INTRODUCTION TO MACHINE LEARNING IN ASTRONOMY

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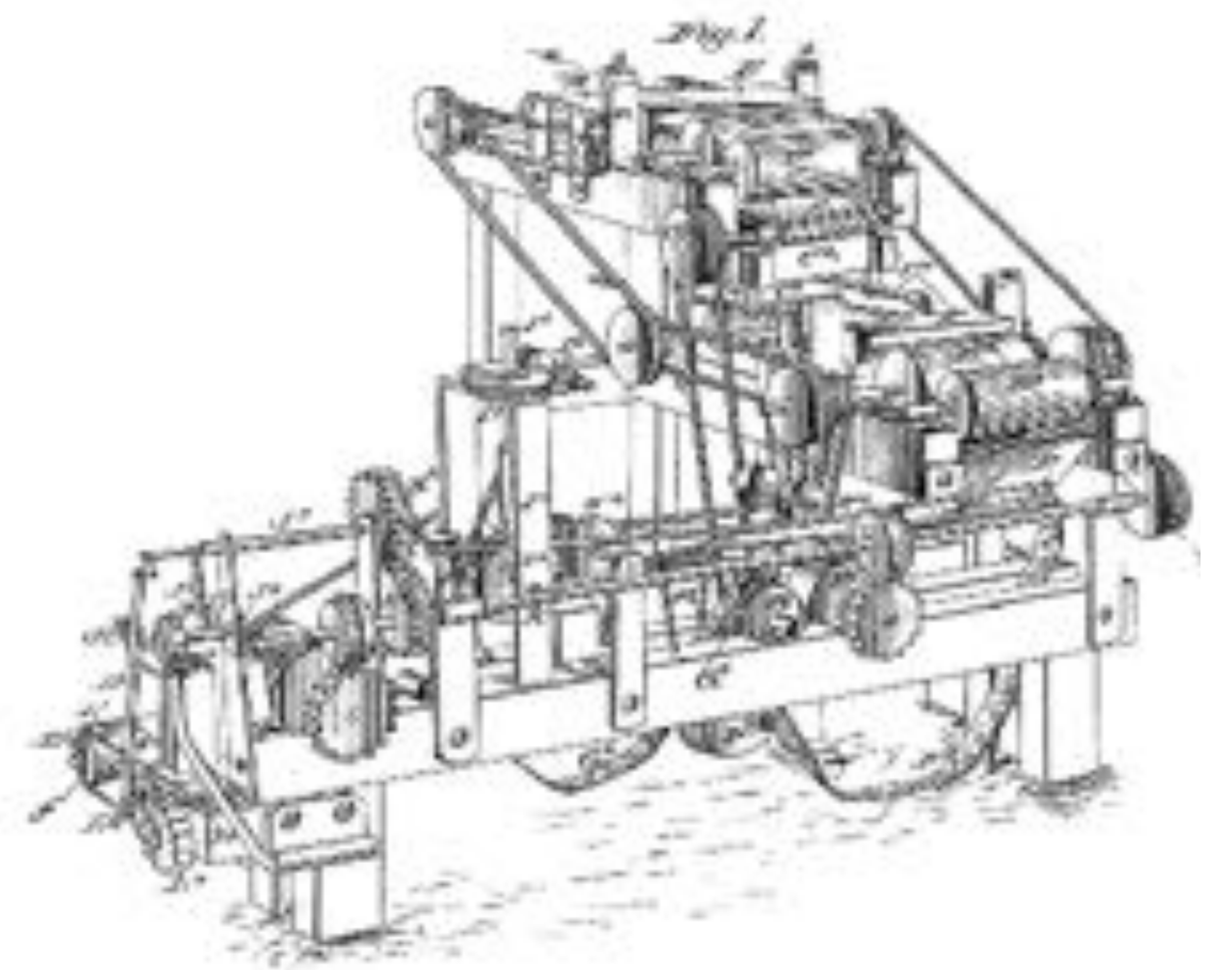
LSSTC Data Science Fellows Program
Caltech, January 2017

ABOUT ME

- Particle Physics
- Cosmology
  - Redshift Surveys (BAO)
    - SDSS (BOSS, eBOSS)
    - DESI
  - Imaging Surveys (WL)
    - LSST
- Data Science, Statistics

MACHINE LEARNING
?



MACHINE LEARNING

GPU +
cuda/opencl

[google TPU]

MACHINE LEARNING

e.g.

Suggest a missing word in a sentence.

Identify a specific person in a photo.

Drive a car automatically.

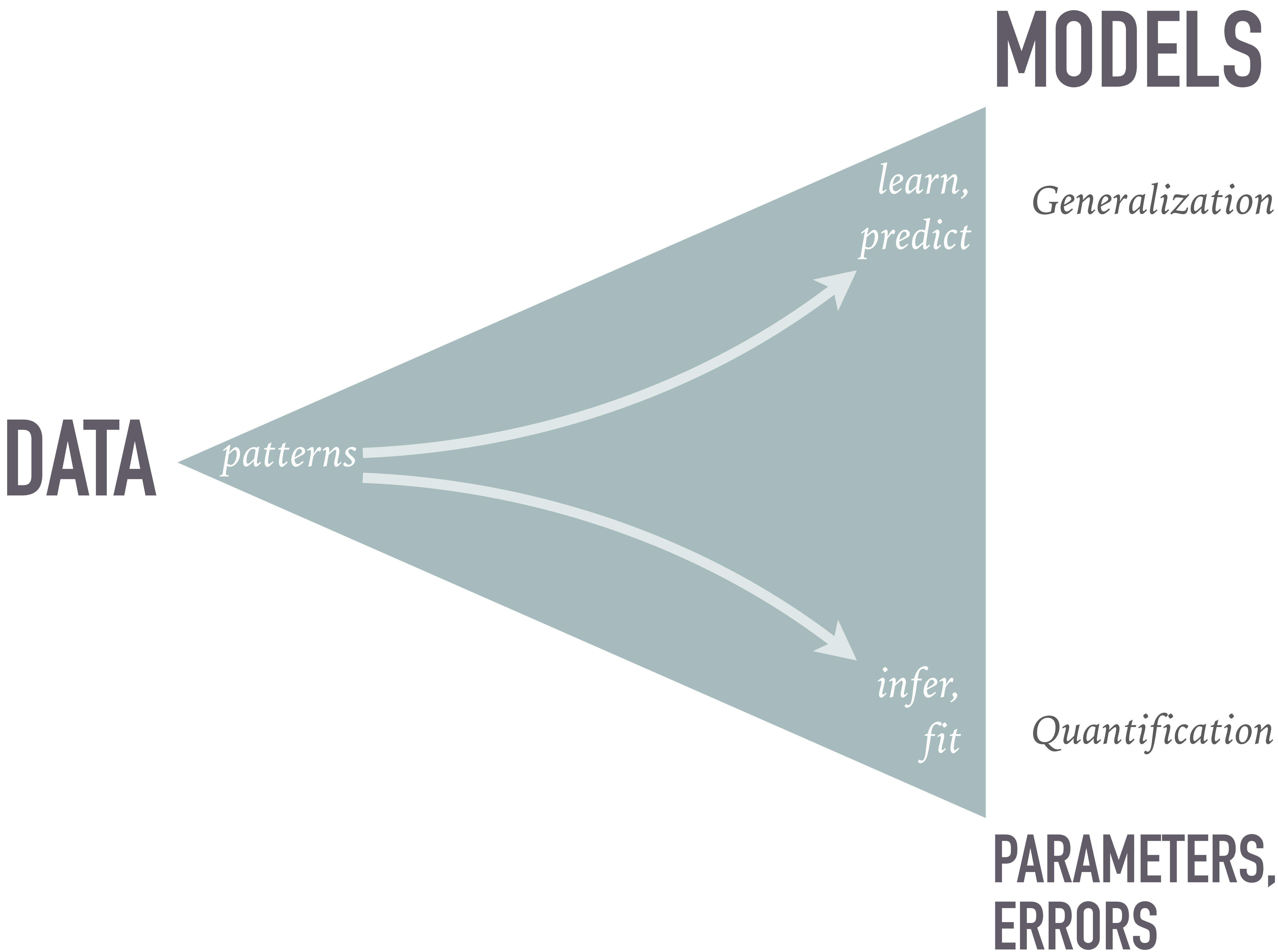
Predict the sky brightness for tomorrow night's observing.

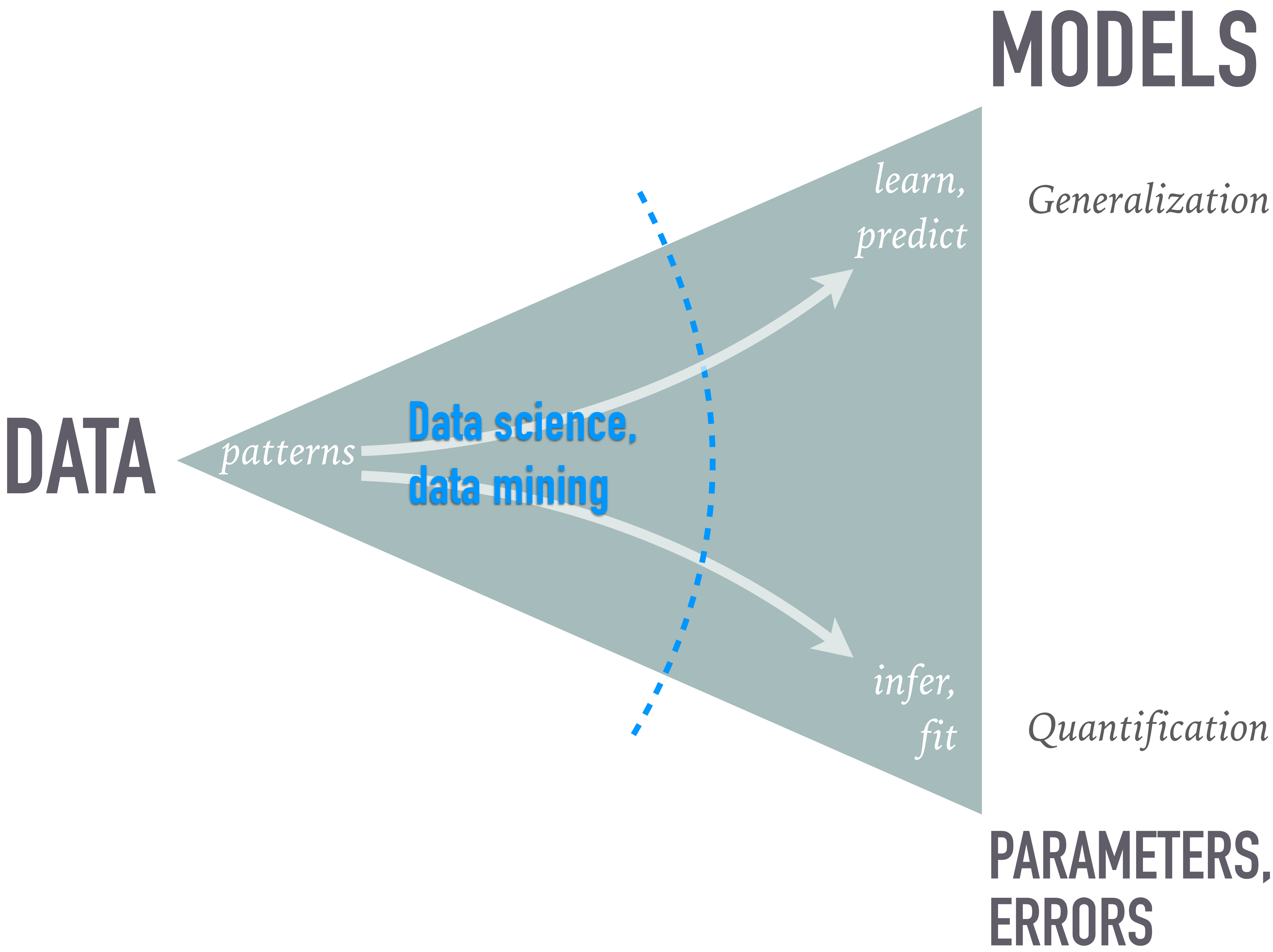
Estimate a galaxy's redshift from its LSST magnitudes.

Describe the relationship between supernovae distance and redshift.

ACTIVITY: DEFINE YOUR TERMS

- What is the relationship between machine learning and statistics?
- What is the difference between a "data scientist" and a "data engineer"?
- Rank these tasks in order of importance for your research:
  - estimating model parameters
  - finding patterns in data
  - predicting new data


MODELS
learn,
predict
Generalization
DATA
patterns
infer,
fit
Quantification
PARAMETERS,
ERRORS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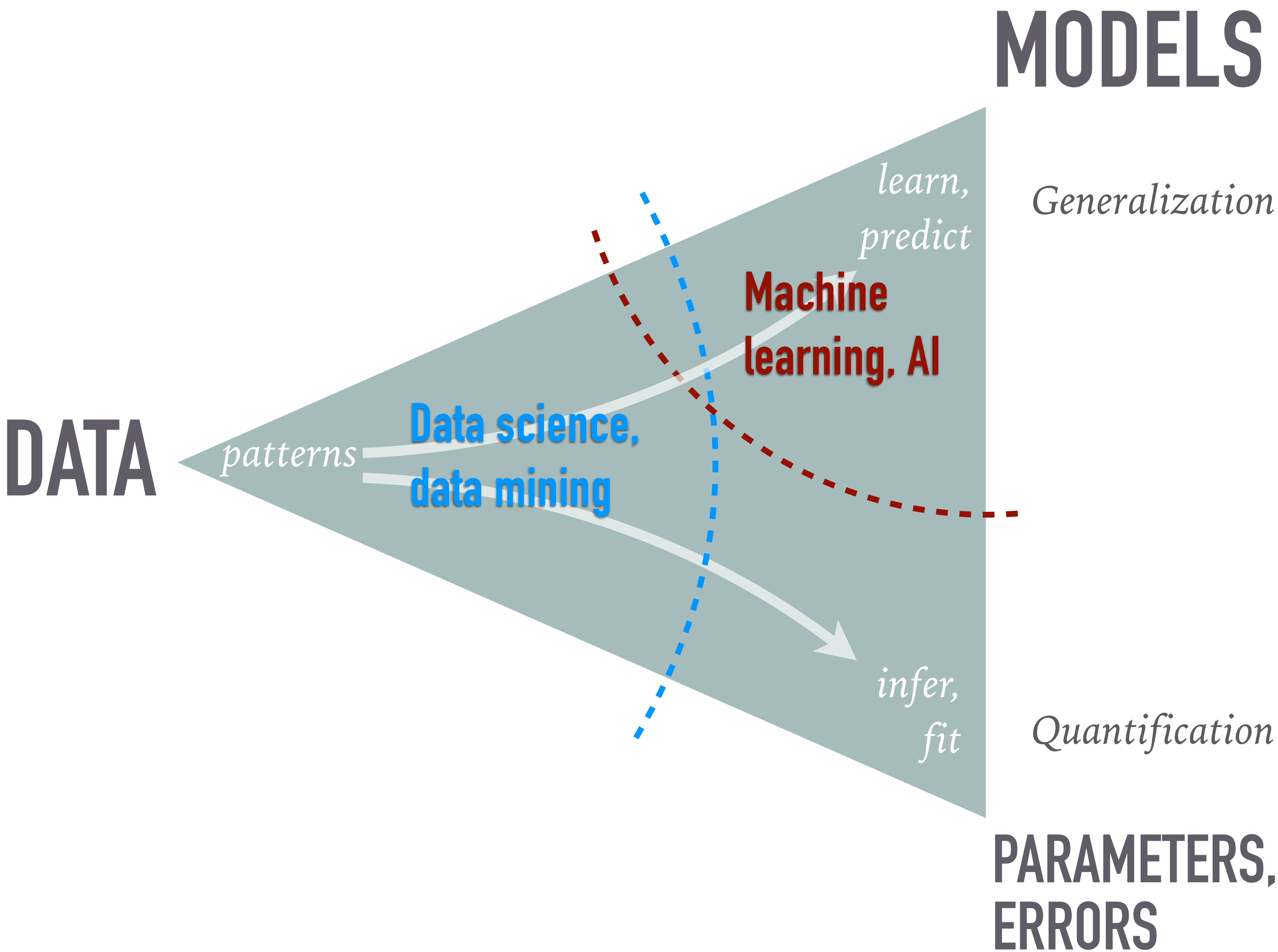
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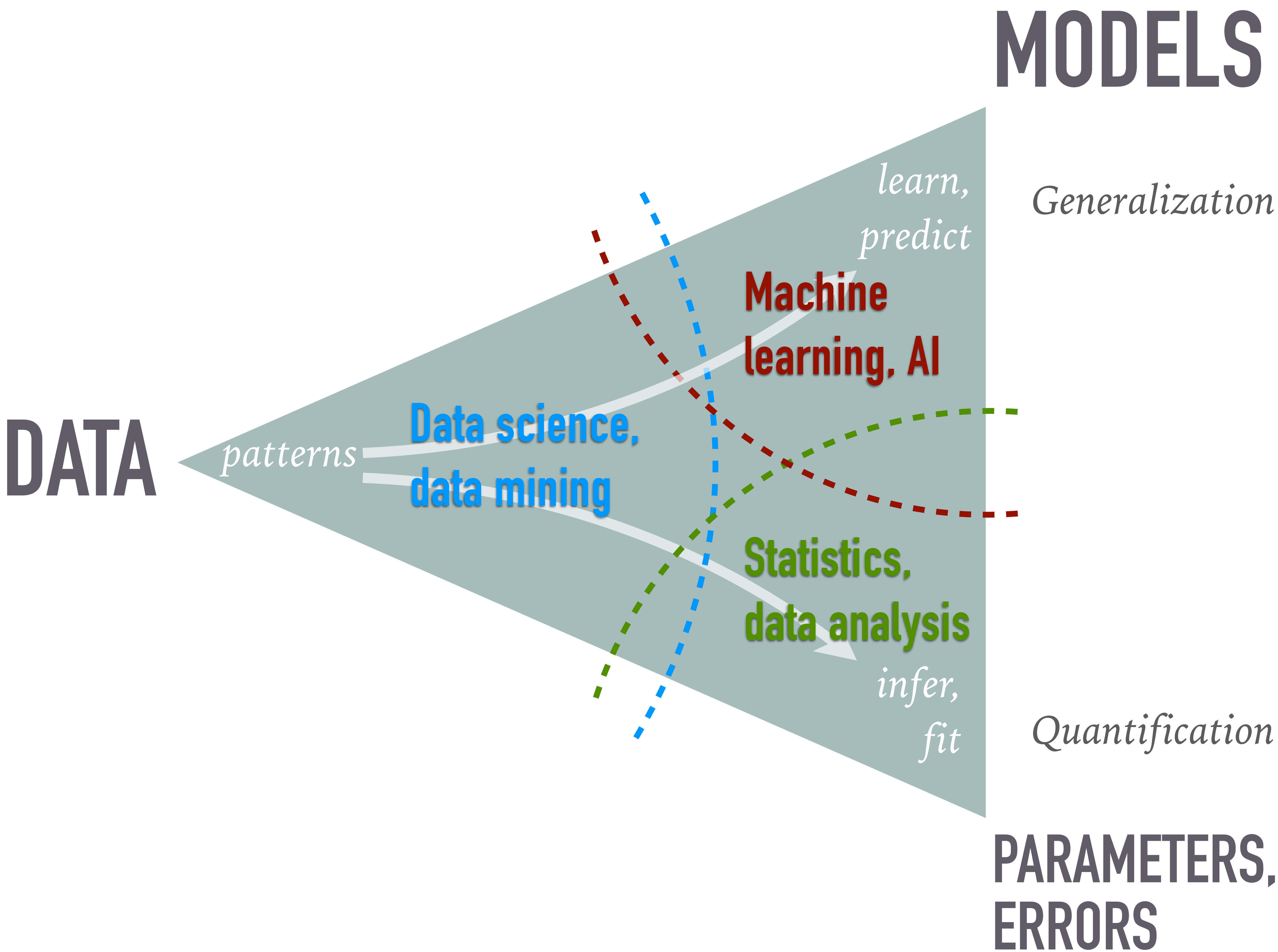
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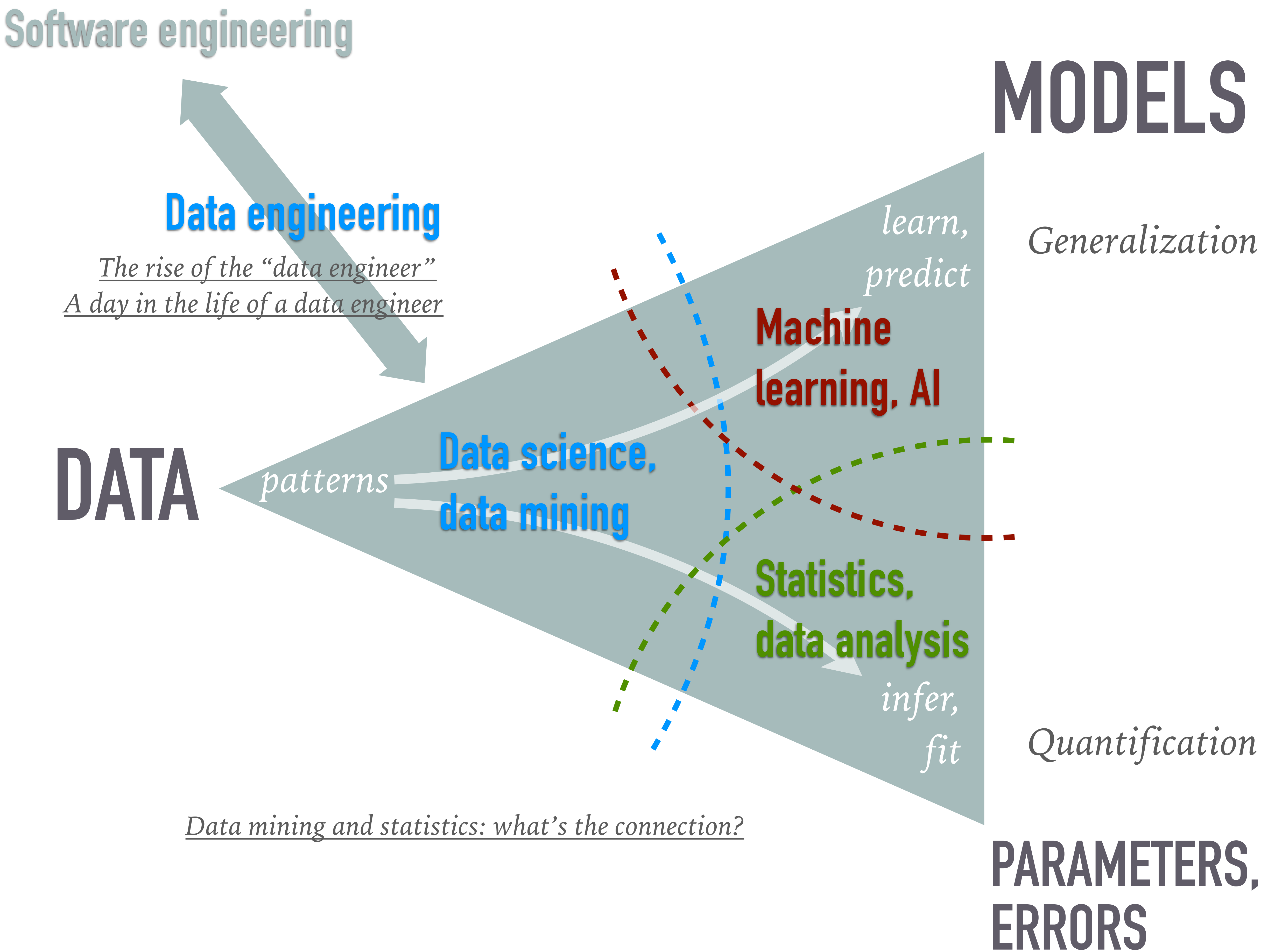
Software engineering
MODELS
Data engineering
The rise of the "data engineer"
A day in the life of a data engineer
learn,
predict
Generalization
Machine
learning, AI
DATA
patterns
Data science,
data mining
Statistics,
data analysis
infer,
fit
Quantification
Data mining and statistics: what's the connection?
PARAMETERS,
ERRORS

Glossary

Machine learning	Statistics
network, graphs	model
weights	parameters
learning	fitting
generalization	test set performance
supervised learning	regression/classification
unsupervised learning	density estimation, clustering
large grant = $1,000,000	large grant= $50,000
nice place to have a meeting: Snowbird, Utah, French Alps	nice place to have a meeting: Las Vegas in August
python	*R*
conference talk	*journal article*

http://statweb.stanford.edu/~tibs/stat315a/glossary.pdf

What's your projection into this state space?

```
['computer engineer',
 'computer scientist',
 'data engineer',
 'data scientist',
 'lsst engineer',
 'lsst scientist']
```

```
['%s %s' % (a,b) for a in ('computer', 'data', 'lsst')
                 for b in ('engineer', 'scientist')]
```

WHAT IS SPECIAL ABOUT MACHINE LEARNING IN ASTRONOMY?

- We are data producers, not data consumers:
  - Experiment / survey design.
  - Optimization of statistical errors.
  - Control of systematic errors.
- Our models are usually traceable to an underlying physical theory:
  - Models constrained by theory and observations.
  - Parameter values linked to universal constants of nature.
- A parameter error estimate is just as important as its value:
  - Prefer methods that handle input data errors and provide error estimates.

MACHINE LEARNING

=

DATA + MODELS

ROADMAP

- ✓ Introduction
- ➤ Data in astronomy
- ➤ Models in astronomy
- ➤ Statistical context of ML
- ➤ Types of learning, problems, solutions
- ➤ The bleeding edge of ML

ACTIVITY: REASONING ABOUT DATA AND MODELS

- Is a CCD raw image <u>data</u>?
- Is a galaxy catalog <u>data</u>?
- Is a histogram a <u>model</u>?
- Do you need a <u>model</u> to calculate an average?
- Does your research focus more on <u>data</u> or <u>models</u>?

DATA + MODELS

"Data" are a finite set of measurements:

- ➤ *e.g., spreadsheet, FITS table, …*
- ➤ *numeric / categorical / mixed?*
- ➤ *ordered? (special role of time, stochastic processes & MCMC)*
- ➤ *independent? identically distributed?*
- ➤ *measurement errors (implicit / explicit)*
- ➤ *binned / un-binned?*
- ➤ *similarity measure?*

columns ~ "features"

rows ~ samples, observations

x	y	z	a	b	c

ASTRONOMICAL DATA + MODELS

Astronomical data:

- measure physical processes (units!)
- low level: images, spectra, time series.
- high level: catalogs.
- results from careful experimental / survey design.
- has quantifiable statistical and systematic uncertainties.

DATA + MODELS

"Models" specify the probability of different outcomes:

- *explicit: probability density function.*
- *implicit: algorithm to generate random outcomes ("forward" model).*
- *observables vs parameters (vs hyper-parameters vs …).*
- *integrability: required to calculate normalized probabilities.*
- *differentiability: required to find most probable (uphill) direction.*
- *hierarchical construction.*
- *variance - bias tradeoffs.*
- *regularization: bias towards "sensible" interpretations.*

DATA + ASTRONOMICAL MODELS

Astronomical models:

- ➤ are usually traceable to an underlying physical theory.
- ➤ parameters often related to universal constants of nature.
- ➤ often have known distribution of measurement errors.
- ➤ need to account for instrumental effects (calibration).
- ➤ prefer models that:
  - ➤ handle input data errors (often via weights),
  - ➤ provide error estimates.

ACTIVITY: REASONING ABOUT ML PROBLEMS

- Rank these ML problems in order of "difficulty".
- List a few possibly relevant data features.

1. *Suggest a missing word in a sentence.*
2. *Identify a specific person in a photo.*
3. *Drive a car automatically.*
4. *Predict the sky brightness for tomorrow night's observing.*
5. *Estimate a galaxy's redshift from its LSST magnitudes.*
6. *Describe the relationship between supernovae distance and redshift.*

A model is trained on, fit to, or inferred from data.

DATA + MODELS

Data is a realization of some model

(but probably not the one you are using).

HOW TO BUILD A MODEL?

Exploratory data analysis & visualization:

- single feature: histogram of PDF, CDF.
- two features: scatter plot.
- multiple features:
  - pair-wise corner plot.
  - local embedding (tSNE, …).

DATA + MODELS

THE LANGUAGE OF ML IS STATISTICS (NOT PYTHON!)

- Key ideas:
  - Bayes theorem.
  - Occam’s razor.

- Given some data:
  - Infer probabilities assuming a model.
  - Compare alternative models.

ACTIVITY: BAYESIAN REASONING

English or not english?

- Write down your best guess: YES/NO.

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- Think about the probability that the answer is YES. Write down a number.

ACTIVITY: BAYESIAN REASONING

English or not english?

- Write down your best guess: YES/NO.
- Think about the probability that the answer is YES. Write down a number.
- Discuss your reasoning with your neighbor, then update your answer.

ACTIVITY: BAYESIAN REASONING

- What do we know?
  - DATA = “wearing an ENGLAND t-shirt”
- What question are we asking?
  - P(english | DATA) ?
- What do we need to assume?
  - MODEL =

```
if english:
  prob[DATA] = 1/3
else:
  prob[DATA] = 1/5
```

  - PRIOR = “20% of astronomers are english”

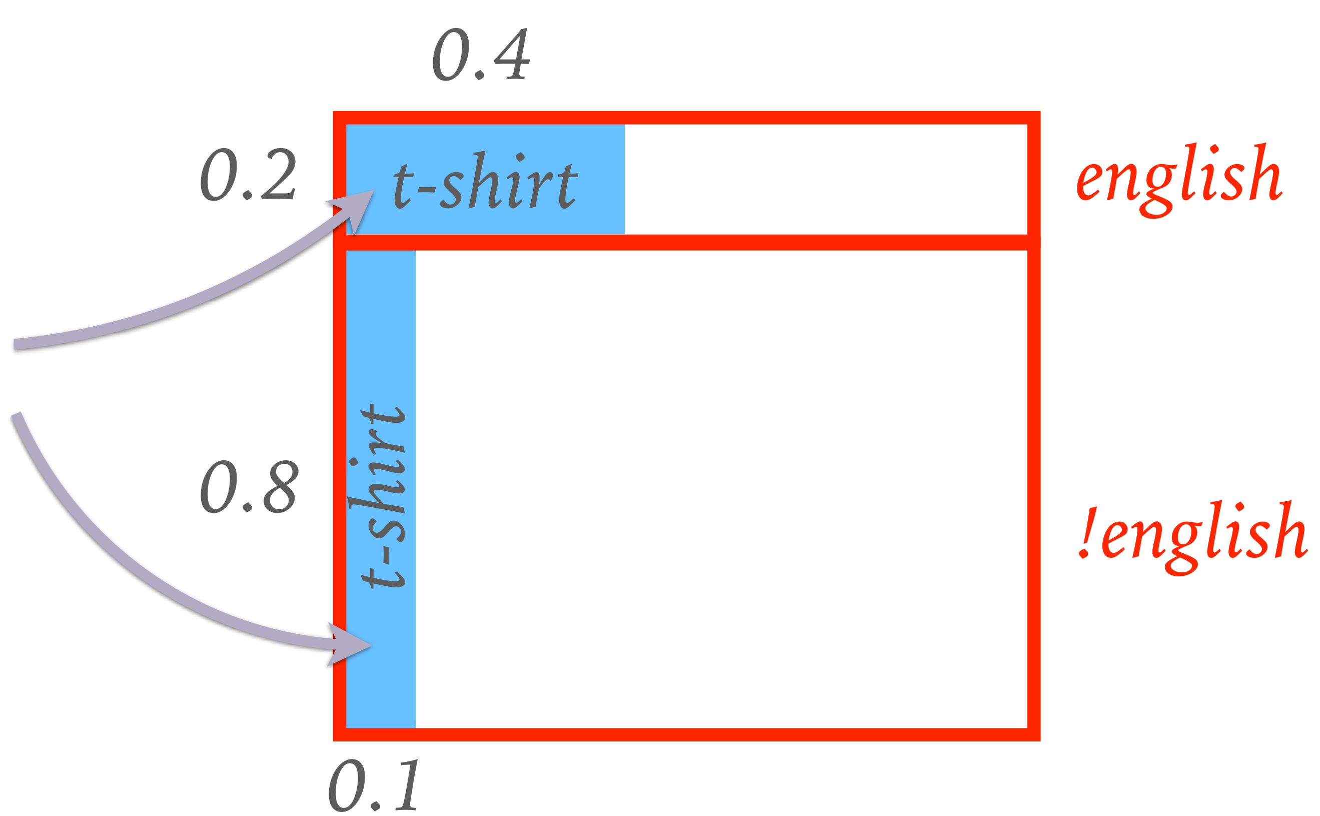
ACTIVITY: BAYESIAN REASONING

- PRIOR = "20% of astronomers are english"
- MODEL =

```
if english:
  prob[DATA] = 0.4
else:
  prob[DATA] = 0.1
```

- DATA = "wearing an ENGLAND tshirt"

P(english | DATA) = ratio of these areas



ACTIVITY: BAYESIAN REASONING

0.4 0.2

$$P(\text{english} \mid \text{tshirt}) = \frac{P(\text{tshirt} \mid \text{english})\ P(\text{english})}{P(\text{tshirt})}$$

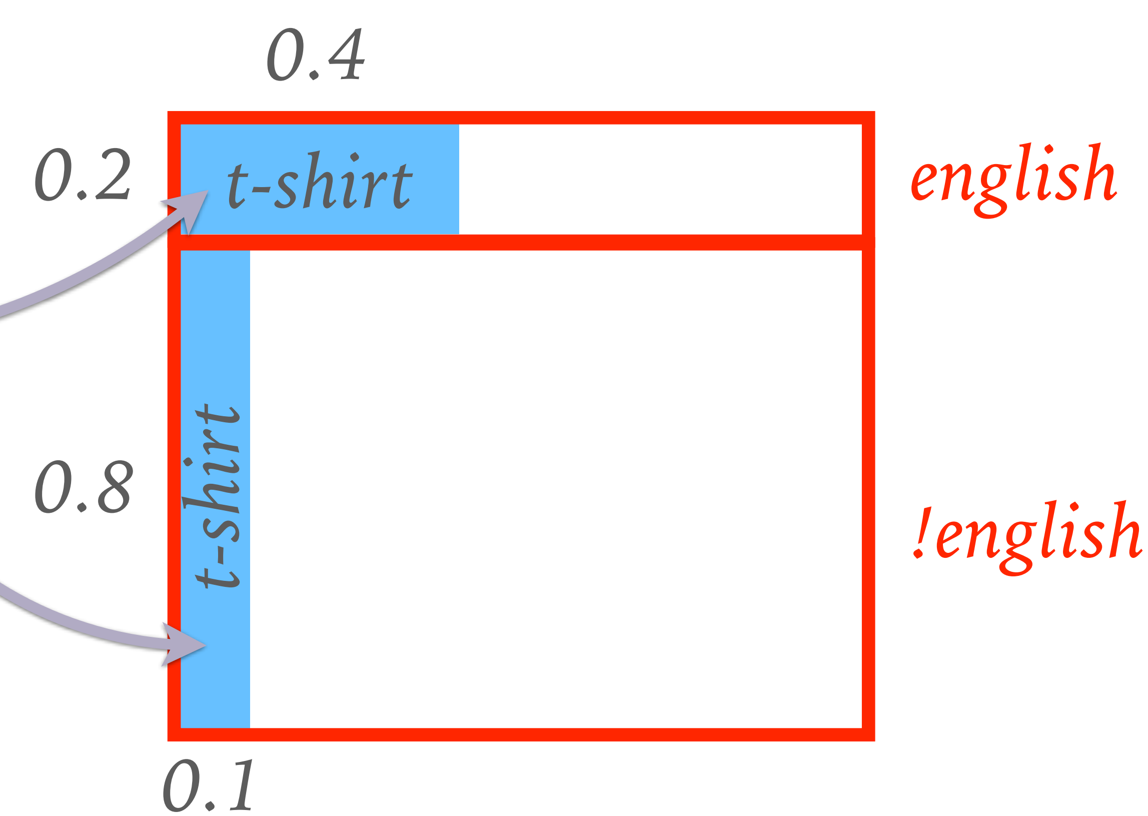
0.5

0.16

$$P(\text{tshirt}) = P(\text{tshirt} \mid \text{english})\ P(\text{english}) + P(\text{tshirt} \mid \text{!english})\ P(\text{!english})$$

0.16 0.4 0.2 0.1 0.8

P(english | DATA) =
ratio of these areas

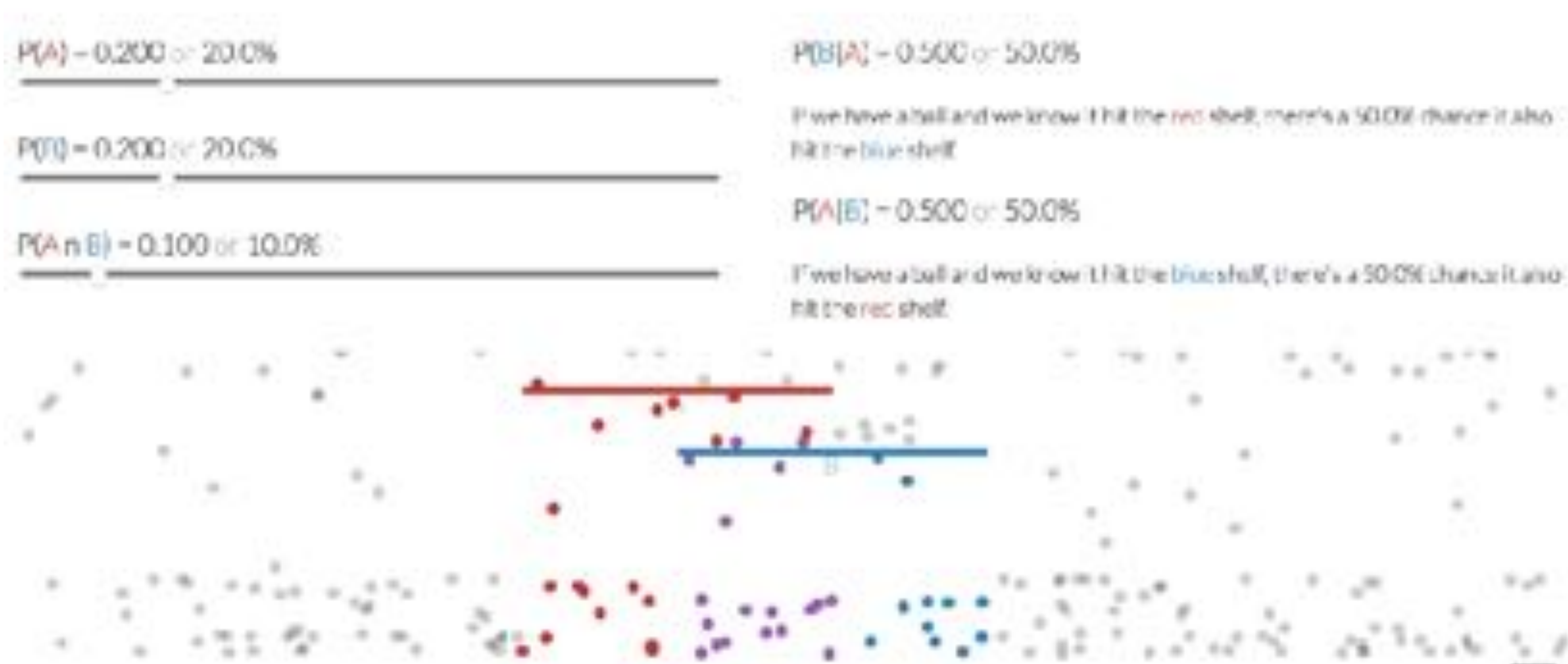


BAYES' THEOREM

http://setosa.io/ev/conditional-probability/

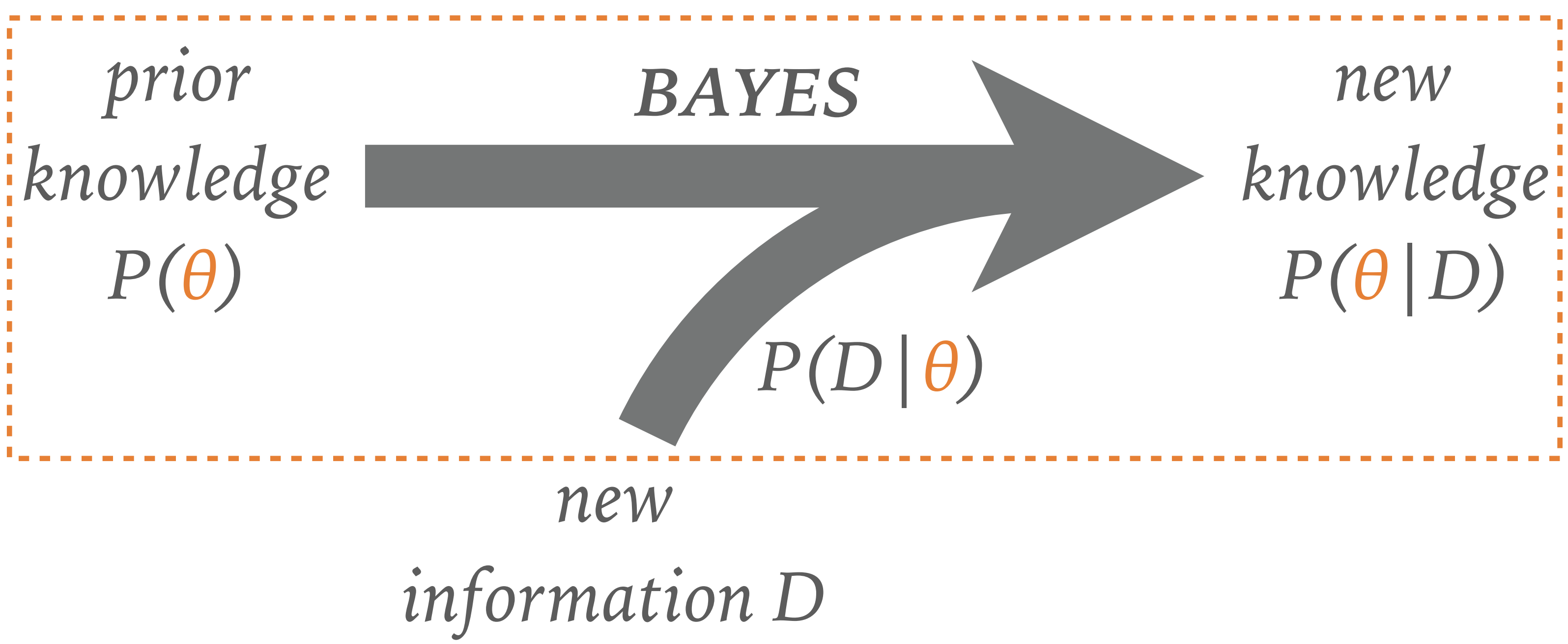
- The theorem has two ingredients:
  - The definition of conditional probability for outcomes.
  - Unified treatment of observables (data) and parameters (model) as outcomes.

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$



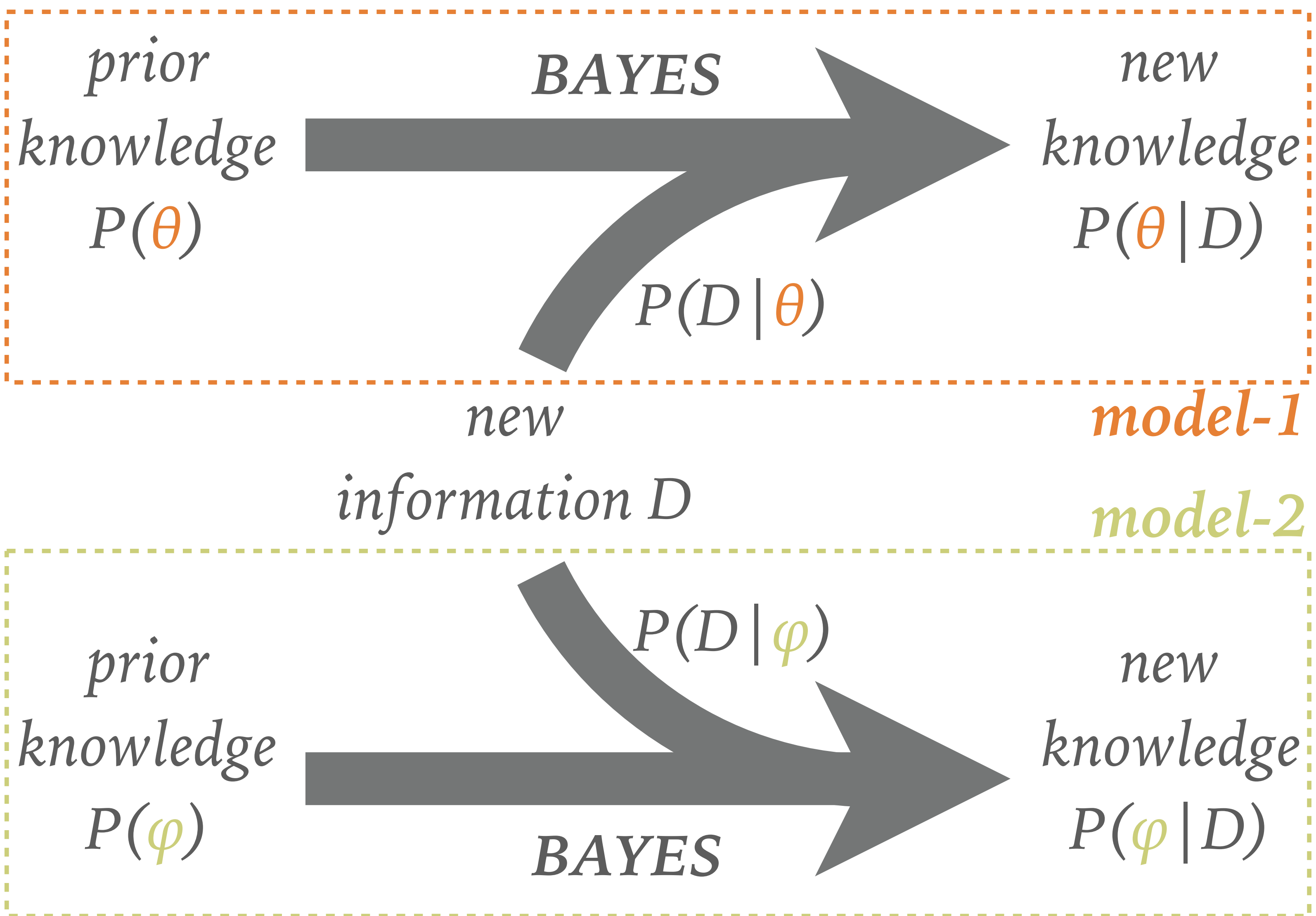
HOW DO WE USE BAYES' THEOREM?

- To update our knowledge based on new information.
  - Must specify a model and priors!



HOW DO WE USE BAYES' THEOREM?

- To update our knowledge based on new information.
  - Must specify a model and priors!
- To compare alternative models that explain the same data.



BAYESIAN MODEL COMPARISON

- We normally use Bayes' rule for the (posterior) probability of data D given specified parameters θ and model M:

$$P(\theta|D,M) = \frac{P(D|\theta,M)\,P(\theta,M)}{P(D,M)}$$

- In order to turn this into a statement about the model without specifying the parameters, we need to marginalize (integrate) them out:

$$P(M|D) = \frac{P(D|M)\,P(M)}{P(D)}$$

(I am skipping many lines of probability calculus here)

BAYESIAN MODEL COMPARISON

$$P(M|D) = \frac{P(D|M)\,P(M)}{P(D)}$$

- The denominator P(D) can only be evaluated if you can fully specify all possible models!
  - Generally cannot make statements about the absolute (posterior) probability of a single model.
  - However, P(D) cancels in probability ratios:

$$\underbrace{\frac{P(M_1|D)}{P(M_2|D)}}_{\textit{Odds ratio}} = \underbrace{\frac{P(D|M_1)}{P(D|M_2)}}_{\textit{Bayes factor}}\;\underbrace{\frac{P(M_1)}{P(M_2)}}_{\textit{Model priors}}$$

BAYESIAN MODEL COMPARISON

- How is the "naturalness" of a model taken into account?
  - Model priors.
  - Occam factor.

$$\frac{P(M_1|D)}{P(M_2|D)} = \underbrace{\frac{P(D|M_1)}{P(D|M_2)}}_{\textit{Bayes factor}} \underbrace{\frac{P(M_1)}{P(M_2)}}_{\textit{Model priors}}$$

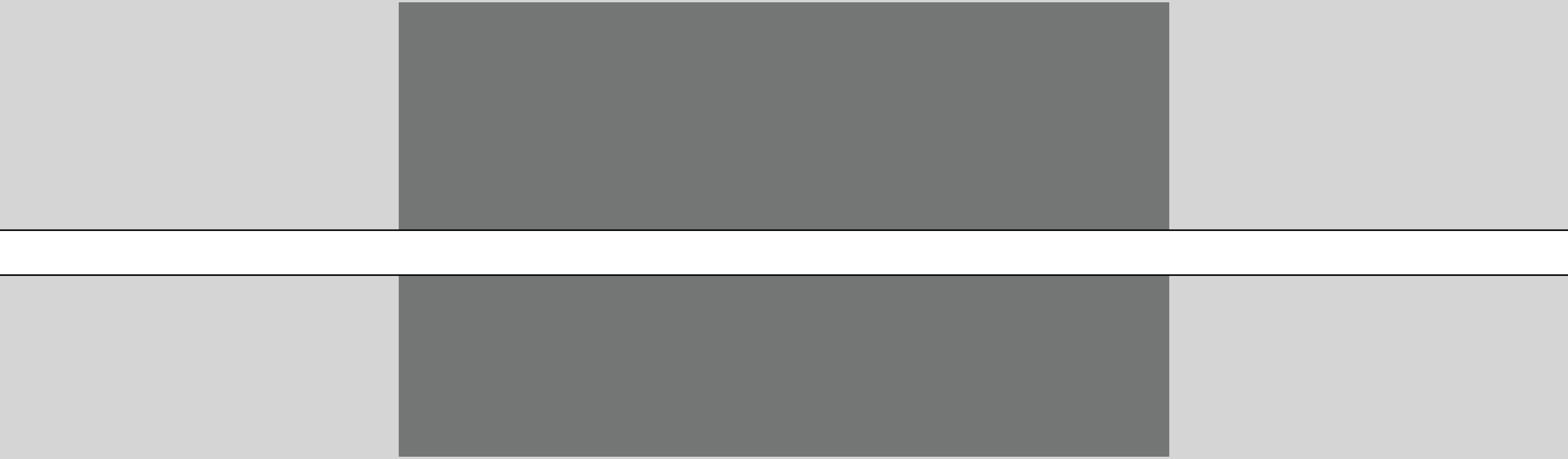
$$\underbrace{\frac{P(D|M_1)}{P(D|M_2)}}_{\textit{Bayes factor}} \propto \underbrace{\frac{(\textit{fraction of } M_1 \textit{ param. space favored by D})}{(\textit{fraction of } M_2 \textit{ param. space favored by D})}}_{\textit{Occam factor}}$$

OCCAM FACTOR

How many large galaxies?

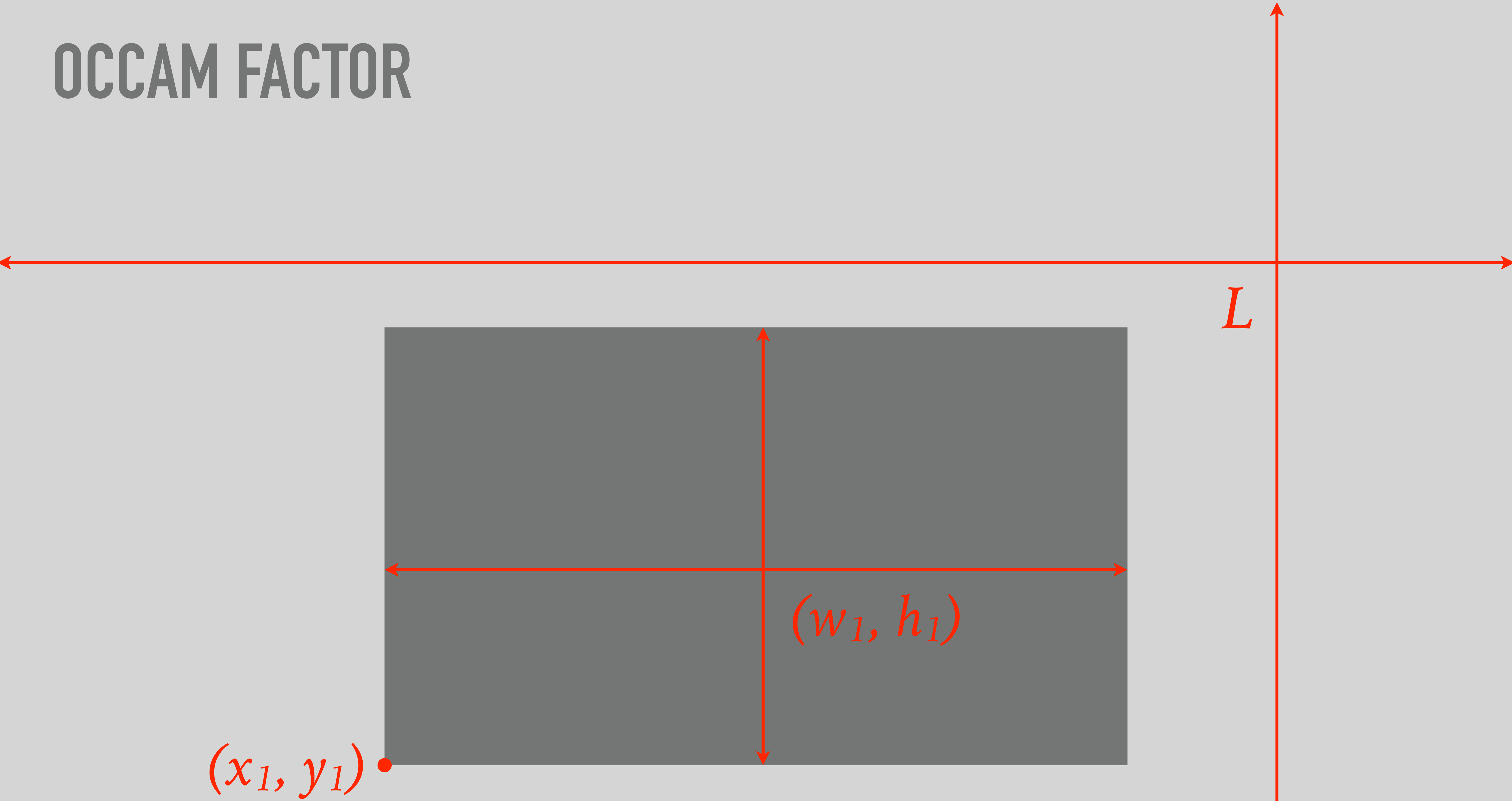
OCCAM FACTOR

- *Is it possible there are two rectangles?*
- *Why are two rectangles an unnatural model?*



How many rectangles?

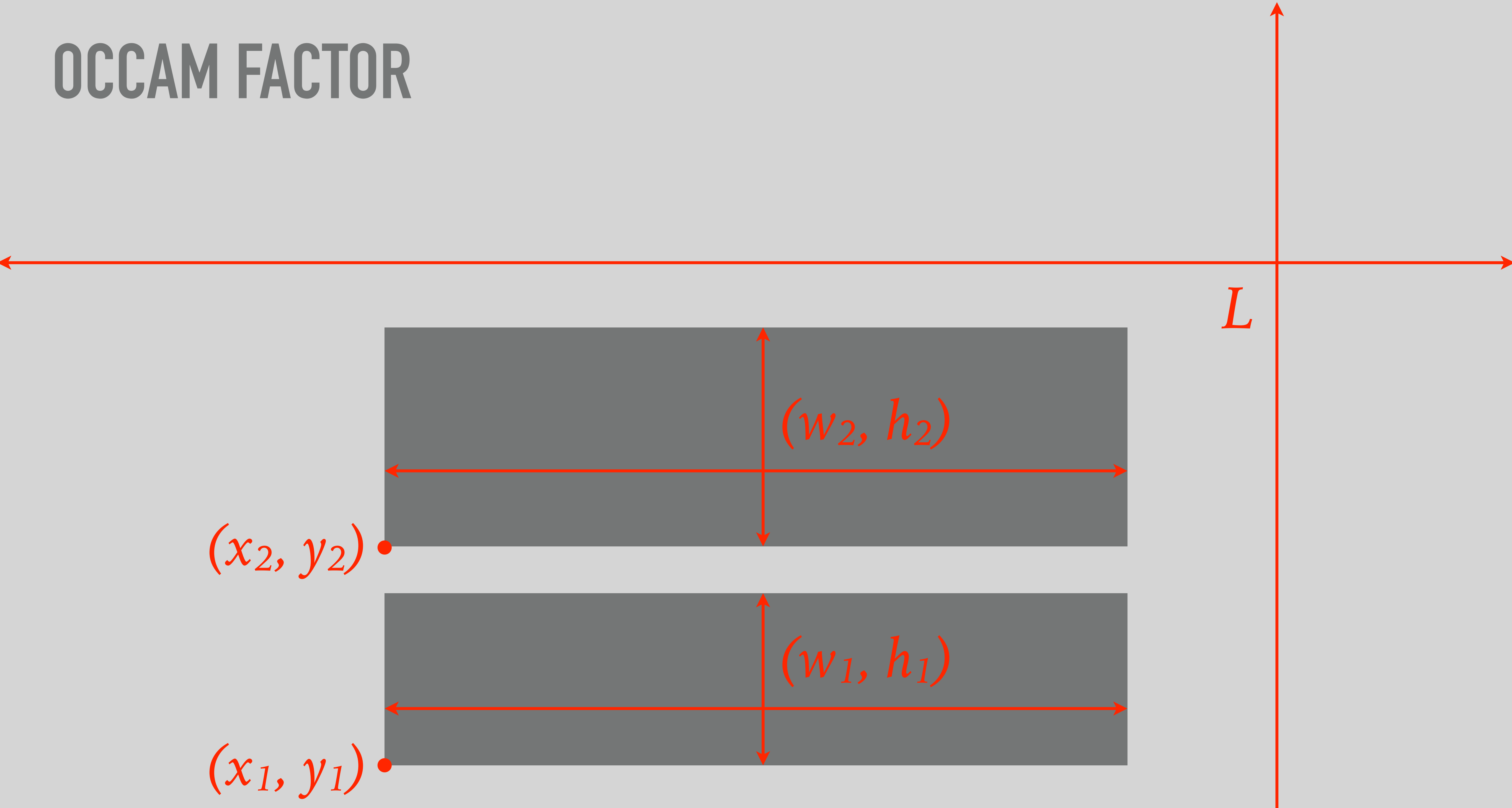
OCCAM FACTOR



$$P(D|M_1) \propto L^{-4}$$

Model-1: one rectangle.

OCCAM FACTOR



$$P(D \mid M_2) \propto L^{-8}$$

Model-2: two rectangles.

OCCAM FACTOR

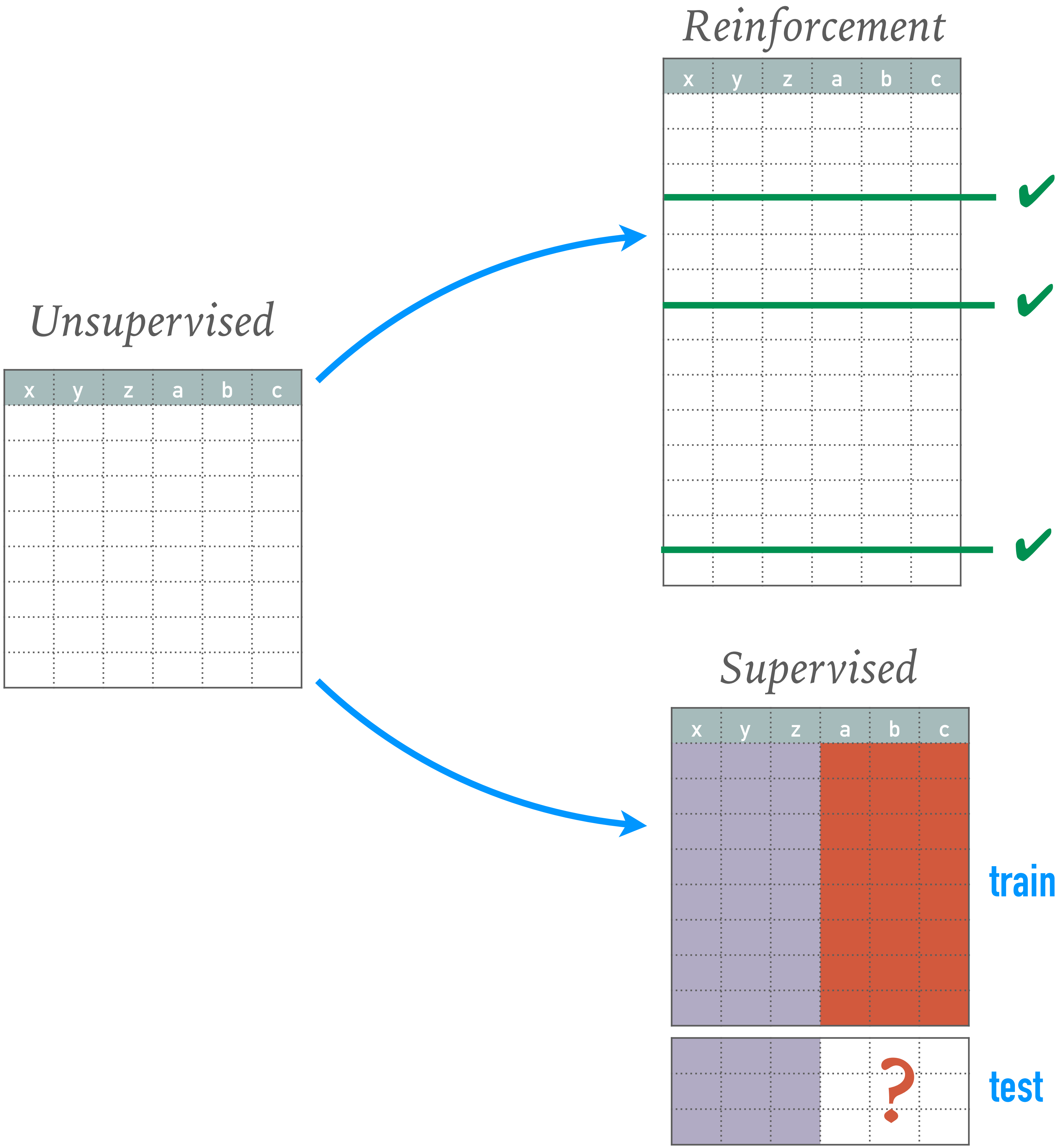
- Two rectangles are possible but extremely unlikely, even if we believe that one vs two rectangles are equally likely a-priori!

$P(D|M_2) \,/\, P(D|M_1) \propto L^{-4} \ll 1$ *Occam factor*

How many rectangles?

TYPES OF LEARNING

- Supervised
- Un-supervised
- Reinforcement
  - Video games, GO (pong example)
  - LSST observing strategy?



Reinforcement
x y z a b c
Unsupervised
x y z a b c
Supervised
x y z a b c
train
test

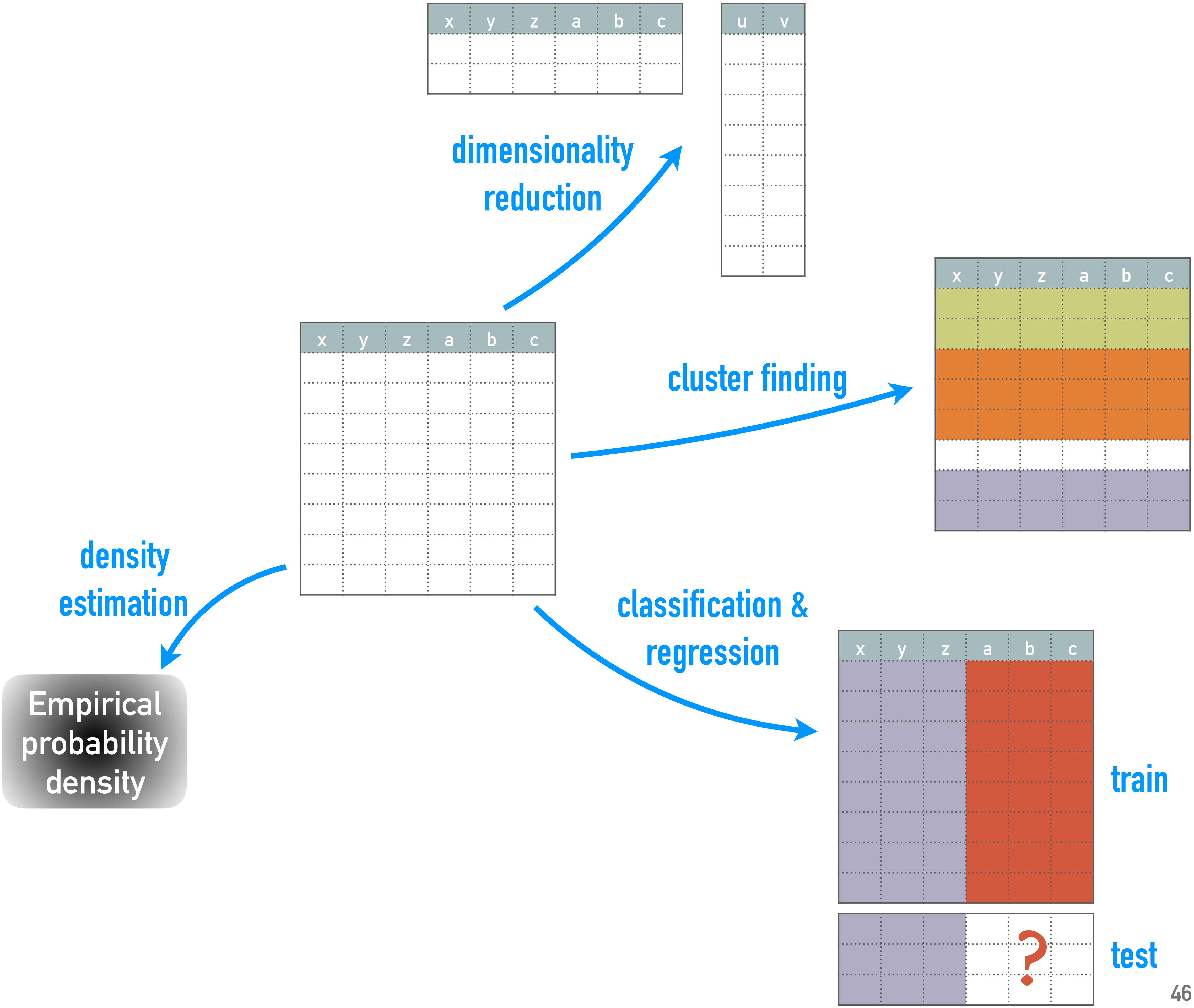
TYPES OF PROBLEM

- Classification.
- Regression.

Supervised

- Cluster finding.
- Density estimation.
- Dimensionality reduction.

Unsupervised



x y z a b c
u v
dimensionality reduction
cluster finding
density estimation
classification & regression
Empirical probability density
train
test
?

GROUP ACTIVITY: REASONING ABOUT ML PROBLEMS

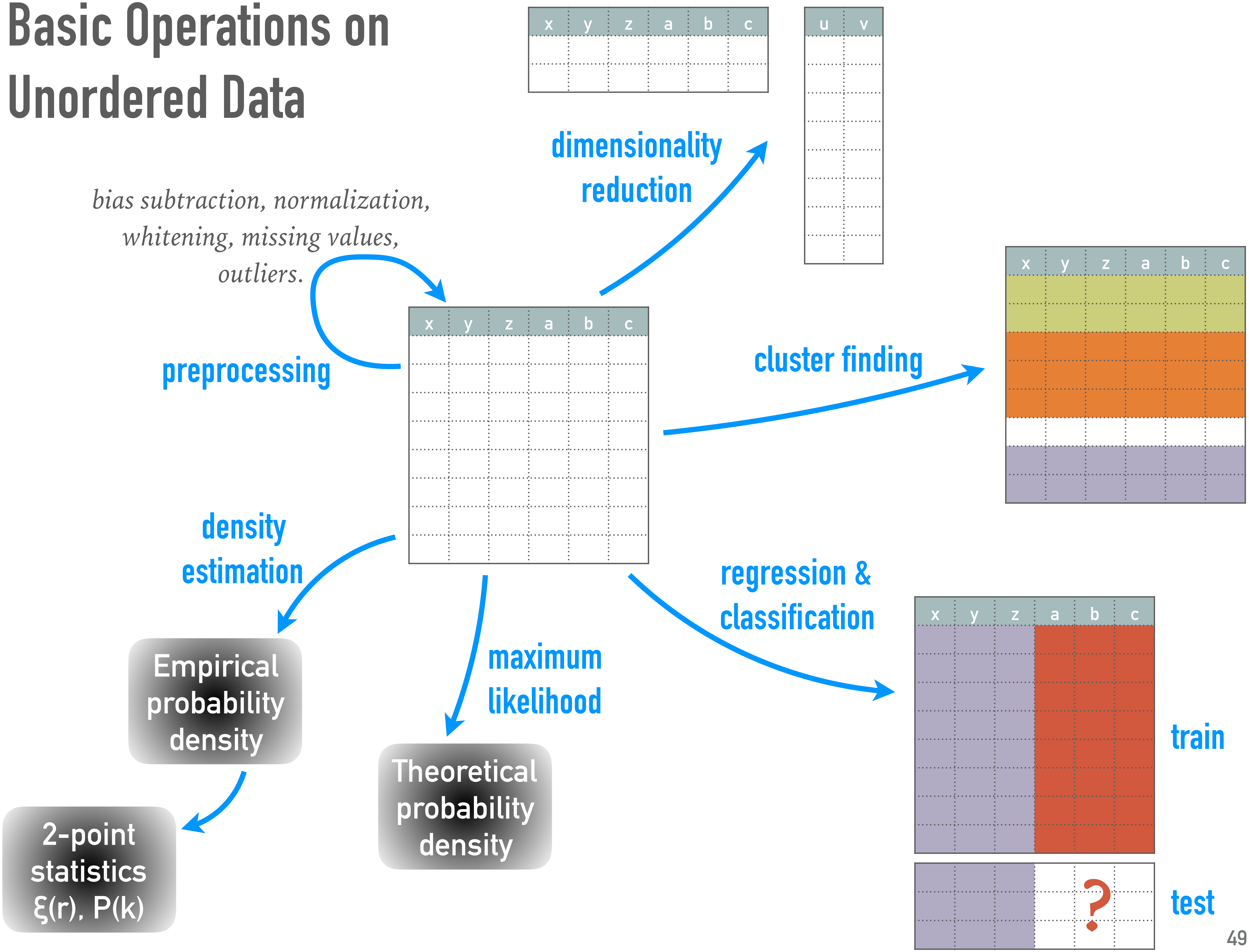
- What type of learning is best suited for these tasks?
- What type of problem best describes each task?

1. *Suggest a missing word in a sentence.*
2. *Identify a specific person in a photo.*
3. *Drive a car automatically.*
4. *Predict the sky brightness for tomorrow night's observing.*
5. *Estimate a galaxy's redshift from its LSST magnitudes.*
6. *Describe the relationship between supernovae distance and redshift.*

TYPES OF SOLUTION

- Fundamental problem: P(D) is difficult to evaluate.
- Exact solution:
  - enumerate all possible outcomes (do it when you can!)
- Approximate solution:
  - Analytic / Deterministic:
    - maximum likelihood (best-fit parameters).
    - Laplace’s approximation (parabolic errors on best-fit params).
    - variational inference (exact results for an approx. posterior).
  - Sampling:
    - Markov-chain MC (approx. results for an exact posterior).

Basic Operations on Unordered Data



RECURRING THEMES OF ML

- Neighbors
- Kernels
- Ensembles
- Regularization
- Entropy

THE MACHINE-LEARNING ZOO

MODELS

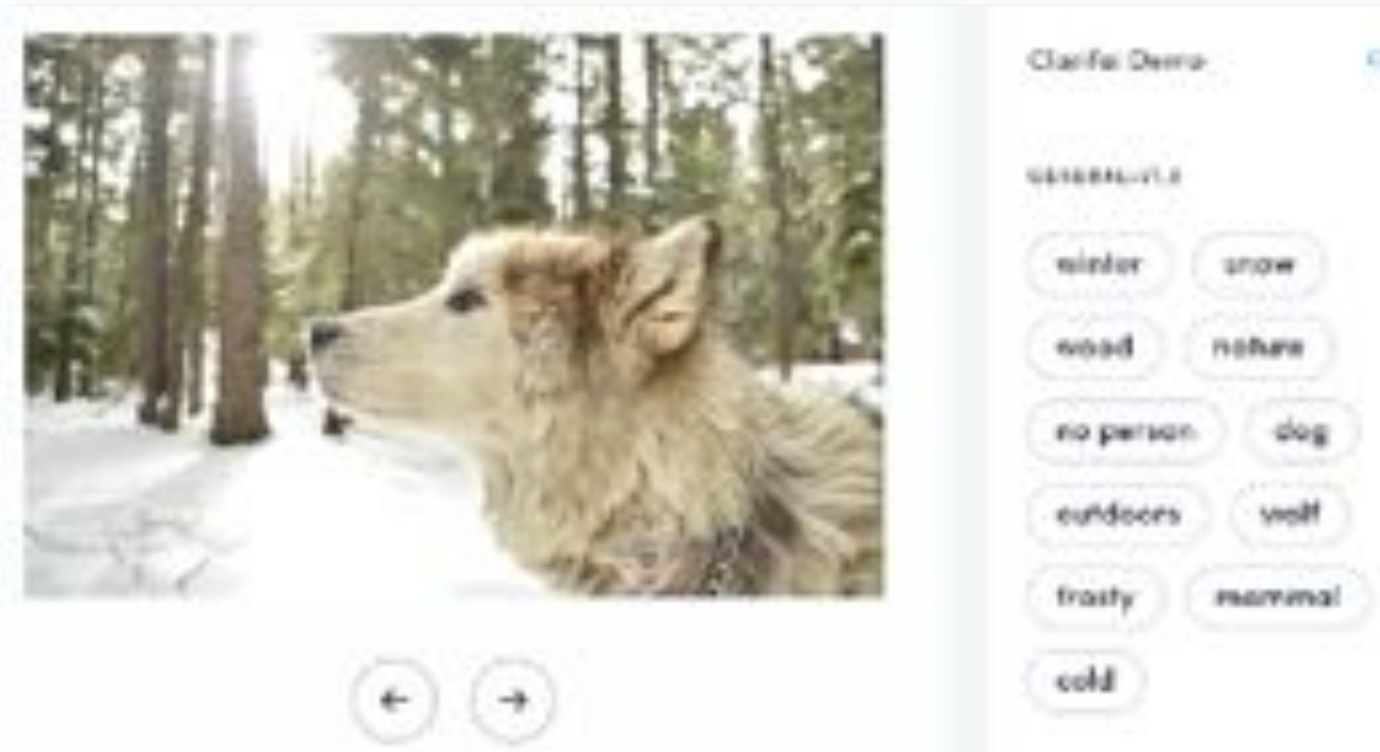
Science *Online Services* *Financial Services*

DATA

PEOPLE

http://insightdatascience.com

BLEEDING EDGE: DEEP LEARNING

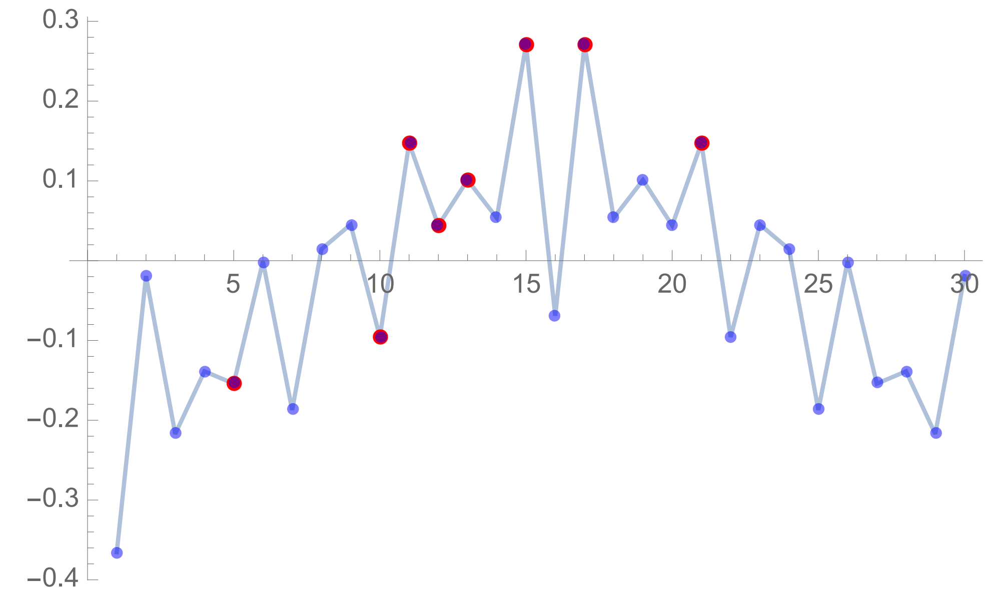


Convolutional neural networks for image classification

Recurrent neural networks for natural language semantics and translation.

BLEEDING EDGE: COMPRESSIVE SENSING

An introduction to compressive sensing

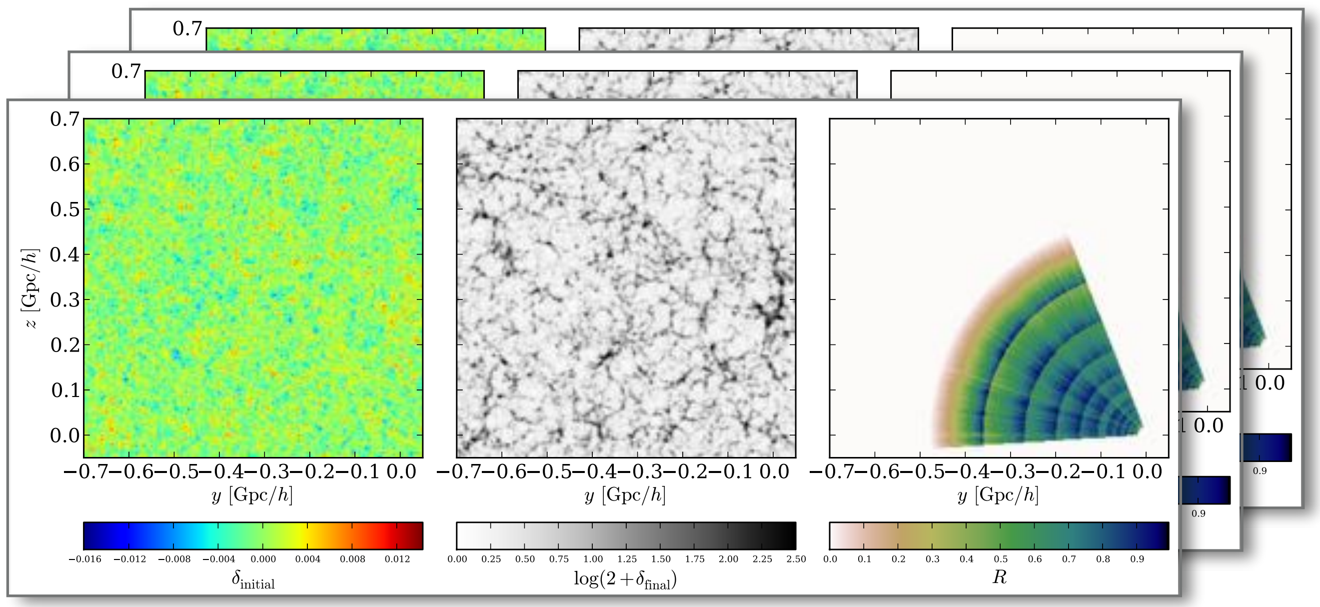


1 x 64Kpix

1300 x 1pix

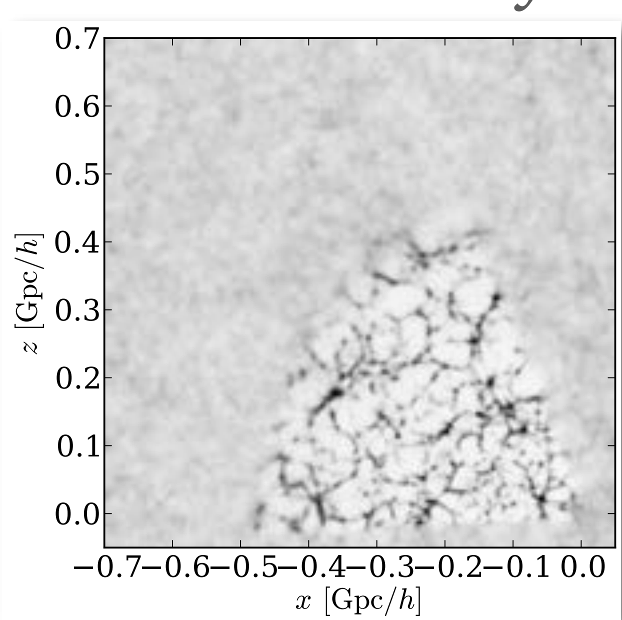
Compressive Imaging: A New Single-Pixel Camera

BLEEDING EDGE: HAMILTONIAN MONTE CARLO

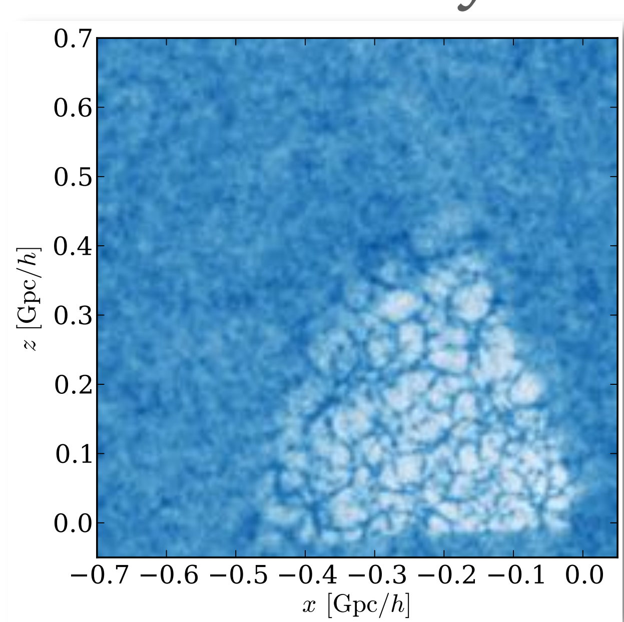


Past and present cosmic structure in the SDSS DR7 main sample

mean density



rms density



LESSONS FROM THE BLEEDING EDGE

- We need to develop & share high-quality building blocks:
  - standard data sets.
  - state of the art pre-trained solutions to low-level tasks.
- Be bold.
- Be persistent.