Machine Learning

for astronomy

Tiana_Athriel

dhuppenkothen

Daniela Huppenkothen

NYU Center for Data Science

Caveat: I am not a machine learning expert.

What is

Machine Learning?

“Field of study that gives computers the ability to learn without being explicitly programmed”

- Arthur Samuel, 1959

Machine learning procedure

feature engineering

cross validation

model evaluation

Machine learning procedure

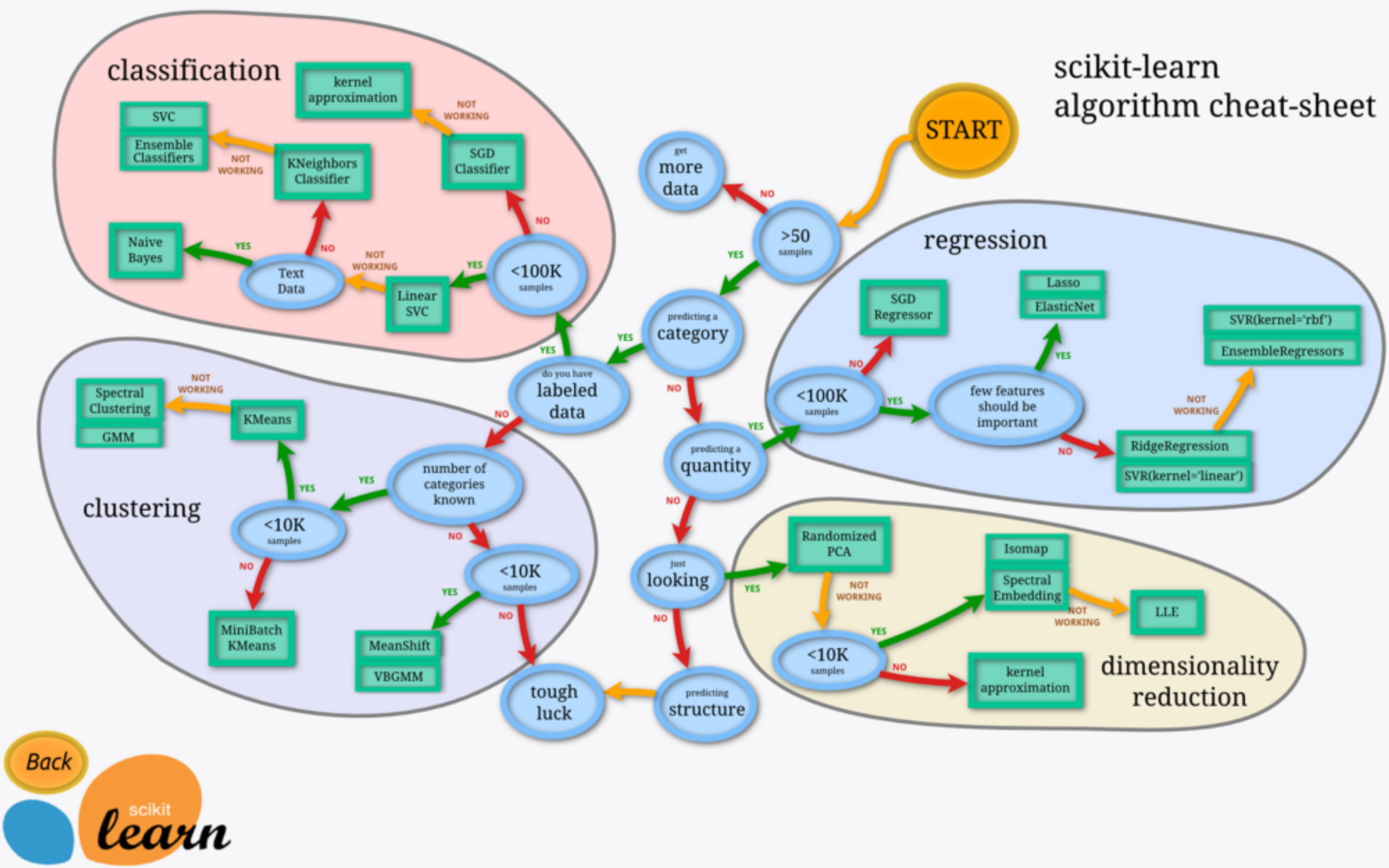
feature engineering

↓

cross validation

↓

model evaluation

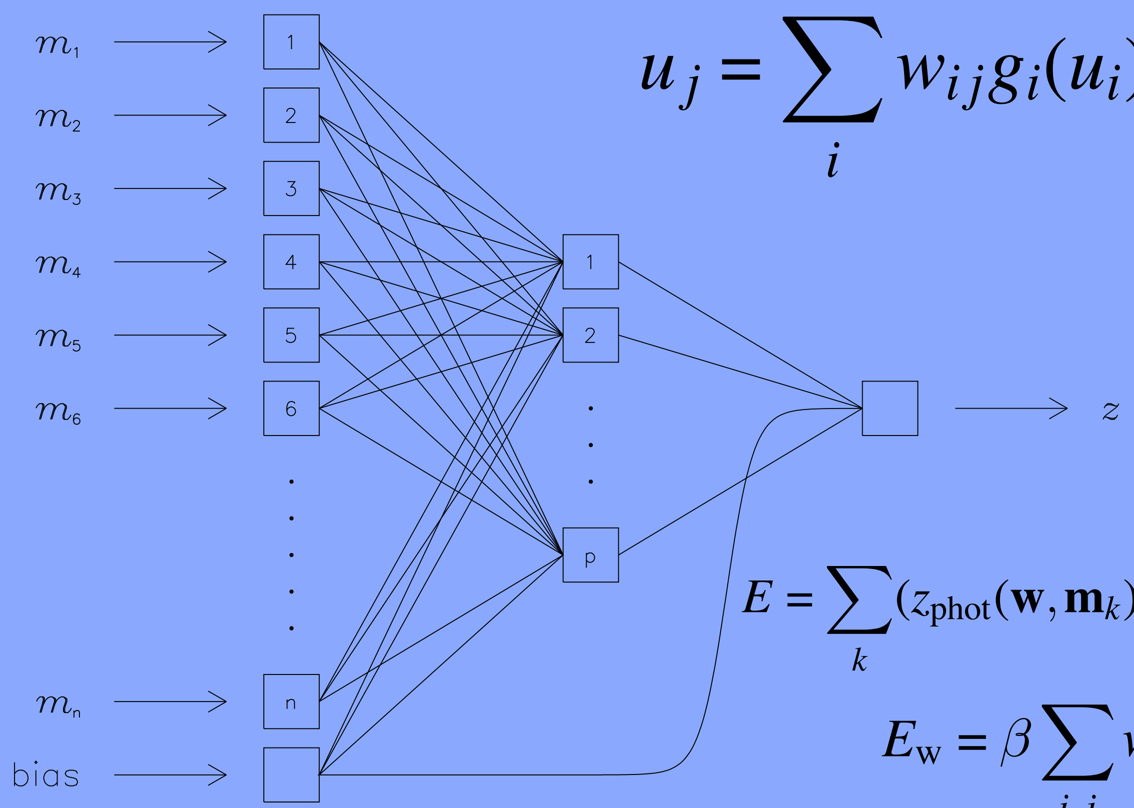


Credit: Andreas Müller

linear model = model linear in the parameters

$$g(z) = \frac{1}{1+e^{-z}} \qquad \text{with}$$

$$z = f(x) = w_0 + w_1 x_1 + \ldots + w_n x_n$$



$$u_j = \sum_i w_{ij} g_i(u_i),$$

$$E = \sum_k (z_{\text{phot}}(\mathbf{w}, \mathbf{m}_k) - z_{\text{spec},k})^2,$$

$$E_{\text{w}} = \beta \sum_{i,j} w_{ij}^2,$$

linear model

non-linear model

non-linear models are far more flexible!

generative model: a model that can generate data

When is

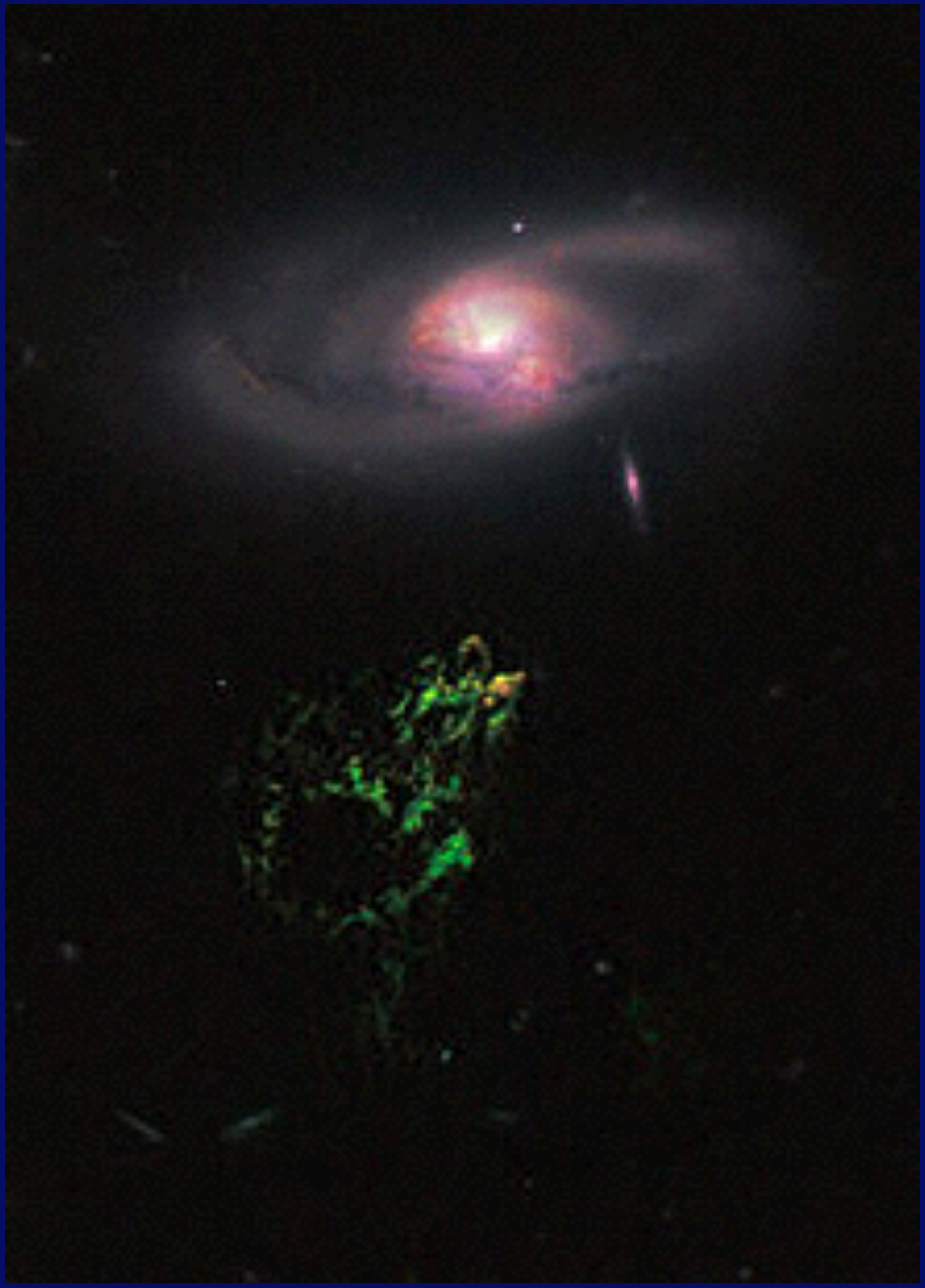
Machine Learning

useful?

Galaxy Zoo classified over 900,000 galaxies!

+ humans are excellent at pattern recognition!

+find the unexpected

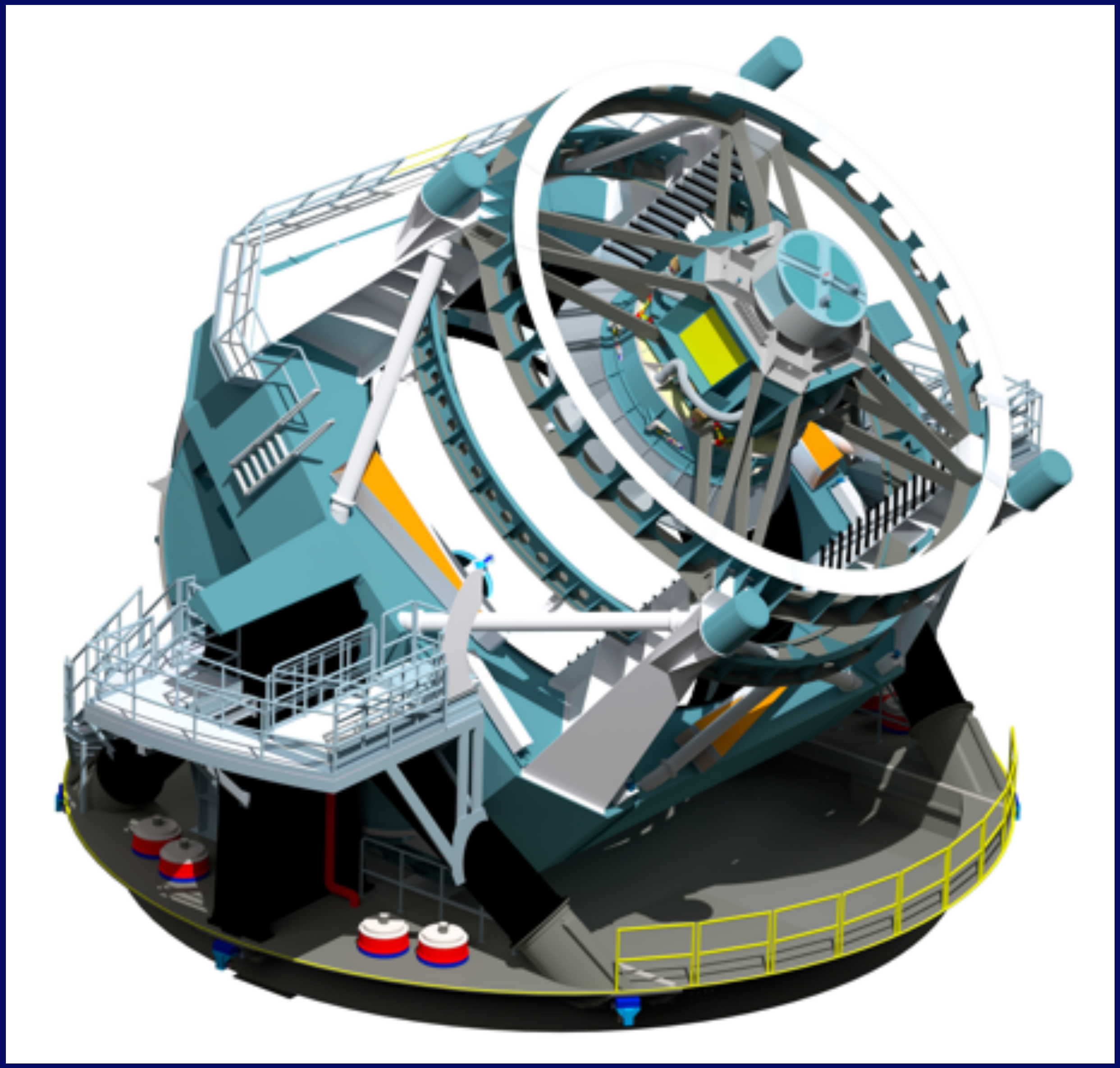


Credit: NASA, ESA, W. Keel (University of Alabama), and the Galaxy Zoo Team

"Hanny's voorwerp"

– doesn’t scale!

Large Synoptic Survey Telescope



Credit: The LSST Corporation

~ 10 million transients per night!

– humans are biased classifiers!

Galaxy Zoo Result: people classify more galaxies as anti-clockwise than clockwise!

https://blog.galaxyzoo.org/2008/01/10/in-the-eye-of-the-beholder/

Future Instruments produce data sets too big to be analysed by hand!

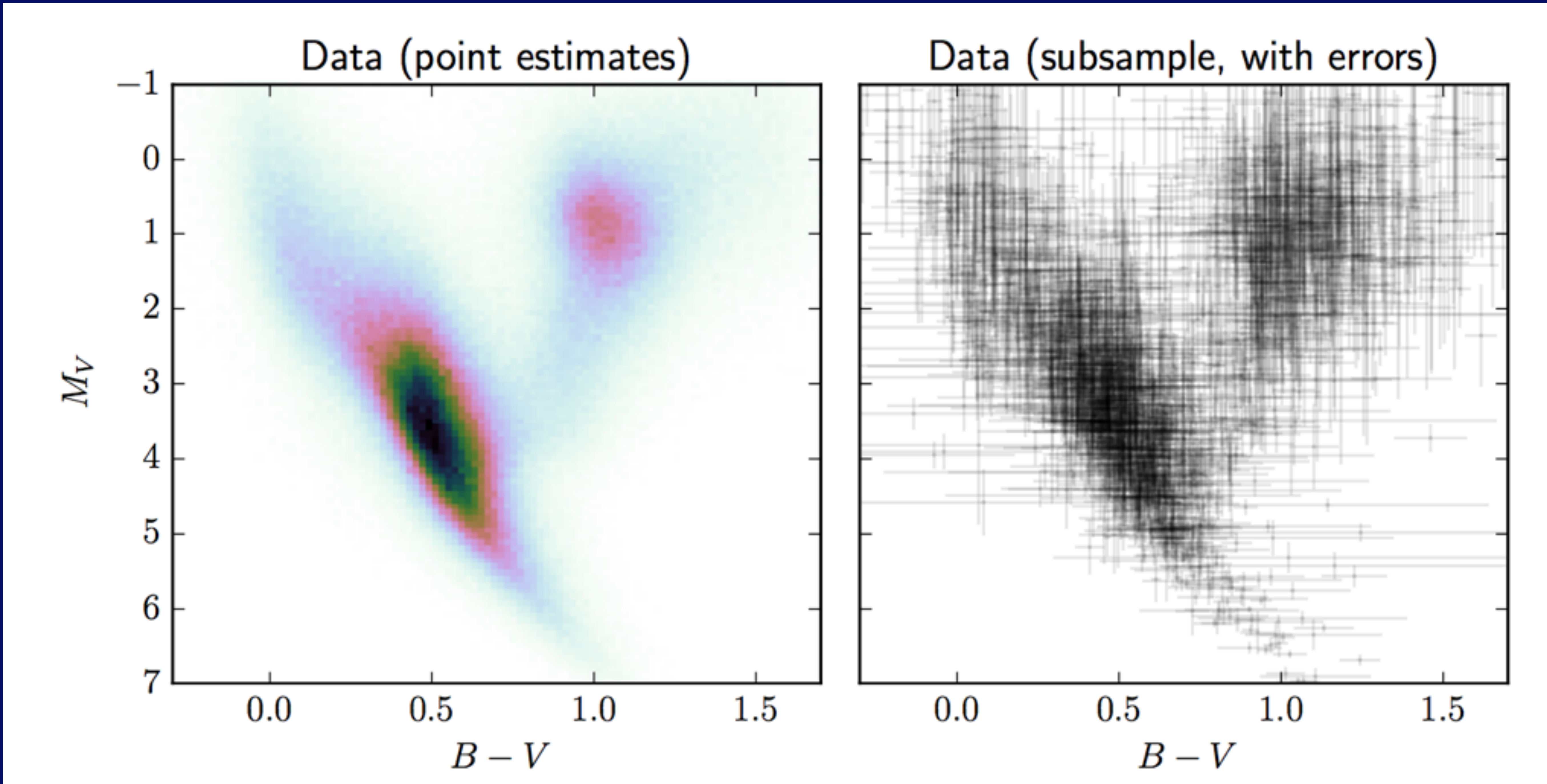
Machine Learning

+ scales to large data sets

+ fewer human biases (except in training data)

– can usually only find what’s been seen **before**

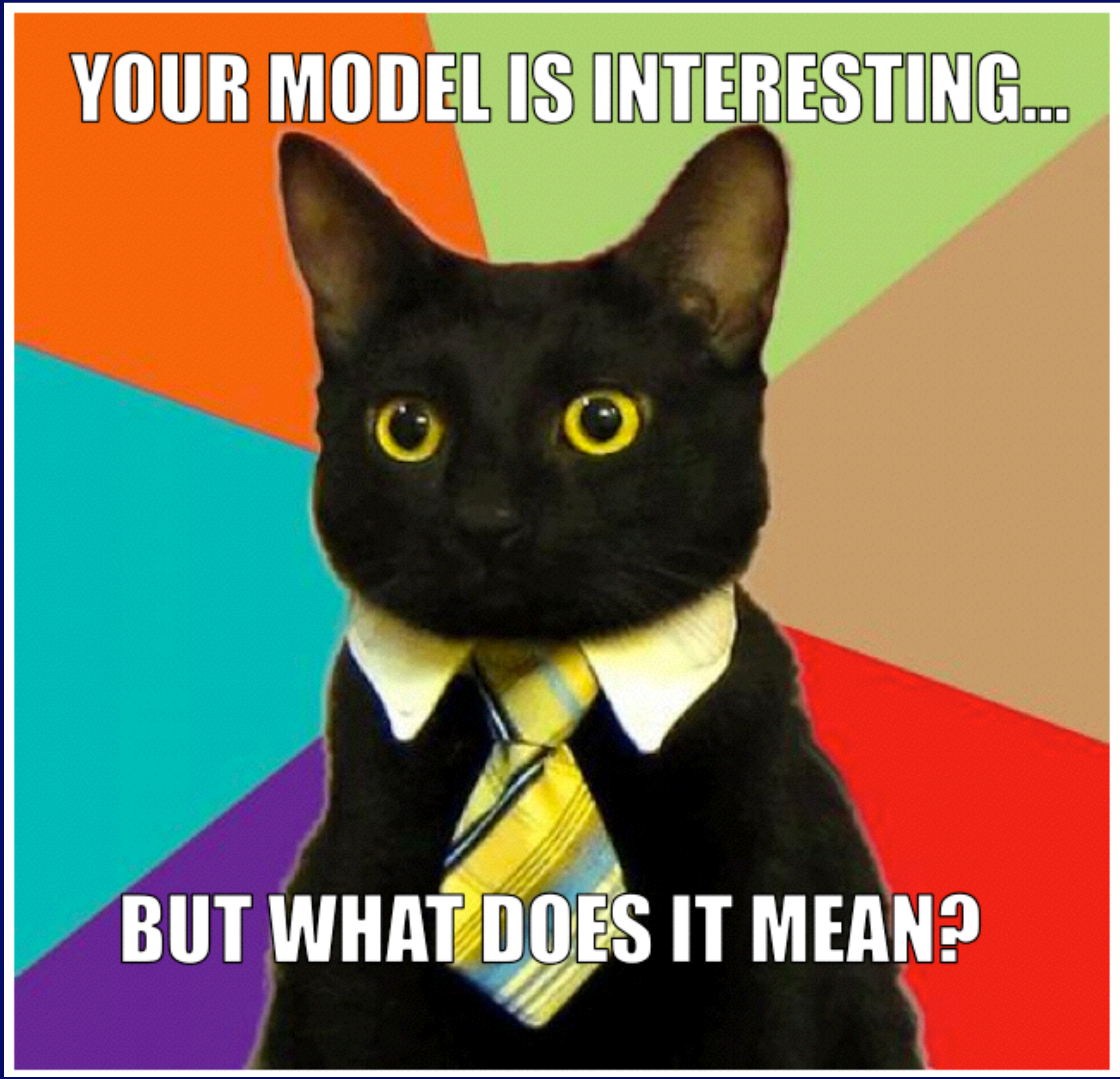
The HR Diagram as seen by GAIA



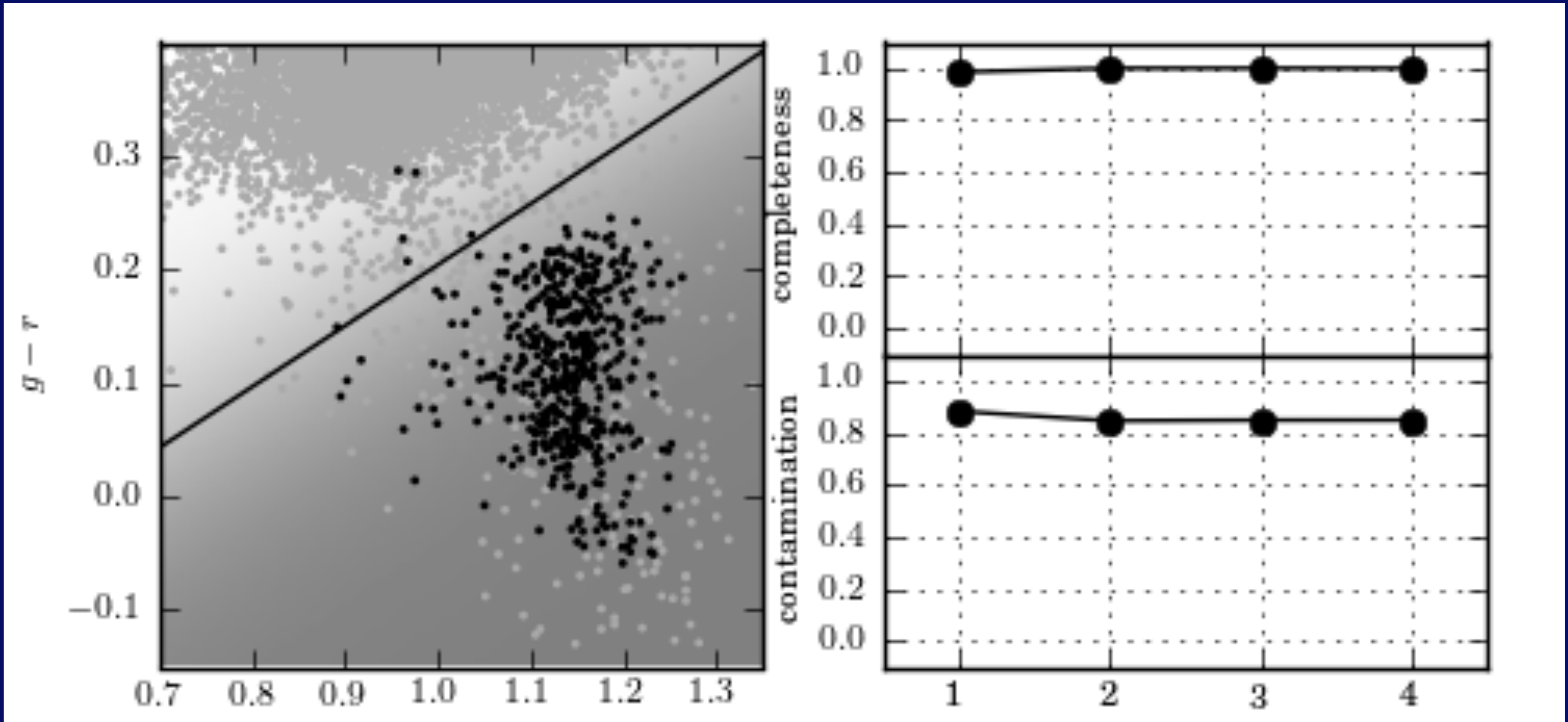
Leistedt + Hogg (2017)

– (sometimes) hard to interpret

Interpretability


YOUR MODEL IS INTERESTING...
BUT WHAT DOES IT MEAN?

Logistic Regression of RR Lyrae Stars



Vanderplas et al, 2012

… now what?

2 main goals:
inference versus prediction

2 main goals:

inference versus prediction

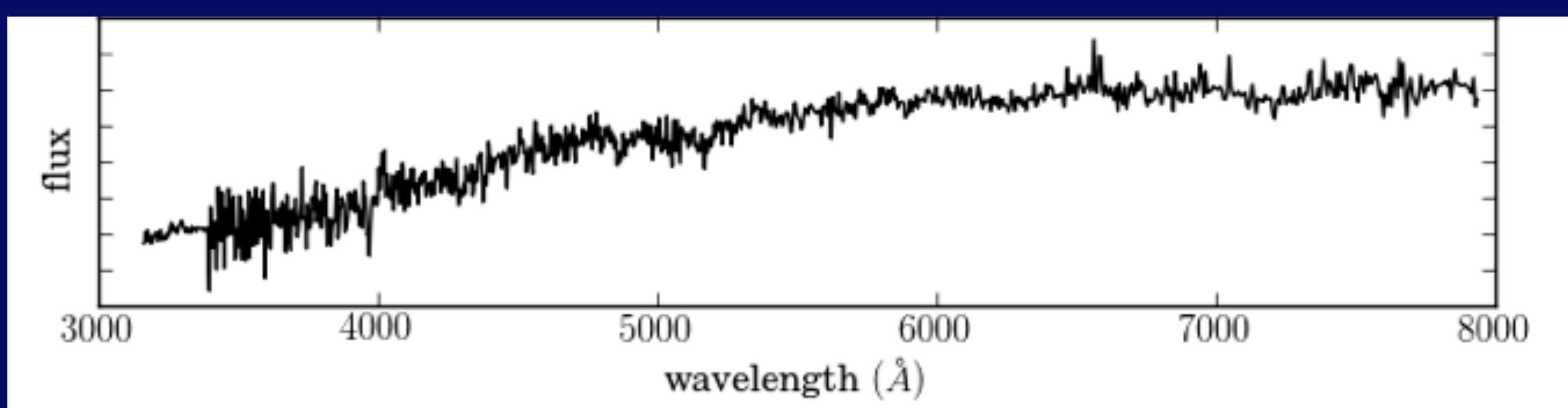
statistics! **machine learning**

Inference

“a conclusion reached on the basis of evidence and reasoning“

Inference

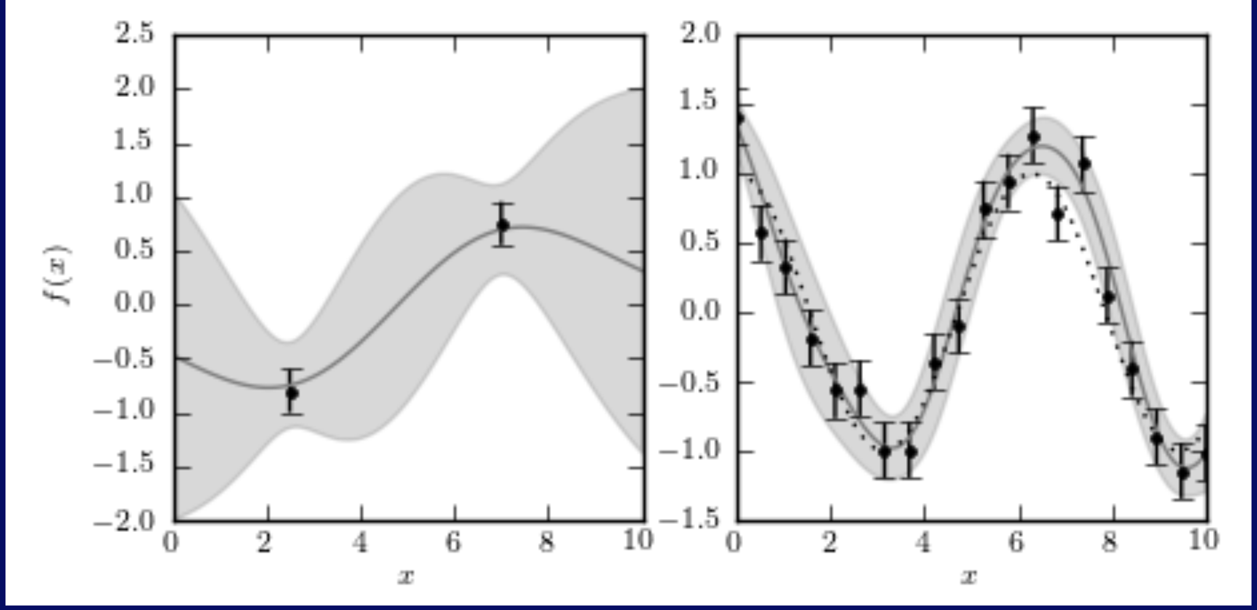
"Why do stars have different colours from galaxies?"



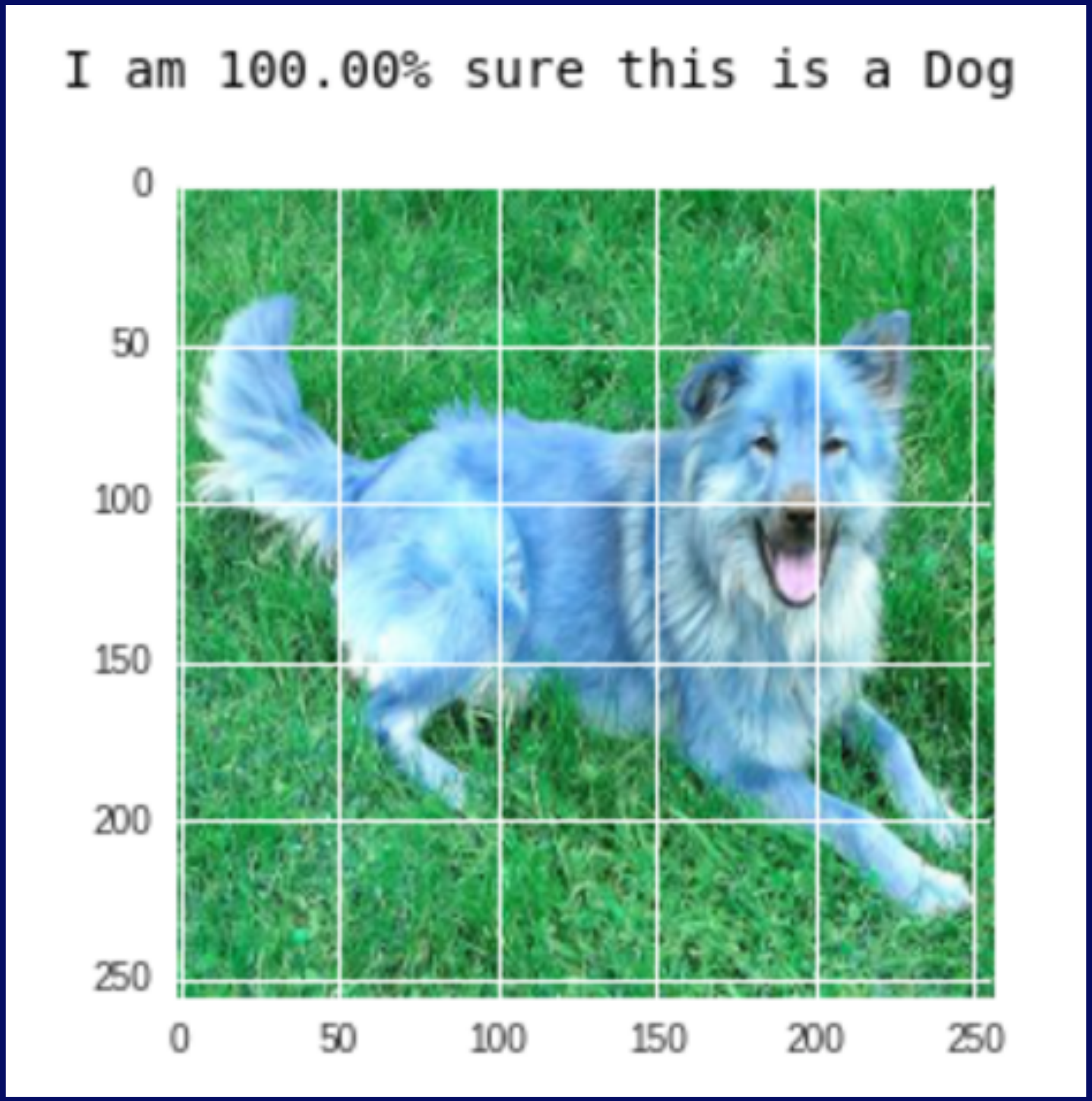
Vanderplas et al, 2012

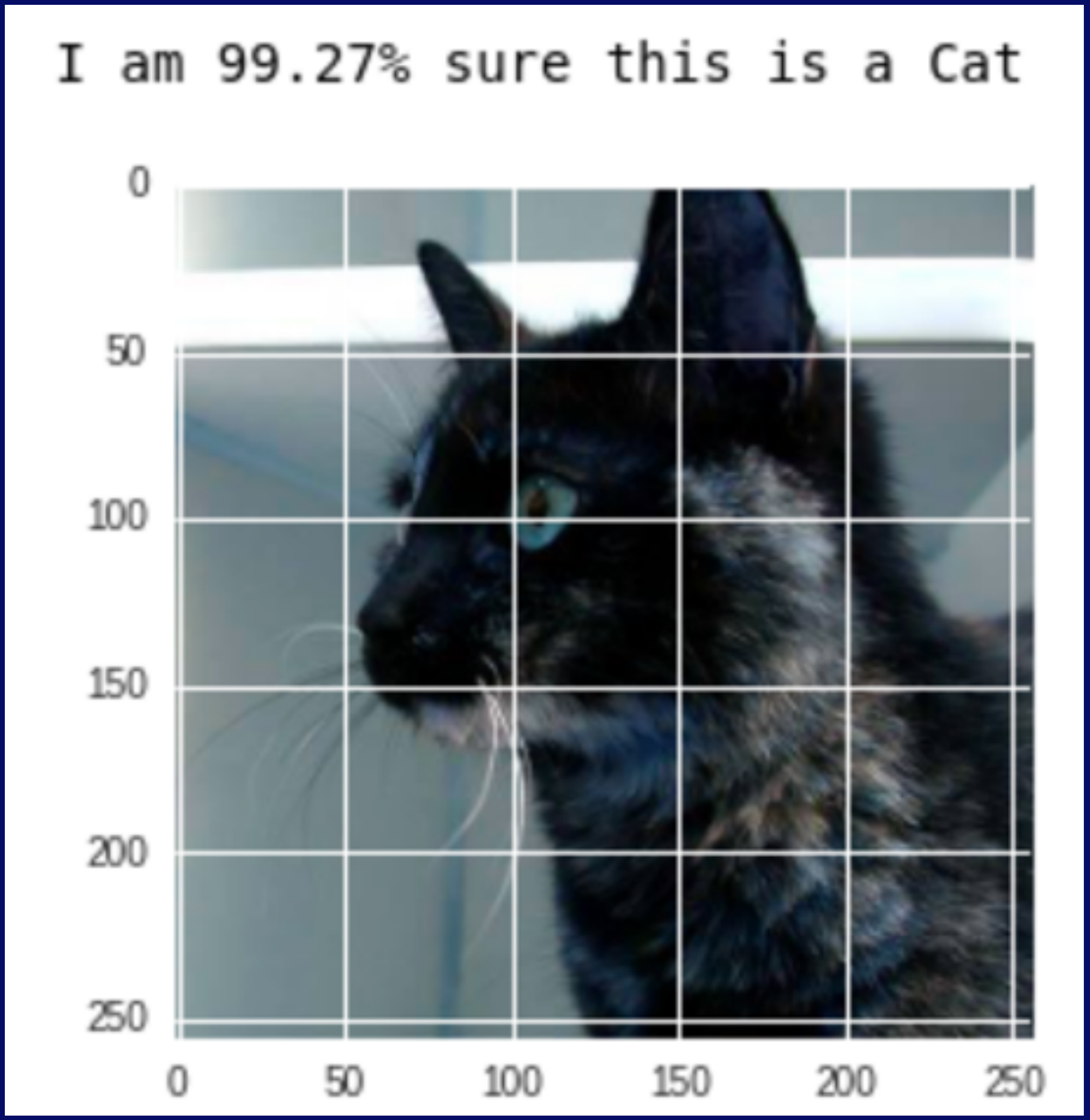
Prediction

"Given my data points X and outcomes y, what outcome will I predict for a new data point x?"



Vanderplas et al, 2012



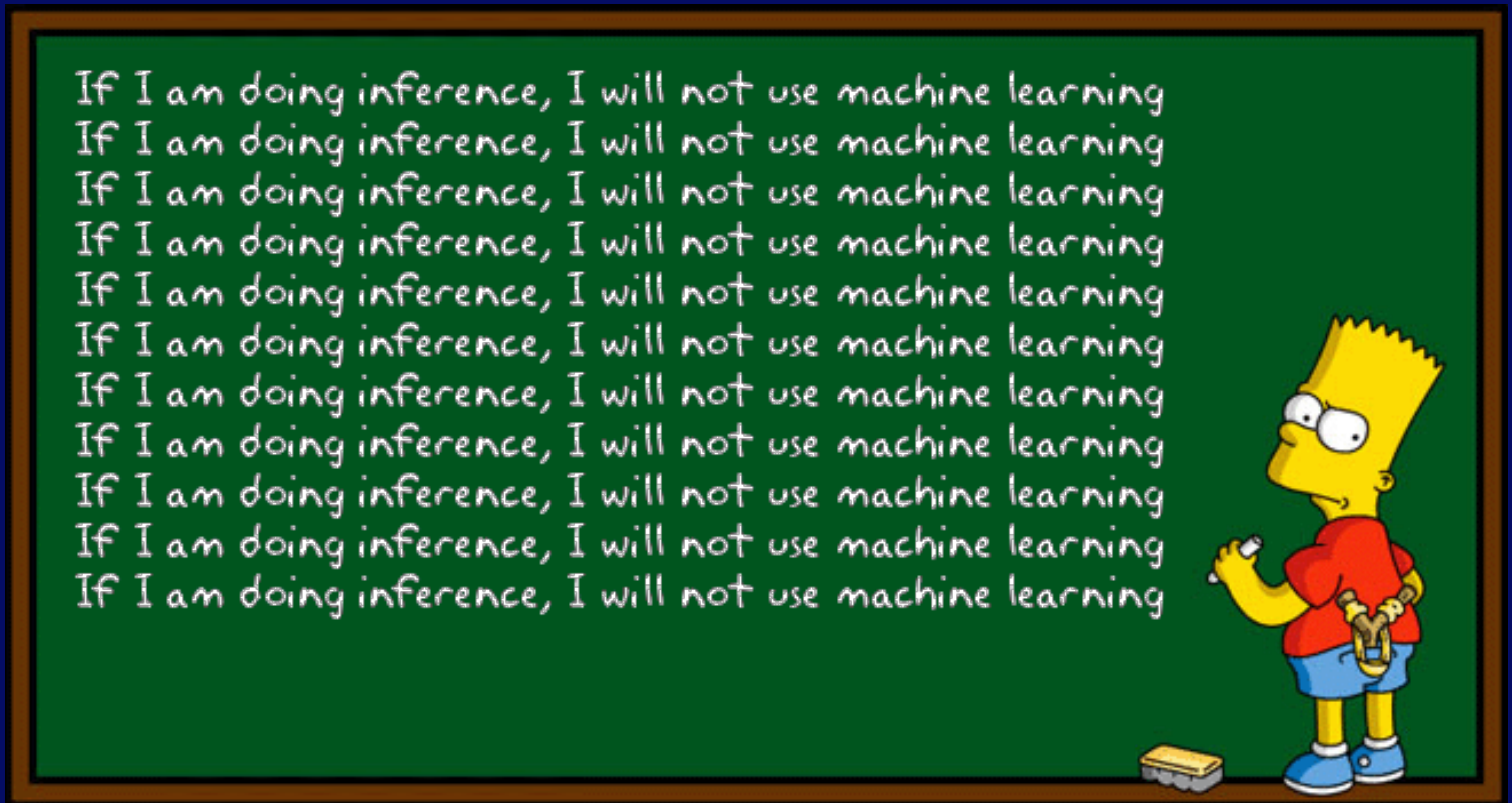


https://www.kaggle.com/jeffd23/catdognet-keras-convnet-starter

Scientific goal: uncover causal relationship

$\neq$

ML goal: minimize prediction error


If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning
If I am doing inference, I will not use machine learning

Caveat: there are probabilistic machine learning models!

e.g.: Gaussian Mixture Models, Hidden Markov Models, Gaussian Processes

Z. Lipton: The Mythos of Model Interpretability

https://arxiv.org/abs/1606.03490

Motives

Trust

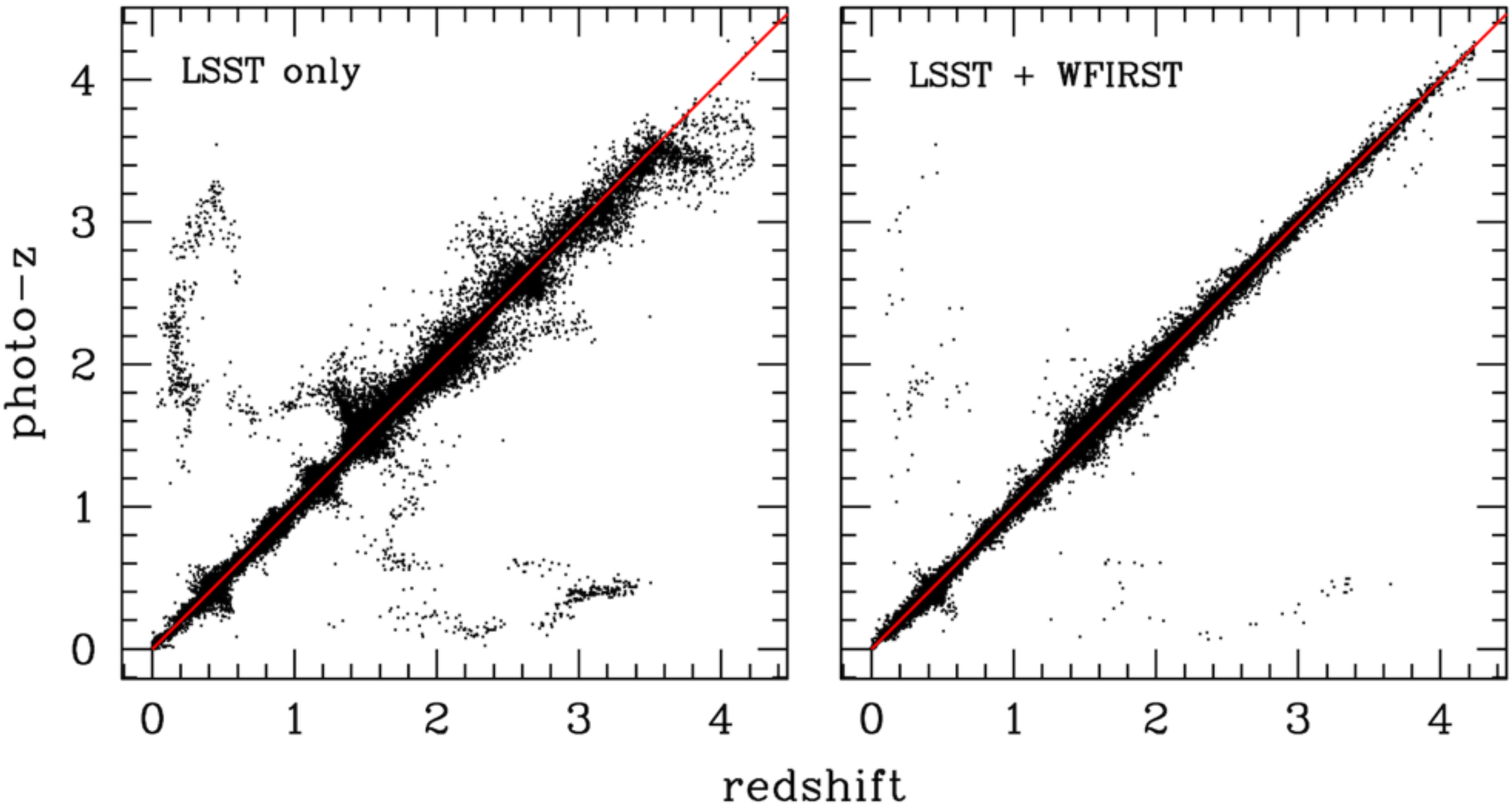
Understandability? Of features? Parameters? Models? Algorithms?

Low test error?

Does training data match deployment environment?

Jain et al, 2015

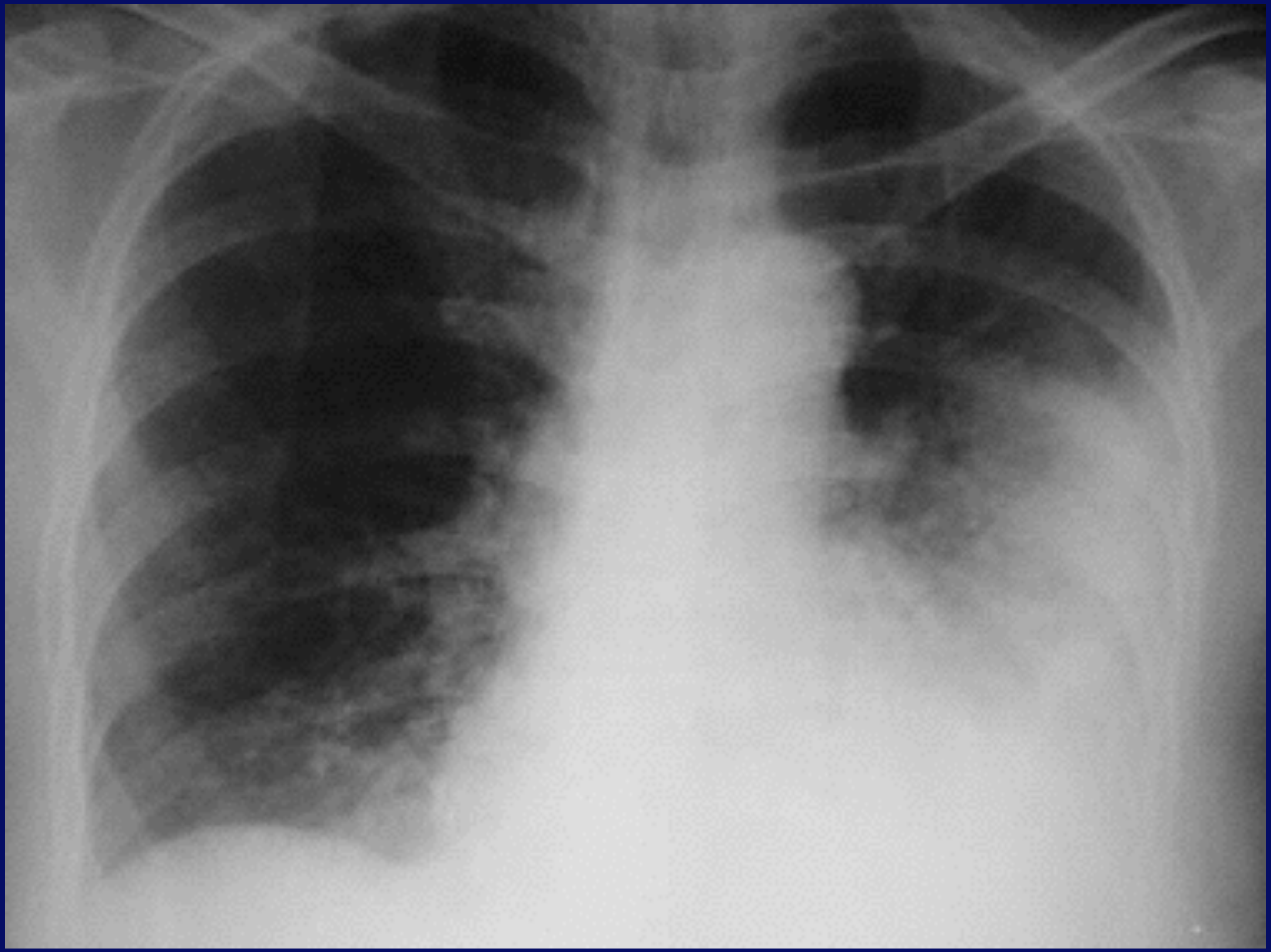
Trust



Jain et al, 2015

Causality

Transferability

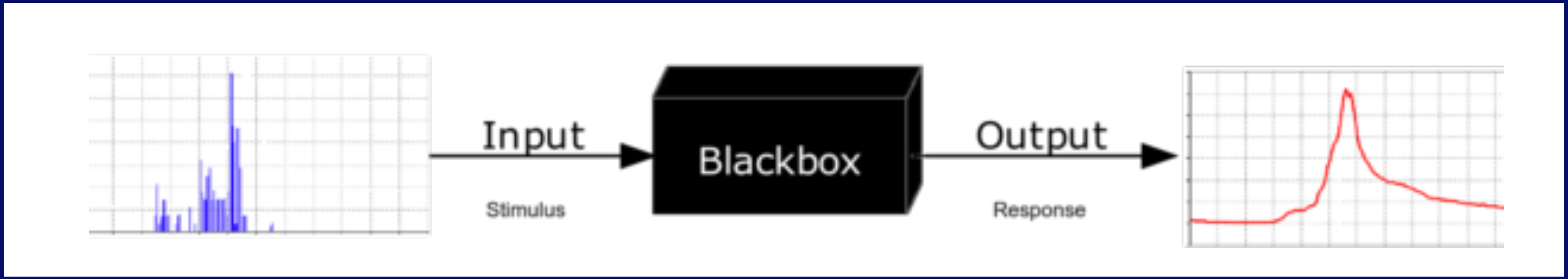


http://emedicine.medscape.com/article/360090-overview

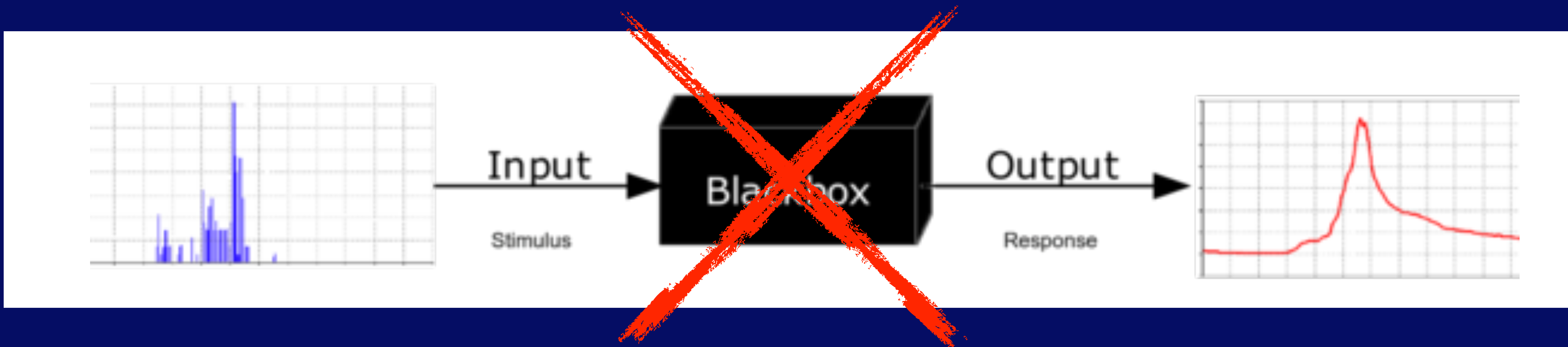
See also: Caruana et al, 2015

Properties of an interpretable model

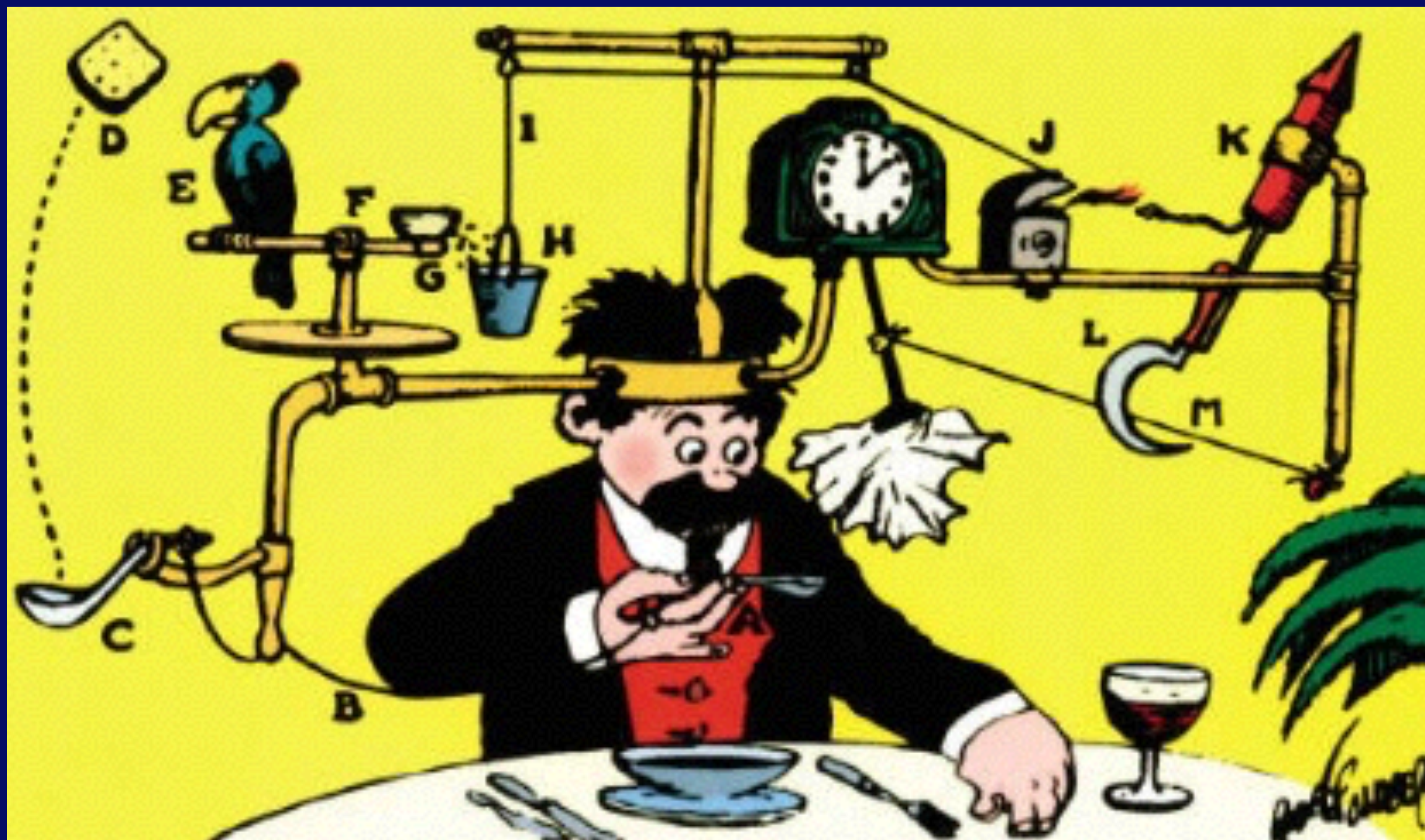
1) Transparency



1) Transparency

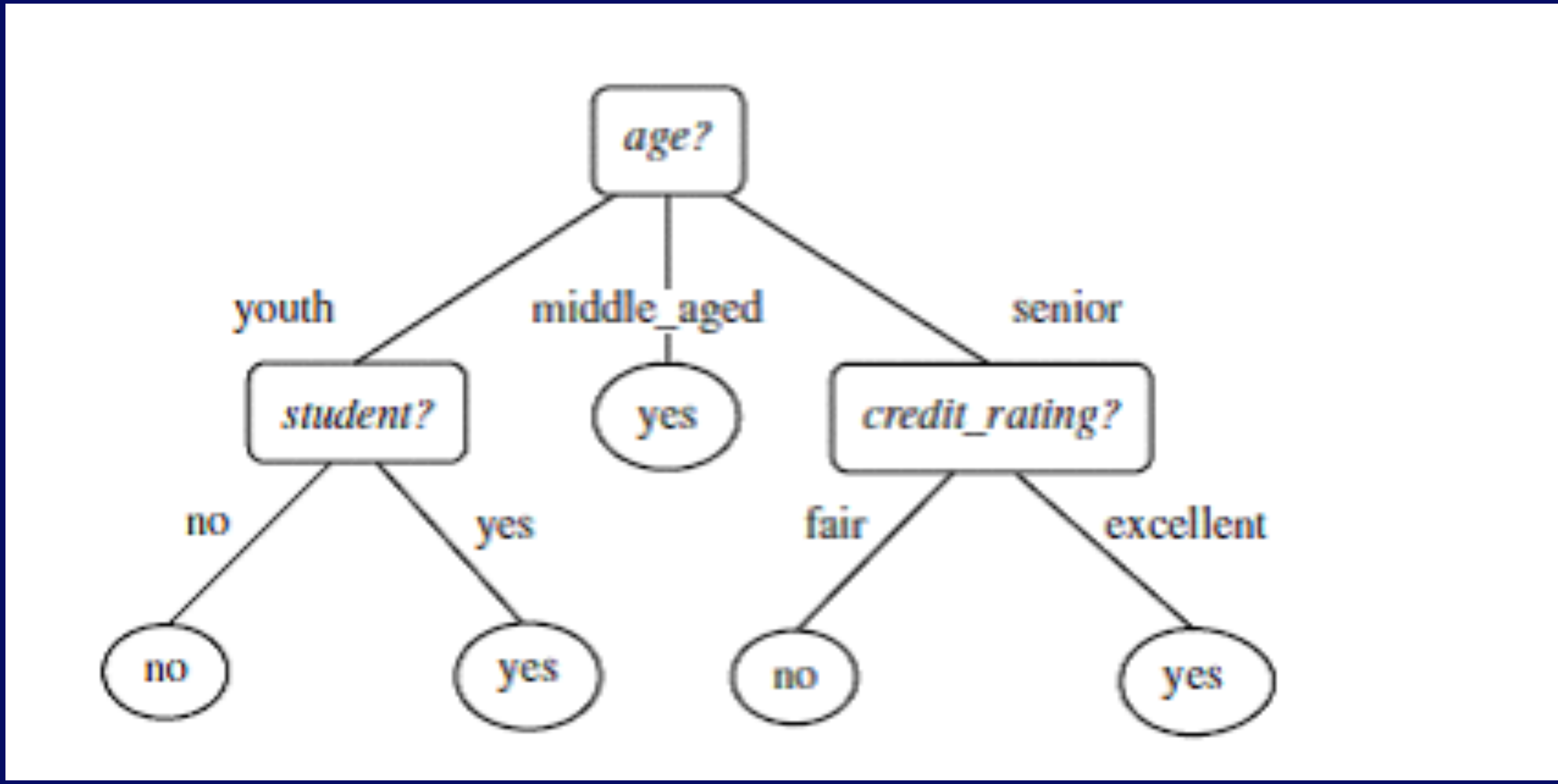


Simulatability

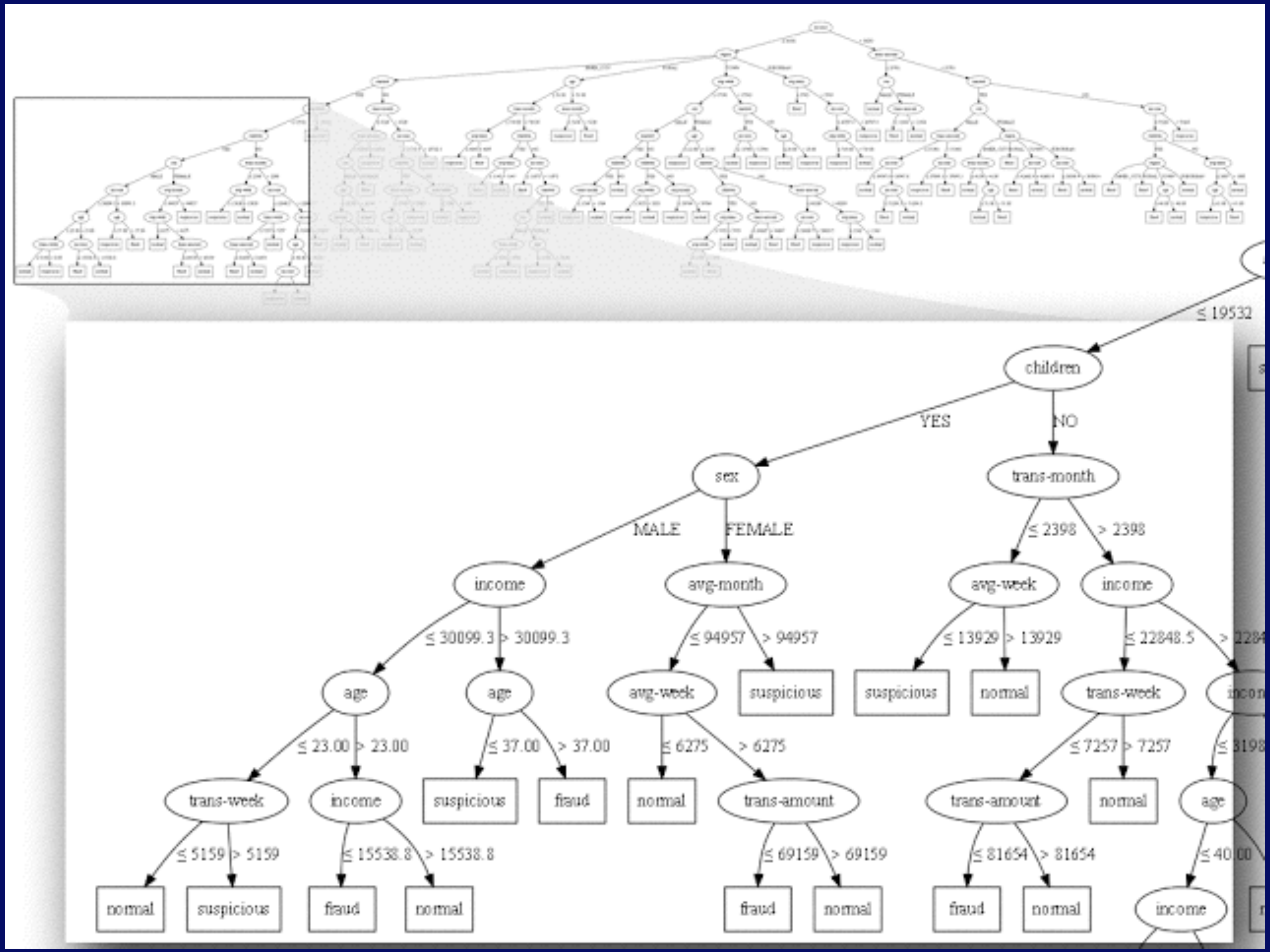


= ability to understand model in your head

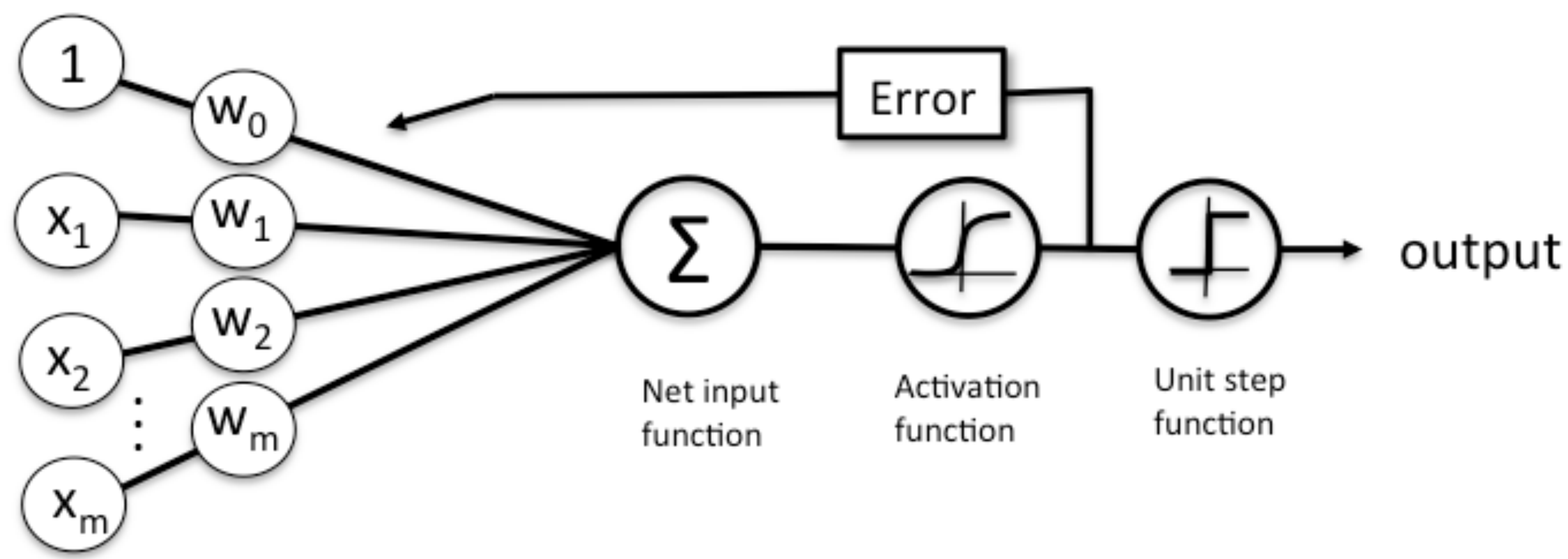
Example: Decision Trees



Example: Decision Trees



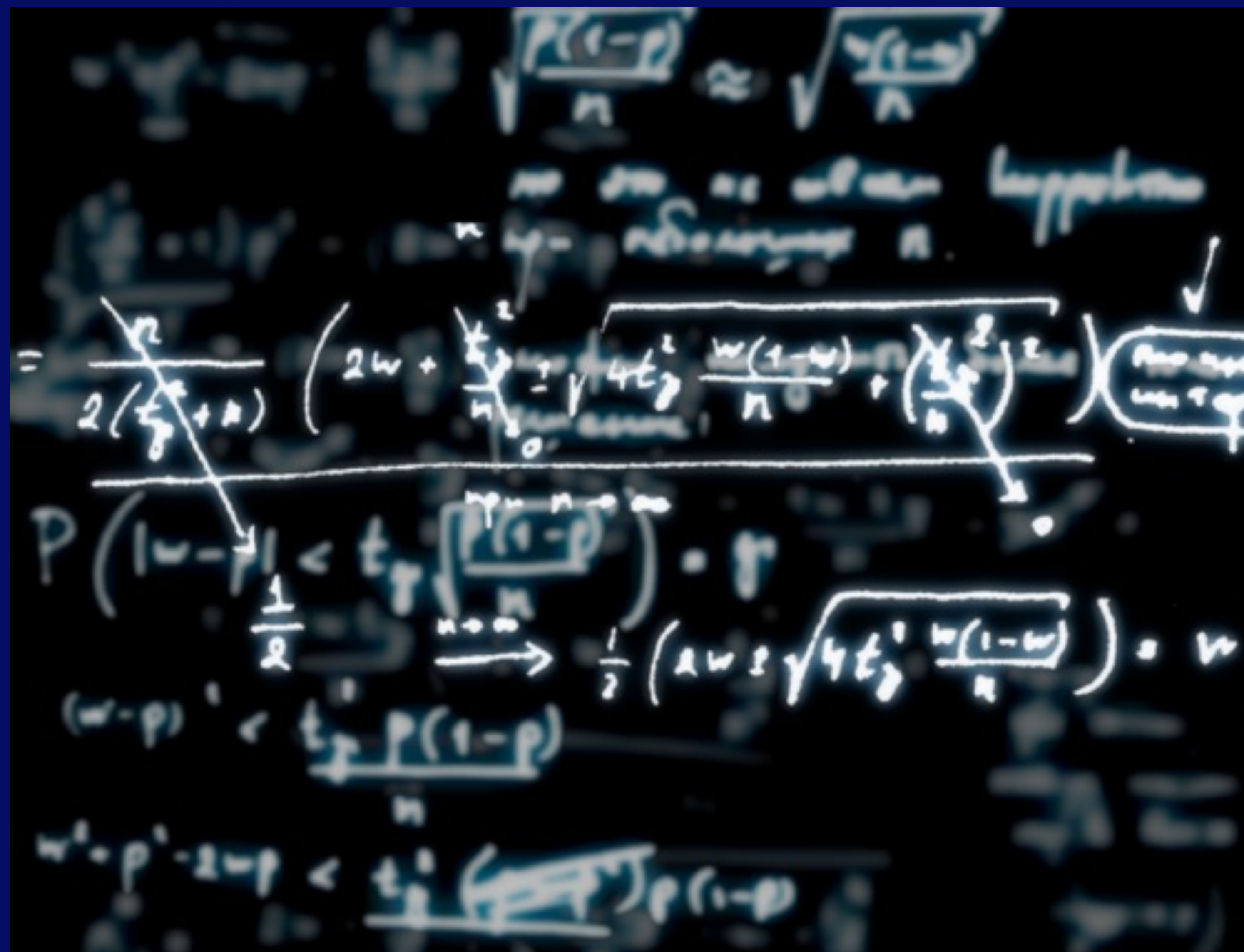
Decomposability



Schematic of a logistic regression classifier.

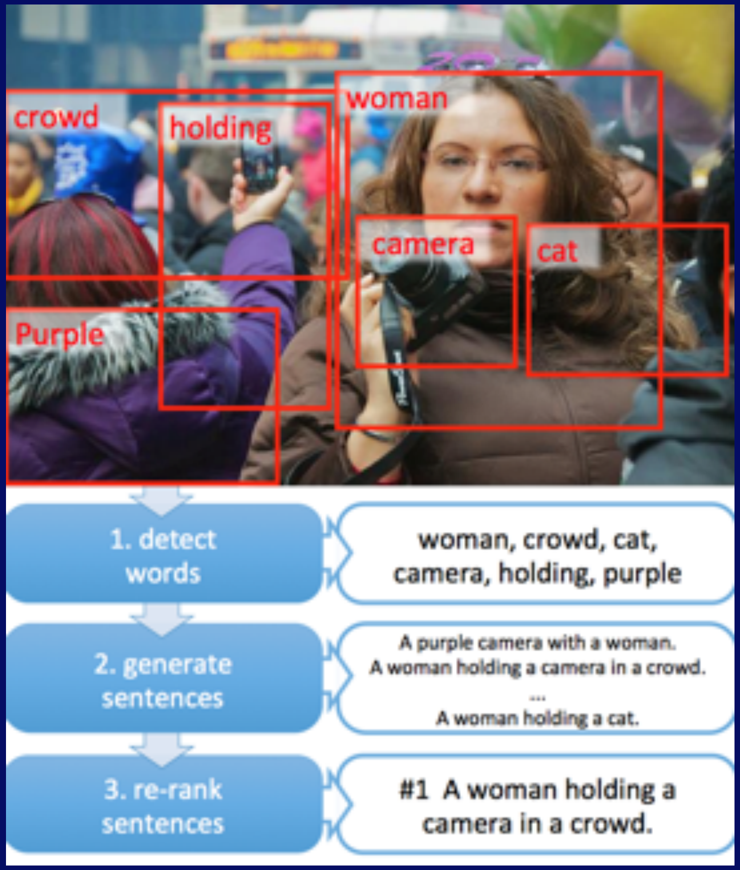
= ability to understand model components

Algorithmic Transparency*

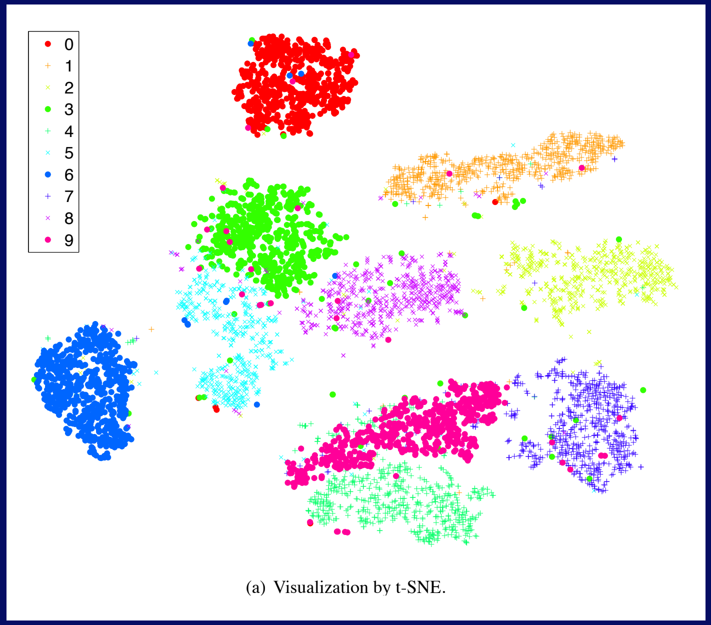


***note: humans have no algorithmic transparency whatsoever!**

2) Post-Hoc Interpretability



natural language explanations

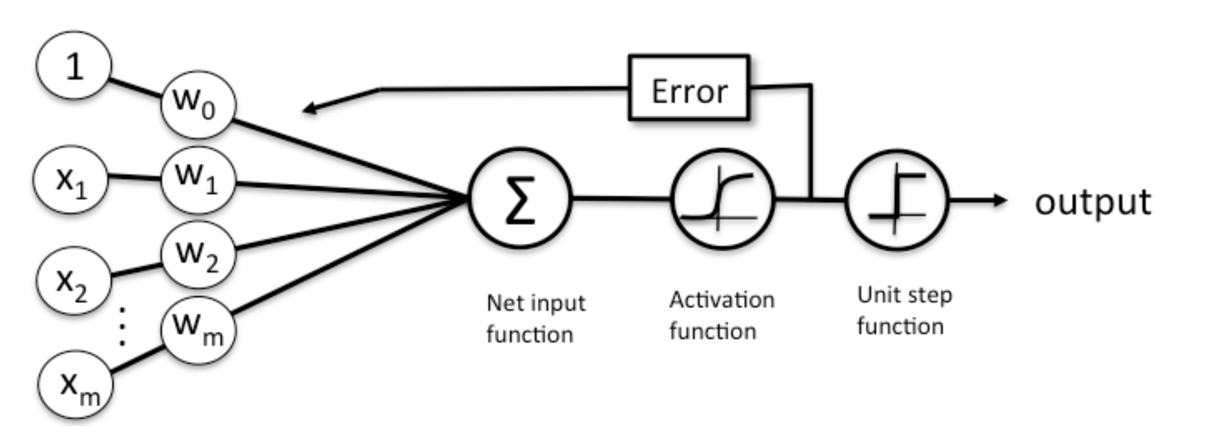


visualization

learning by example

How to make your model more interpretable (maybe)

Black Box Benchmarking



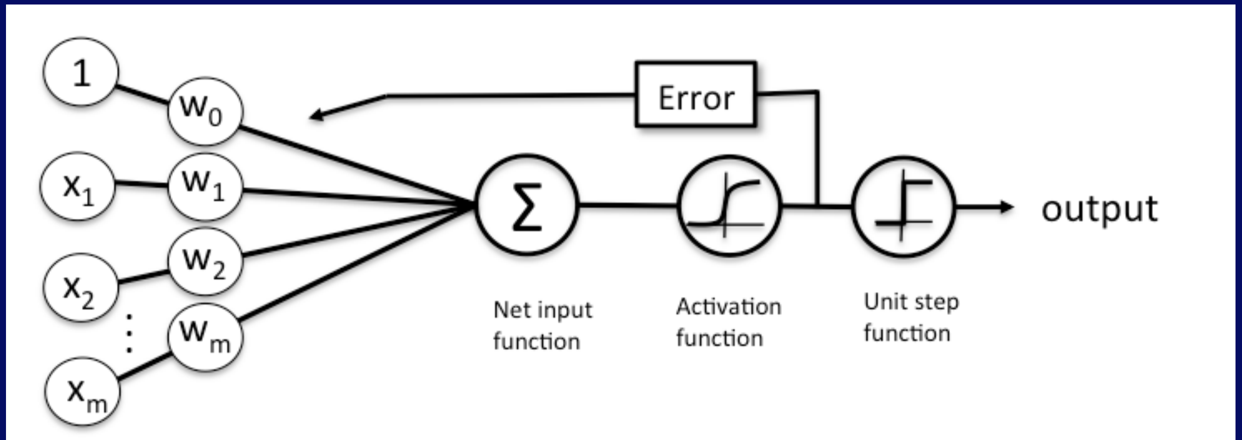
Schematic of a logistic regression classifier.

1) train linear model

2) train blackbox model

compare!

Surrogate Models



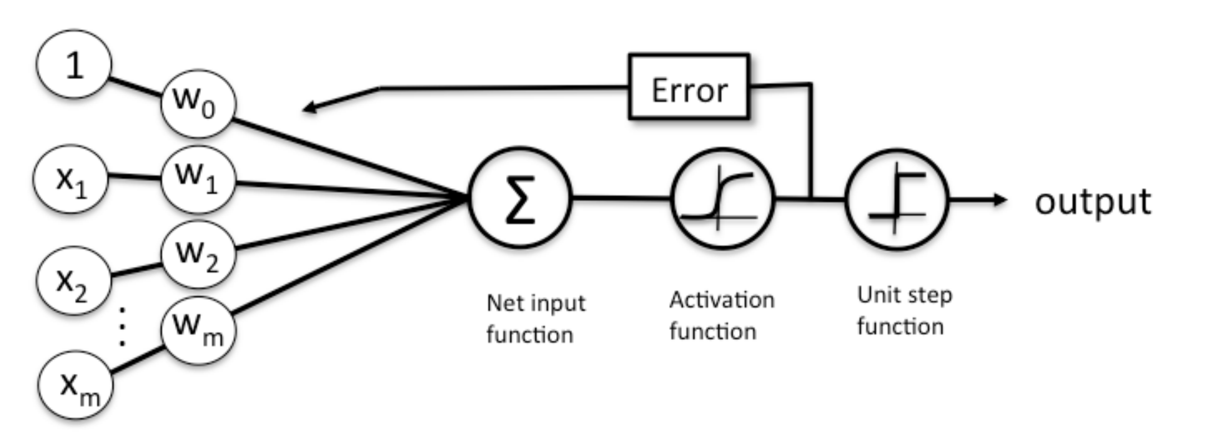
Schematic of a logistic regression classifier.

1) train blackbox model

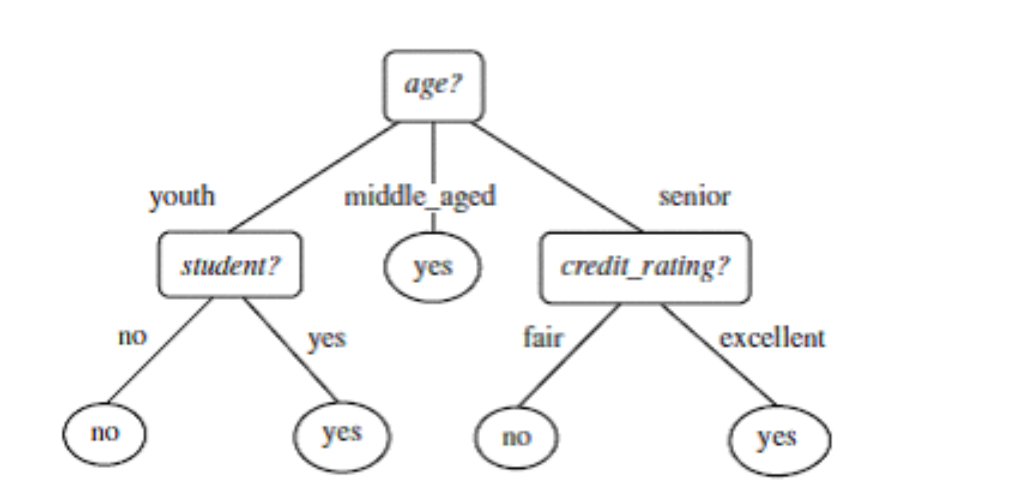
2) train interpretable model on predictors

interpret

Ensemble of Models



Schematic of a logistic regression classifier.

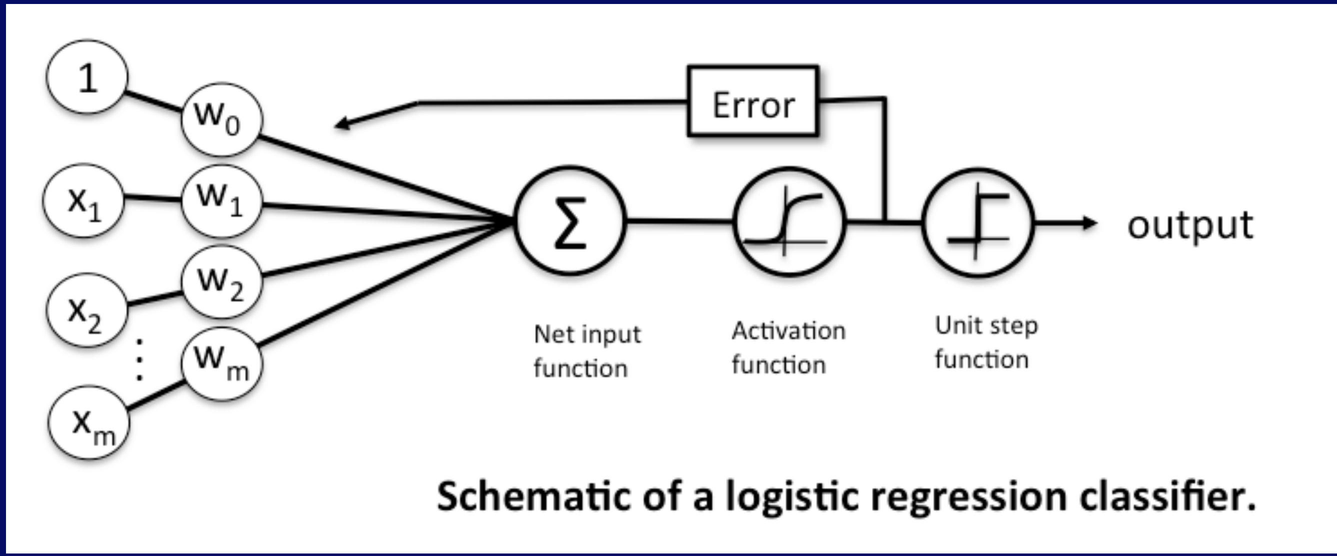


1) train interpretable linear model

2) train interpretable decision tree

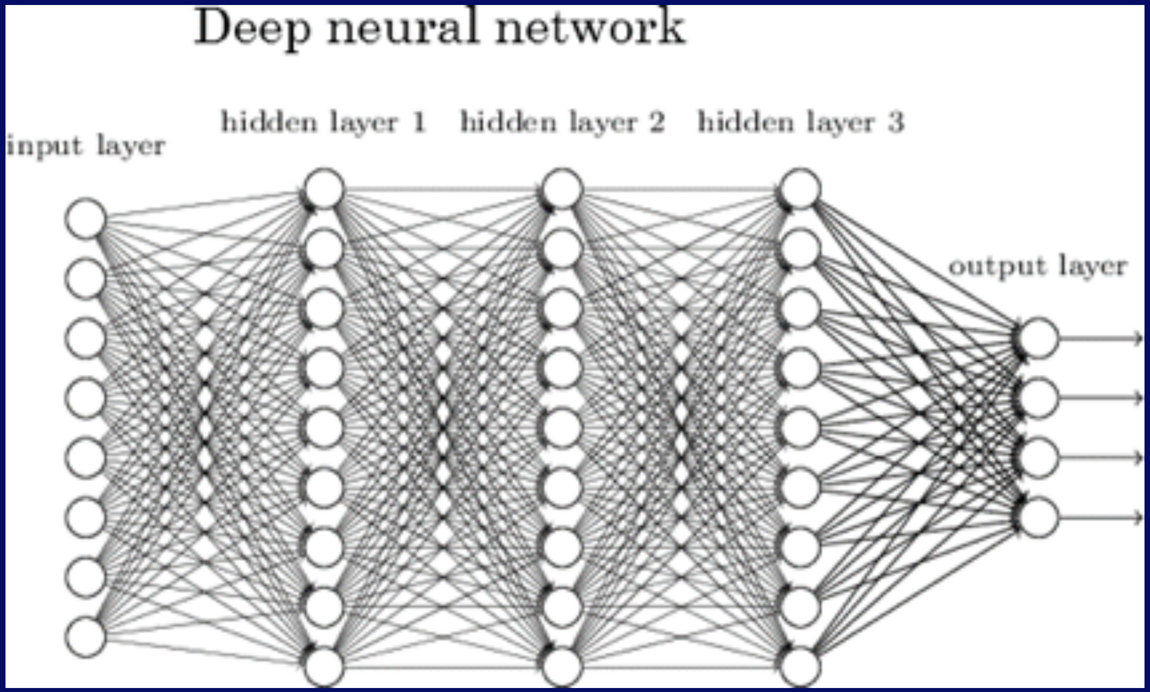
compare

Which is easier to interpret?



Schematic of a logistic regression classifier.

or



Answer: it depends!

A linear model with highly engineered features and high-dimensional variables may not be very interpretable

but: linear models have a better track record for modelling the natural world and identifying weaknesses in the training data

Think carefully about your goals, your features, and your feature engineering!