PHYS 142/242

Lecture 23: Preview of PHYS 139/239

Javier Duarte — March 6, 2024

Course Evaluations!

- https://academicaffairs.ucsd.edu/Modules/Evals?e11230304
- Available until **Wednesday, March 27 at 8:00 AM**
- If we reach above 80% submitted evaluations, extra credit on final projects

Final Presentations

- 1 person per group fill out the form ASAP: https://forms.gle/RVSJ2RNAoAL83n286
- Discuss amongst yourselves then fill it out by Friday lecture
- Limited to 15+5 minutes
- Example presentations from previous years: https://docs.google.com/presentation/d/1jkIBqTkAAXtWCO88Lm4ulzRwCAi8nwUU/edit?usp=sharing&ouid=117156458781940750638&rtpof=true&sd=true
- Presentations will take place Tuesday - Friday in Lab/Lecture
- **All groups are expected to be present to give feedback via form: https://forms.gle/9w36yFgoB8PqwZPE9**

Final Presentations Schedule

Tuesday Lab	Wednesday Lecture	Thursday Lab	Friday Lecture
Double Well Potential with MCMC (B)	Double Well Potential with MCMC (A)	Drell-Yan Production with VEGAS (C)	2D Ising Model with MCMC (B)
Drell-Yan Production with VEGAS (A)	***Drell-Yan Production with VEGAS (B)***	***2D Ising Model with MCMC (C)***	***Drell-Yan Production with VEGAS (D)***
2D Ising Model with MCMC (A)		Double Well Potential with MCMC (C)	

Final Report

- Template: https://www.overleaf.com/read/drwctbrvmzfs#705aa6
- Due Friday of Finals Week

Manuscript Title: Subtitle

Ann Author* and Second Author†
University of California San Diego

(Group: Double Well Potential with MCMC (A))
(Dated: March 6, 2024)

An article usually includes an abstract, a concise summary of the work covered at length in the main body of the article.

I. INTRODUCTION

Introduce the problem you are solving. Discuss the physics behind the project and introduce the computational methods you will use. Also, mention and cite any papers you use [1].

Describe the main objective of your project.

II. METHODS

Describe methods, e.g. Markov chain Monte Carlo with Metropolis-Hastings algorithm. Here's an example of an equation for the path integral

$$K(x_b, t_b; x_a, t_a) = \int \mathcal{D}x(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} L(x(t))dt\right] \quad (1)$$

Make sure you define all variables in any equations you write!

Describe and discuss any parameters you choose for your computational method, e.g. burn-in steps, etc.

Provide the link to your software in GitHub repository [2].

III. RESULTS

Report the results of your simulations. Add figures showing your results, as in Fig. 1.

Discuss significance of results. In particular answer questions posed in the assignment, e.g. explain the connection to statistical mechanics.

IV. CONCLUSION

Brief summary of the project and results. Describe any lessons learned or possible future work.

V. CONTRIBUTIONS

Briefly describe contributions from each team member.

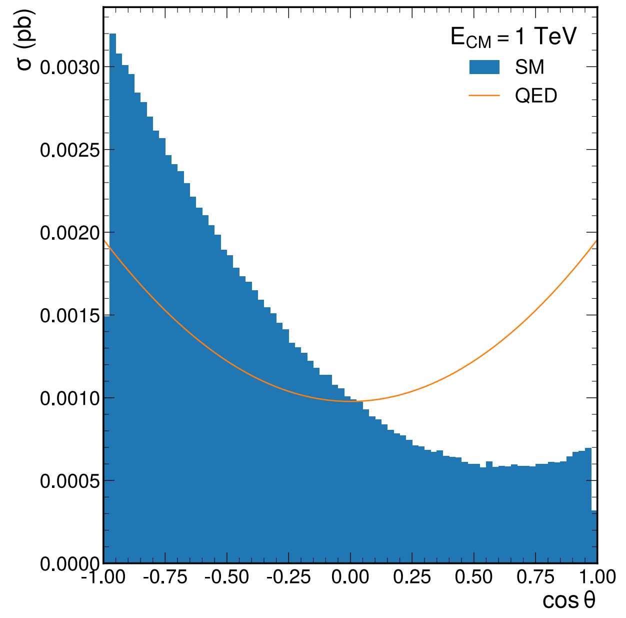

FIG. 1. Describe your figure in full.

ACKNOWLEDGMENTS

Add any acknowledgments (optional).

[1] S. Mittal, M. J. Westbroek, P. R. King, and D. D. Vvedensky, Path integral Monte Carlo method for the quantum anharmonic oscillator, Eur. J. Phys. **41**, 055401 (2020).
[2] J. M. Duarte, UCSD PHYS 142 GitHub (2024).

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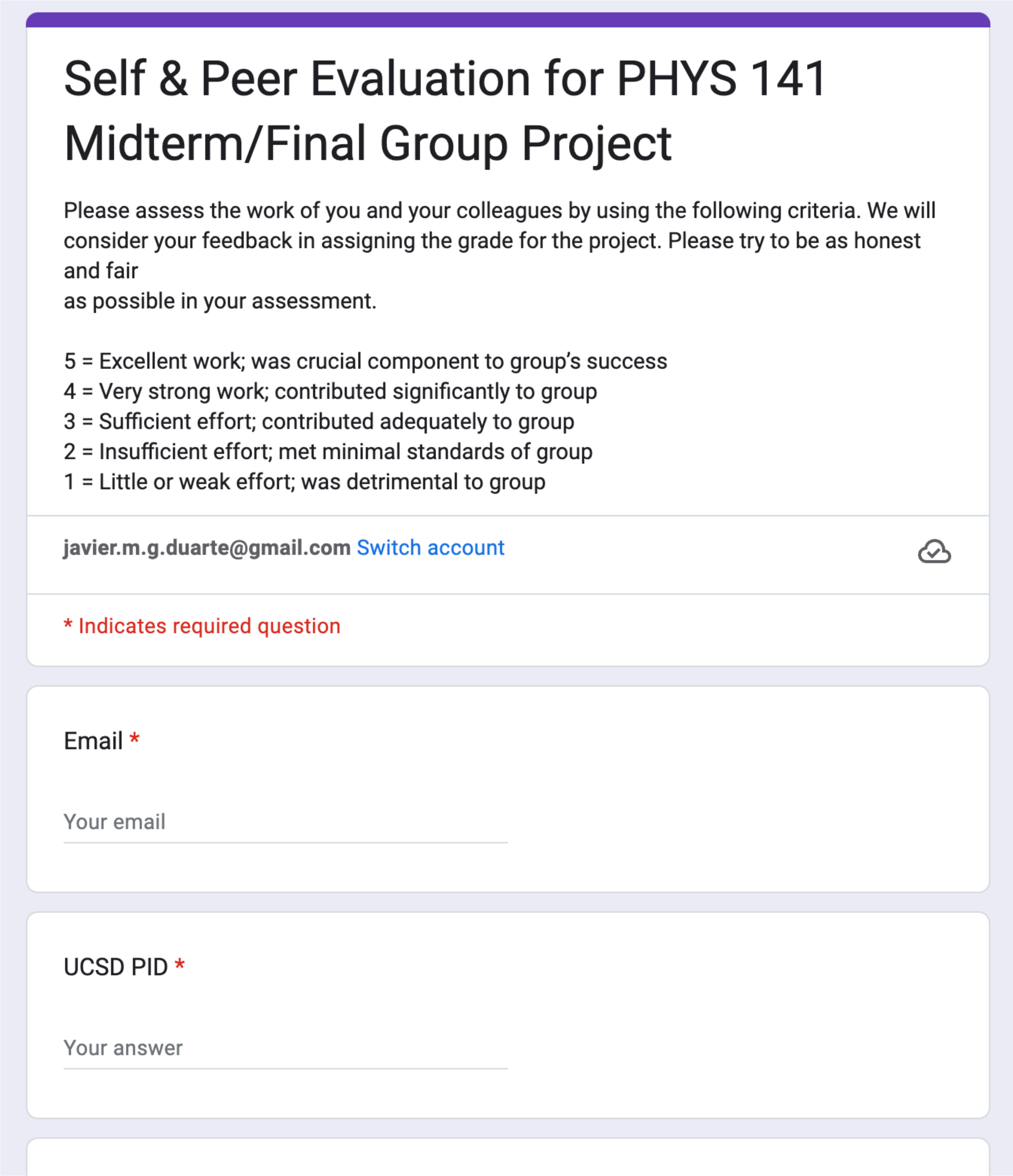
Self & Peer Evaluations

- Form: https://forms.gle/P9C7E9jYrmn4hEHZ7
- Due Friday of Finals Week



Self & Peer Evaluation for PHYS 141 Midterm/Final Group Project

Please assess the work of you and your colleagues by using the following criteria. We will consider your feedback in assigning the grade for the project. Please try to be as honest and fair
as possible in your assessment.

5 = Excellent work; was crucial component to group's success
4 = Very strong work; contributed significantly to group
3 = Sufficient effort; contributed adequately to group
2 = Insufficient effort; met minimal standards of group
1 = Little or weak effort; was detrimental to group

javier.m.g.duarte@gmail.com Switch account

* Indicates required question

Email *

Your email

UCSD PID *

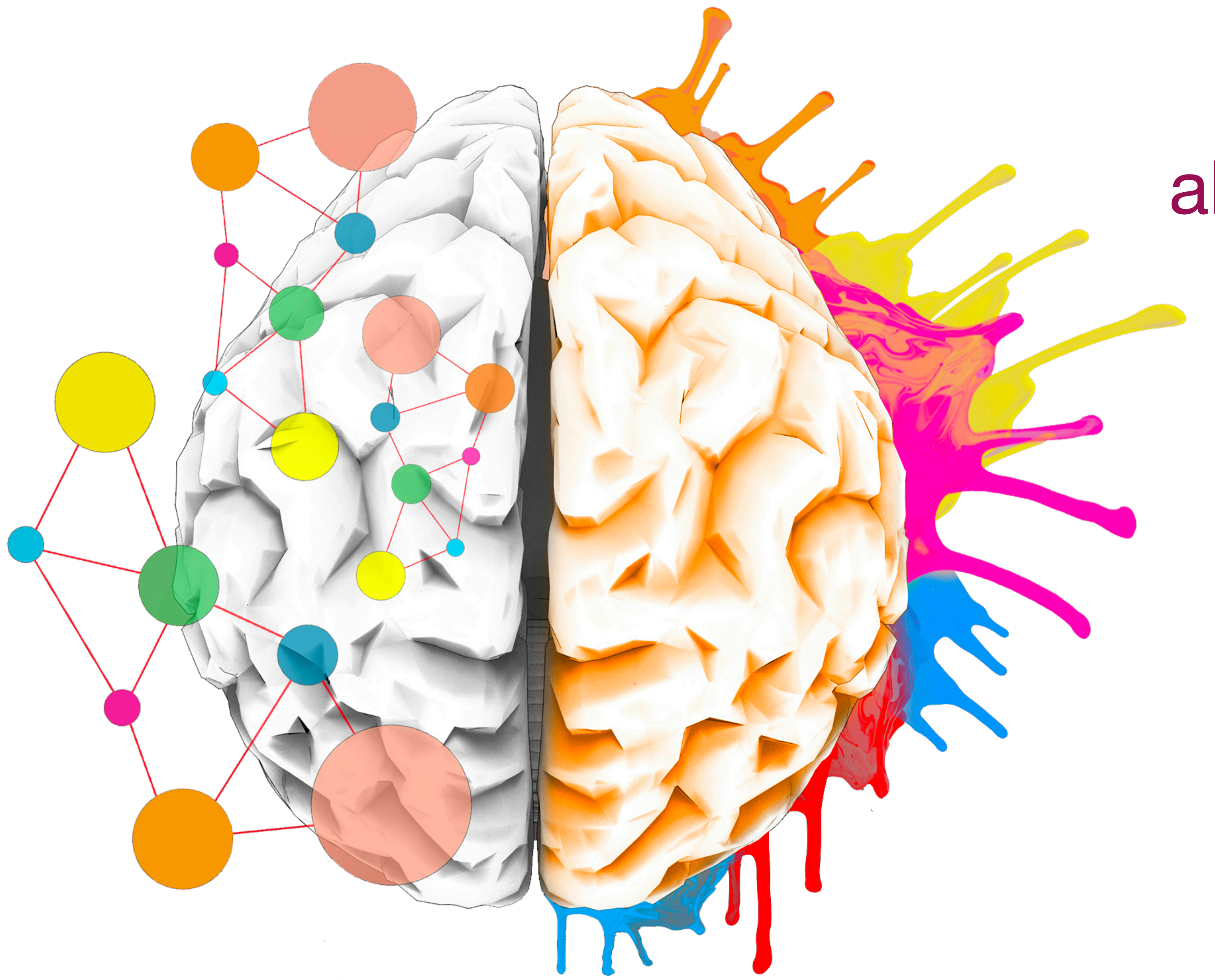
Your answer

PHYS 143/243: Machine Learning in Physics

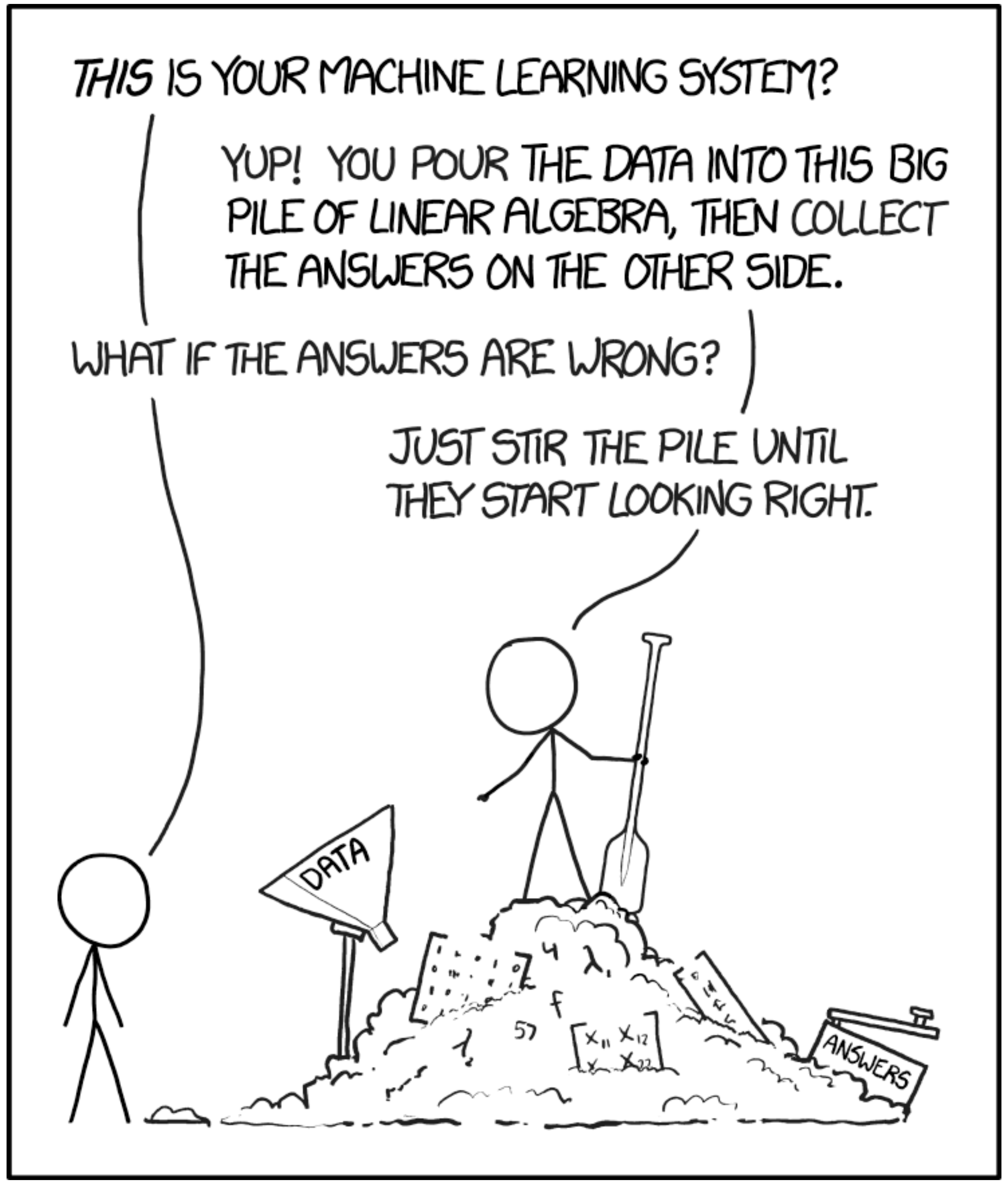
- Study of machine learning methods applied to physics
- Currently offered as a 139/239 Special Topics
- Overview:
    - Supervised learning
    - (Boosted) decision trees — tabular data
    - (Deep) neural networks — tabular data
    - Convolutional neural networks — image-like data
    - Graph neural networks — graph-like data and point clouds
    - Unsupervised learning
    - (Variational) autoencoders for anomaly detection
    - Model compression
    - Special topics via guest lectures (TBD)
        - Equivariant models
        - Generative models
        - Reinforcement learning
        - Explainability
        - Uncertainty
    - Final team projects

What is machine learning?

- Science and art of learning automatically from data and experience



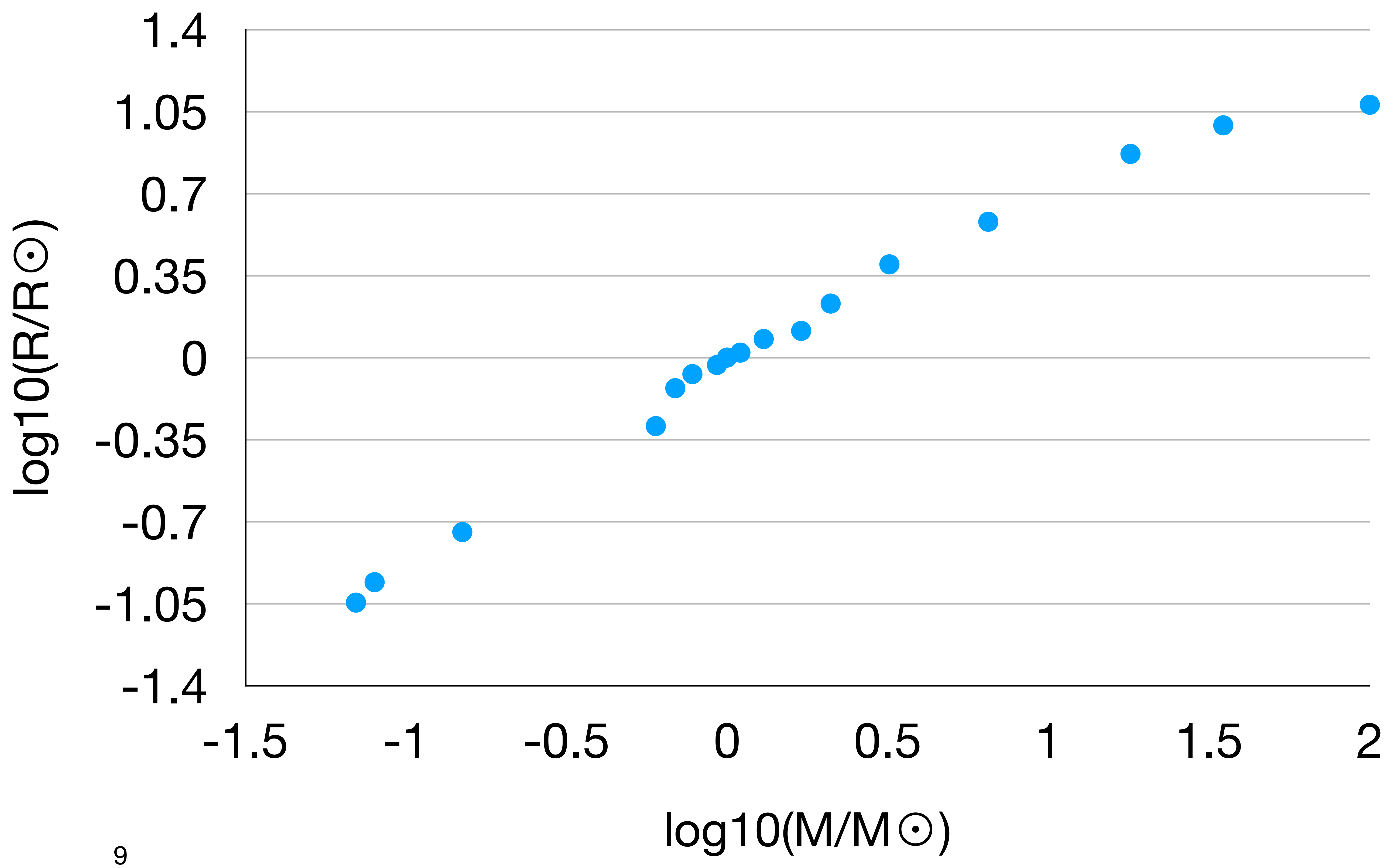
Also, a lot of calculus, linear algebra, statistics, group theory, …



- Large overlap with data mining:
  - ML focuses on algorithms, DM on discovering patterns

Supervised learning

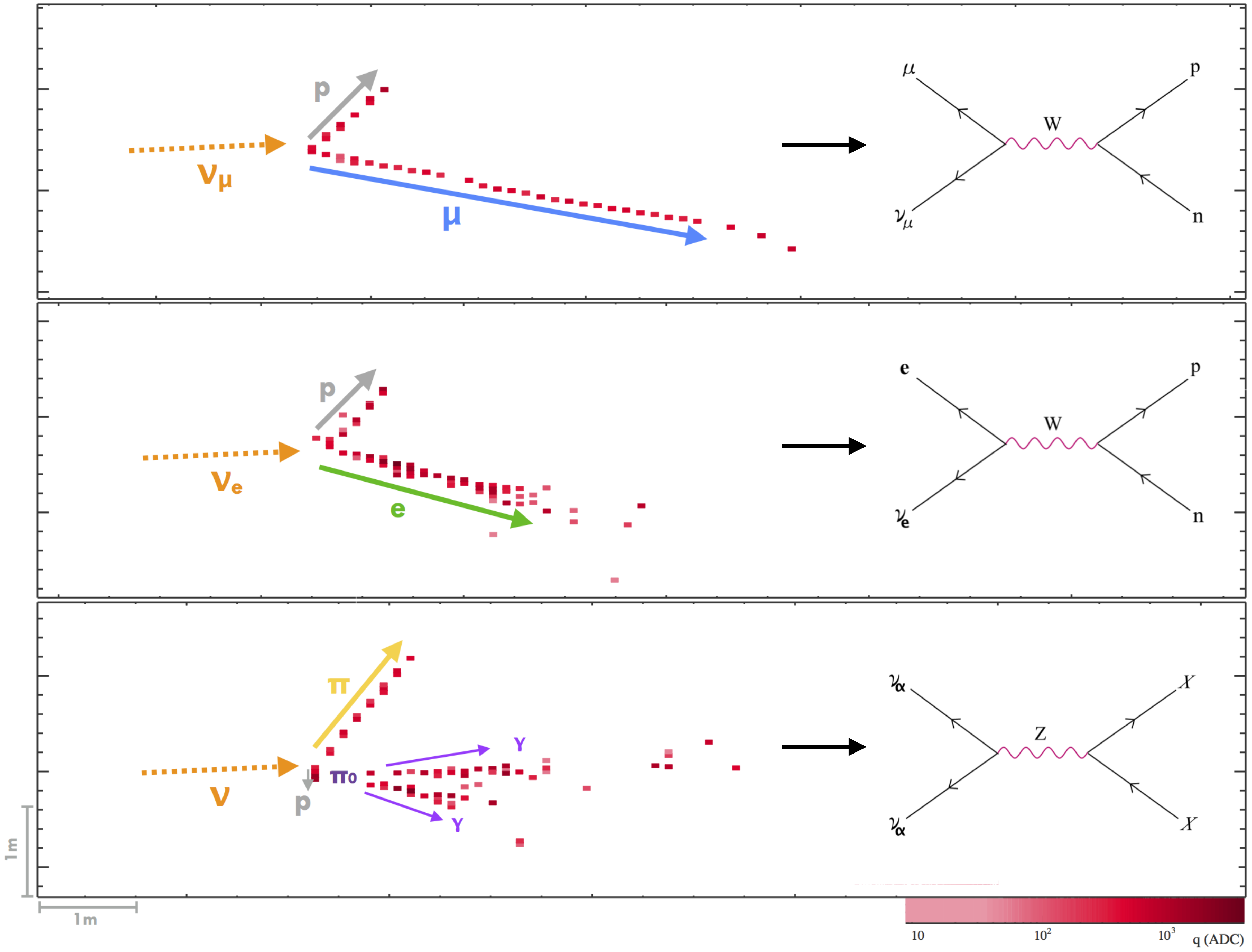
- Learn a function $f : X \to Y$ from an input space X (observations) to an output space Y (targets), using a set of labeled examples$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$.
- Example 1: Predict stellar radius given stellar mass



Supervised learning

- Learn a function $f : X \rightarrow Y$ from an input space X (observations) to an output space Y (targets), using a set of labeled examples$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$.

- Example 2: Classify images of neutrino interactions



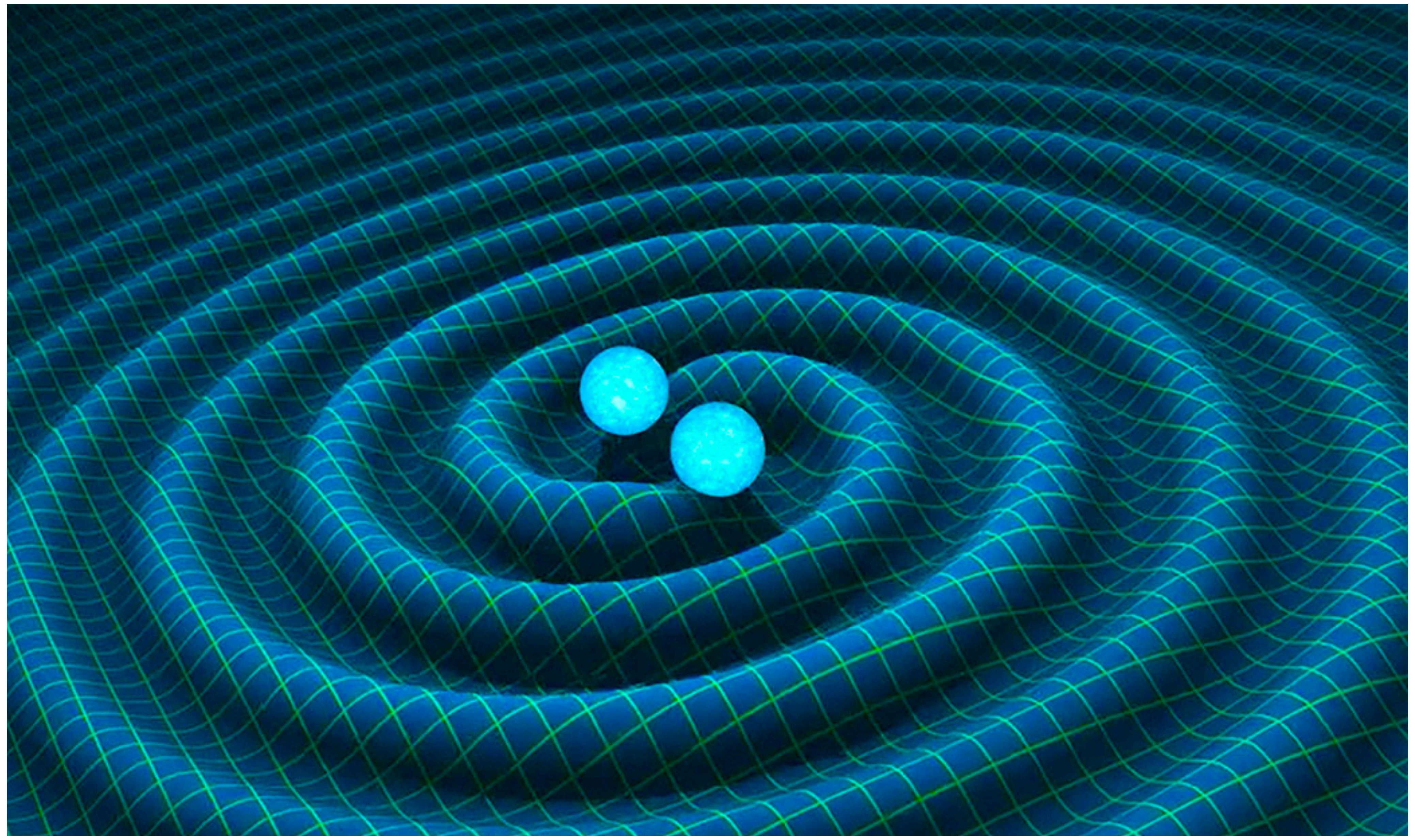
arXiv:1604.01444

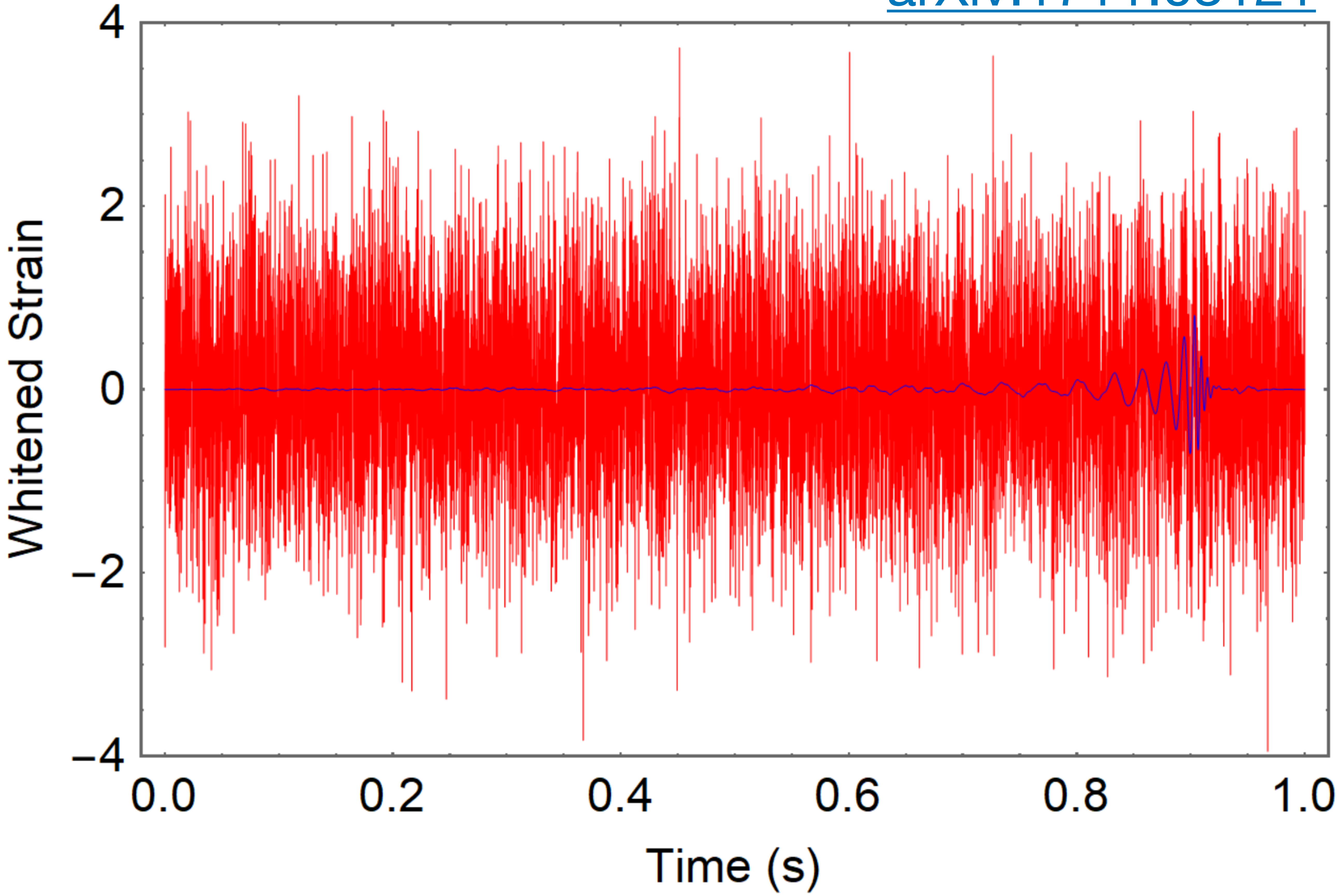
Supervised learning

- Learn a function $f: X \to Y$ from an input space X (observations) to an output space Y (targets), using a set of labeled examples$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$.

- Example 3: Reduce noise in a time-series trace to identify a gravitational wave signal

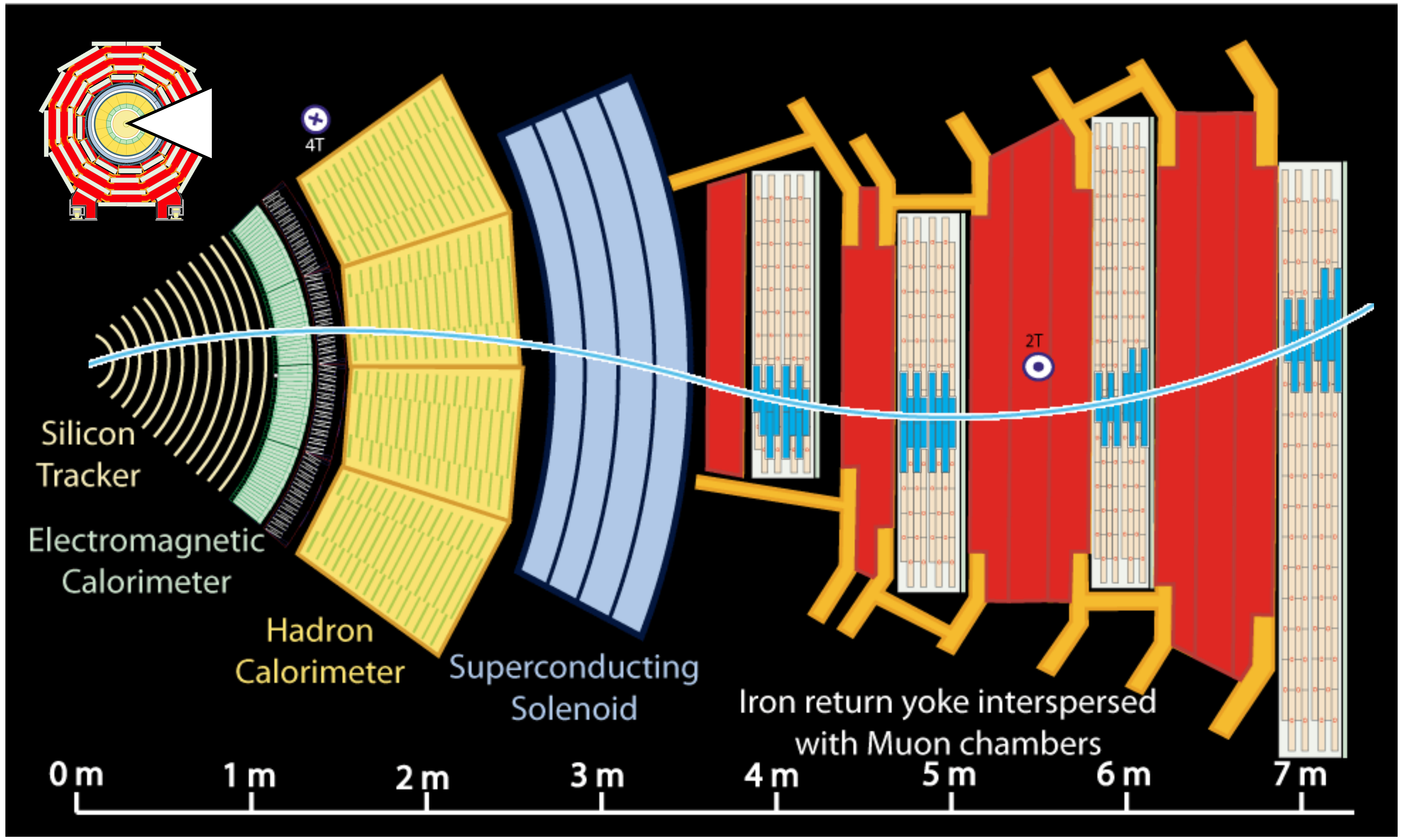
arXiv:1711.03121





Supervised learning

- Learn a function $f : X \to Y$ from an input space X (observations) to an output space Y (targets), using a set of labeled examples$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$.
- Example 4: Estimate particle momentum, charge, type, etc. from detector hits



$$\to \begin{pmatrix} E \\ p_x \\ p_y \\ p_z \end{pmatrix}, q, \text{type}, p_{\text{pileup}}, \ldots$$

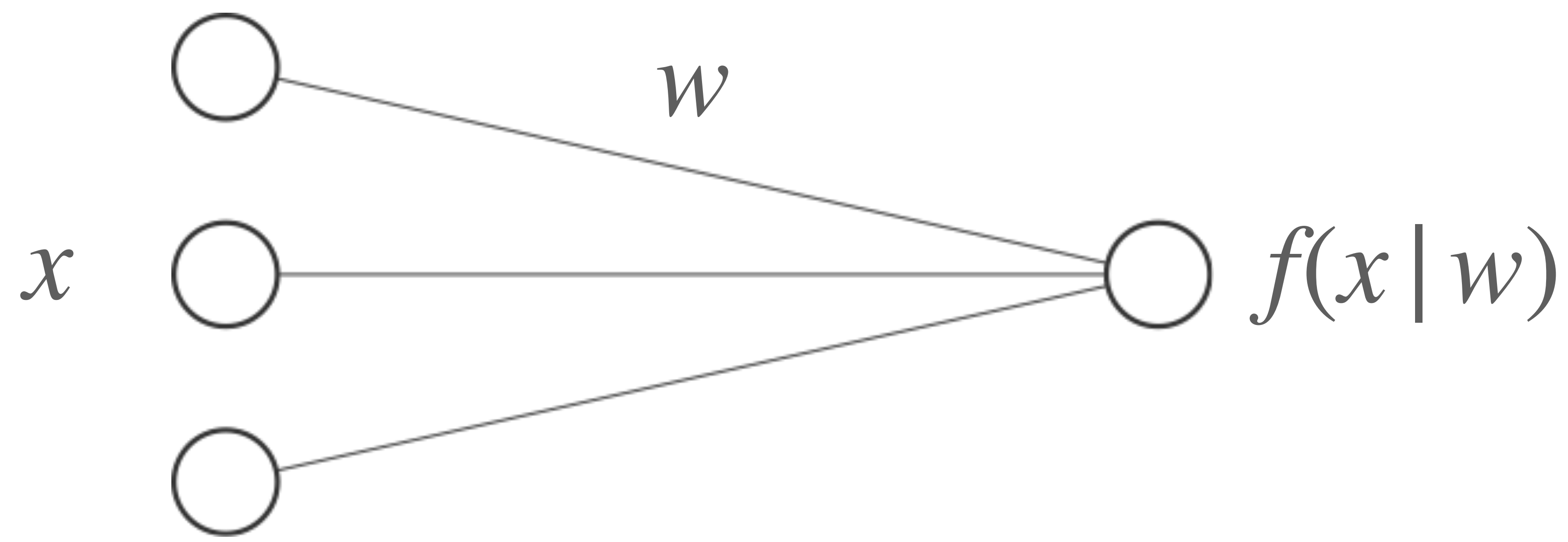
arXiv:2101.08578

Linear models: workhorse of machine learning

- Linear models on top of good features can yield excellent results

- More complex model classes (e.g., neural networks) have linear models as their basic building block

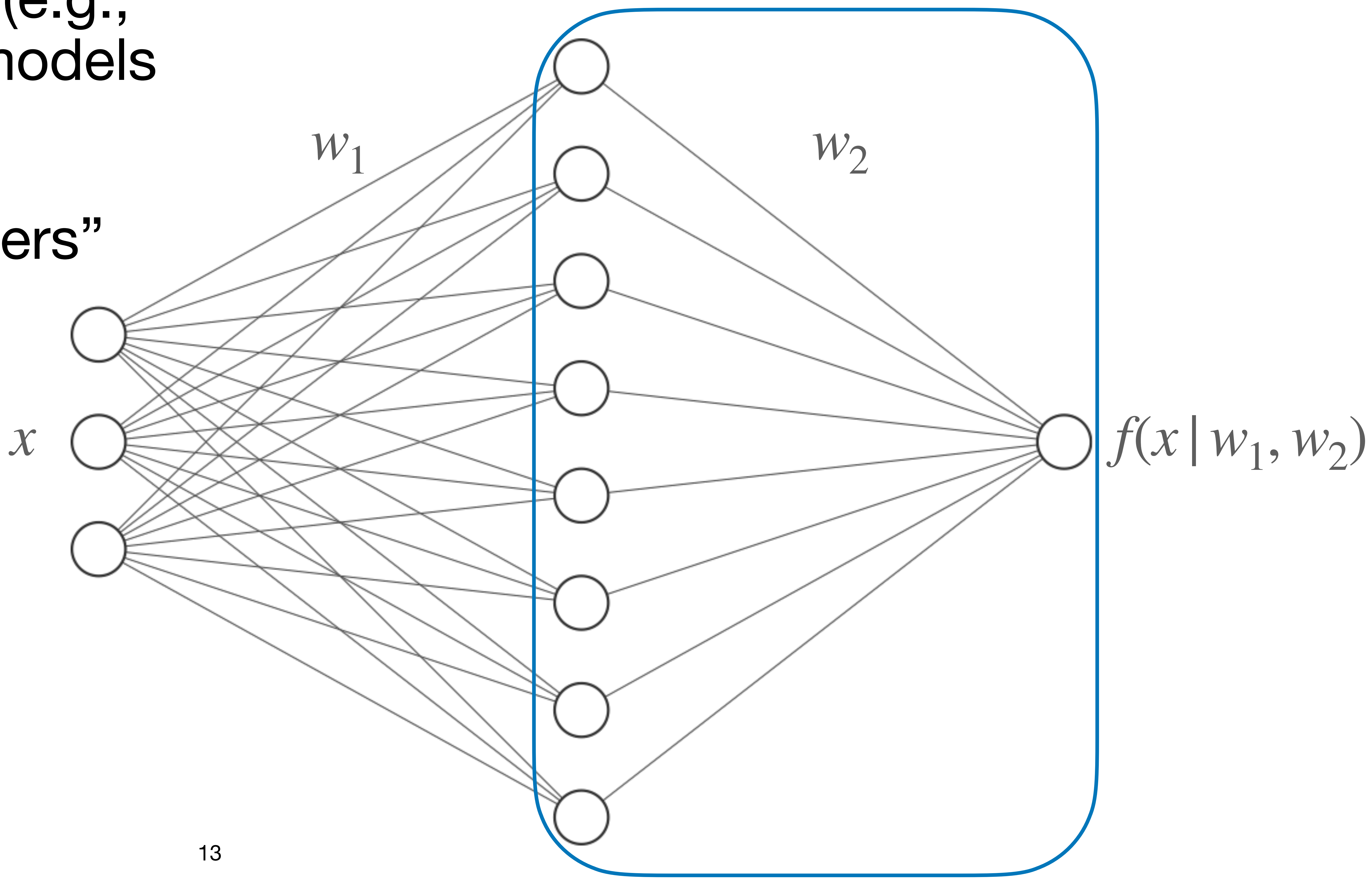
  - NNs are "automatic featurizers"



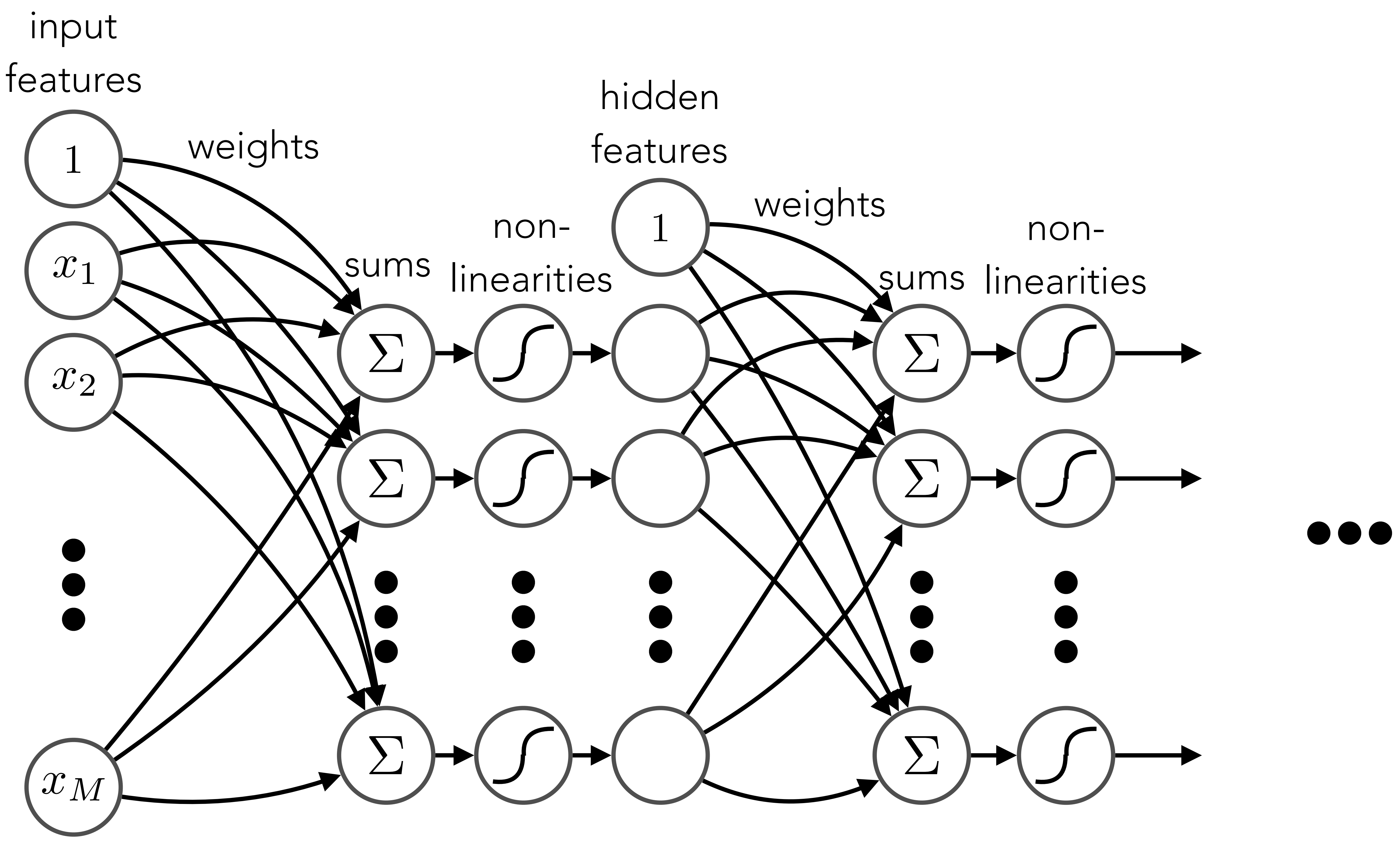
Linear model: $f(x \mid w) = w^\intercal x$

Neural network: linear model after inputs are mapped to features through a nonlinear transformation

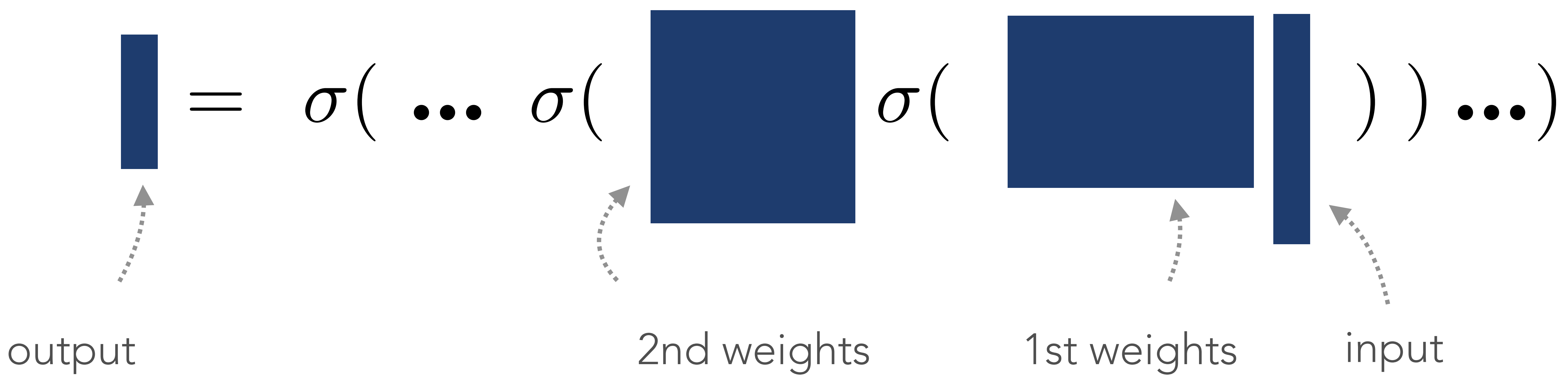
$f(x \mid w_1, w_2) = w_2^\intercal \sigma(w_1^\intercal x)$



Neural networks



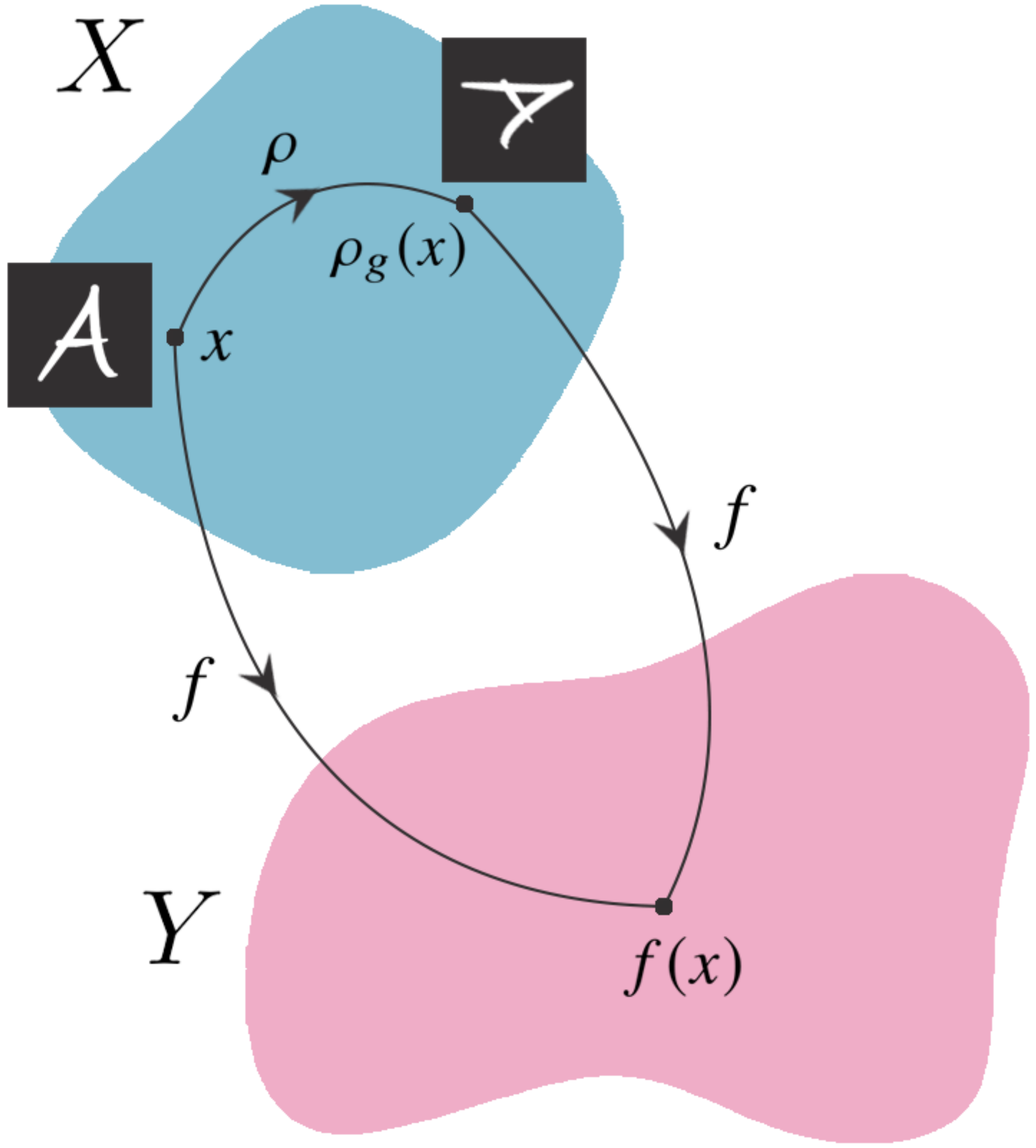
network: *sequence of parallelized weighted sums and non-linearities*



Symmetries

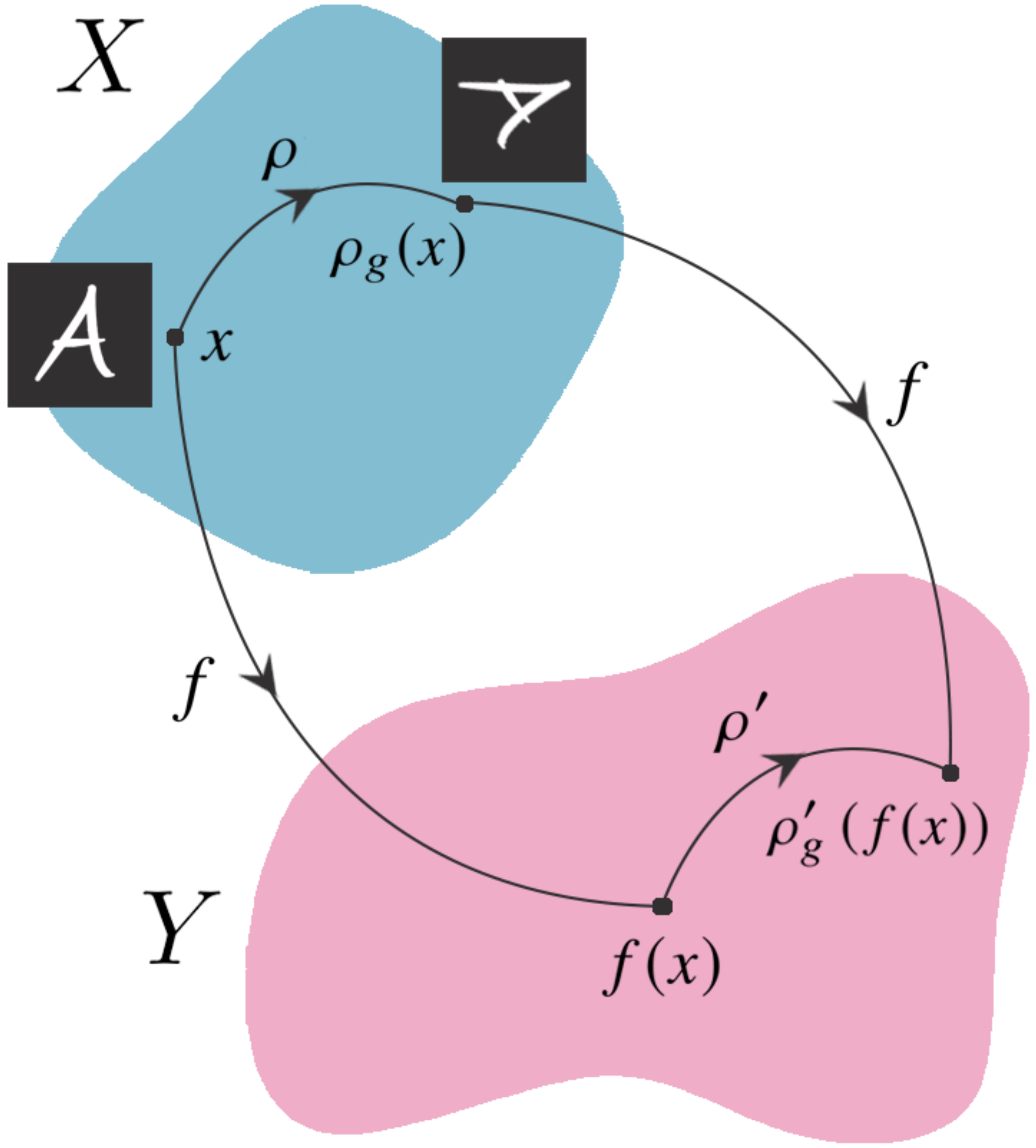
Invariance

$$f(\rho_g(x)) = f(x)$$



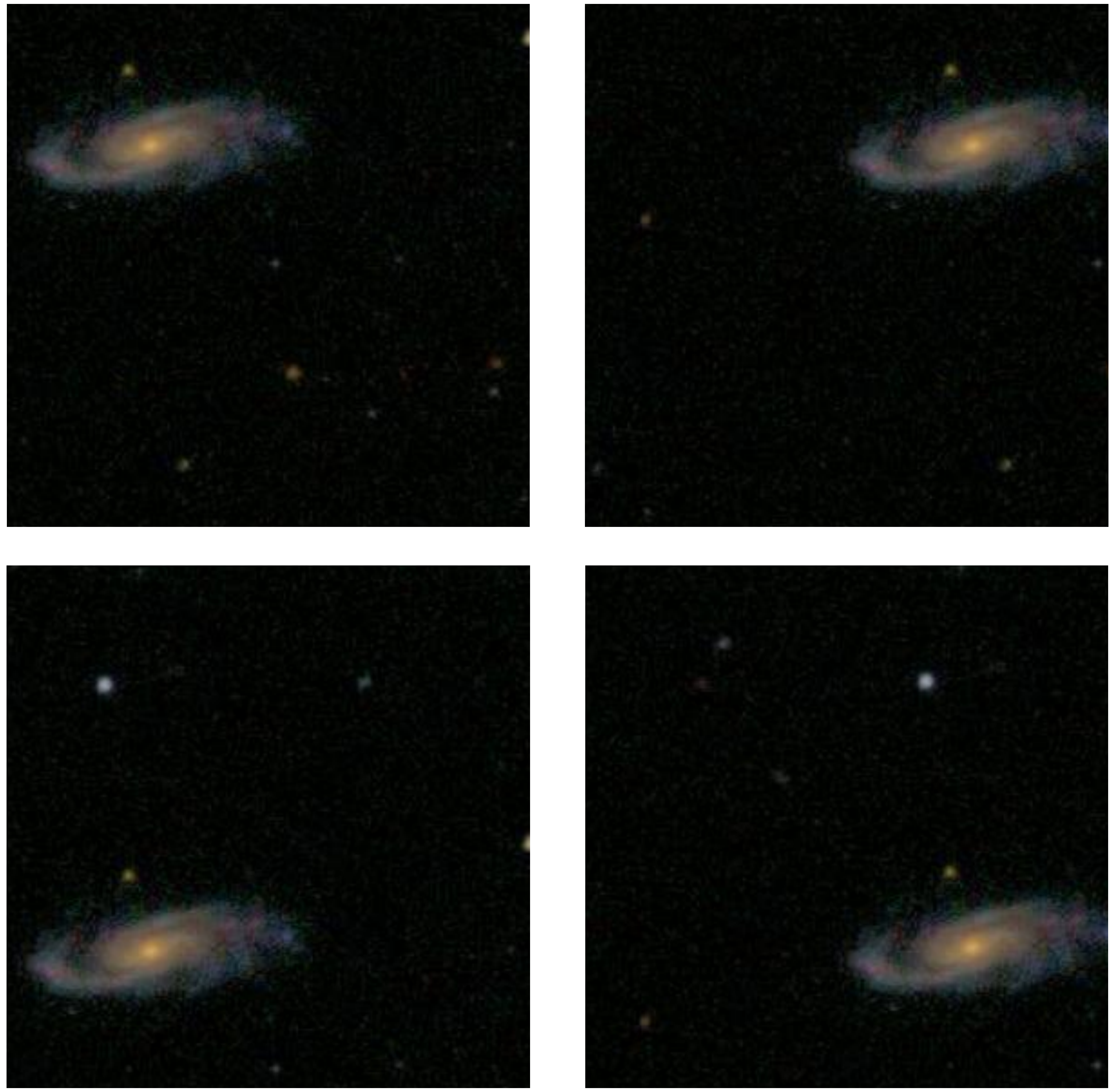
Equivariance

$$f(\rho_g(x)) = \rho'_g(f(x))$$



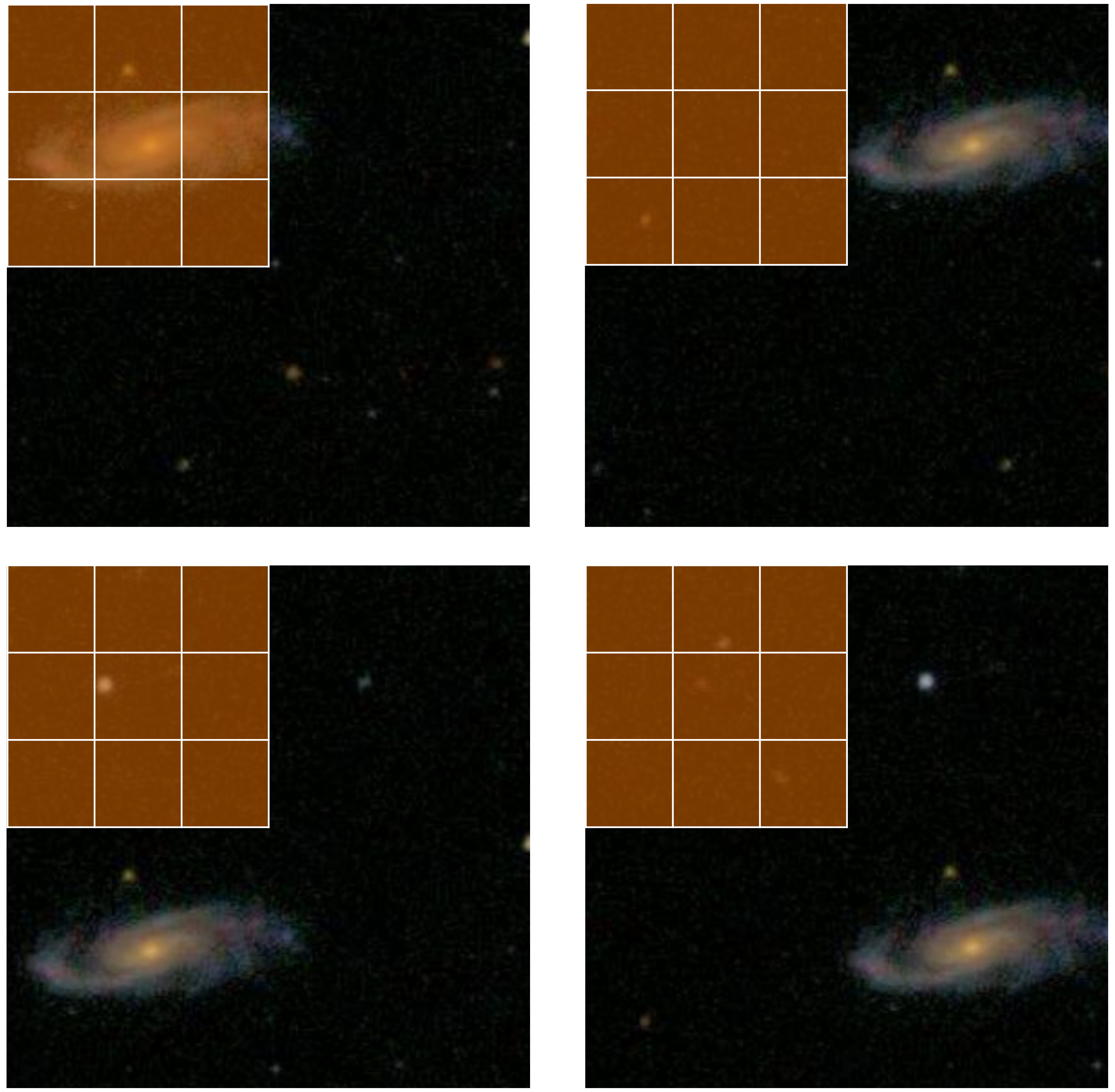
Translational invariance

- For the purpose of classifying galaxy morphologies (e.g. spiral), the answer shouldn't depend on the absolute location of the pixels
- For simplicity, imagine there are 4 possible locations the galaxy might show up (top left, top right, bottom left, and bottom right)



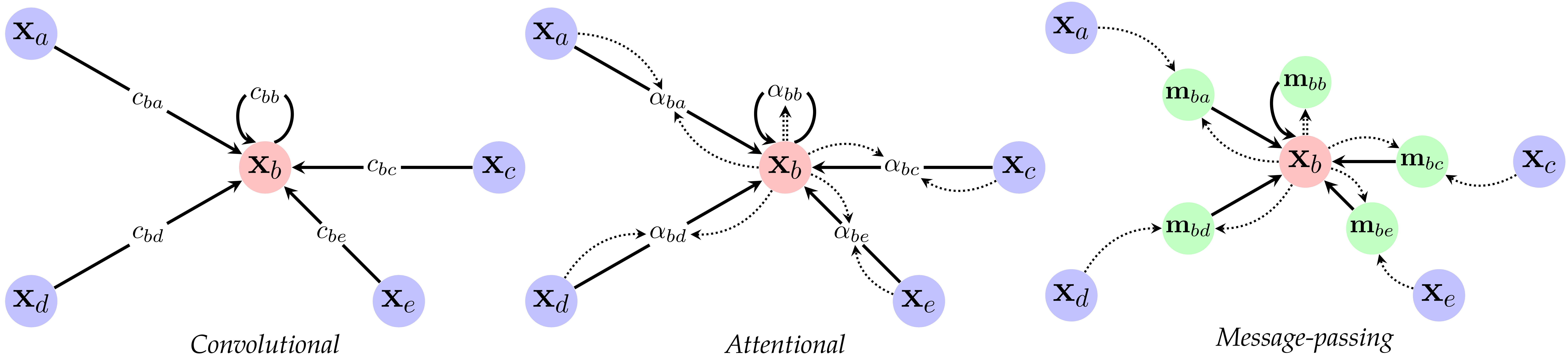
Convolutional neural networks

What if the *same* fully-connected neural network is applied to each corner?



Graph neural networks

arXiv:104.13478



- Convolutional: sender node features are multiplied with a constant
- Attentional: multiplier is implicitly computed via an attention mechanism of the receiver over the sender
- Message-passing: vector-based messages are computed based on both the sender and receiver