Introduction to machine learning

Thomas Stoeger, Northwestern University

Slides:

https://bit.ly/3bKMrhM

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demystify

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orientation

demystify

orientation

coding

demystify → understand conceptual possibilities

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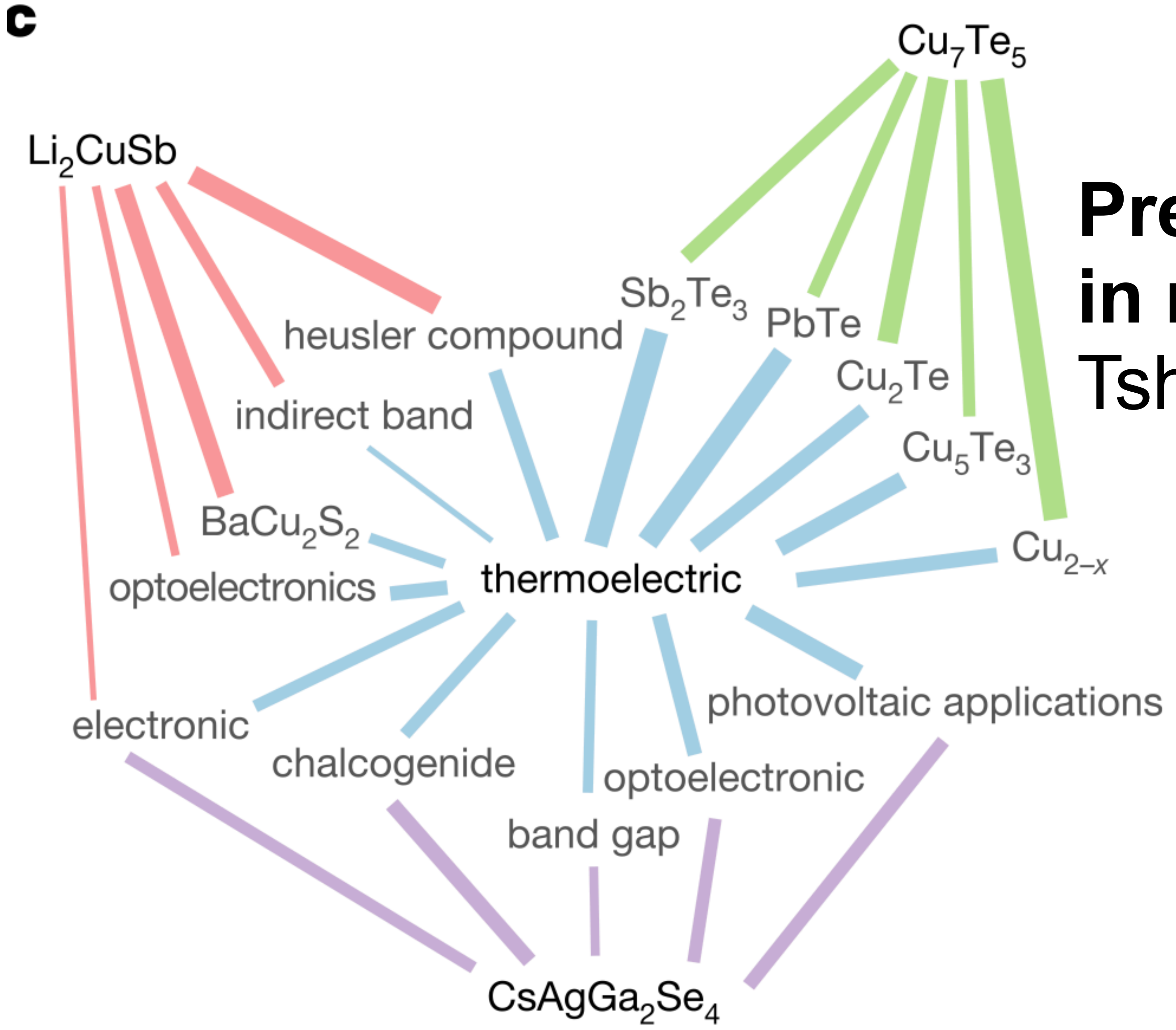
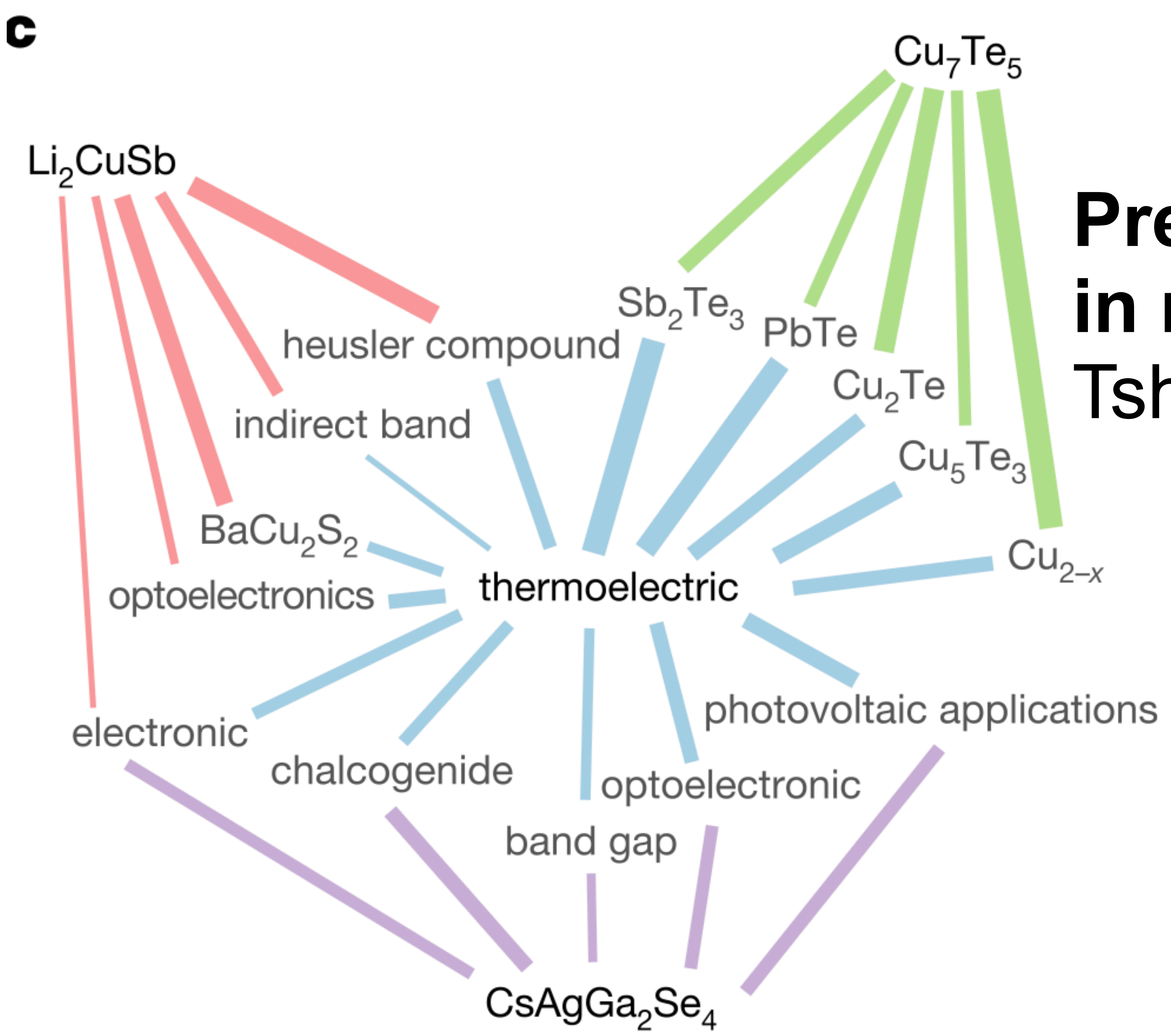


Predict future discoveries in material science

Tshitoyan et al., Nature, 2019



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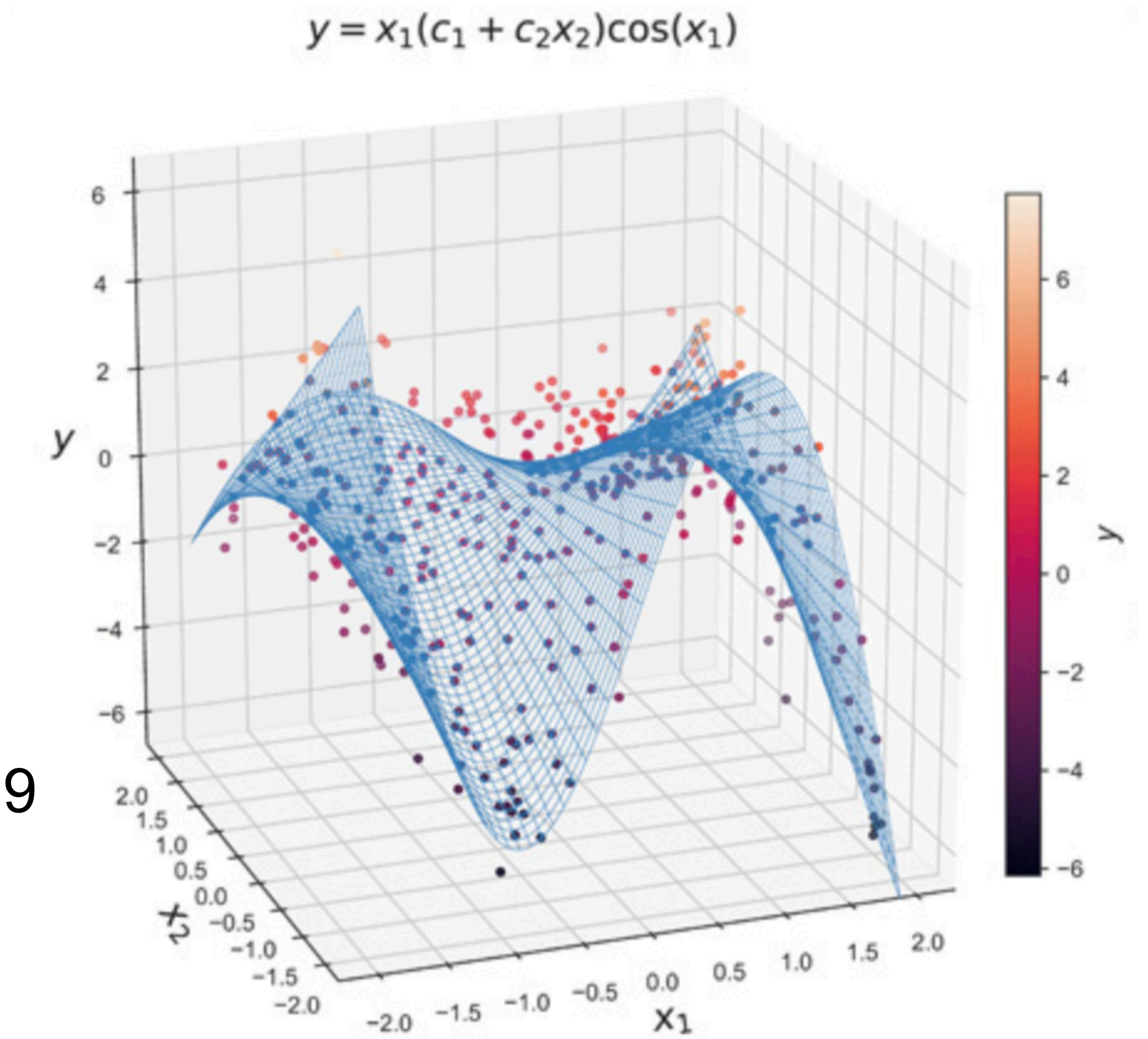
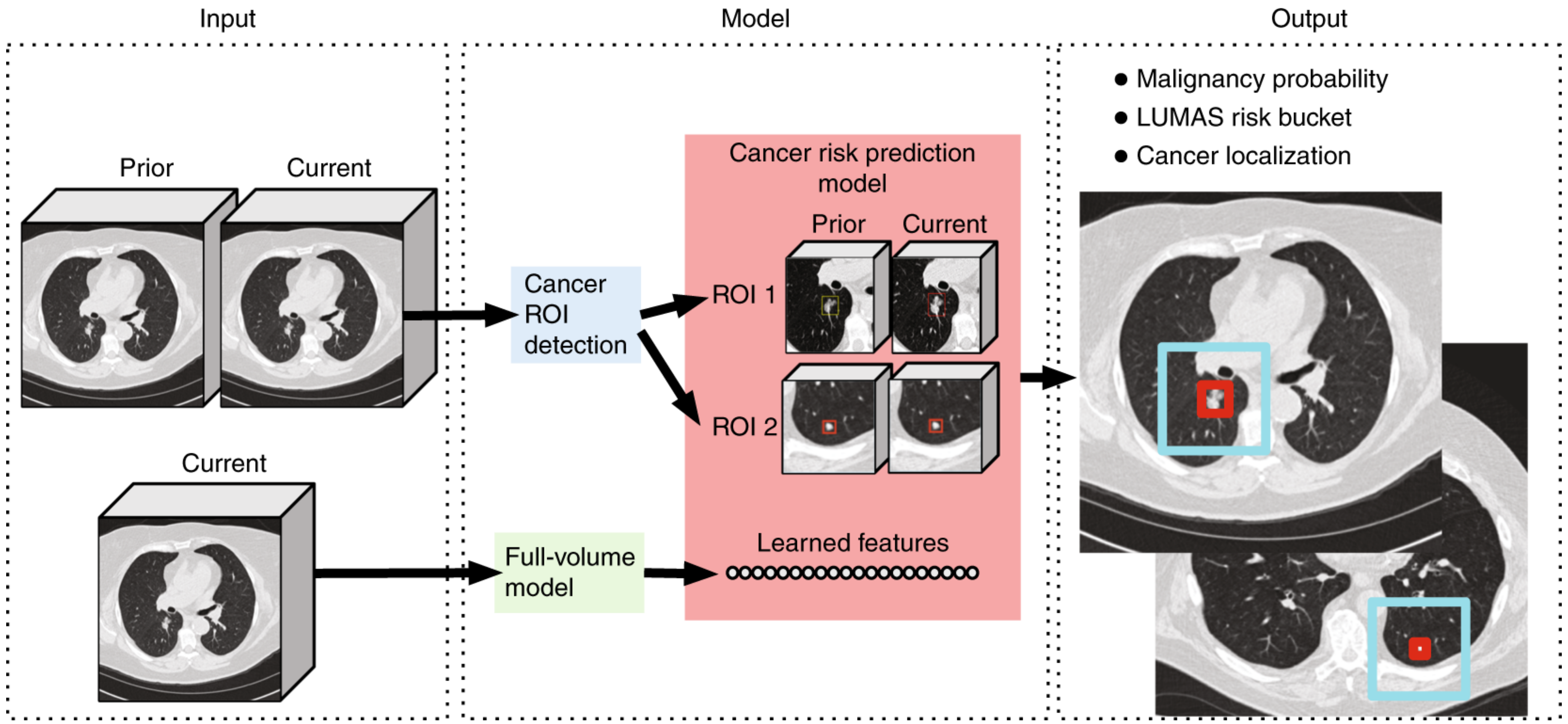
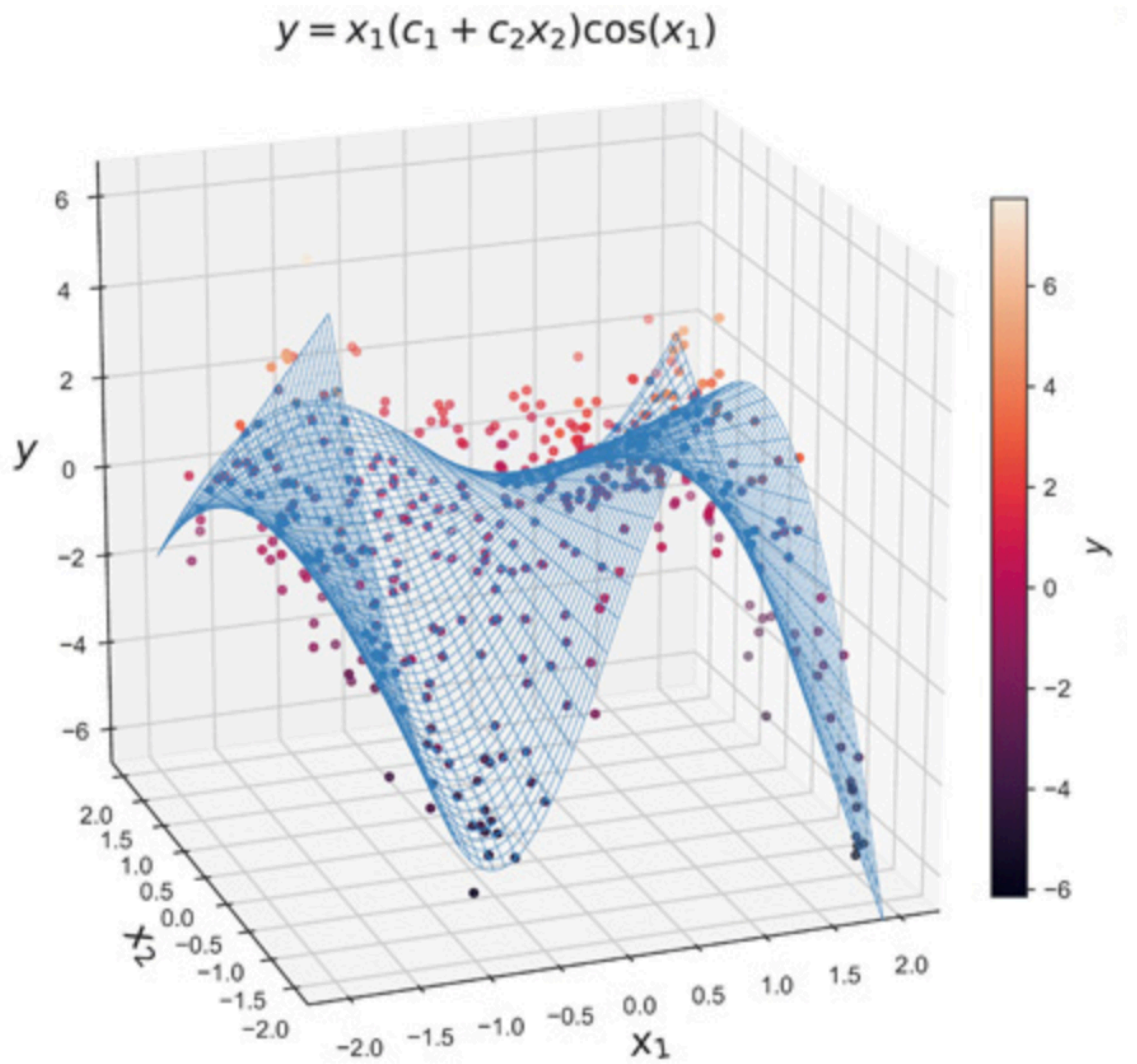
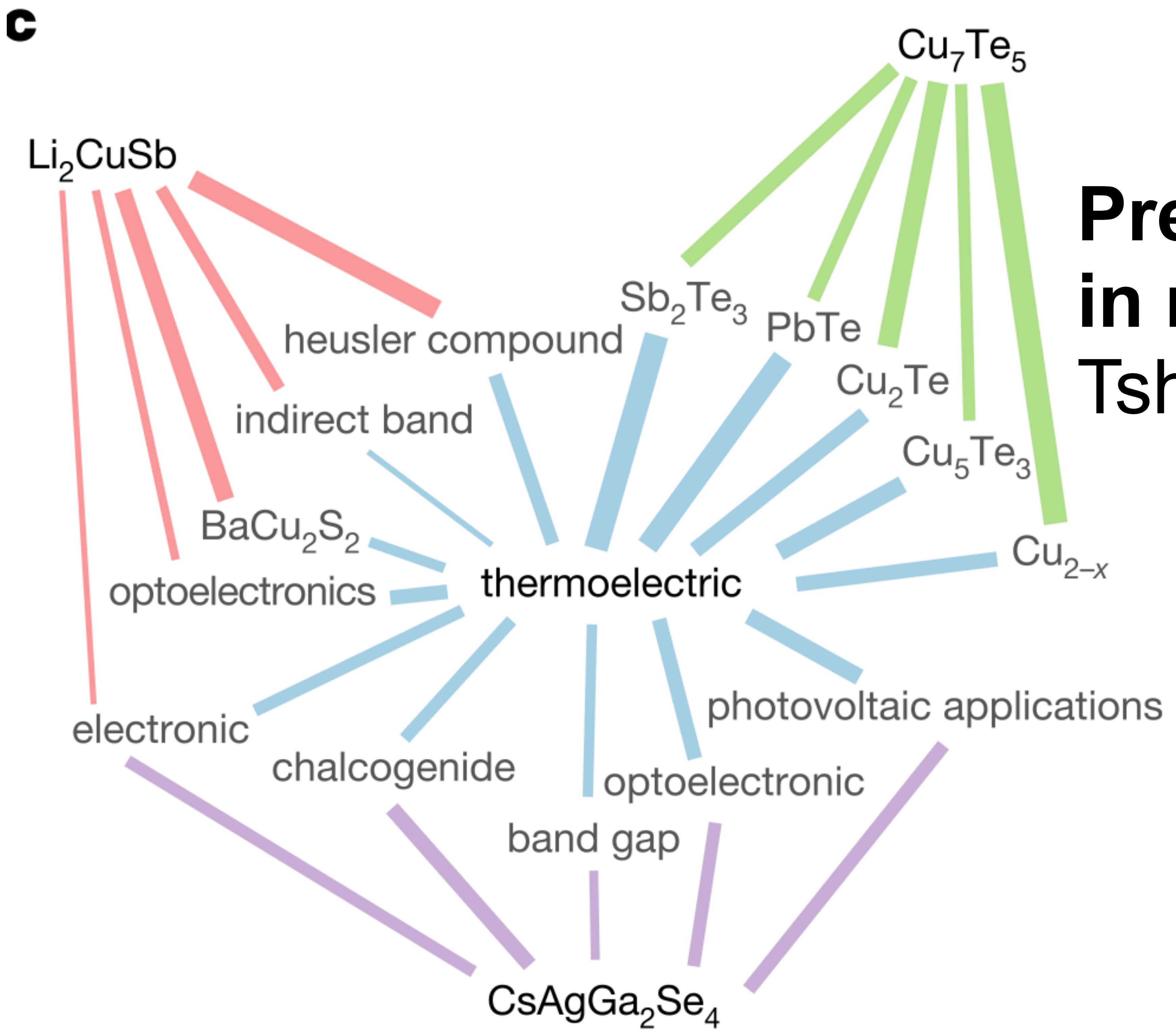


A Bayesian machine scientist to aid the solution of challenging scientific problems.
Guimera et al., Science Advances, 2020



Predicting lung cancer
Ardila et al., Nature Medicine, 2019





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example: Salganik et al., PNAS, 2020:

How well are life outcomes of children understood?

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How well are life outcomes of children understood?

	Birth	Age 1	Age 3	Age 5	Age 9
Core mother survey	●	●	●	●	●
Primary caregiver survey			●	●	●
Core father survey	●	●	●	●	●
In-home assessment			●	●	●
Child survey					●
Child care provider survey			●		
Teacher survey				●	●

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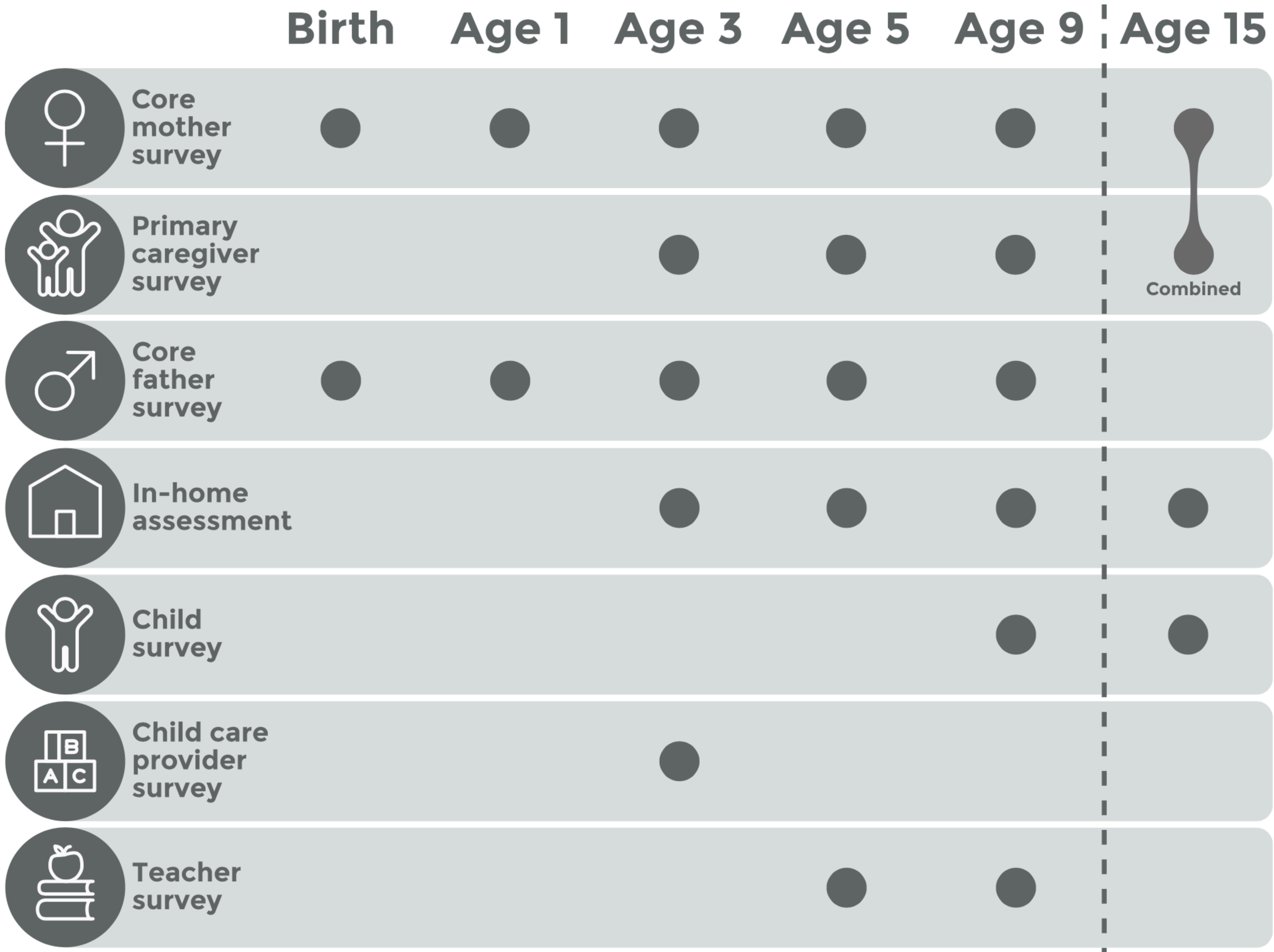

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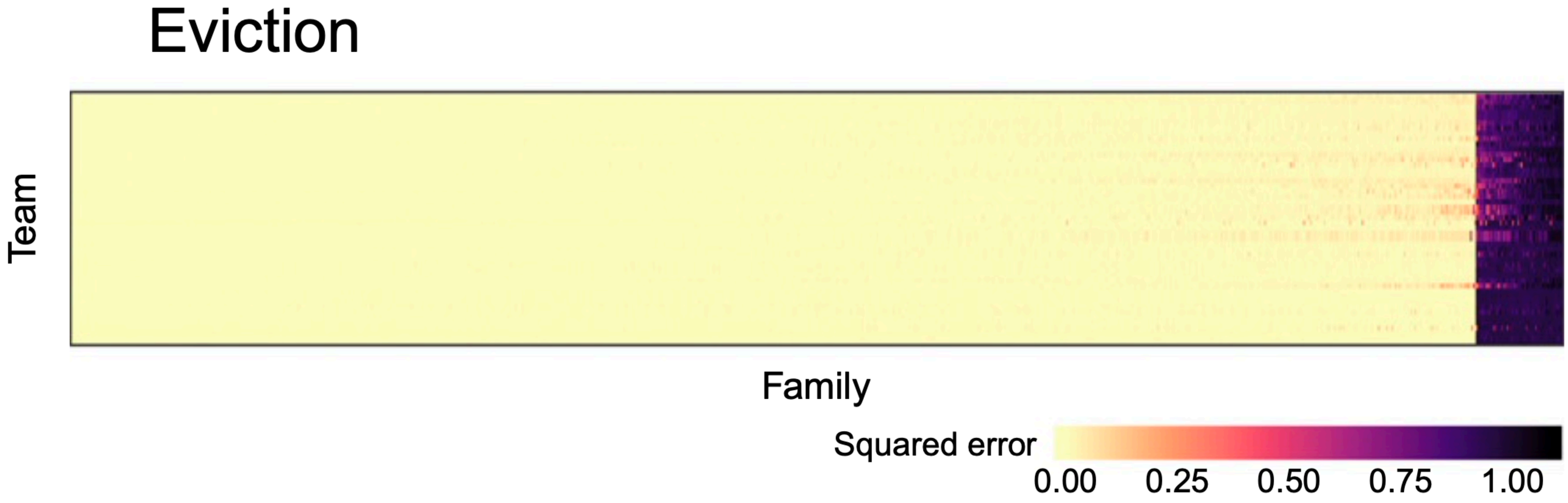

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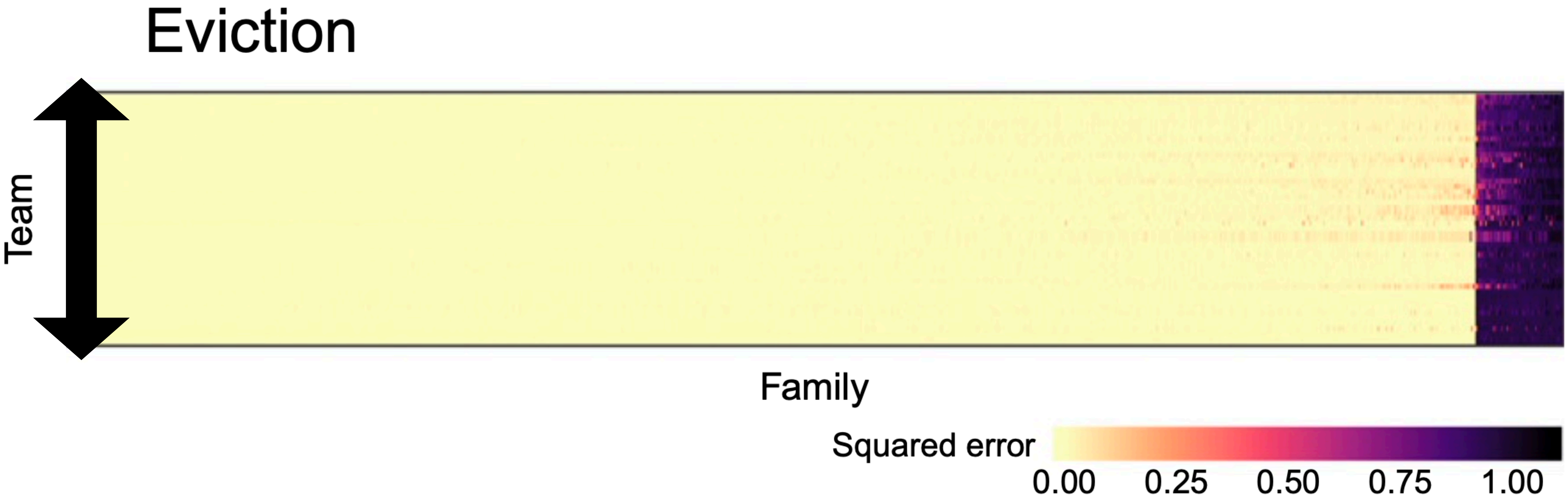

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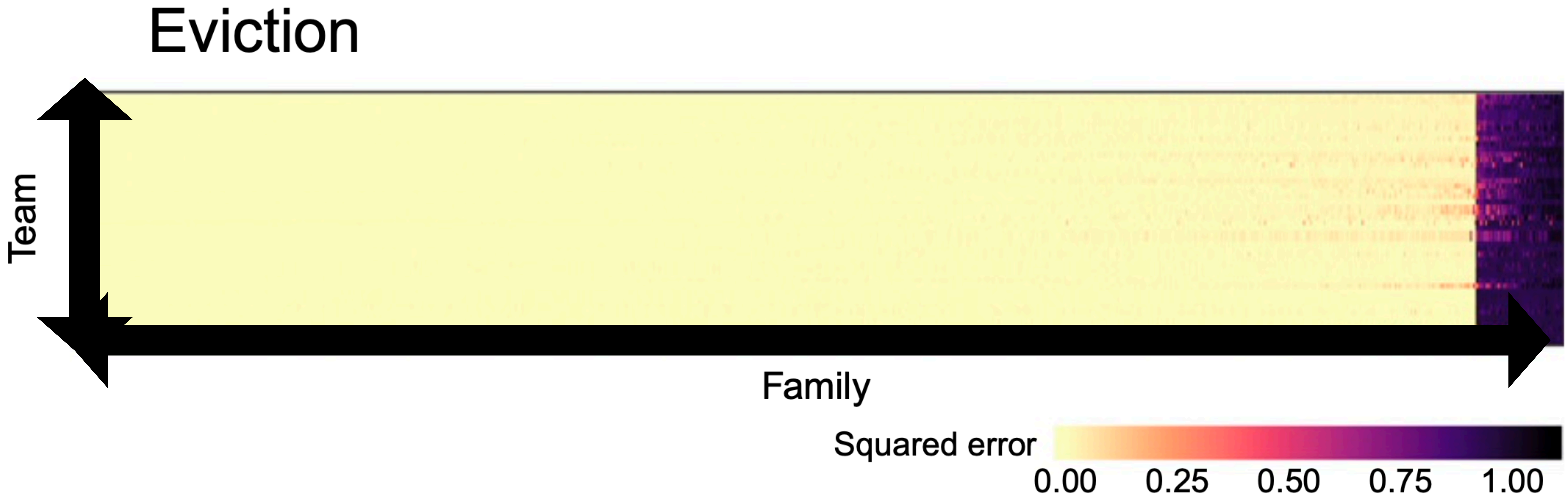

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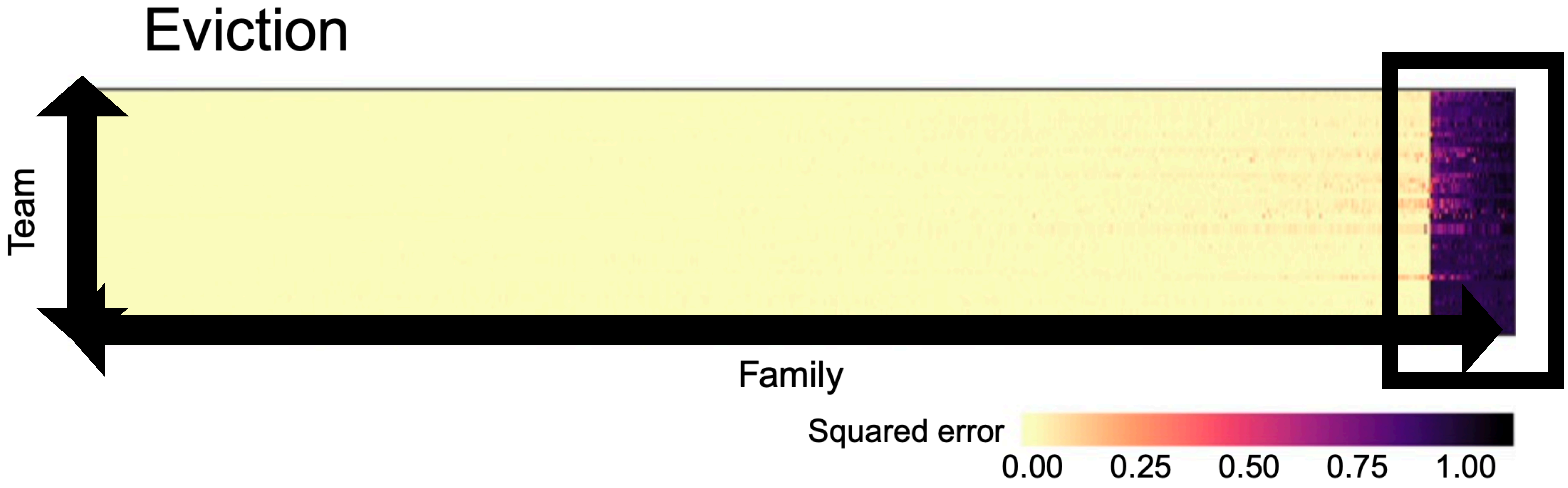

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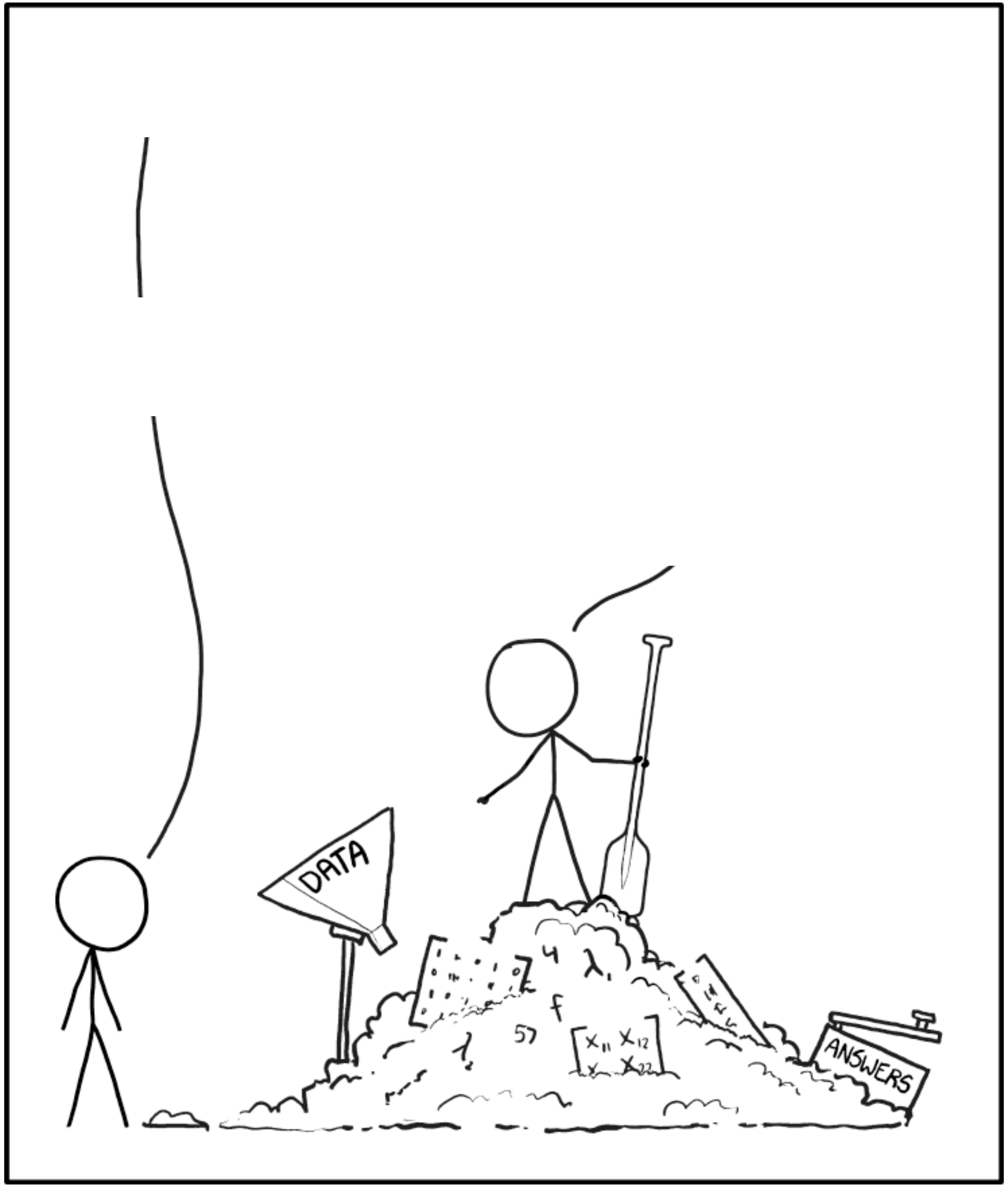
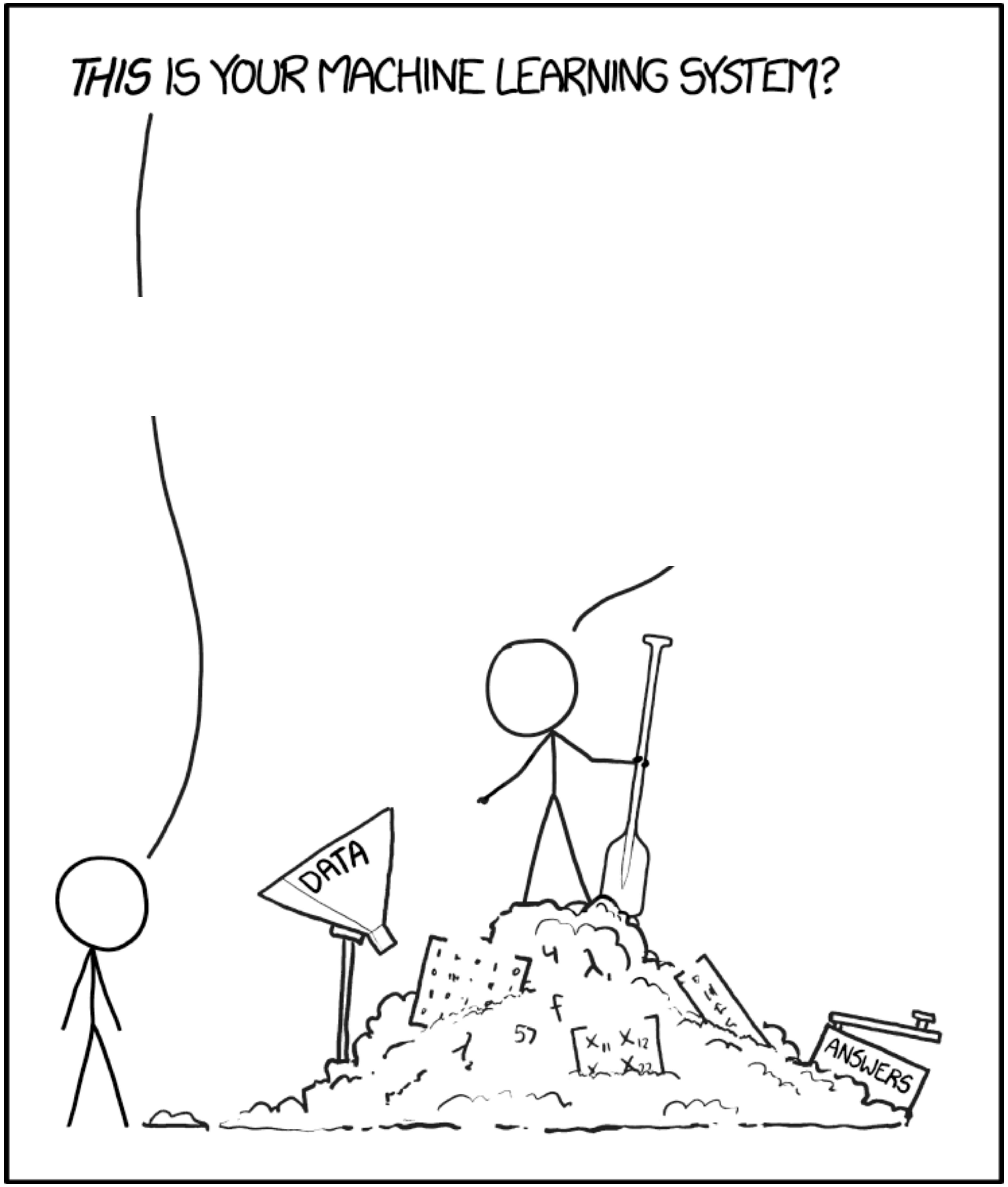


xkcd.com



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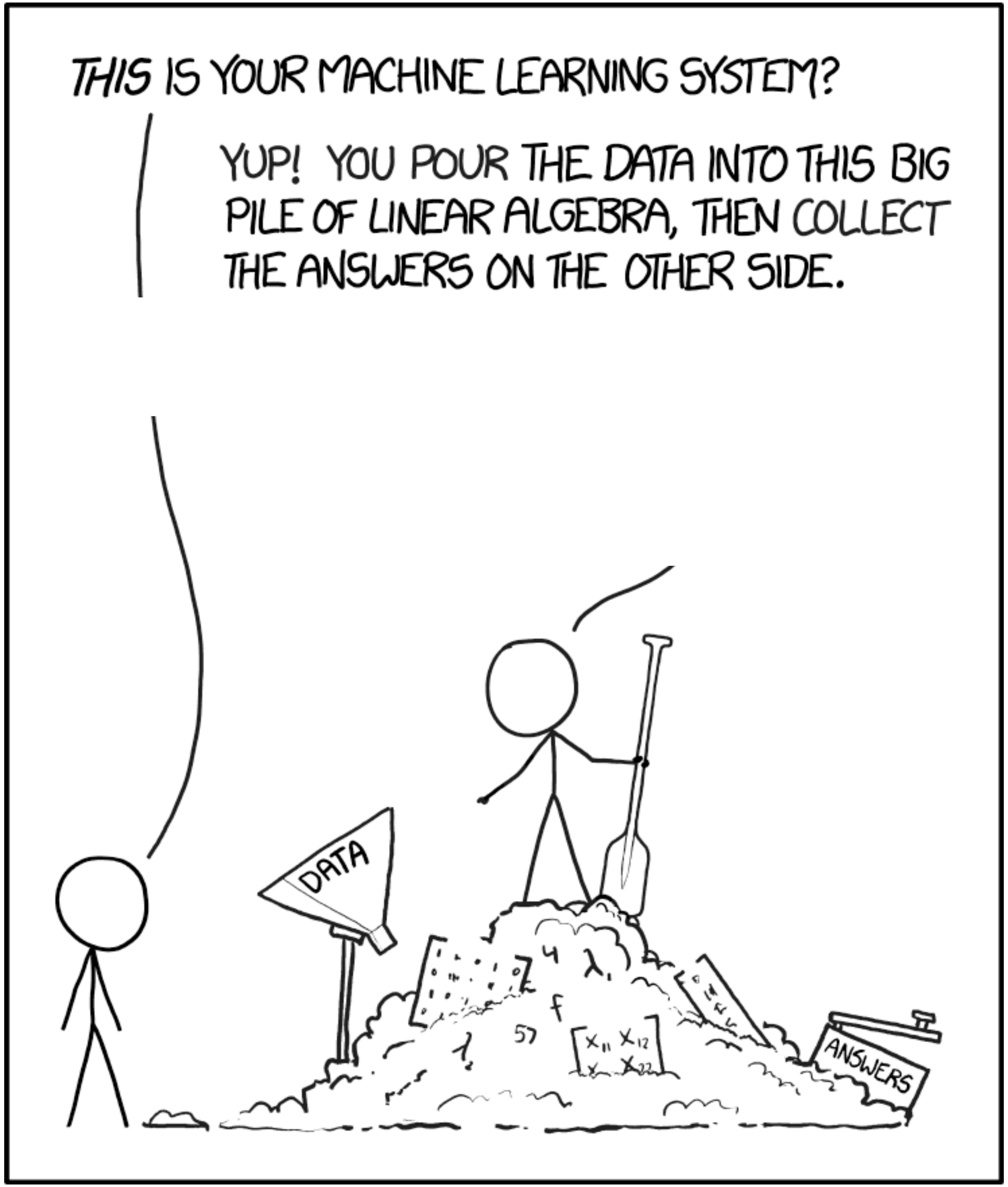
THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
DATA
ANSWERS

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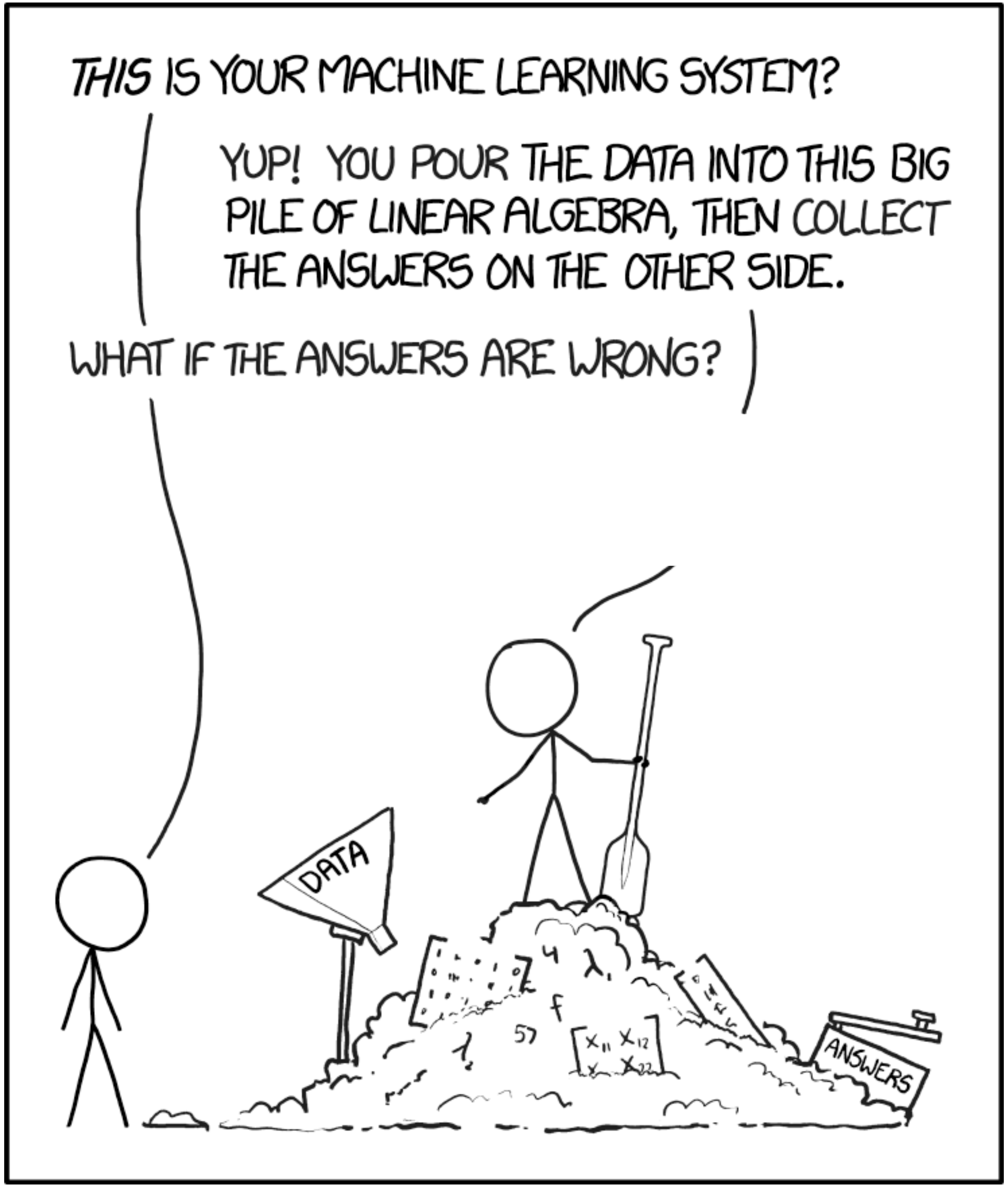
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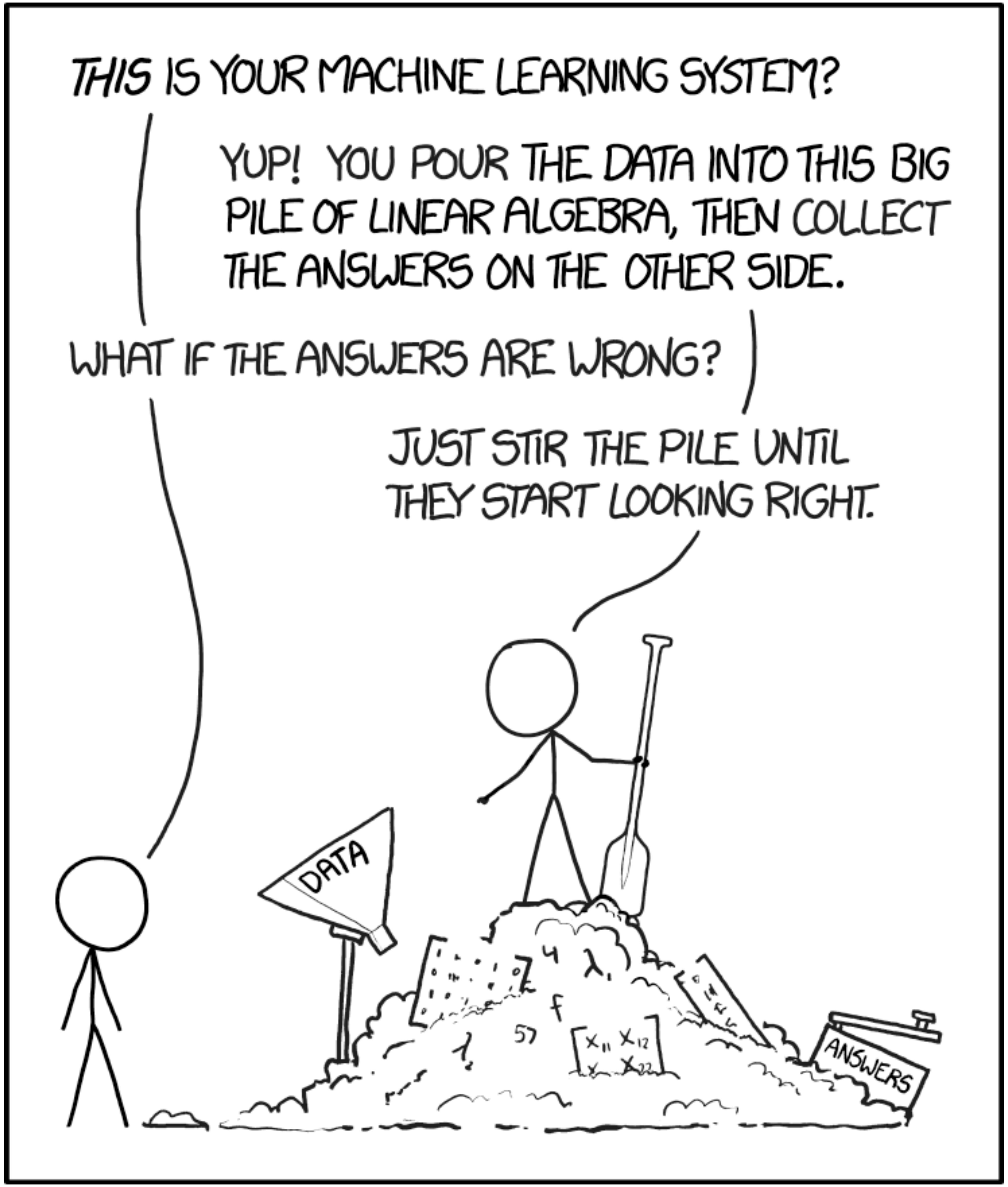
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WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

xkcd.com

Two tricks to avoid misleading models:

Machine learning

Two tricks to avoid misleading models:

Data cleaning

Machine learning

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Data cleaning

Separation of training- and test-set

Machine learning

Two tricks to avoid misleading models:

recommended start:
1) Broman et Woo, 2017: Data Organization in spreadsheets;
2) "tidy data"

Data cleaning

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Machine learning

Two tricks to avoid misleading models:

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Data cleaning

e.g.: different experimental series, or subsample data

Separation of training- and test-set

Machine learning

Machine learning is based on **features**.

features ➞ model ➞ inference

e.g.: measurements

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- generally, qualitatively diverse features are better

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features → model → inference

e.g.: measurements

- generally, qualitatively diverse features are better

- generally, number of independent features should be smaller than observations

Feature engineering may help or be needed.

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Note: feature engineering may also do harm.

A nice guide to feature engineering:
https://towardsdatascience.com/feature-engineering-for-machine-learning-3a5e293a5114

Which machine learning approach should I follow?

Supervised and unsupervised approaches form the two major families of machine learning algorithms.

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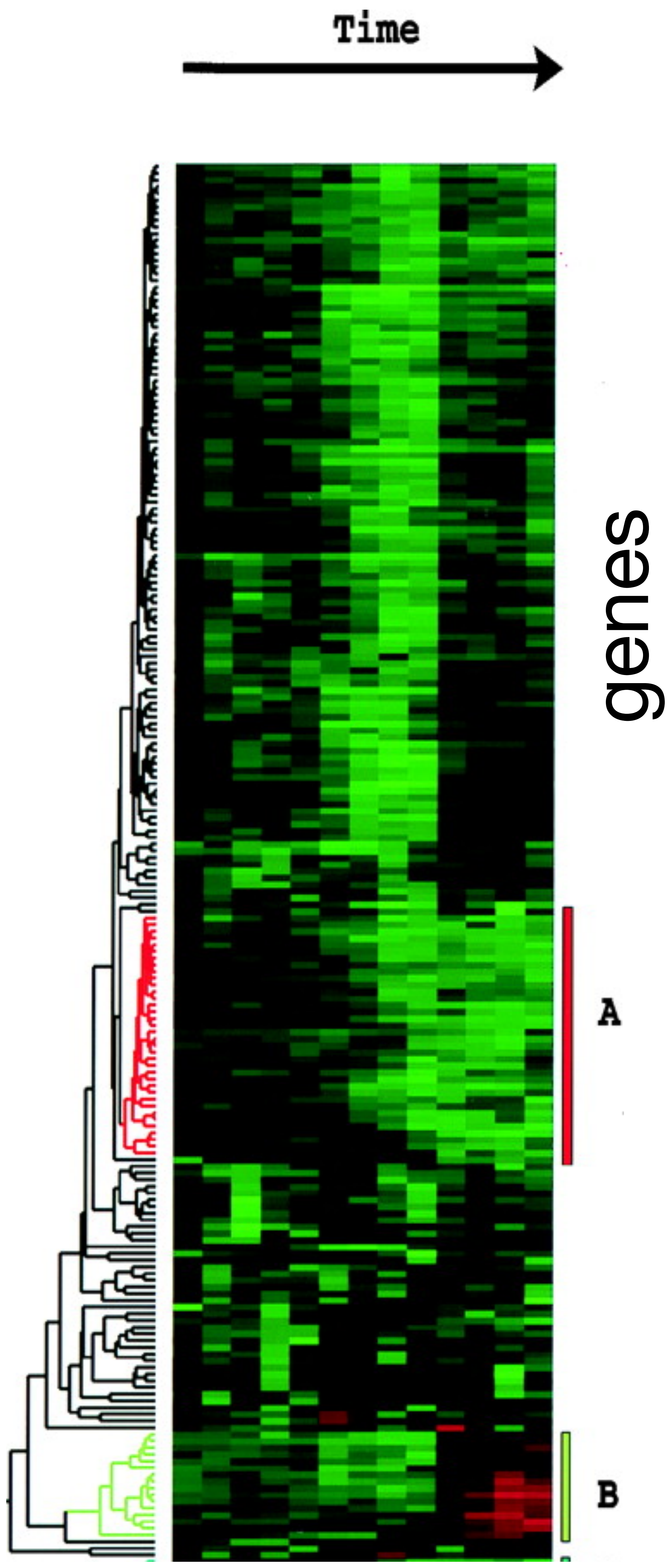
unsupervised:
e.g.: clustergram



Eisen et al. 1998

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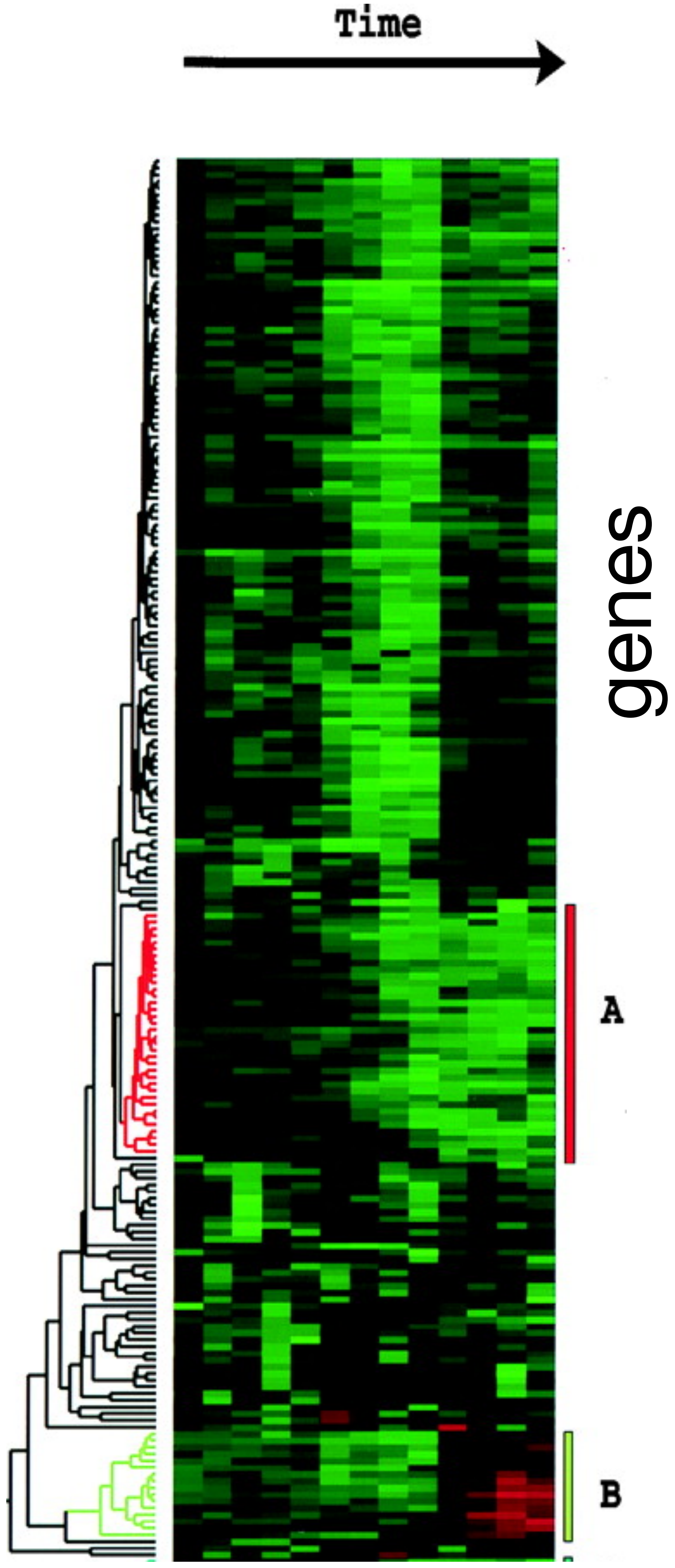

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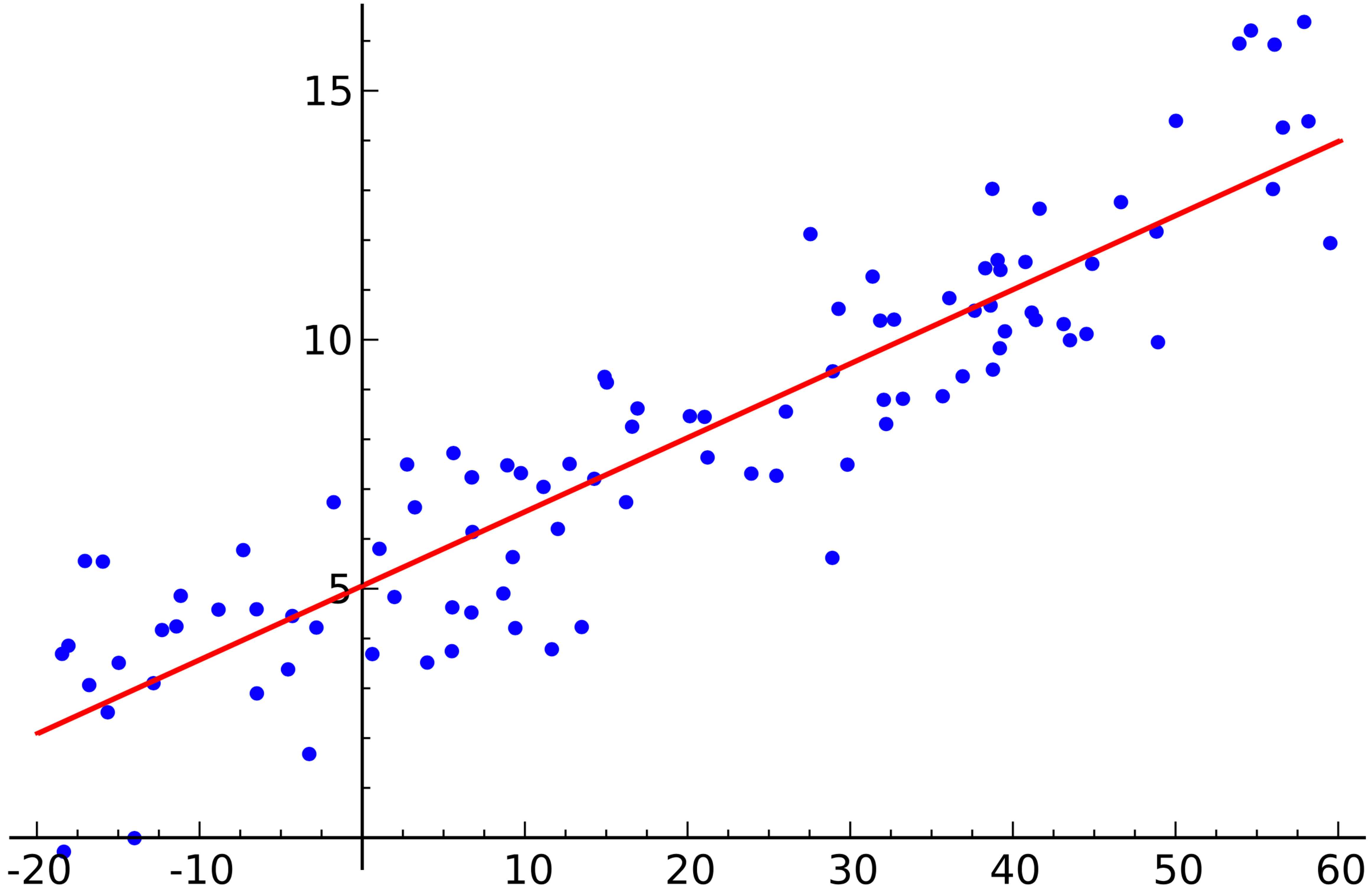
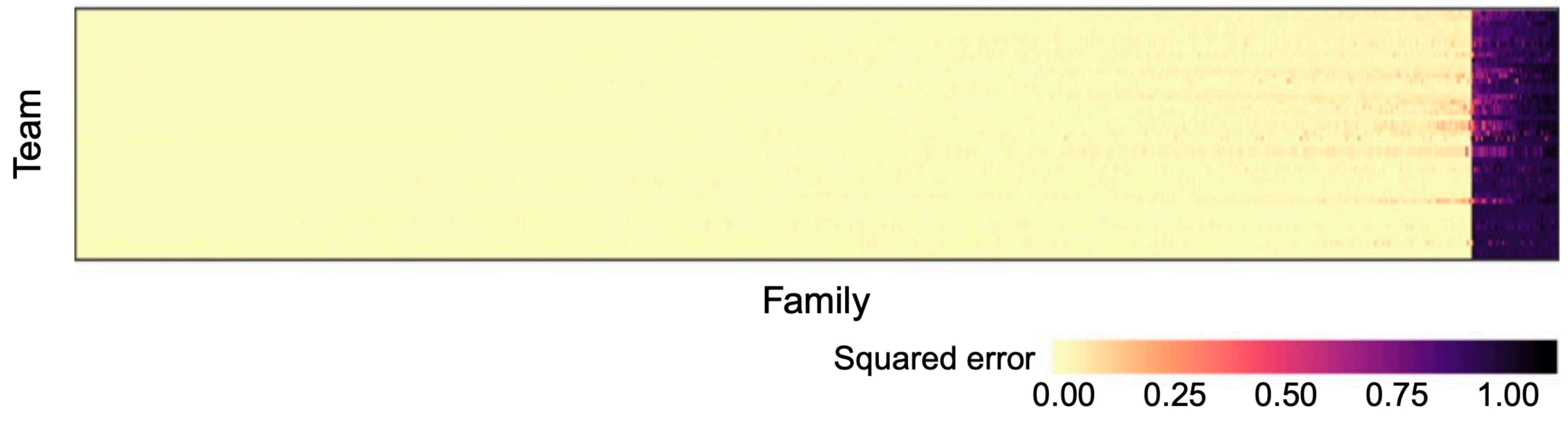


supervised:
e.g.: linear regression

Which specific machine learning approach should I follow?

Which <u>specific</u> machine learning approach should I follow?

*It may not matter. Remember the following?



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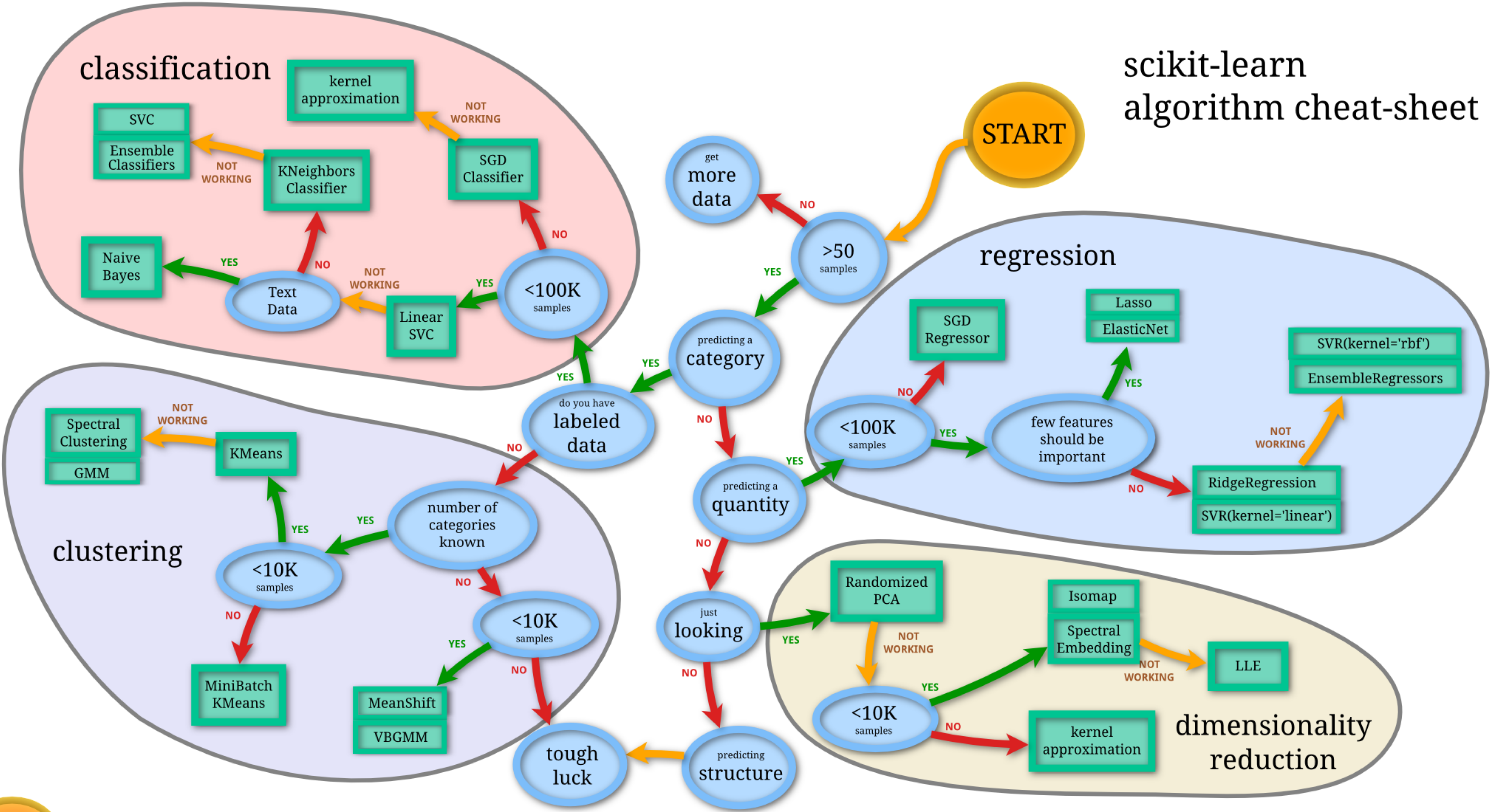

Back

https://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

Note: above webpage is interactive, revealing more details on distinct approaches

Automated machine learning

nice summary:
https://heartbeat.fritz.ai/automl-the-next-wave-of-machine-learning-5494baac615f

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Automated machine learning

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- Good start is auto-sklearn

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Beth1126

PDA Python DataFrames and Graphs Webinar 2020

cloned from **Beth526/PDA-Python-Webinar**

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FORK THIS PROJECT

Make a fork of this project and run your own experiments.

A UIC Postdoctoral Association webinar by a postdoc who is learning python

Last updated: April 23rd, 2020

Python DataFrames and Basic Graphs

Python is a popular programming language that can be used for analysis and graphing of large datasets. There are a lot of **free resouces online** to learn python:

- https://www.codecademy.com
- https://www.datacamp.com
- https://docs.python.org/3.8/tutorial/index.html
- Coursera courses such as "Programming for Everybody (Getting Started with Python)" from University of Michigan
- Linkedin Learning courses (free with UIC login) such as "Learning Python"

To use this Jupyter Notebook you *do not have to download anything*, but a way to download and use Python and many of the Python packages is by downloading the **Anaconda platform**:

- https://www.anaconda.com/distribution/

In this short walk-through we are going to focus on practical Python packages for data analysis called **Pandas** and **Seaborn**. Packages add functionality to basic Python. Here are links to the

Remember? Last week's lecture from Bethany Baumann.

https://notebooks.ai/Beth1126/pda-python-dataframes-and-graphs-webinar-2020-54351877)

NOTEBOOKS_

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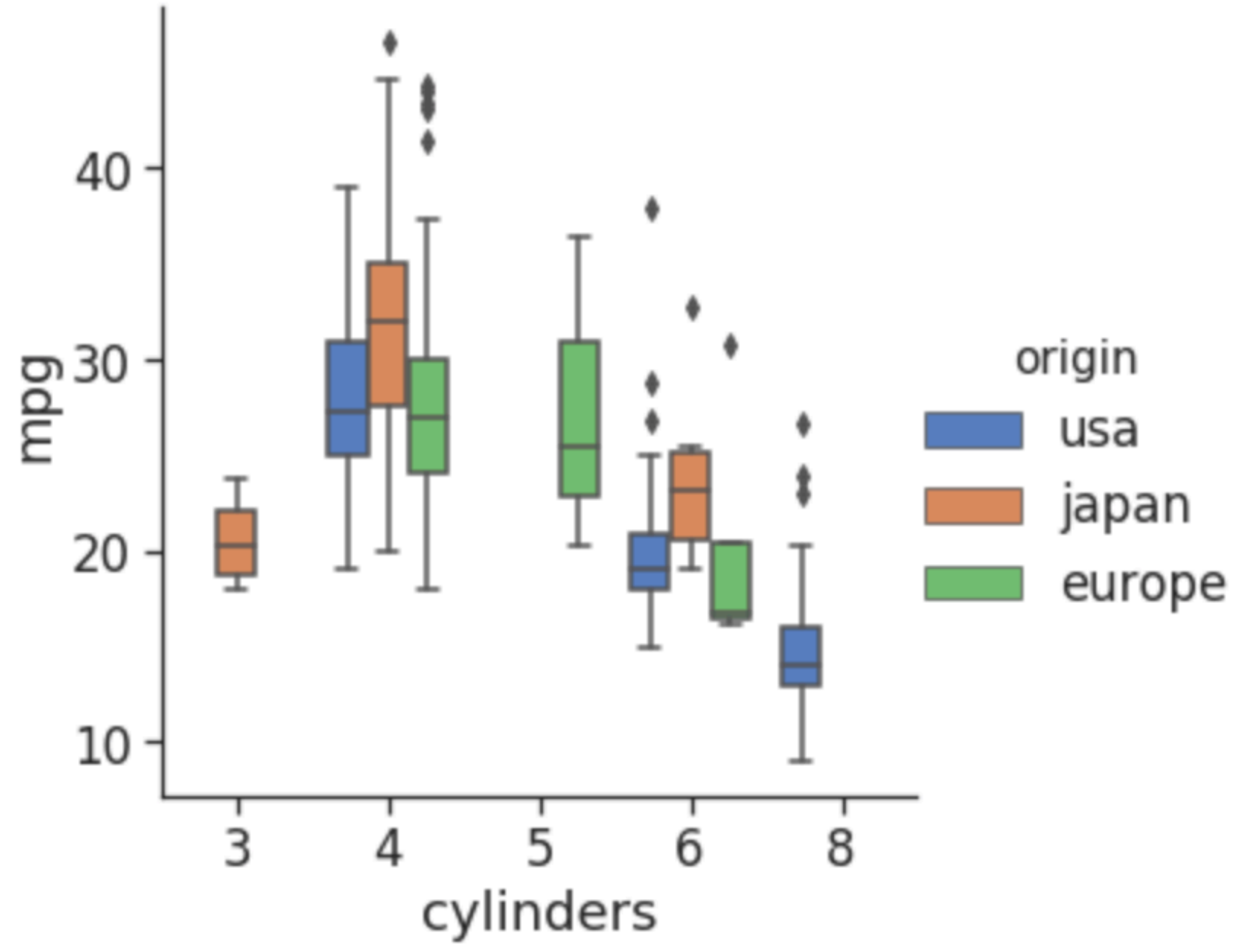
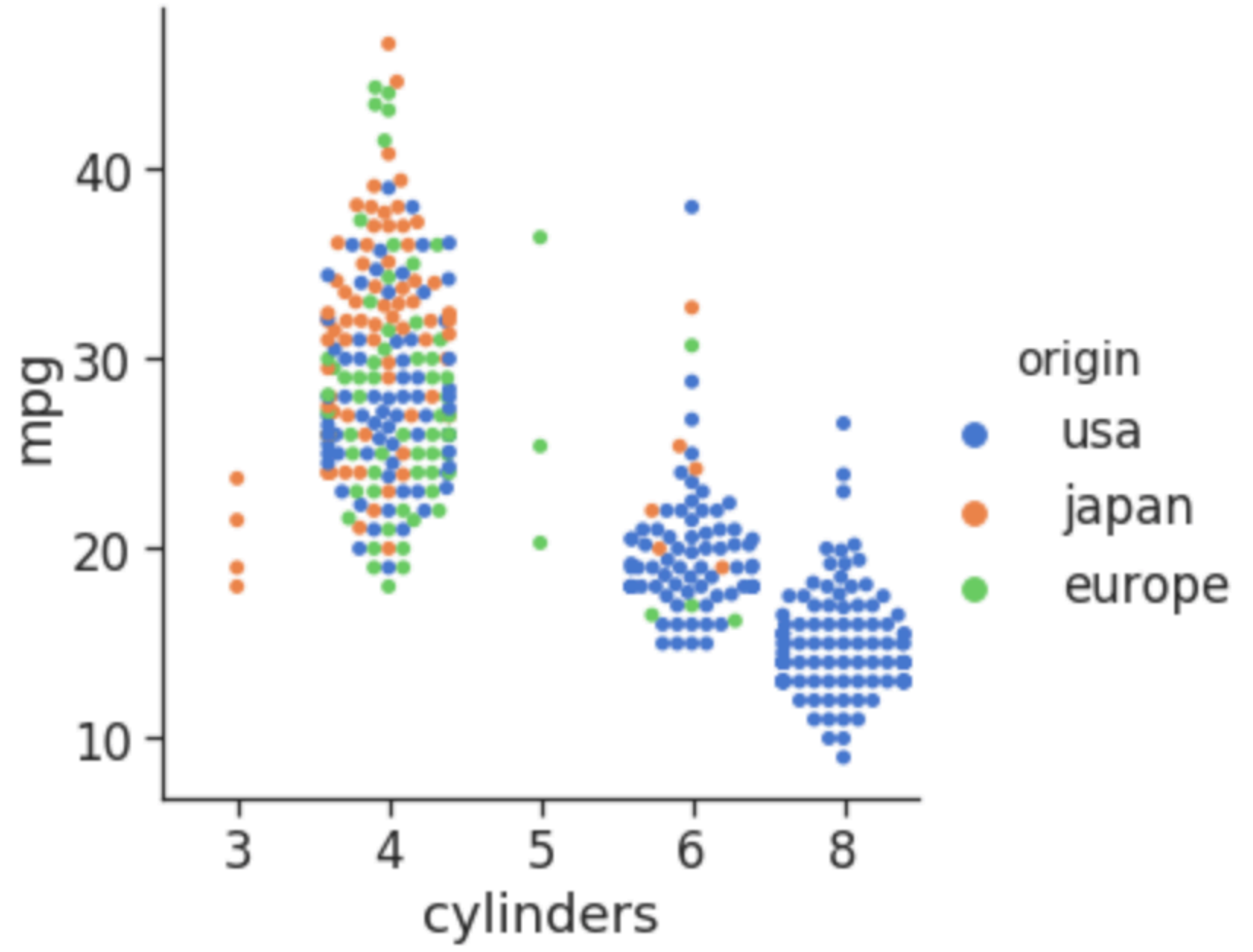
```
<seaborn.axisgrid.FacetGrid at 0x7f65293f9640>
```




```
sns.catplot(x = 'cylinders', y = "mpg", hue = "origin", data = df, kind = 'swarm')
```

OUTPUT

```
<seaborn.axisgrid.FacetGrid at 0x7f65272f42e0>
```



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mpg	cylinders	displacement	horsepower	weight	acceleration	model_year	origin	name
18.0	8	307.0	130.0	3504	12.0	70	usa	chevrolet chevelle malibu
15.0	8	350.0	165.0	3693	11.5	70	usa	buick skylark 320
18.0	8	318.0	150.0	3436	11.0	70	usa	plymouth satellite
16.0	8	304.0	150.0	3433	12.0	70	usa	amc rebel sst
17.0	8	302.0	140.0	3449	10.5	70	usa	ford torino

to predict: miles per gallon

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https://notebooks.ai/tstoeger/predict-miles-per-gallon-1342dcb1/