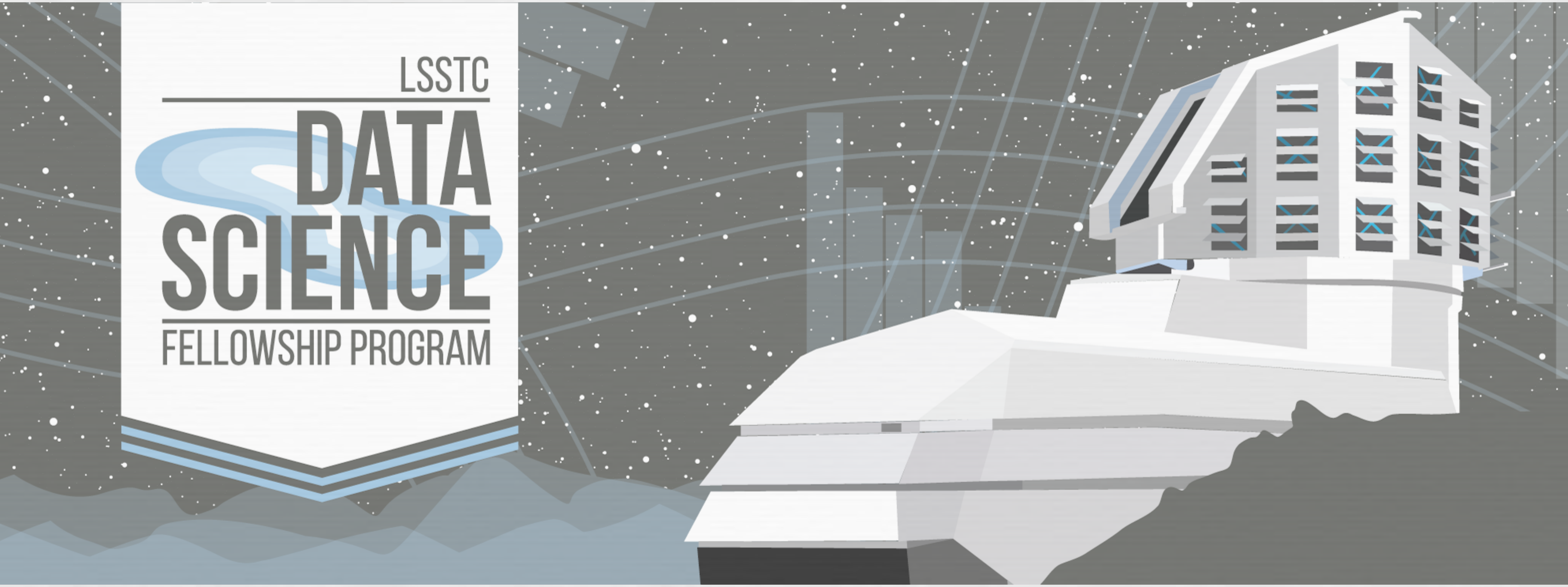
Developing the Machine Learning Workflow



Adam A Miller

Northwestern/Adler Planetarium

2017 LSSTC DSFP
27 Jan 2016

CIERA
Center for Interdisciplinary Exploration and Research in Astrophysics

ADLER
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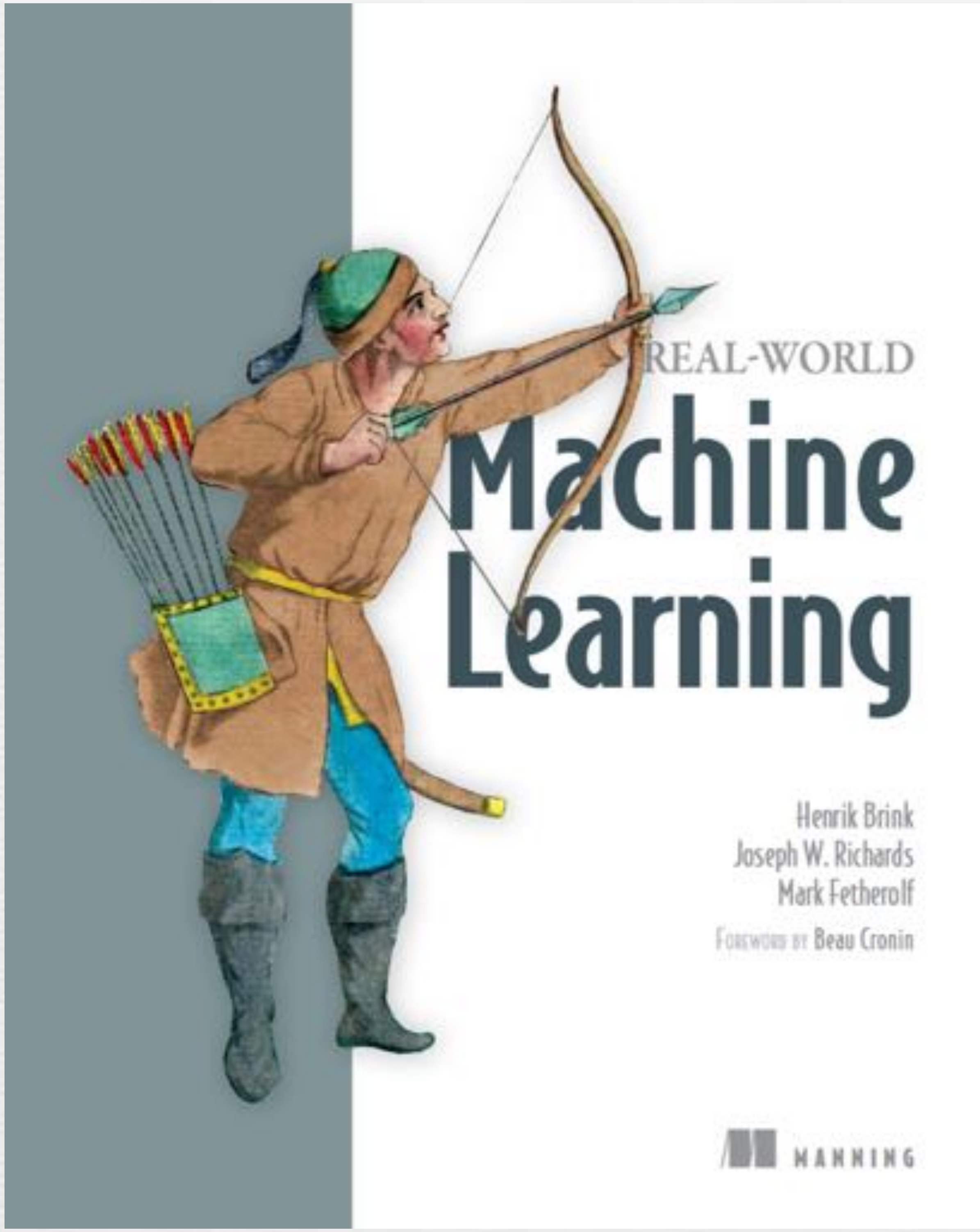
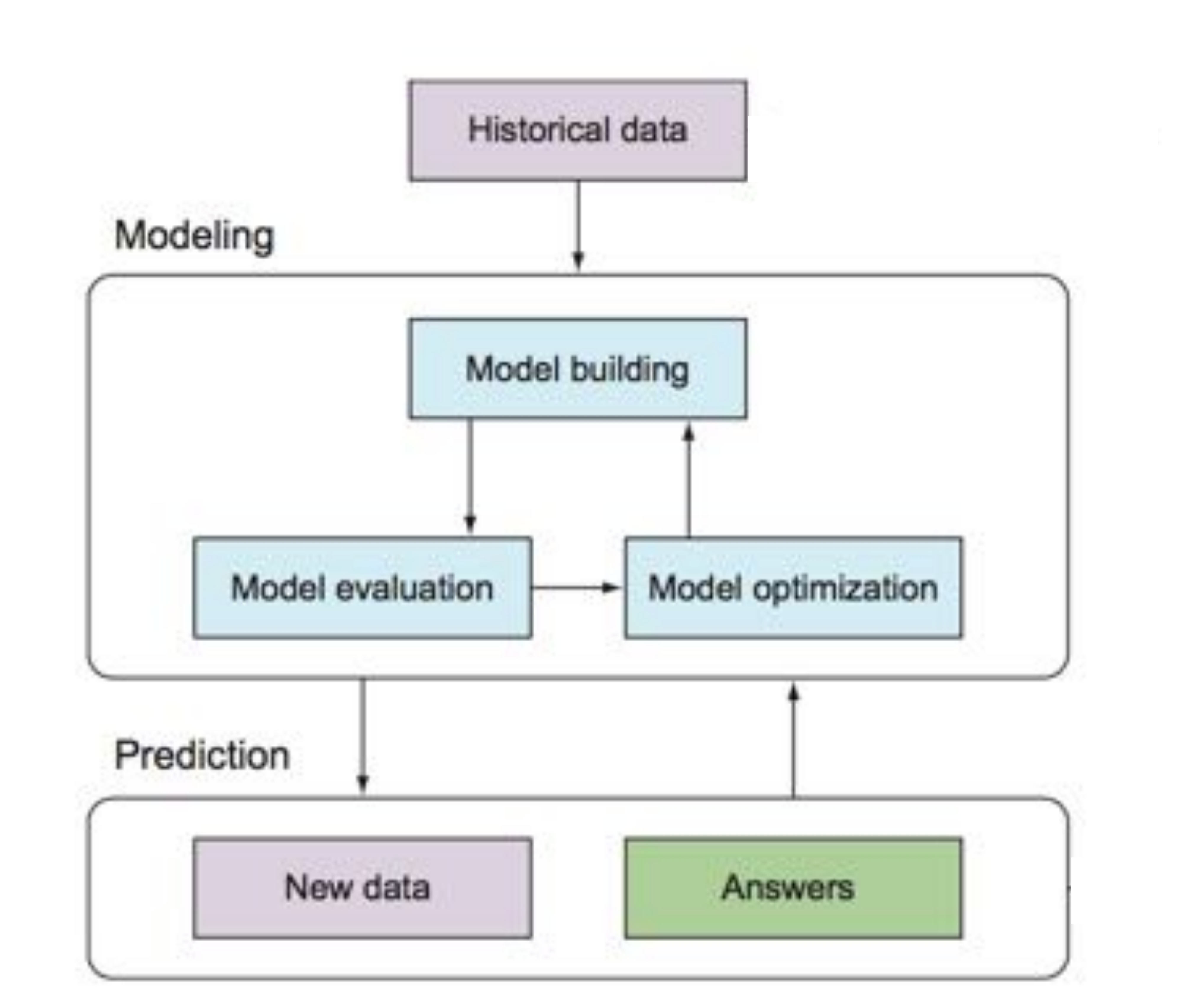


Brink, Richards, & Fetherolf 16

The Machine Learning Workflow



BRF16

Data Preparation

Query, observe, simulate, etc. - collect data that needs to be modeled

Worry About The Data

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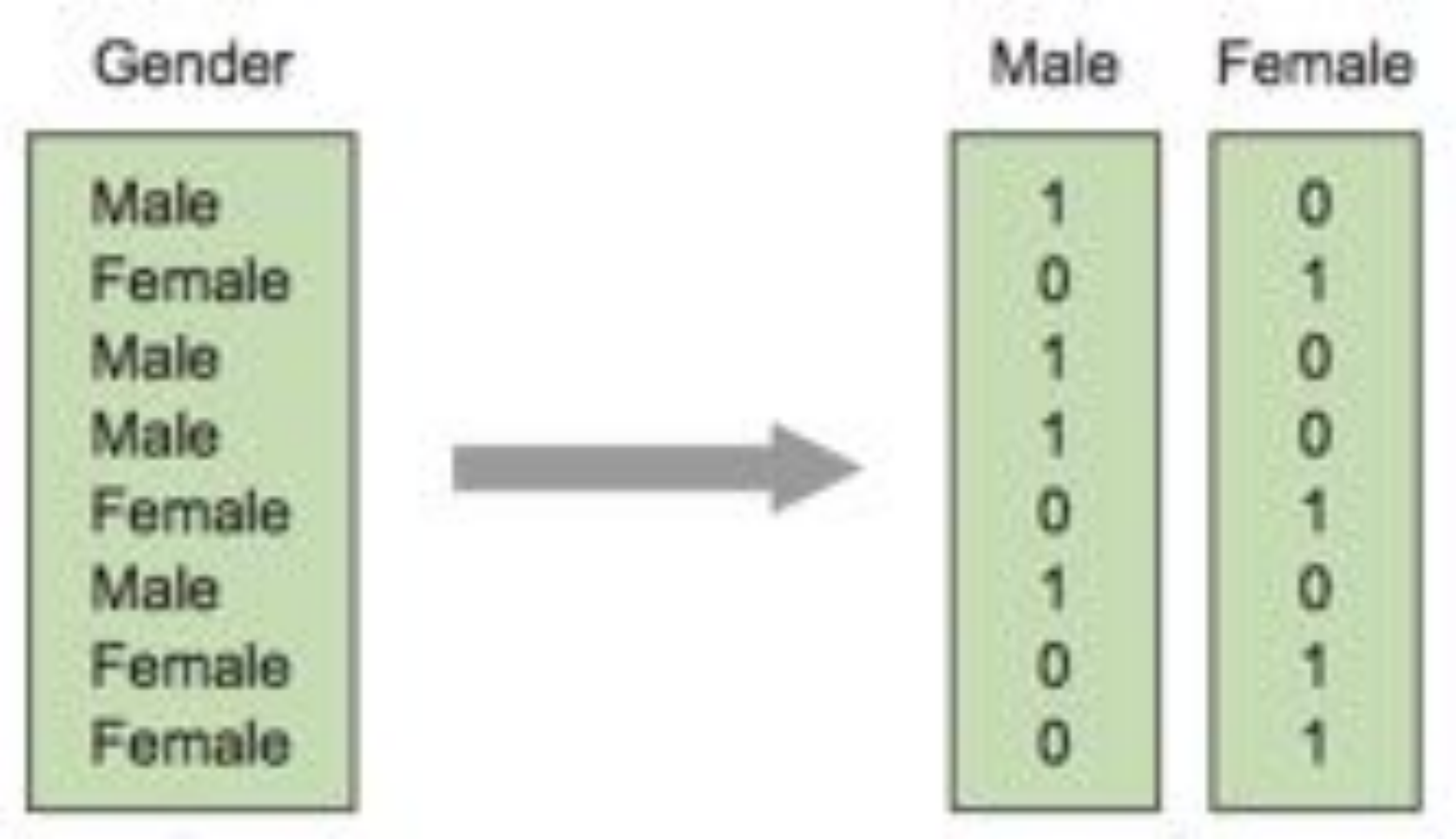

Gender
Male
Female
Male
Male
Female
Male
Female
Female

Male	Female
1	0
0	1
1	0
1	0
0	1
1	0
0	1
0	1

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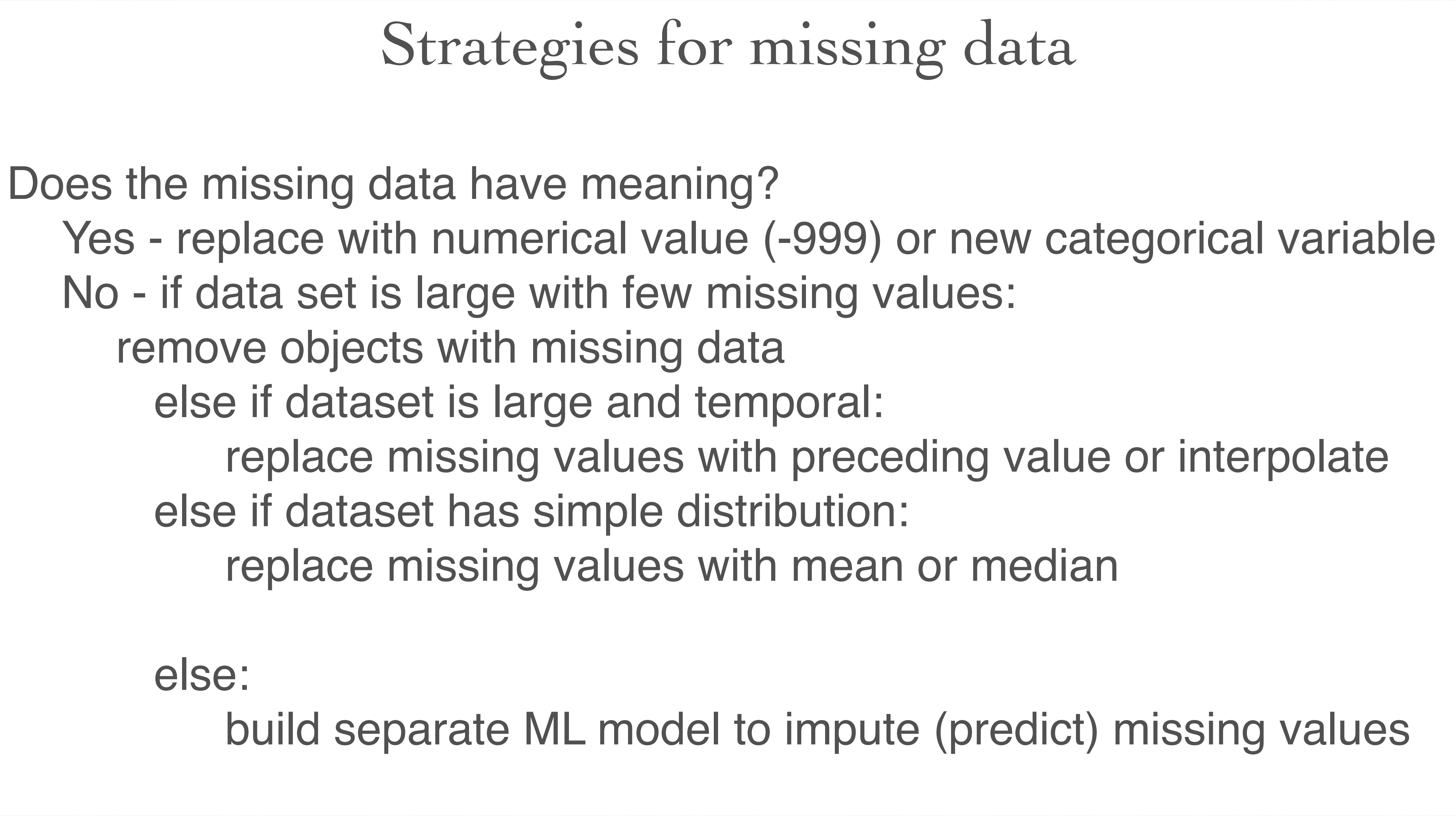

Strategies for missing data

```
Does the missing data have meaning?
    Yes - replace with numerical value (-999) or new categorical variable
    No - if data set is large with few missing values:
        remove objects with missing data
           else if dataset is large and temporal:
                replace missing values with preceding value or interpolate
           else if dataset has simple distribution:
                replace missing values with mean or median

           else:
                build separate ML model to impute (predict) missing values
```

Data Preparation

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Normalize the features

Data Preparation

Query, observe, simulate, etc. - collect data that needs to be modeled

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Normalize the features

Visualize the data

Worry About The Data

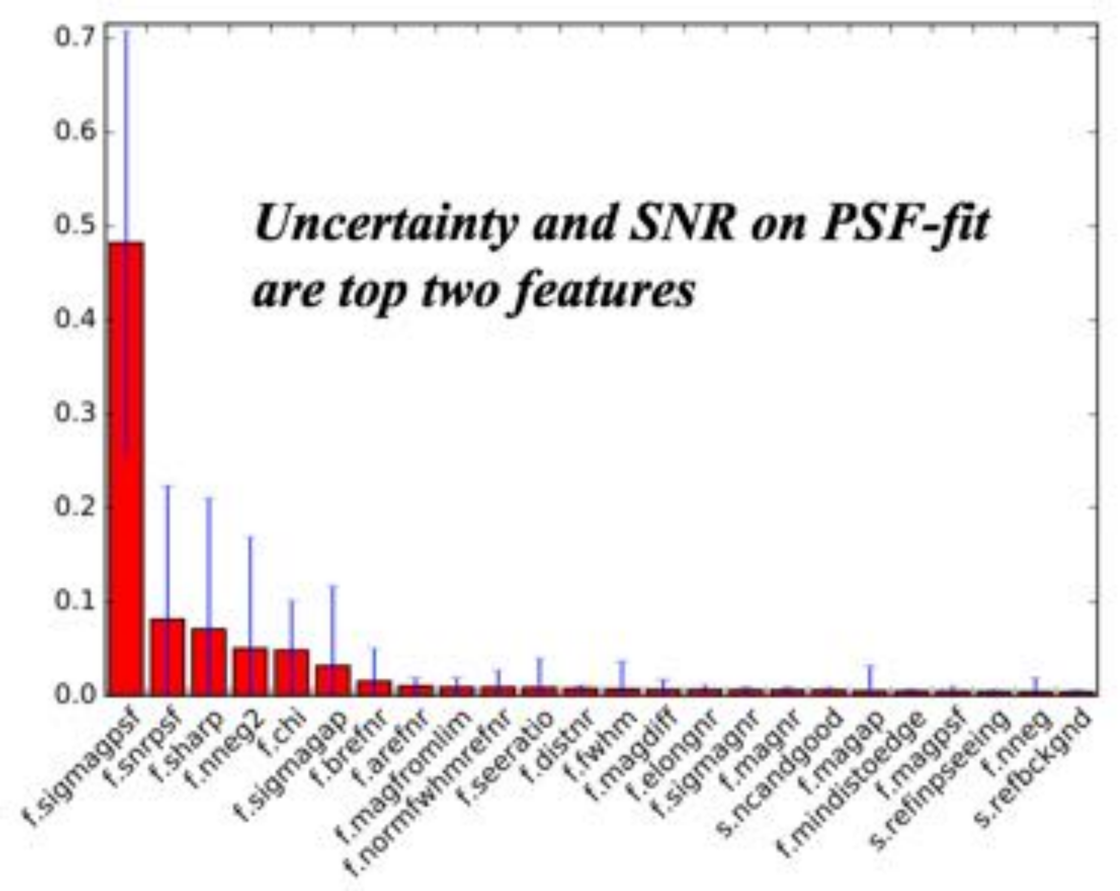
Feature Engineering

Add new features - if necessary

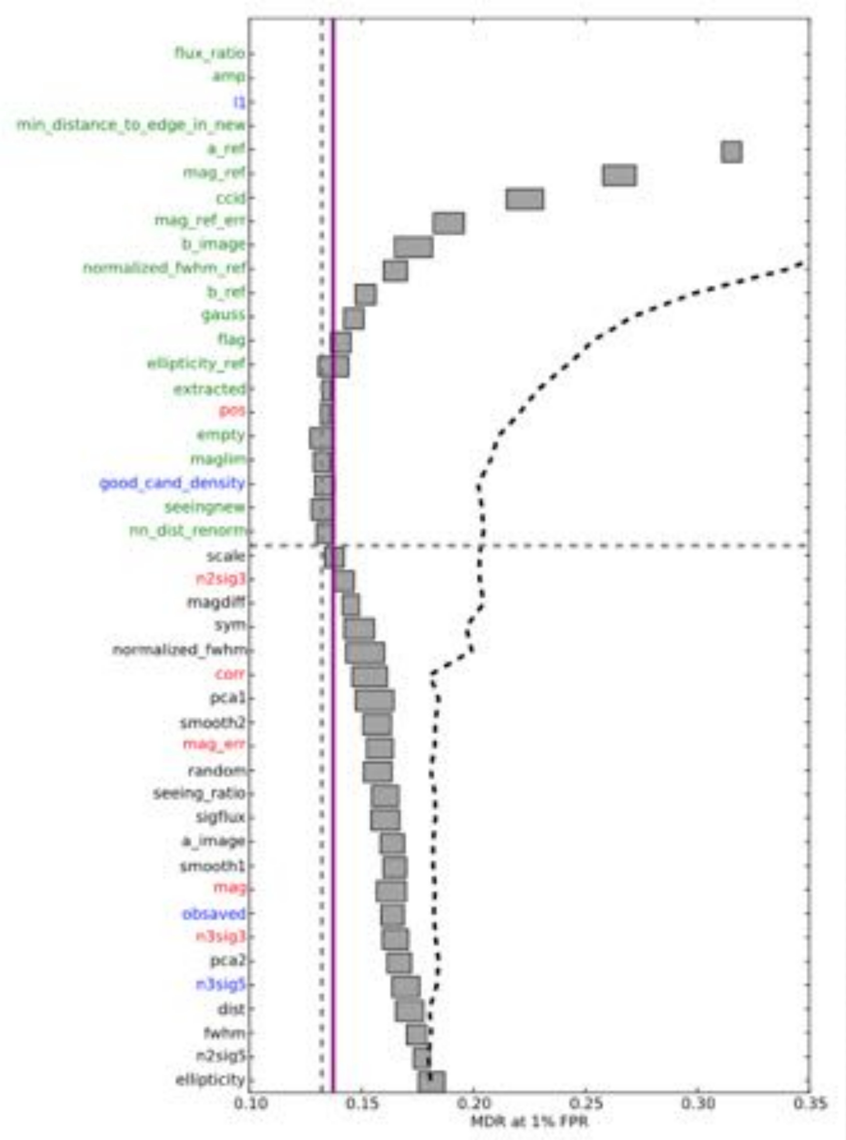
- Utilize domain knowledge to create/compute new features
- Combine features or represent in an alternative fashion

Remove noisy/uniformative features - if necessary

- Determine feature importance (RF)
- Forward/backward selection to iteratively remove features

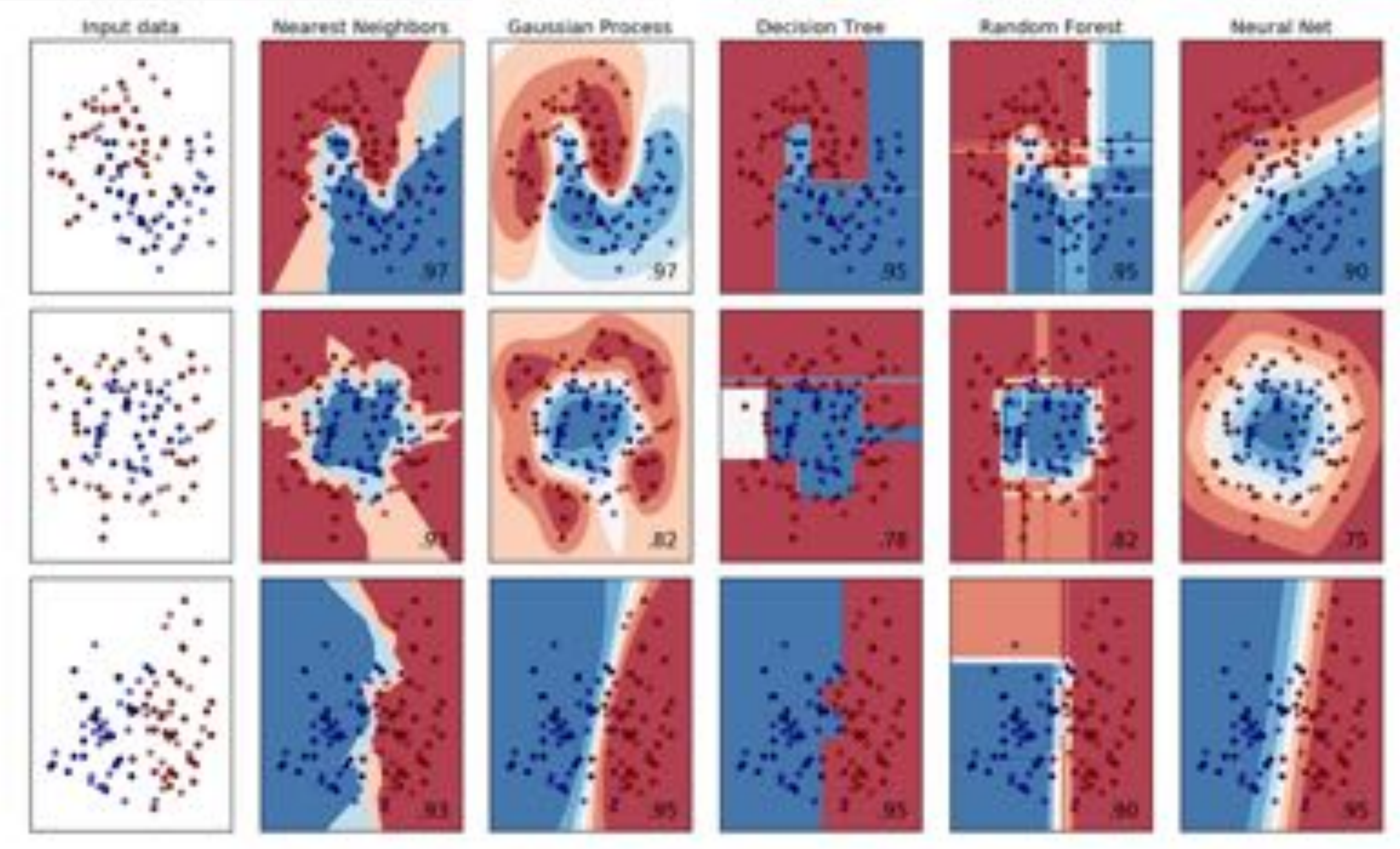


Rebbapragada+16



Brink+13

Model Selection

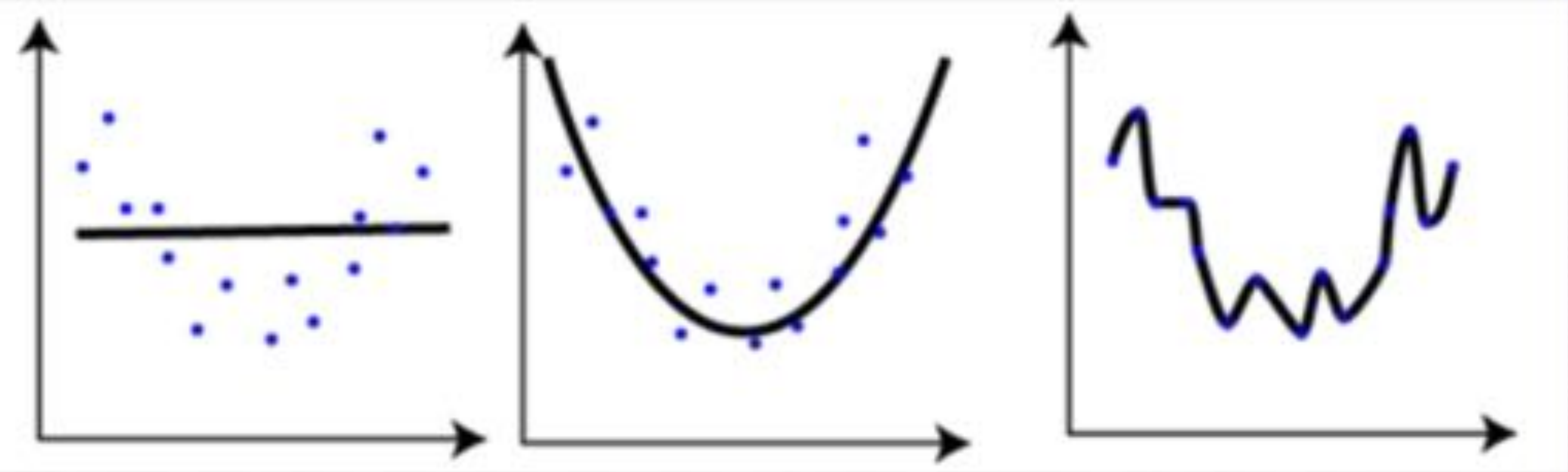


credit:scikit-learn

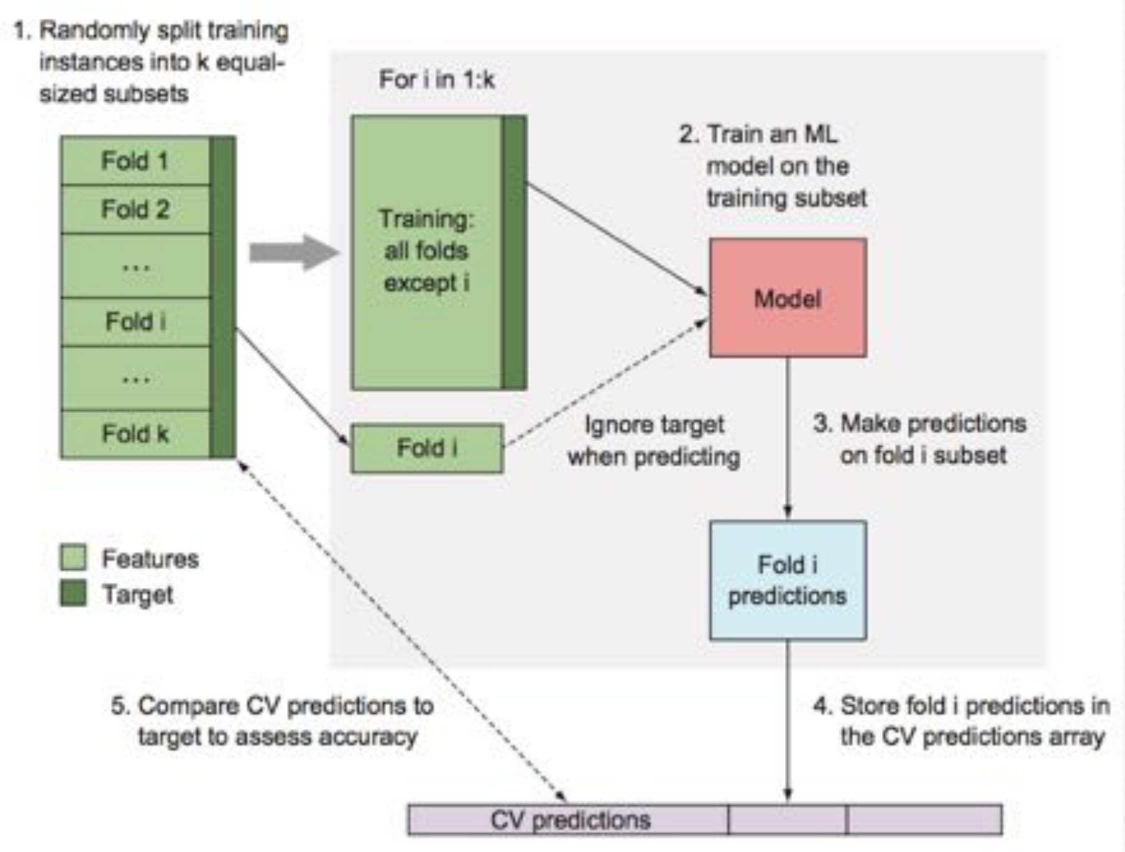
Worry About The Data

Model Evaluation

Avoid under- and over-fitting



Daniela’s lecture (Day 2)



1. Randomly split training instances into k equal-sized subsets

For i in 1:k

2. Train an ML model on the training subset

3. Make predictions on fold i subset

4. Store fold i predictions in the CV predictions array

5. Compare CV predictions to target to assess accuracy

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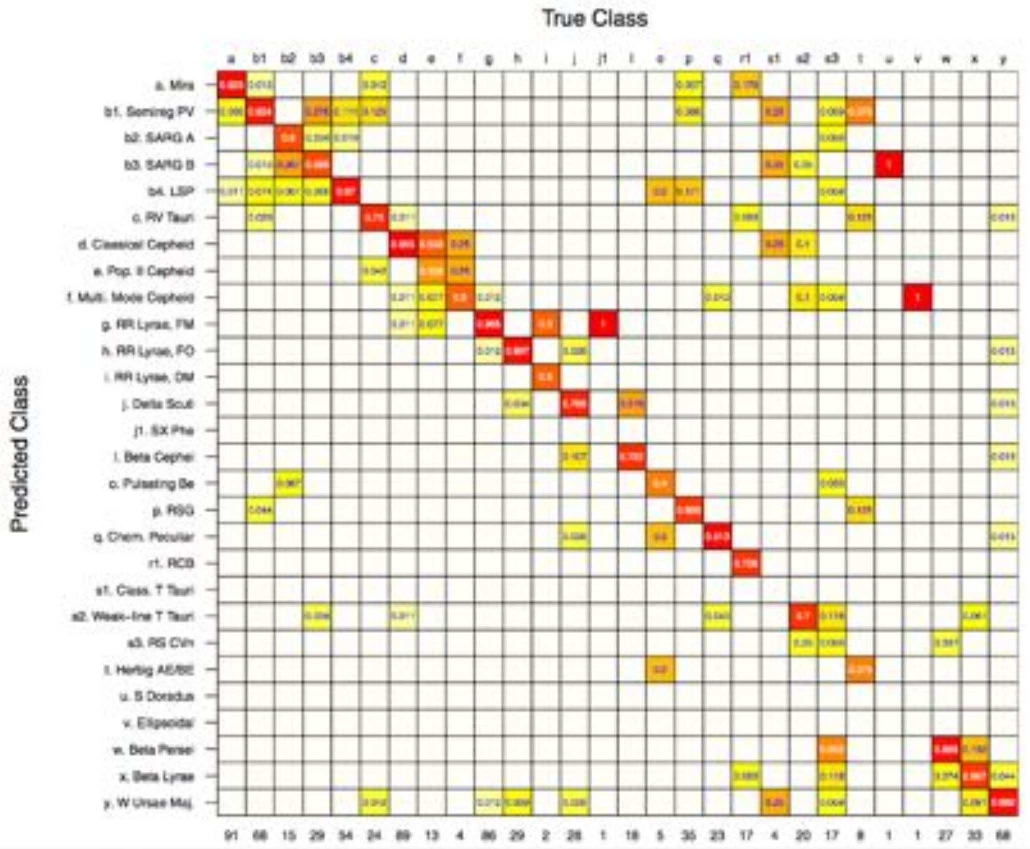
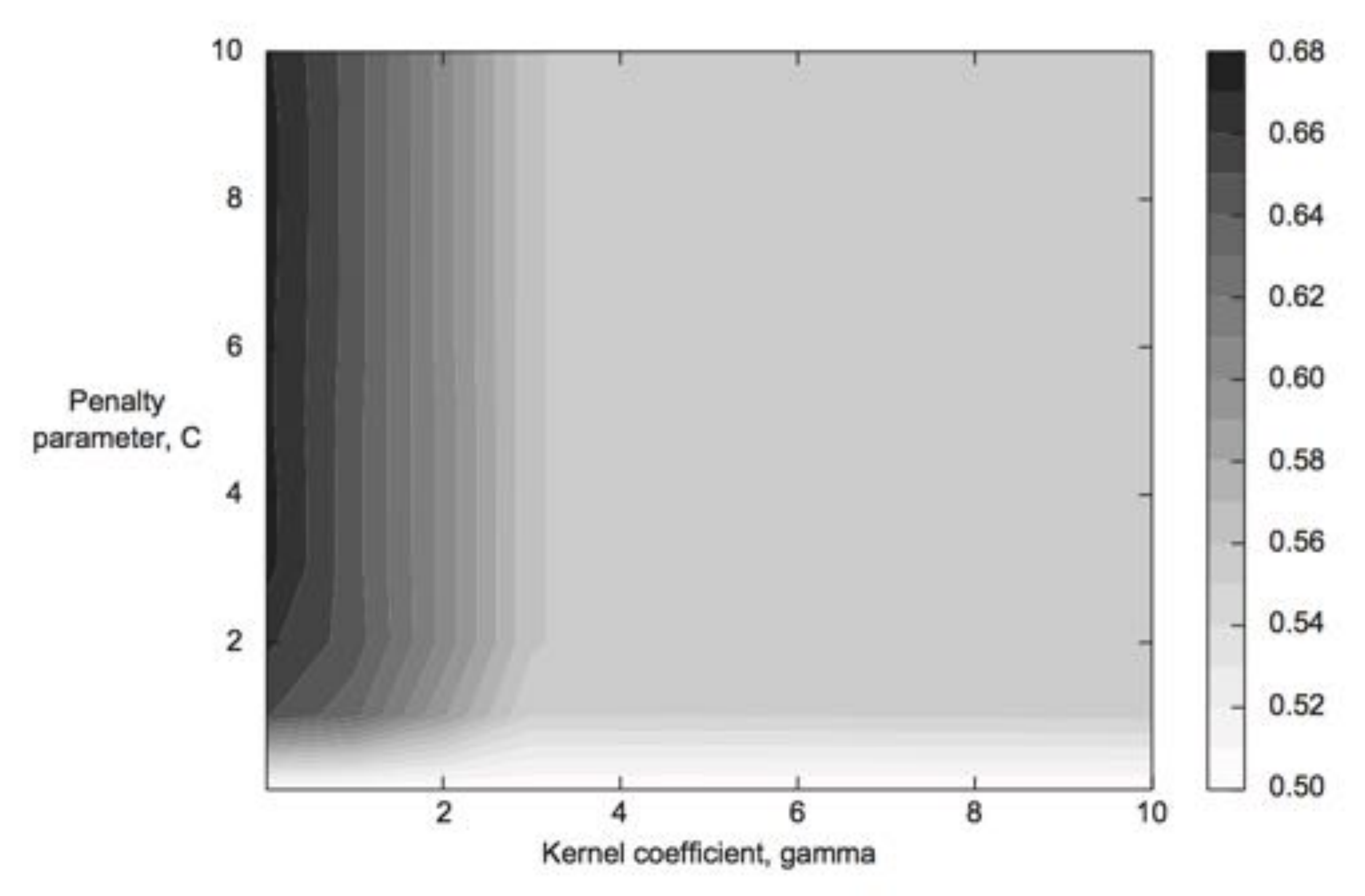


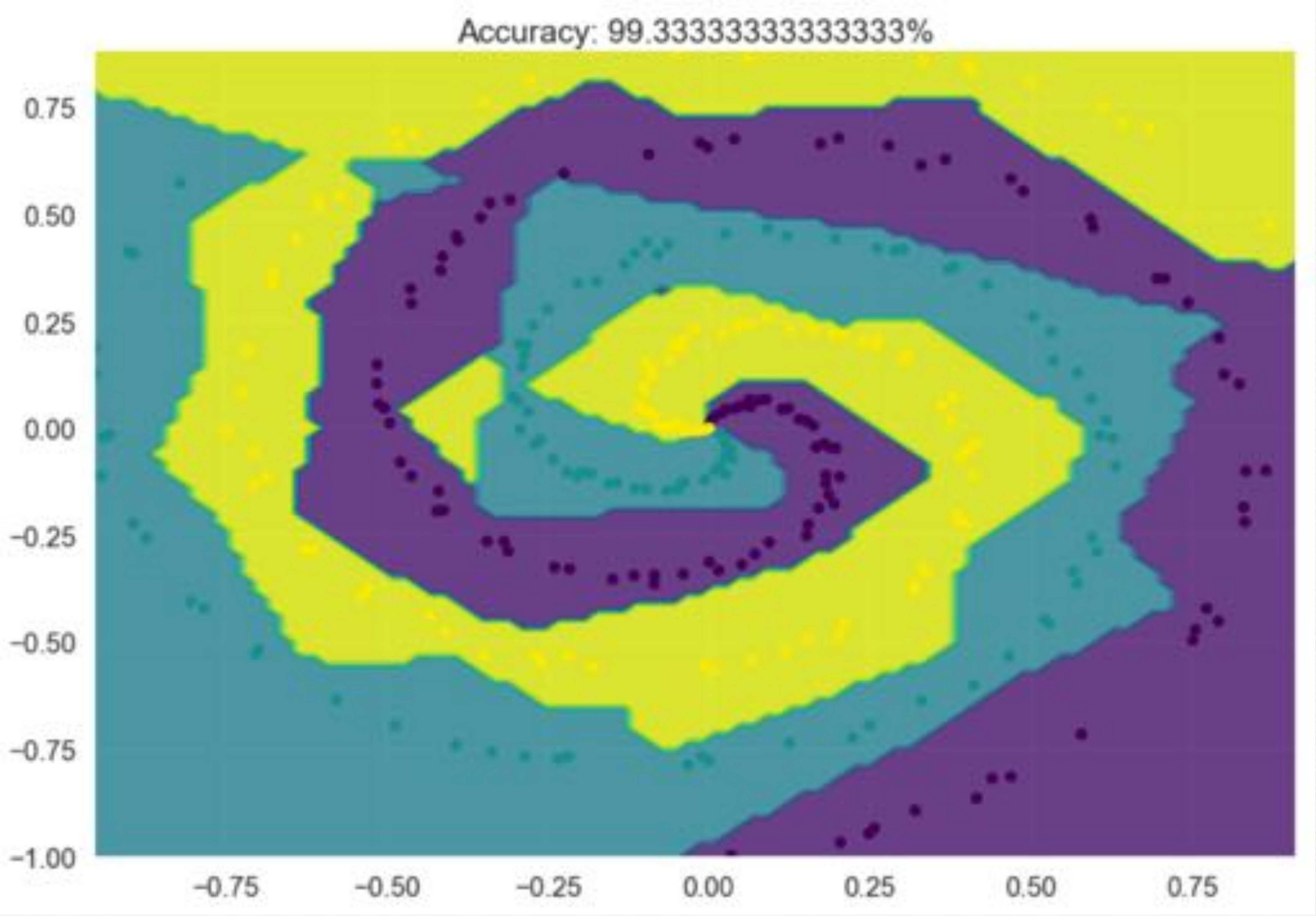
Richards+12

Model Optimization

Identify optimal tuning parameters via grid search



Model Prediction



Worry About The Data

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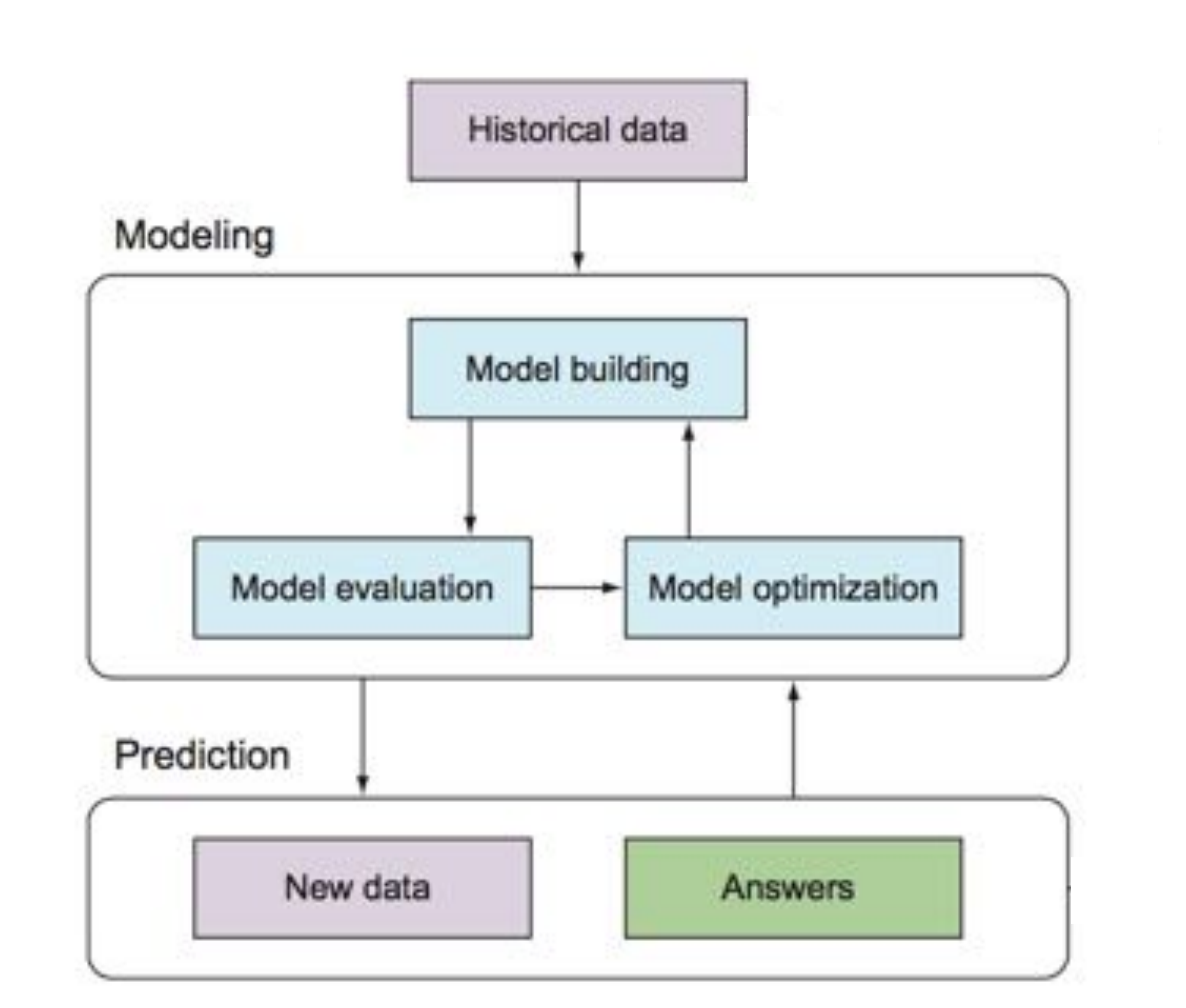

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