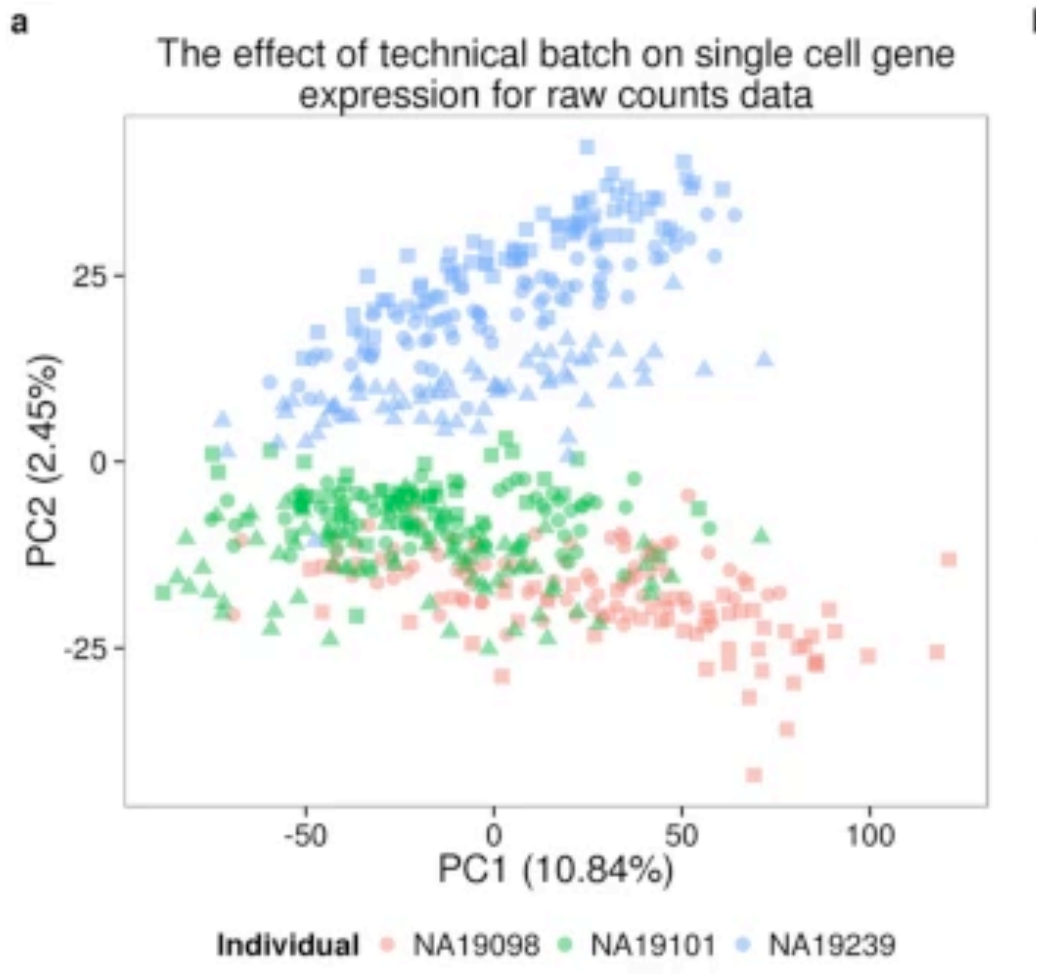

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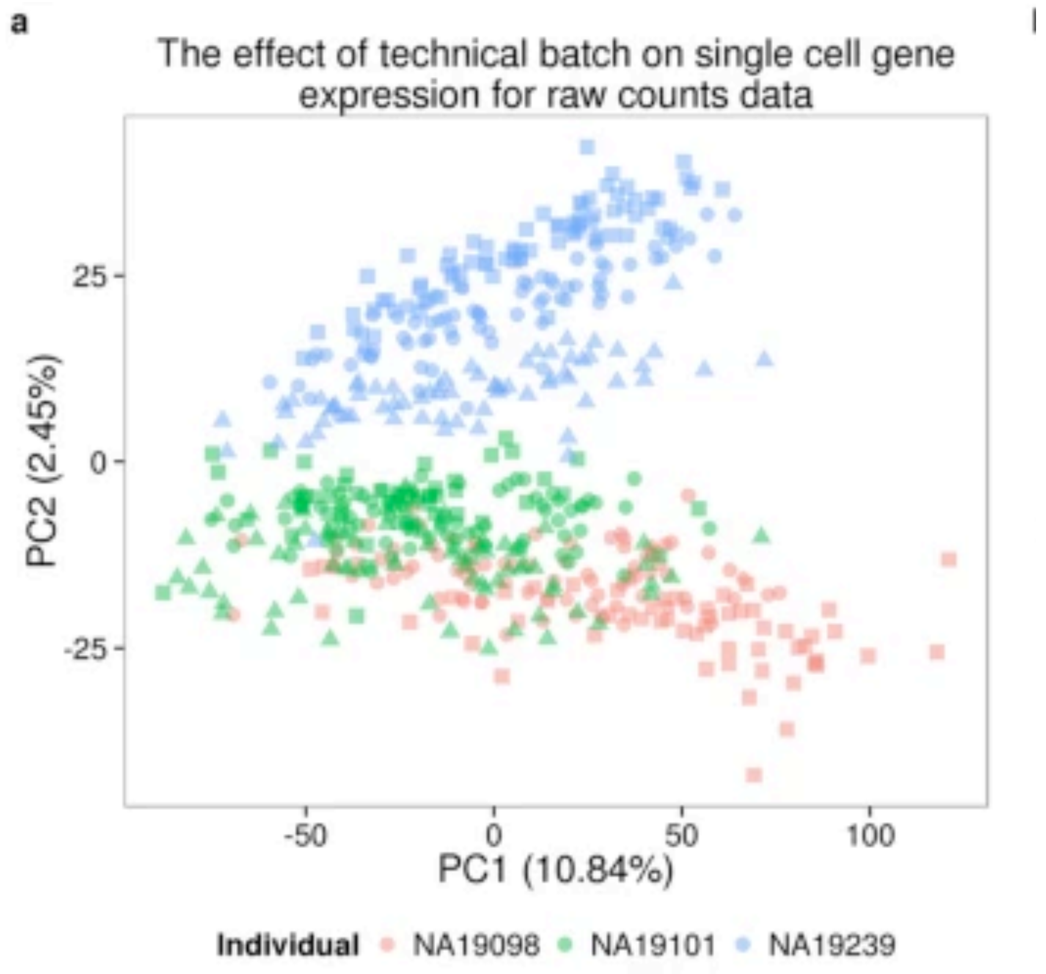

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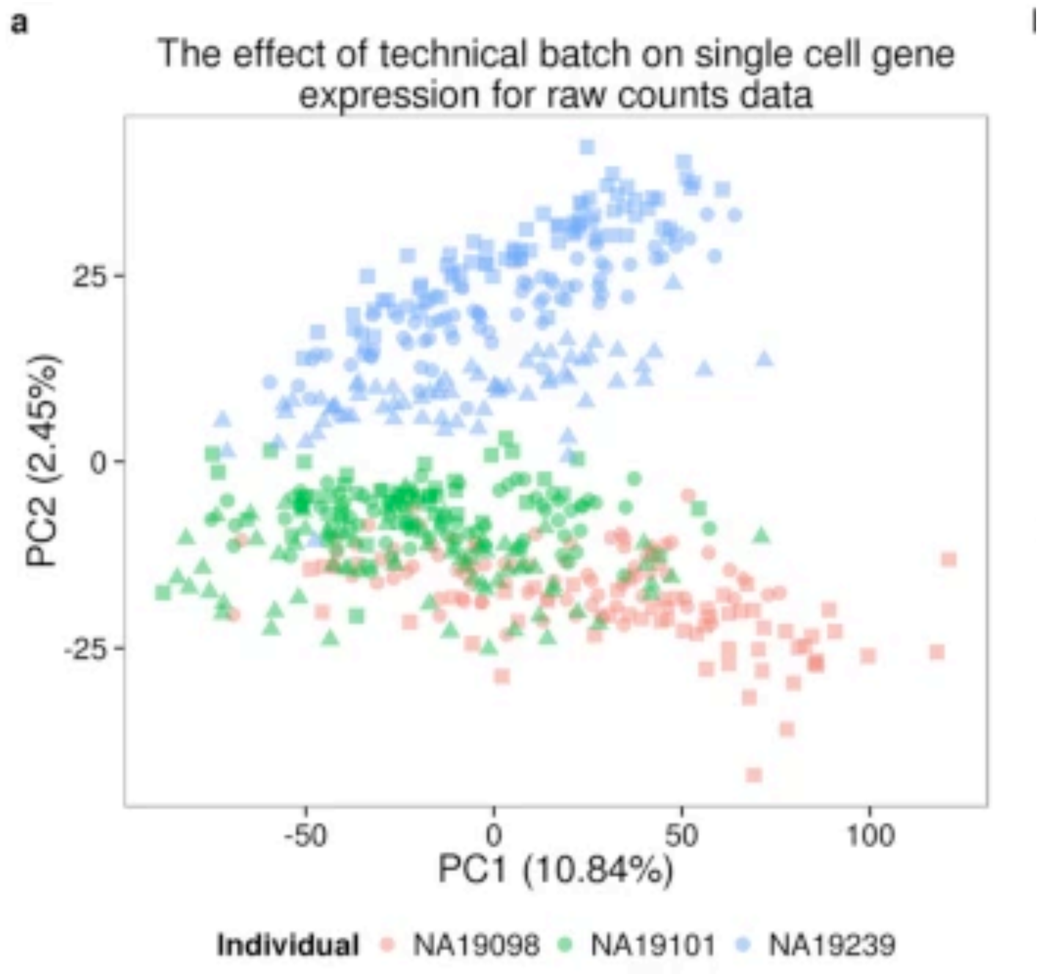
- Sampling bias



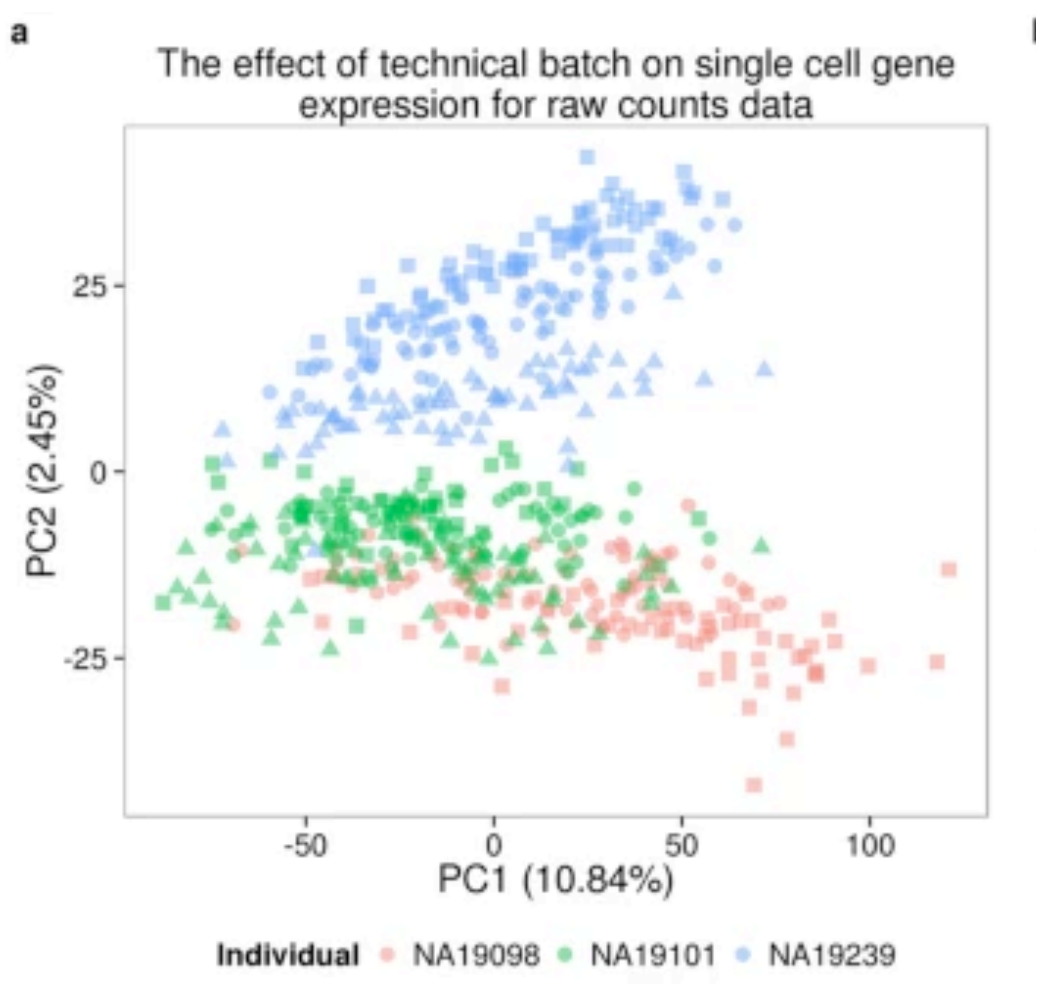
Images: pngrepo.com, Tung et al. (2017), OpenMoji.org

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…



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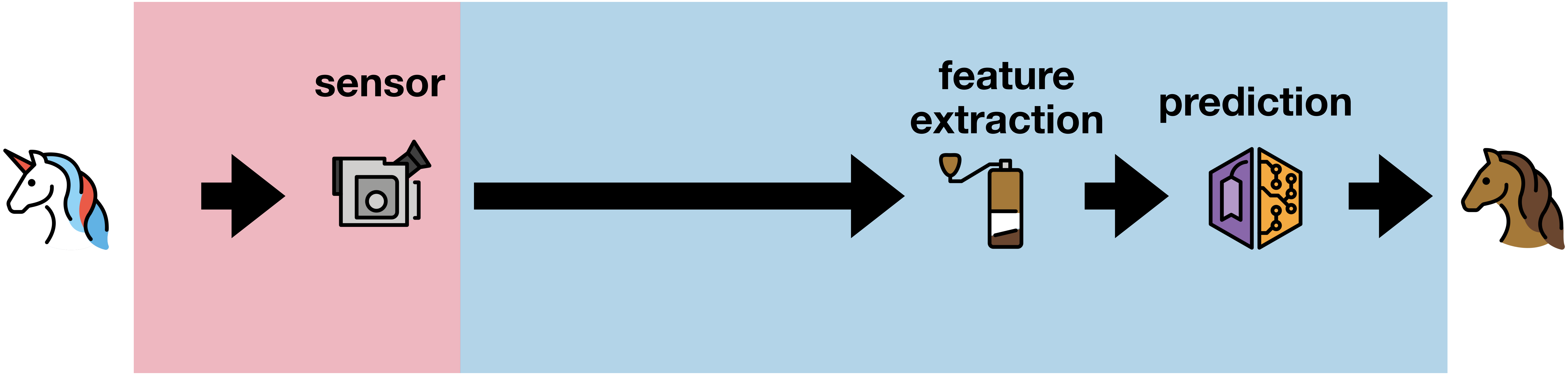
Pushing the kitchen sink backwards

Sensors, instrumentation, and decision support



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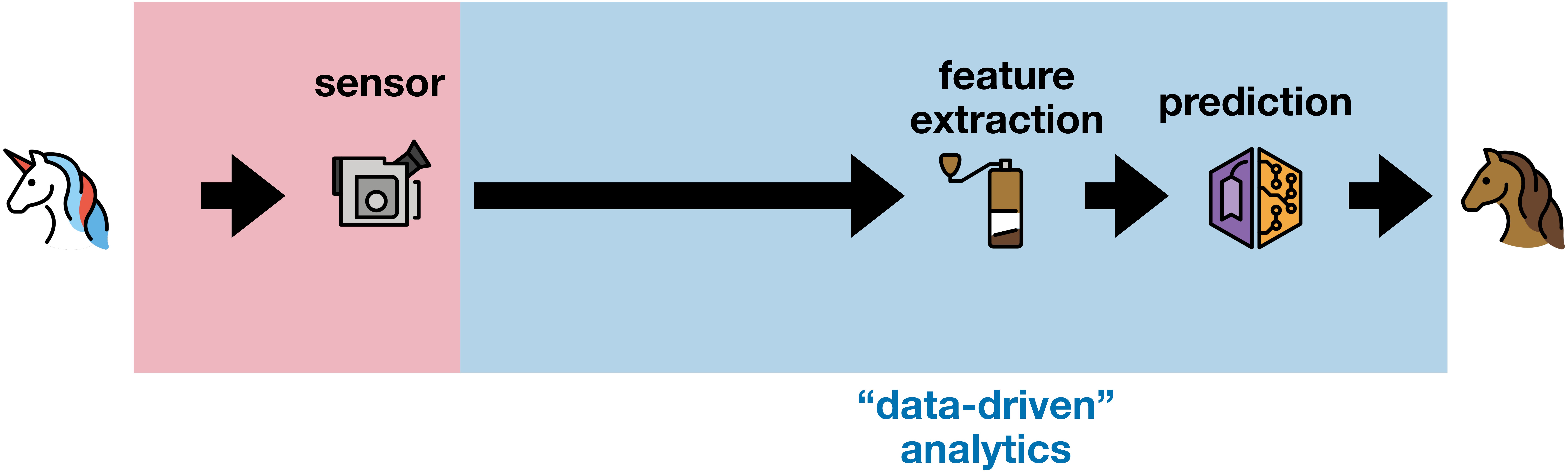

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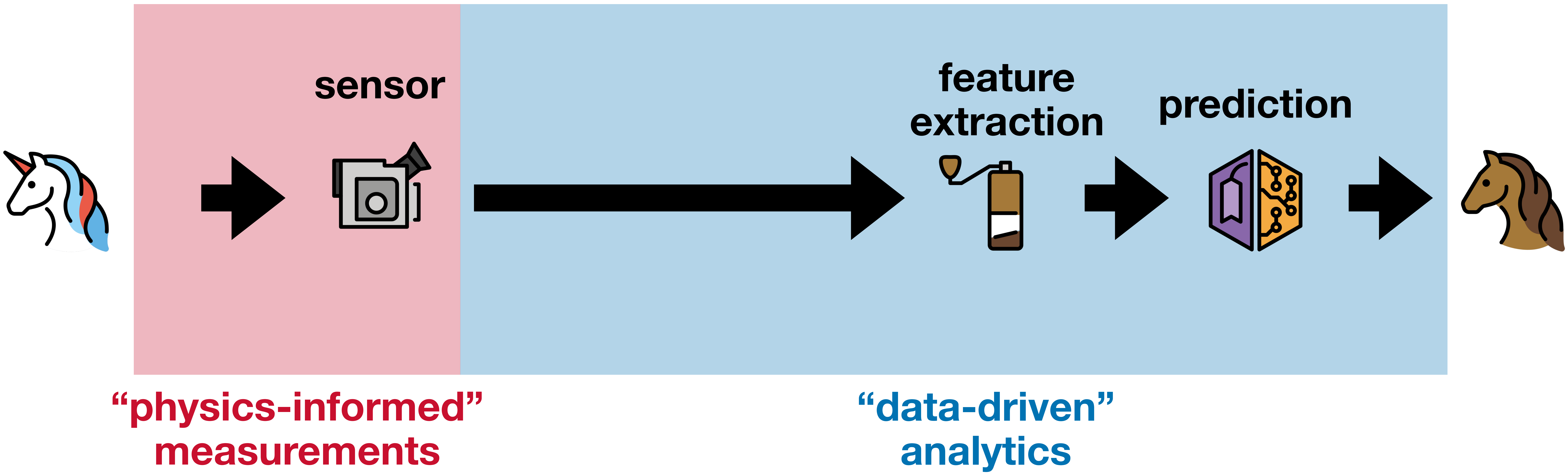
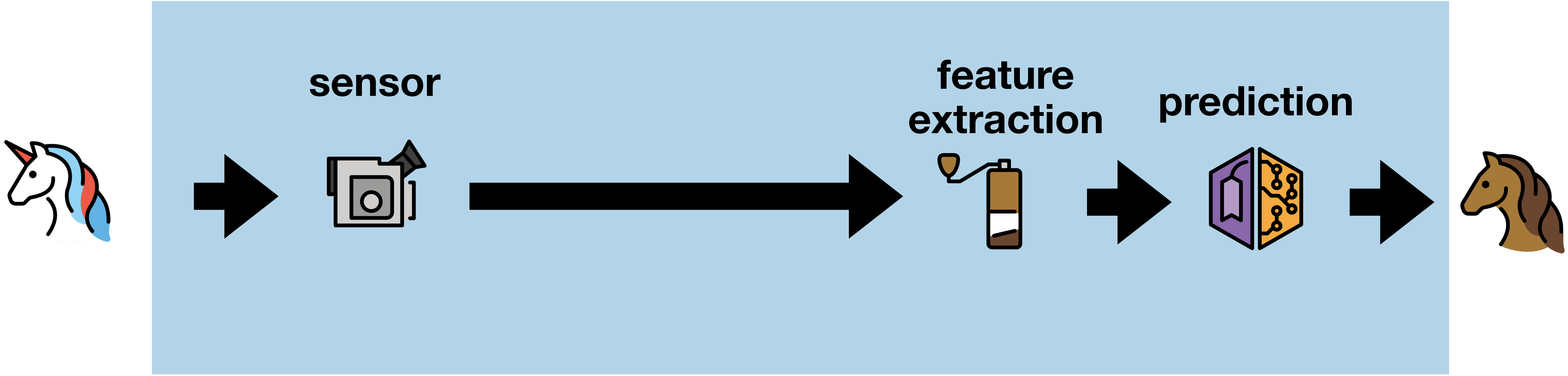


Do we even need to understand physics?

(Asking for an undergrad friend)



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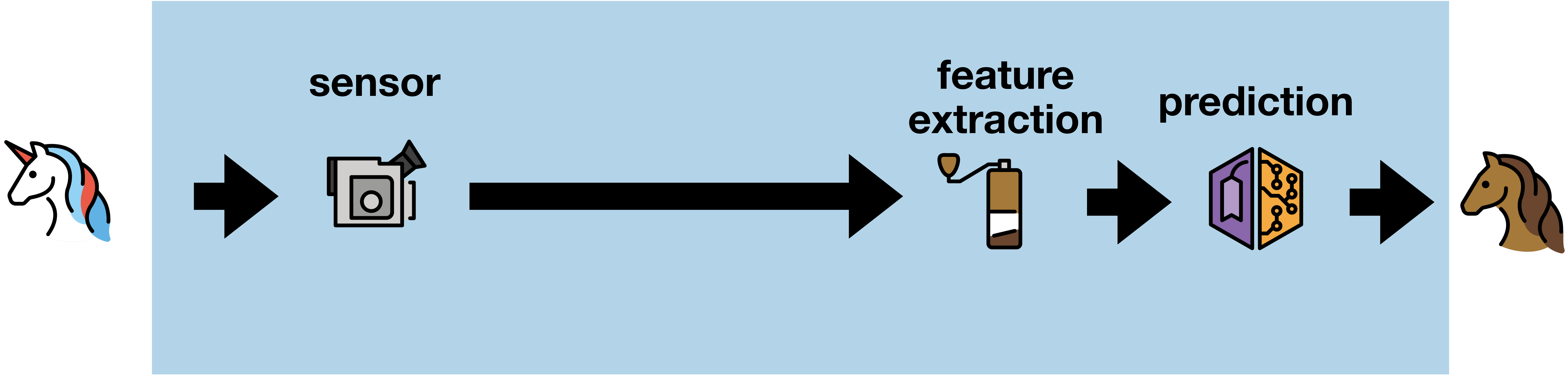


“data-driven”
scientific instrumentation

What about our assumptions?

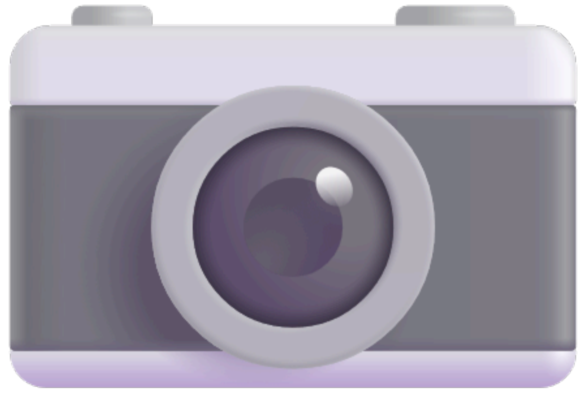
What would it mean of them to hold (if they do)?

iOS 8.3

iOS 18.4

HarmonyOS 4.0

Samsung UI 7.0



MS 3D Fluent

SerenityOS

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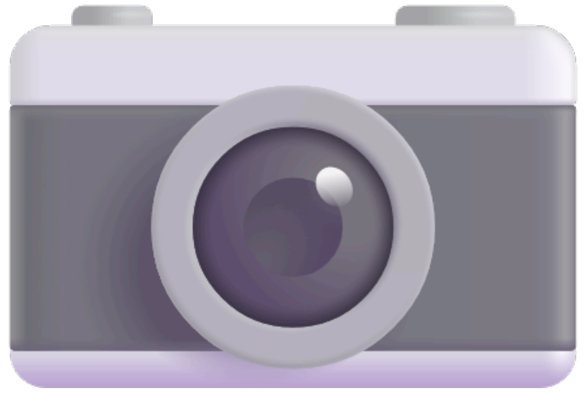

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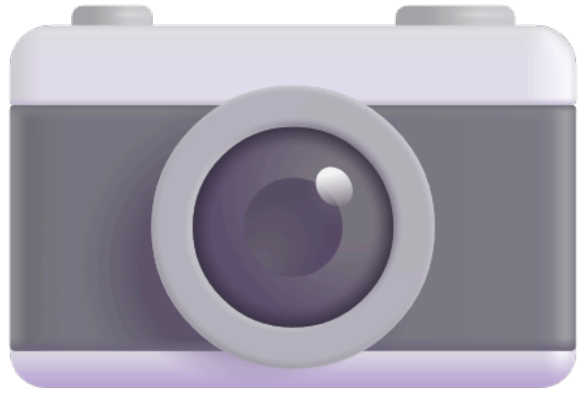

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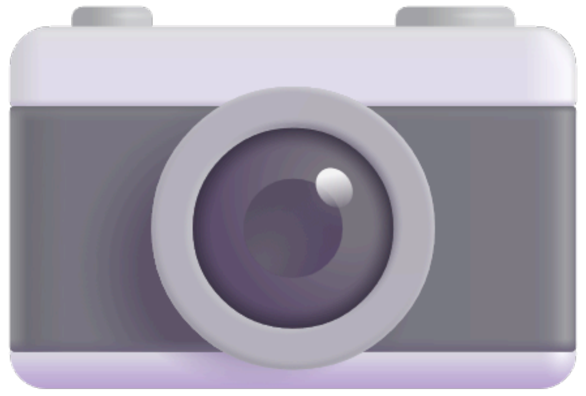

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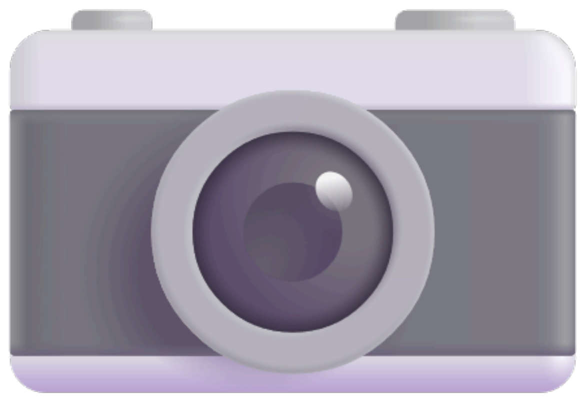
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<u>**These questions are not new!**</u> We can use “classical” tools to try and understand them.


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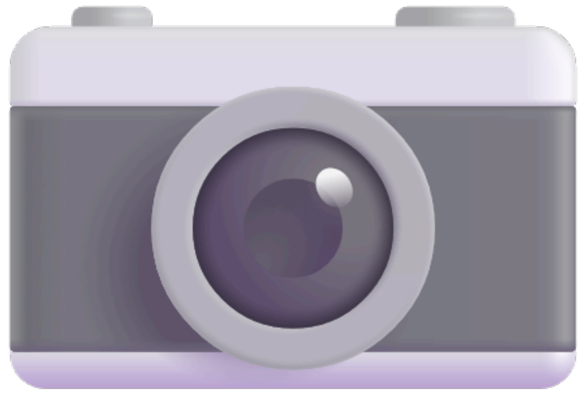
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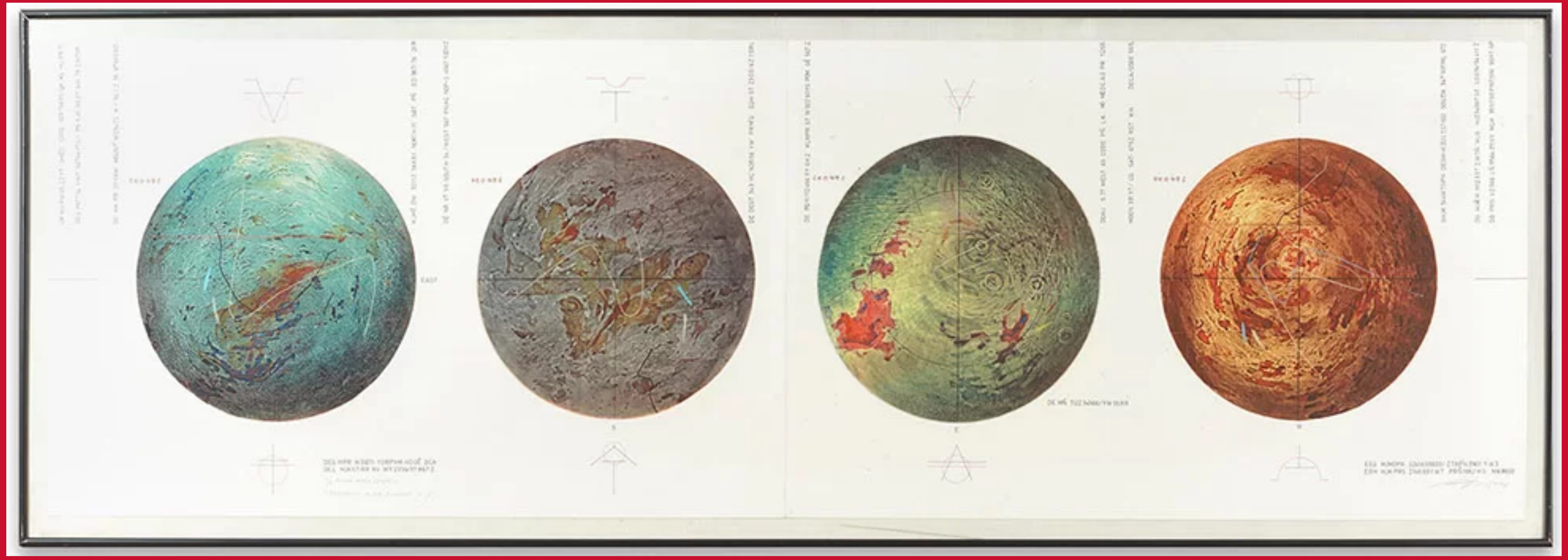
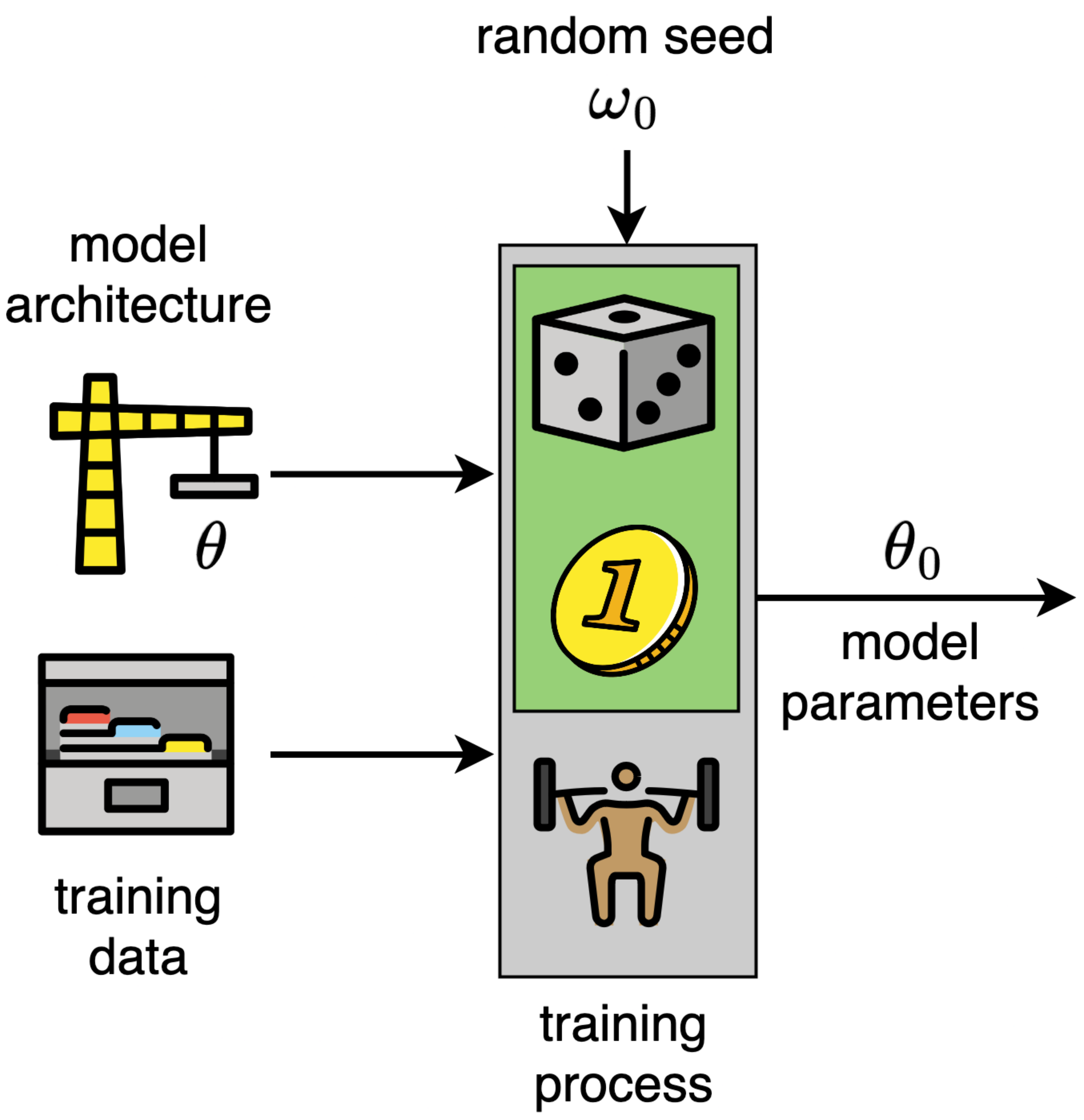
Some preliminaries



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

The standard statistical setup for modern ML

Machine learning as function-fitting



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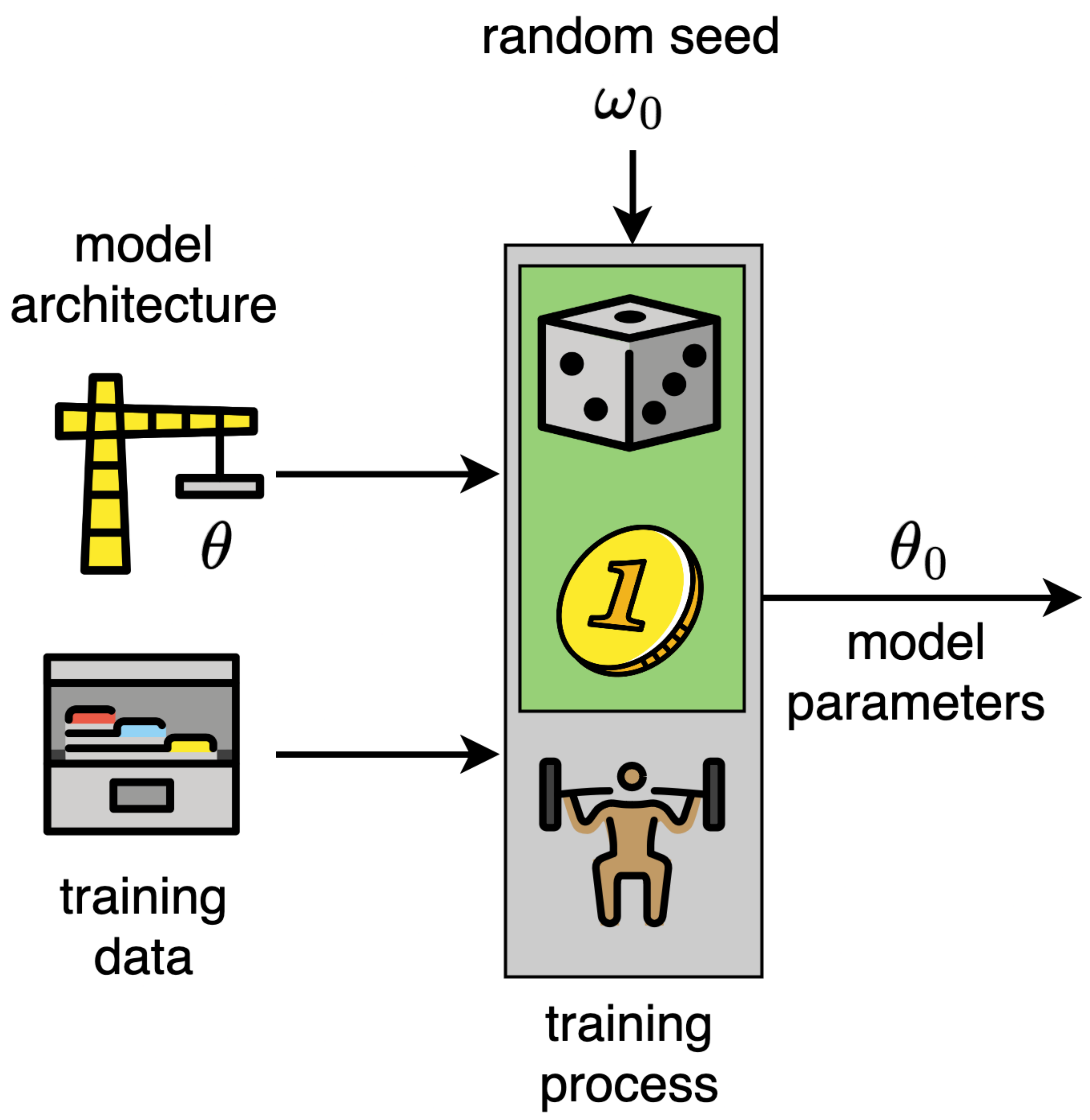

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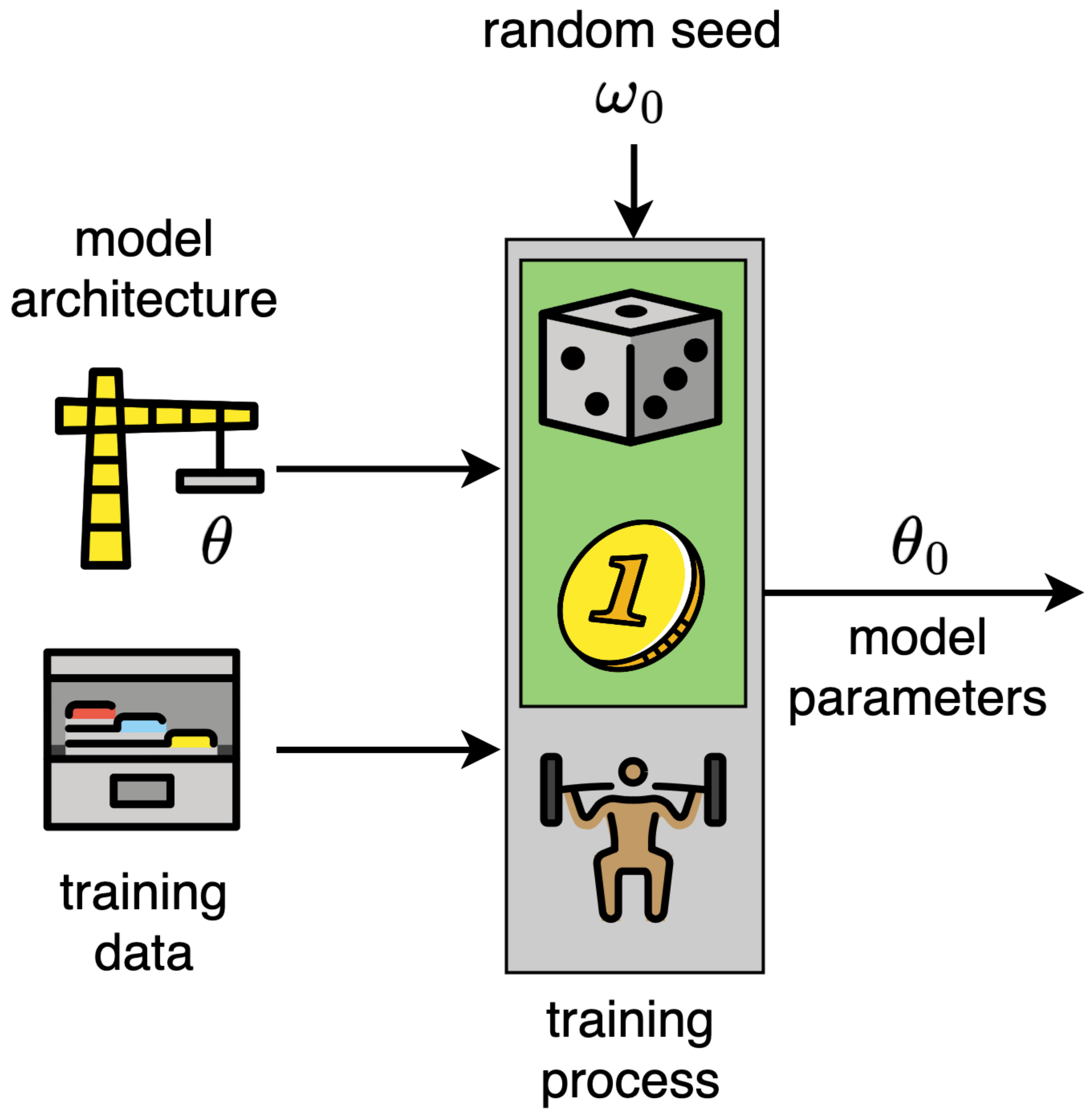

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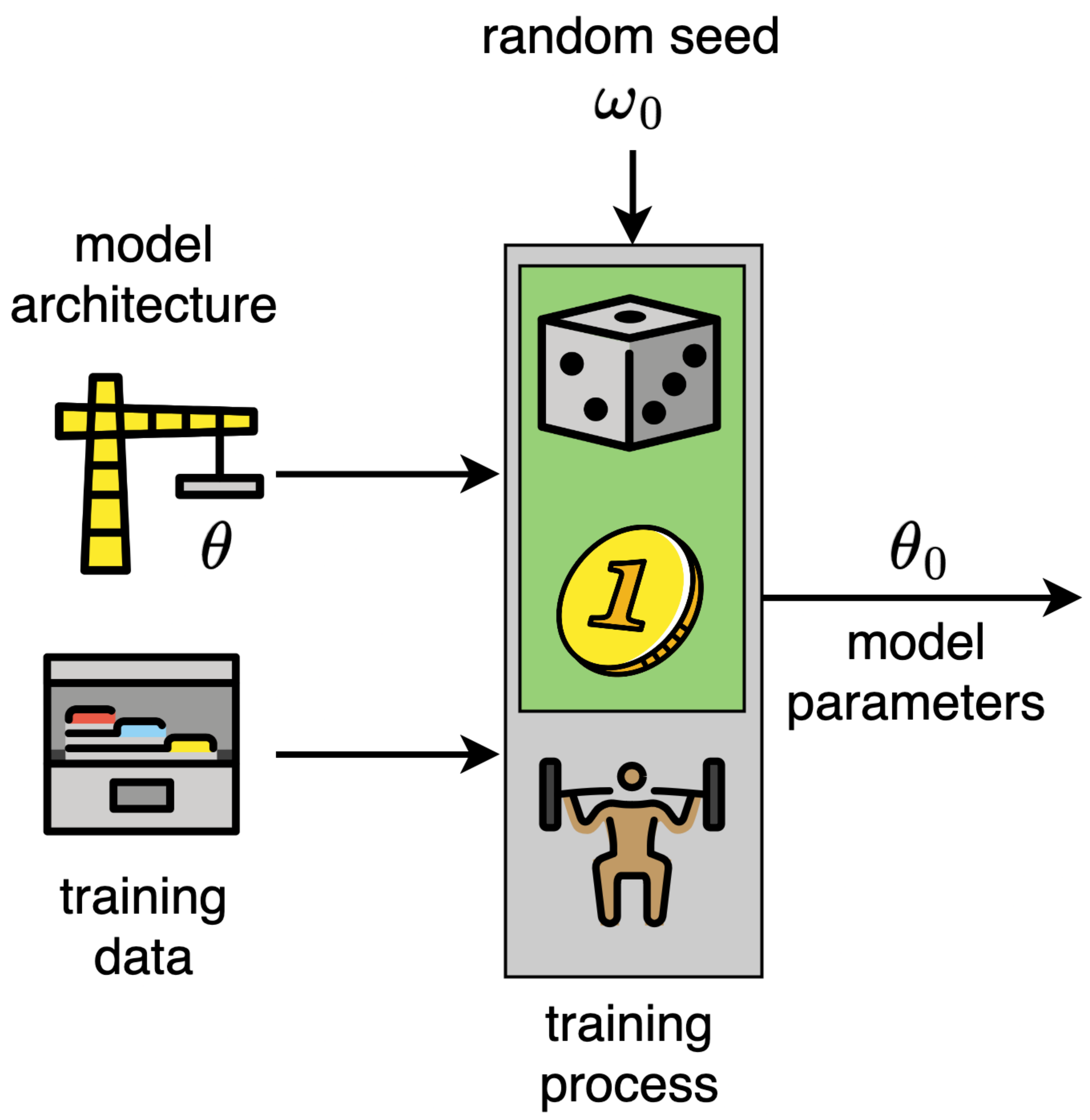

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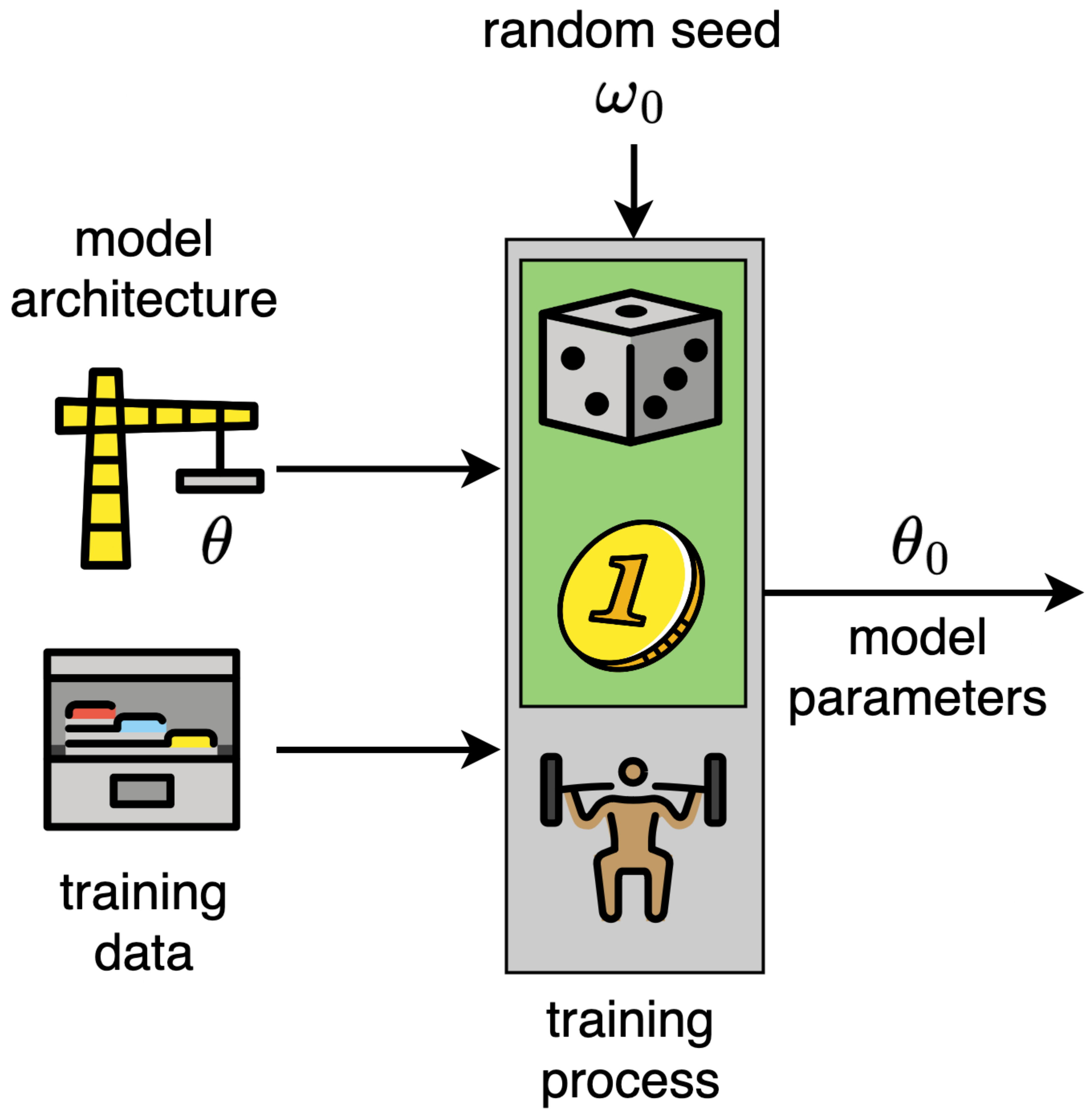

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- Parameterized set of functions/models $\{f(x \mid \theta) : \theta \in \Theta\}$.
- Training data used to estimate the parameters by minimizing some objective function.
- Stochastic optimization algorithm that does the actual minimization.

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Drawing samples from the function space

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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

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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?

HarmonyOS 4.0

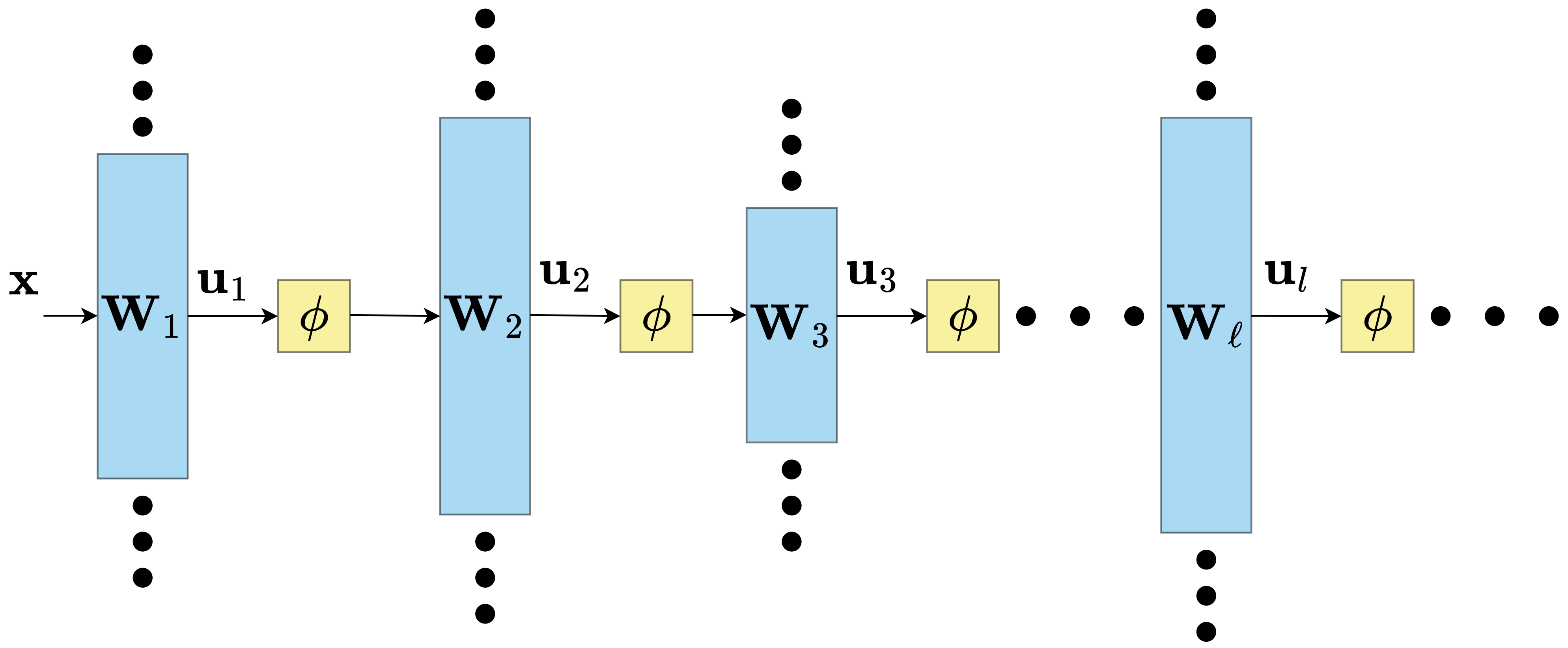
Samsung UI 7.0

If we have two different architectures $\mathscr{F}$ and $\mathscr{G}$ 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?



$$\approx$$

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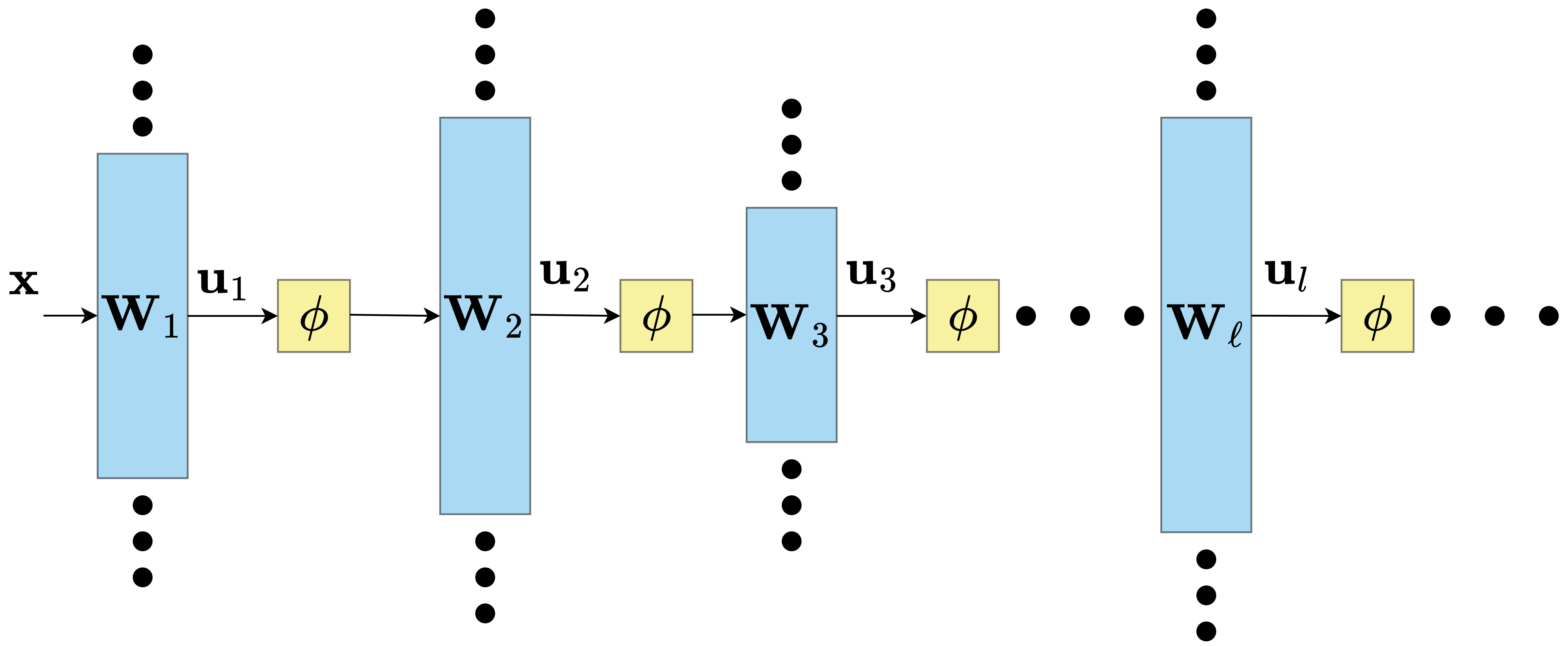

$\approx$

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).

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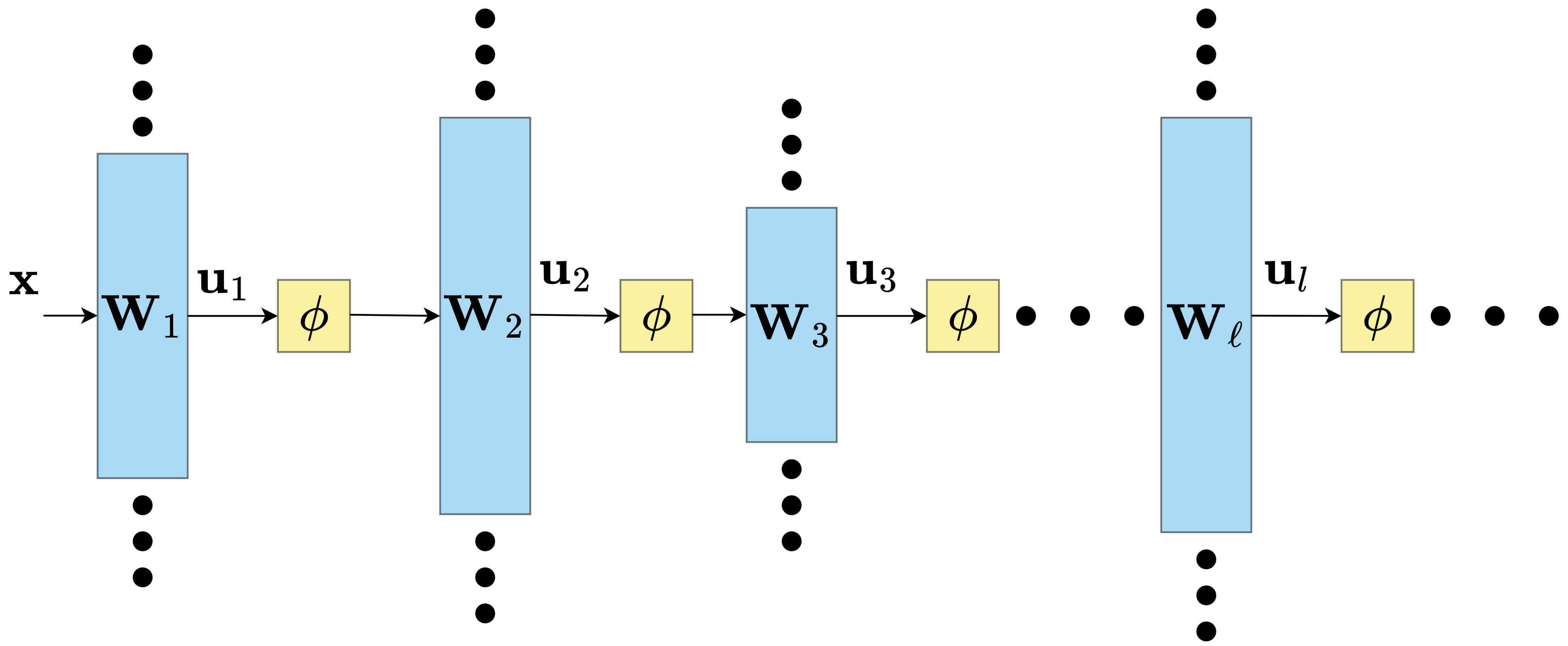

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One example: the **neural tangent kernel**.

Neural Networks as Kernel Machines

Approximating an NN with a “simpler” model

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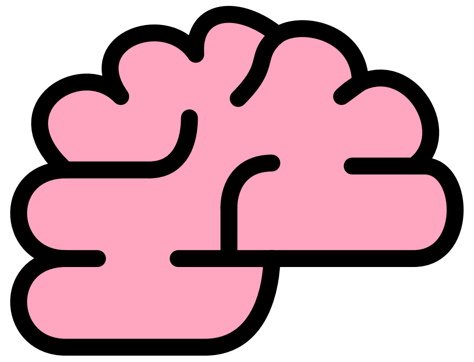
$\text{NTK} \neq$  

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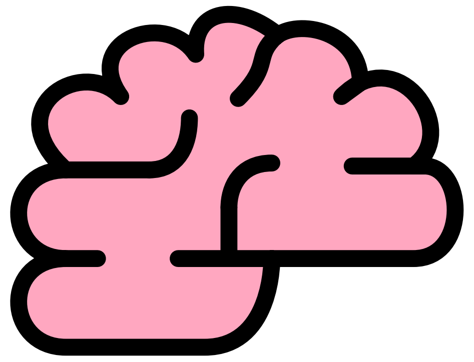
NTK $\neq$  

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

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

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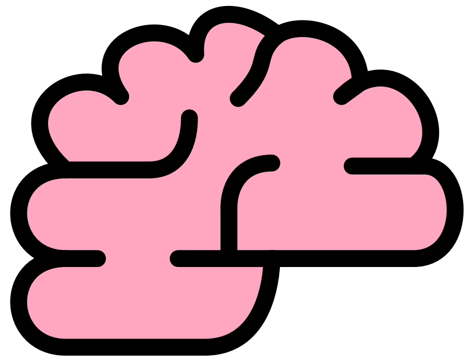
NTK $\neq$  

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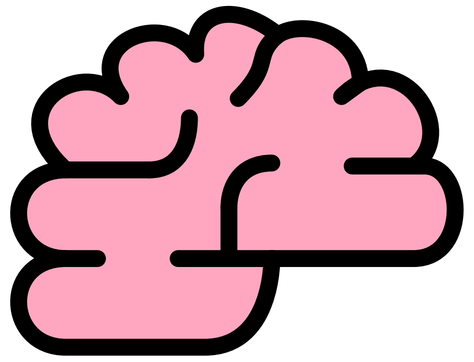
NTK ≠  

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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:

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

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.

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

Trace NTK: a proxy for the eNTK

Much lower computational overhead needed

We look at a simplification of the NTK:

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

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

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Embedding spaces and model comparisons

Rm Palaniappan, *Alien Planet-B*
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A question of interoperability

Challenges in collaborating with AI instruments

HarmonyOS 4.0

Samsung UI 7.0

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Challenges:

- To the human eye, they are functionally similar.

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HarmonyOS 4.0

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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**.

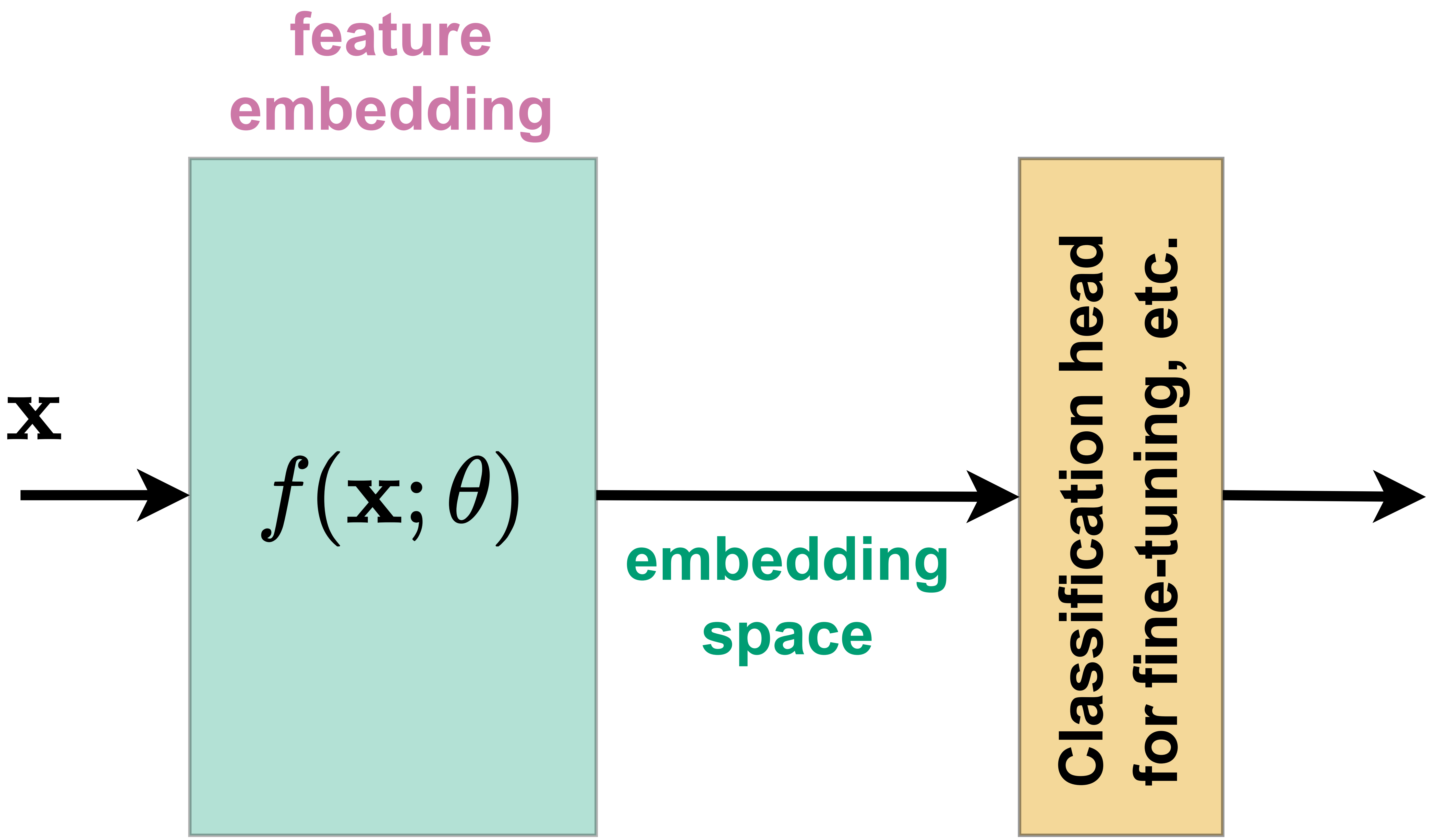
Are these models producing outputs that **“look the same?”**

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



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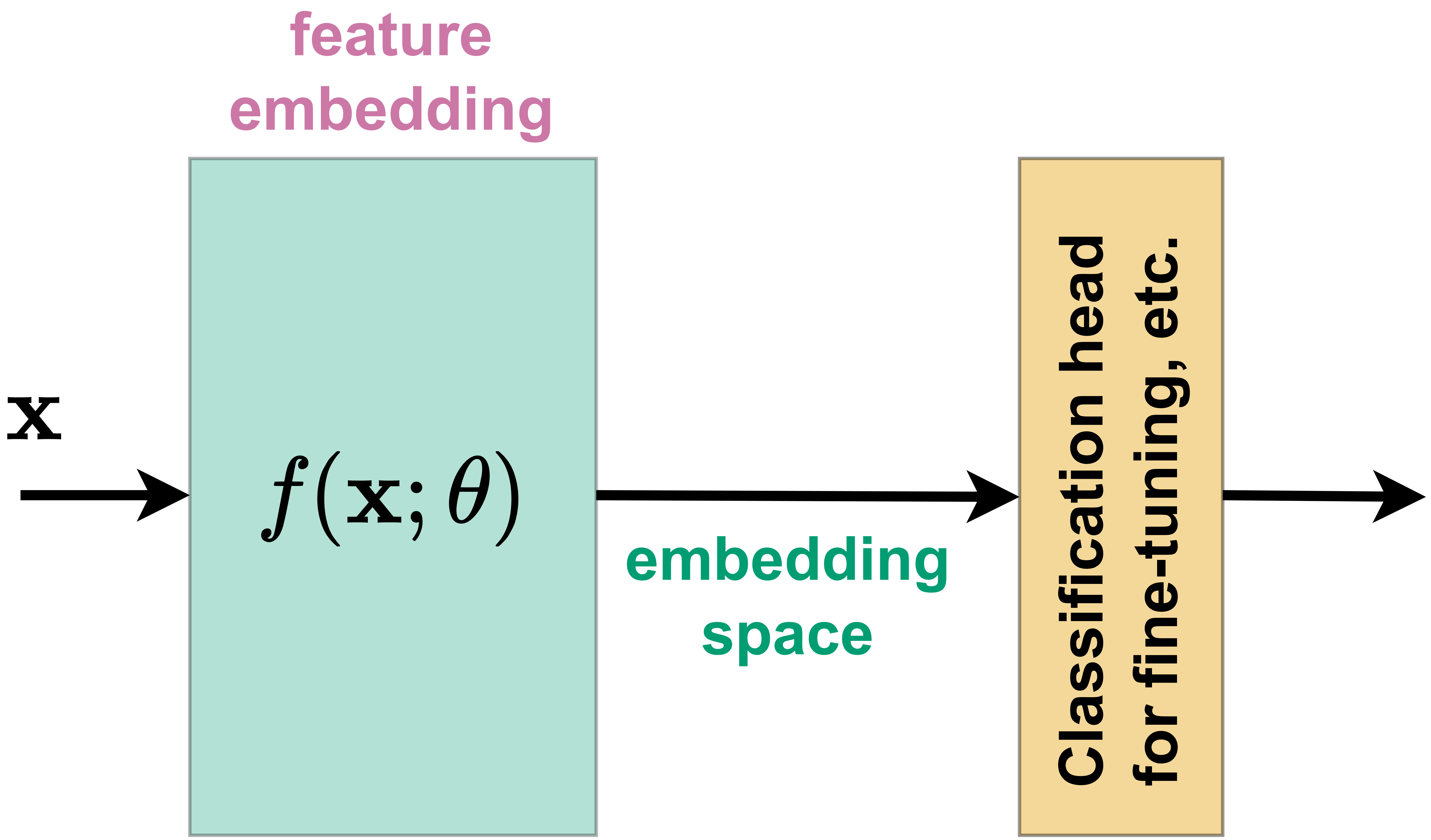

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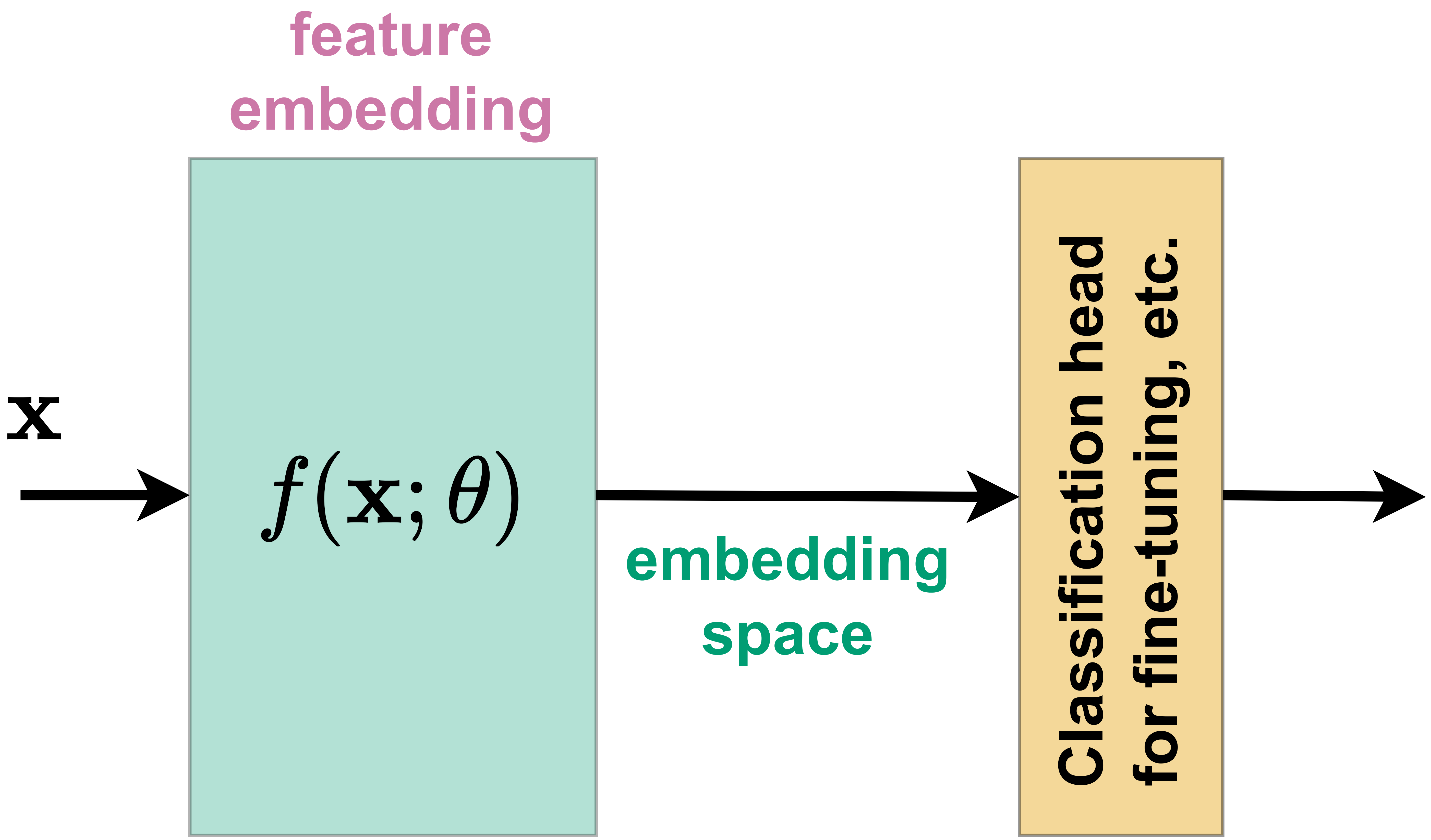

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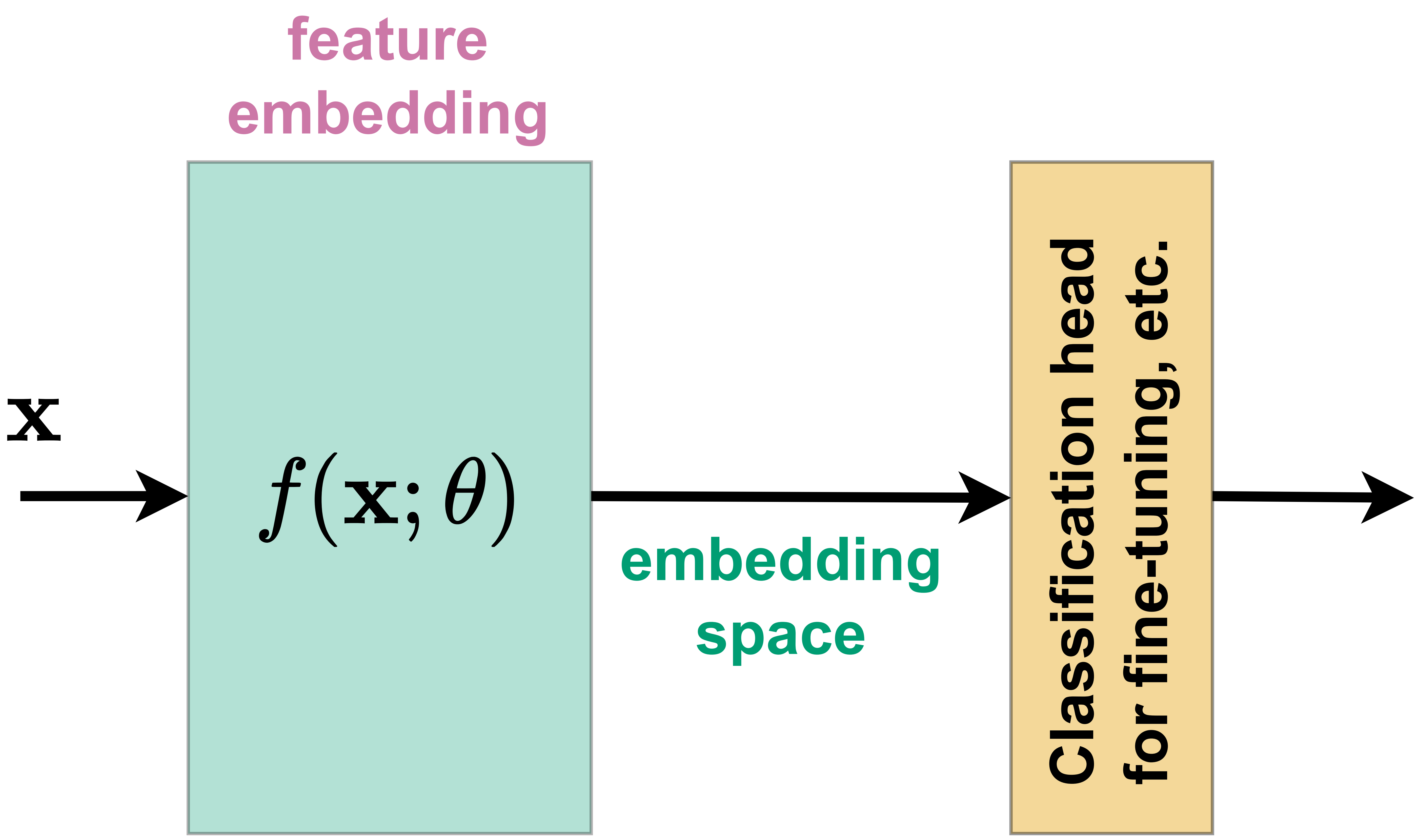


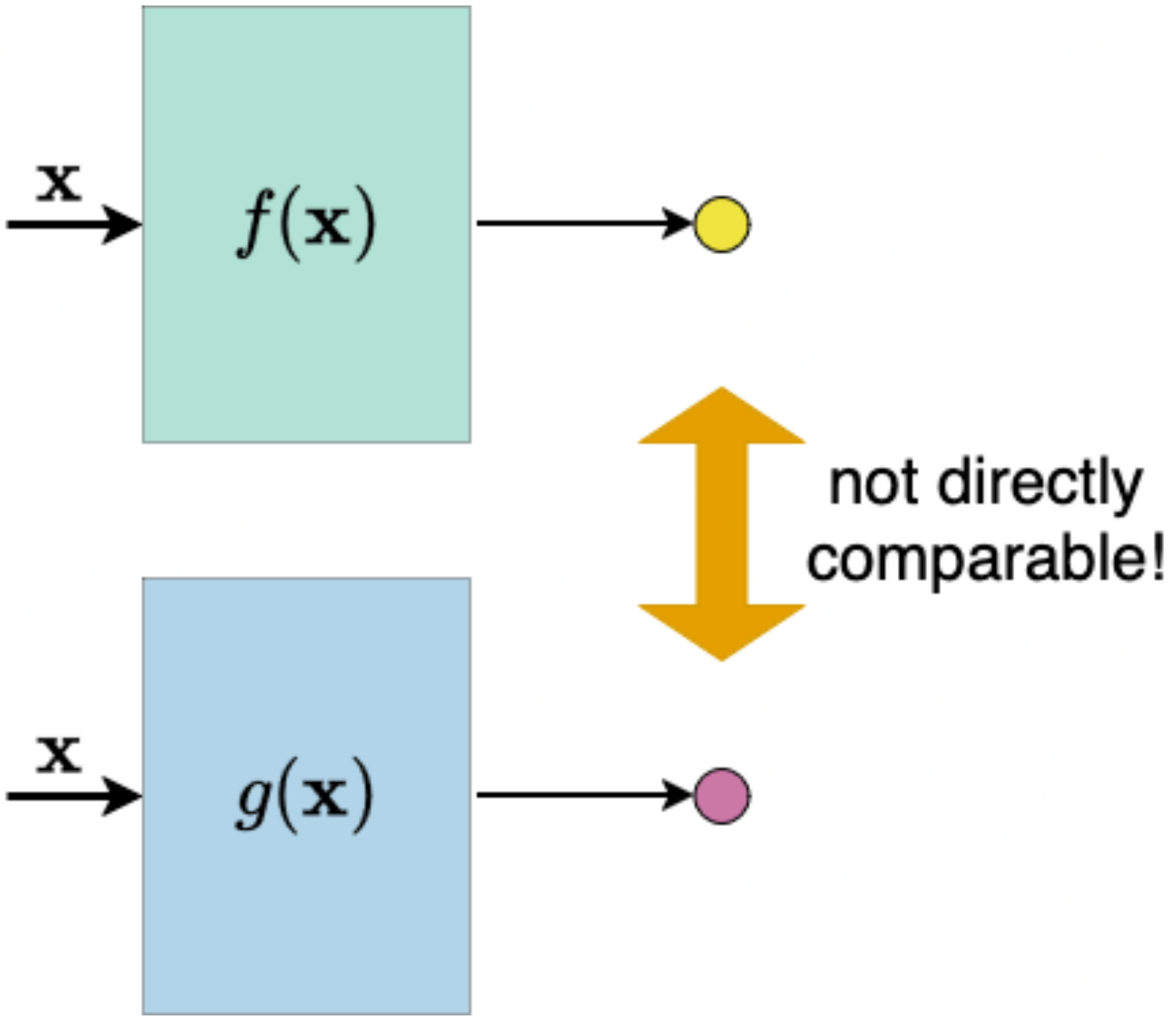
We can think of many models as having “feature embedding” stage followed by “downstream tasks.”

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



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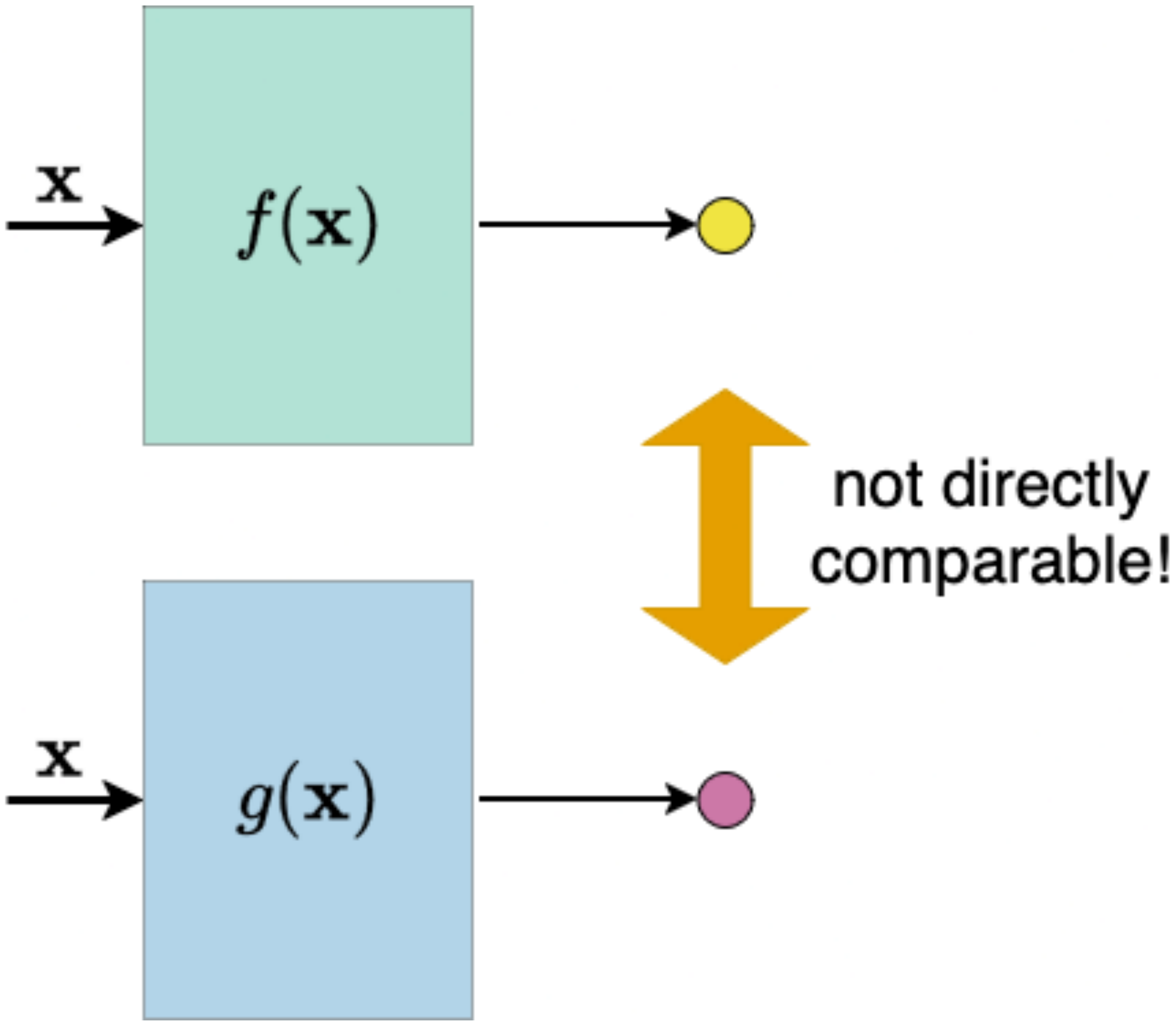

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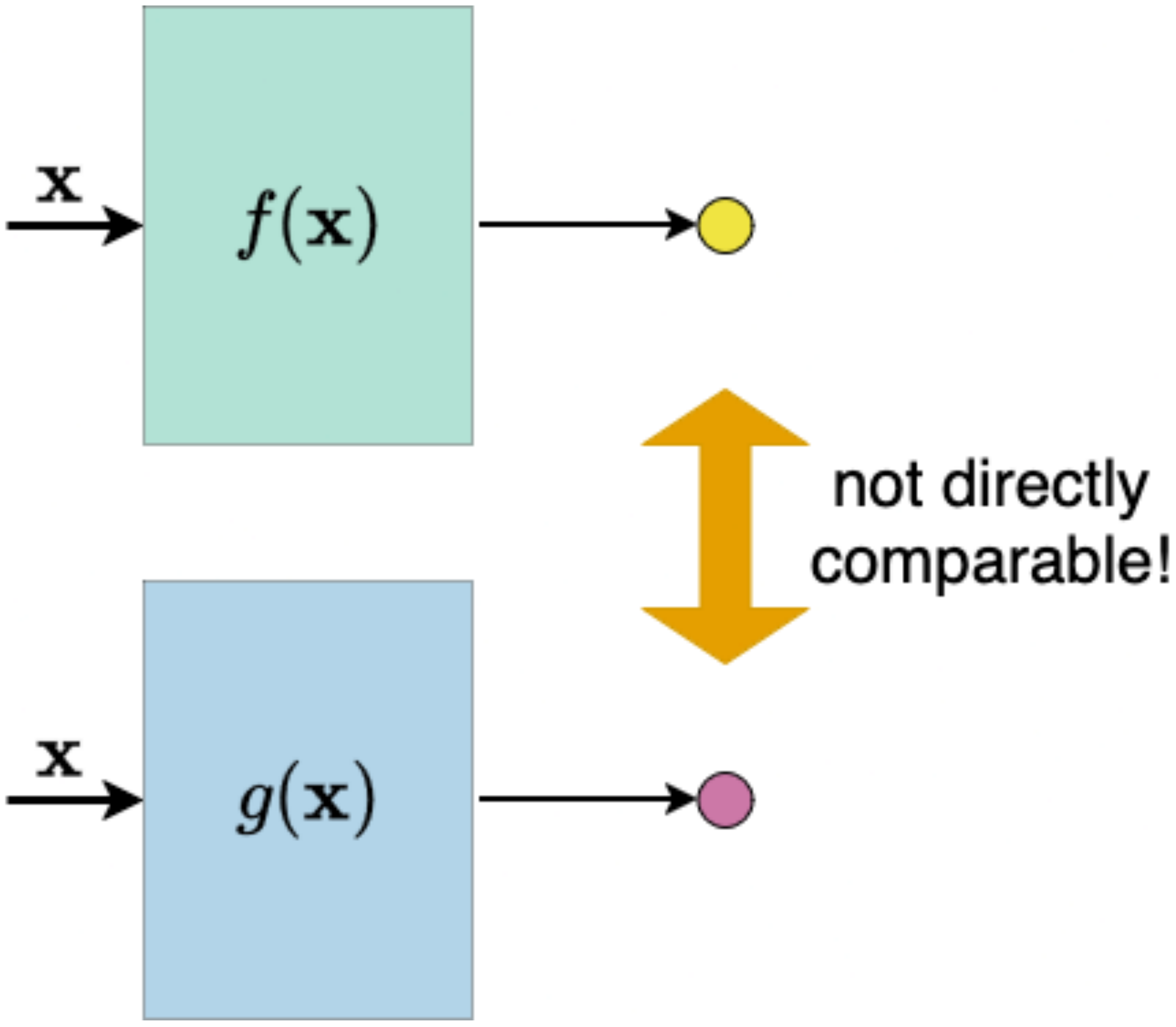

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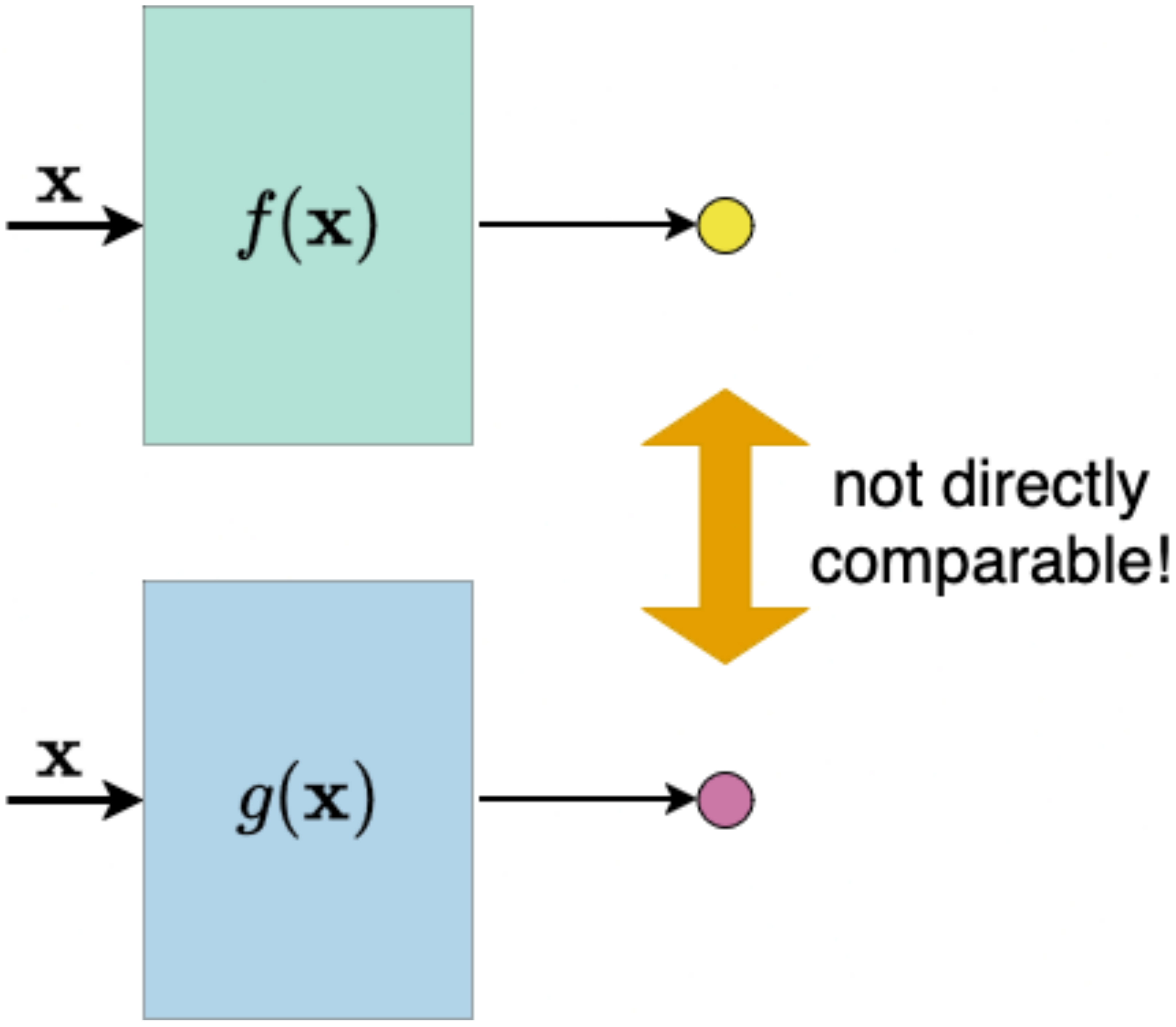

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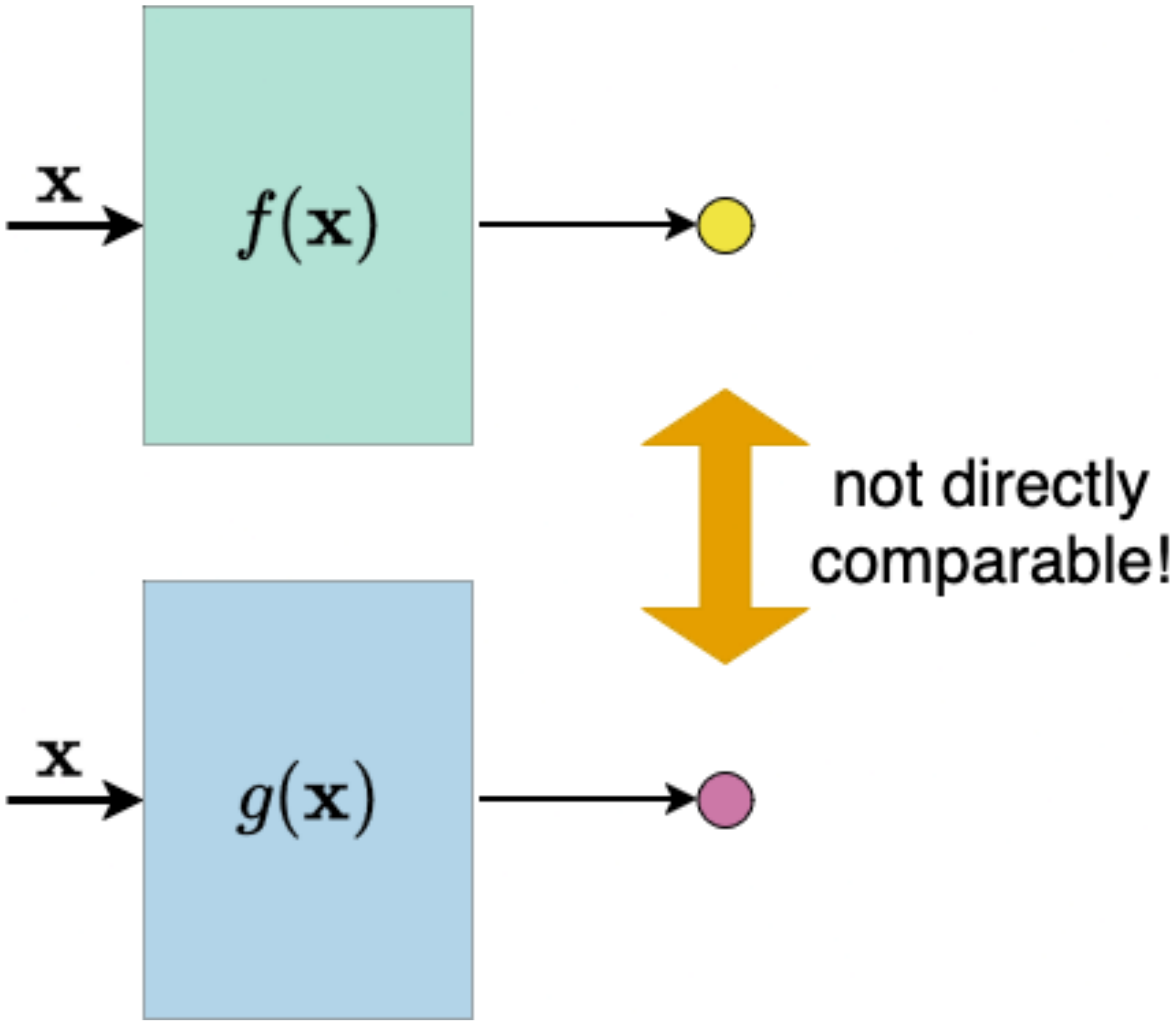

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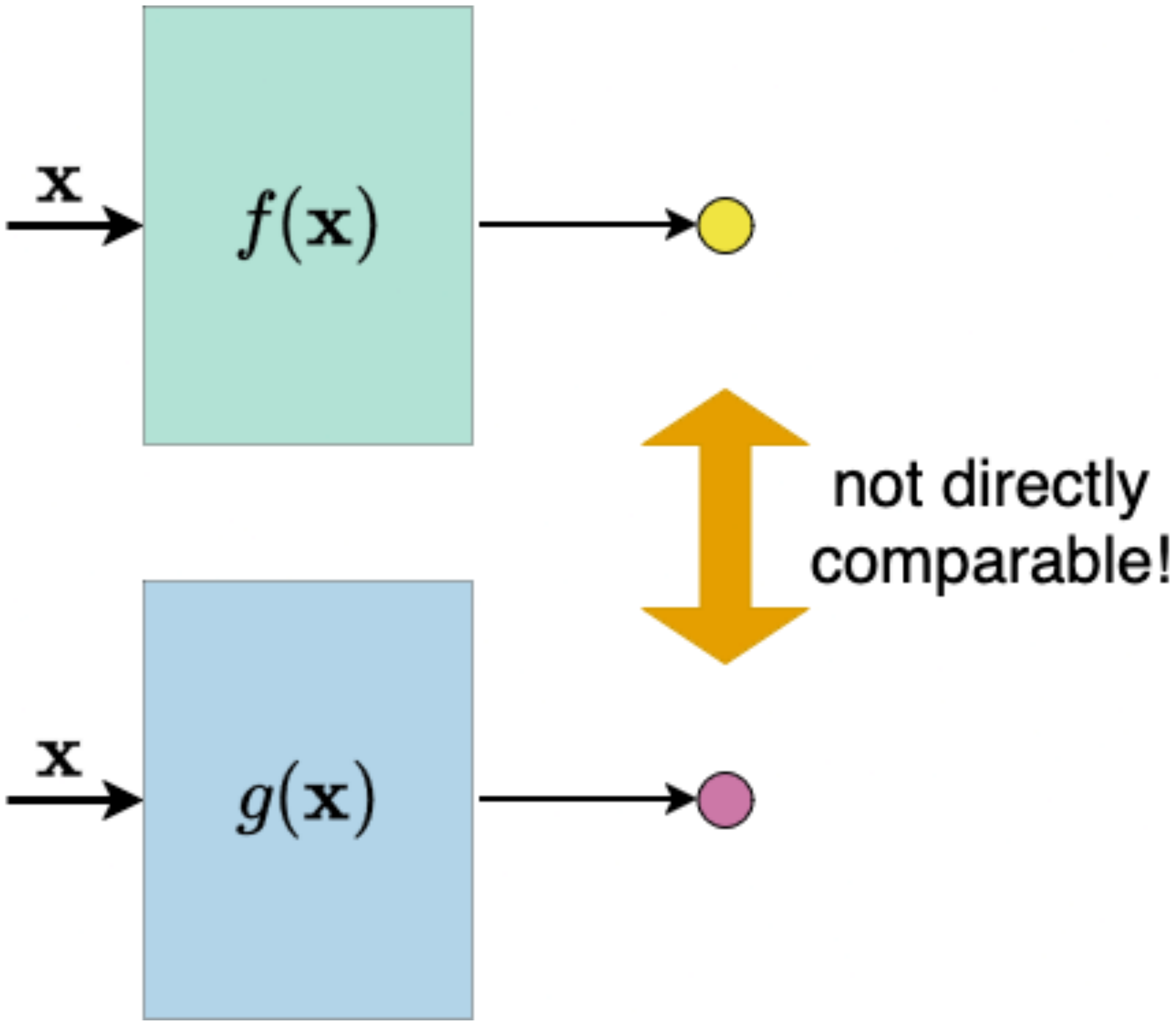

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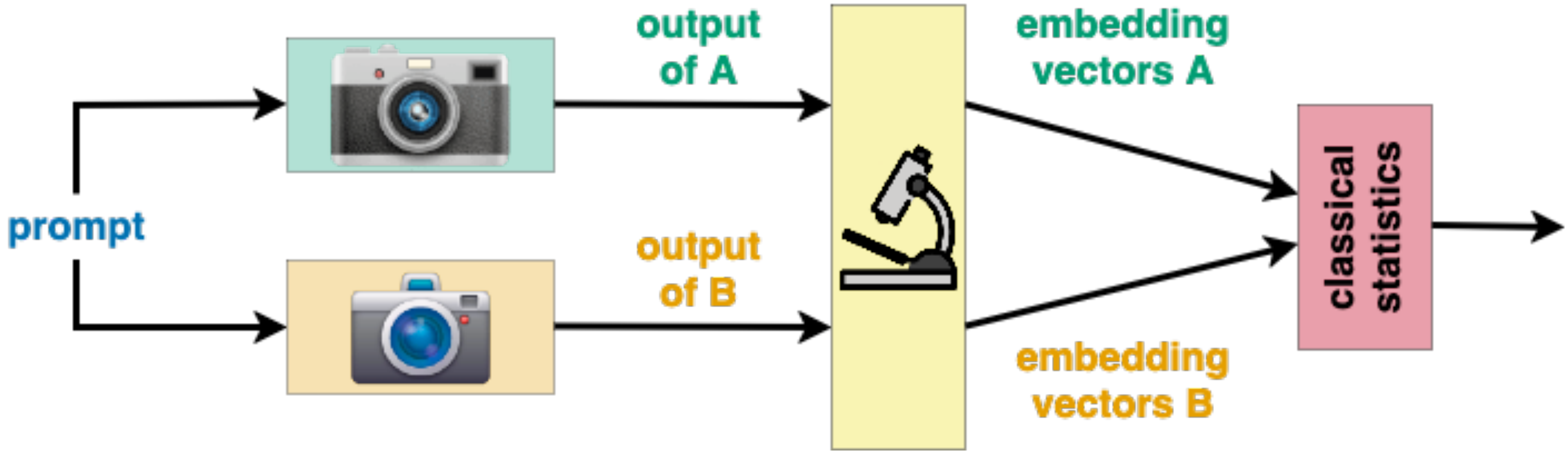
Unlike with classification, we need to compare the outputs of the generative models.

Using a pre-trained model to distinguish

Use the embedding space to compare outputs of models



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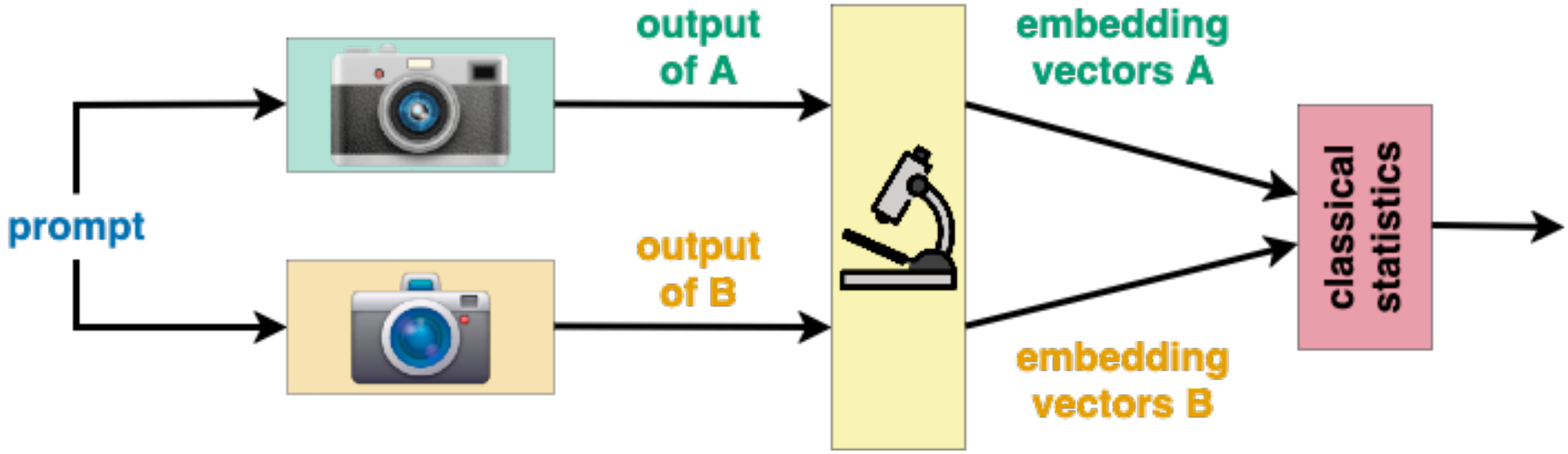
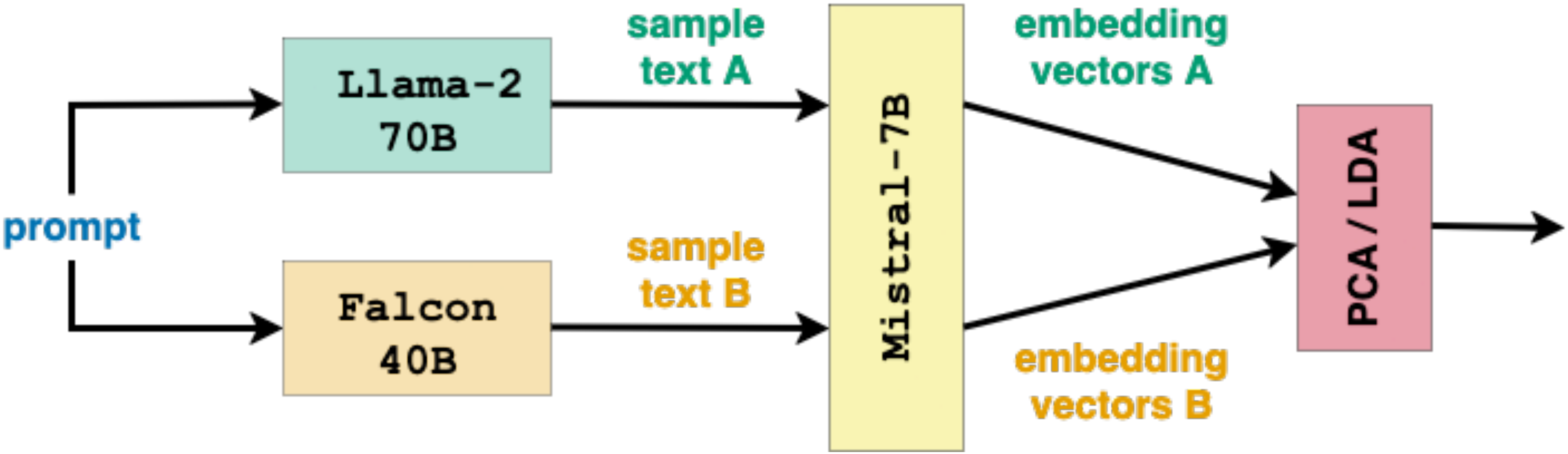


New idea: use the embedding space of a **third AI model** as a “microscope” to compare the outputs of two AI models.s

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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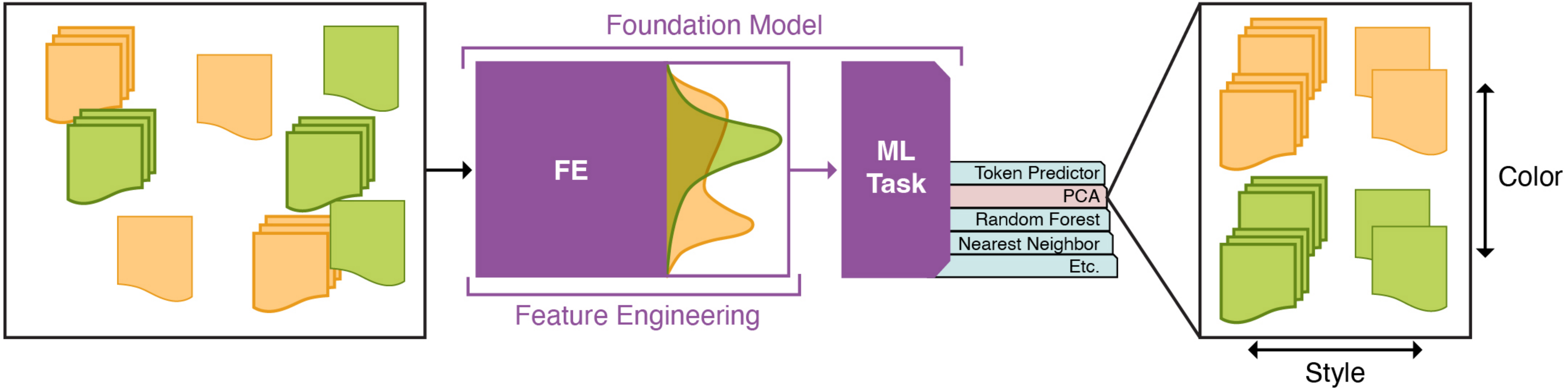
- `Multilingual-e5-large`: extracts sentence embeddings from text in different languages to 1024-dimensional embedding vectors. 60M parameters, context window of 512 tokens and long text is truncated to fit within this window.
- `Data Filtering Network`: a CLIP model trained on 5B images that were filtered 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

A.



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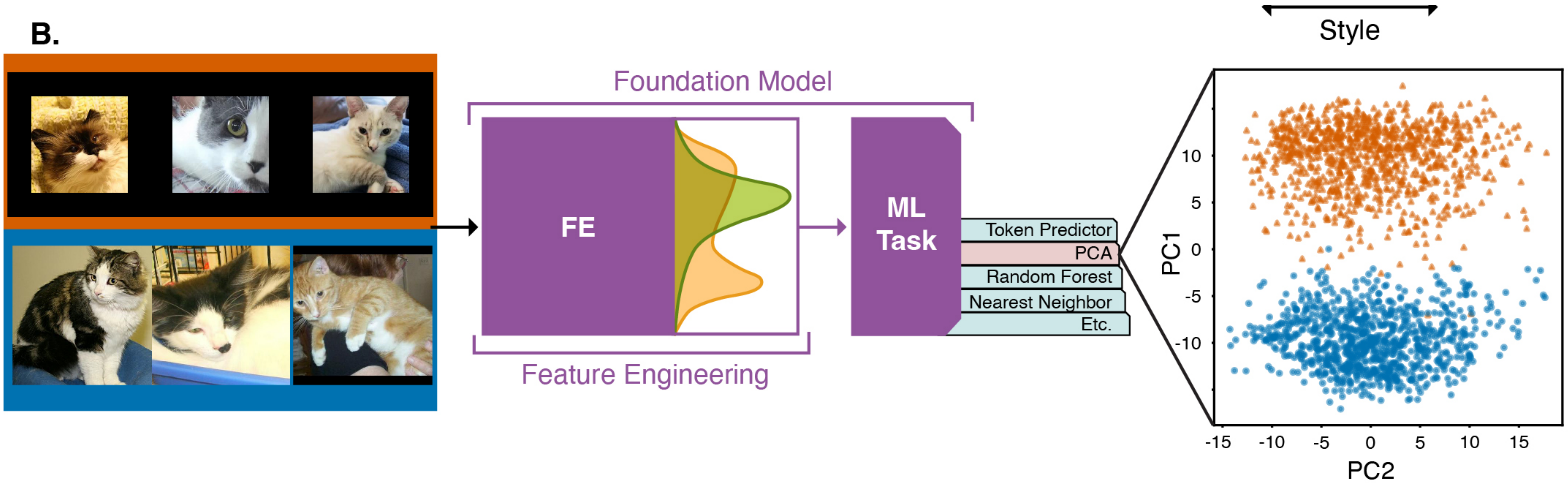

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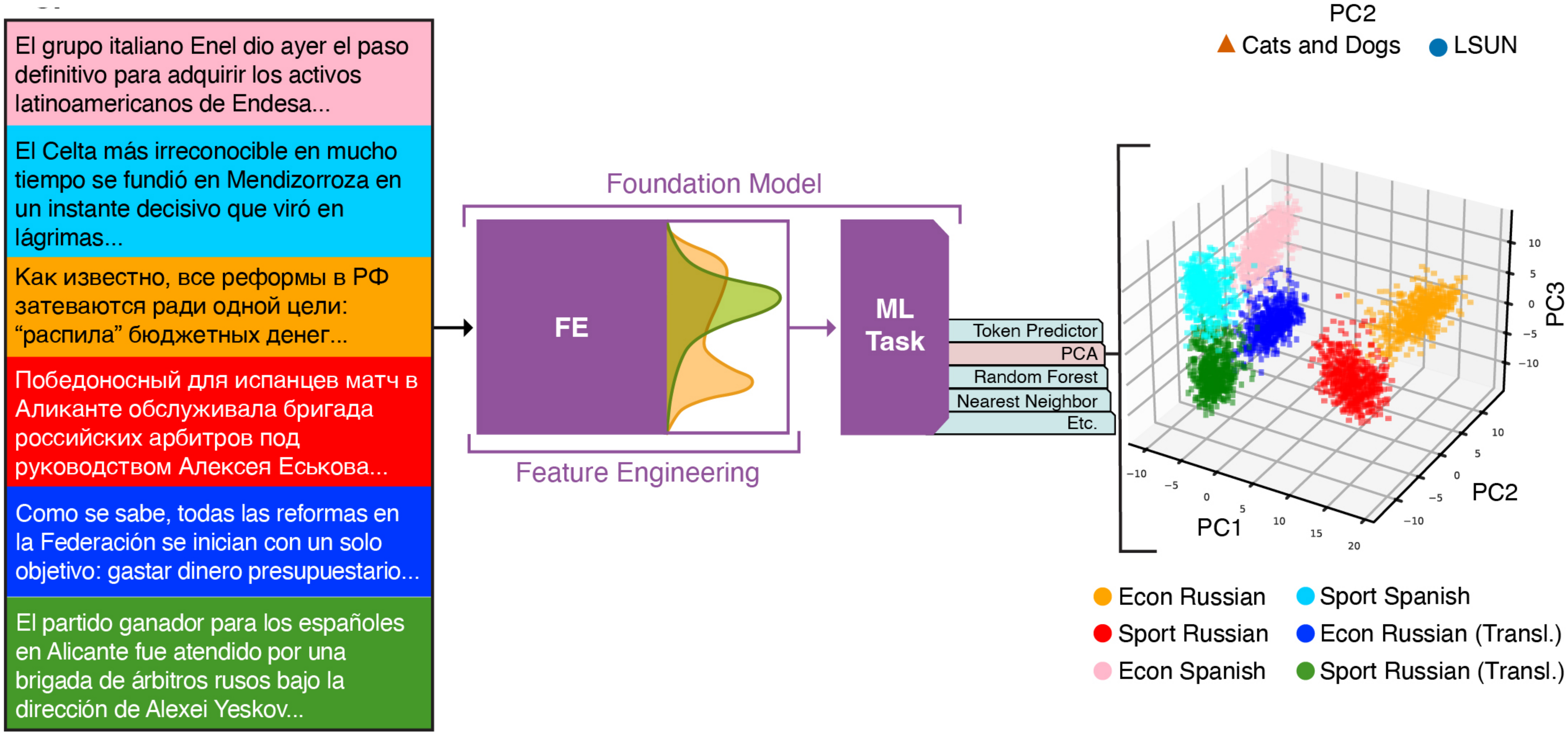

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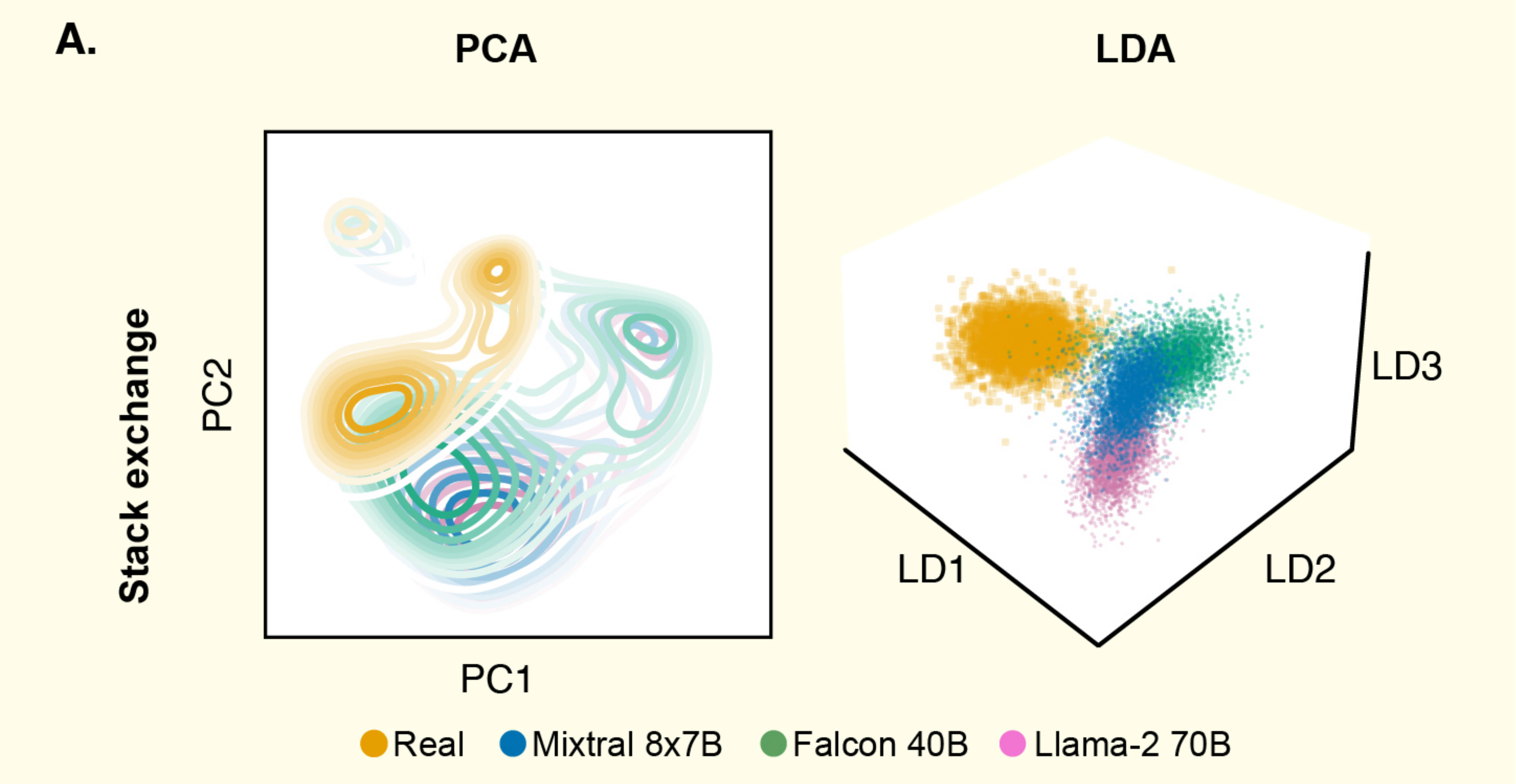
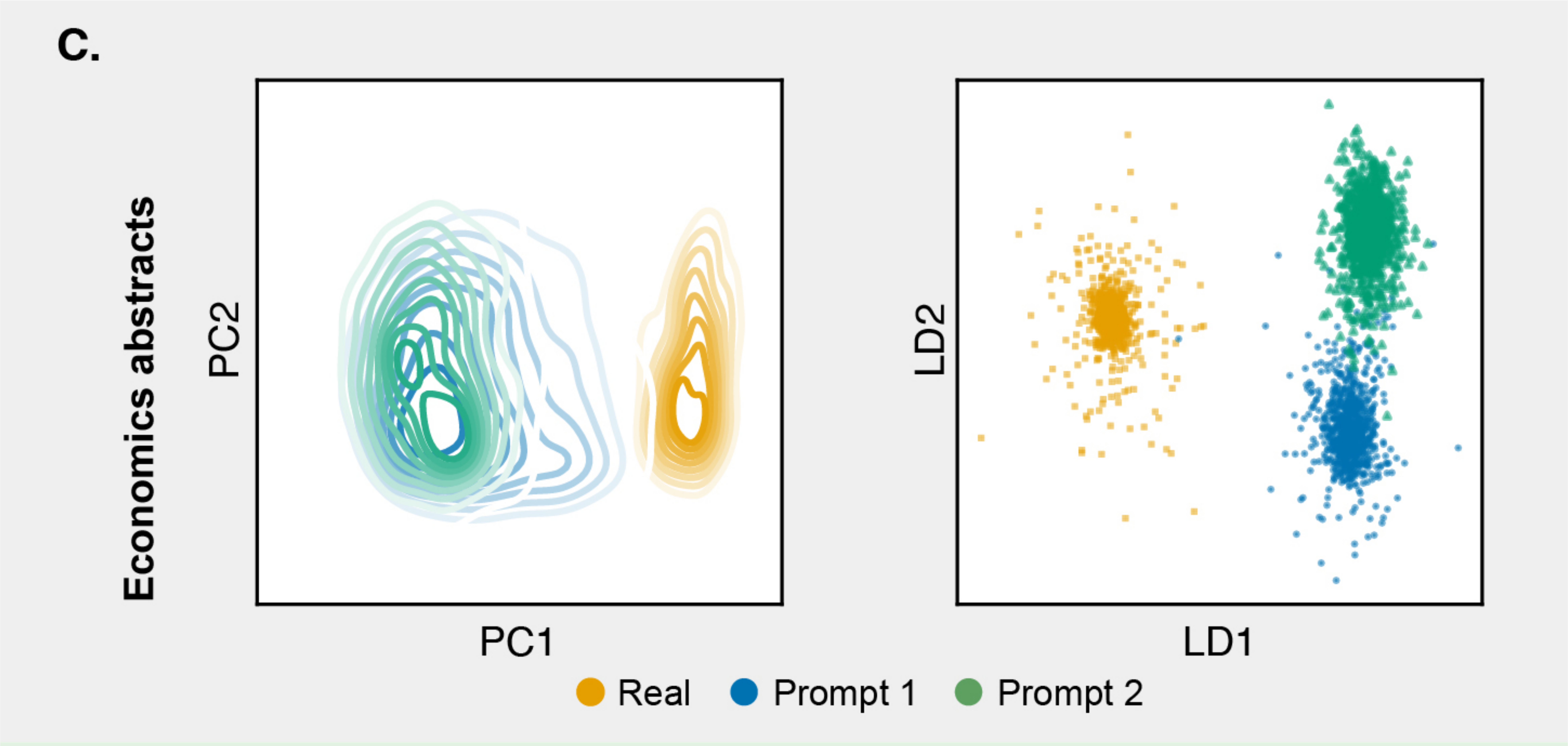
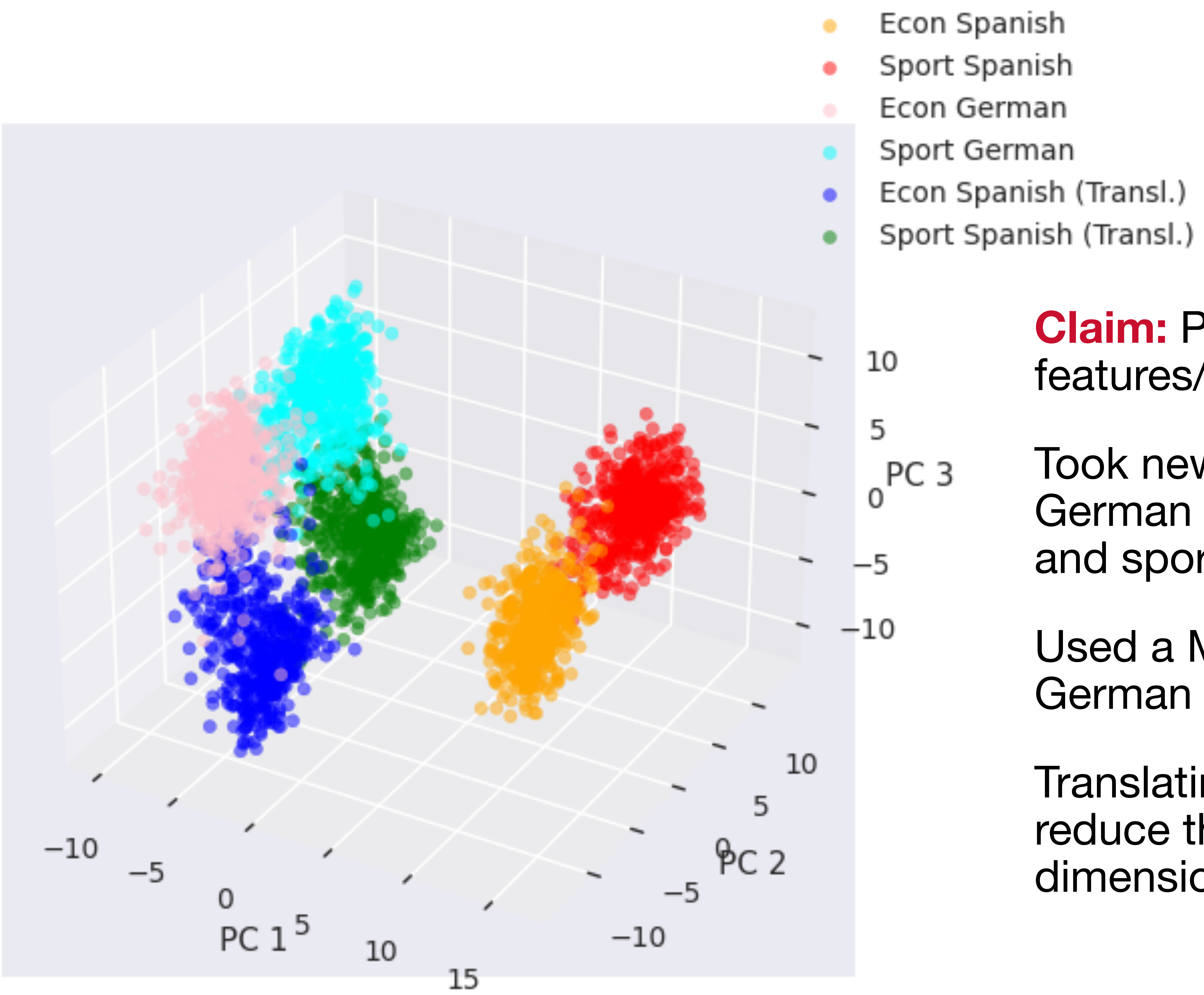
1. Embed real data and AI-generated data to see if the embedding vectors cluster.

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

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


A.
PCA
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

HarmonyOS 4.0

Samsung UI 7.0

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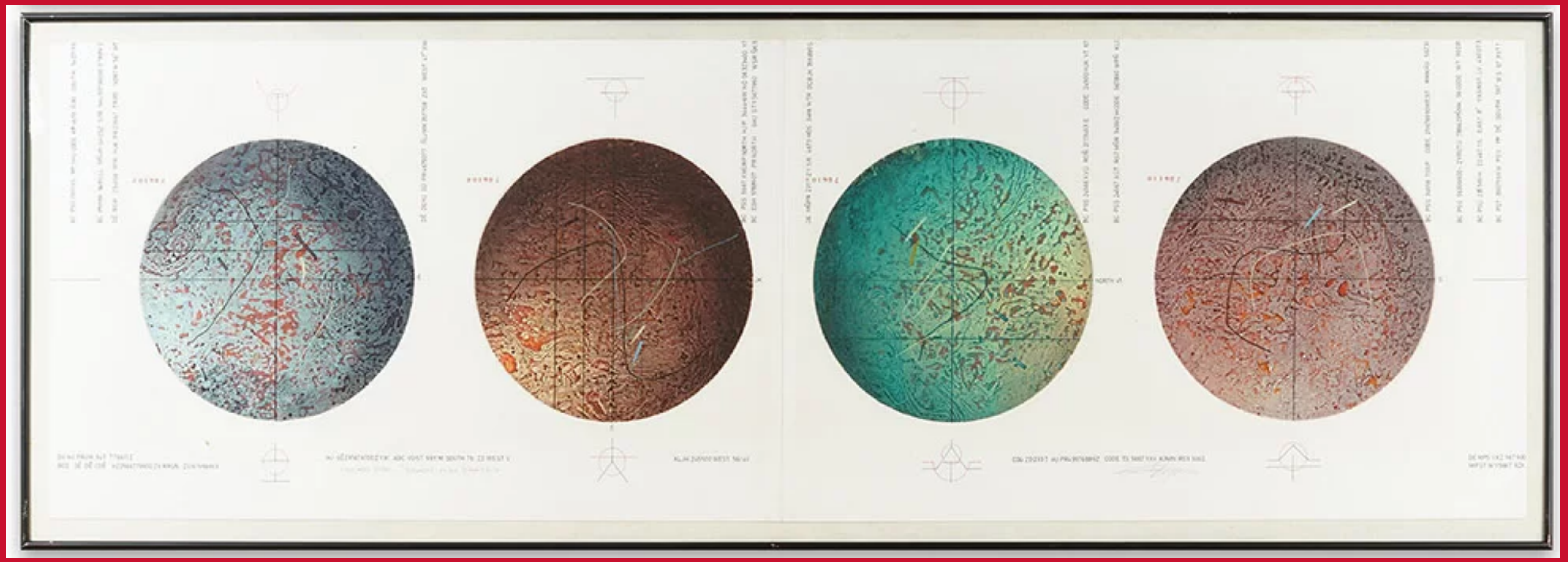
- Forensics applications: comparing models, detecting deepfakes, etc.
- “Model DNA”: fine-tuned or “lightly modified” models make minor modifications to the embeddings.
- Use post processing to “align” embeddings for calibration, ensembling, federated learning, etc.

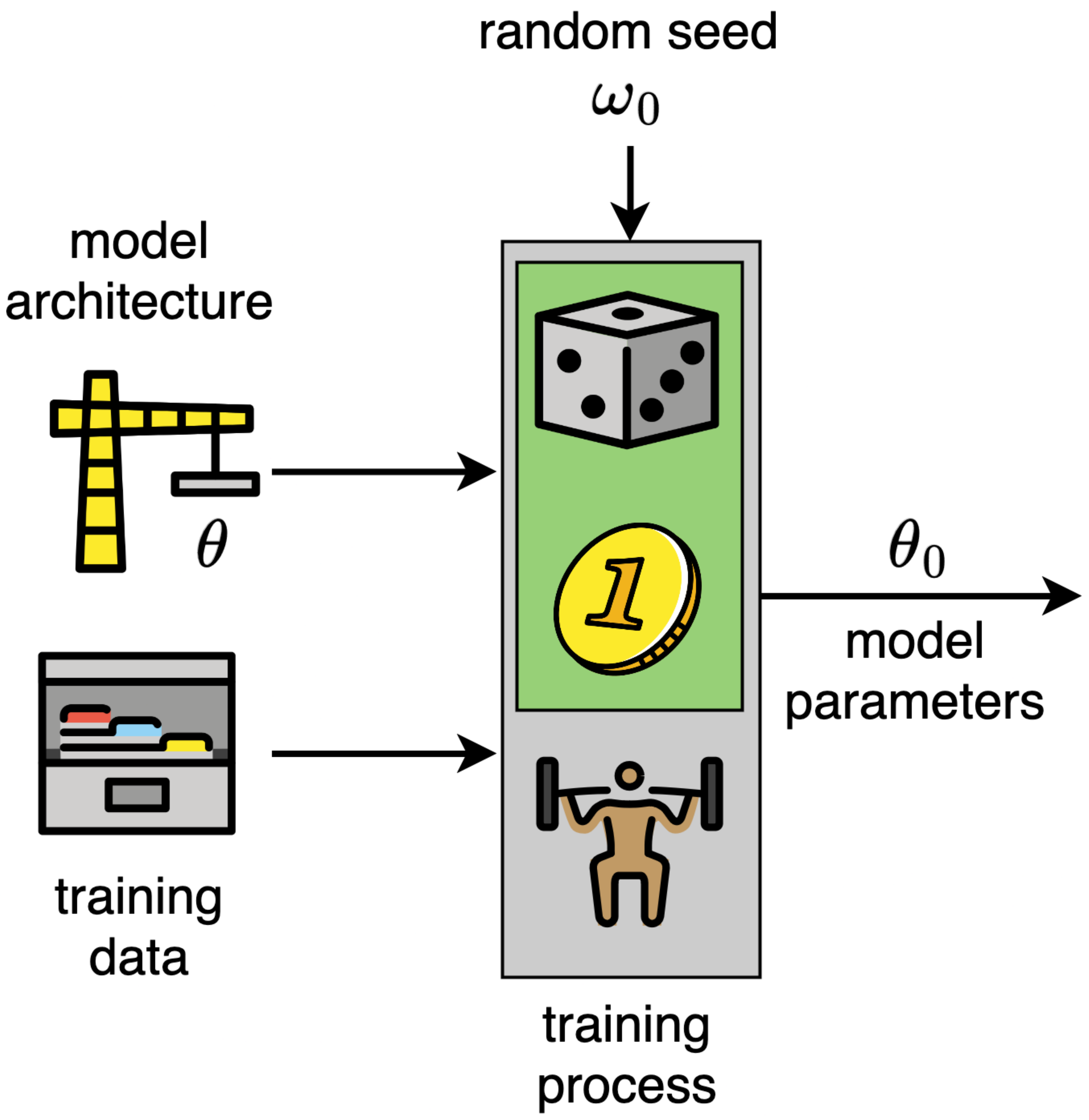
Model comparisons in training



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

Variability in the training process

Is training reliable?



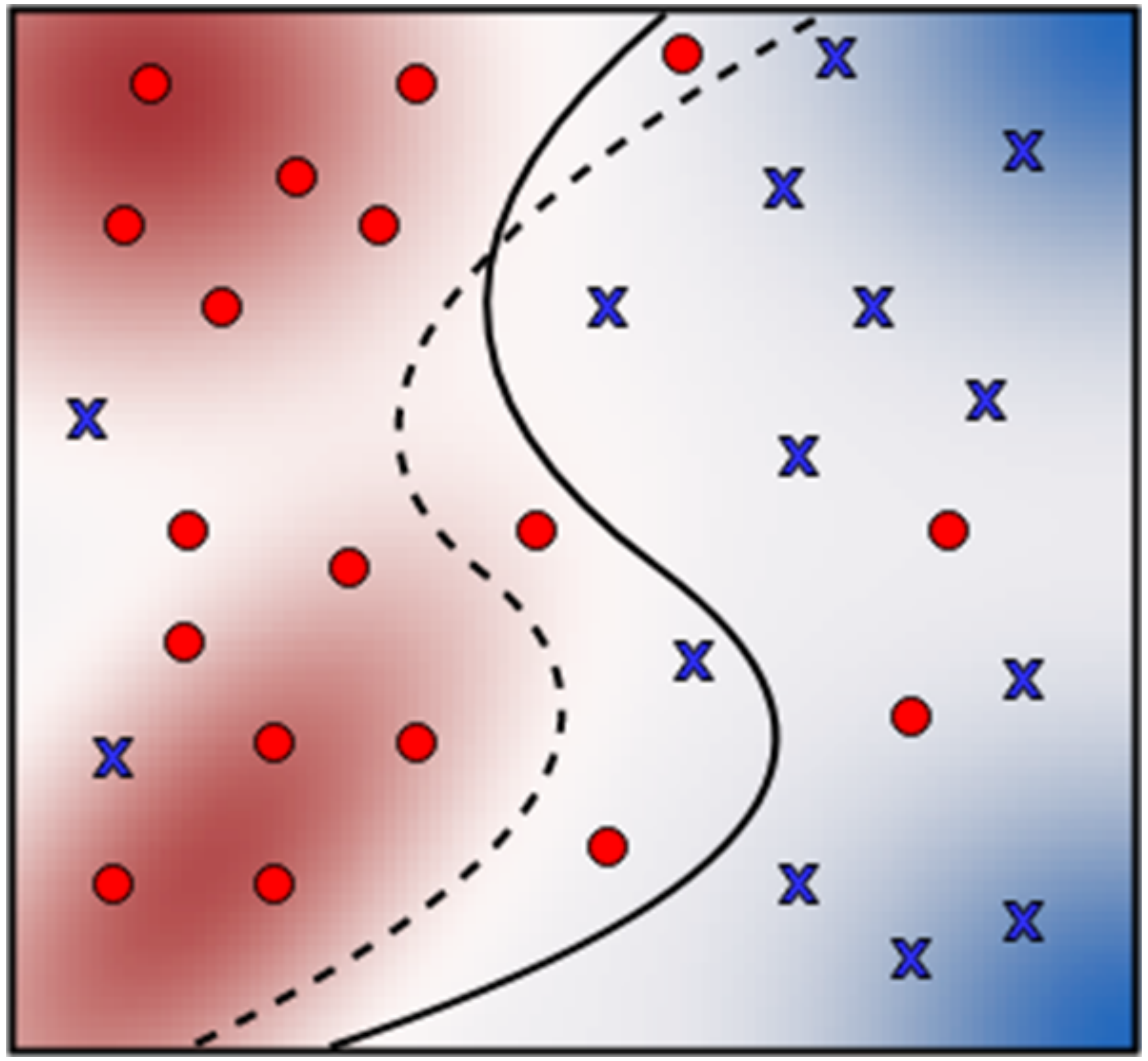
Each time we run the training algorithm on the **same training set**, **same architecture**, **same algorithm**, we still use (pseudo-)**independent randomness**.

- Each training run is a **sample** from $\mathscr{F}$.
- 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



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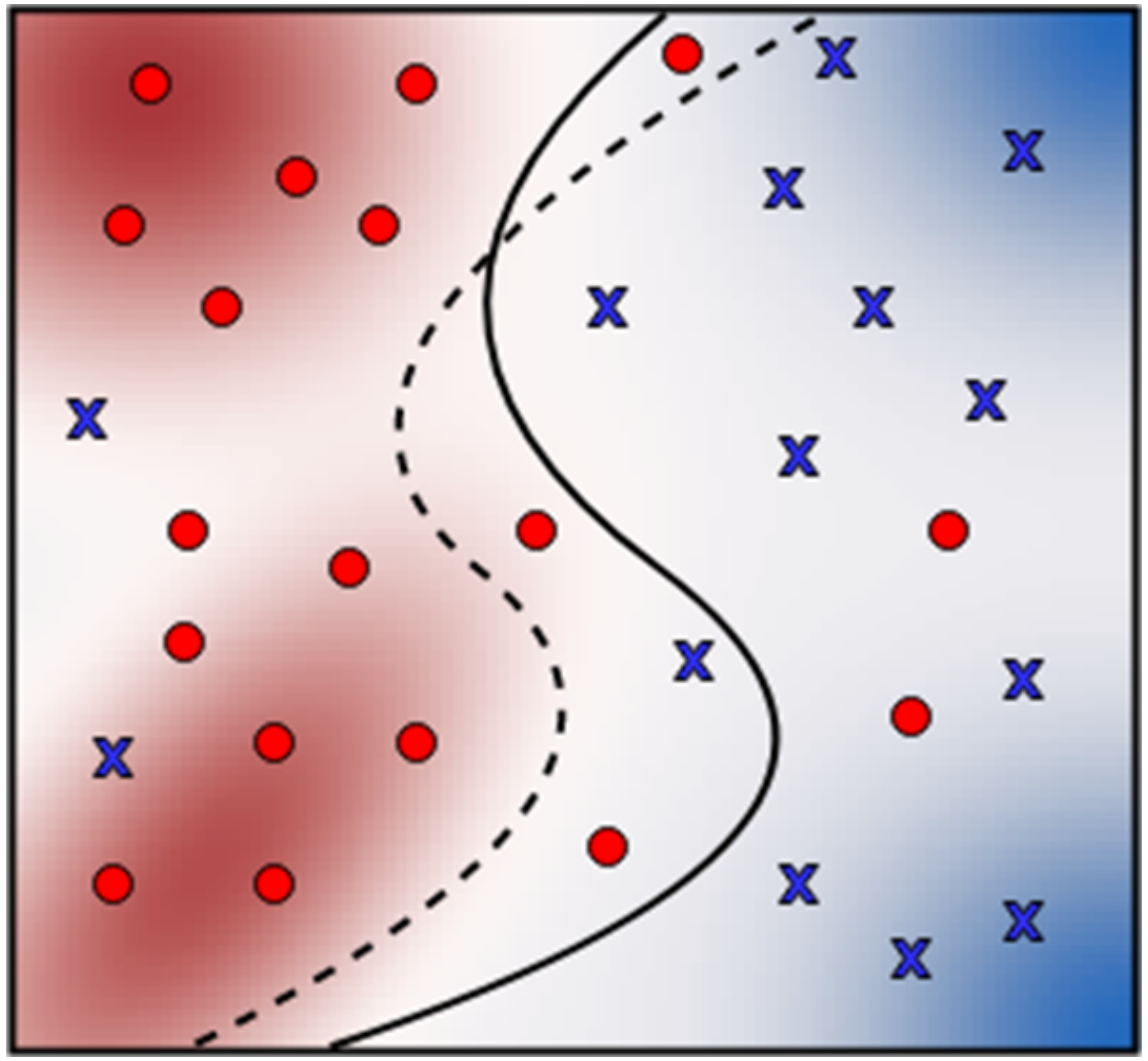
Model comparisons are ad hoc and waste energy

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



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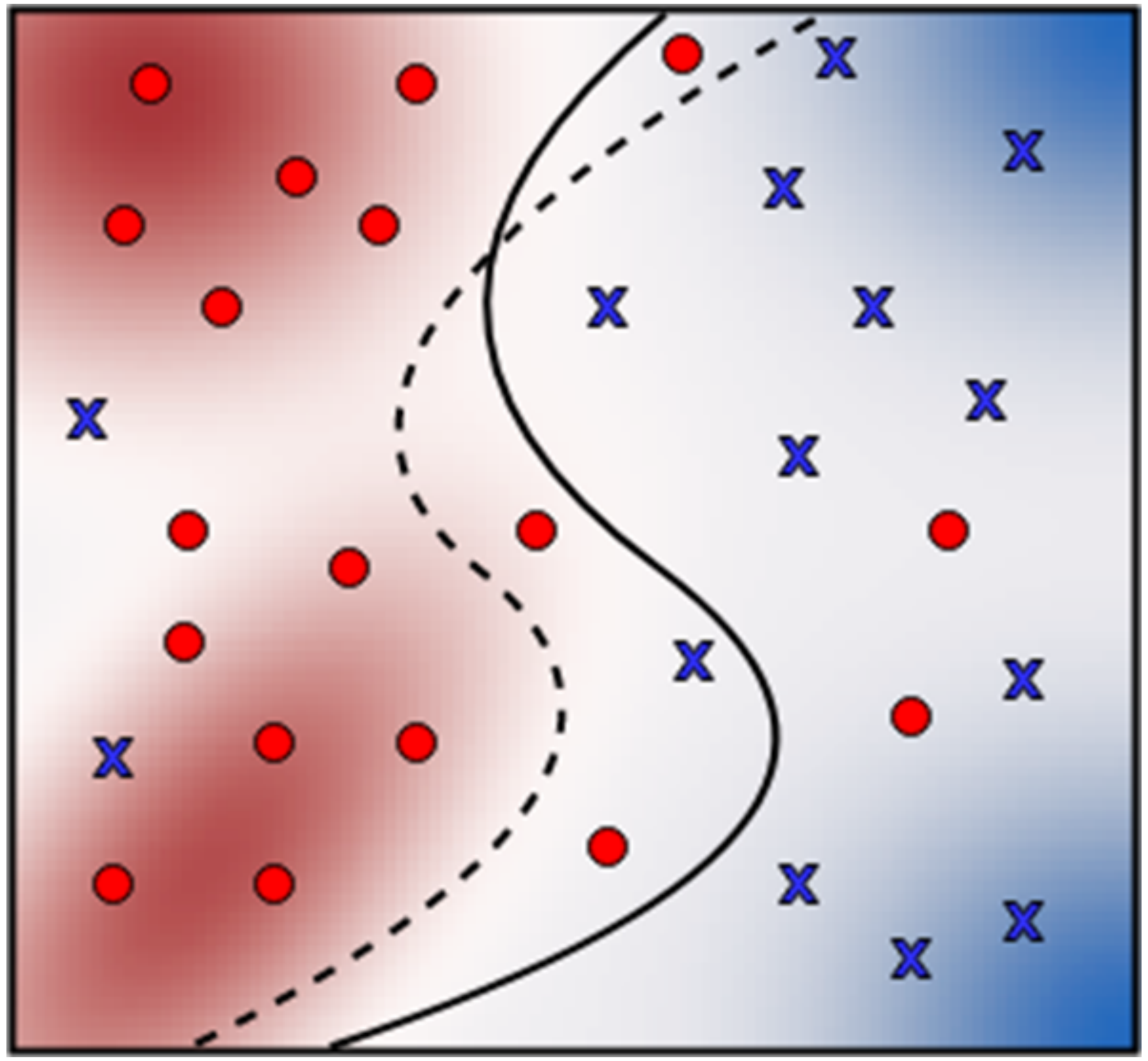

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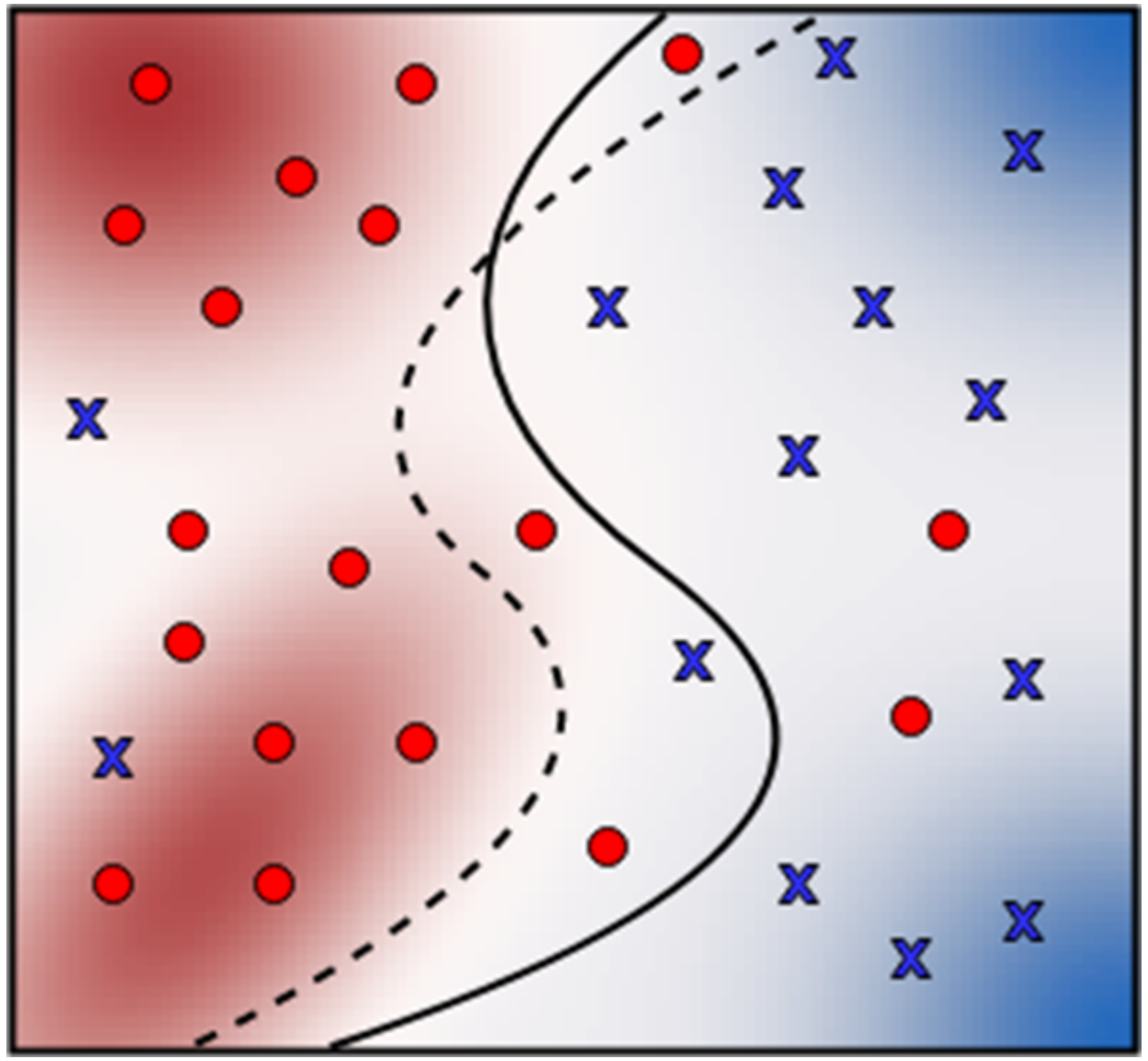
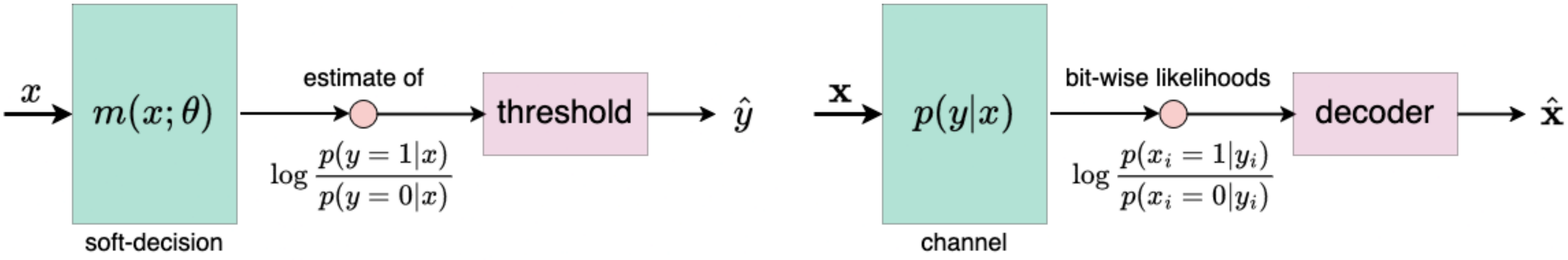


Terms like the **Rashomon effect**[1][2][3], **predictive multiplicity**[4], or **prediction churn**[5] have been used to describe this phenomena.

[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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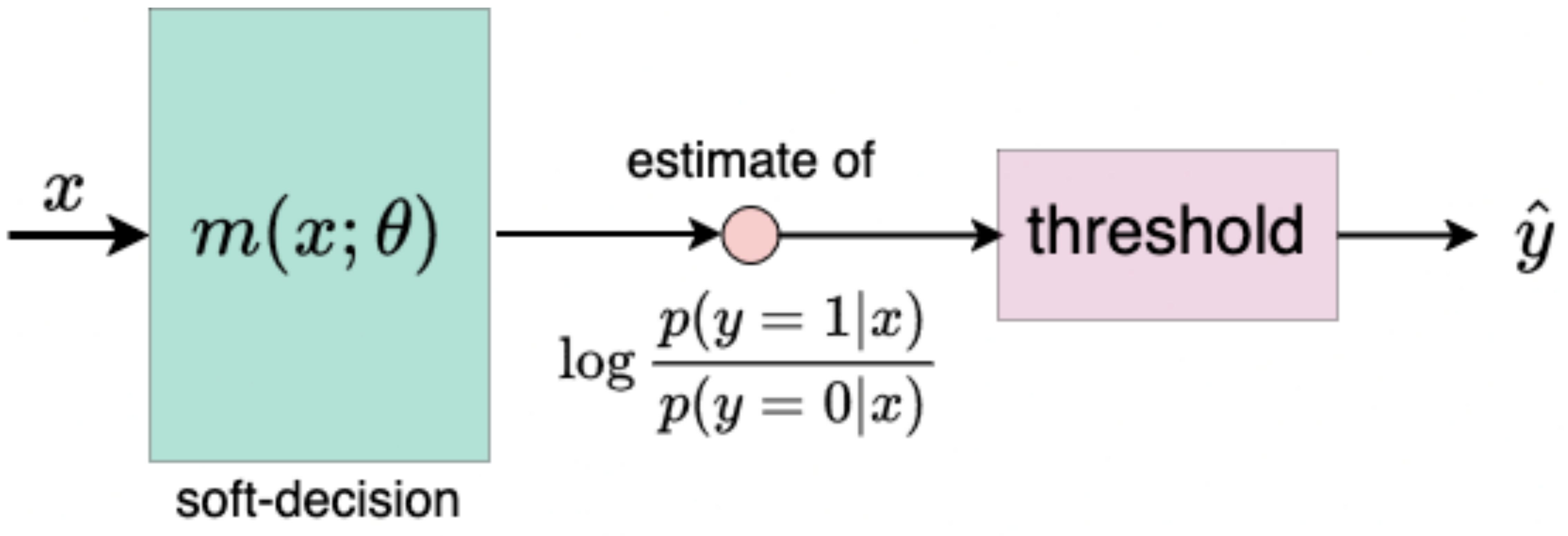

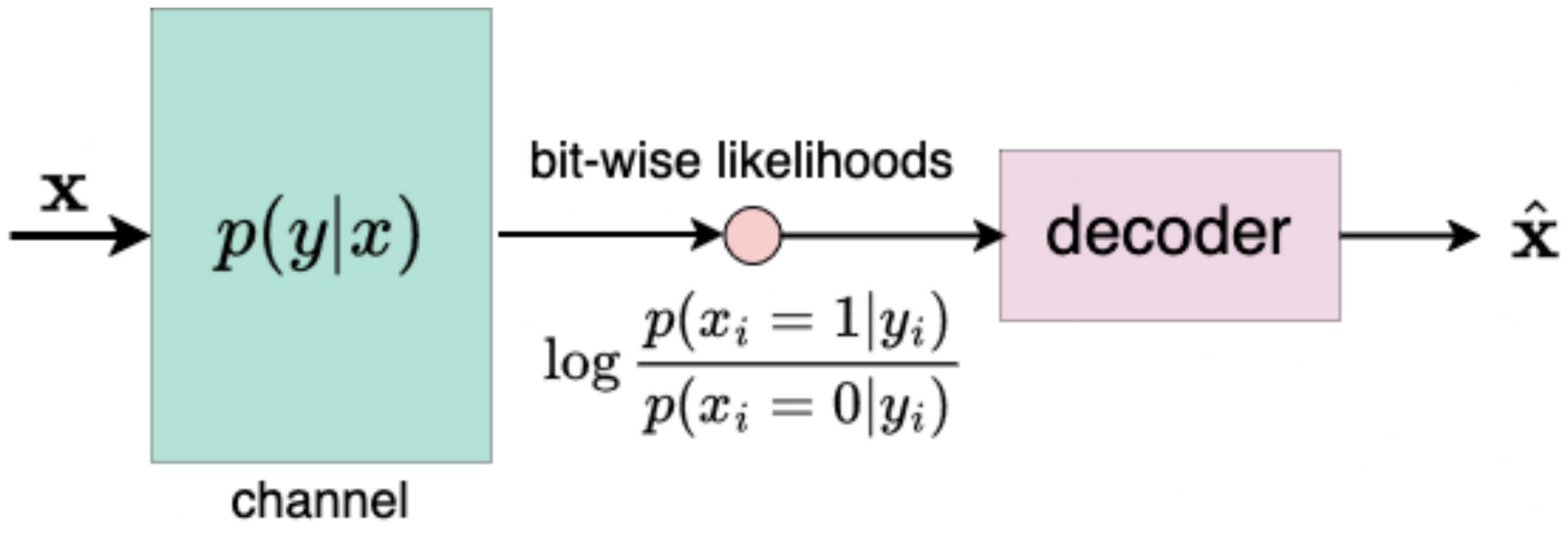

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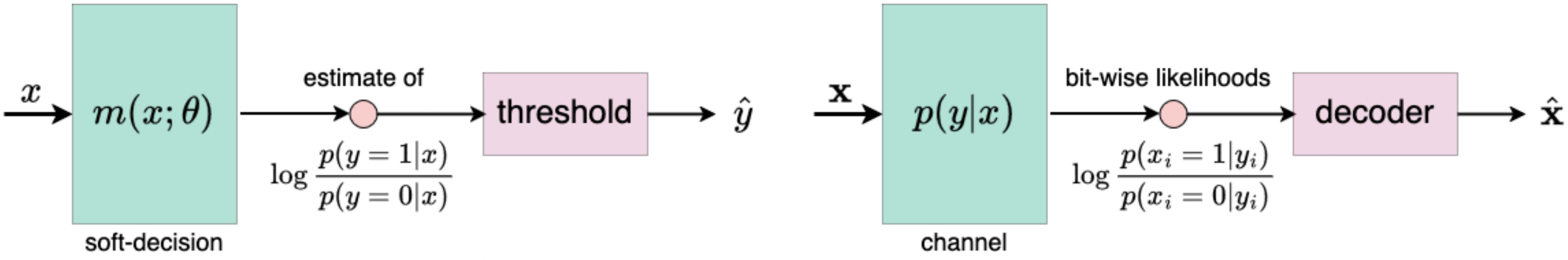

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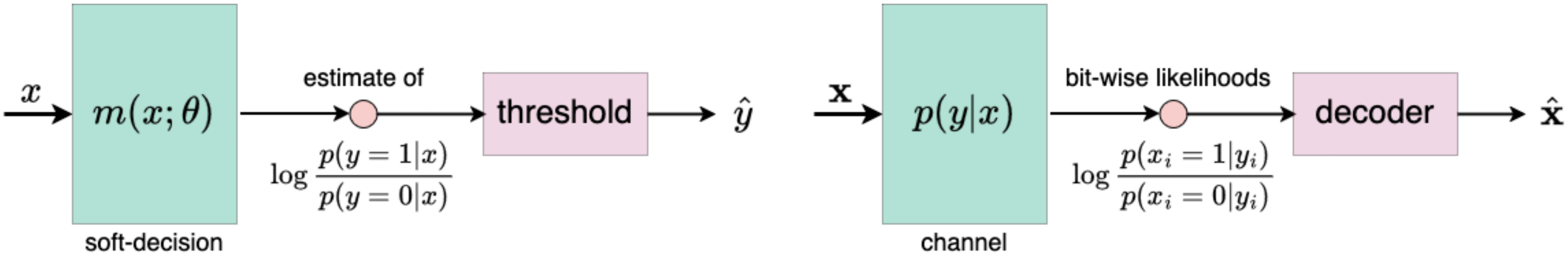

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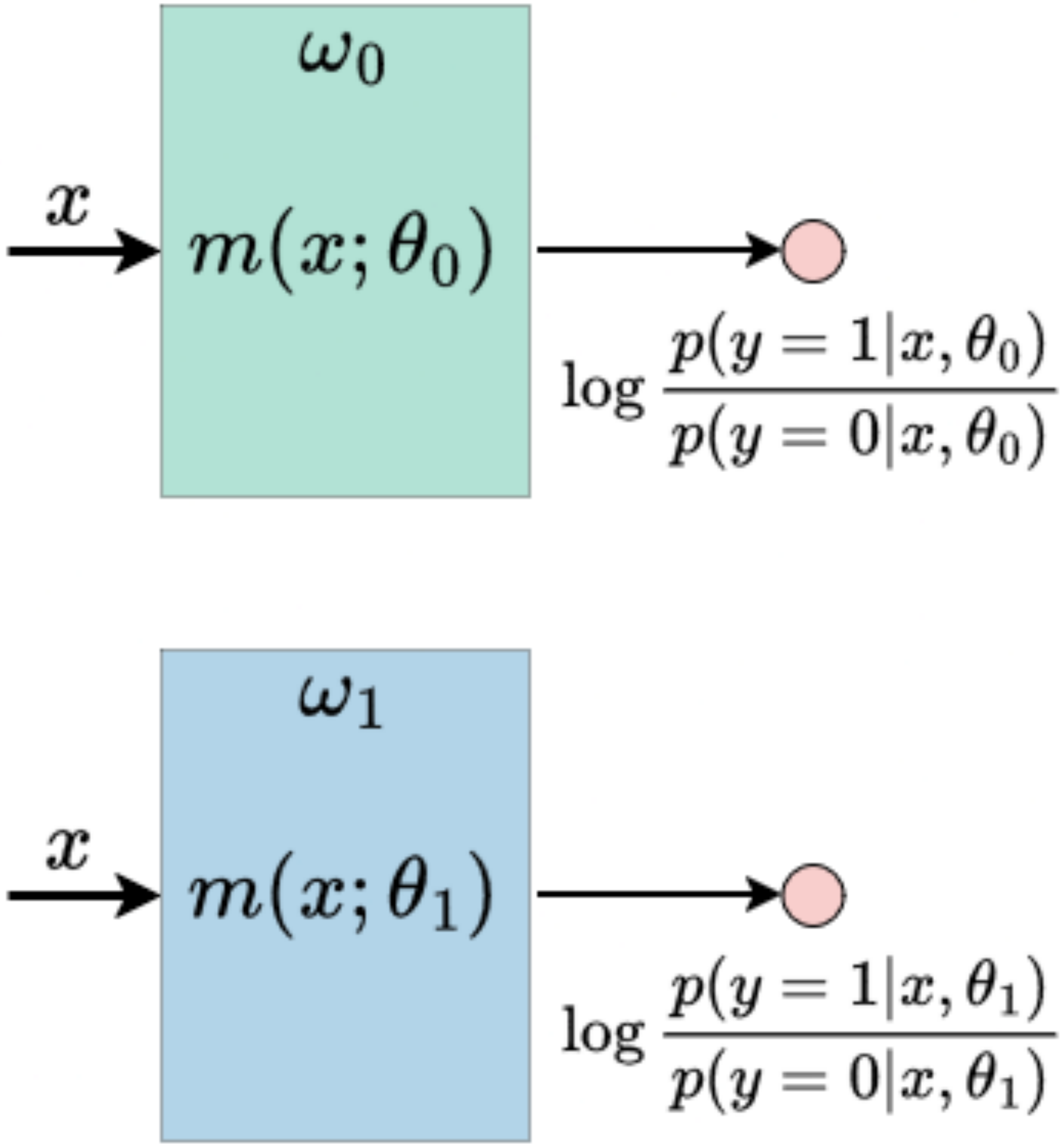
- These are usually made using (softmax) probability estimates $\hat{p}(y \mid x, \theta)$.
- Instead look at **pre-threshold "soft decision"** $m(x \mid \theta)$ for the model.

Comparing two binary classifiers

Soft decisions are different even if decisions are the same



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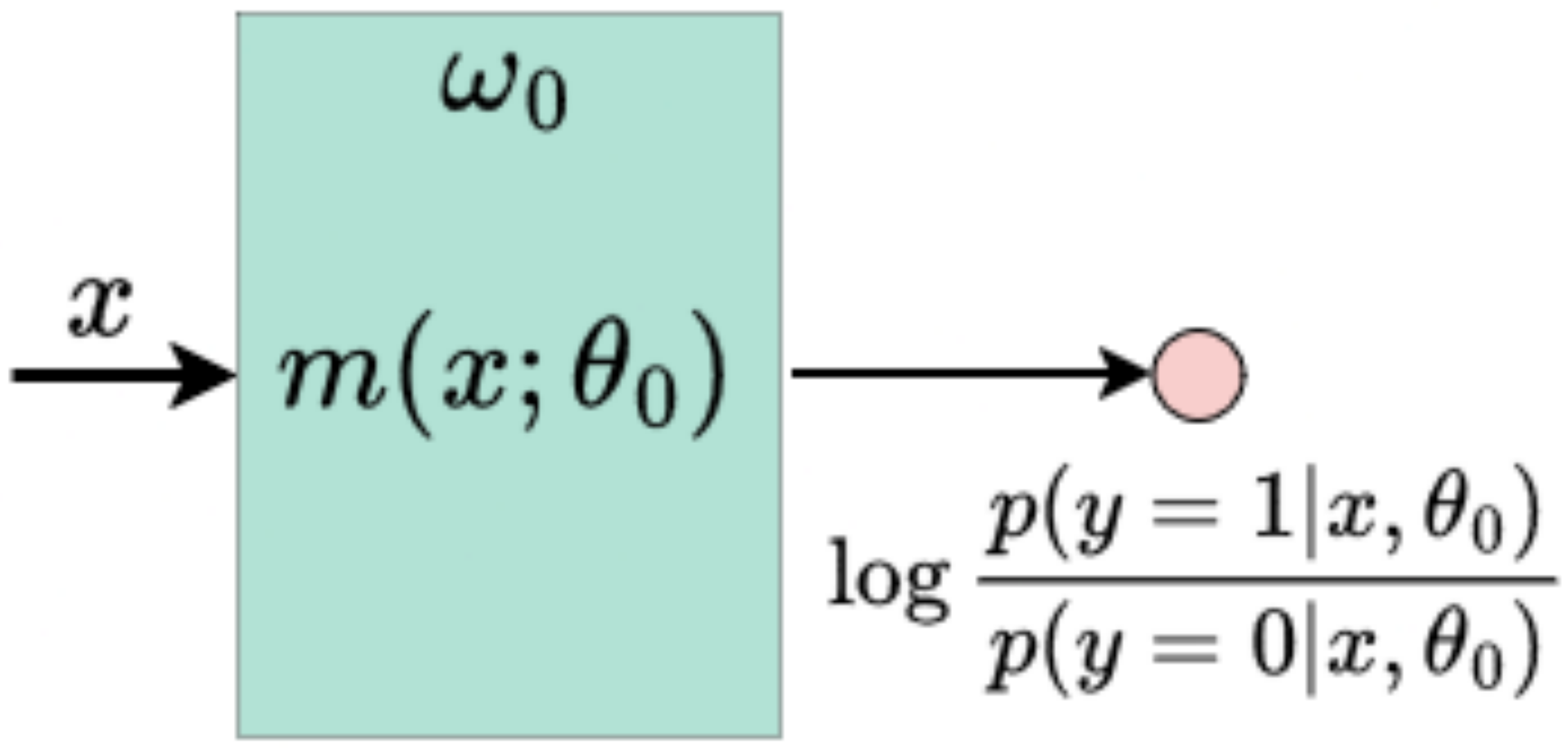
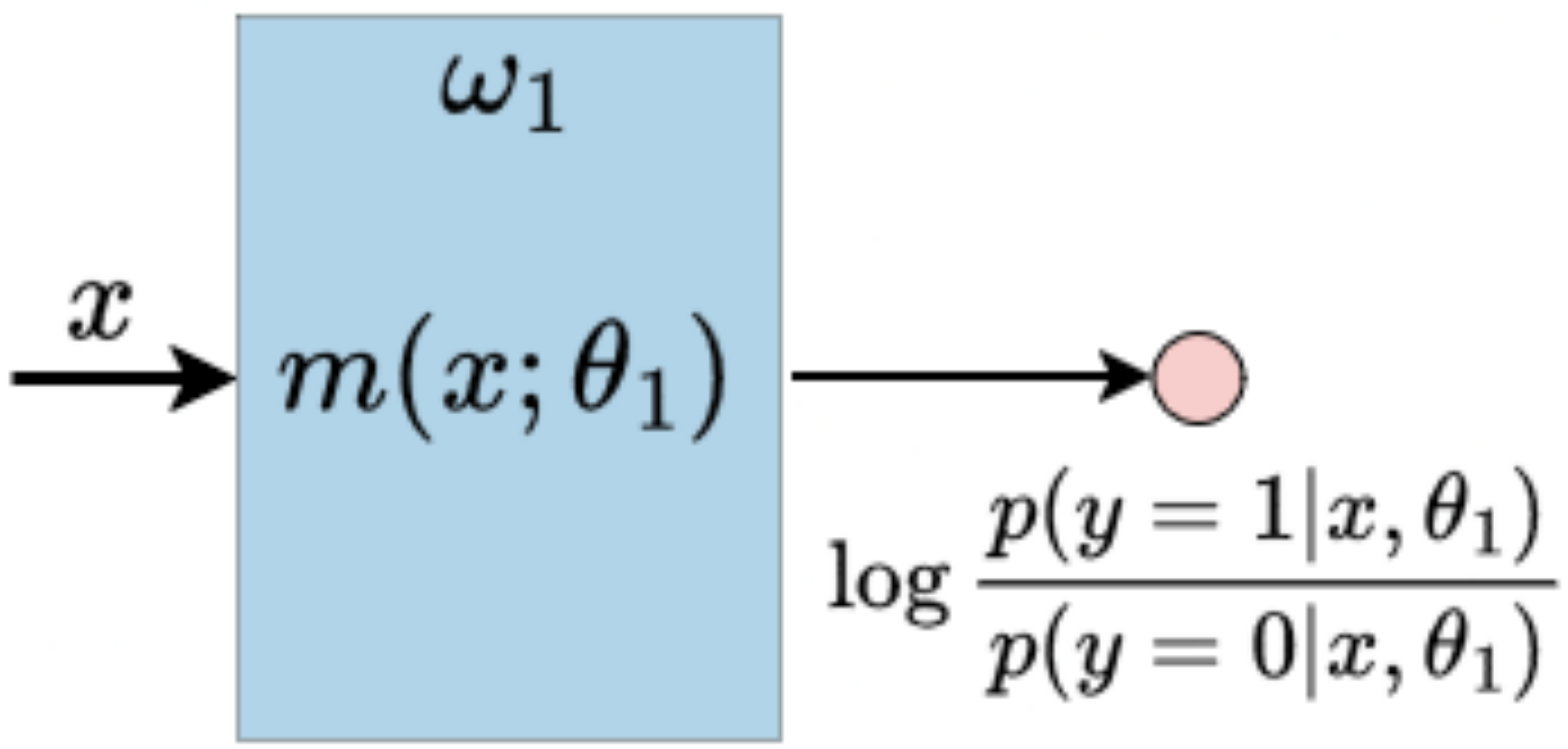




Measure the difference between the **soft decisions/LLRs**.

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

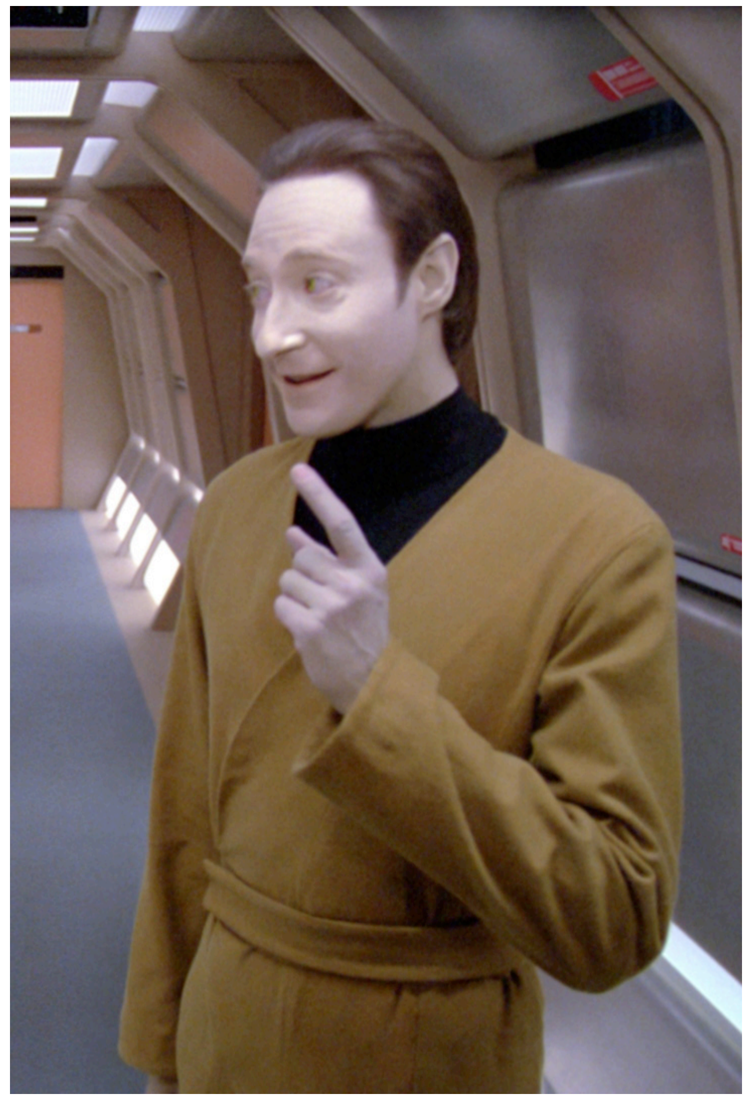
Assume the test set is made of i.i.d. draws from the input distribution.

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

Two-sample tests for model similarity

Back to simple tools: hypothesis testing

VS.



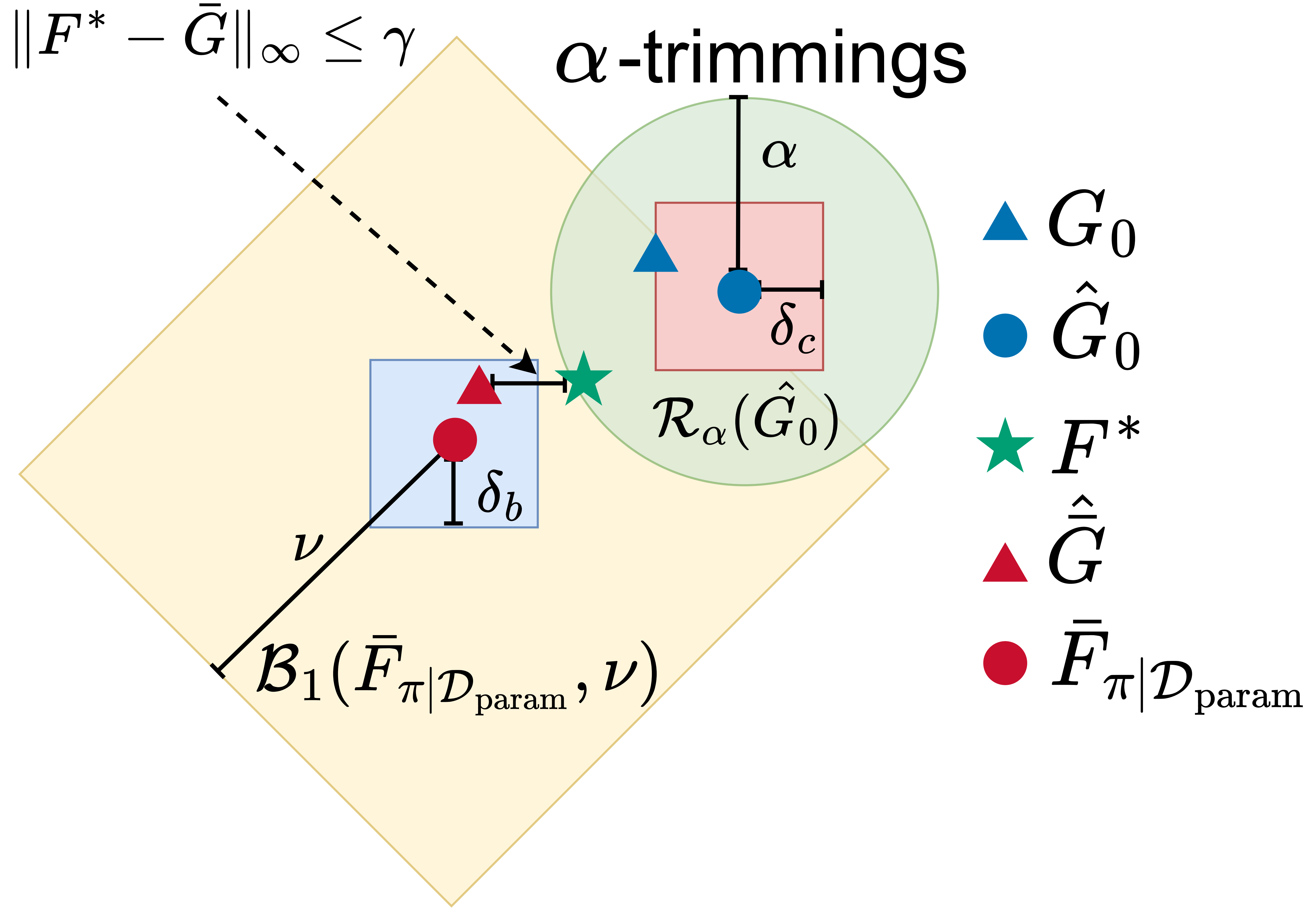
Are the models the same are different? Answer this by testing:

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

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

Hypothesis testing for model comparisons

Use the test's threshold as a measure of difference



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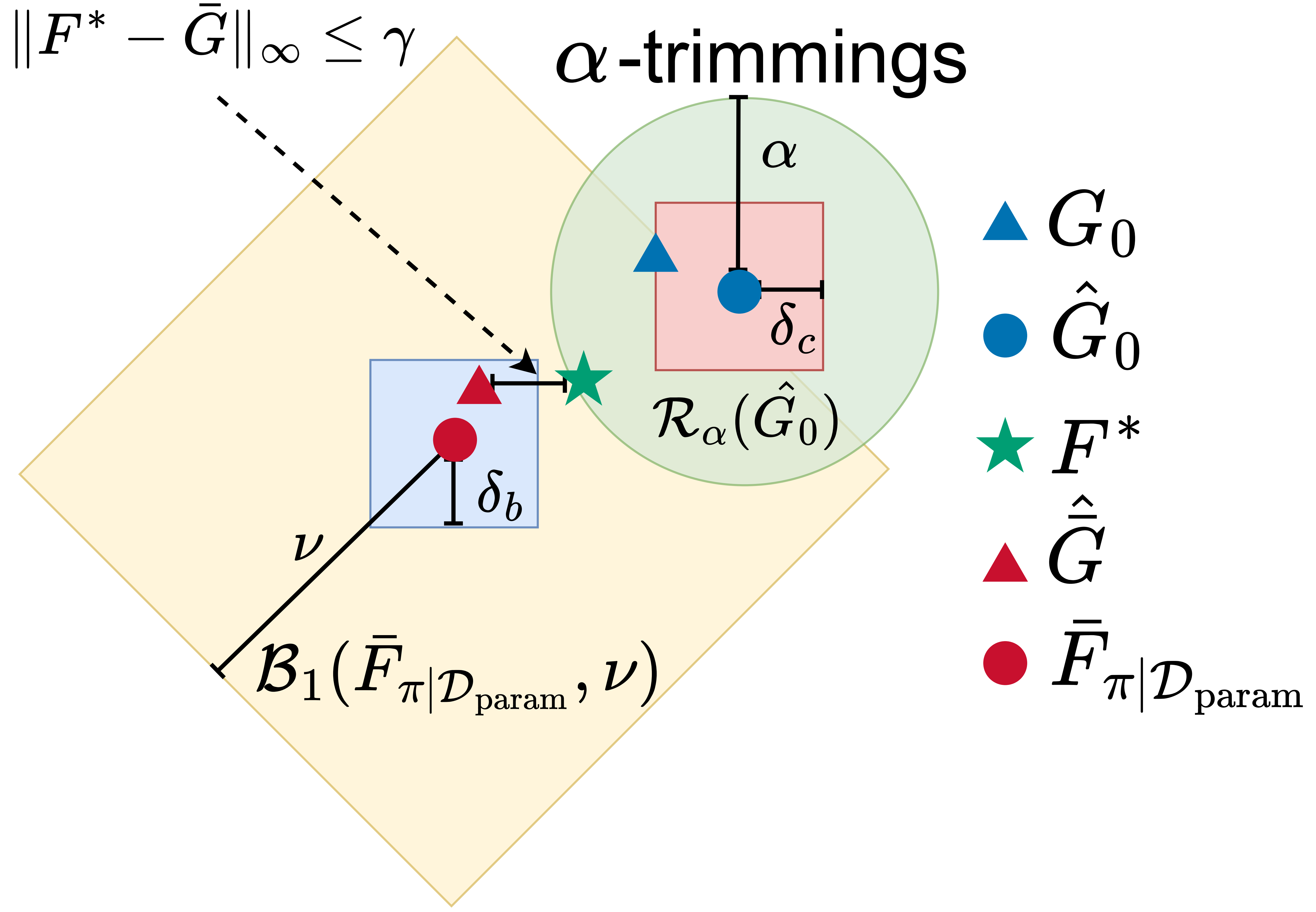

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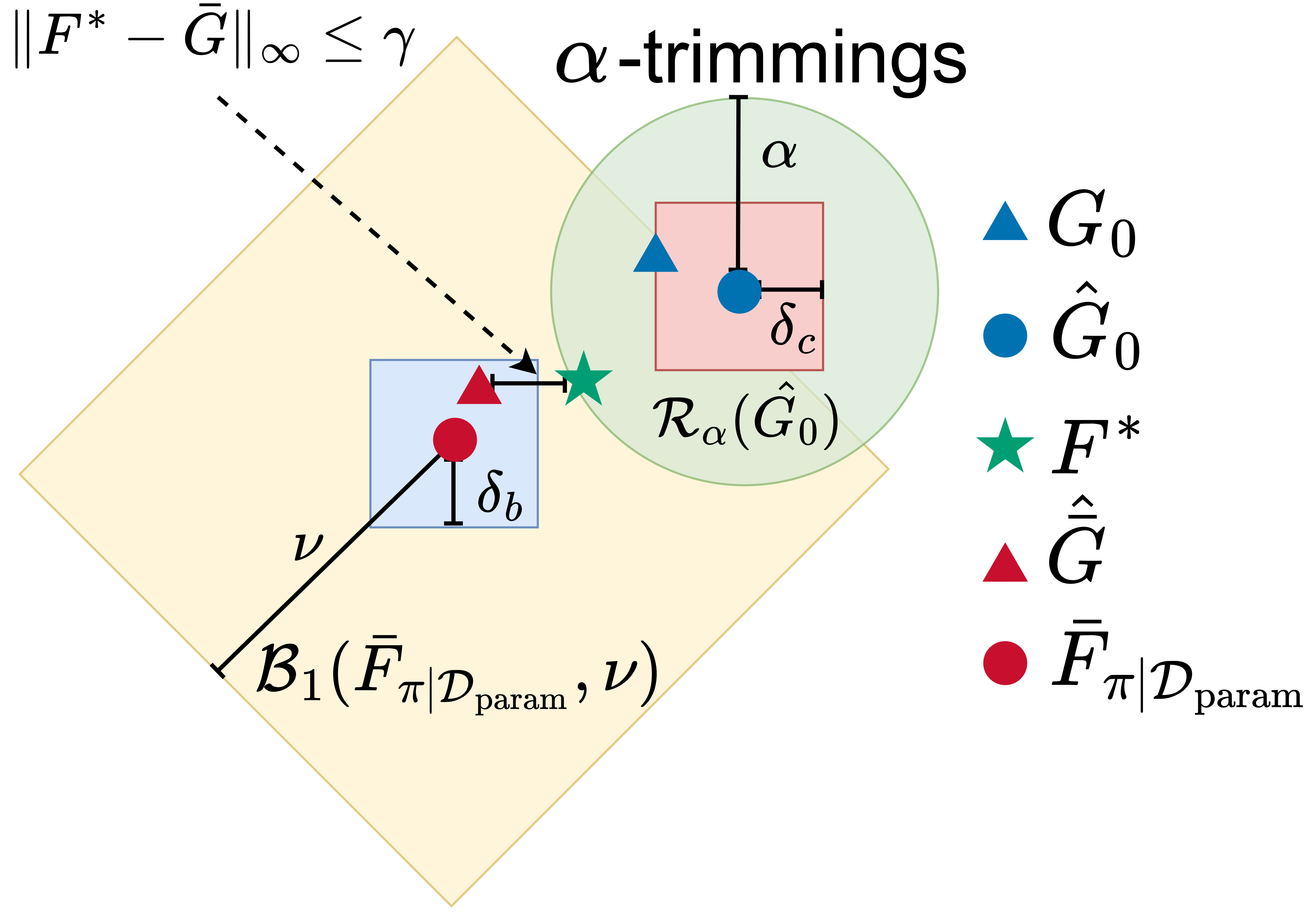

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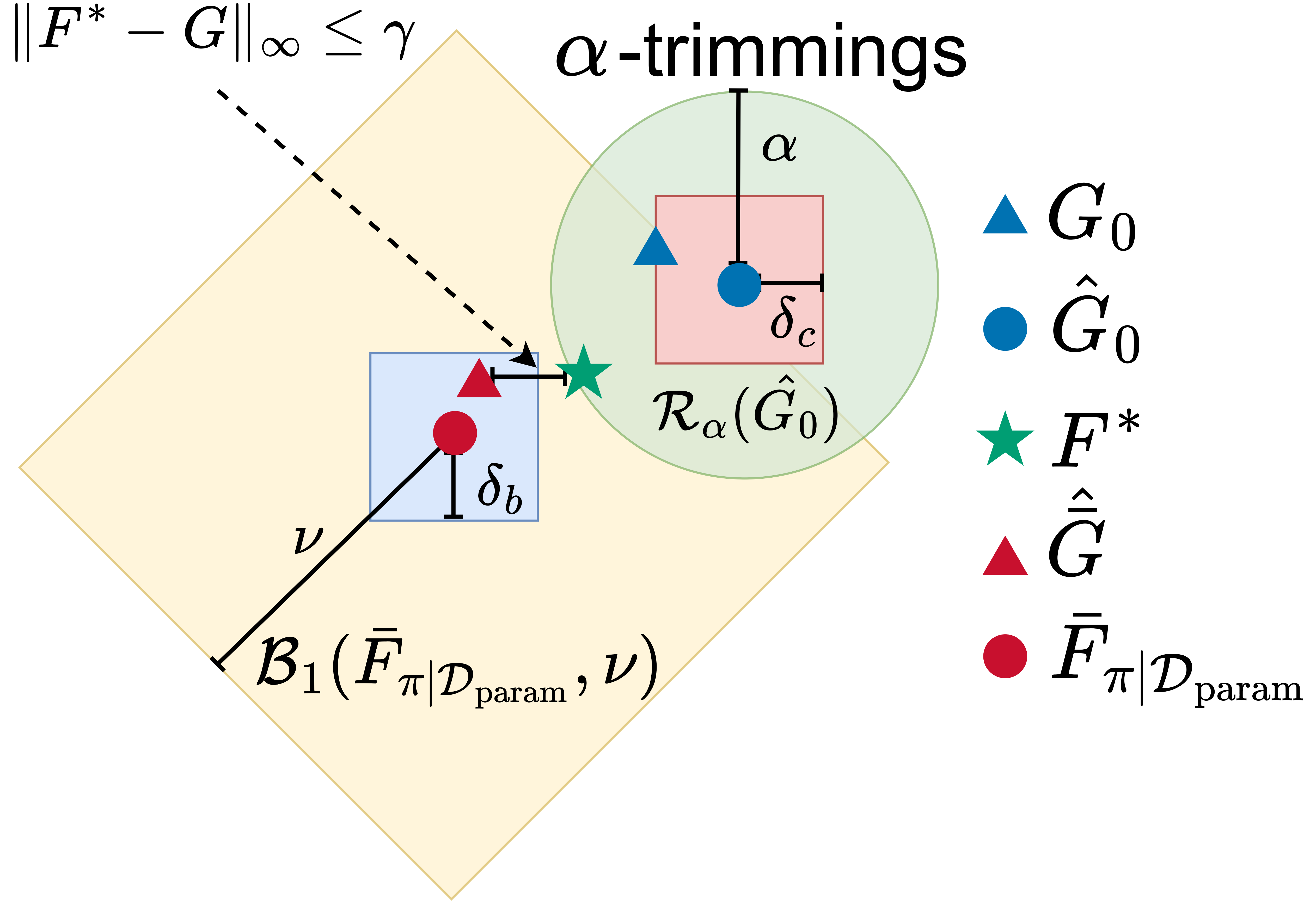

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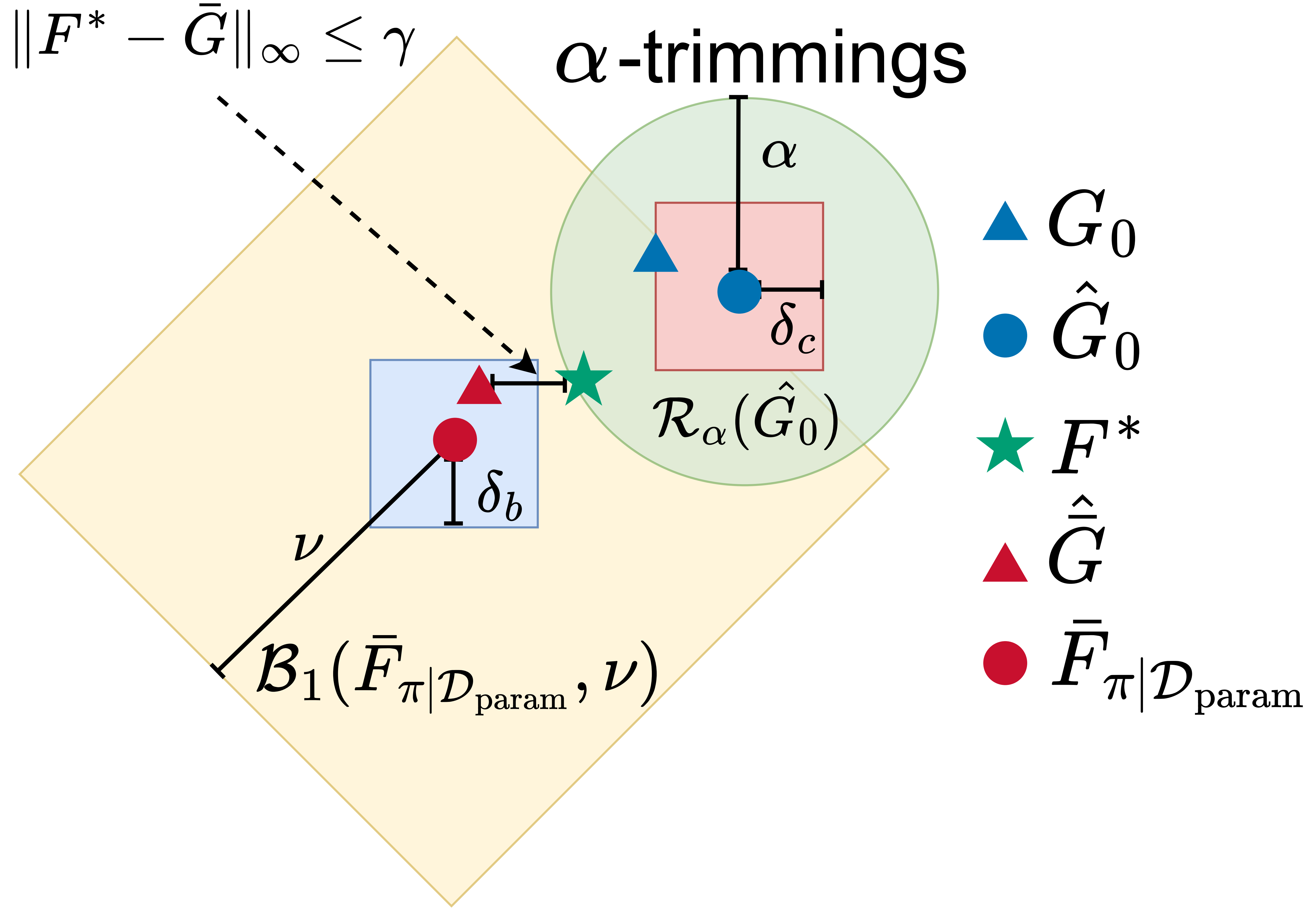
Define a new discrepancy measure $\hat{\alpha}$ as the minimum level for the test (= radius of the ball) to accept.



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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.

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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

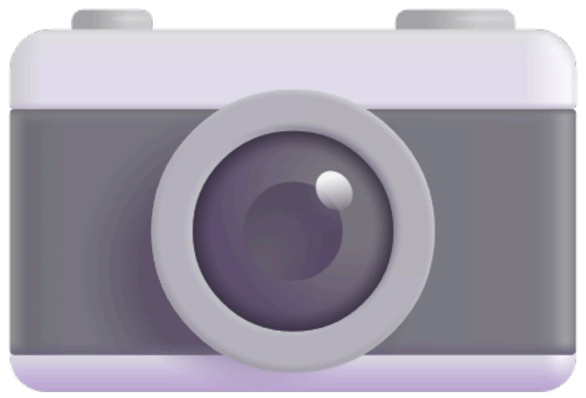
“Reliable” training algorithm should produce “typical” models

iOS 8.3

iOS 18.4

HarmonyOS 4.0

Samsung UI 7.0



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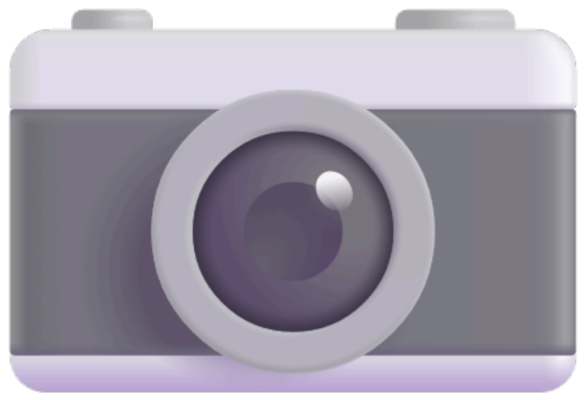

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Measures like $\hat{\alpha}$ (using ℓ_1 balls, Wasserstein balls, etc.) can let us **measure “atypicality.”**

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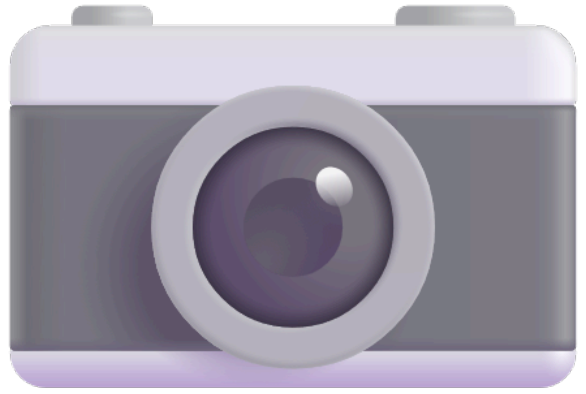

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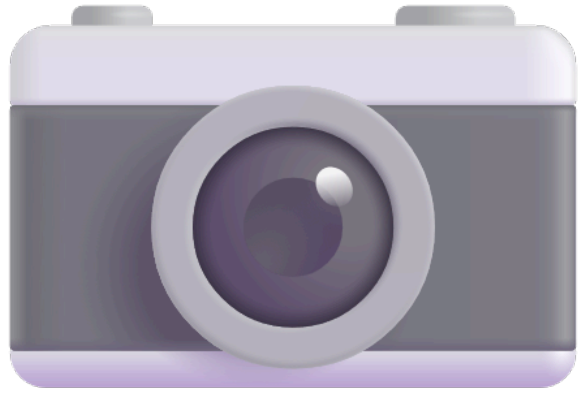

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- Apply it to **other features of trained models** (e.g. NTK spectra) to find model differences.

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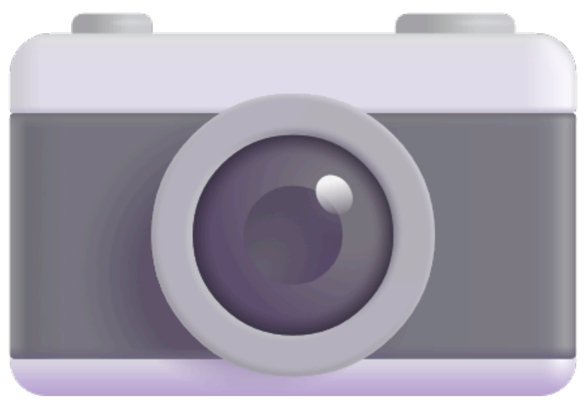

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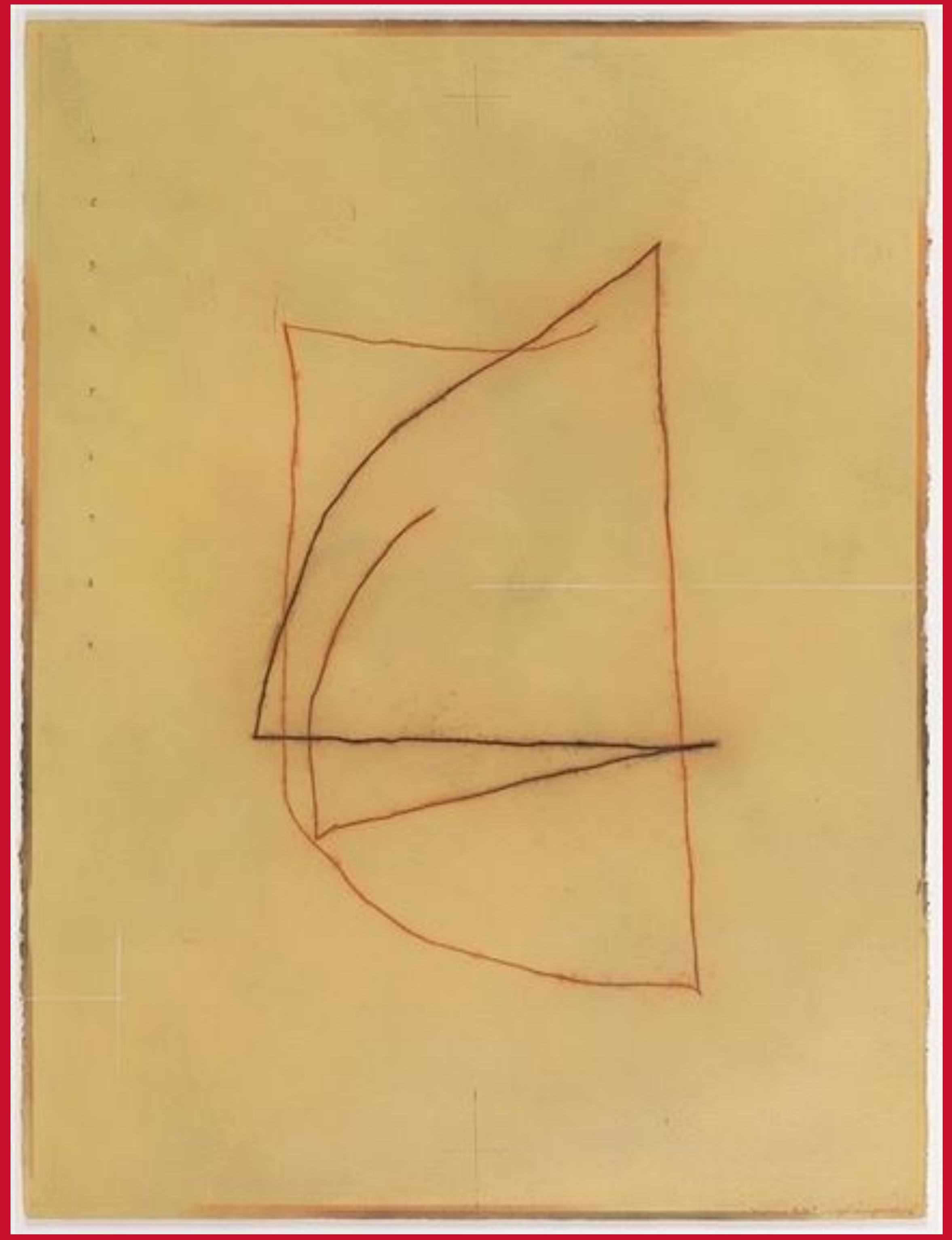
- Use this to design **new methods for model ensembling**.
- Apply it to **other features of trained models** (e.g. NTK spectra) to find model differences.
- Connect it to **process engineering** and other industrial production ideas.

Some final remarks



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

Back to the original question

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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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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!