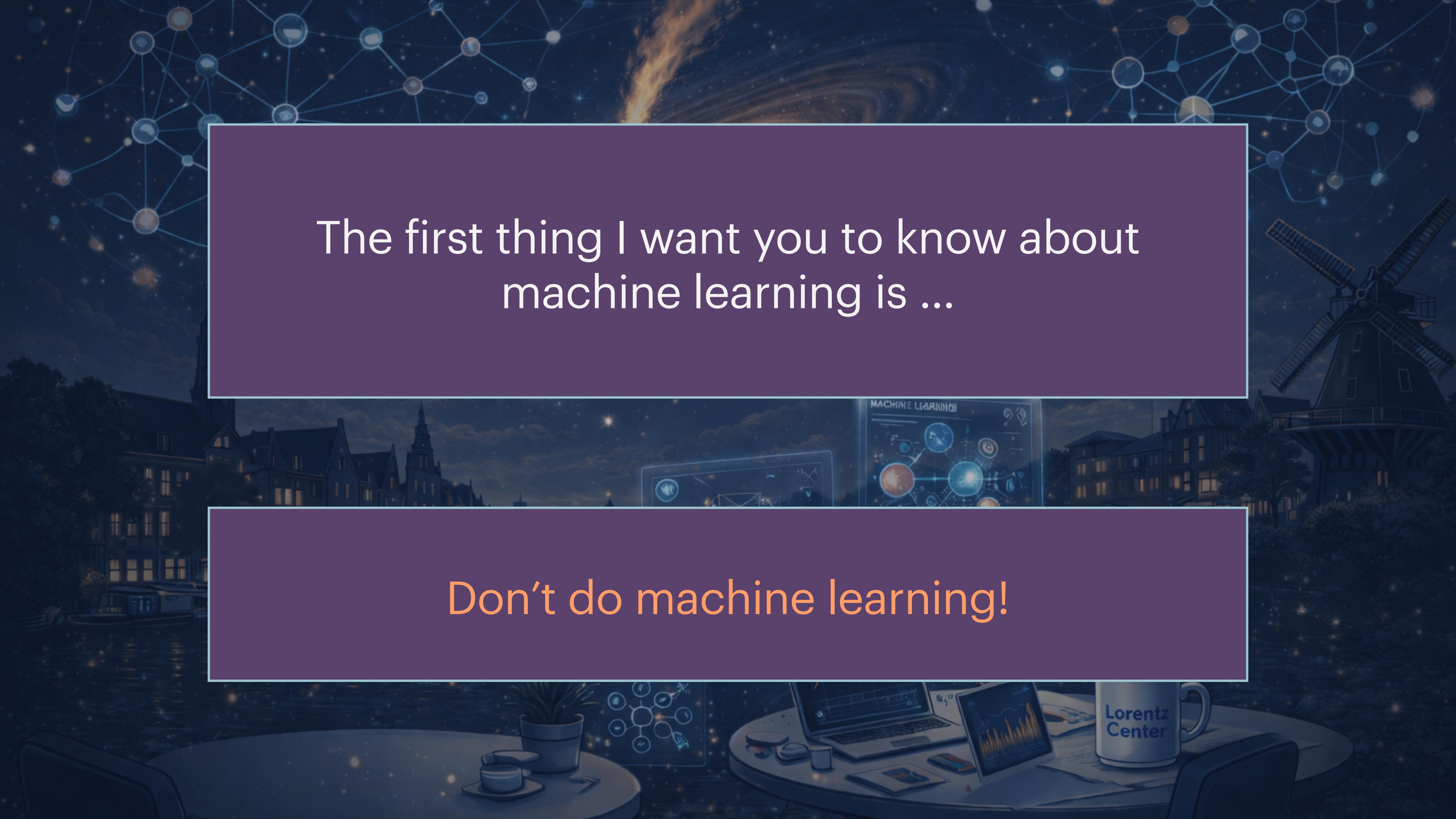


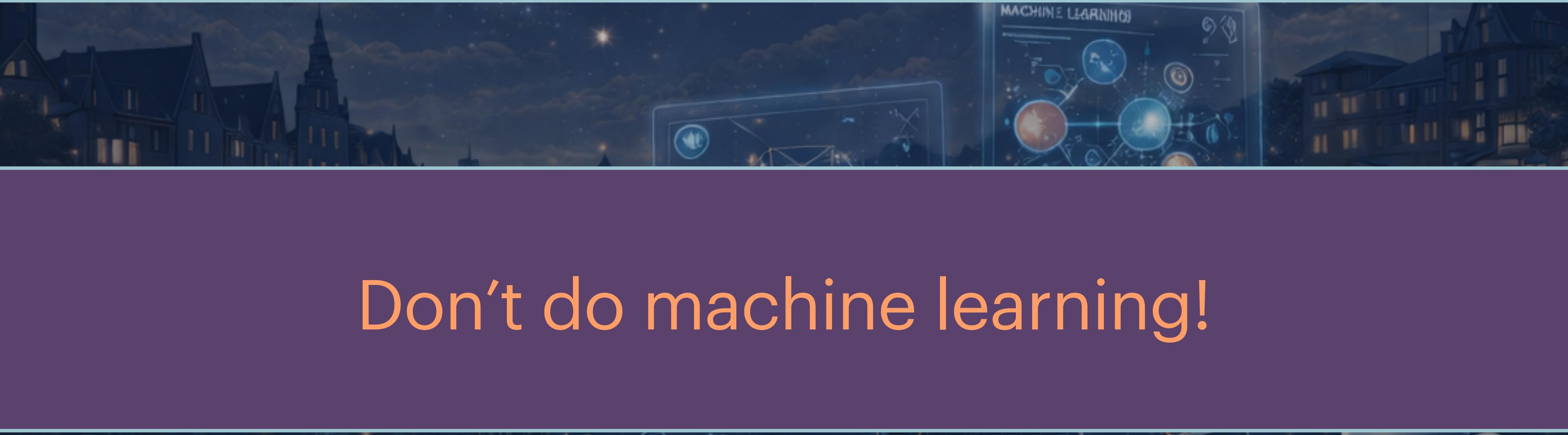
# Machine Learning in X-ray Spectral Timing

DANIELA HUPPENKOTHEN

[d.huppenkothen@uva.nl](mailto:d.huppenkothen@uva.nl)



The first thing I want you to know about machine learning is ...



Don't do machine learning!



Lorentz  
Center

# Types of Machine Learning

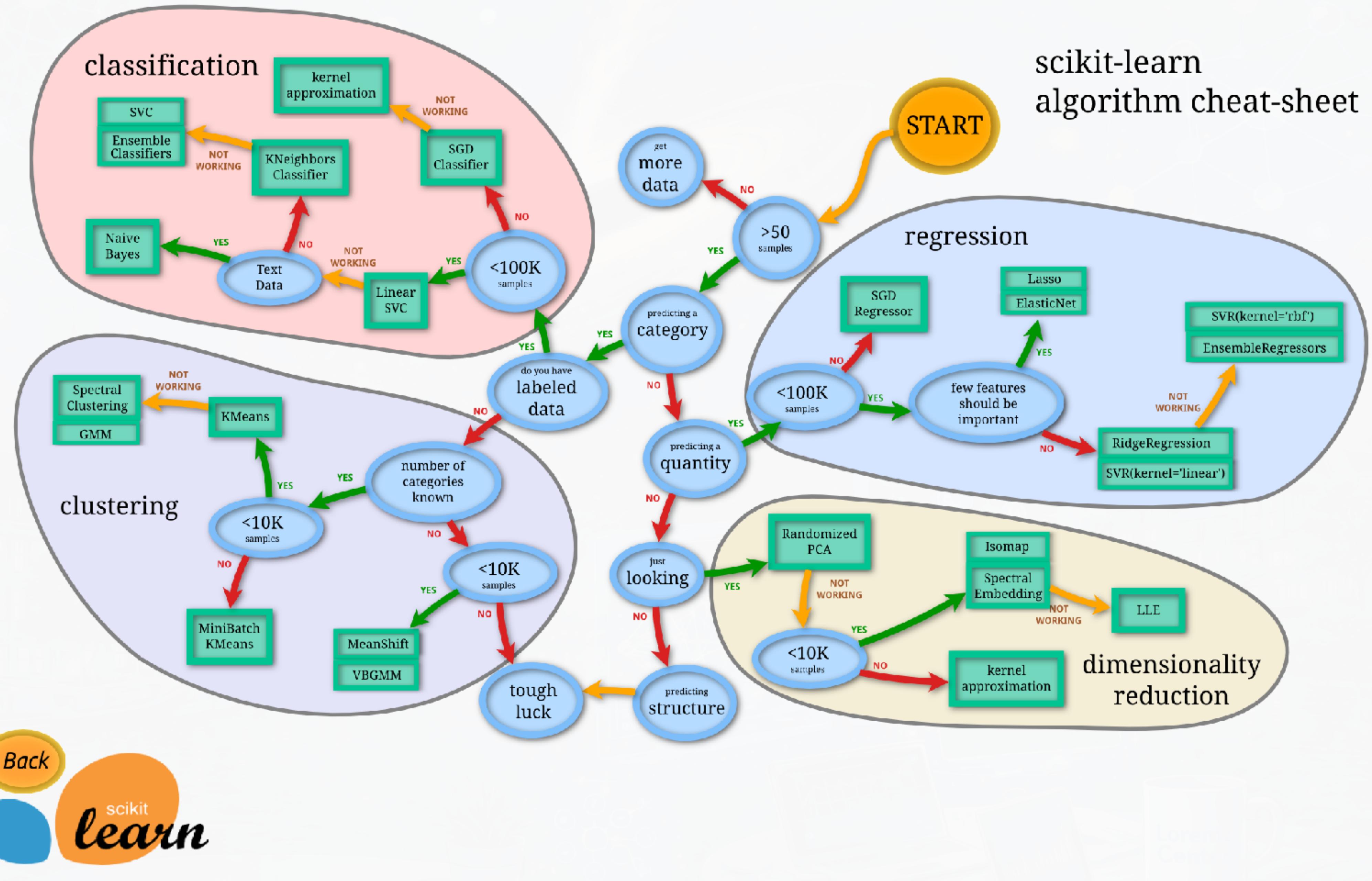
Supervised learning = learn explicit relationships between input data and known outputs (e.g. image labels, photometric redshifts, ...)

Unsupervised learning = infer labels from data (mainly clustering, some anomaly detection, dimensionality reduction, density estimation, ...)

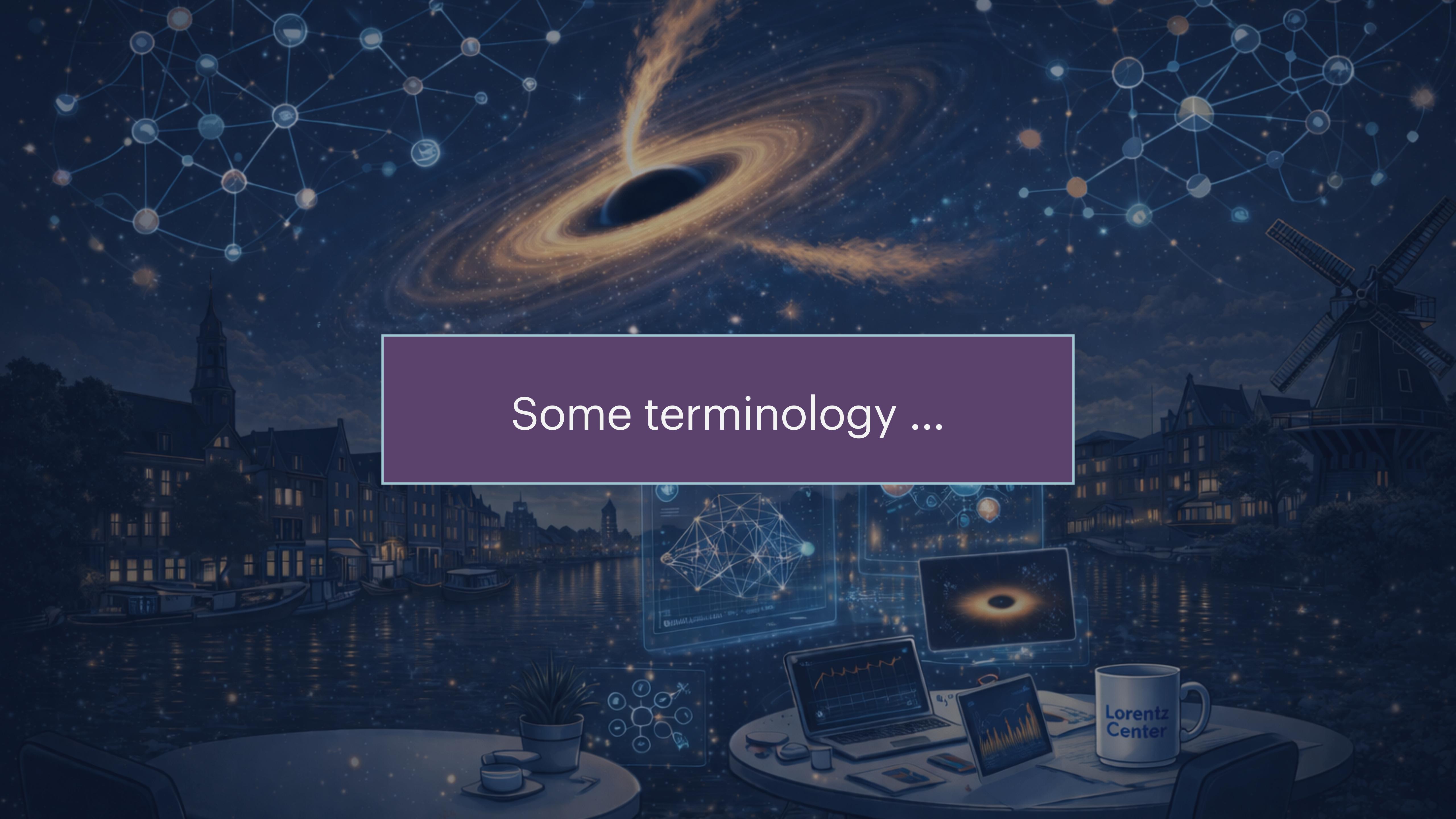
Semi-supervised learning = uses both labelled and unlabelled data simultaneously

Reinforcement learning = learning method that interacts with the environment by producing actions and discovering errors (trial, error, delay)

# scikit-learn algorithm cheat-sheet



Credit: Andreas Müller

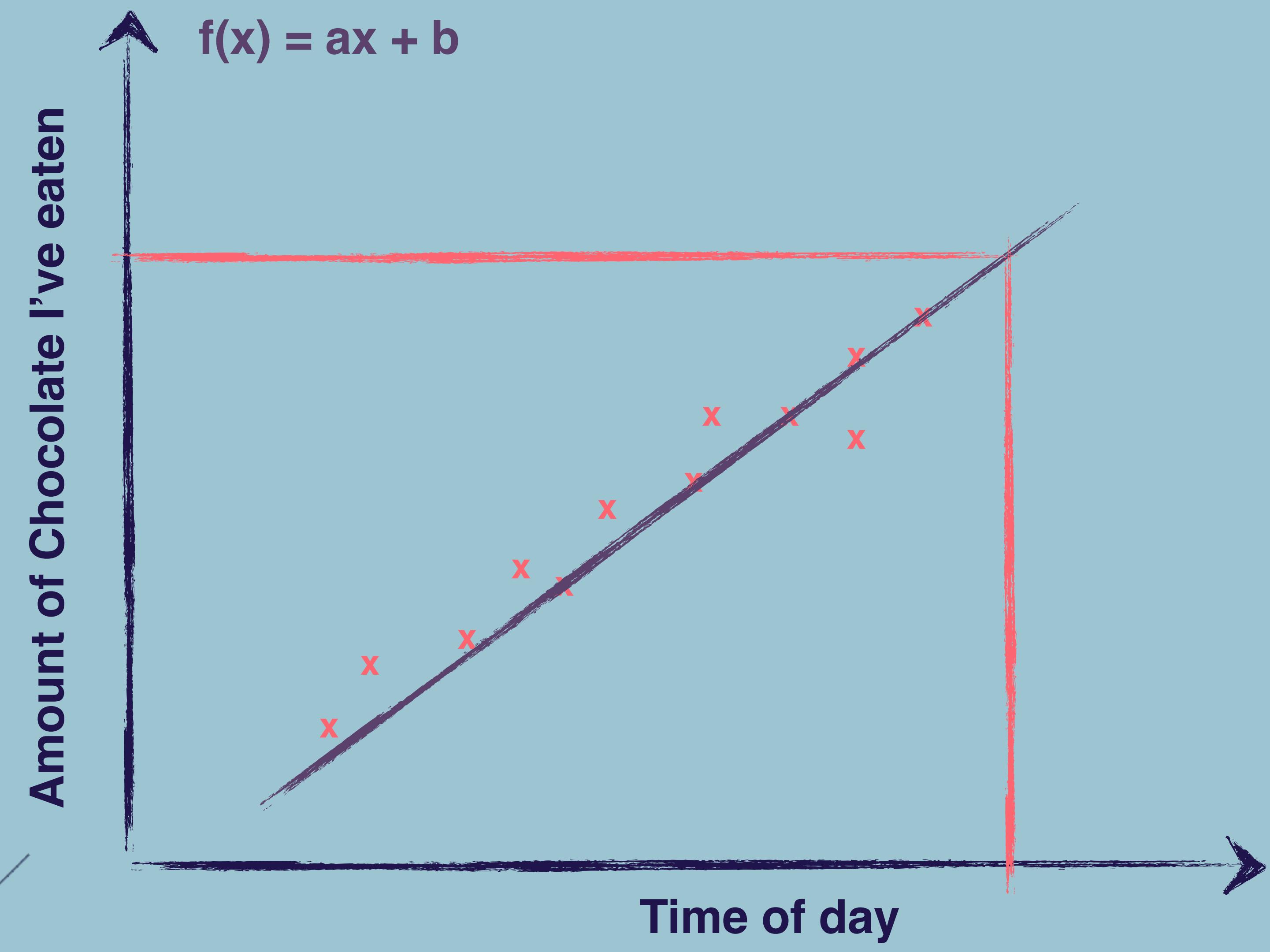
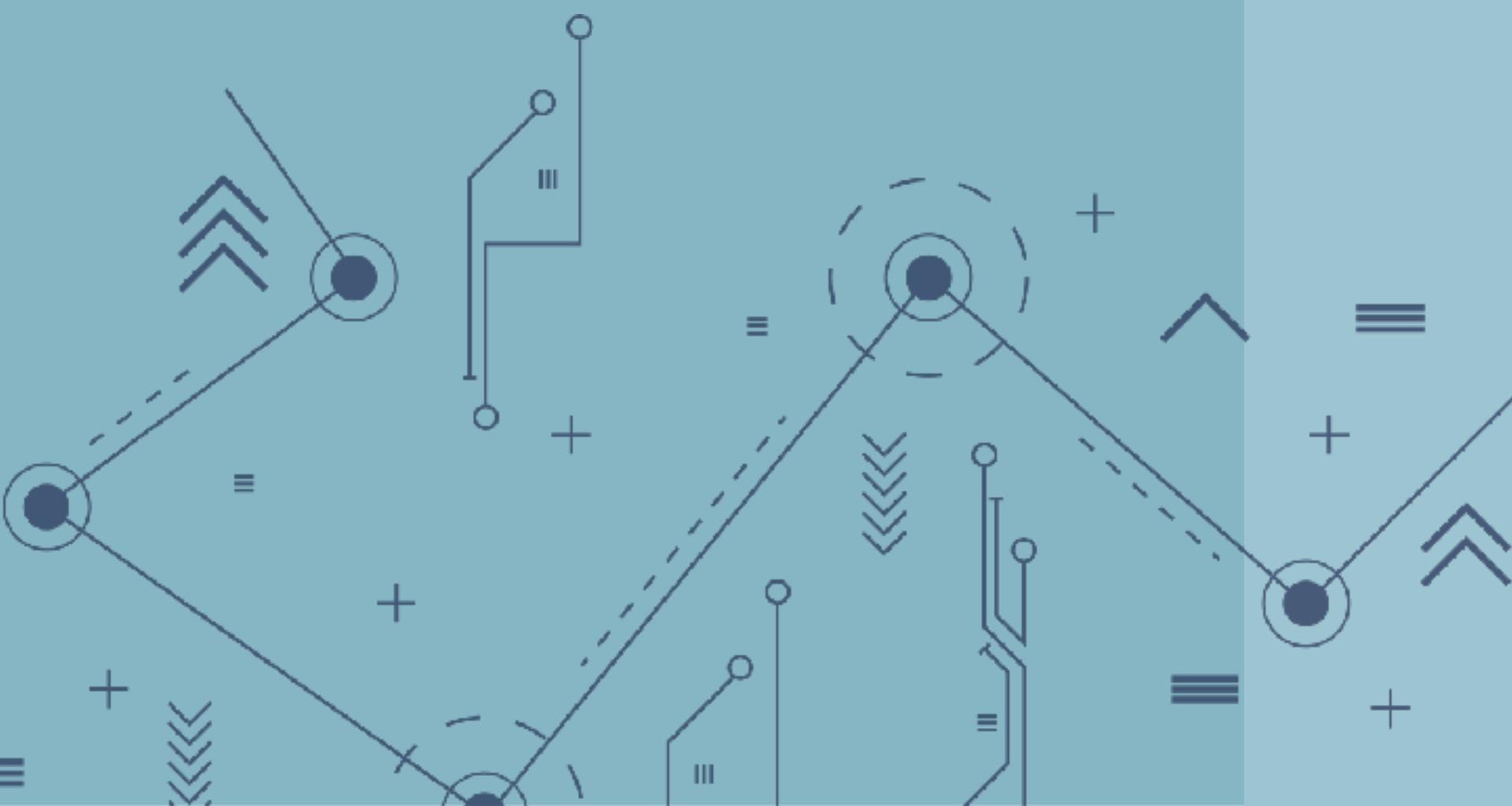


The background of the slide features a composite image. The upper portion shows a dark blue night sky filled with stars and a prominent yellow and orange spiral galaxy. The lower portion depicts a traditional Dutch town at night, with a church tower on the left and a windmill on the right. In the foreground, there's a desk setup with a laptop, a tablet, a smartphone, a mug labeled 'Lorentz Center', and a small potted plant. Several floating windows show scientific data: a network graph, a black hole simulation, a brain scan, a heart rate monitor, and a molecular structure.

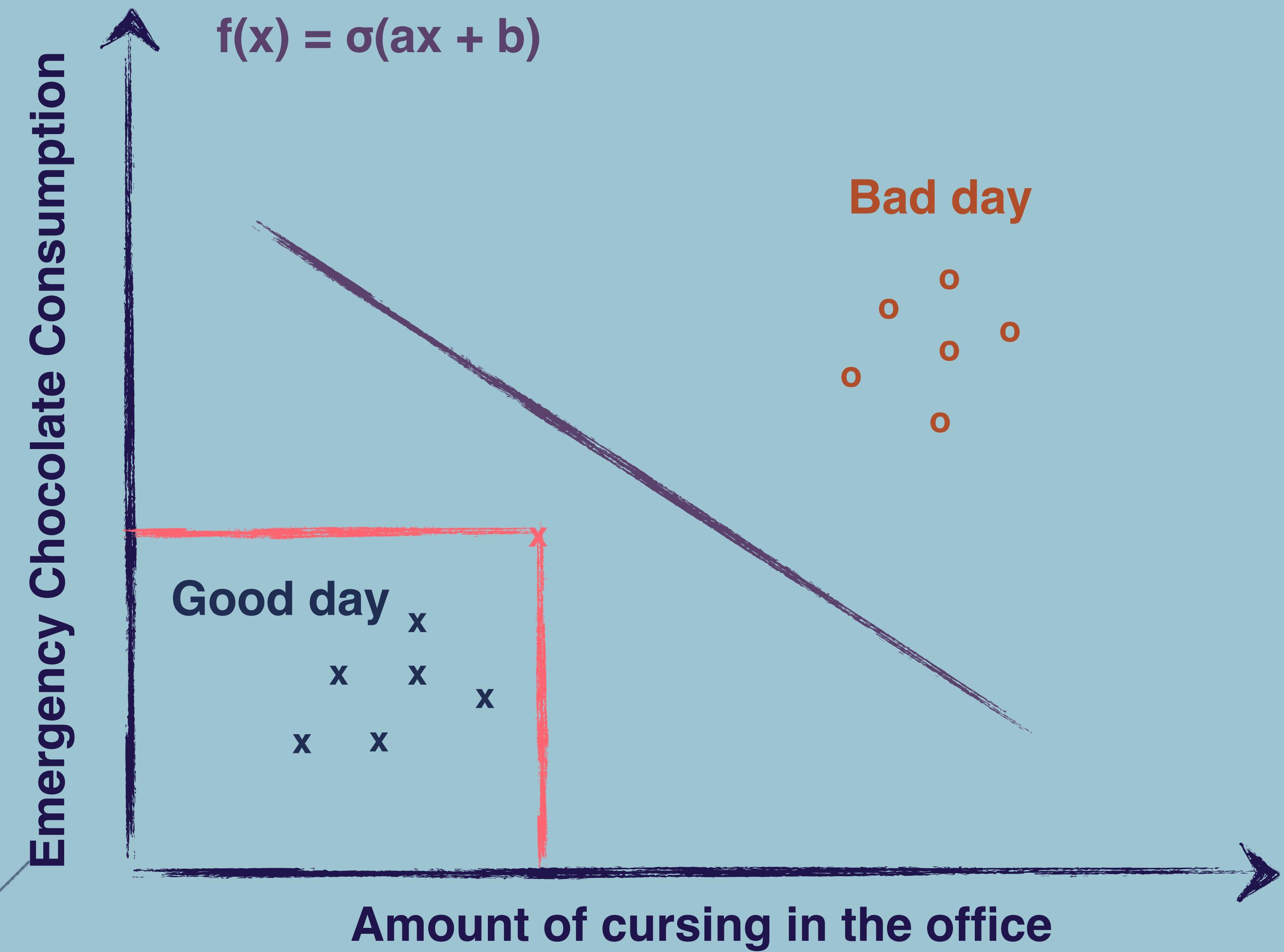
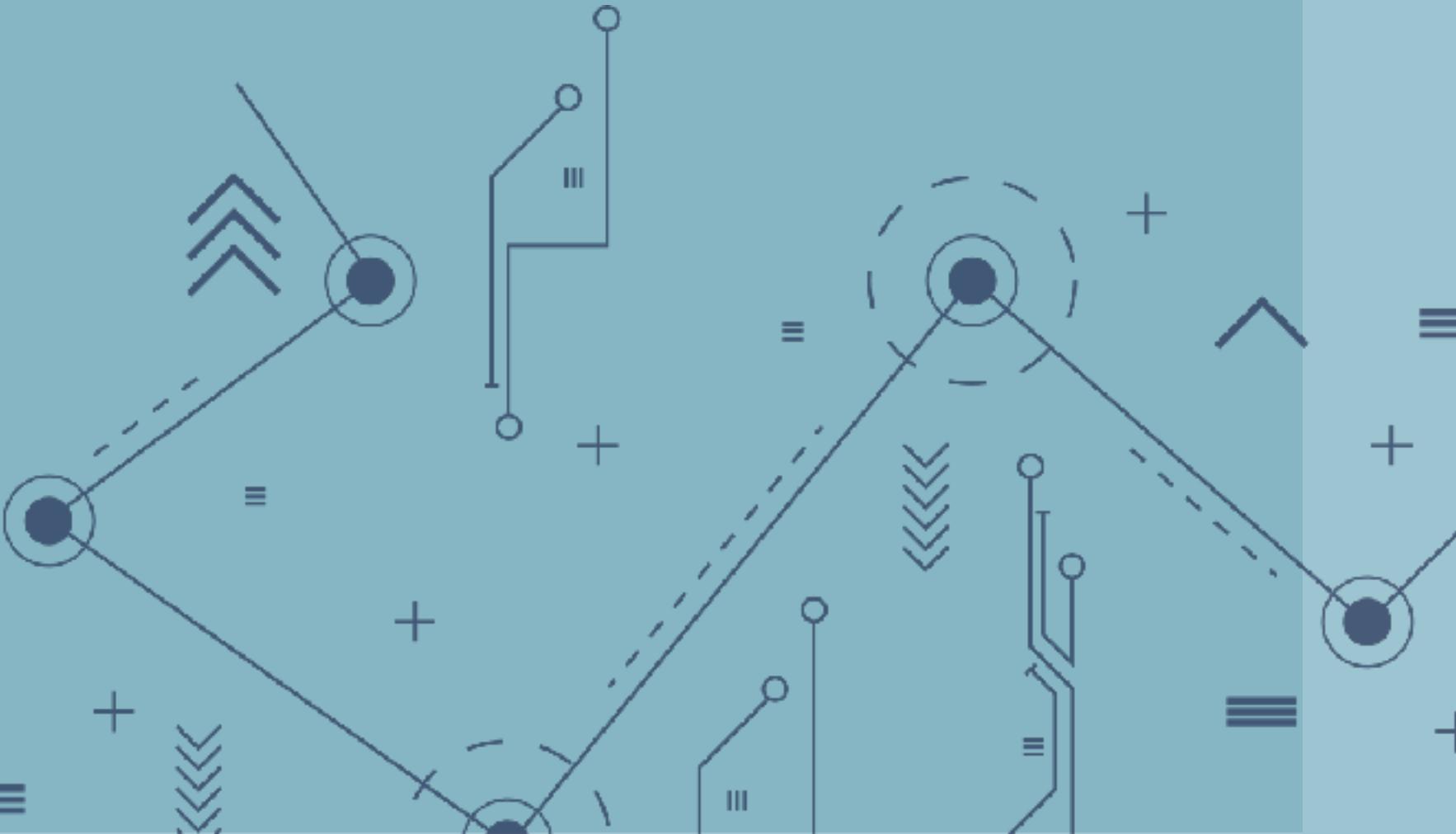
Some terminology ...

# Learning Patterns from Data:

## Regression

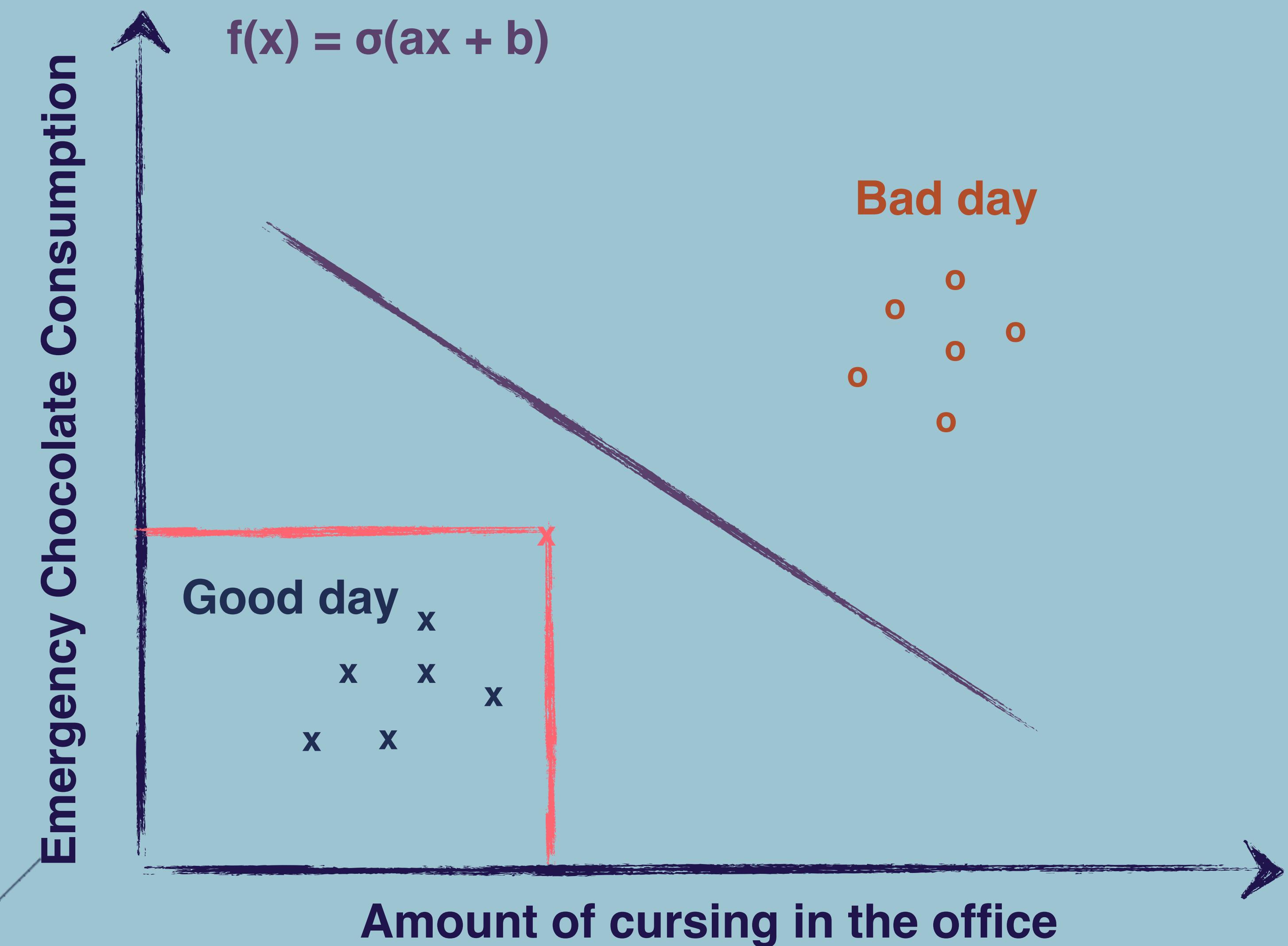
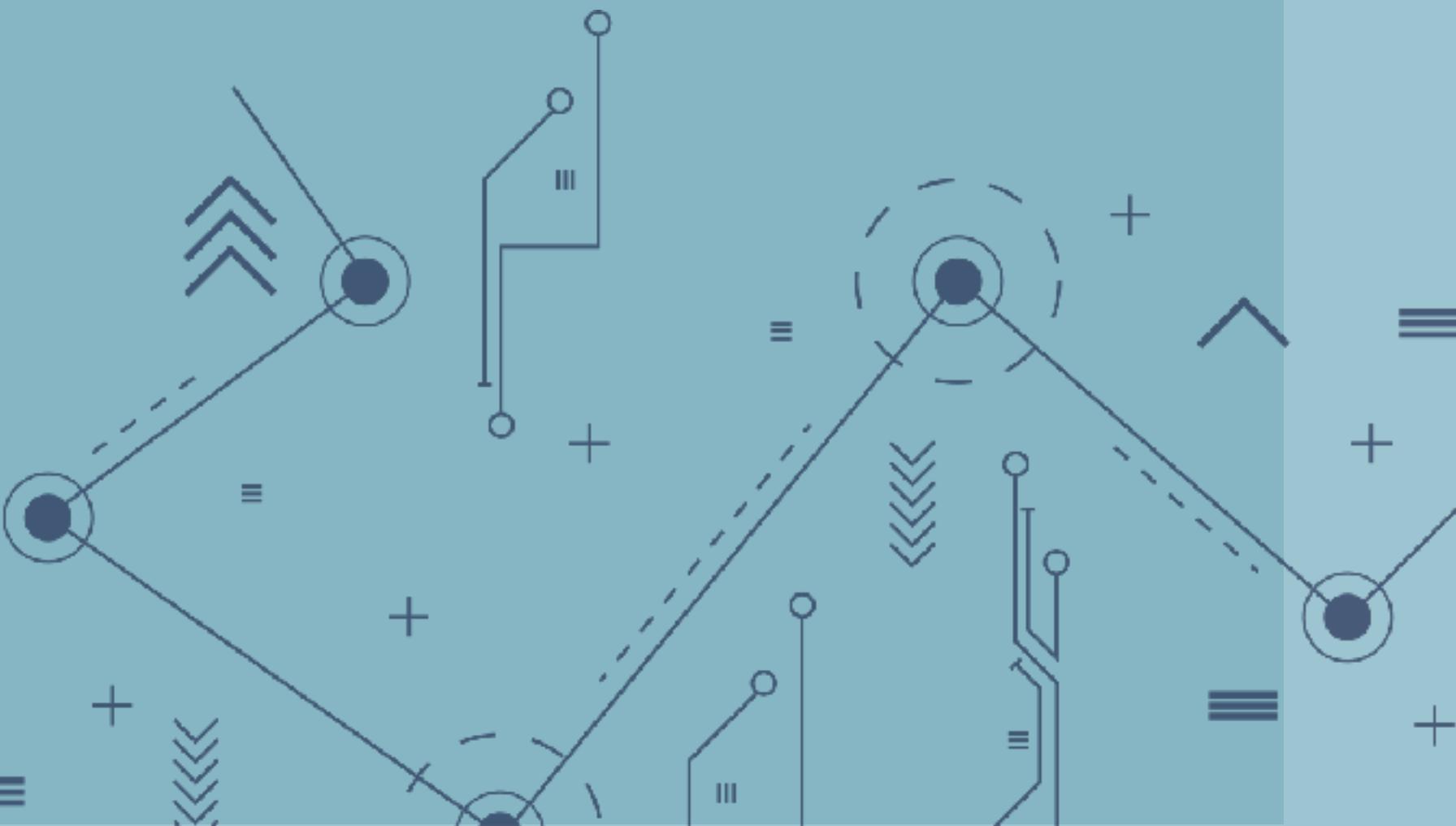


# Learning Patterns from Data: Classification

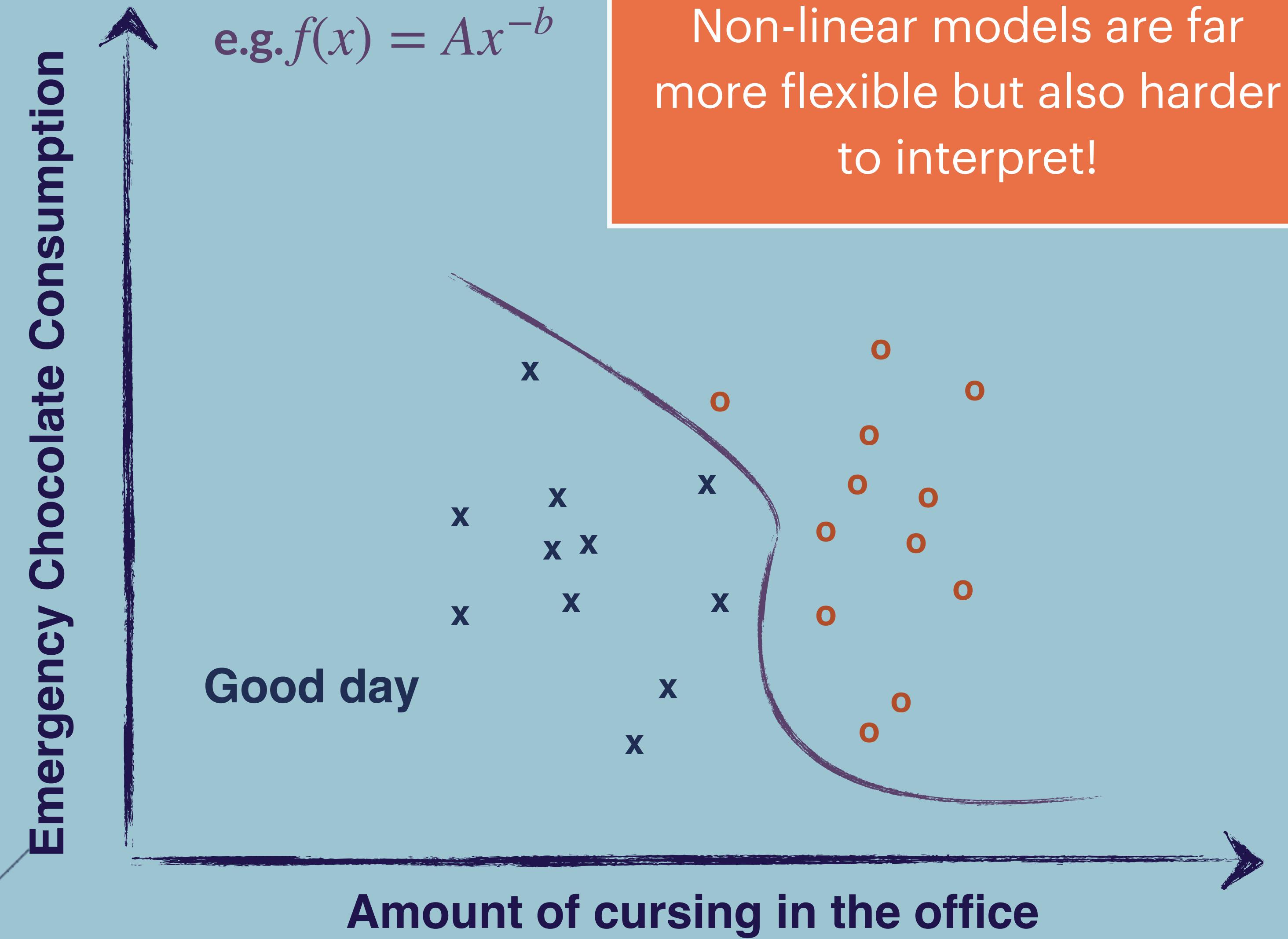
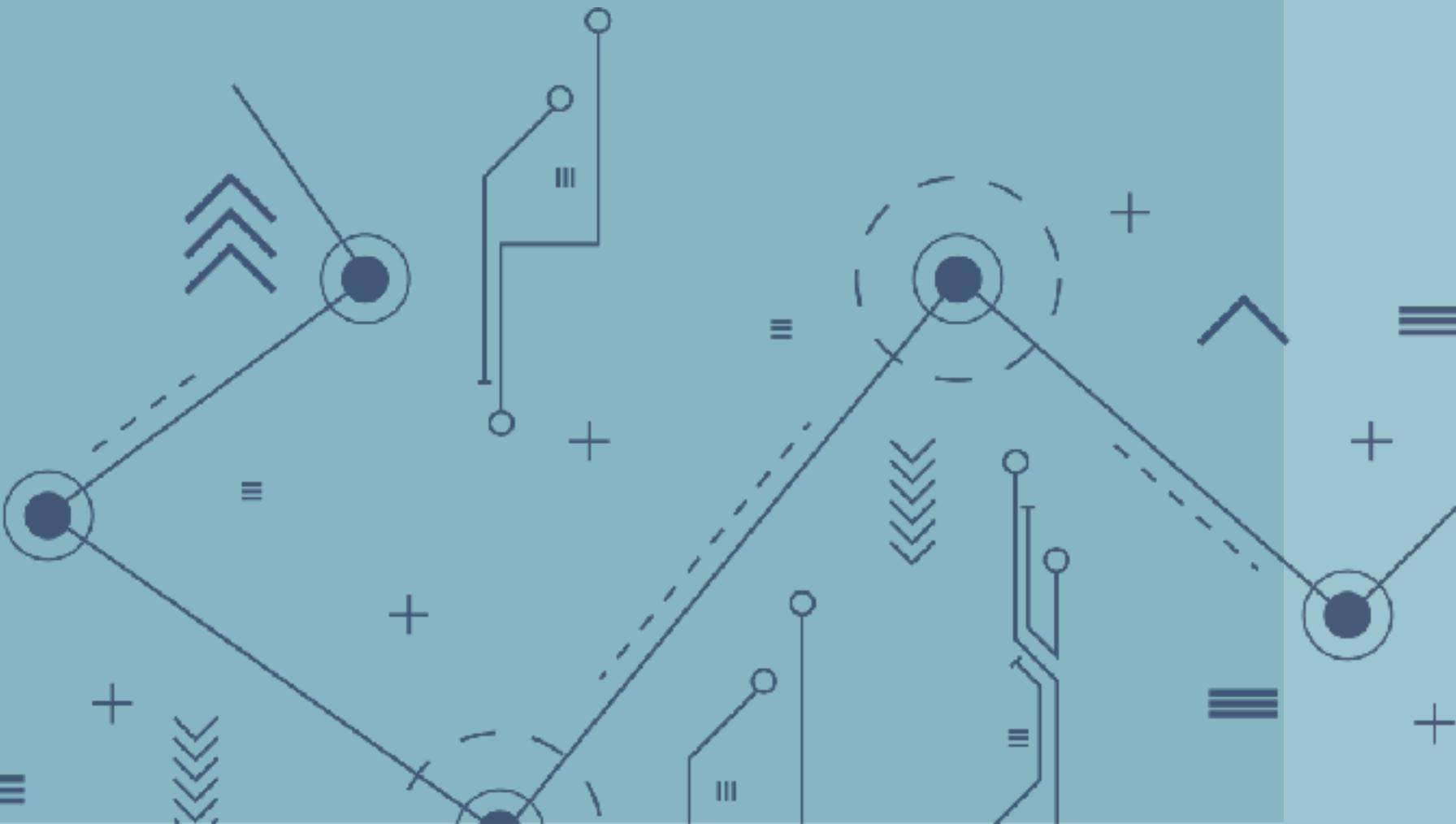


# Linear model:

A model that is linear in the parameters

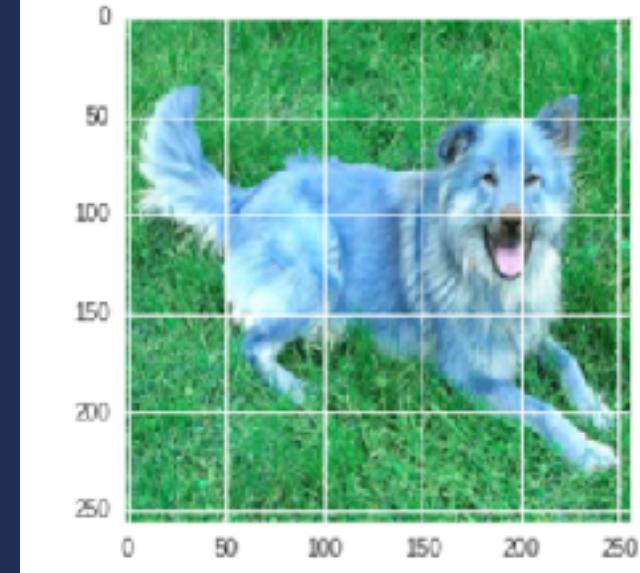


# Non-Linear models

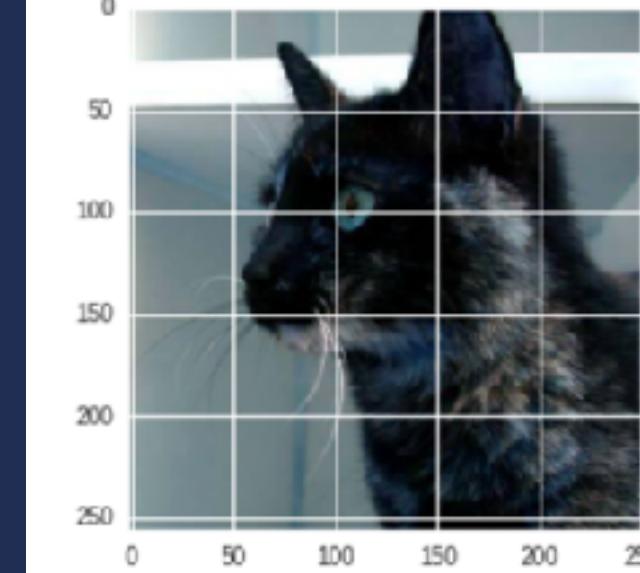


# The perceptron

I am 100.00% sure this is a Dog

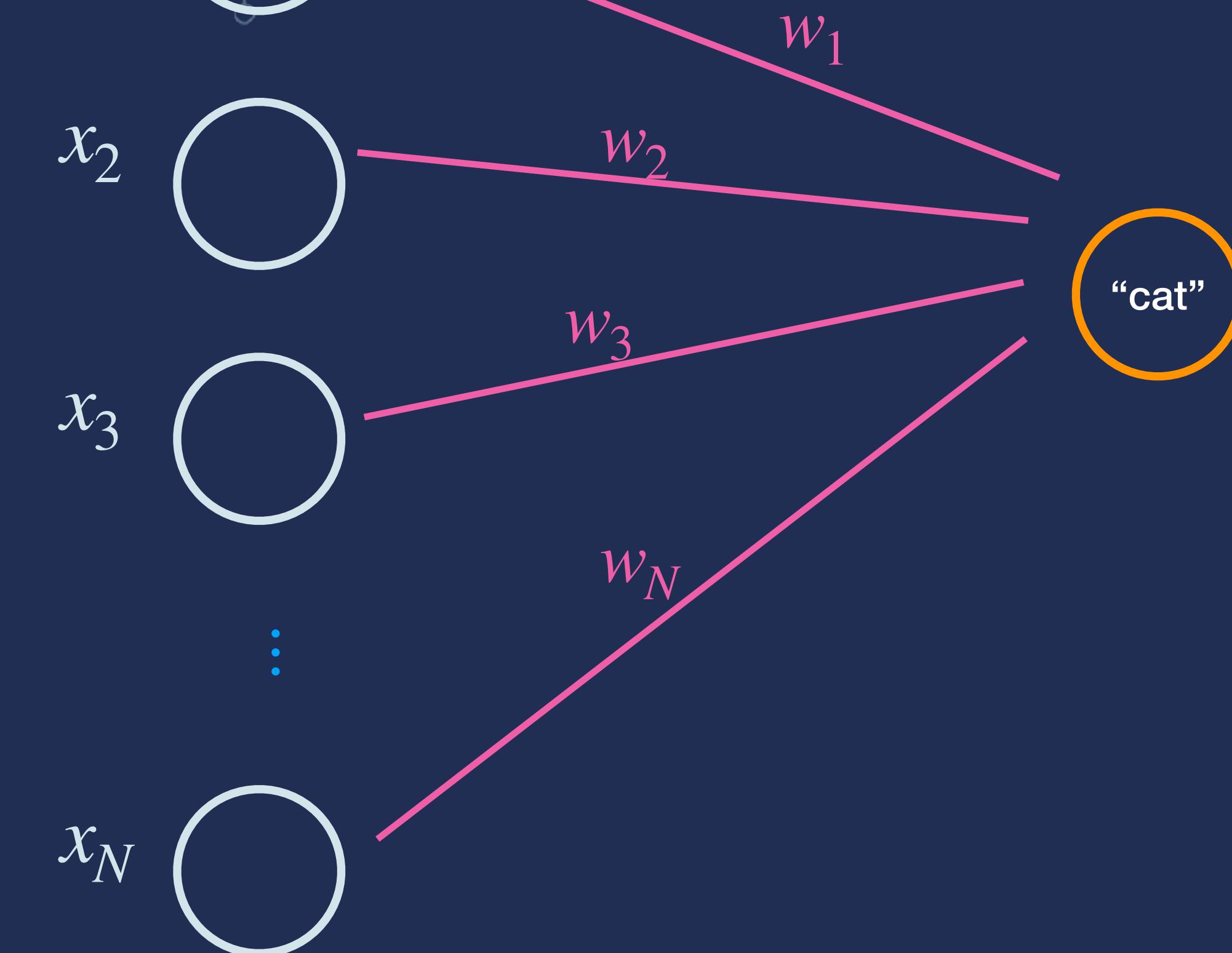


I am 99.27% sure this is a Cat



Input Layer

Output Layer



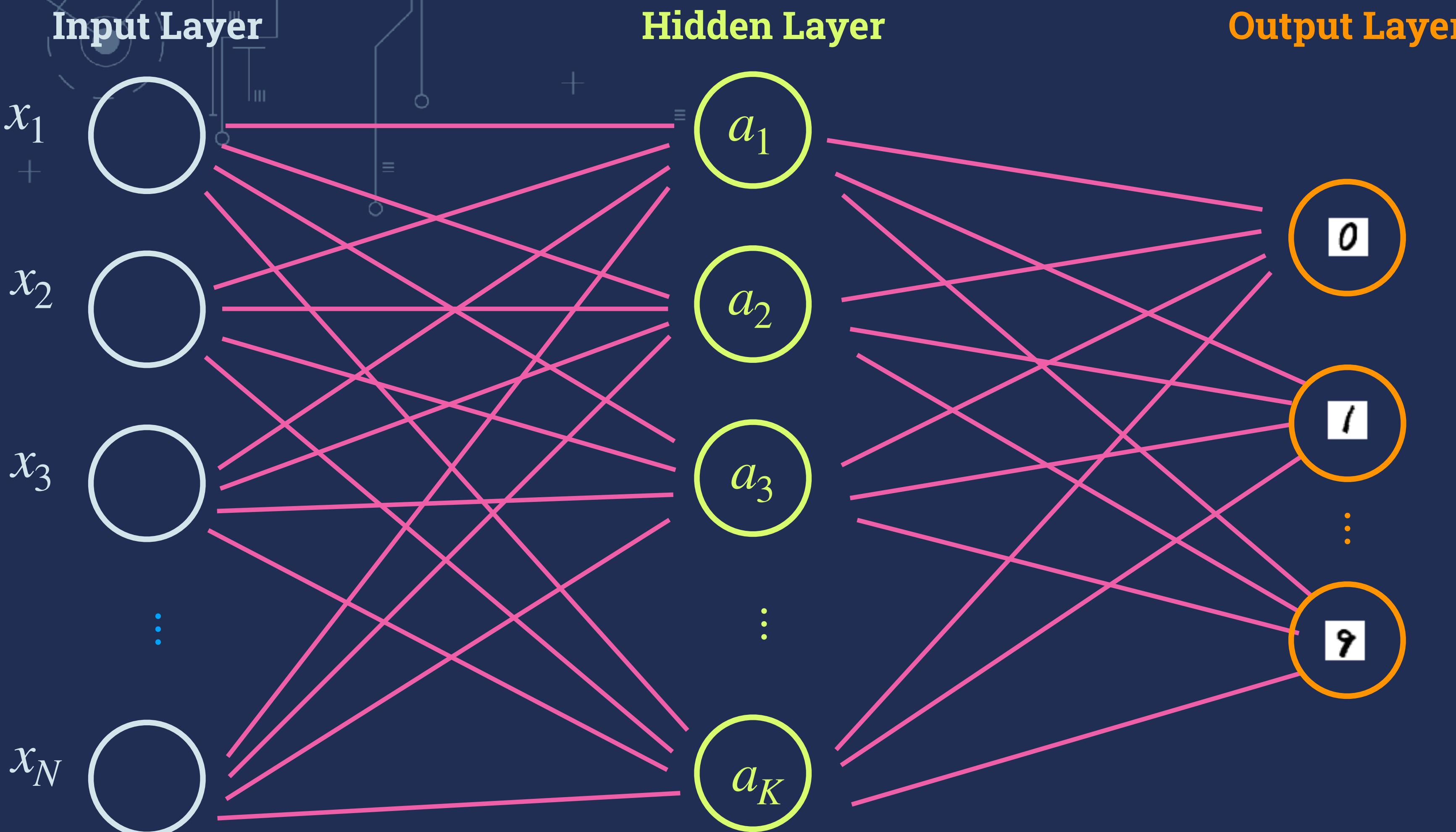
$$y = \sigma \left( \sum_k w_k x_k + b \right)$$

"weights"      "biases"

$\sigma(z) = \text{Activation function}$

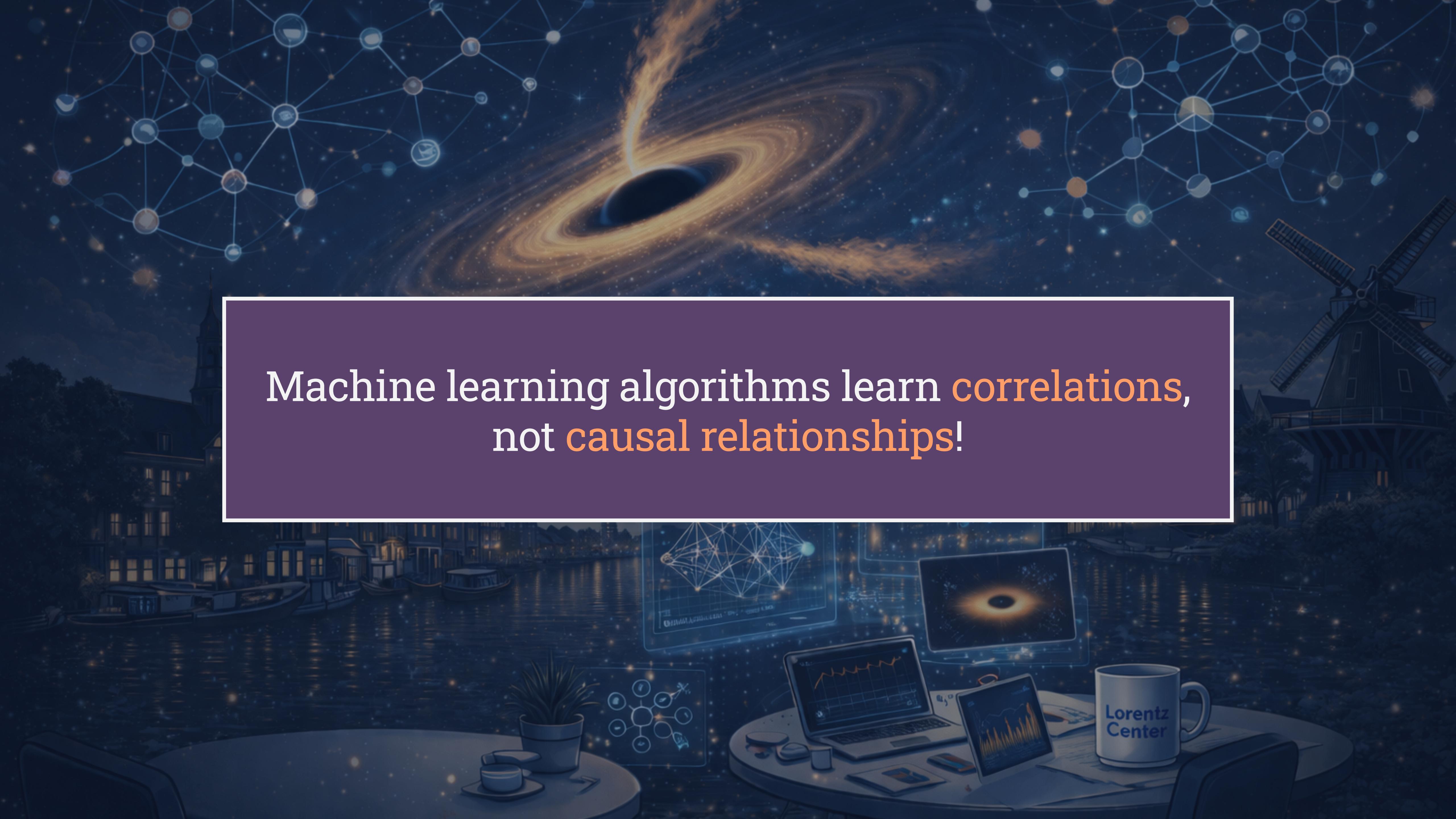
$$\text{Example: } \sigma(z) = \frac{1}{1 + e^{-z}}$$

# Building a Feed-Forward Neural Network



$$a_k = \sigma \left( \sum_j w_{kj}^1 x_j + b_k \right)$$

$$y_l = \sigma \left( \sum_k w_{lk}^2 x_k + b_l \right)$$



Machine learning algorithms learn correlations,  
not causal relationships!

Lorentz  
Center

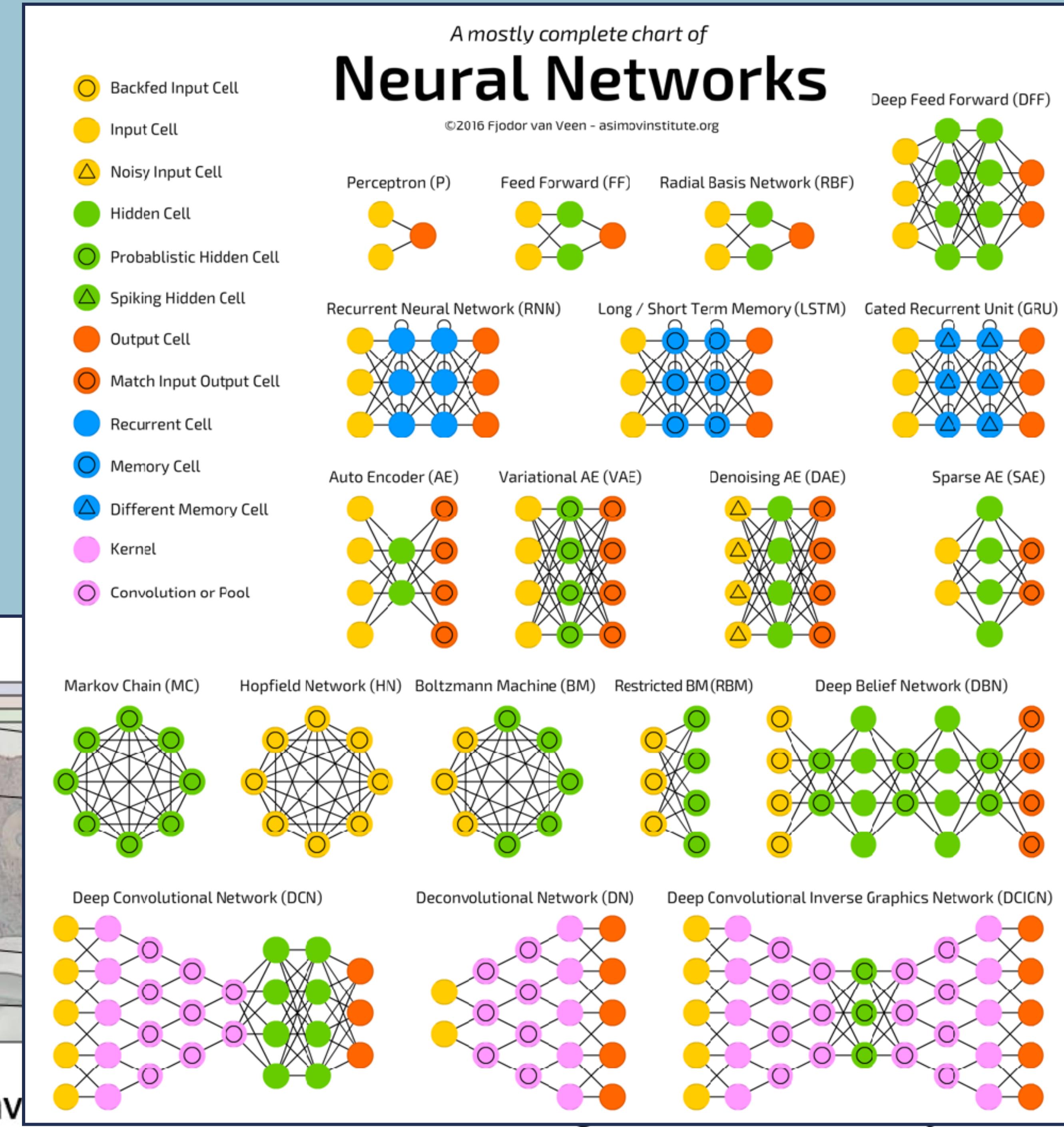
# Clever Additions Make Neural Networks Work Efficiently



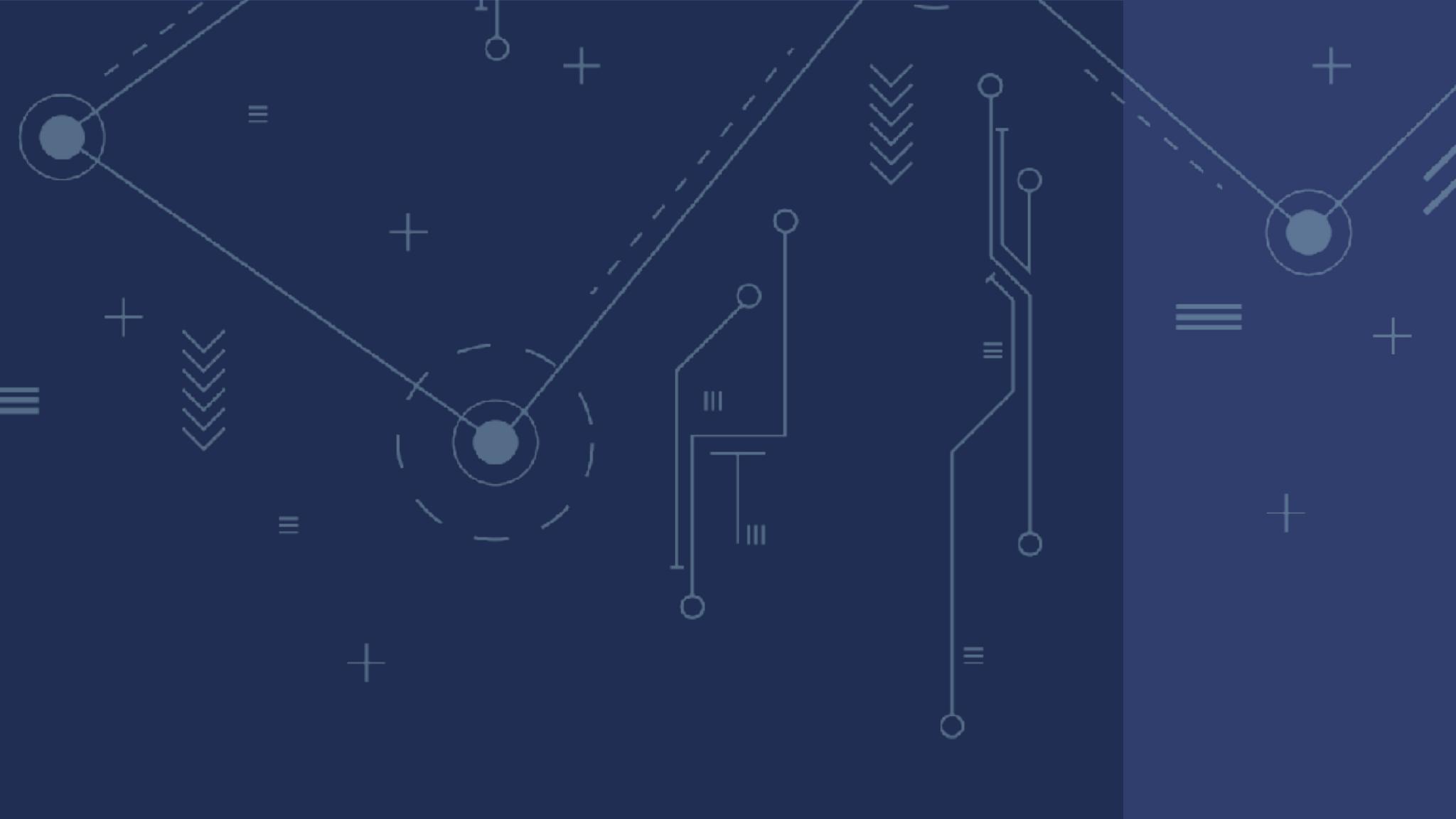
Input image



Conv



ected



## When to be cautious about machine learning

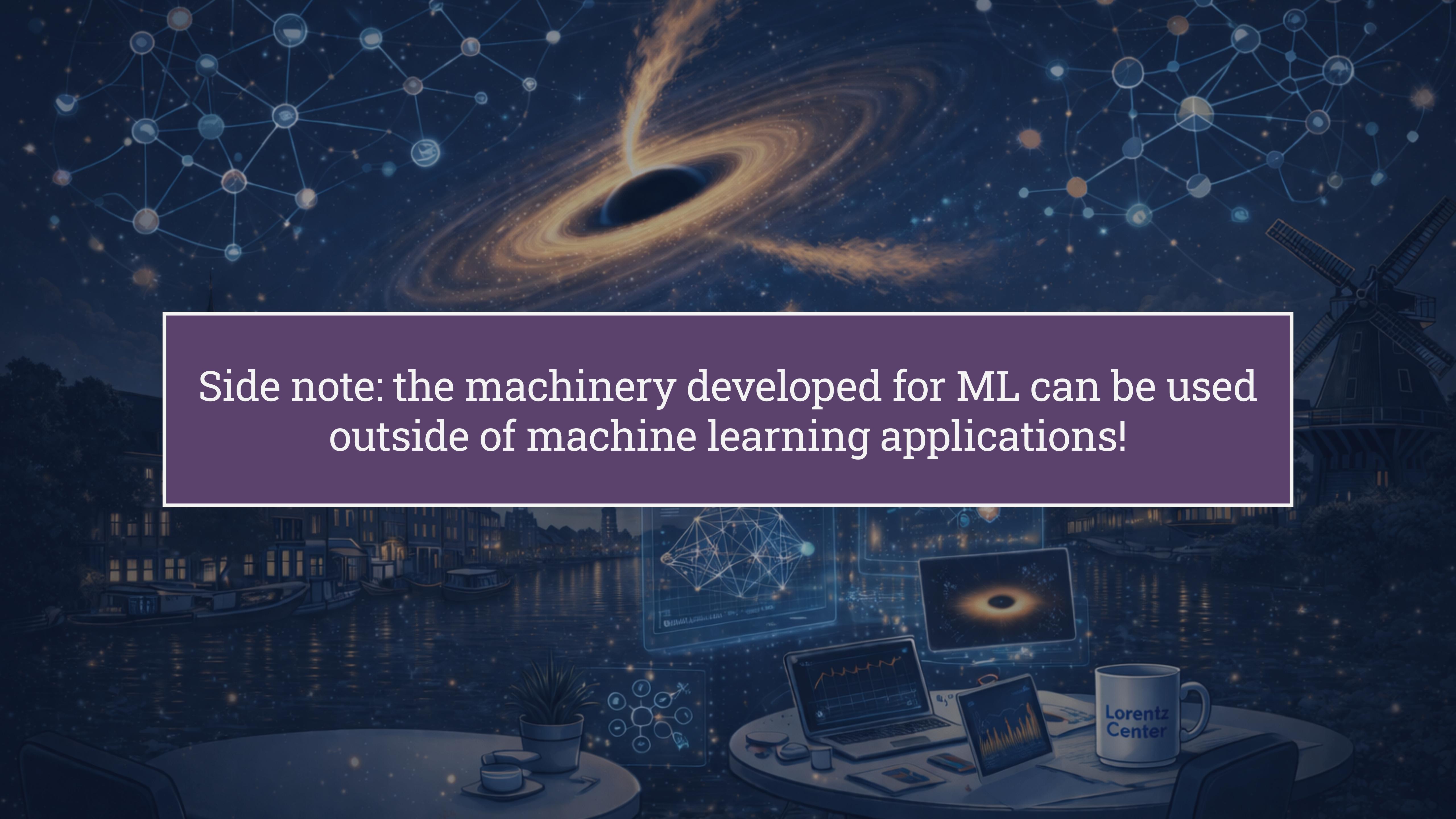
1. Are there ethical implications for using machine learning on your problem?
2. Is your problem really a statistics problem?
3. Do you have enough training data? Does your training data look like your target data?
4. Would (unrecognised) biases in your ML model significantly affect downstream analyses?



# I (Still) Can't Believe It's Not Better! Workshop

ICBINB@NeurIPS 2021 - A Workshop for "beautiful" ideas that \*should\* have worked

Lorentz  
Center



Side note: the machinery developed for ML can be used outside of machine learning applications!



= “differentiable NumPy that  
runs on accelerators”

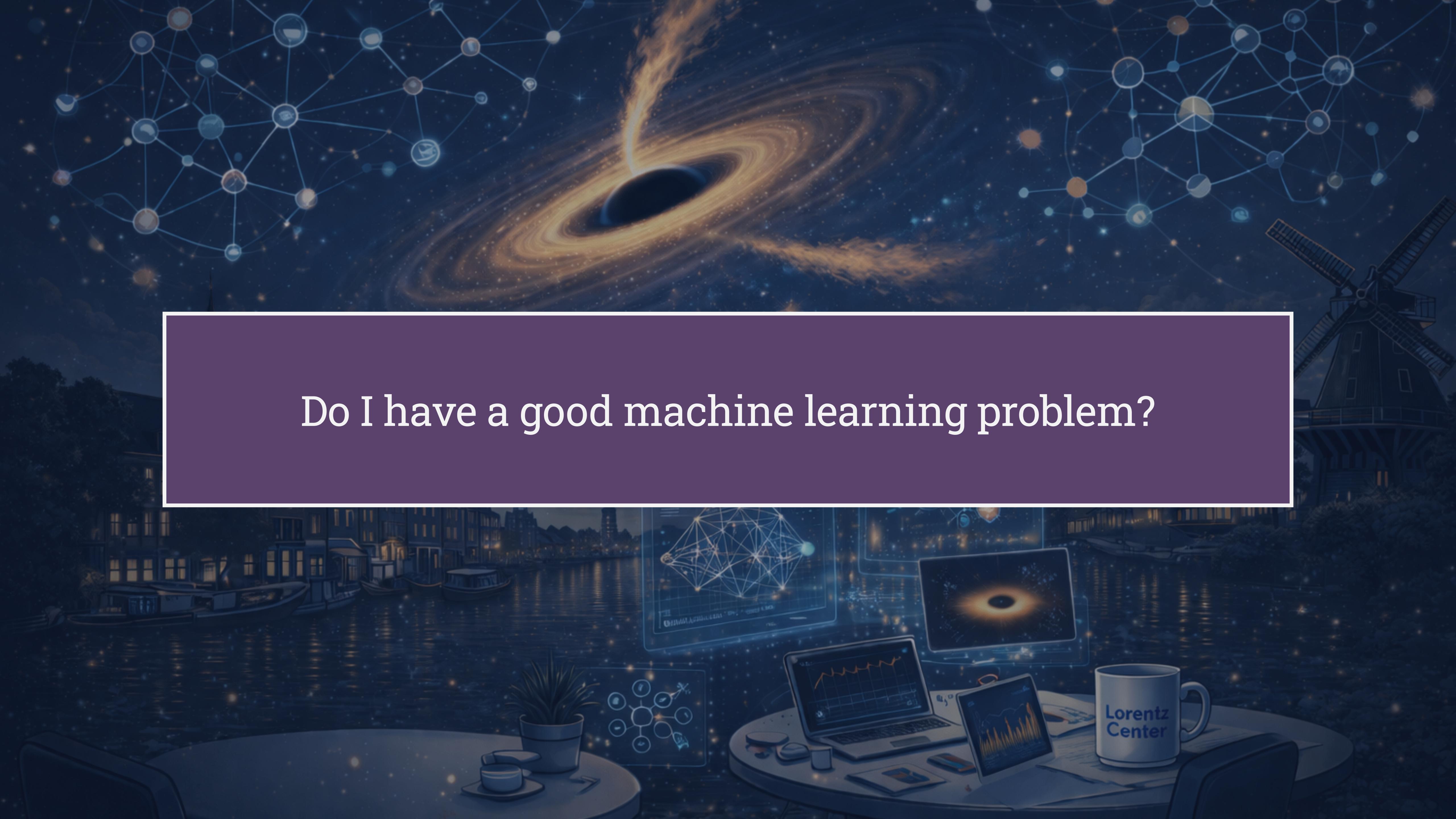


= optimizing compiler for  
machine learning



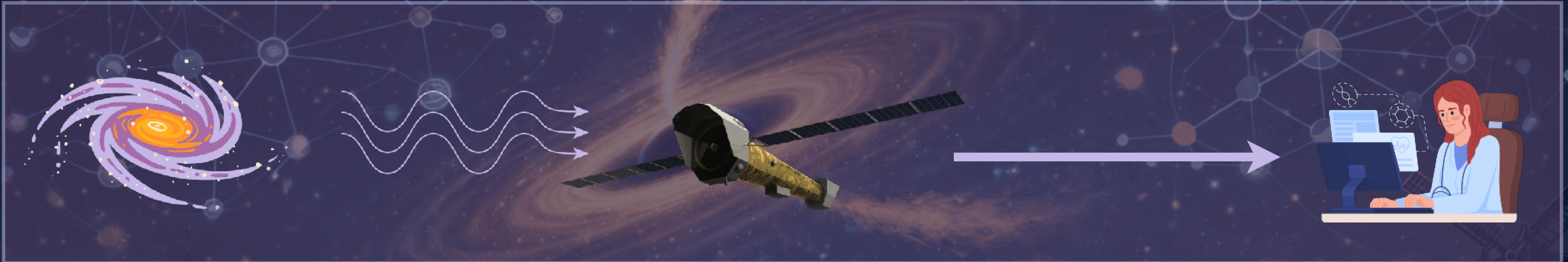
## Other cool things:

- just-in-time compilation with XLA
- Automatic parallelisation
- Distributed arrays

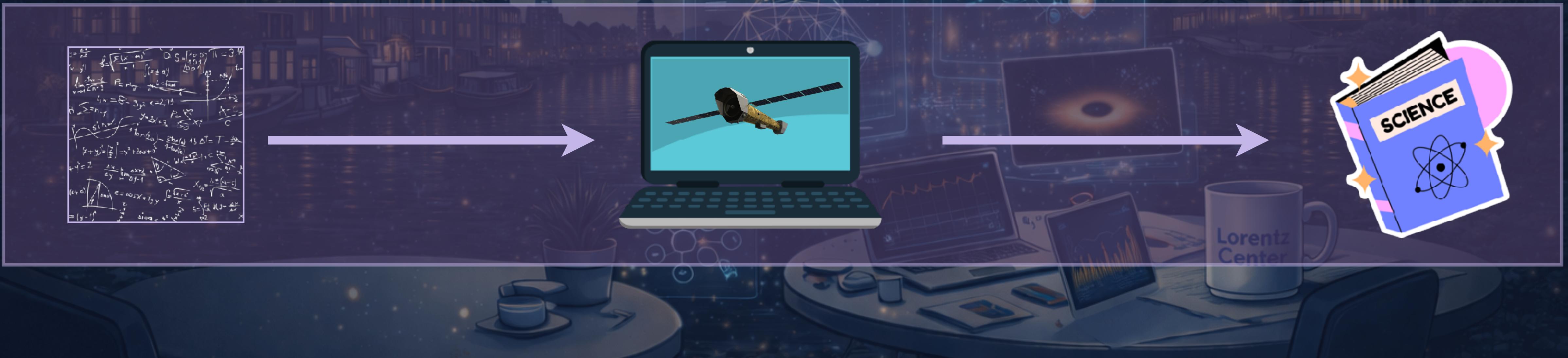


Do I have a good machine learning problem?

Lorentz  
Center



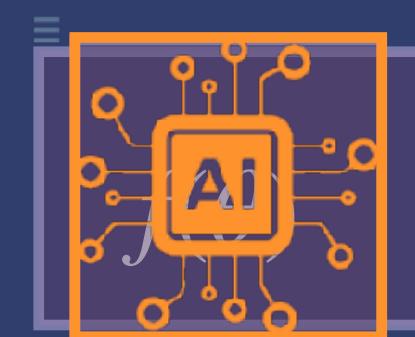
$$p(\theta | D) = \frac{p(D | \theta)p(\theta)}{p(D)}$$



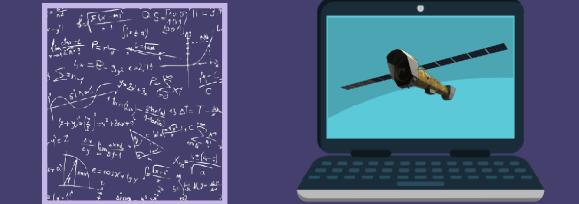


Might be expensive  
to compute!

$$p(\theta | D) = \frac{p(D | f(\theta))p(\theta)}{p(D)}$$



= a physics model with parameters  $\theta$



$D$  = the data

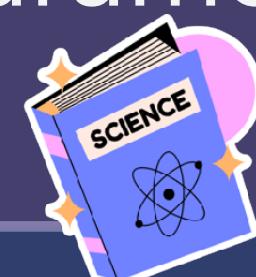


$p(D | f(\theta))$  = how to generate data from a known set of parameters using physics model  $f(\theta)$

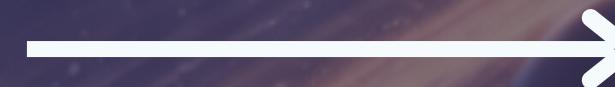
$p(\theta)$  = everything we know about the parameters **before** we look at the data

## Inference

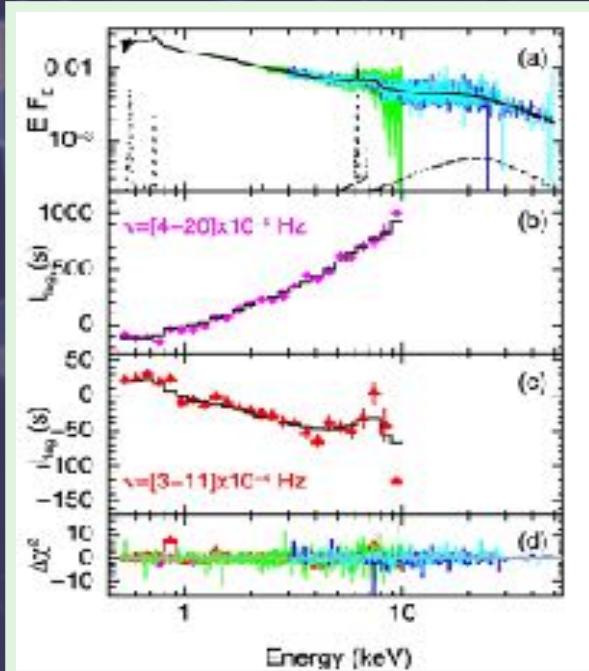
$p(\theta | D)$  = the probability of the parameters **after** we've looked at the data



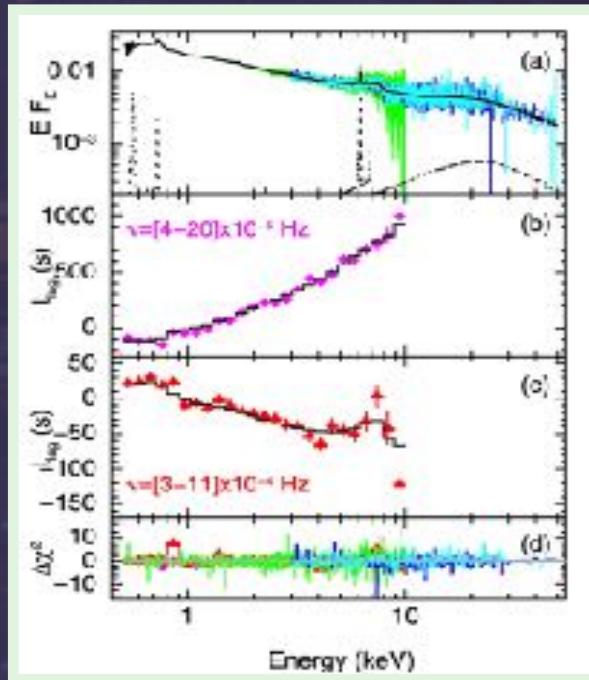
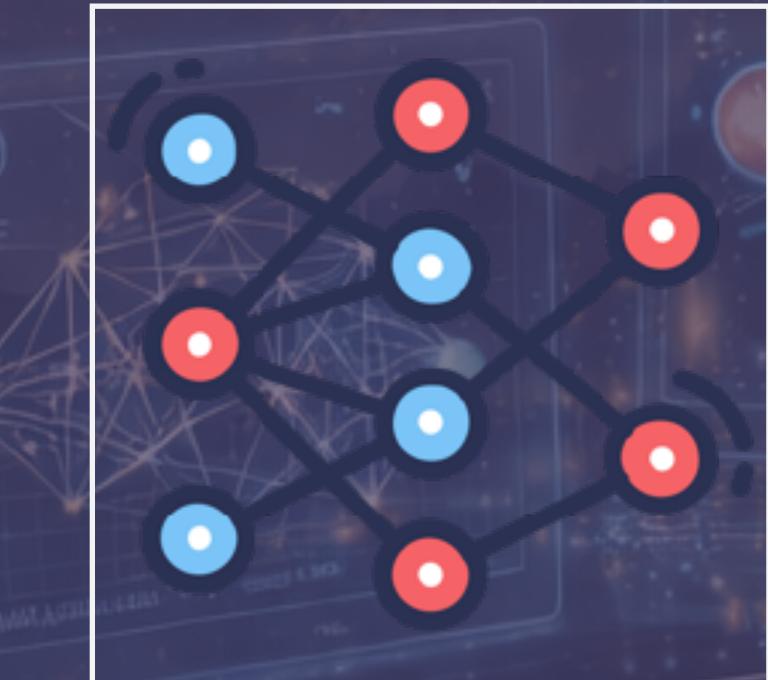
black hole +  
accretion flow  
parameters

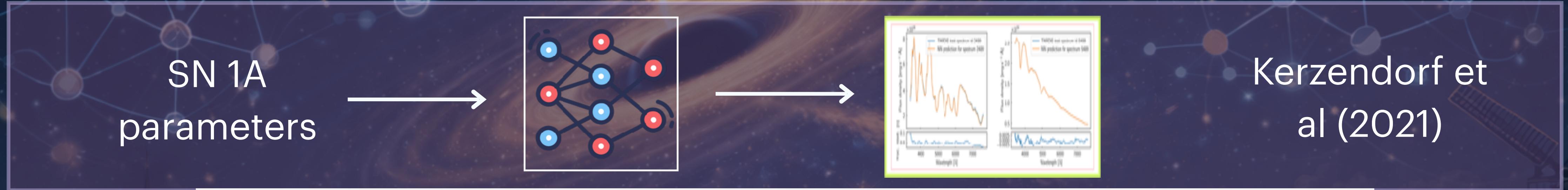


The diagram contains several mathematical equations and diagrams. At the top, there's a diagram of a black hole with an accretion disk. Below it are several equations, including:  
$$P = \frac{2\pi}{\omega}$$
  
$$\delta = \sqrt{\sum (x_i - \bar{x})^2}$$
  
$$Q = S = \int_{10}^{100} \int_{10}^{100} \dots$$
  
$$R = \frac{P}{\omega}$$
  
$$e = \sqrt{1 - \frac{v^2}{c^2}}$$
  
$$y = \frac{r}{a}$$
  
$$x = \frac{r}{a}$$
  
$$t = \frac{P}{2\pi}$$
  
$$\Delta t = T - \frac{P}{2\pi}$$
  
$$(x+y)^2 = \left(\frac{y}{z}\right)^2 = x^2 + 2ax + a^2$$
  
$$x = \frac{a(1-e^2)}{1-e}$$
  
$$y = \frac{a(1-e^2)}{e}$$
  
$$z = \sqrt{1 - \frac{2a}{r}}$$
  
$$e = \cos x, z = \sin x$$



black hole +  
accretion flow  
parameters





black  
hole  
mass

One of the few problems in astronomy where  
we have **reliable training data!**

de Gucht  
(2022)

This section contains a large text box with the message 'One of the few problems in astronomy where we have **reliable training data!**'. To the left is a small image of a black hole, and to the right is a reference to 'de Gucht (2022)'.





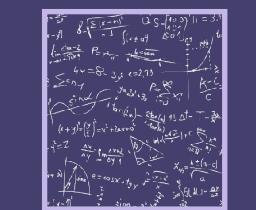
Might not be analytically tractable



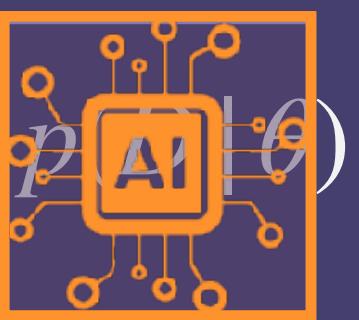
## Inference

$$p(\theta | D) = \frac{p(D | \theta)p(\theta)}{p(D)}$$

$f(\theta)$  = a physics model with parameters  $\theta$



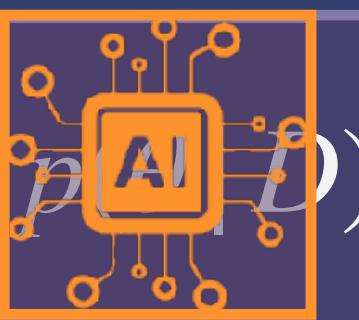
$D$  = the data



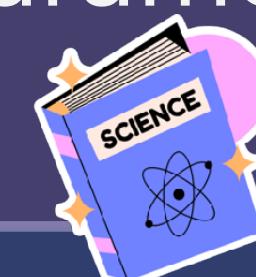
= how to generate data from a known set of parameters

$p(\theta)$

= everything we know about the parameters **before** we look at the data



= the probability of the parameters **after** we've looked at the data



# Why Simulation-Based Inference?

You have a stochastic numerical model

You have instrumental biases or selection effects you can simulate but not parametrize

Fast inference with Normalising Flows



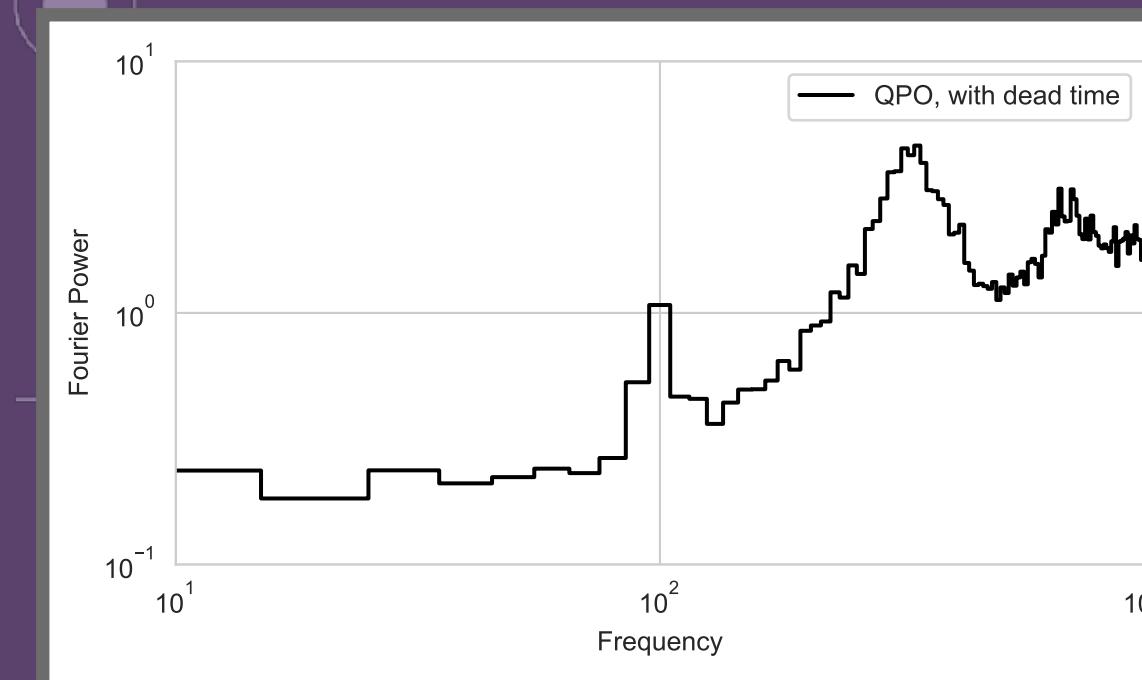
Step 1: draw parameters from prior

Step 2: simulate data sets

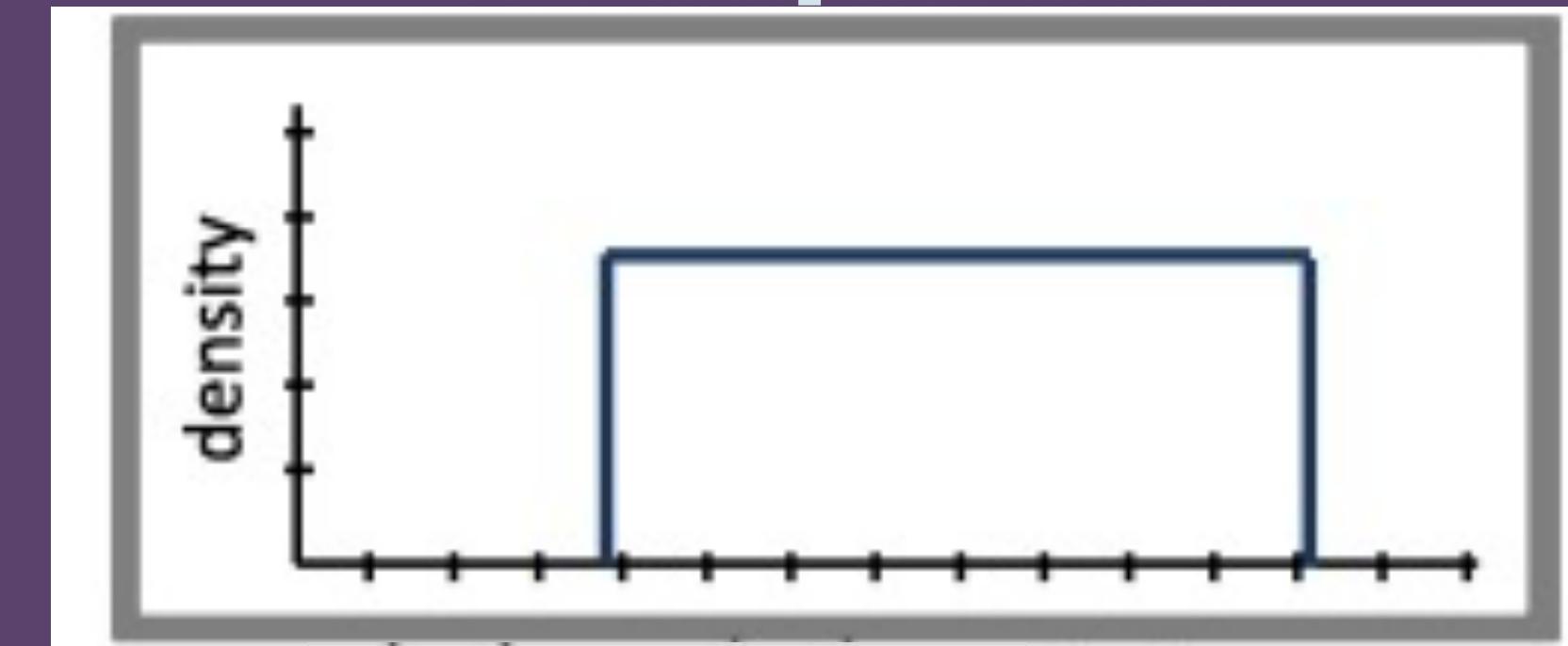
Step 3: compare simulated to observed data

Step 4: keep parameters that produce simulations similar to the data

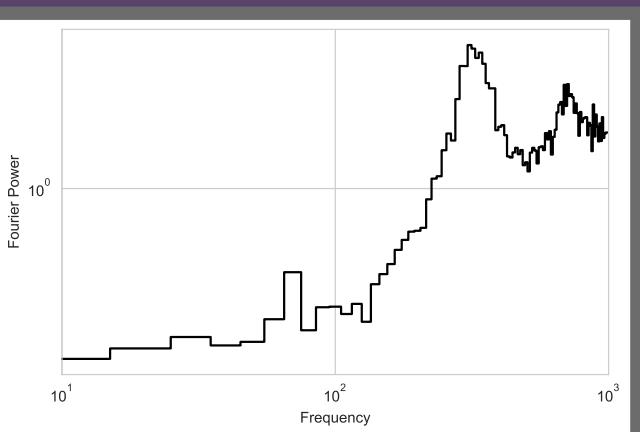
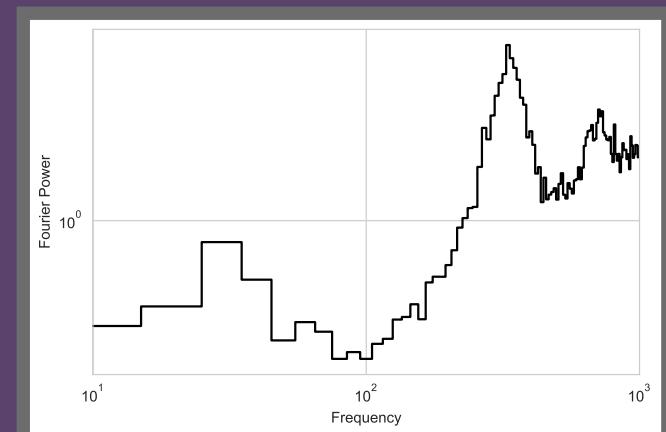
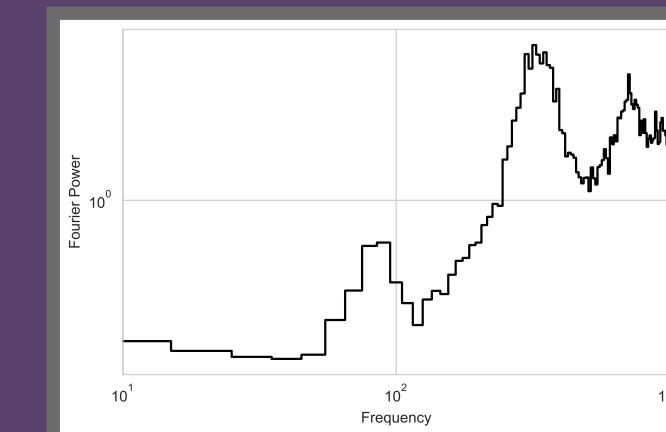
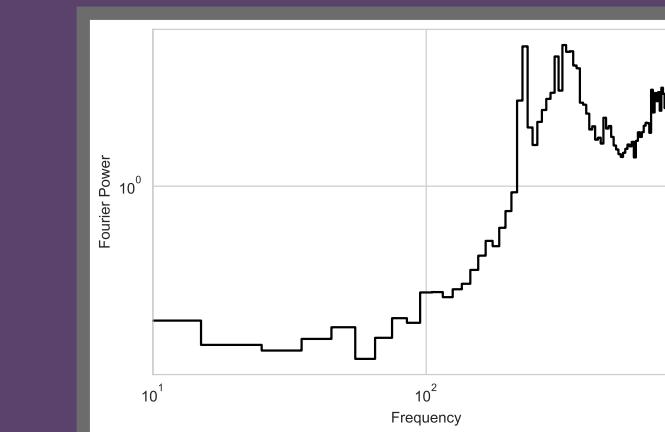
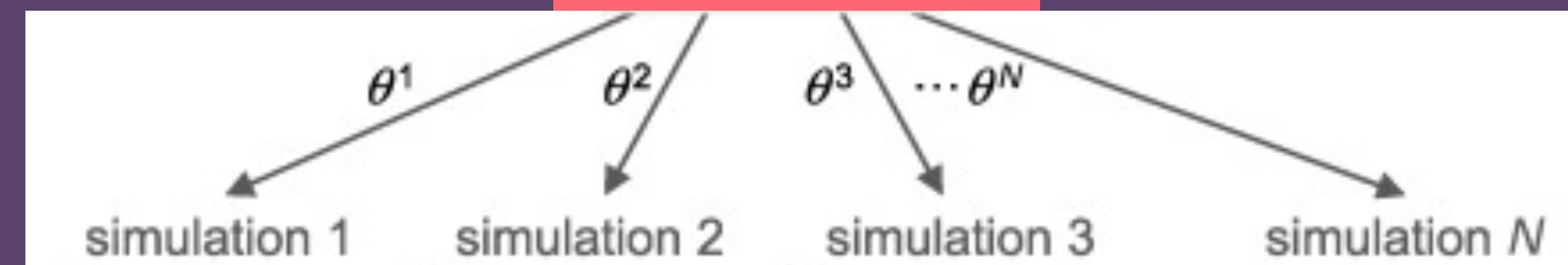
Observed data



Prior on parameters  $\theta$



Physics + telescope simulator



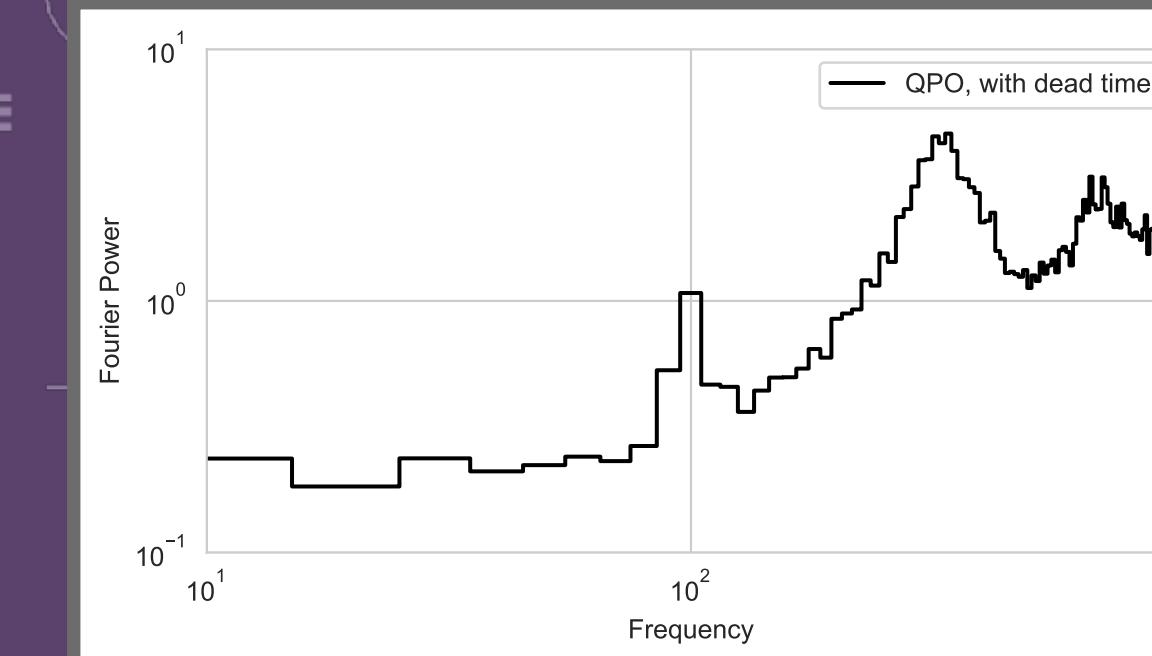
Step 1: draw parameters from prior

Step 2: simulate data sets

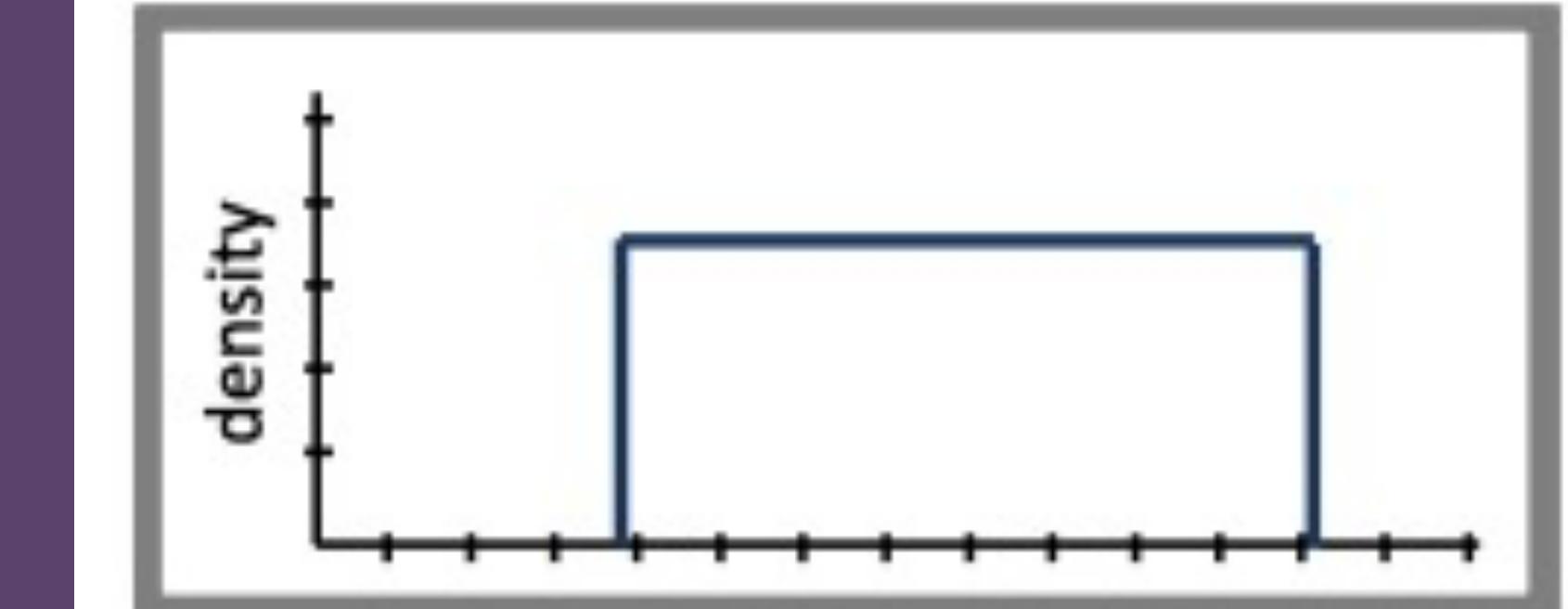
Step 3: compare simulated to observed data

Step 4: keep parameters that produce simulations similar to the data

Observed data



Prior on parameters  $\theta$



Physics + telescope simulator

$\theta^2$

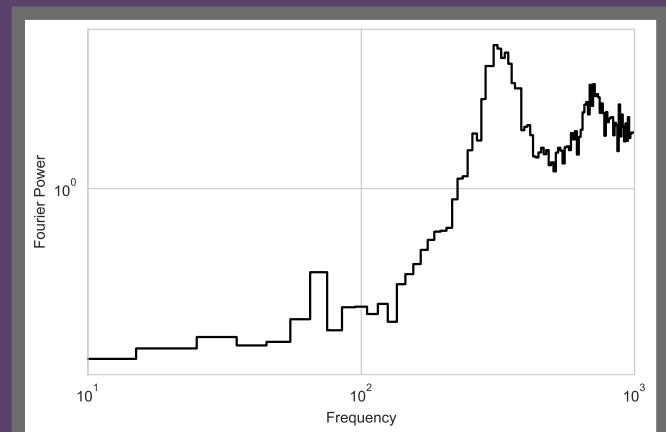
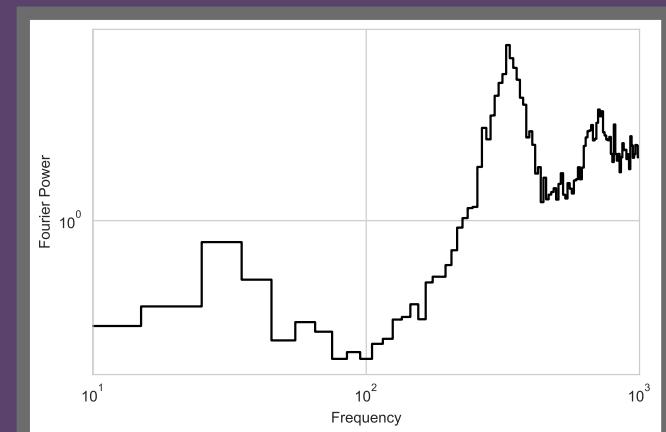
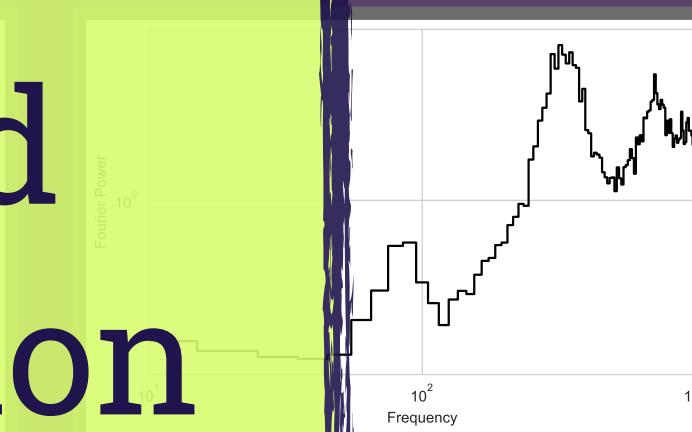
$\theta^3 \dots \theta^N$

simulation 2

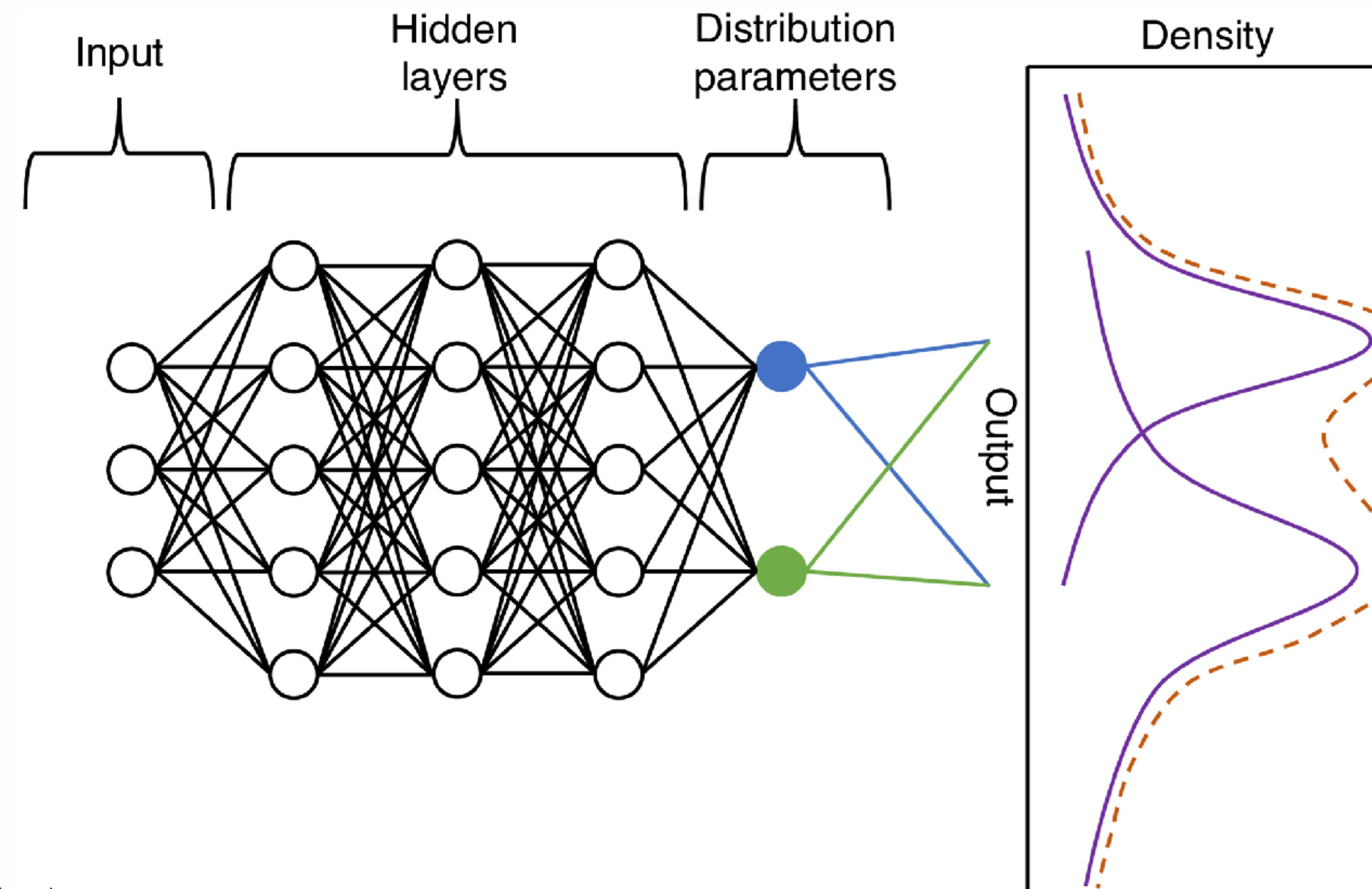
simulation 3

simulation  $N$

Can be efficiently addressed by neural network-based density estimation

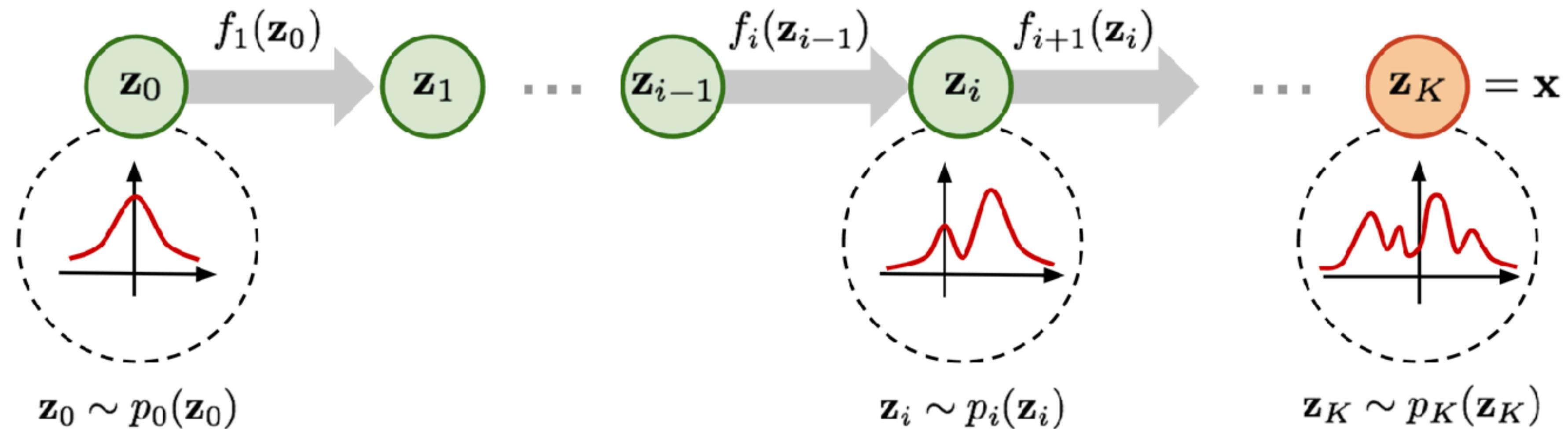


# Mixture Density Networks



# Normalizing Flows

- map simple base distribution (e.g. Gaussian) to a much more complex output distribution through a sequence of invertible transformations



# Simulation Based Inference



## Neural Posterior Estimation

$$p(\theta | D) = \frac{p(D | \theta) p(\theta)}{p(D)}$$

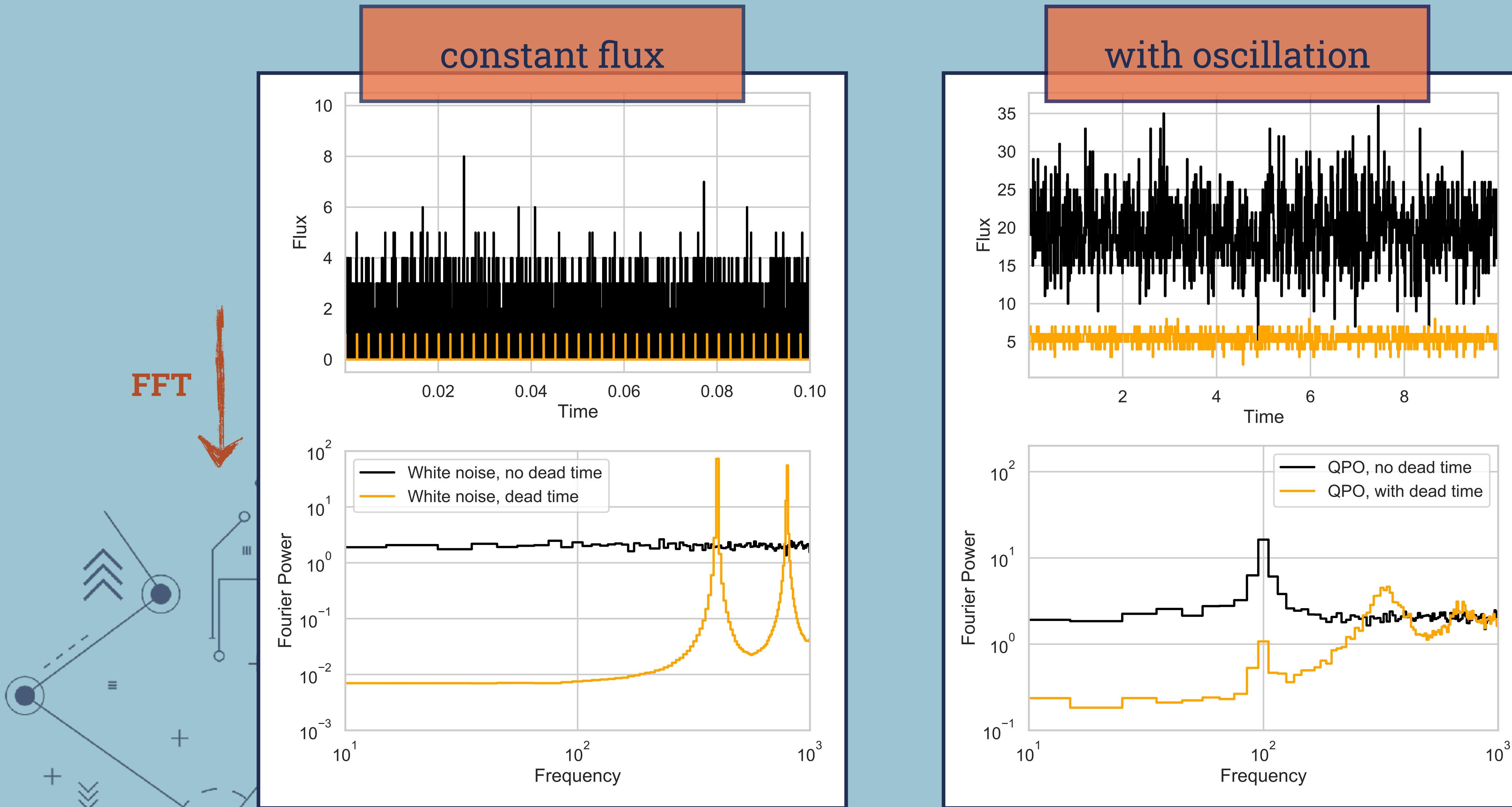
## Neural Likelihood Estimation

$$p(\theta | D) = \frac{p(\theta)}{\int p(\theta) p(D | \theta) d\theta}$$

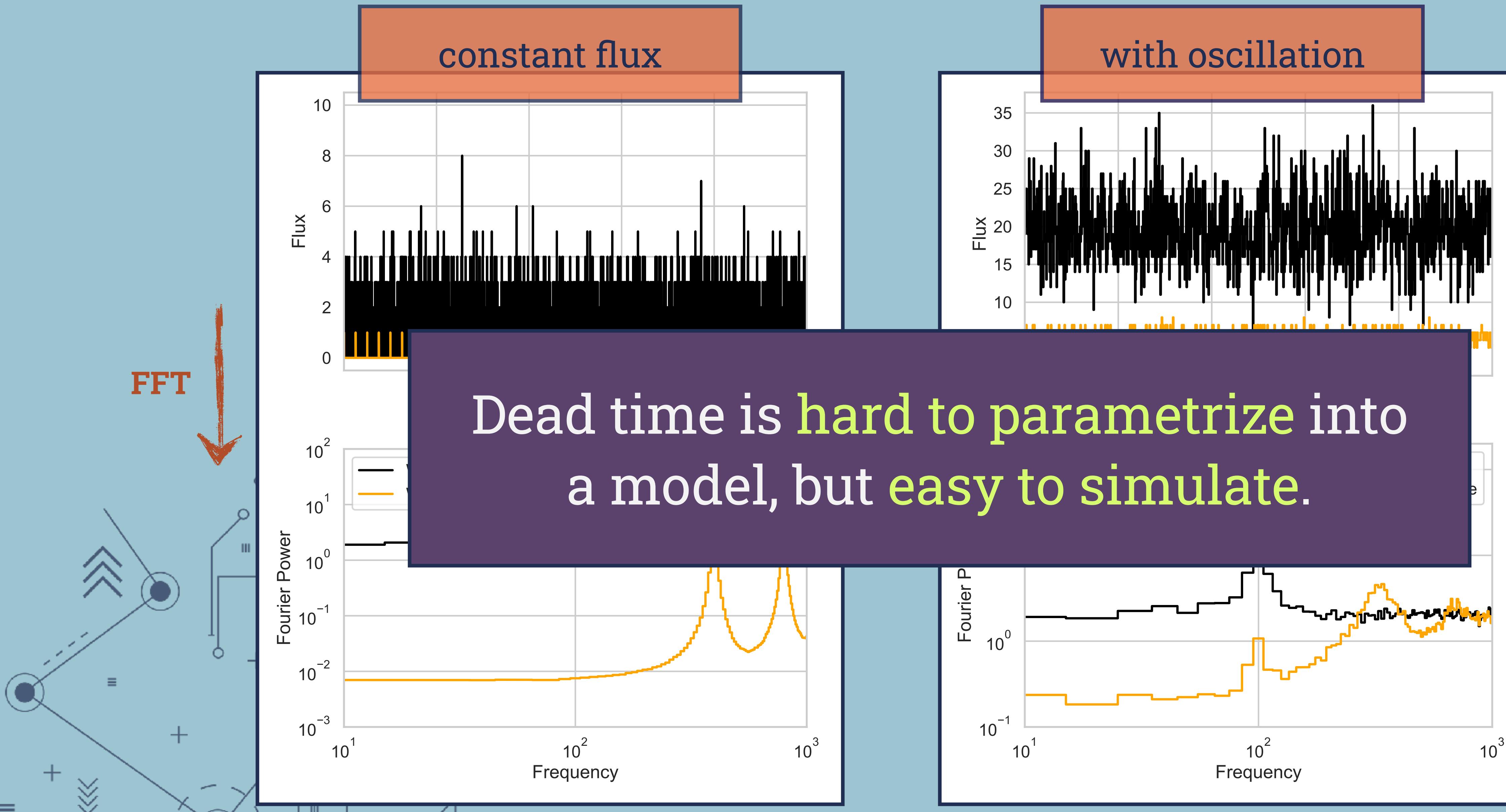
## Neural Ratio Estimation

$$p(\theta | D) = \frac{p(D | \theta)}{\int p(D | \theta) d\theta} p(\theta)$$

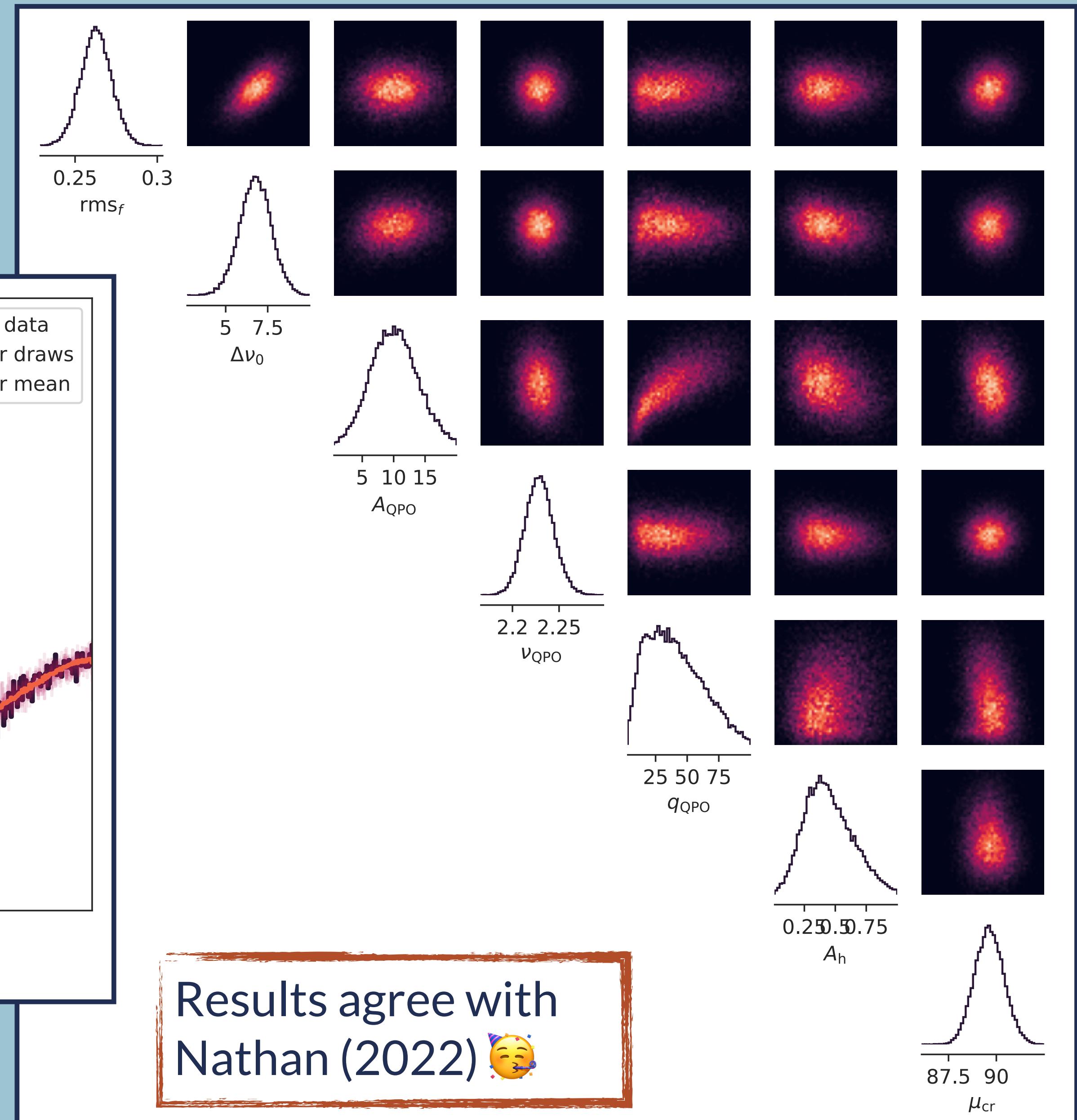
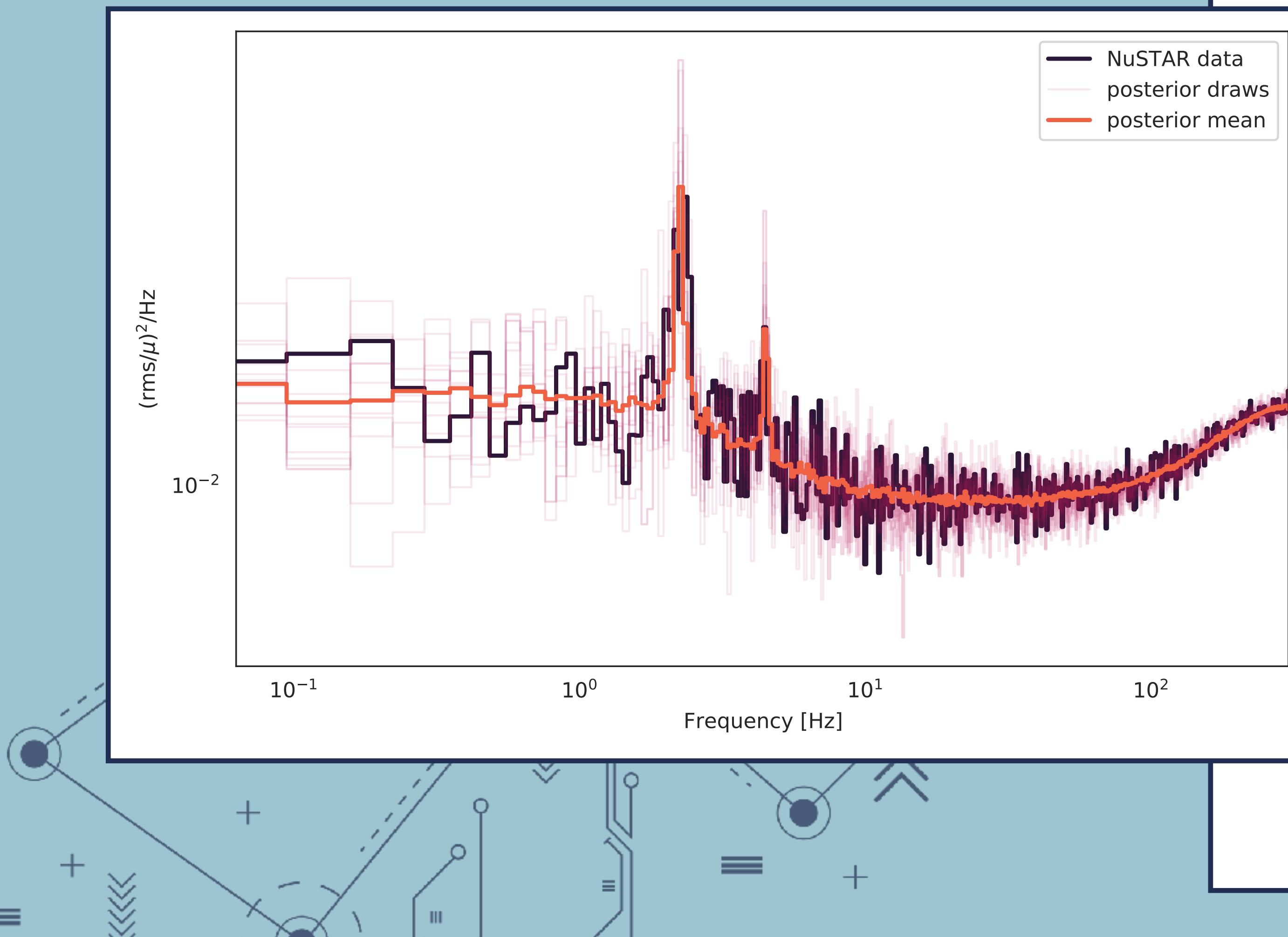
# Dead Time in X-ray Detectors



# Dead Time in X-ray Detectors

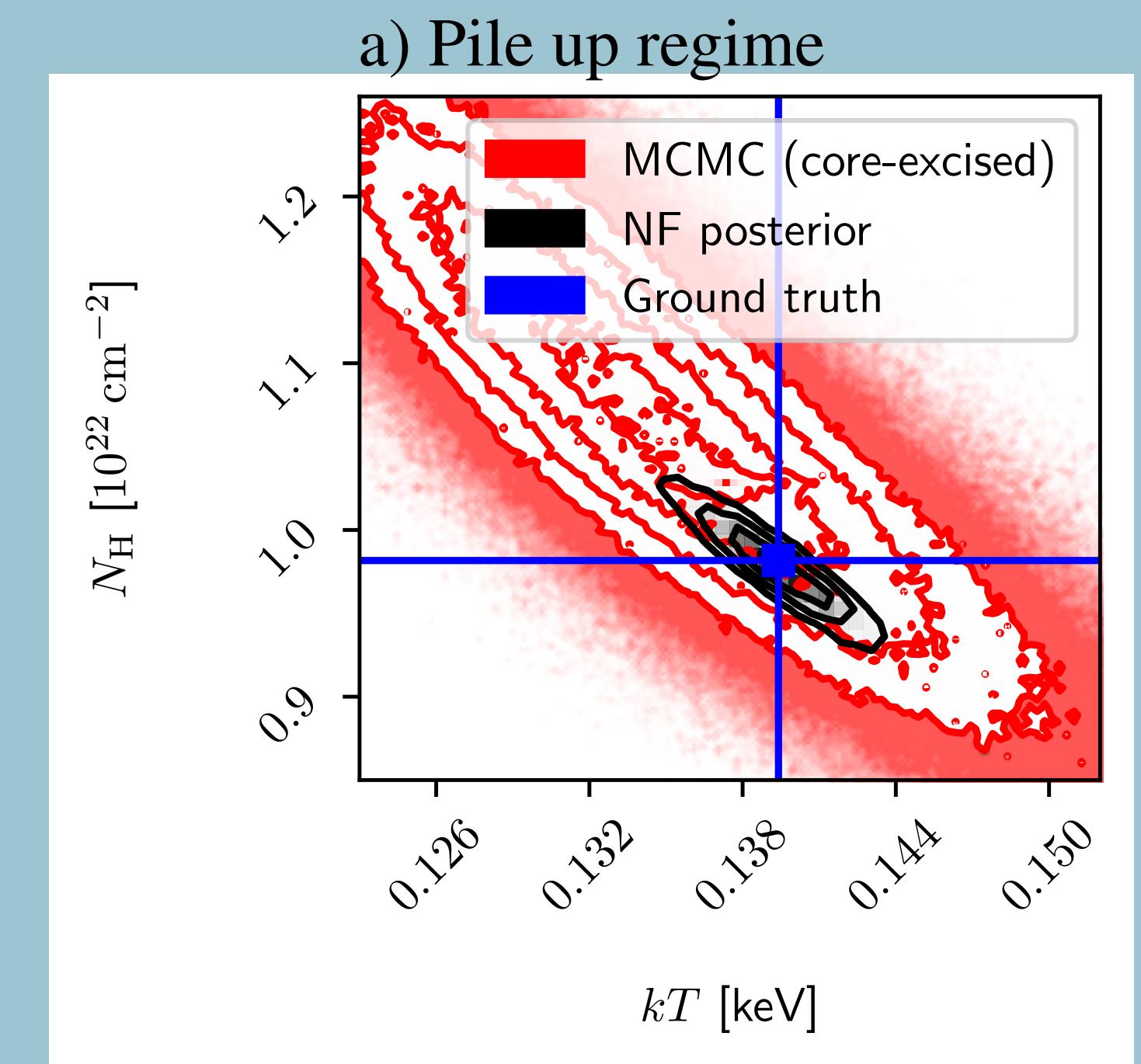
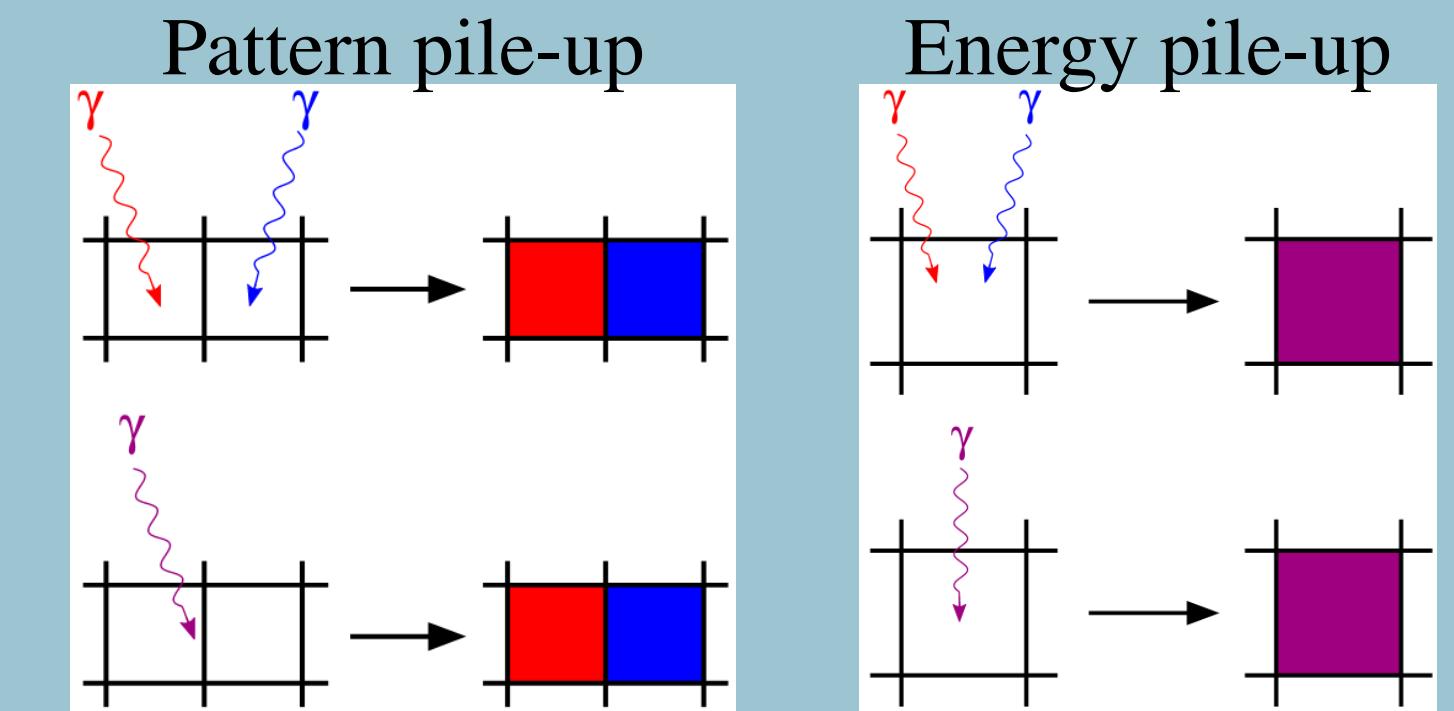
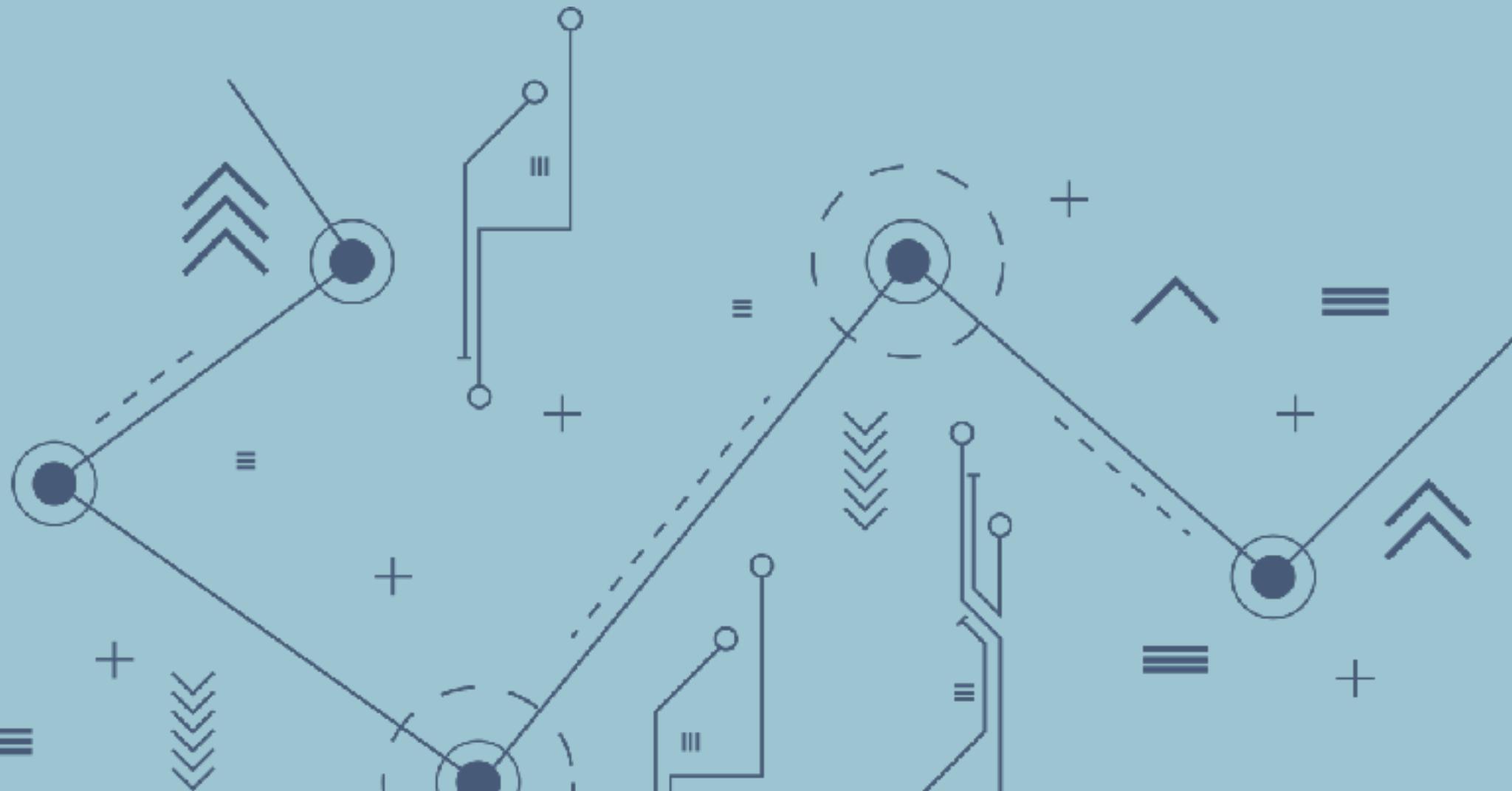
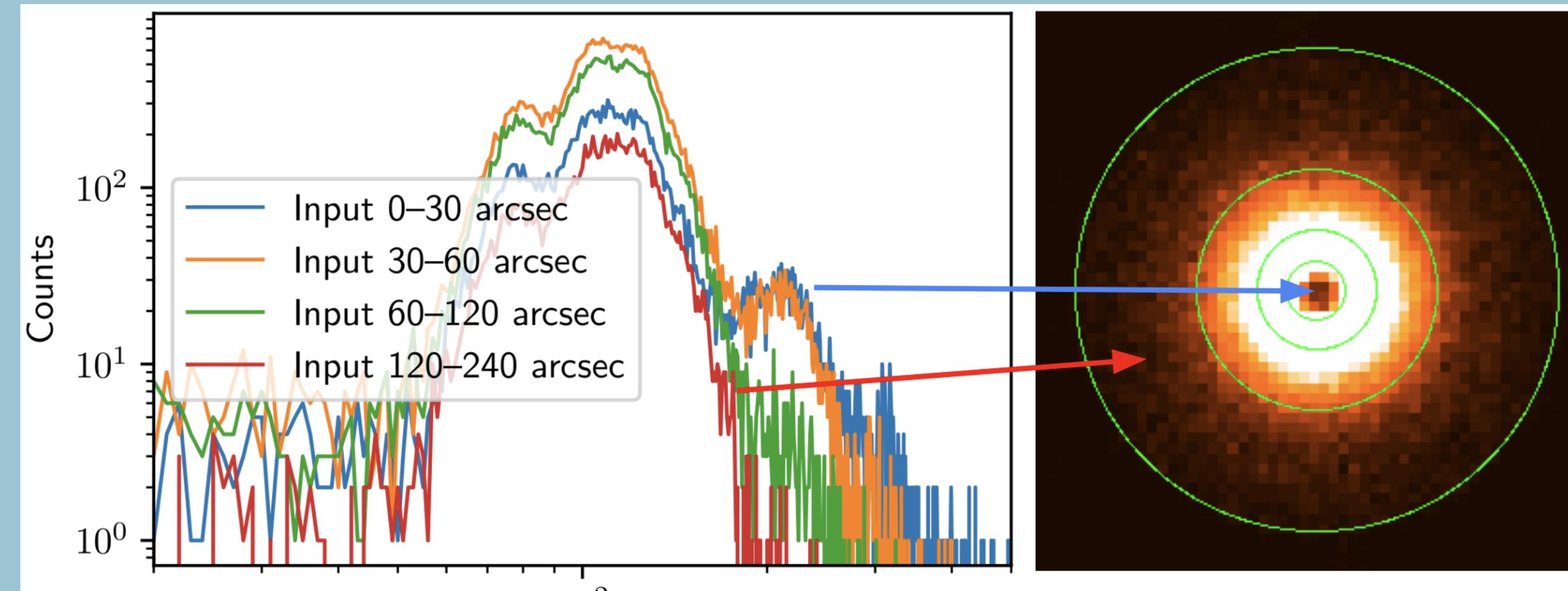


# Simulation-Based Inference for Instrumental Biases



Results agree with  
Nathan (2022) 😊

# Simulation-Based Inference for Instrumental Biases: Pile-up



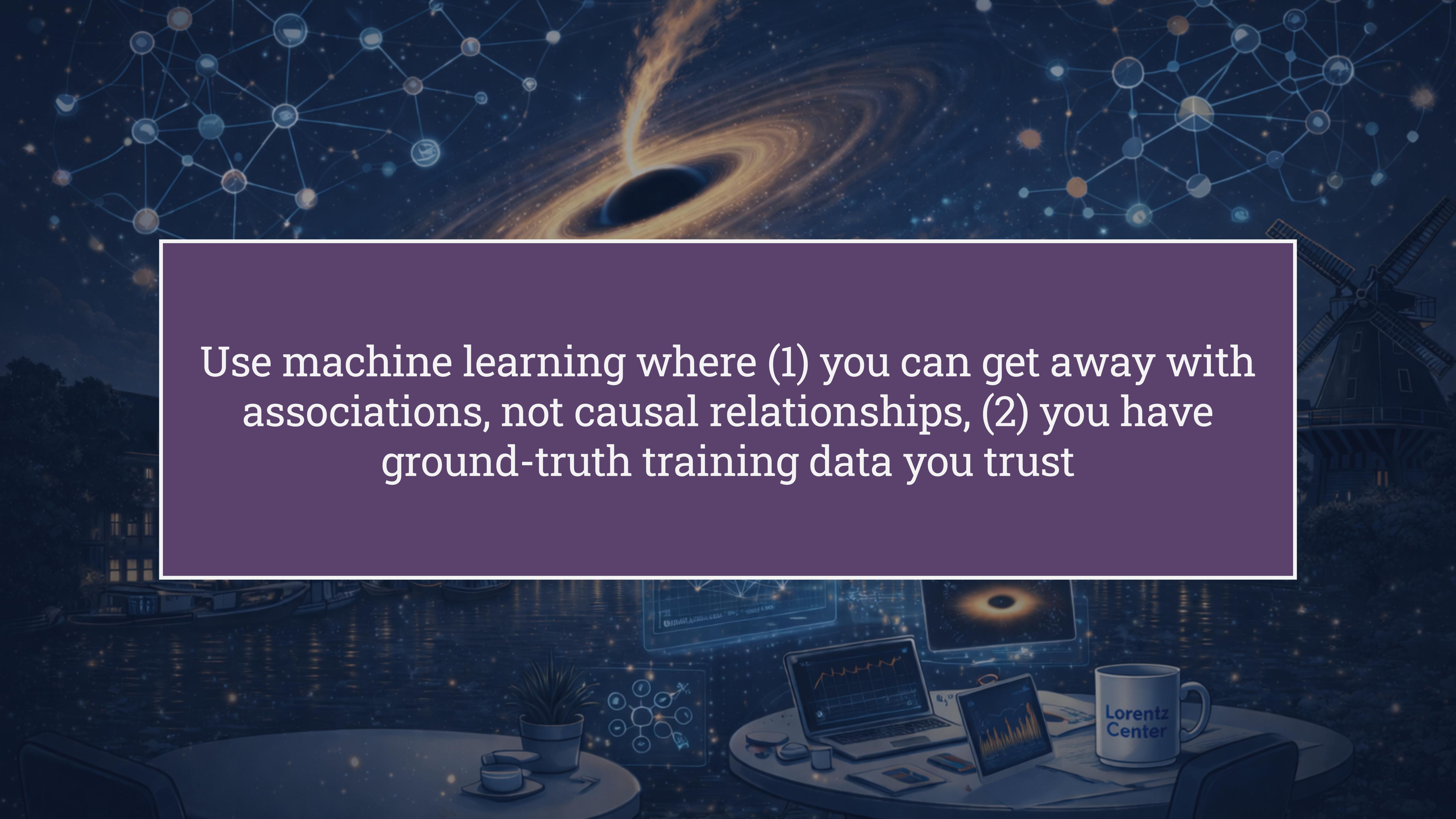
# Should you use machine learning

If you can do it with regular statistics: no! Statistics gives you mathematical guarantees!

Machine learning can be used to significantly accelerate numerical models (but at an accuracy trade-off)

Simulation-based inference is a principled way to infer (less biased) parameter distributions with complex simulators

Some of the technology that underpins machine learning is useful outside of ML, too!



Use machine learning where (1) you can get away with associations, not causal relationships, (2) you have ground-truth training data you trust

Lorentz  
Center



Extra advice:  
the newest algorithms aren't always the best  
suited for scientific applications!

# Things I haven't talked about

Classification tasks

Representation learning/unsupervised learning/clustering

Foundation models

Physics-informed machine learning

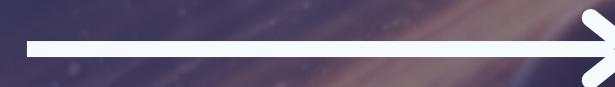
The many, many biases and pitfalls you can fall into while doing machine learning!



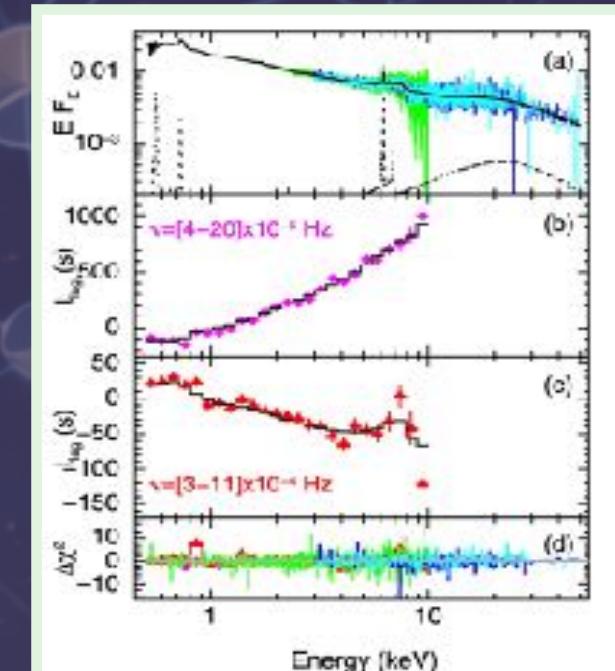
Let's meet our problem!

Lorentz  
Center

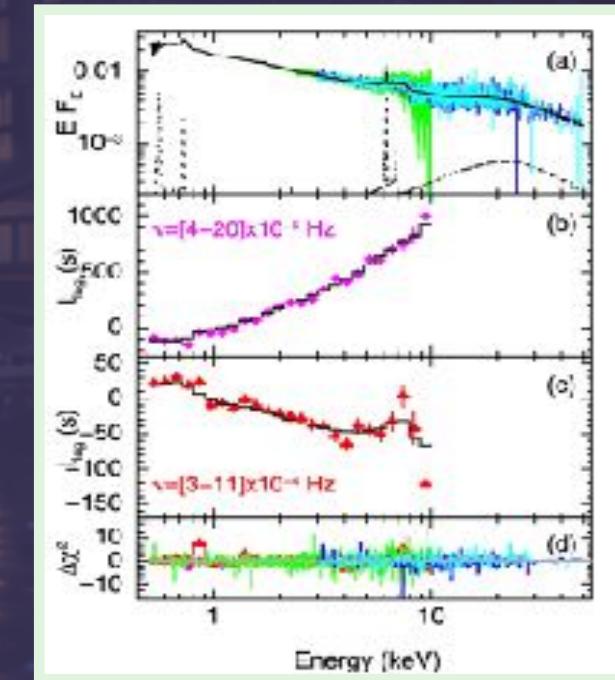
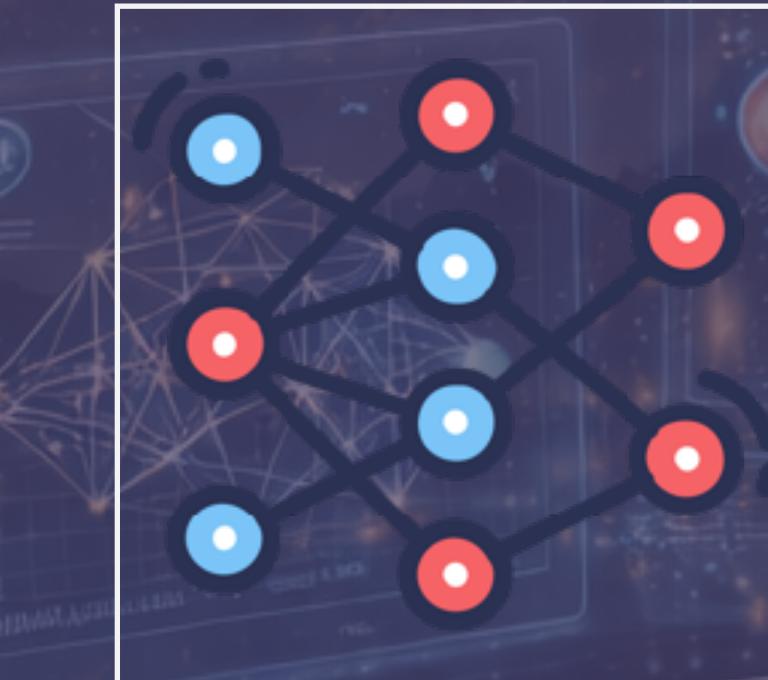
Power law  
parameters



$$\begin{aligned} & \text{Derivation steps include: } \\ & \text{1. } \frac{\partial}{\partial x} \left( \sum_{i=1}^n (x_i - \bar{x})^2 \right) = 0 \Rightarrow \sum_{i=1}^n 2(x_i - \bar{x}) = 0 \Rightarrow \sum_{i=1}^n x_i = n\bar{x} \\ & \text{2. } \text{Simplifying: } \sum_{i=1}^n x_i = n\bar{x} \Rightarrow \bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \\ & \text{3. } \text{Defining variance: } \sigma^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 \\ & \text{4. } \text{Simplifying variance: } \sigma^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i^2 - \bar{x}^2) = \frac{1}{n-1} \left( \sum_{i=1}^n x_i^2 - \bar{x}^2 \right) = \frac{1}{n-1} \left( \sum_{i=1}^n x_i^2 - \frac{1}{n} \sum_{i=1}^n x_i \cdot \sum_{i=1}^n x_i \right) = \frac{1}{n-1} \left( \sum_{i=1}^n x_i^2 - \frac{1}{n} \sum_{i=1}^n x_i \cdot n\bar{x} \right) = \frac{1}{n-1} \left( \sum_{i=1}^n x_i^2 - \bar{x} \cdot n\bar{x} \right) = \frac{1}{n-1} \left( \sum_{i=1}^n x_i^2 - \bar{x}^2 \right) \end{aligned}$$



Power law  
parameters





Important: supervised classification requires  
ground-truth training data

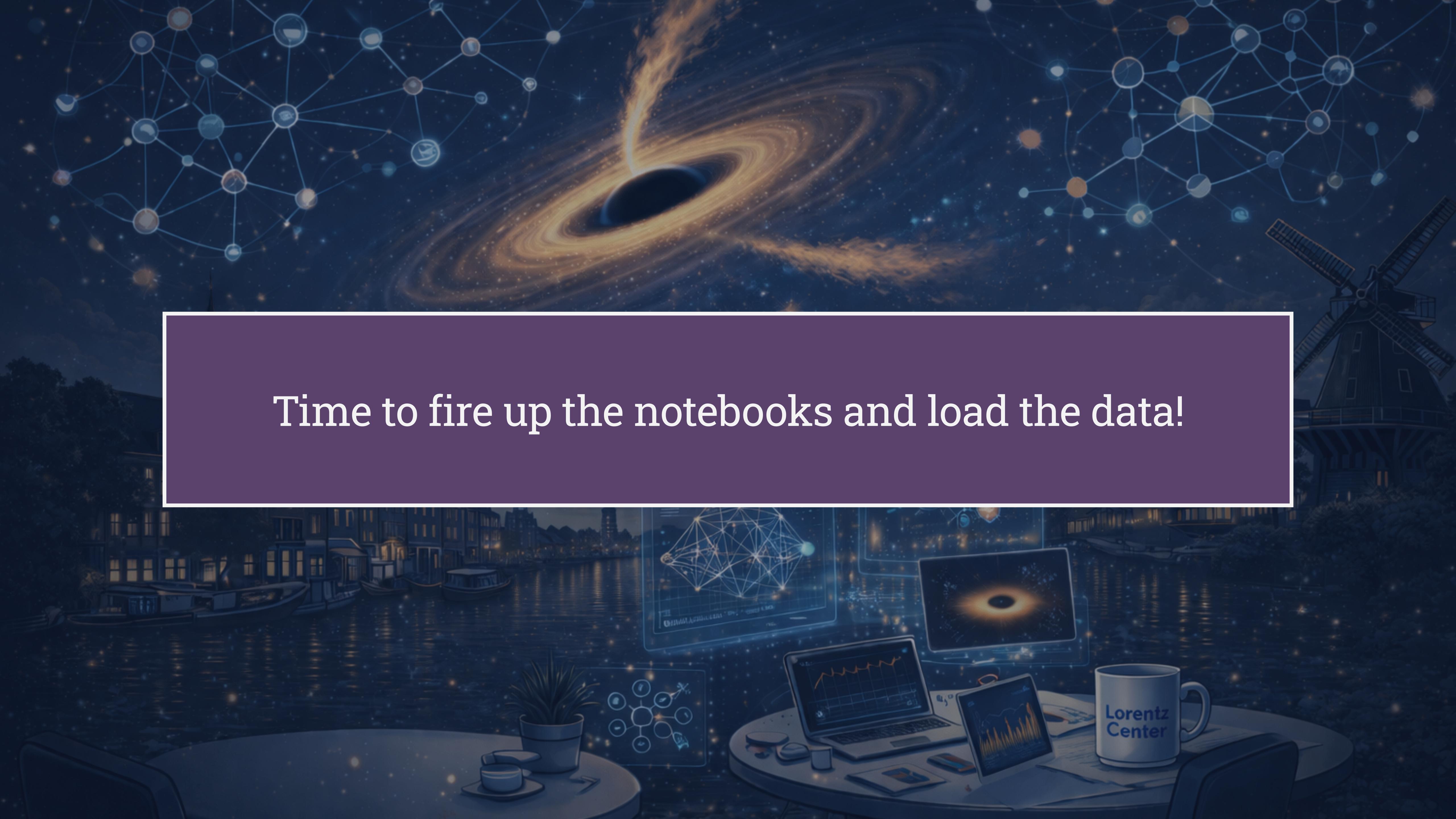
Lorentz  
Center

## ML Jargon

**Features:** informative summaries of the data used in ML tasks

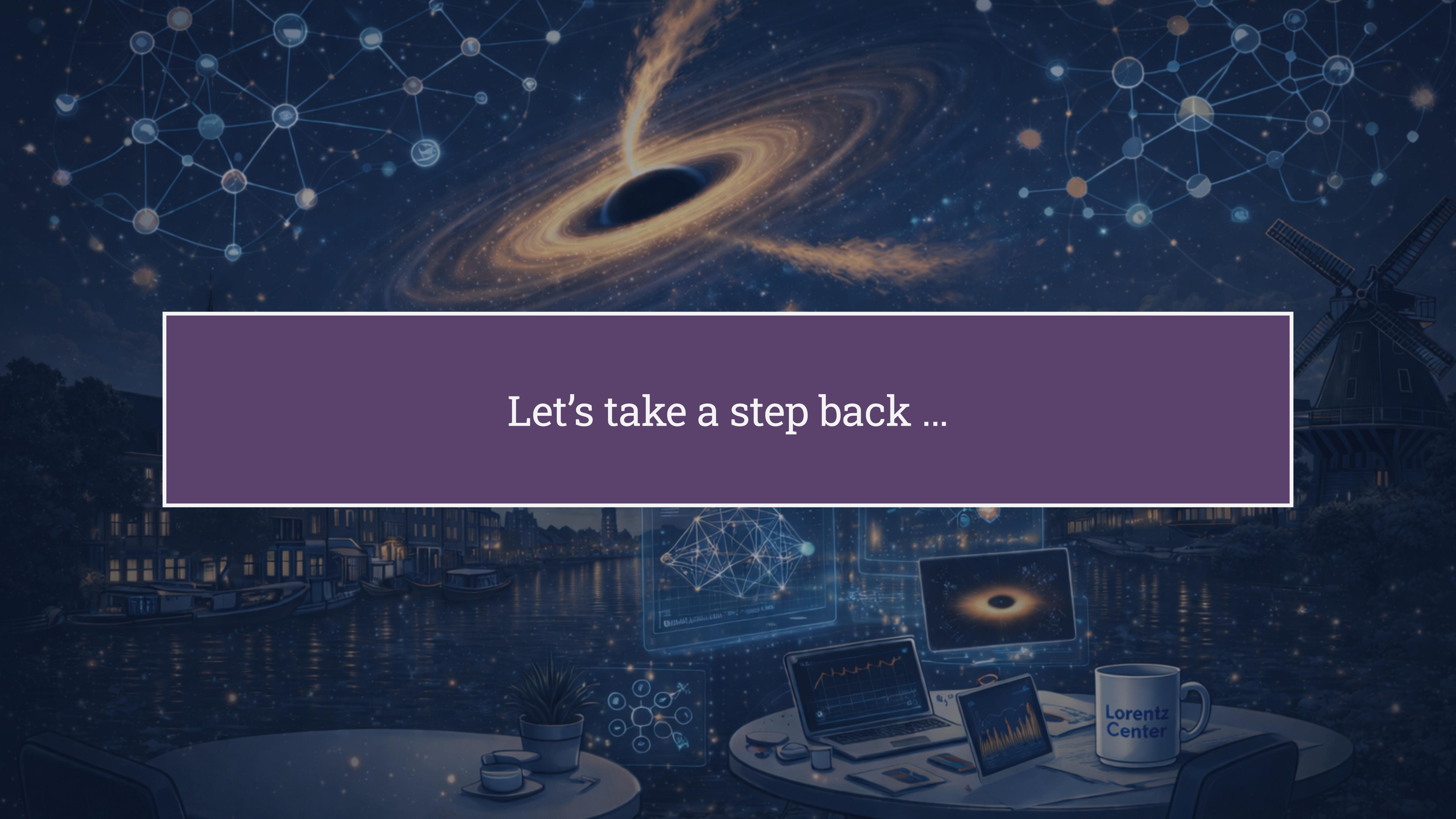
**Labels:** the true (known) outputs that the ML model is trying to reproduce. For classification, these are discrete class labels, for regression continuous quantities

**Sample:** a single example in your training data



Time to fire up the notebooks and load the data!





Let's take a step back ...

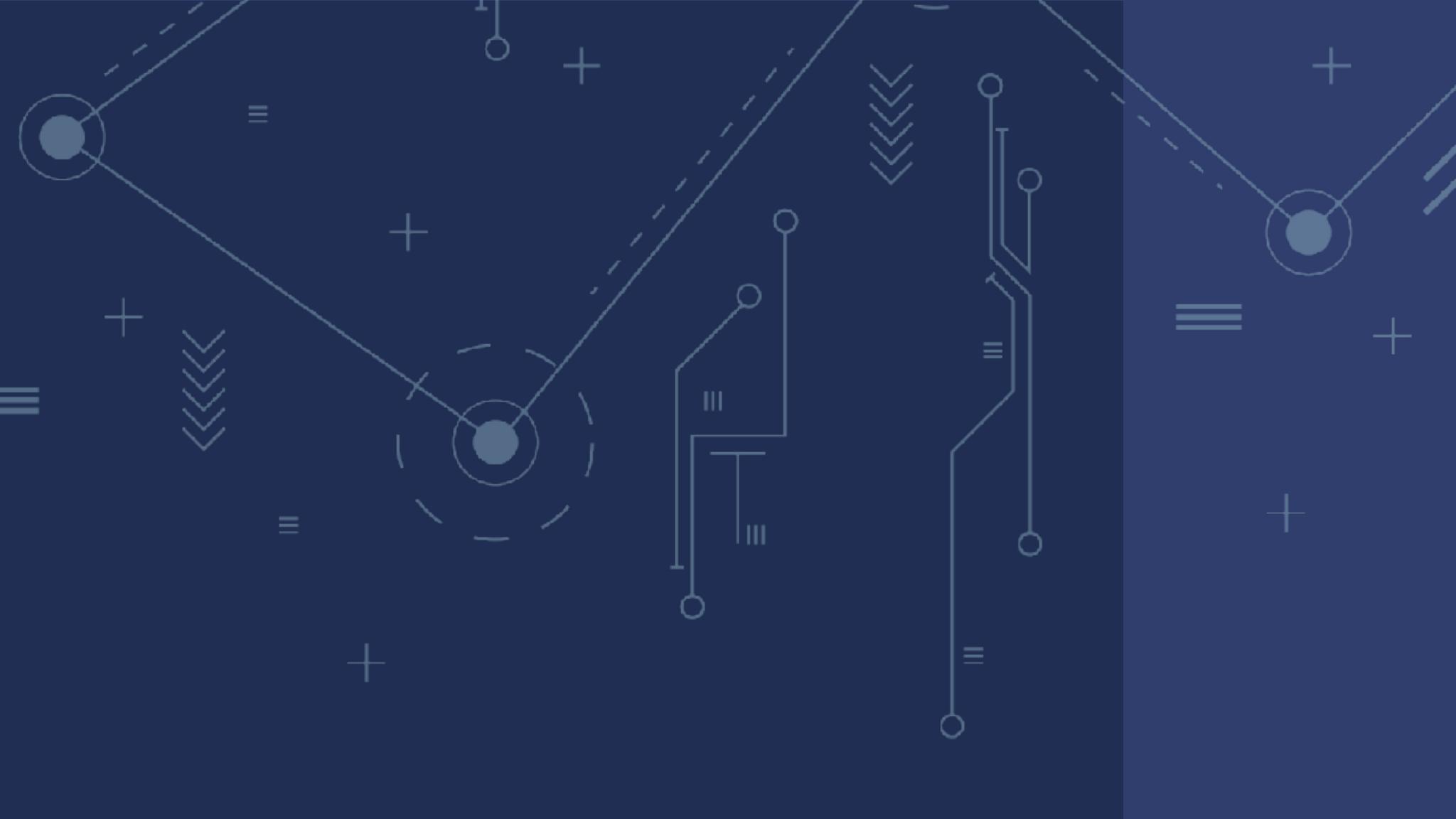
Lorentz  
Center

# Machine Learning Overview

1. Figuring out what we want to learn, and why!
2. Exploring the Data, Part I
3. Train-validation-test set splits
4. Exploring the Data, Part II
5. Data Pre-Processing: Dimensionality Reduction, Scaling the Data
6. Choose an evaluation metric
7. Choosing a (simple) algorithm + fit the model
8. Explore results
9. Choose a (more complex?) algorithm, explore results
10. Hyperparameter tuning, explore results
11. Interpret outcomes
12. Science! 🎉

# Machine Learning Overview

1. Figuring out what we want to learn, and why!
2. Exploring the Data, Part I
3. Train-validation-test set splits
4. Exploring the Data, Part II
5. 90% of your time will be spent on data exploration, data processing, visualising your model, critiquing and interpreting your results, 10% on actually applying a ML algorithm to data
- 6.
- 7.
- 8.
9. results
10. Hyperparameter tuning, explore results
11. Interpret outcomes
12. Science! 🎉



Use best practices  
in machine learning  
to establish trust in  
results

1. Designing and preparing data sets
2. Choosing algorithms
3. Choosing evaluation metrics
4. Exploring and reporting outputs

Machine learning is not just a set of algorithms,  
but a **community of practice** with **rules**,  
**conventions** and **best practices** to guard against  
challenges (e.g. overfitting, lack of generalisation)

# Figuring Out What We Want to Learn



## Considerations before starting

1. Do we only care about **predictions**, or also the **parameters** of the model? Do we need the model to be **interpretable**?
2. How **similar** is our **training data** to our **target data**? Do they come from the same instrument?
3. What **biases** do you know exist in your **training data**? Is there a **part of feature space** that's **not covered**?
4. What **physics knowledge** do you have about the data and the problem? Can that knowledge guide you in **constructing features** and choosing **algorithms/evaluation metrics**?

# Exploring + Pre-Processing Data



# Algorithm Spotlight: Logistic Regression

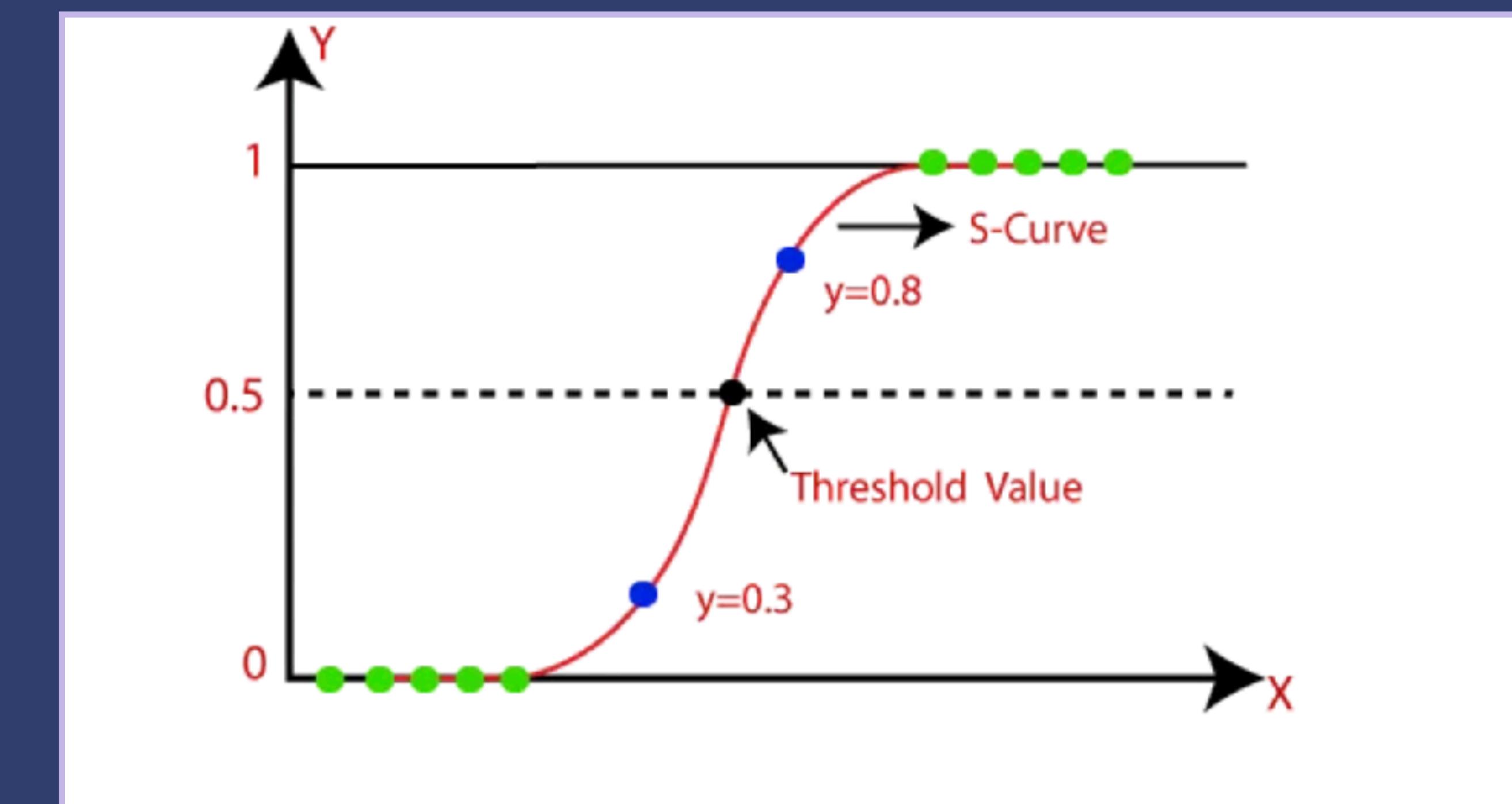




## Logistic Regression

$$p(\vec{X}_k) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 \vec{X}_k)}}$$

- Binary classification, e.g. with GALAXY=0, and STAR=1





## Logistic Regression

$$l = \sum_k l_k$$

Loss function

$$\ell_k = \begin{cases} -\ln p_k & \text{if } y_k = 1, \\ -\ln(1 - p_k) & \text{if } y_k = 0. \end{cases}$$

- Binary classification, e.g. with GALAXY=0, and STAR=1

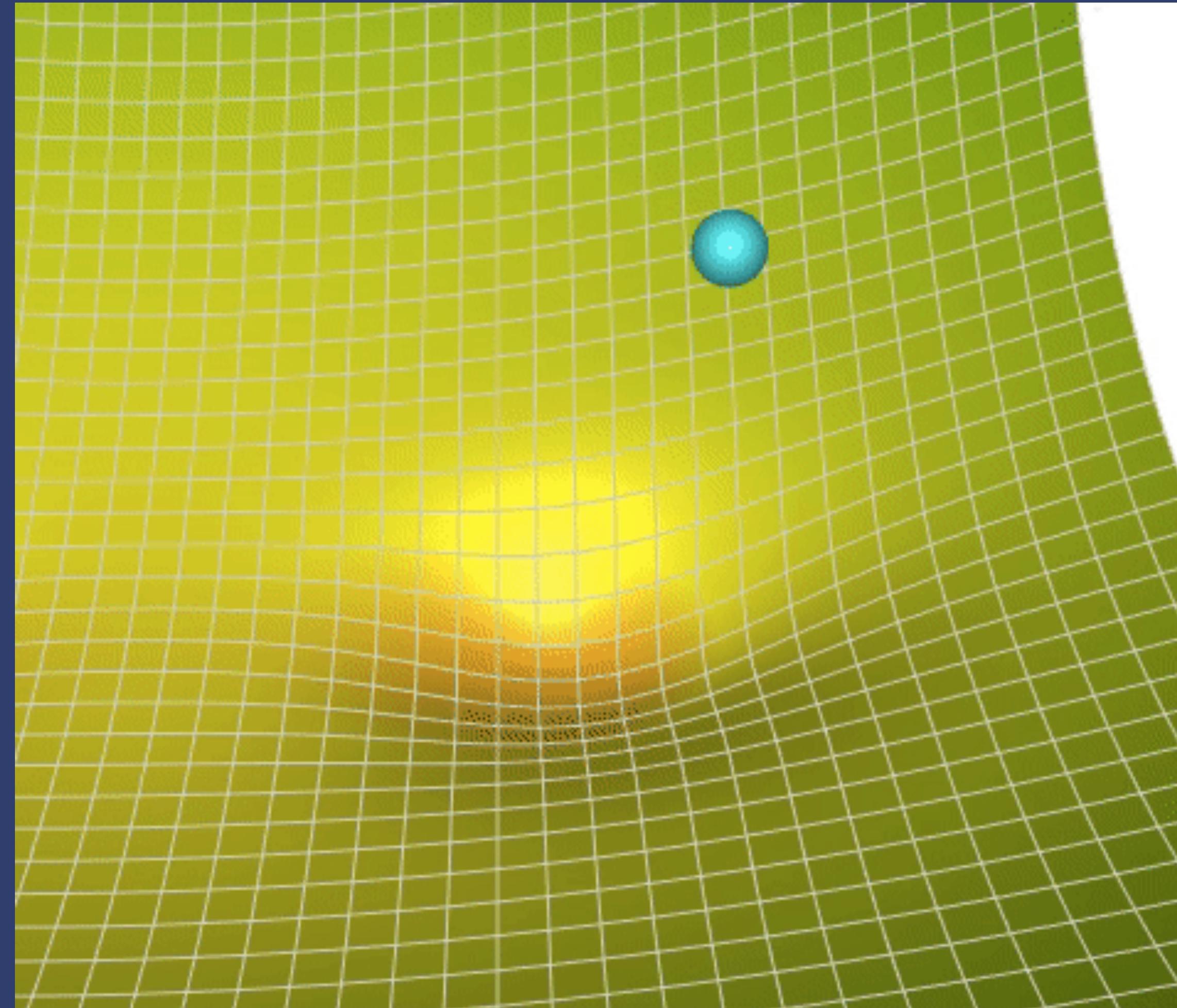
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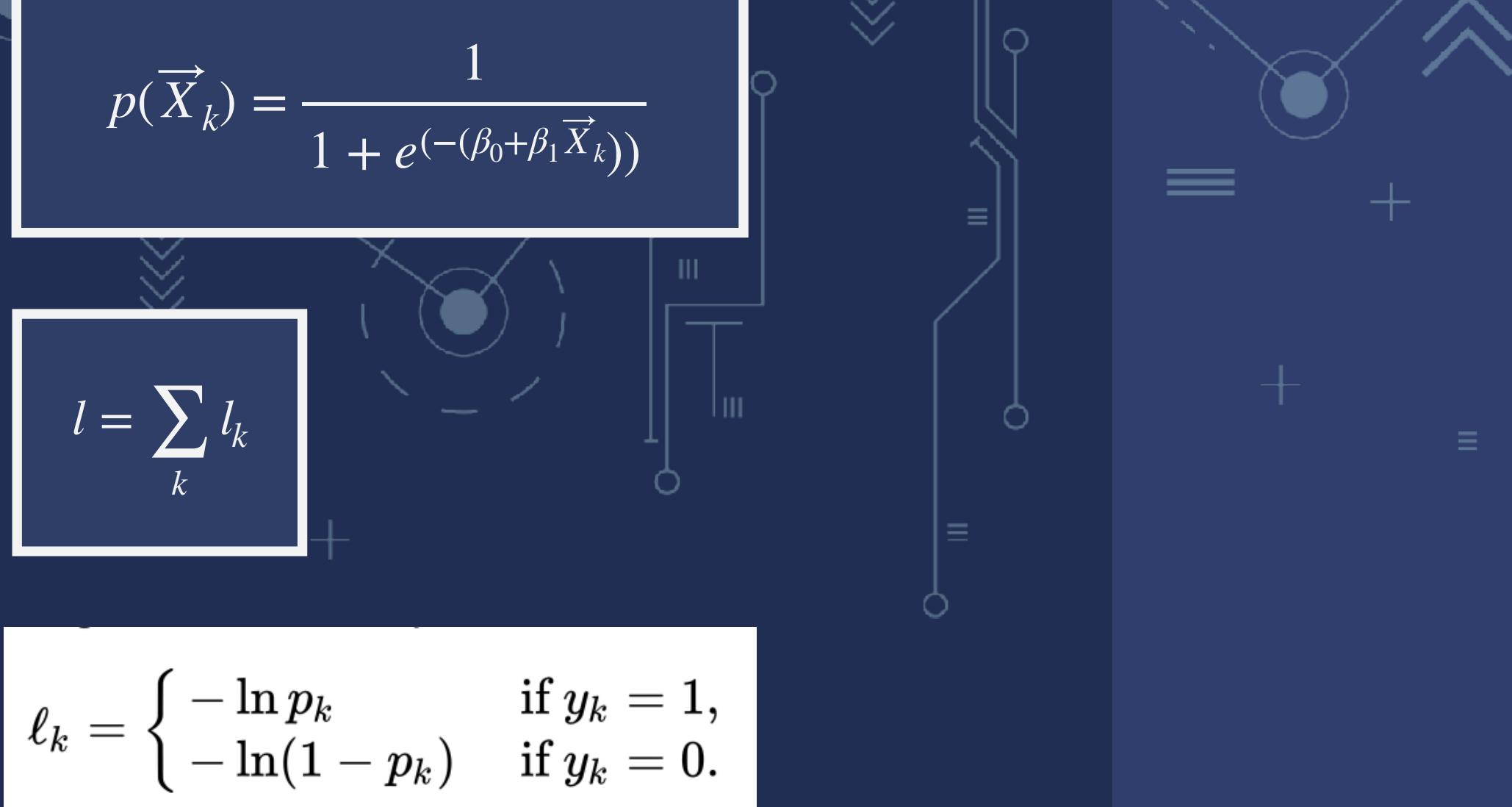
$$l = \sum_k l_k$$

$$\ell_k = \begin{cases} -\ln p_k & \text{if } y_k = 1, \\ -\ln(1 - p_k) & \text{if } y_k = 0. \end{cases}$$

## Gradient Descent

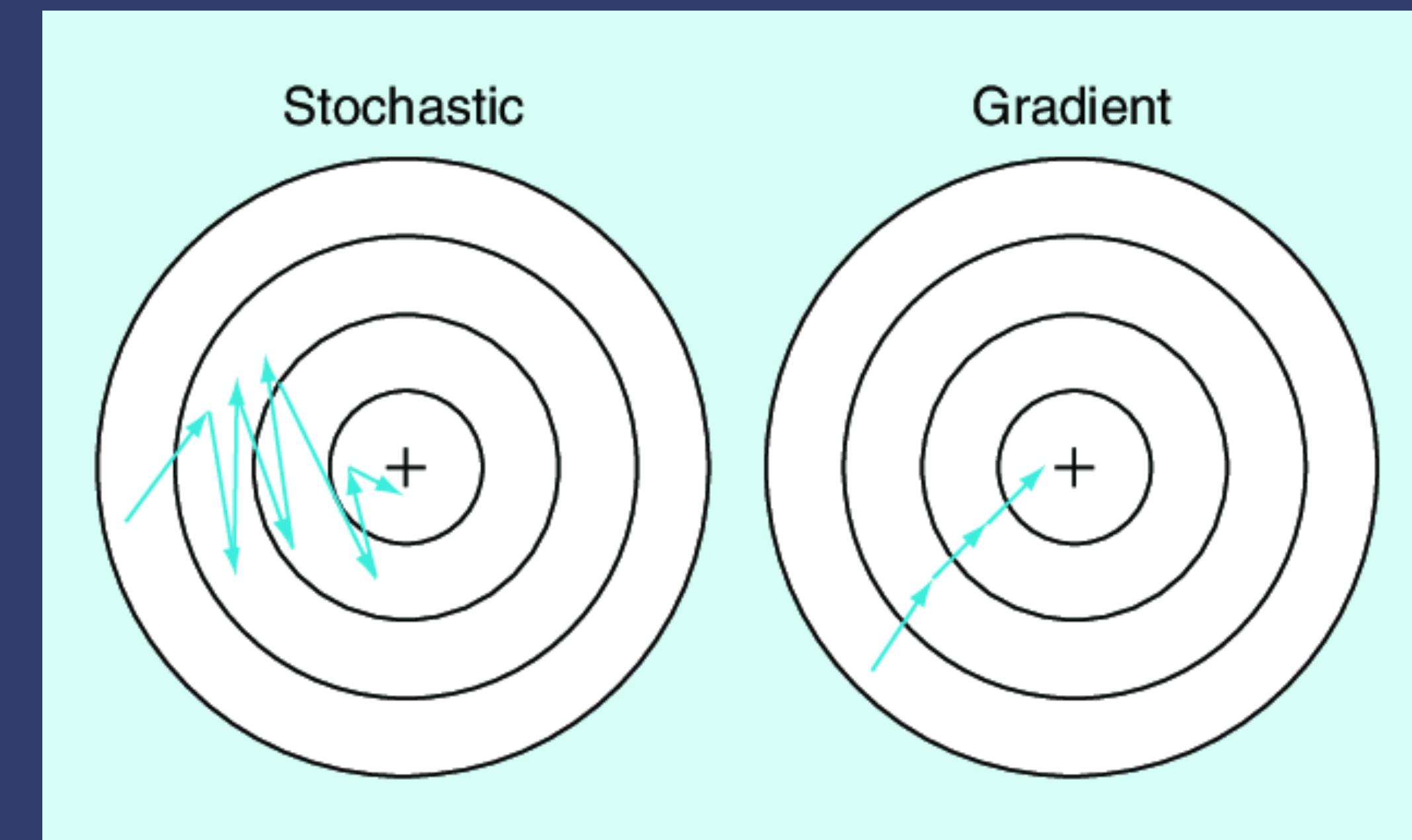


# Stochastic + Mini-batch Gradient Descent

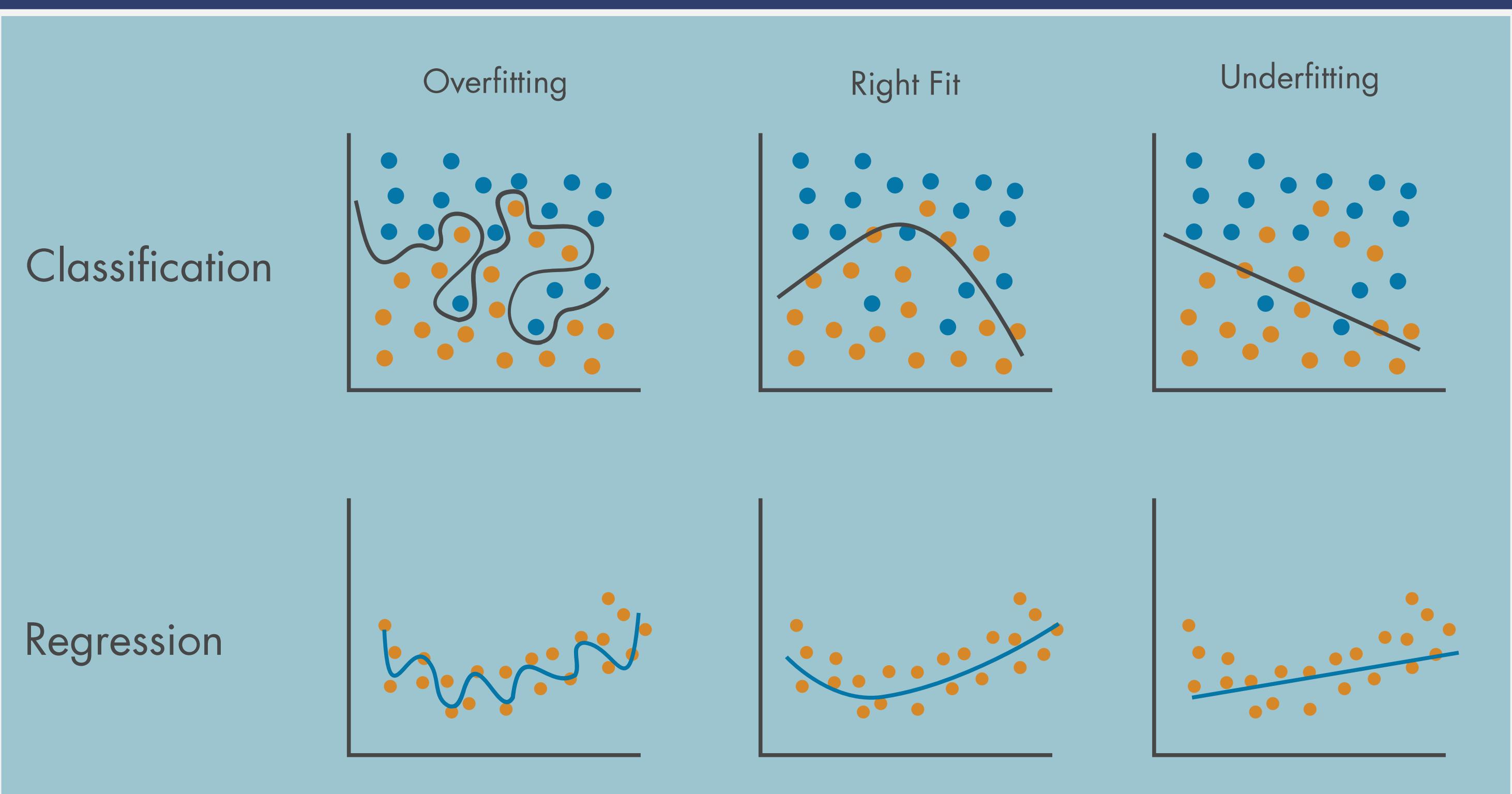


**Stochastic Gradient Descent** = Update parameters and compute gradients based on a single random training example

**Mini-batch SGD** = Update parameters based on mean gradient over a mini-batch, i.e. a small subset of the training data



# Overfitting versus underfitting





L2 Norm (ridge regression):

## Solution: Regularisation

L1-Norm (LASSO):

$$l = \sum_k l_k + C \sum_{j=1}^n |\beta_j|$$

$$l = \sum_k l_k + C \sqrt{\left( \sum_{j=1}^n |\beta_j|^2 \right)}$$

$$l = \sum_k l_k + C \left( \sum_{j=1}^n |\beta_j|^p \right)^{1/p}$$



L2 Norm (ridge regression):

## Solution: Regularisation

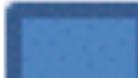
p-norm:

$$l = \sum_k l_k + C \sum_{j=1}^n |\beta_j|$$

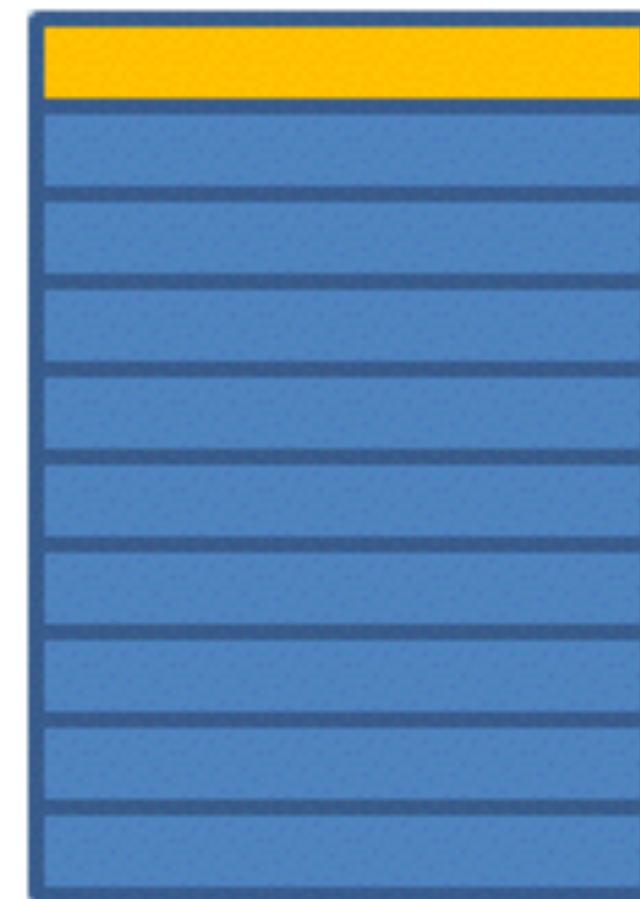
$$l = \sum_k l_k + C \sqrt{\left( \sum_{j=1}^n |\beta_j|^2 \right)}$$

$$l = \sum_k l_k + C \left( \sum_{j=1}^n |\beta_j|^p \right)^{1/p}$$

# K-Fold Cross Validation

 Validation Set  
 Training Set

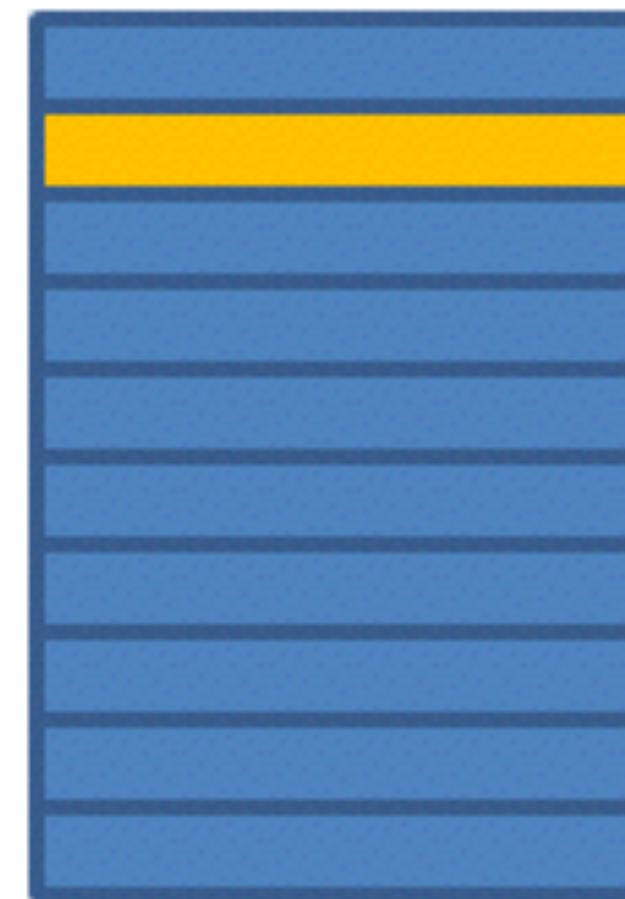
Round 1



Validation Accuracy:

93%

Round 2



90%

Round 3



91%

Round 10



95%

...

Final Accuracy = Average(Round 1, Round 2, ...)

# Evaluation Metrics

Lorentz  
Center



## Evaluation

	<b>Positive Prediction (STAR)</b>	<b>Negative Prediction (GALAXY)</b>
<b>Positive class (STAR)</b>	True positive (TP)	False negative (FN)
<b>Negative class (GALAXY)</b>	False positive (FP)	True negative (TN)

Sensitivity = True Positive / (True Positive + False Negative)

Specificity = True Negative / (False Positive + True Negative)

Precision = True Positive / (True Positive + False Positive)

Recall = True Positive / (True Positive + False Negative)

F-score =  $(2 * \text{Precision} * \text{Recall}) / (\text{Precision} + \text{Recall})$

# General Advice



**Rule 1:** Compare against a domain reference and put result into larger context

**Rule 2:** Adopt best practices from the ML community

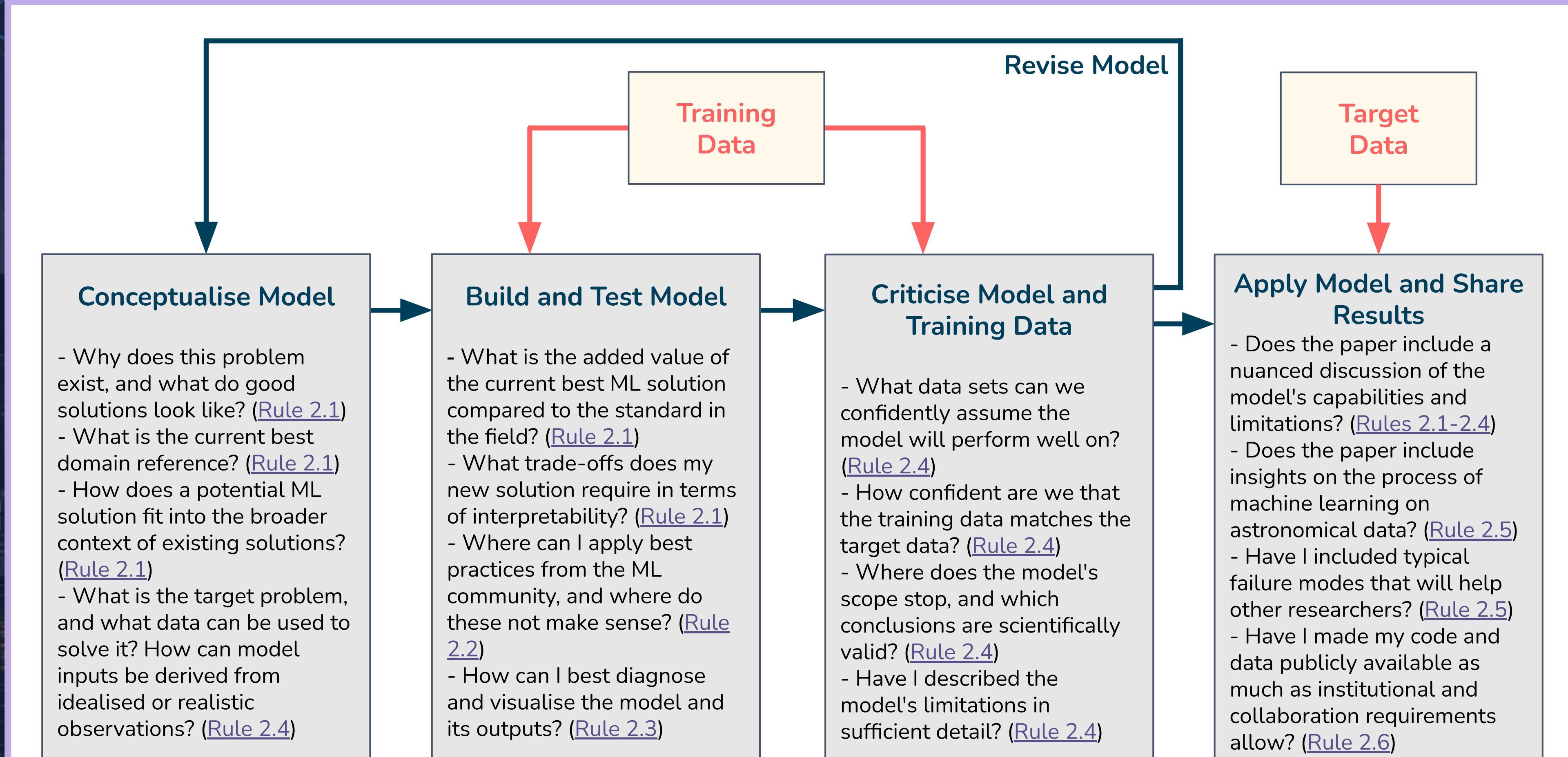
**Rule 3:** Interpret, Diagnose and/or Visualise Models

**Rule 4:** Explore limits and scope of the model

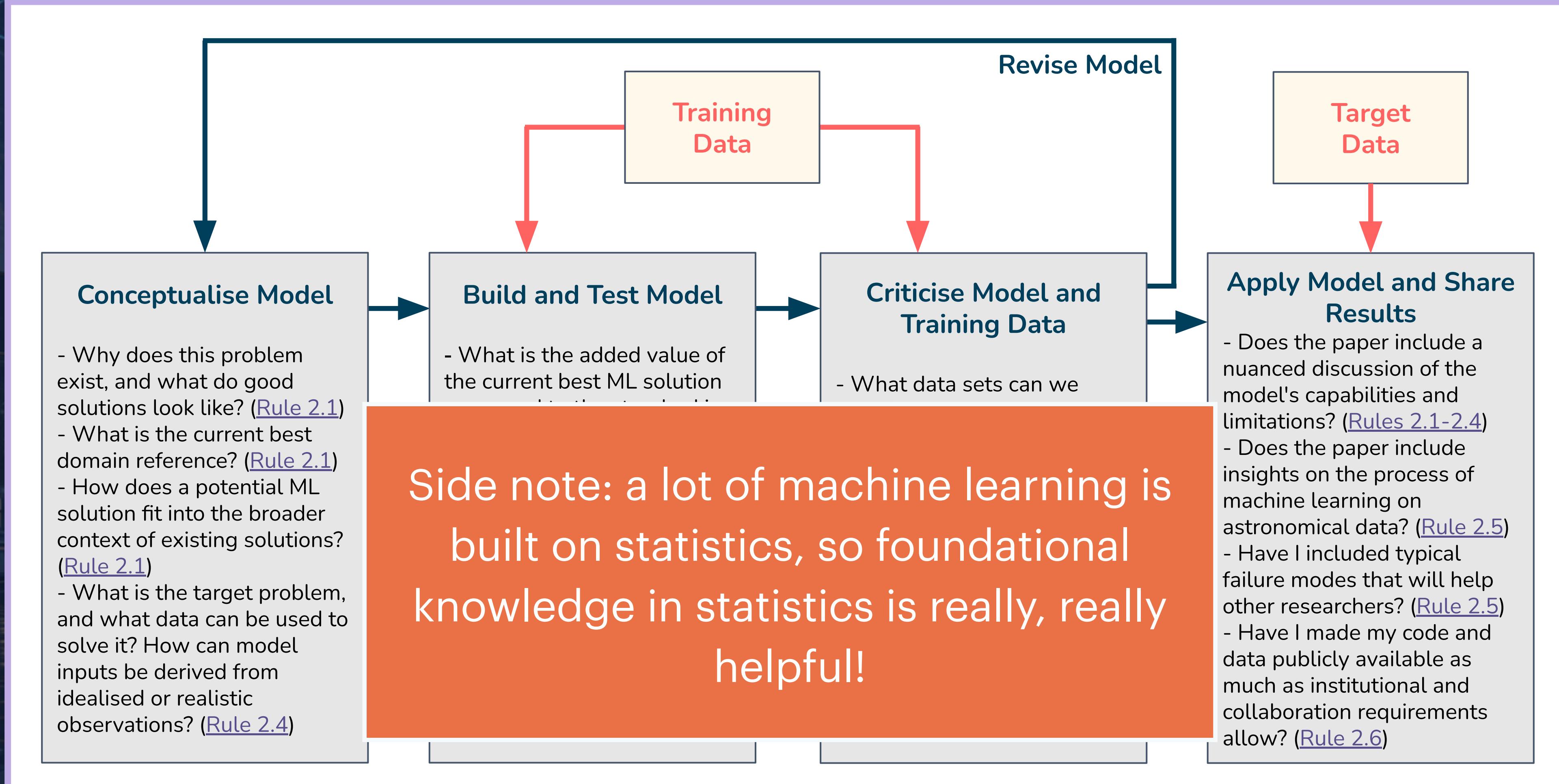
**Rule 5:** Share and Discuss Lessons Learned

**Rule 6:** Make Software and Data Publicly Available

# Box Loop for Machine Learning in Astronomy



# Box Loop for Machine Learning in Astronomy



## What to try next



- Viviana Acquaviva, "Machine learning for Physics and Astronomy", <https://press.princeton.edu/books/paperback/9780691206417/machine-learning-for-physics-and-astronomy>
- Also chalkboard colloquium: <https://www.youtube.com/watch?v=f8NlkChOg2oY>
- Buchner + Fotopoulou: How to set up your first machine learning project in Astronomy, <https://arxiv.org/html/2502.08222v1>
- Baron, Machine Learning in Astronomy: A Practical Overview, <https://arxiv.org/abs/1904.07248>
- Huppenkothen, Ntampaka et al, Constructing Impactful Machine Learning Research in Astronomy, <https://arxiv.org/pdf/2310.12528>
- Fotopoulou: A review of Unsupervised Learning in Astronomy, <https://arxiv.org/pdf/2406.17316>
- Scikit-learn tutorials and examples: <https://scikit-learn.org/stable/>
- Great tutorials by the folks at MPIA: [https://mfouesneau.github.io/astro\\_ds/chapters/datascience/chapter1-introML.html](https://mfouesneau.github.io/astro_ds/chapters/datascience/chapter1-introML.html)
- NeurIPS and ICML workshops on machine learning for physics and astronomy, e.g. <https://ml4physicalsciences.github.io/2024/>
- NeurIPS tutorials on specific topics: e.g. at <https://neurips.cc/virtual/2024/events/tutorial>
- Kaggle competitions on astronomy problems, e.g. <https://www.kaggle.com/search?q=astronomy+in:competitions>
- Millions of good online resources, e.g. <http://www.r2d3.us/visual-intro-to-machine-learning-part-1/>
- Great resource: <https://distill.pub/>
- NASA's Hello Universe initiative: <https://archive.stsci.edu/hello-universe>



# ML Beyond Astronomy: Ethical Considerations





But we are **astronomers**!  
Why should we care  
about **ethics** when it  
comes to **algorithms** and  
**artificial intelligence**?

- Our lives are affected every day by predictions made by algorithms
- Technology and algorithms can be misused
- There is a growing number of studies about the astronomy community
- You might have a future job or side project that is not in astronomy



Algorithms are designed by people, and people embed (unconscious) biases in algorithms, data collection and interpretation of results.



## UTK Faces Dataset



## Biases in training data sets

### Labels

The labels of each face image is embedded in the file name, formated like

`[age]_[gender]_[race]_[date&time].jpg`

- `[age]` is an integer from 0 to 116, indicating the age
- `[gender]` is either 0 (male) or 1 (female)
- `[race]` is an integer from 0 to 4, denoting White, Black, Asian, Indian, and Others (like Hispanic, Latino, Middle Eastern).
- `[date&time]` is in the format of `yyyymmddHHMMSSFFF`, showing the date and time an image was collected to UTKFace

## Ethical Concerns in using Algorithms

- purposeful harm or manipulation
- technological solutionism
- ubiquity, trust
- limited perspective of algorithm writer
- errors in algorithm's implementation
- unrepresentative data sets
- insufficient evaluation metrics
- faulty representations (e.g. in language)
- fairness
- privacy and data rights
- ...

# Deepfake Videos Are Getting Real and That's a Problem

The damaging impact and destabilizing potential of sophisticated video fakery

By Hilke Schellmann

Oct. 15, 2018 11:30 am



Computer-generated videos are getting more realistic and even harder to detect thanks to deep learning and artificial intelligence. As WSJ's Jason Bellini finds in this episode of Moving Upstream, these so-called deepfakes can be playful, but can also have real, damaging consequences for people's lives.



'I was shocked it was so easy': meet the professor who says facial recognition can tell if you're gay



## How a Self-Driving Uber Killed a Pedestrian in Arizona

By TROY GRIGGS and DAISUKE WAKABAYASHI | UPDATED MARCH 21, 2018

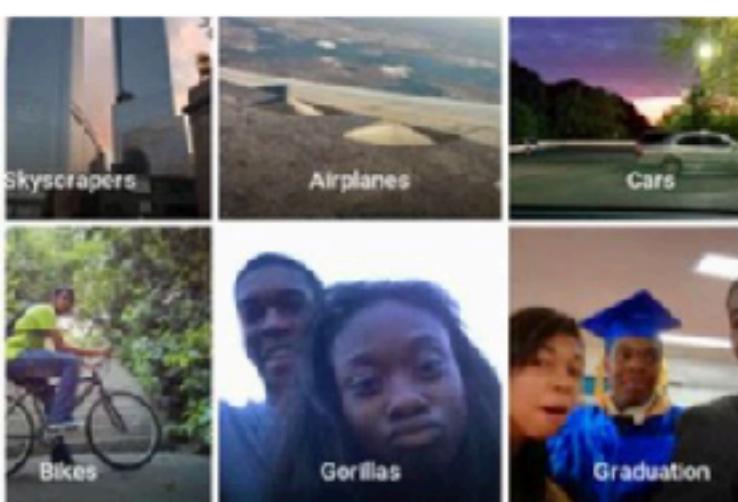
A woman was [struck and killed](#) on Sunday night by an autonomous car operated by Uber in Tempe, Ariz. It was believed to be the first pedestrian death associated with self-driving technology.

DIGITS

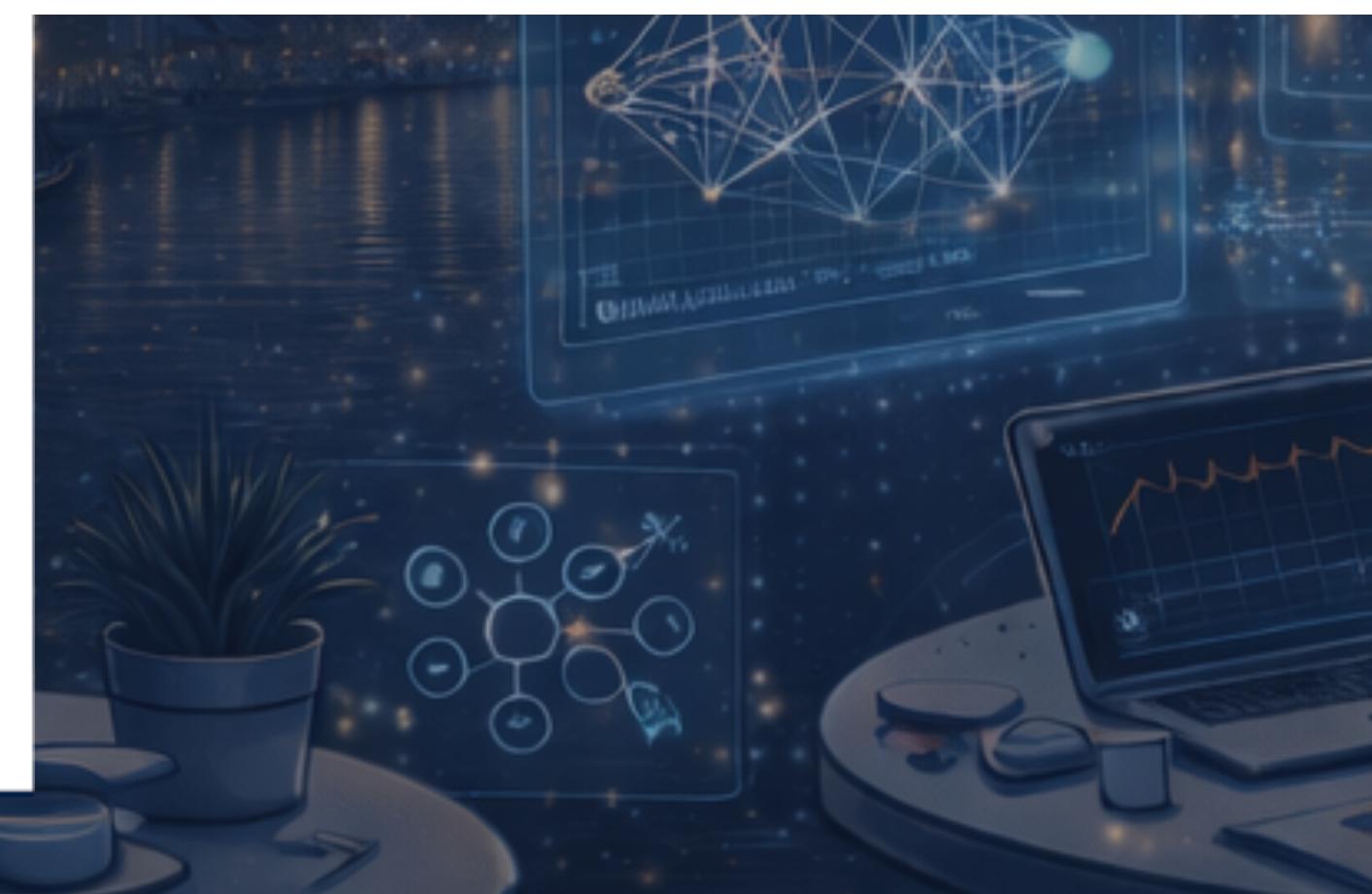
## Google Mistakenly Tags Black People as 'Gorillas,' Showing Limits of Algorithms

By Alistair Barr

Jul 1, 2015 3:40 pm ET

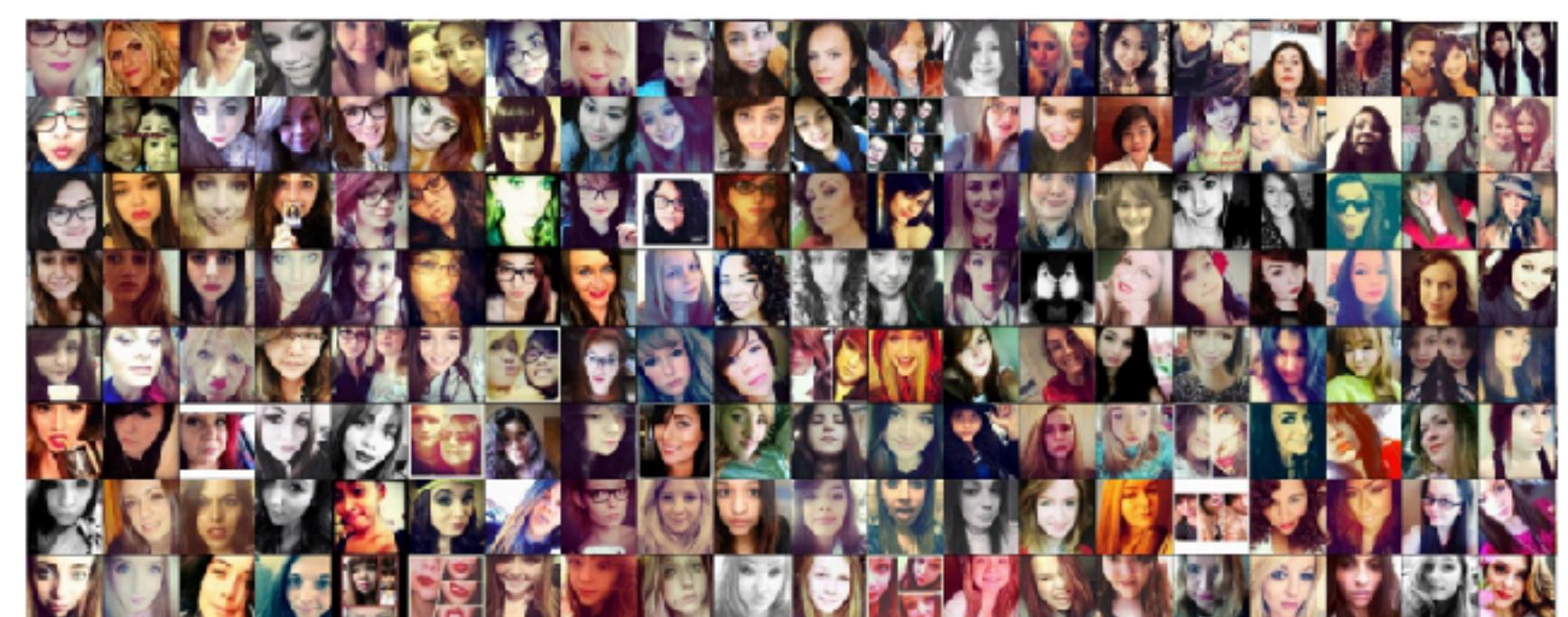


Black programmer Jacky Alcine said on [Twitter](#) that the new Google Photos app had tagged photos of him and a friend as gorillas. JACKY ALCINE AND TWITTER



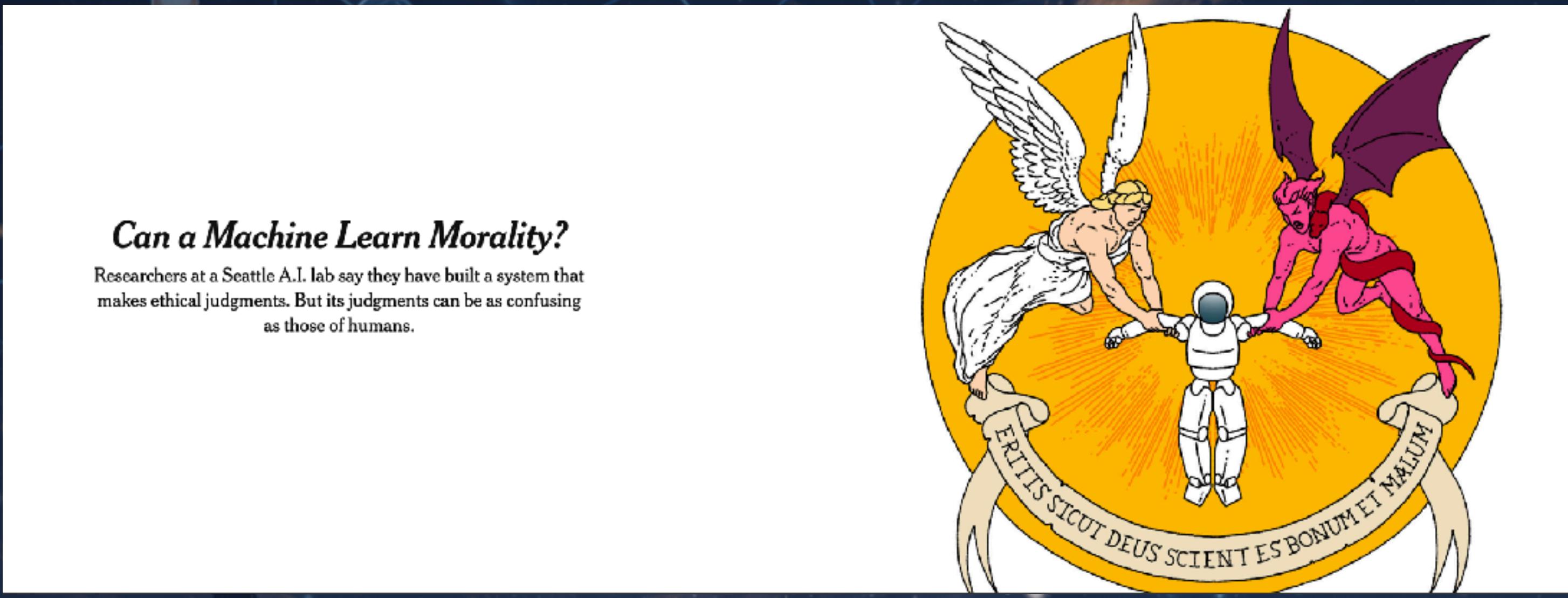
## What a Deep Neural Network thinks about your #selfie

Oct 25, 2015



About Hacker's guide to Neural Networks

Andrey Karpathy blog



## Can a Machine Learn Morality?

Researchers at a Seattle A.I. lab say they have built a system that makes ethical judgments. But its judgments can be as confusing as those of humans.

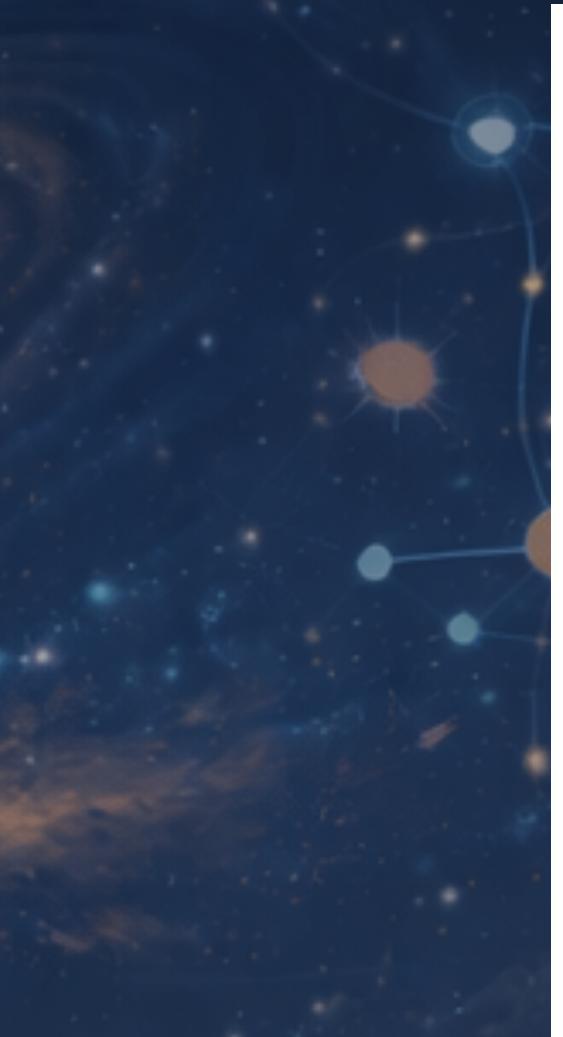
Kate MacKay @KLMacKay · Nov 23  
I just checked out the **Delphi** Morality AI. I asked **#Delphi** 'should people ask computers for **moral** advice?'  
**Delphi** speculates:  
"People shouldn't"  
[delphi.allenai.org/?a1=should+peo...+](http://delphi.allenai.org/?a1=should+peo...+)

\* Input a situation for Delphi to ponder:  
Procrastinating.  
Ponder

Delphi speculates:  
Delphi's responses are automatically extrapolated from a survey of US crowd workers and may contain inappropriate or offensive results.  
"Procrastinating."  
**- It's bad**

Delphi says:

"Bring back dinosaurs  
using genetic  
engineering to create  
theme park jobs."  
**- It's good**



Previously, Delphi said:  
"Being a white man"  
- **is more morally acceptable than** -  
"Being a black woman"

Being a black woman vs. Being a white man

The original prototype of  
Delphi made a number of  
racist, sexist,  
homophobic statements

## Ethical Concerns in using Algorithms



What makes the application of  
algorithms **ethical**?

Why is this **important** at all?

What can we do to ensure that  
we are applying algorithms  
**ethically and responsibly**?



## Data Values & Principles

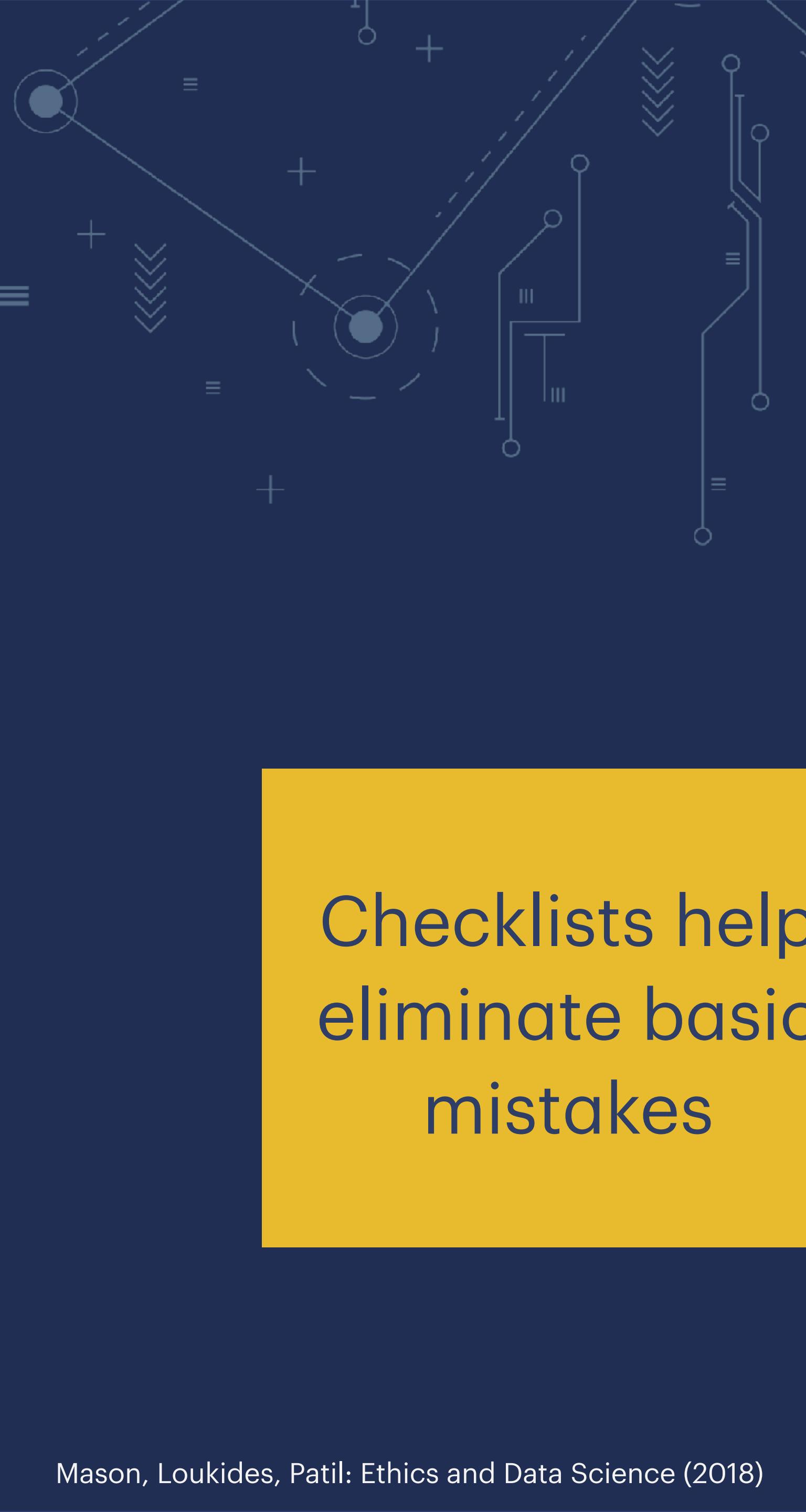
These values and principles, taken together, describe the most effective, ethical, and modern approach to data teamwork.

[READ AND SIGN](#)

## Data Practices Courseware

Consume and collaborate on free and open courses designed to help everyone from the novice to the expert data practitioner.

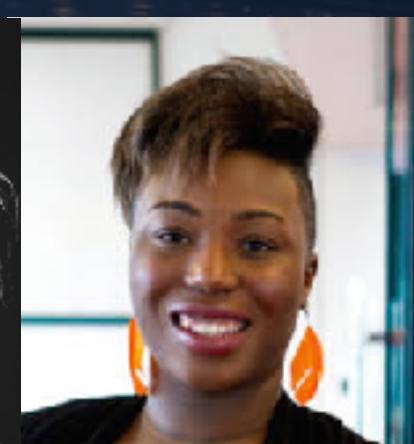
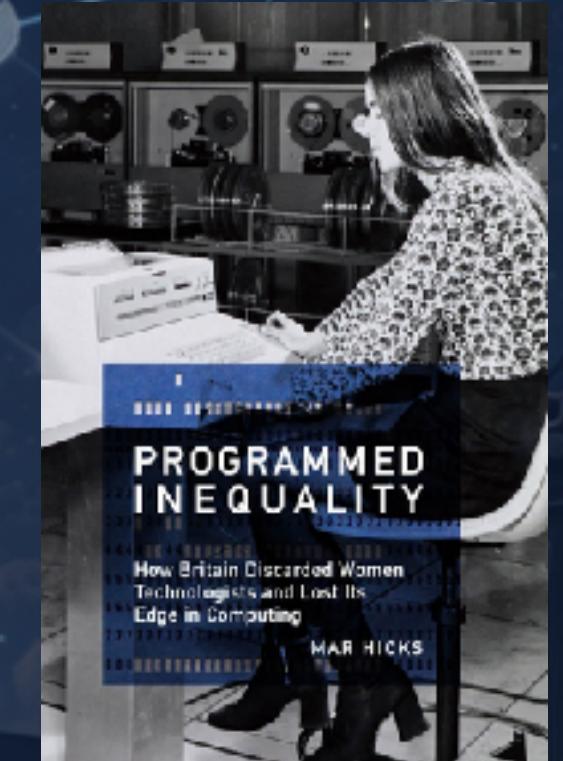
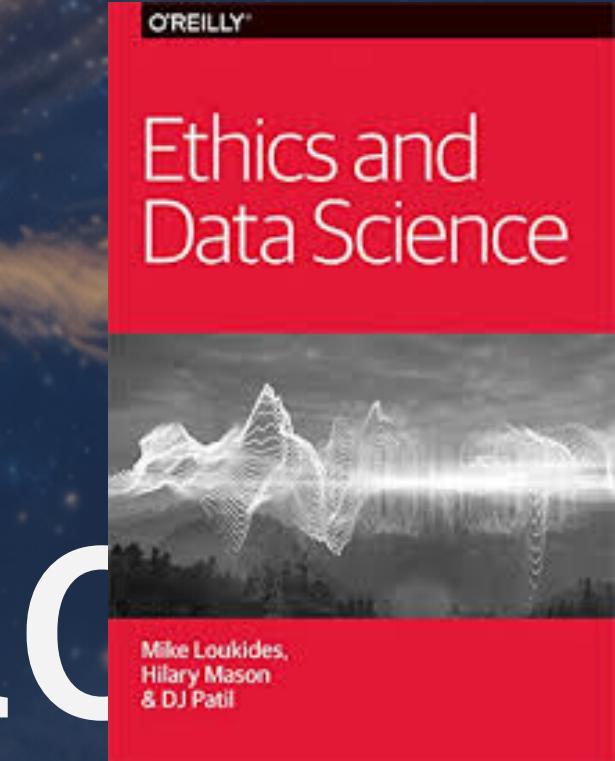
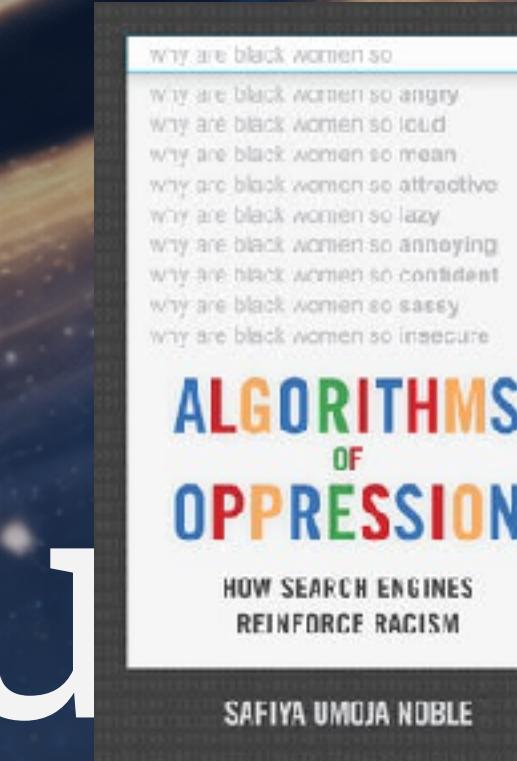
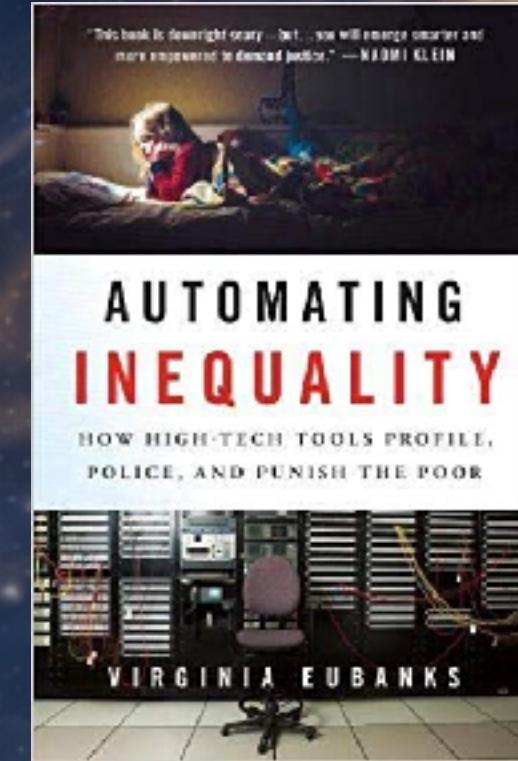
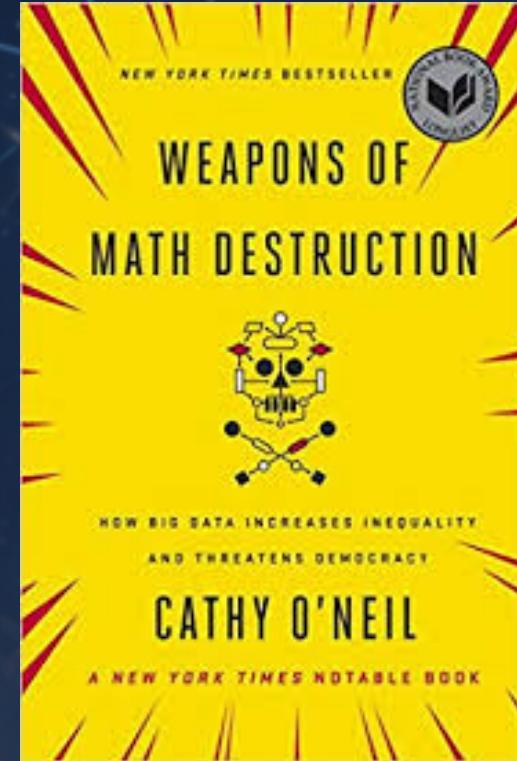
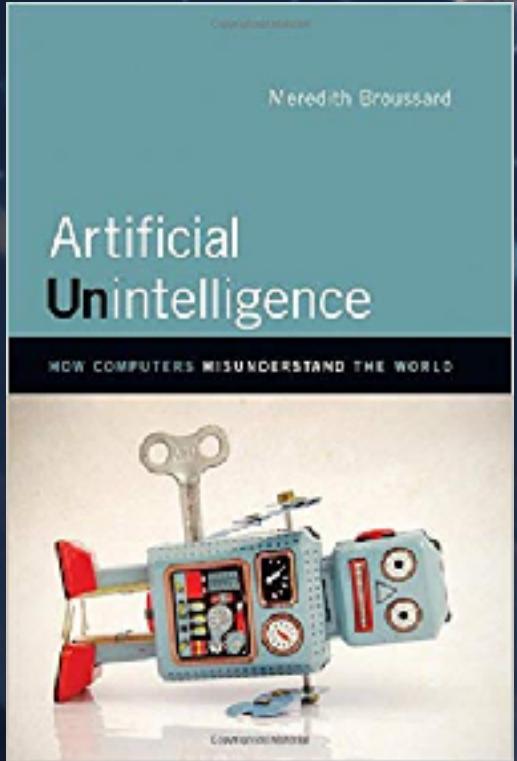
[EXPLORE COURSES](#)



## Checklists help eliminate basic mistakes

- Have we listed how this technology can be attacked or abused?
- Have we tested our training data to ensure it is fair and representative?
- Have we studied and understood possible sources of bias in our data?
- Does our team reflect diversity of opinions, backgrounds, and kinds of thought?
- What kind of user consent do we need to collect to use the data?
- Do we have a mechanism for gathering consent from users?
- Have we explained clearly what users are consenting to?
- Do we have a mechanism for redress if people are harmed by the results?
- Can we shut down this software in production if it is behaving badly?
- Have we tested for fairness with respect to different user groups?
- Have we tested for disparate error rates among different user groups?
- Do we test and monitor for model drift to ensure our software remains fair over time?
- Do we have a plan to protect and secure user data?

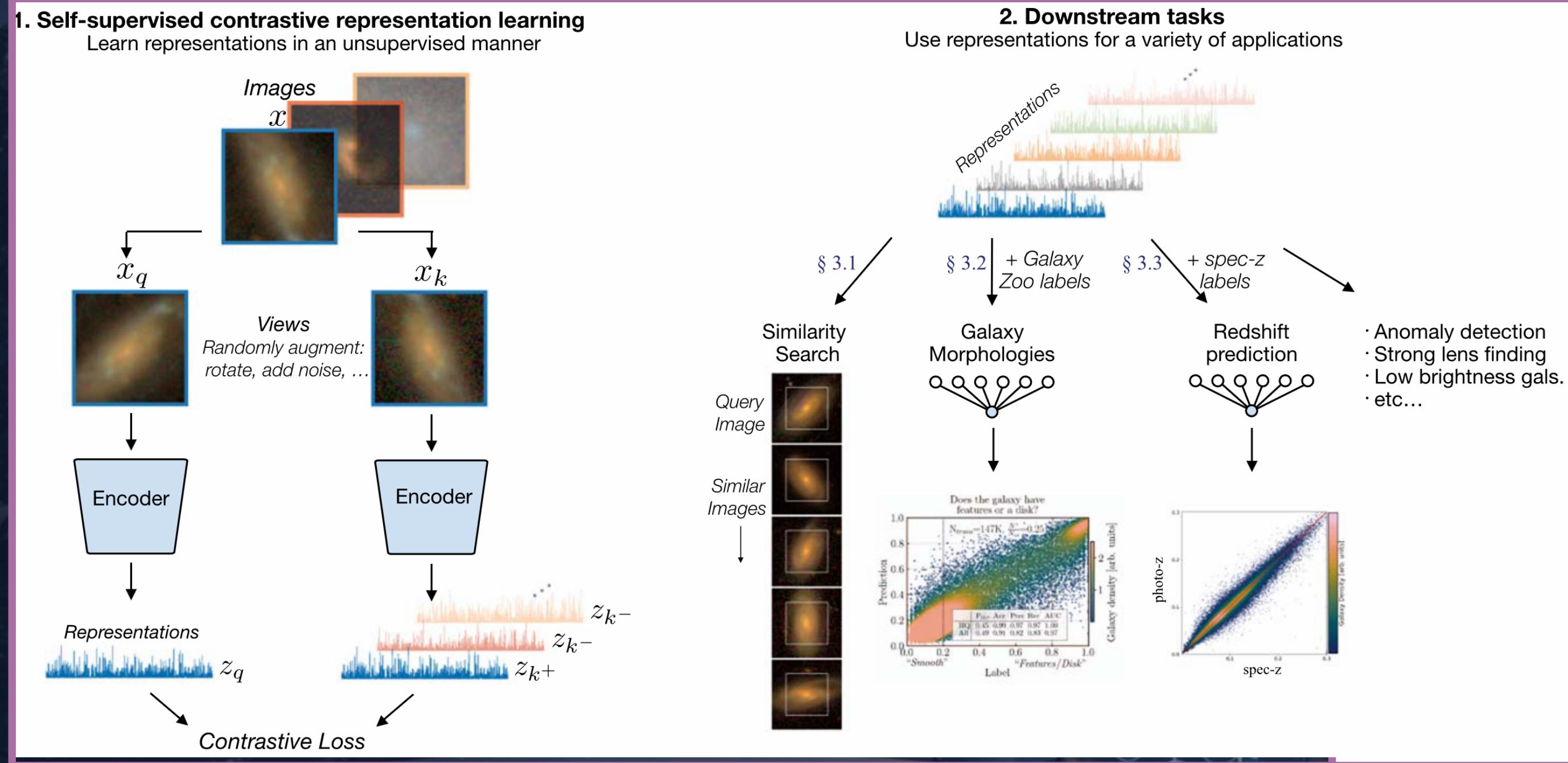
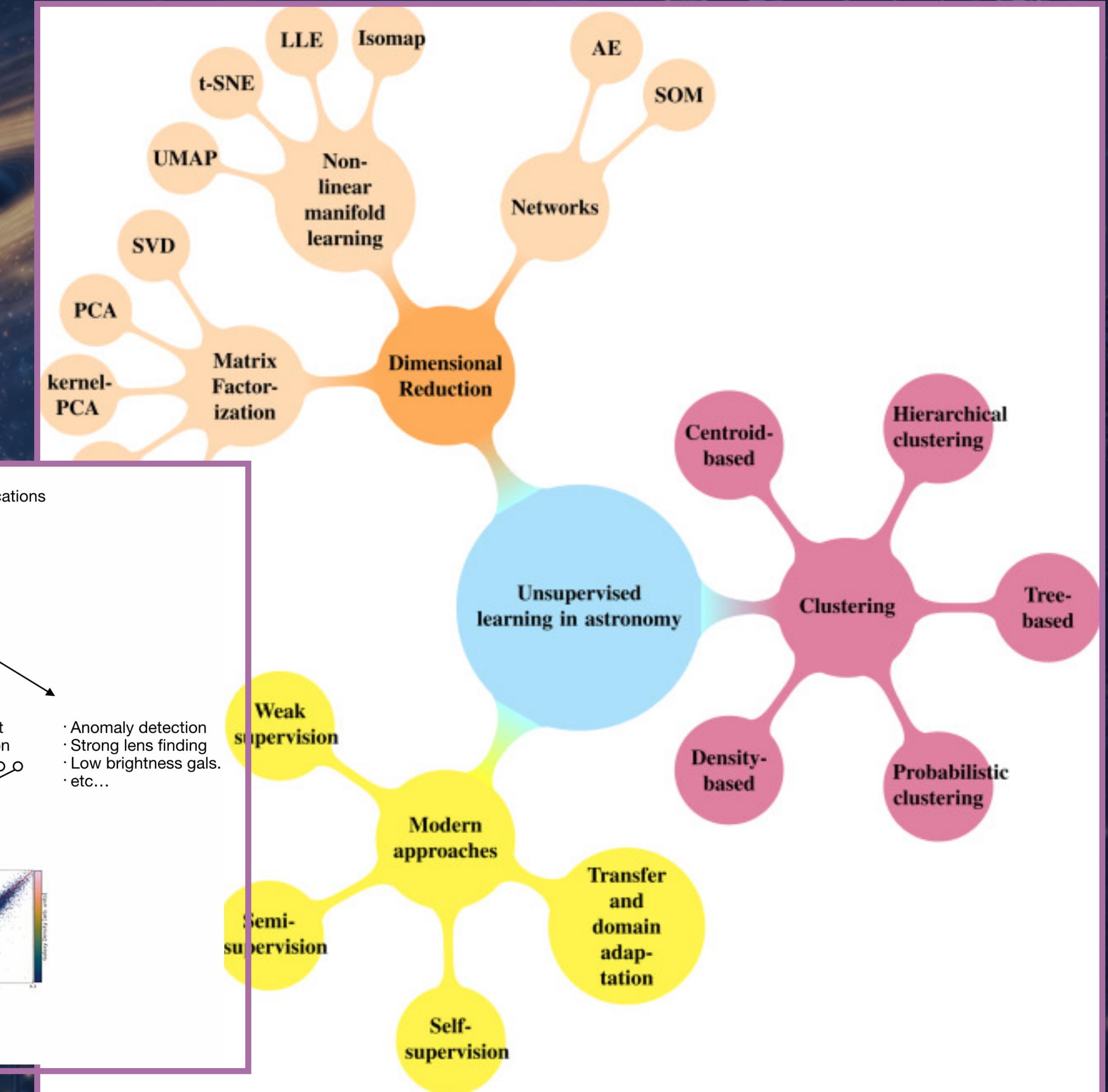
# Resources



# Questions!



# Unsupervised Learning



Hayat et al (2021)

Fotopoulou (2024, arXiv:2406.17316)

# Data Science Challenges in Astronomy

adapted from Hernan (2019)



## Description

How can we split supernovae into different classes?

- Eligibility criteria
- Features
- Representation learning
- Dictionary learning
- Clustering
- ...

## Prediction

What is the probability of an observed supernova to be Type Ia?

- Eligibility criteria
- Features
- Training examples
- (Linear) Regression
- Decision trees
- Neural networks
- ...

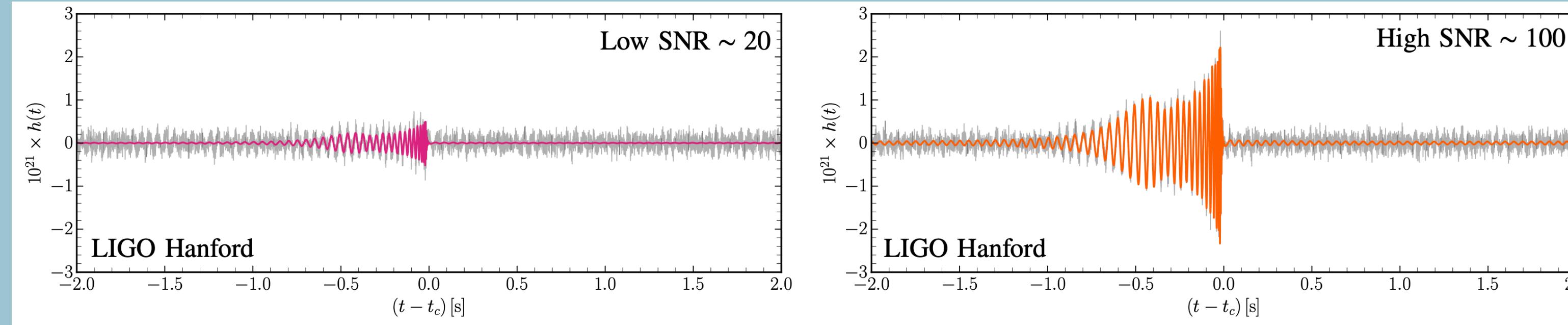
## Inference

Are Type Ia supernovae caused by the explosion of white dwarfs?

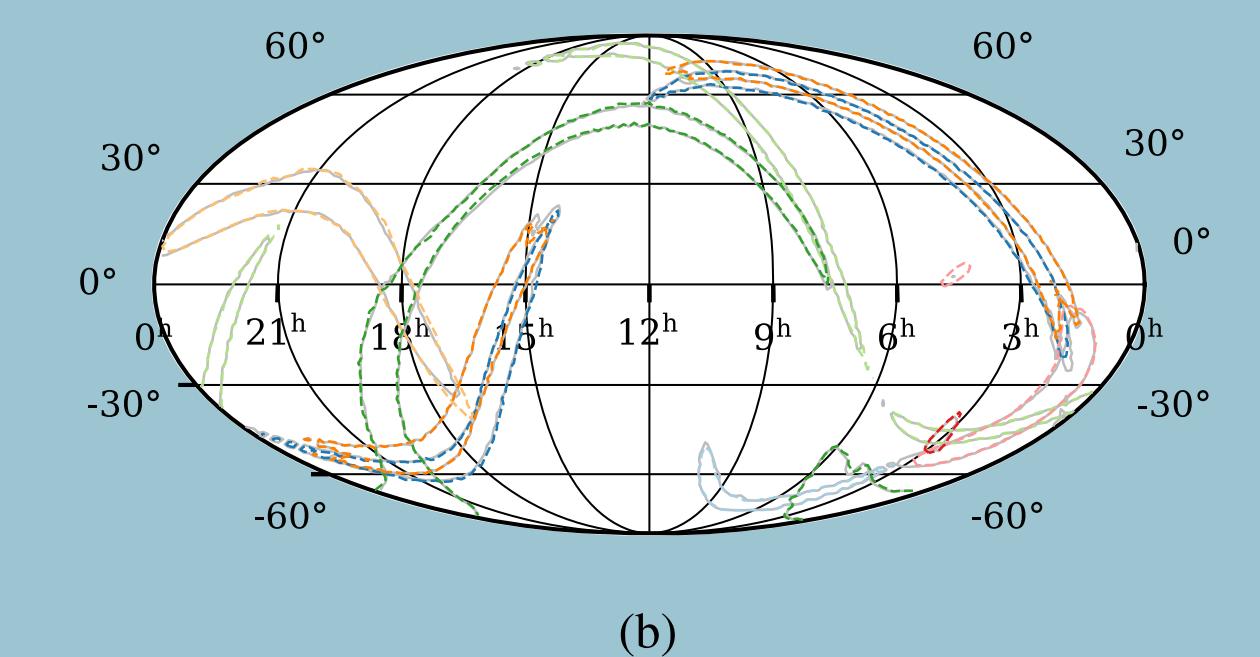
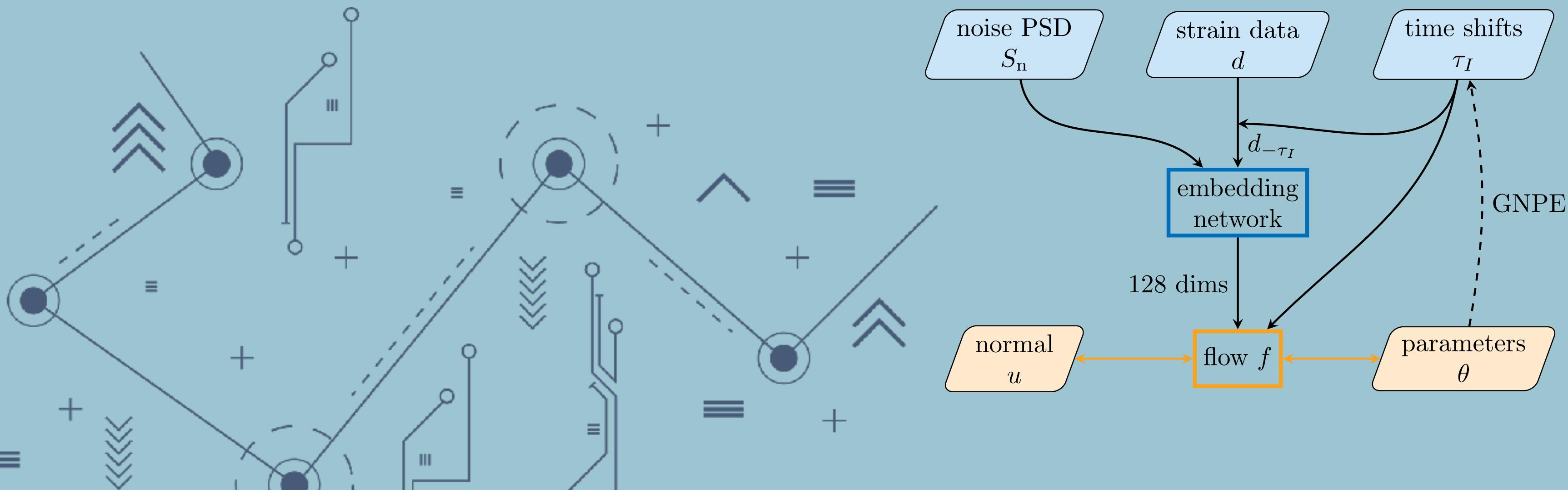
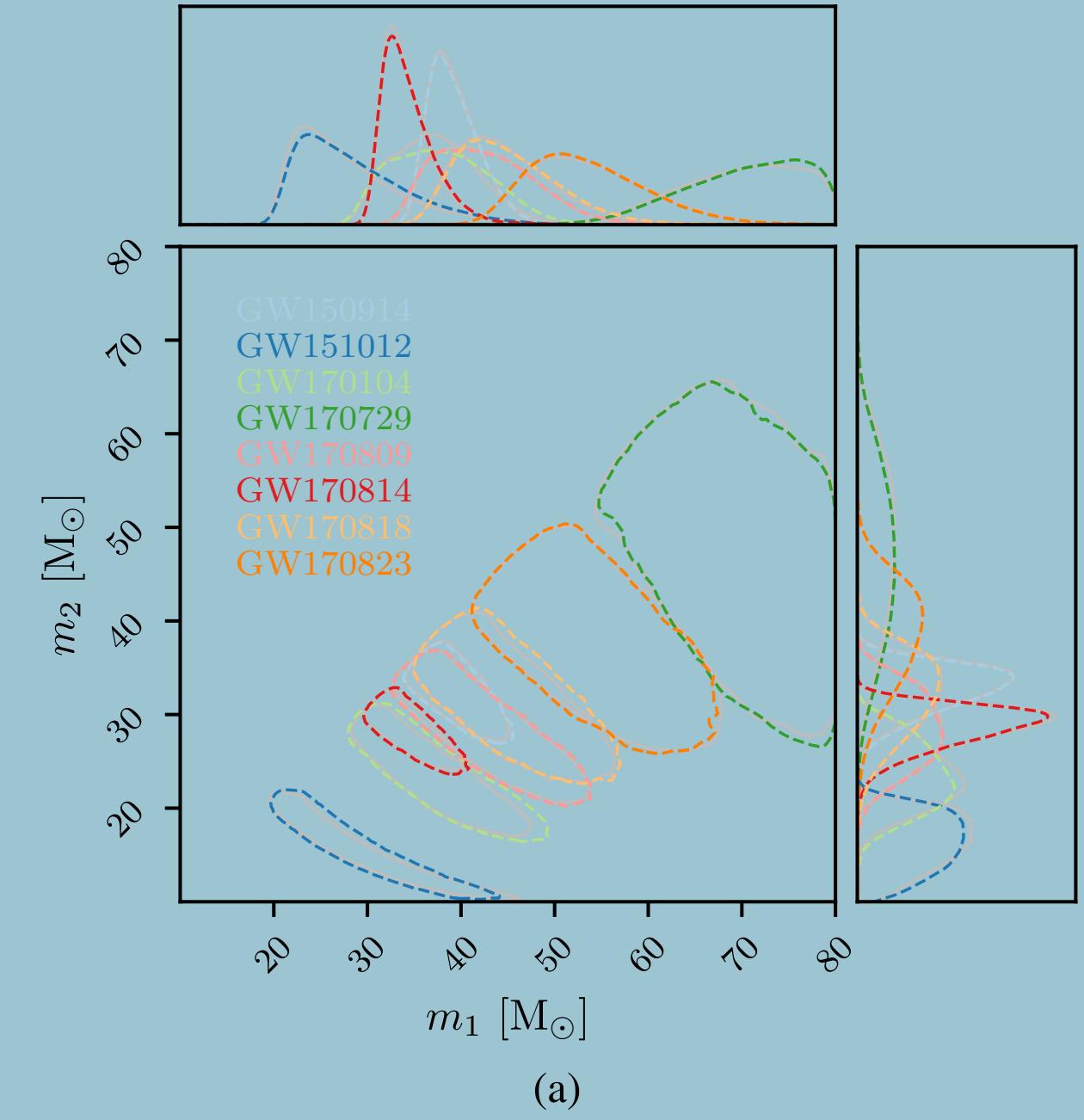
- Eligibility criteria
- Features
- White dwarf explosion model
- (Linear) Regression
- Maximum Likelihood
- Bayesian inference
- Simulation-based inference
- Physics-informed ML

# Gravitational Wave Inference

Bhardwaj et al (2023)



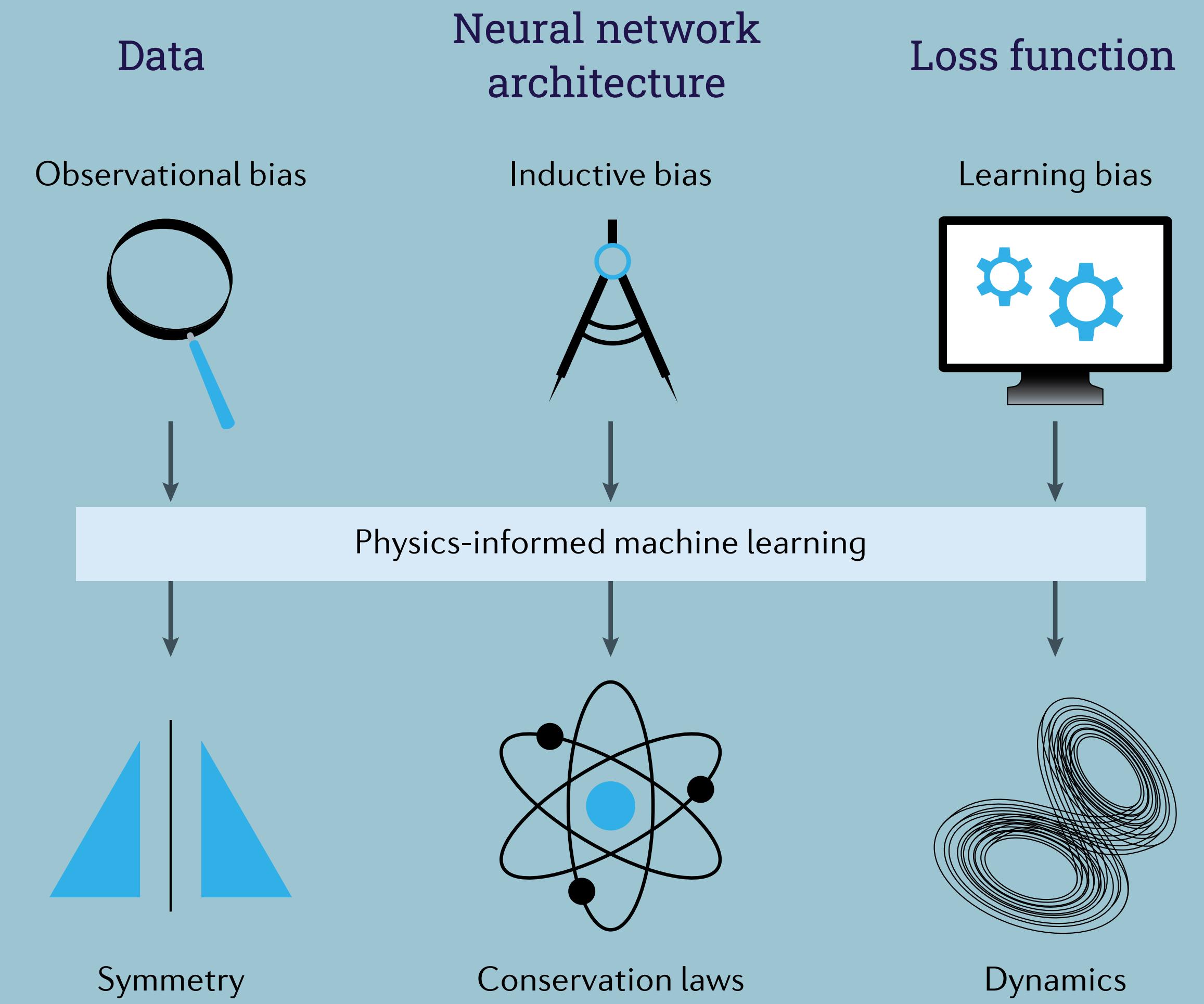
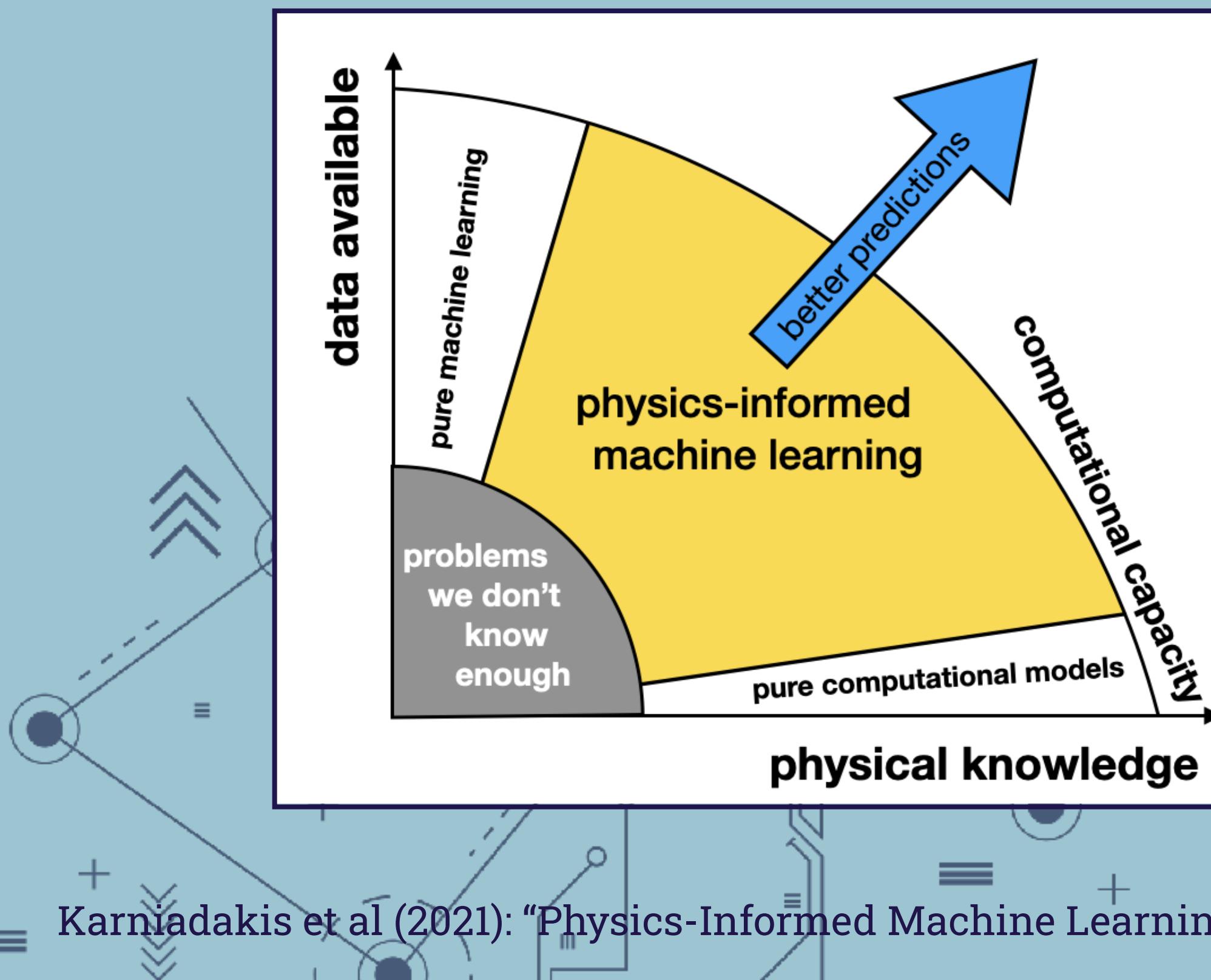
- signals that arrive coincidentally in detectors
- longer signals that are in the presence of non-stationary noise or other shorter transients
- noisy, potentially correlated, coherent stochastic backgrounds



Dax et al (2021)

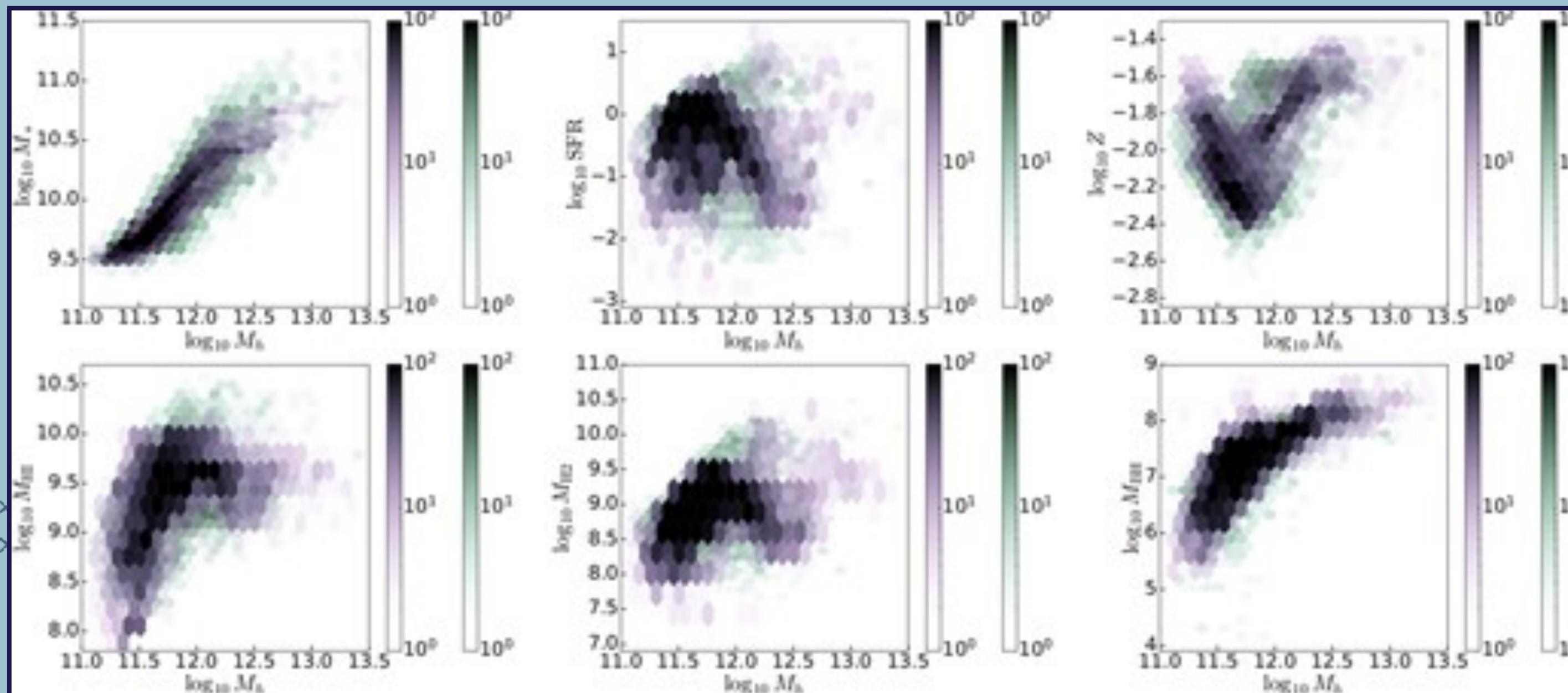
# Physics-Informed Machine Learning

- seamlessly integrate data and mathematical physics models, even in partially understood, uncertain and high-dimensional contexts.
- Learn solutions from severely limited data by constraining neural network architecture and loss functions

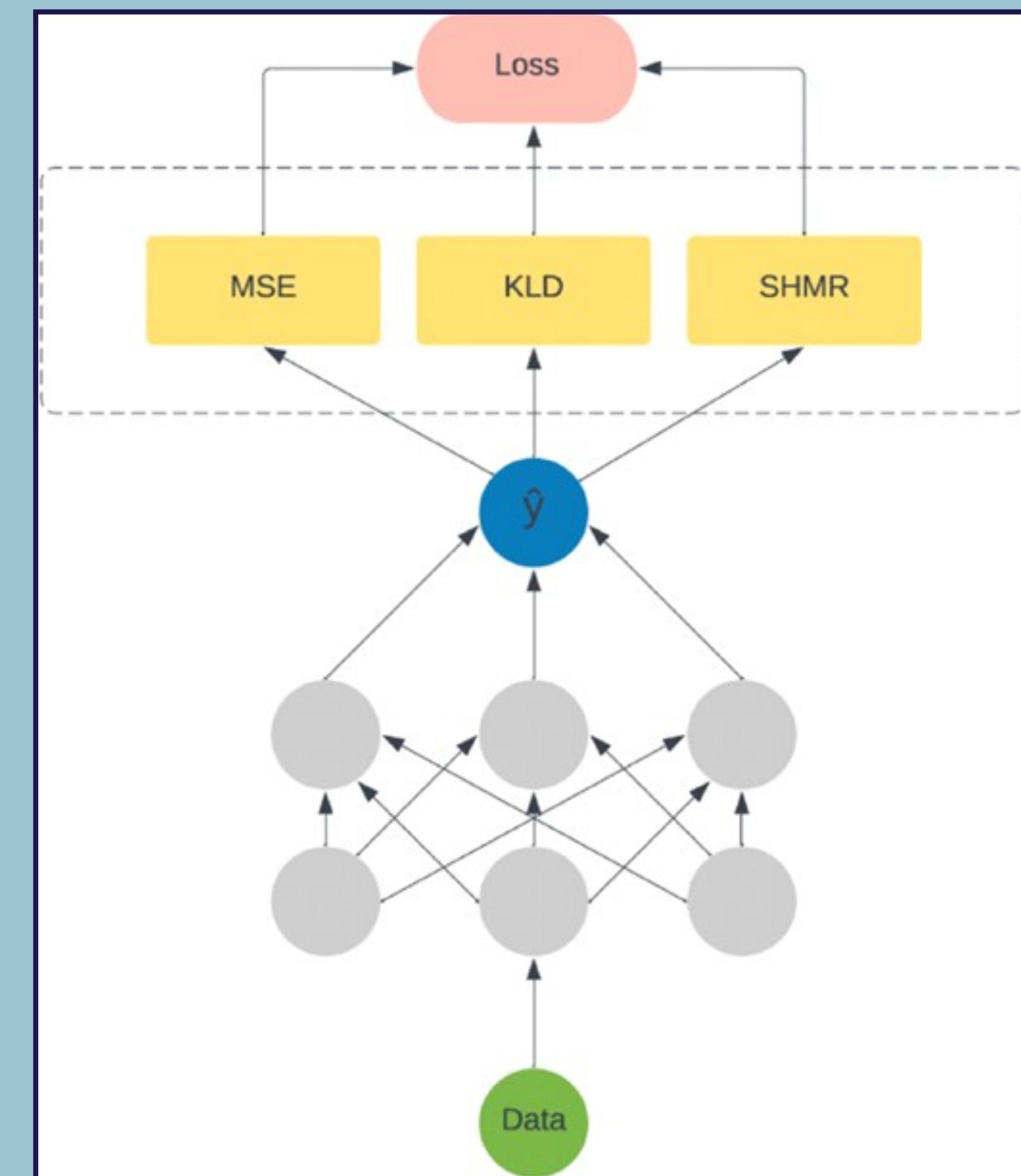


# Baryon Inpainting in Dark Matter Simulations

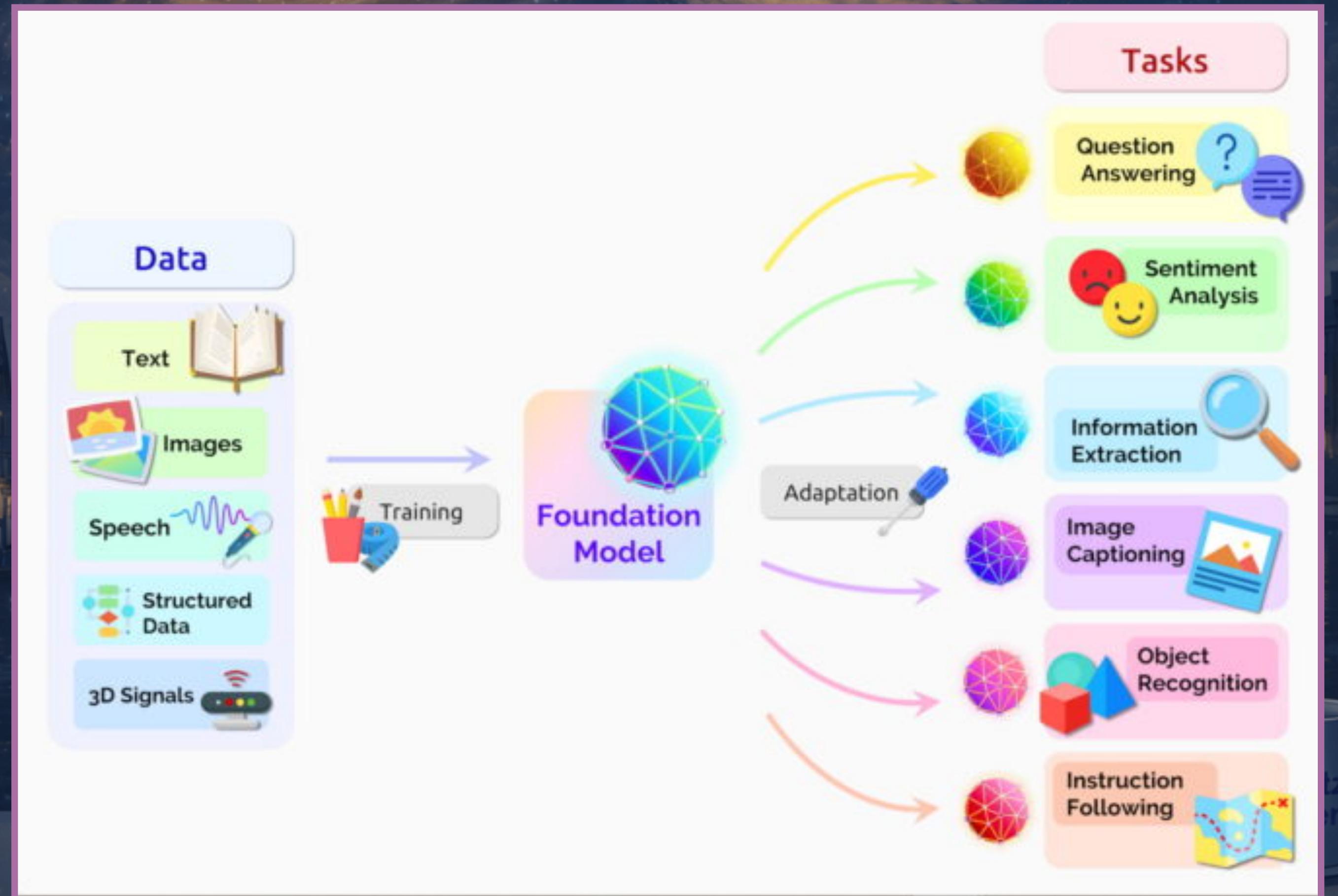
- Dark matter simulations are relatively fast and cheap, but hydrodynamic simulations of baryons are expensive
- Predict limited set of baryon properties from analytical models, then combine with halo properties to predict the complete set of baryons using machine learning
- Incorporate stellar-to-halo mass relation (SHMR) and baryon conversion efficiency into training process



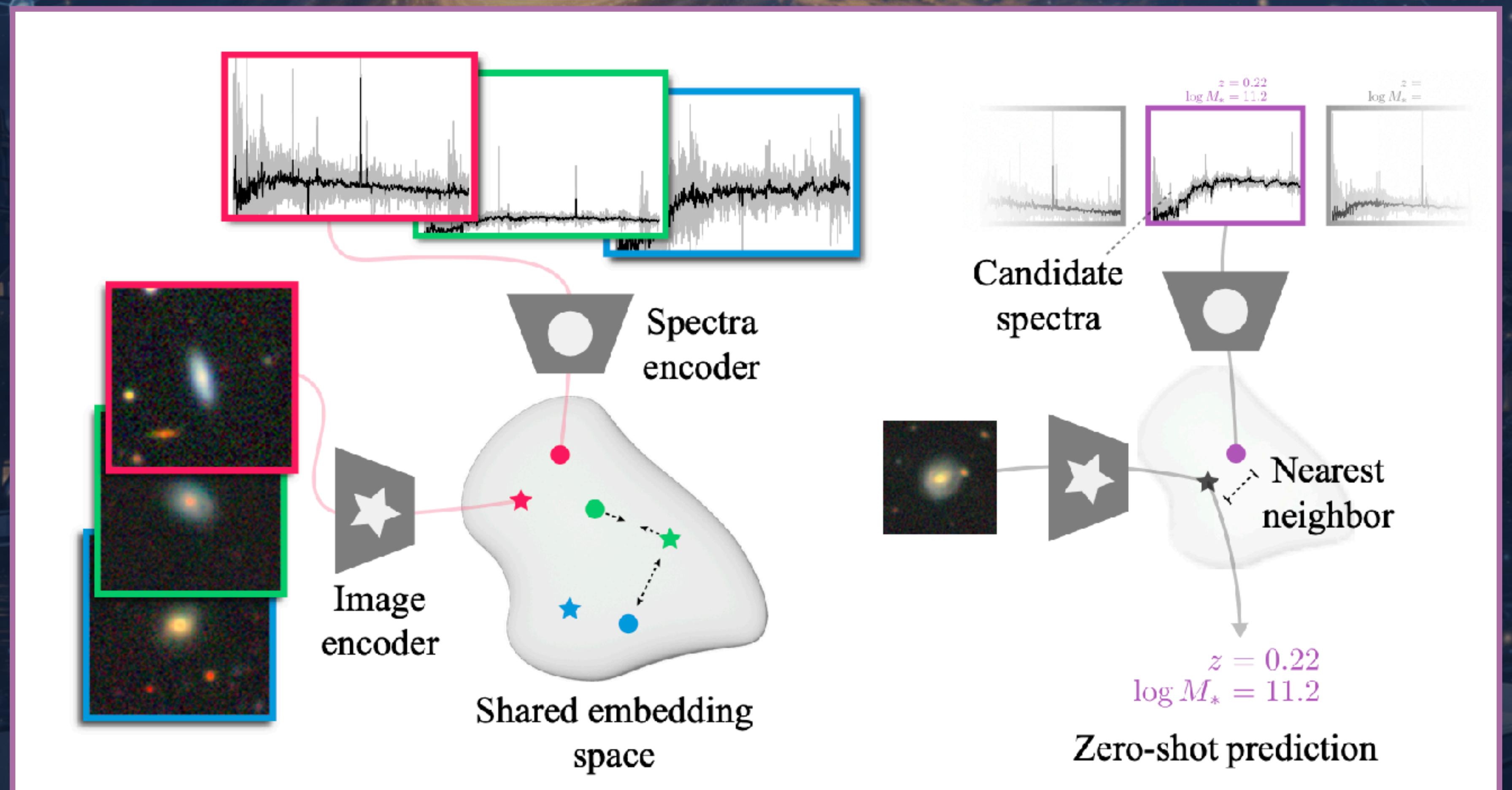
Dai et al (2024)



# Foundation Models



# AstroCLIP



# Challenges

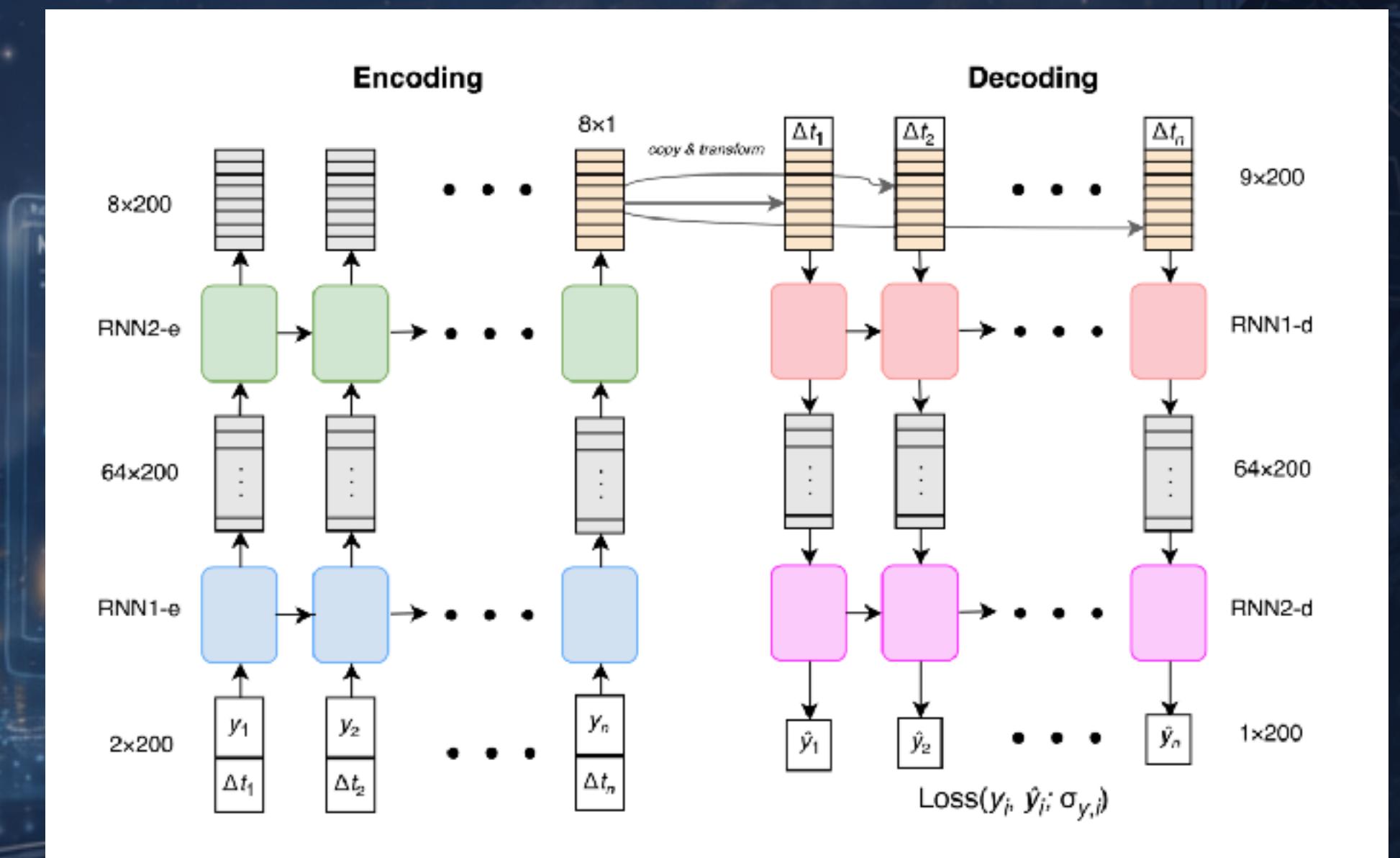
Lorentz  
Center

# Features or no features, that's the question!

Feature	Description
amplitude	Half the difference between the maximum and the minimum magnitude
beyondistd	Percentage of points beyond one st. dev. from the weighted mean
flux_percentile_ratio_mid20	Ratio of flux percentiles (60th - 40th) over (95th - 5th)
flux_percentile_ratio_mid35	Ratio of flux percentiles (67.5th - 32.5th) over (95th - 5th)
flux_percentile_ratio_mid50	Ratio of flux percentiles (75th - 25th) over (95th - 5th)
flux_percentile_ratio_mid65	Ratio of flux percentiles (82.5th - 17.5th) over (95th - 5th)
flux_percentile_ratio_mid80	Ratio of flux percentiles (90th - 10th) over (95th - 5th)
linear_trend	Slope of a linear fit to the light curve fluxes
max_slope	Maximum absolute flux slope between two consecutive observations
median_absolute_deviation	Median discrepancy of the fluxes from the median flux
median_buffer_range_percentage	Percentage of fluxes within 20% of the amplitude from the median
pair_slope_trend	Percentage of all pairs of consecutive flux measurements that have positive slope
percent_amplitude	Largest percentage difference between either the max or min magnitude and the median
percent_difference_flux_percentile	Diff. between the 2nd & 98th flux percentiles, converted to magnitude <sup>a</sup>
QSO	Quasar variability metric in Butler & Bloom (2010)
non_QSO	Non-quasar variability metric in Butler & Bloom (2010)
skew	Skew of the fluxes
small_kurtosis	Kurtosis of the fluxes, reliable down to a small number of epochs
std	Standard deviation of the fluxes
stetson_j	Welch-Stetson variability index J <sup>b</sup>
stetson_k	Welch-Stetson variability index K <sup>b</sup>

<sup>a</sup> Butler & Bloom (2005)

Richards et al (2011)



Naul et al (2017)

# Biased Training Data

ars TECHNICA

BIZ & IT TECH SCIENCE POLICY CARS GAMING & CULTURE FOR



This stop sign has been covered by a full-size replica that includes subtle camo marks. This was 100 percent effective at fooling their machine into thinking it was also a 45mph speed limit sign.

# Biased Training Data

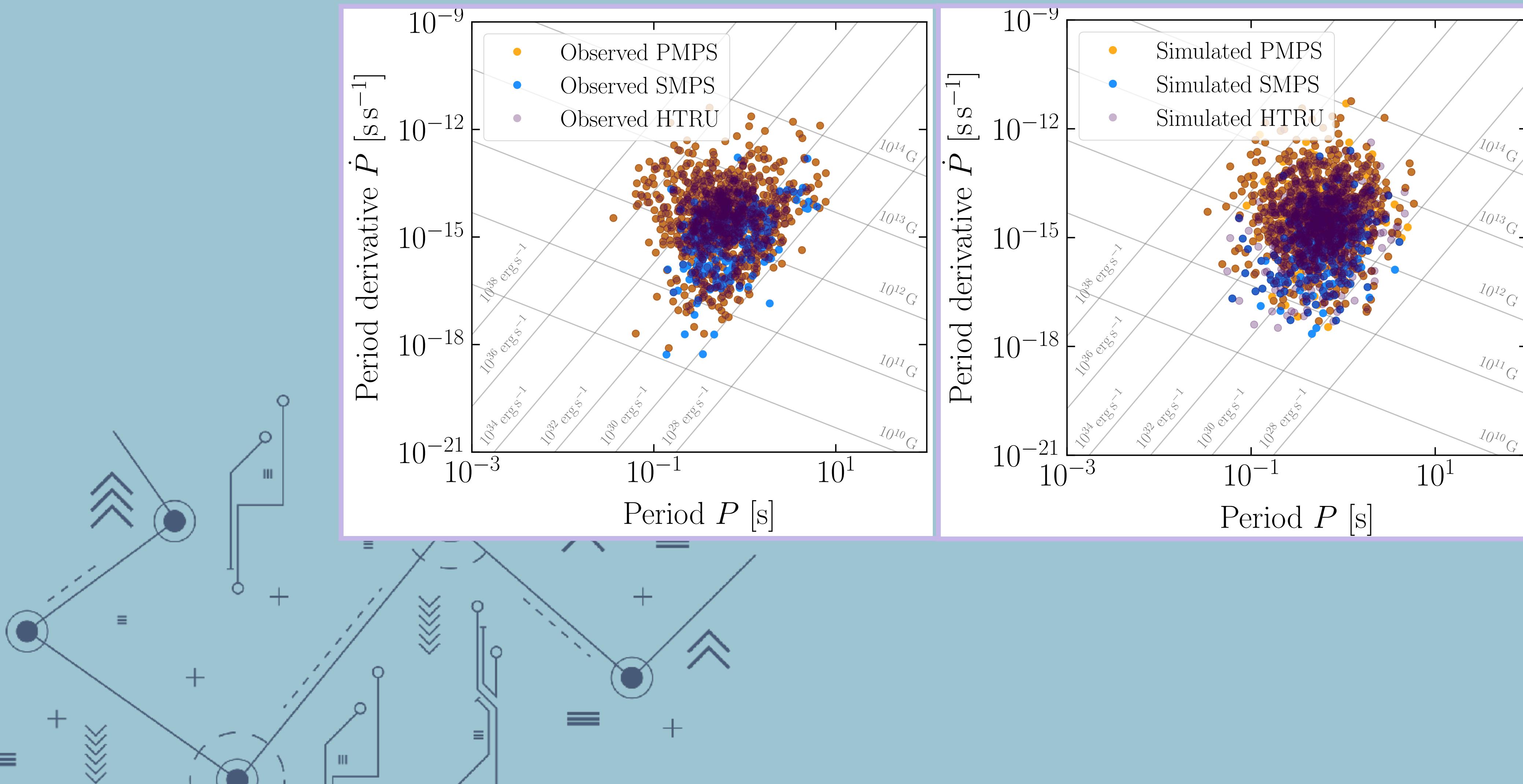
## GALAXY ZOO: MORPHOLOGICAL CLASSIFICATION AND CITIZEN SCIENCE

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The results of the mirror image bias testing are discussed extensively in Land et al. (2008). They showed a significant bias in favour of anti-clockwise direction arms (in both the original and mirrored images). The interpretation of this bias could be due to psychological effects (possibly related to the preference for right handedness amongst the population), or possibly site design (it being easier to click the anti-clockwise button for example). However, once this bias was corrected for, the data could still be used (see below).

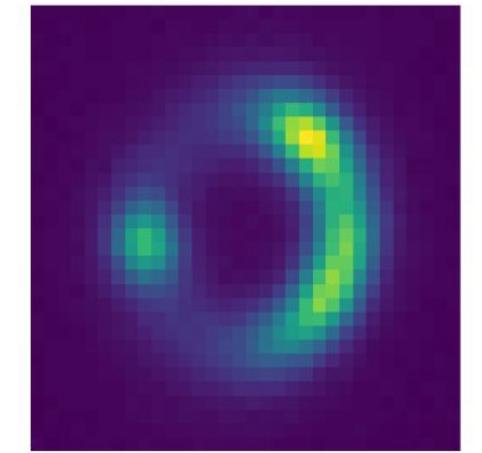
# Challenge: Out-of-domain target data



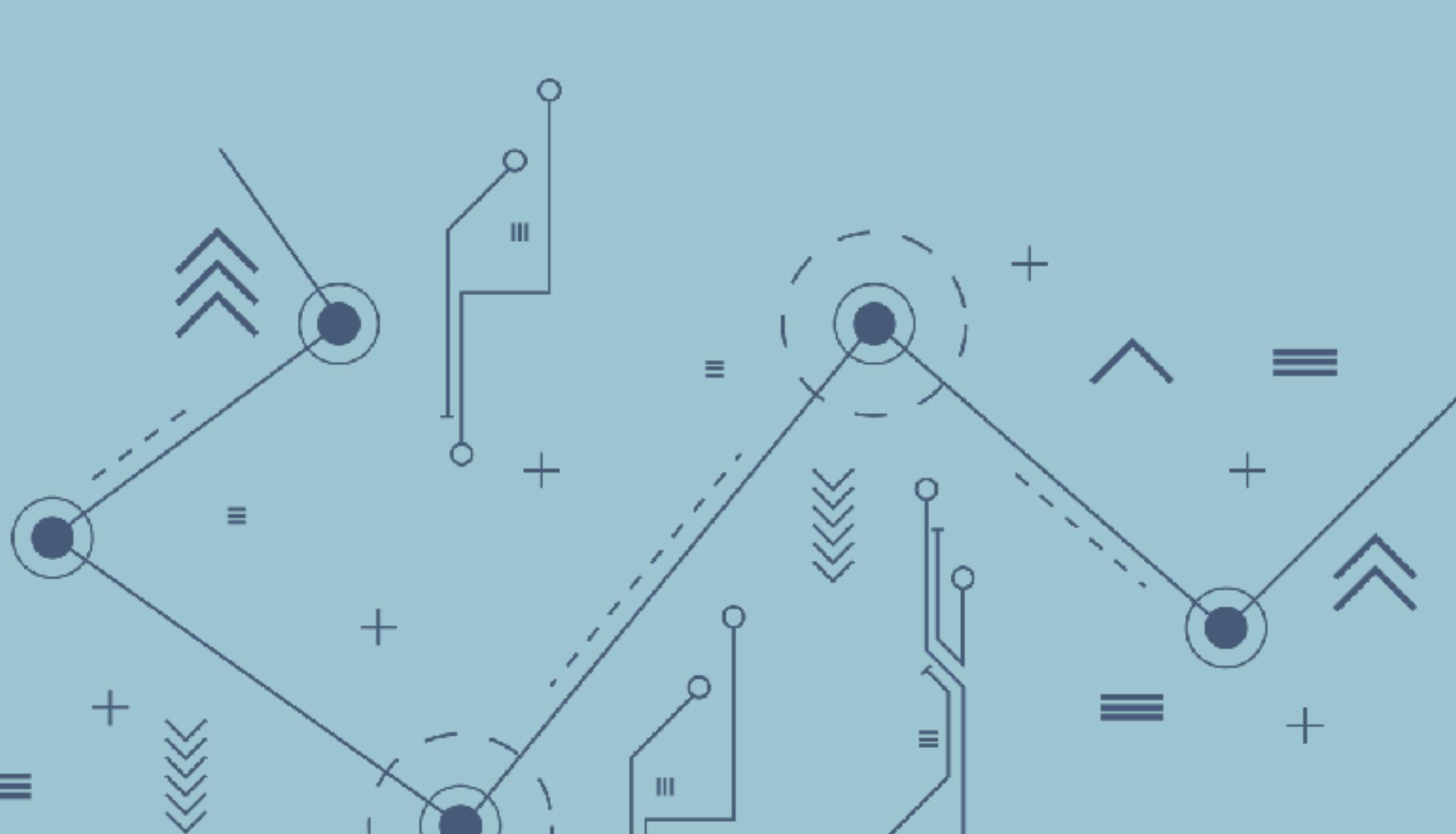
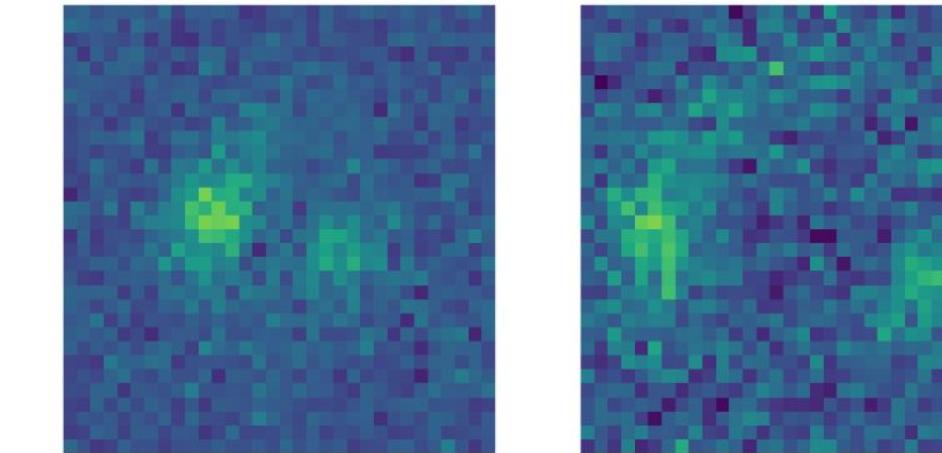
# Solution: Unsupervised Domain Adaptation

(a)

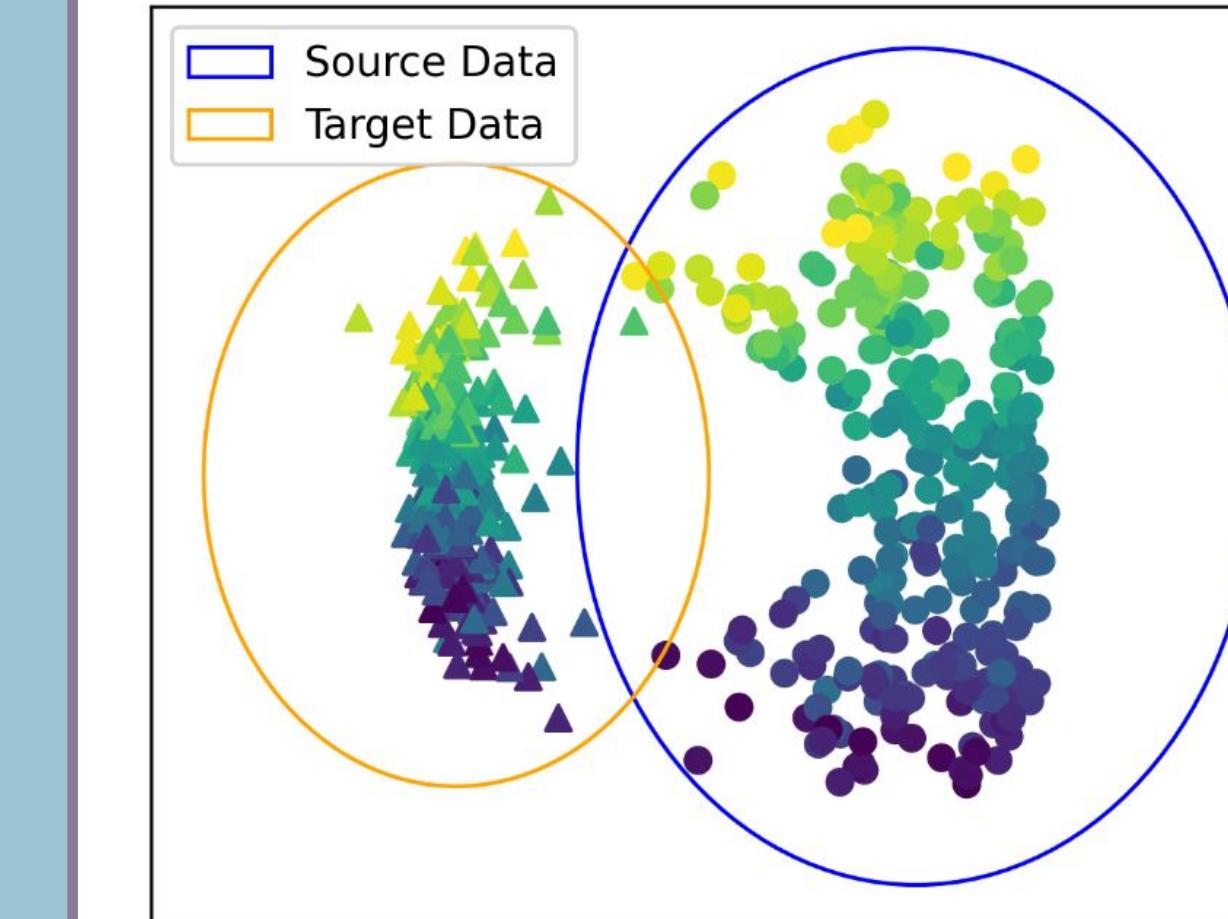
Source



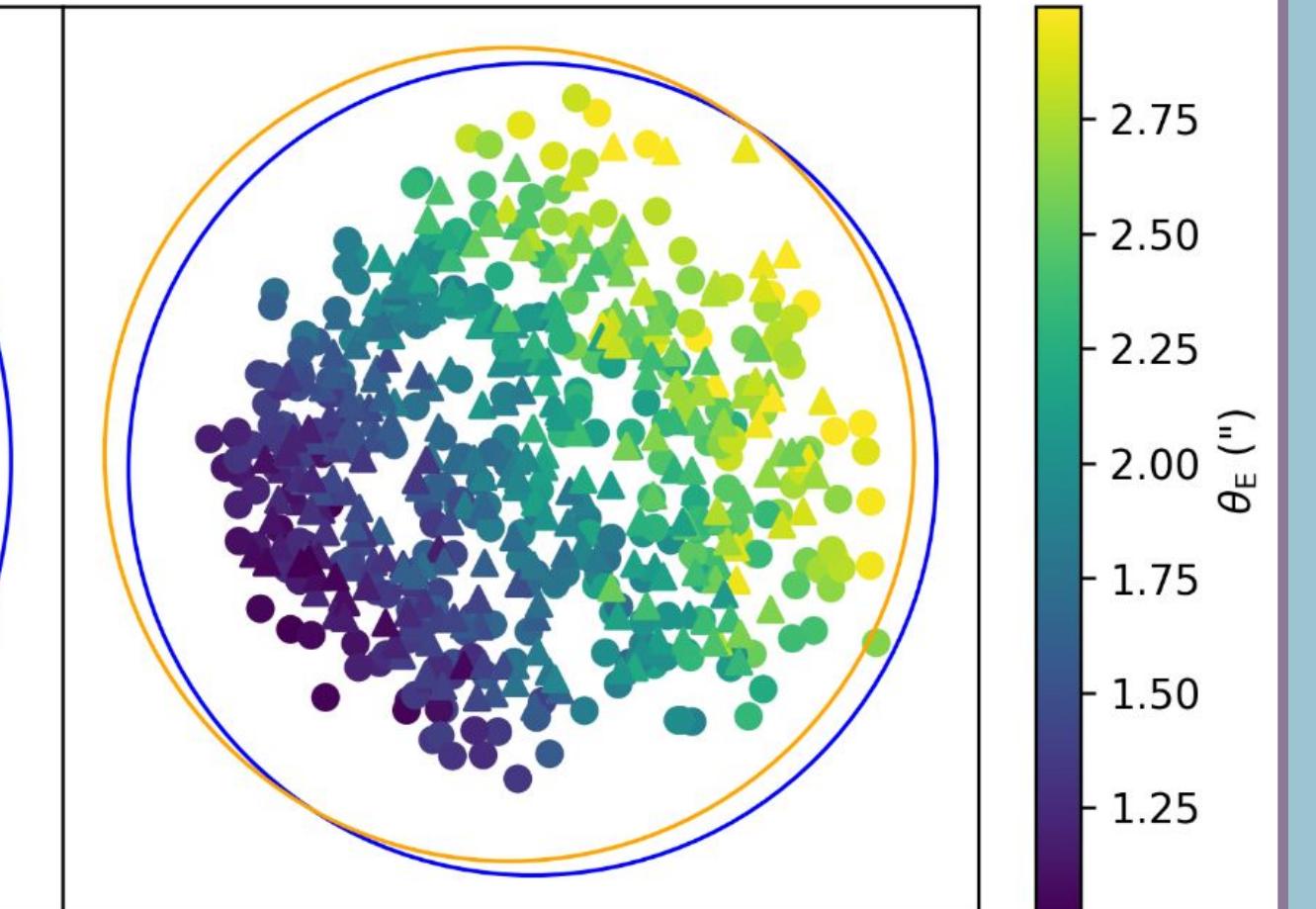
Target



NPE-only



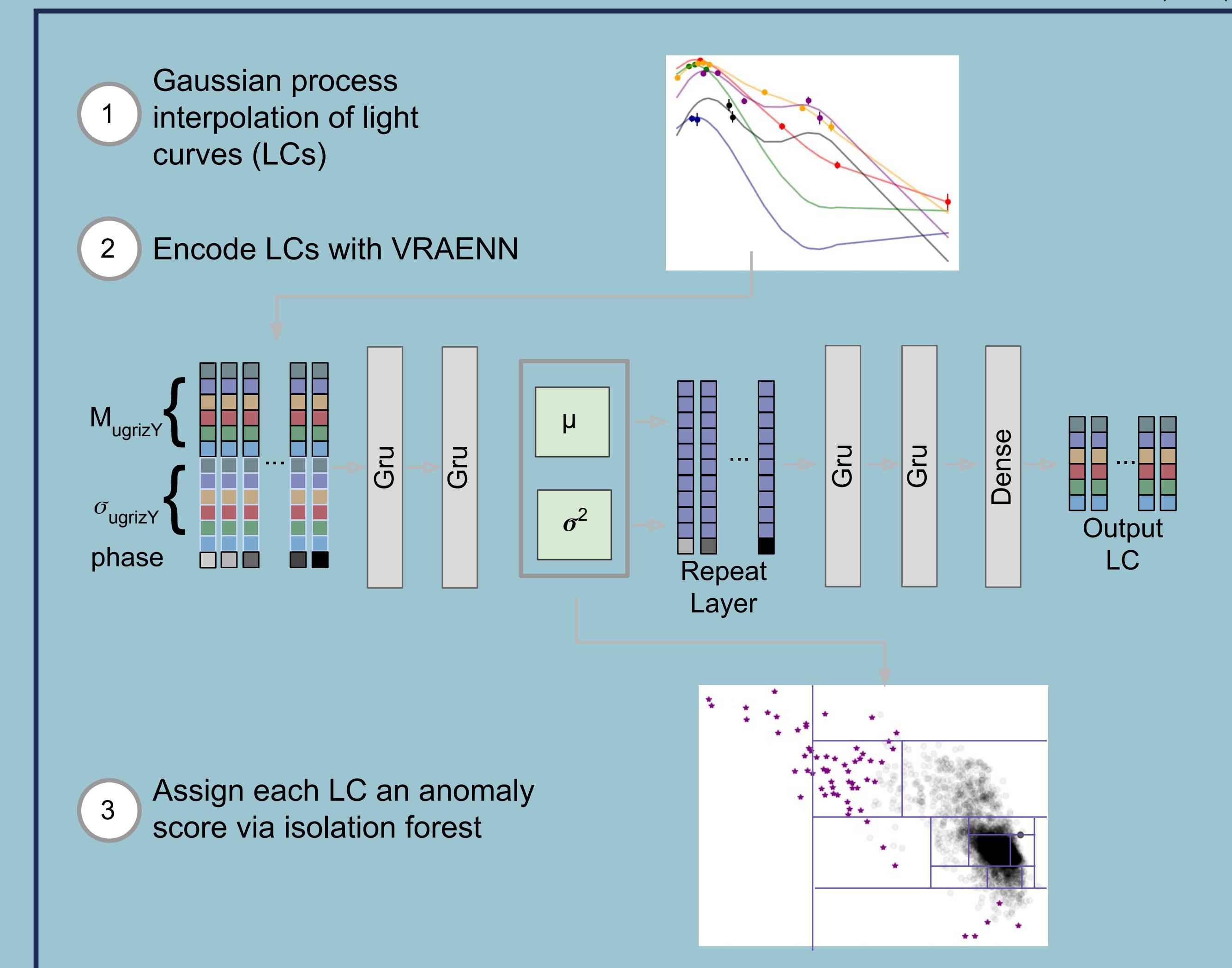
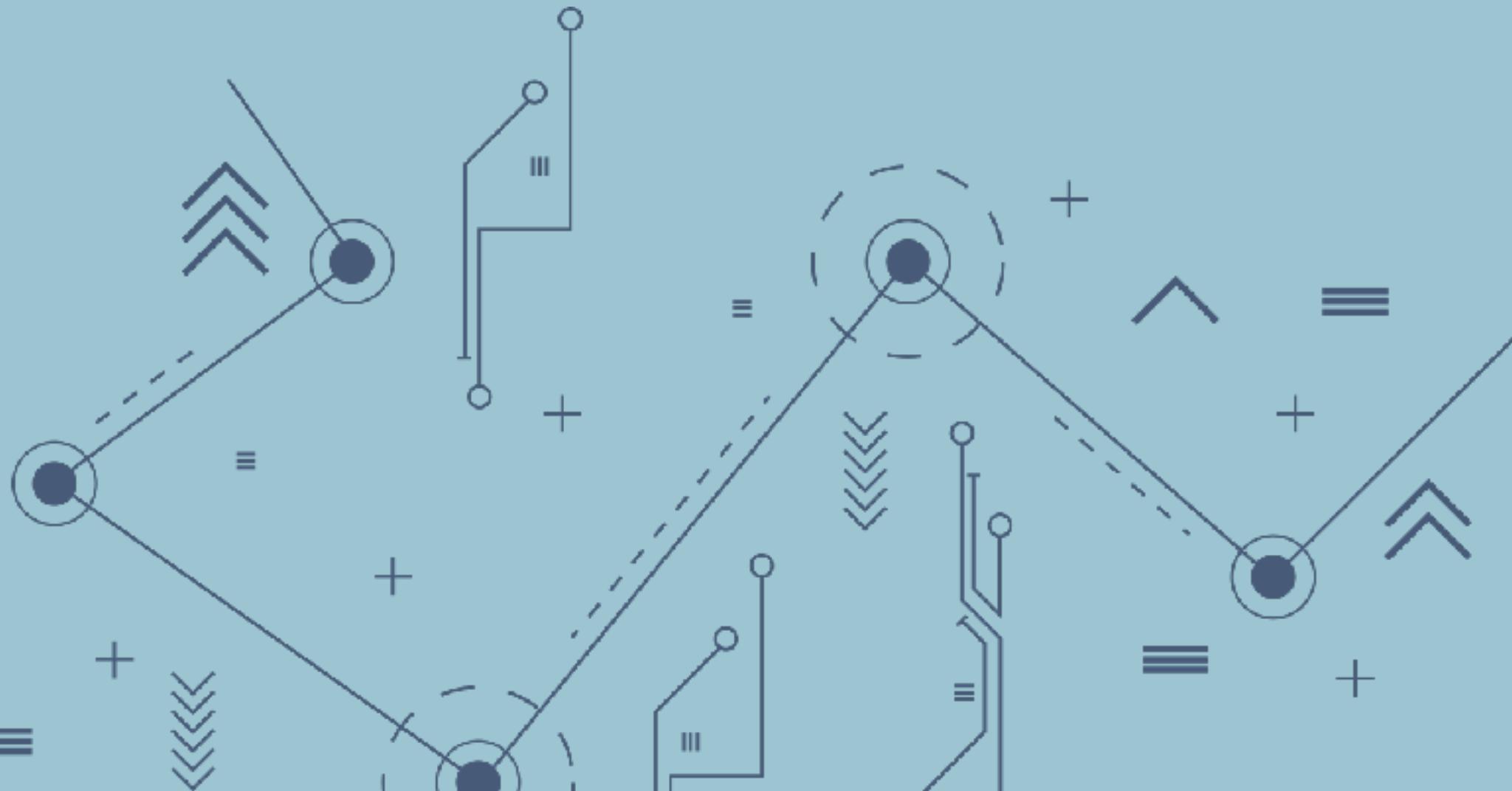
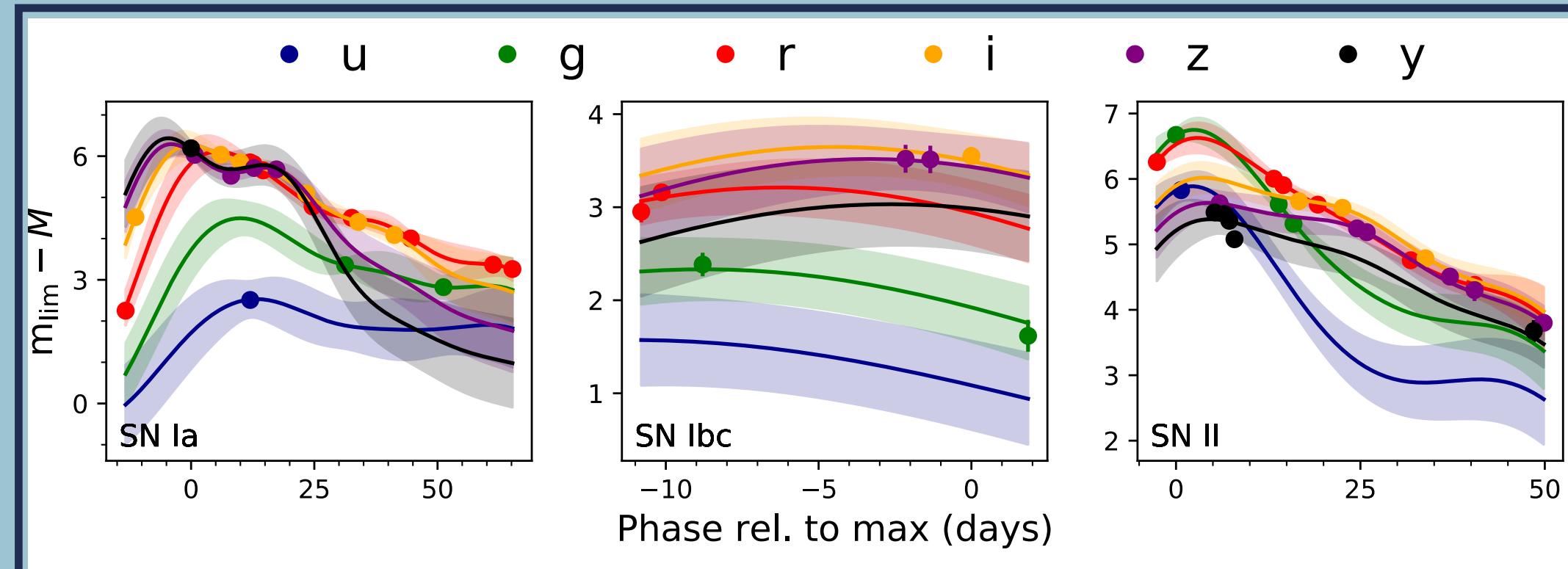
NPE-UDA



Swirl et al (2024)

# Out-of-distribution data: Anomaly detection in transients

Villar et al (2020)



# Confirmation bias

If simulations are prohibitively expensive, we might only check a neural network emulator's results if they are surprising.

(See also: David Hogg “Is Machine learning Useful for Astrophysics?”)

