

# Big Data Inference

Combining Hierarchical Bayes and Machine Learning  
to Improve Photometric Redshifts

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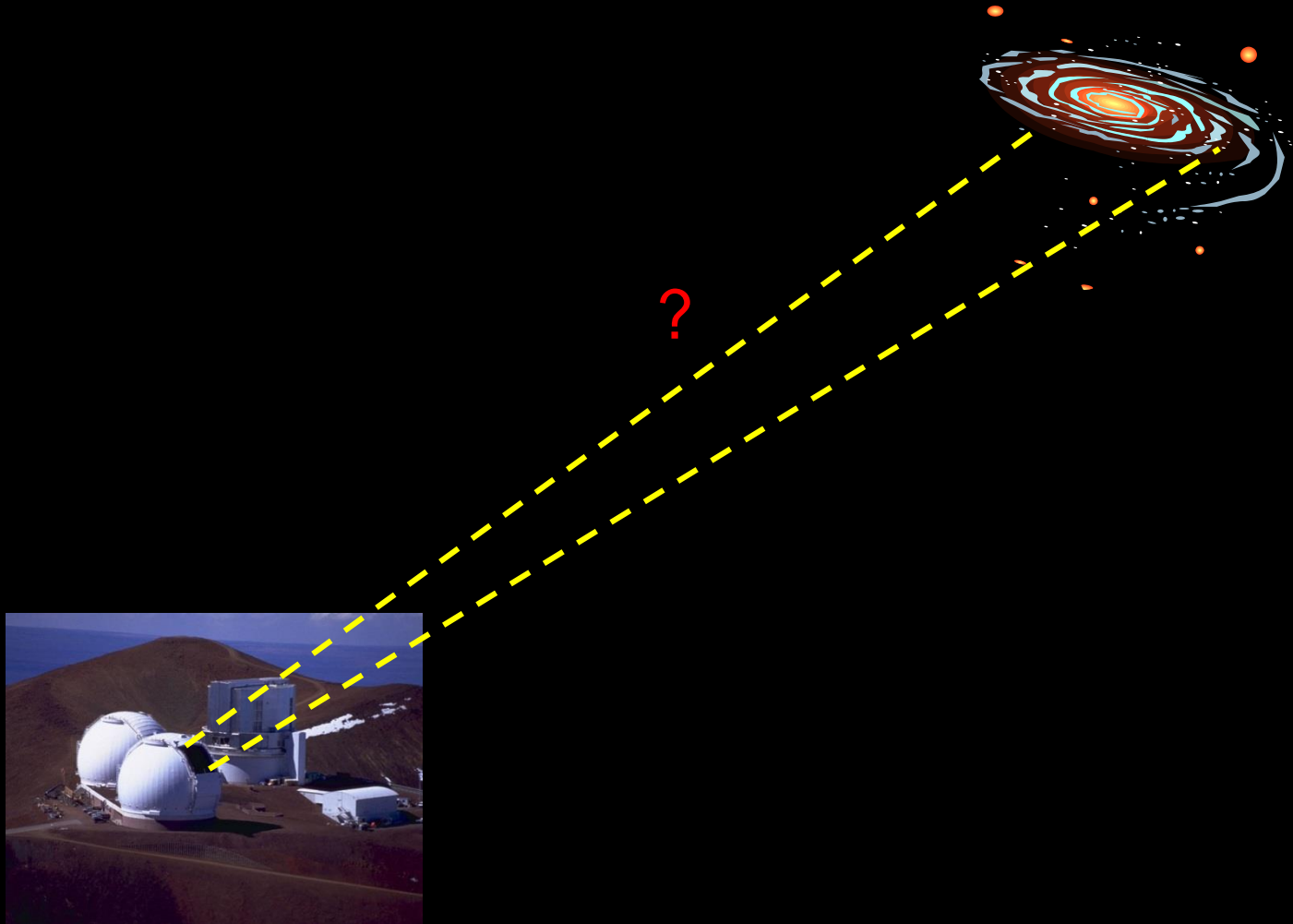
In collaboration with:

Boris Leistedt<sup>2</sup>, Alexie Leauthaud<sup>3</sup>, Daniel Eisenstein<sup>1</sup>, Kevin Bundy<sup>3,4</sup>,  
Peter Capak<sup>5</sup>, Ben Hoyle<sup>6</sup>, Daniel Masters<sup>5</sup>, Daniel Mortlock<sup>7</sup>, and Hiranya Peiris<sup>8,9</sup>

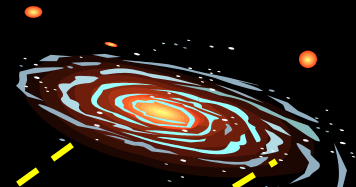
<sup>†</sup>NSF Graduate Research Fellow, <sup>1</sup>Harvard University, <sup>2</sup>NYU, <sup>3</sup>UC Santa Cruz, <sup>4</sup>UC Observatories, <sup>5</sup>IPAC,  
<sup>6</sup>LMU Munich, <sup>7</sup>Imperial College London, <sup>8</sup>University College London, <sup>9</sup>Oskar Klein Centre for Cosmoparticle  
Physics

What are Photometric Redshifts?

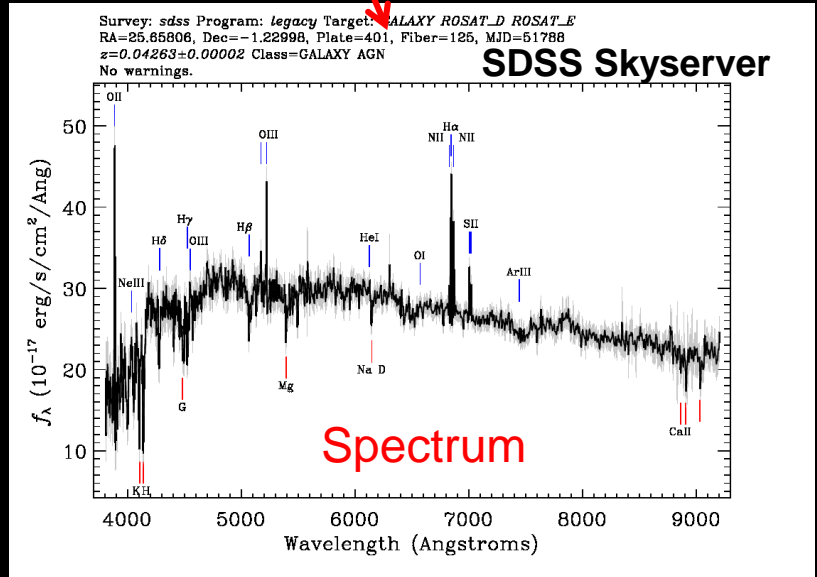
# Basic Concept



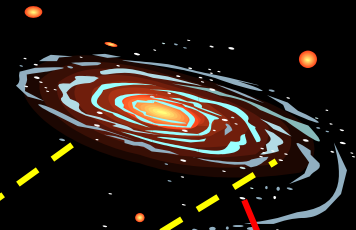
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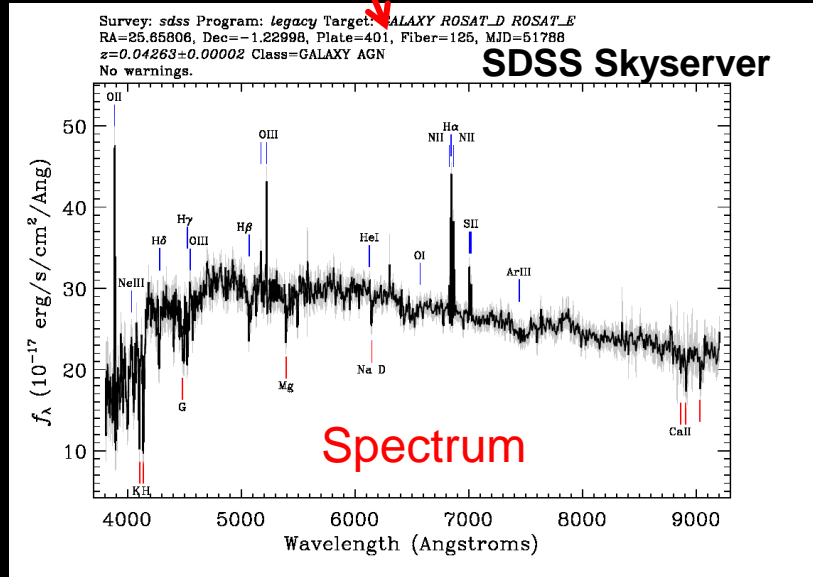
?



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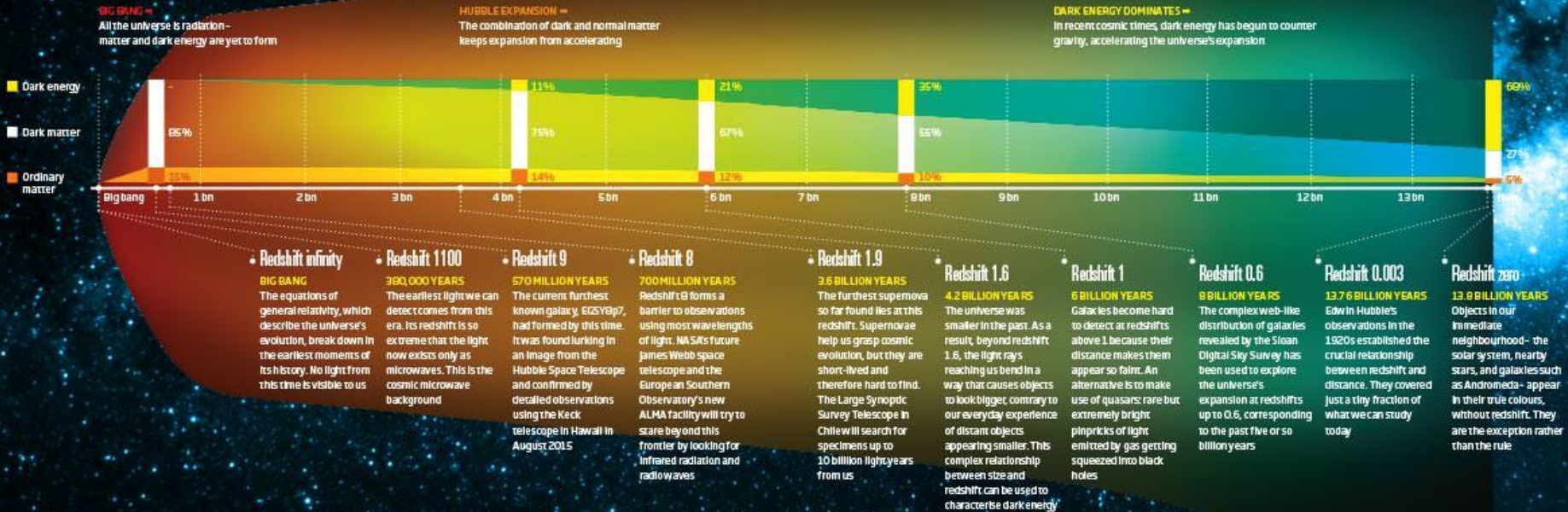


Spec-z



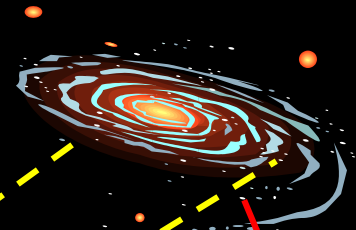
## The cosmic story

Redshift measurements reveal how the tussle between matter and dark energy has

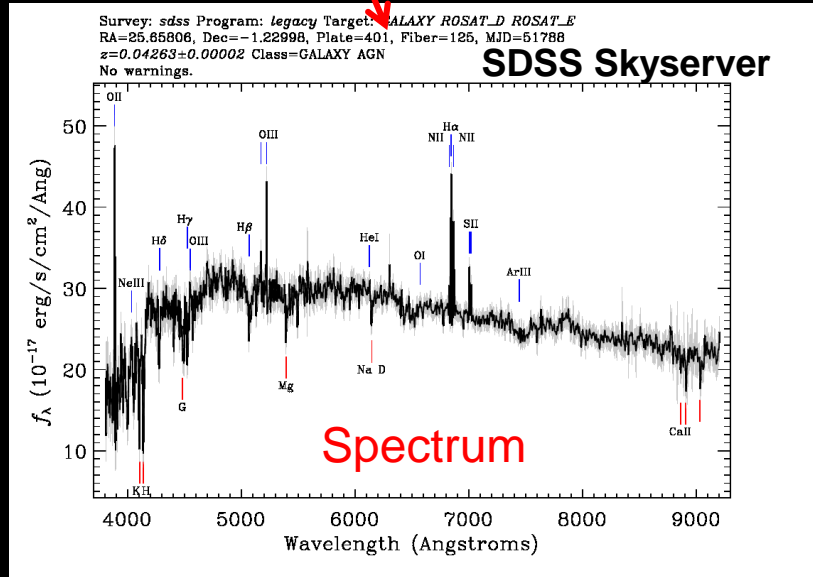




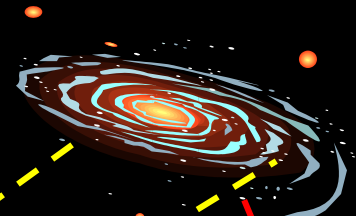
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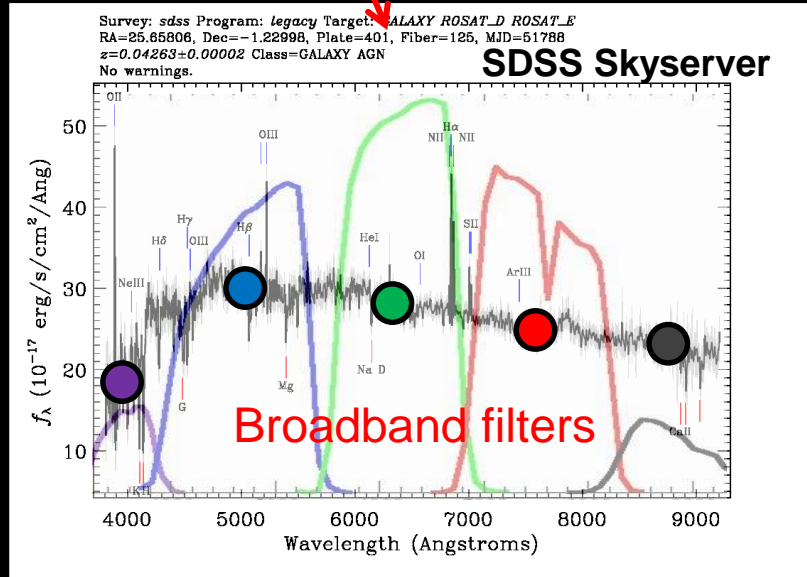
Spec-z



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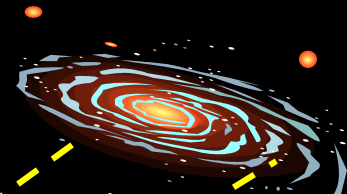
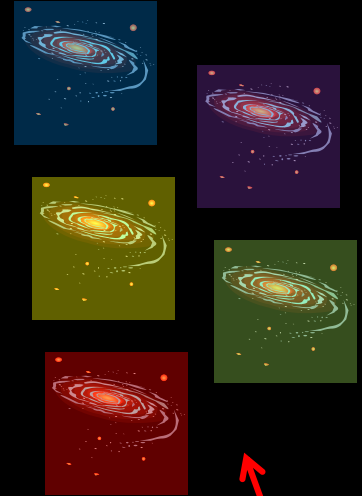
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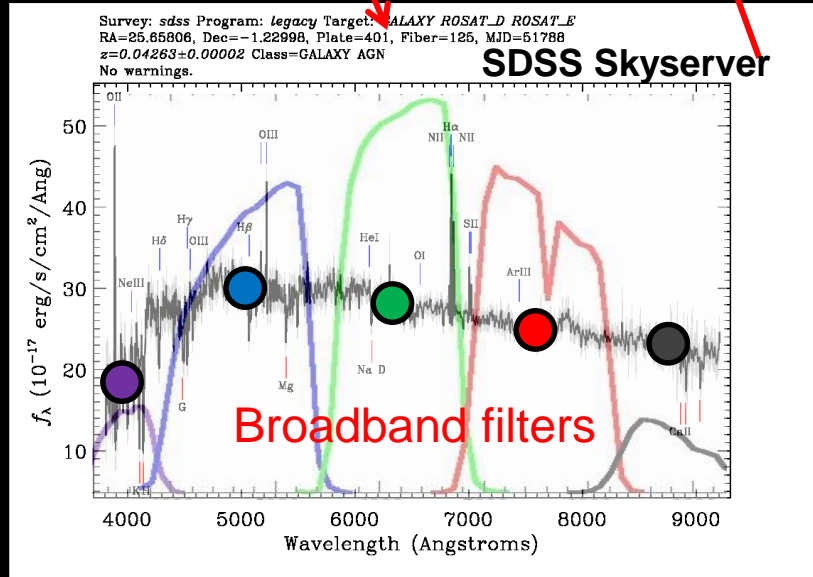


# Basic Concept

Spectral Energy Distribution (SED)



?

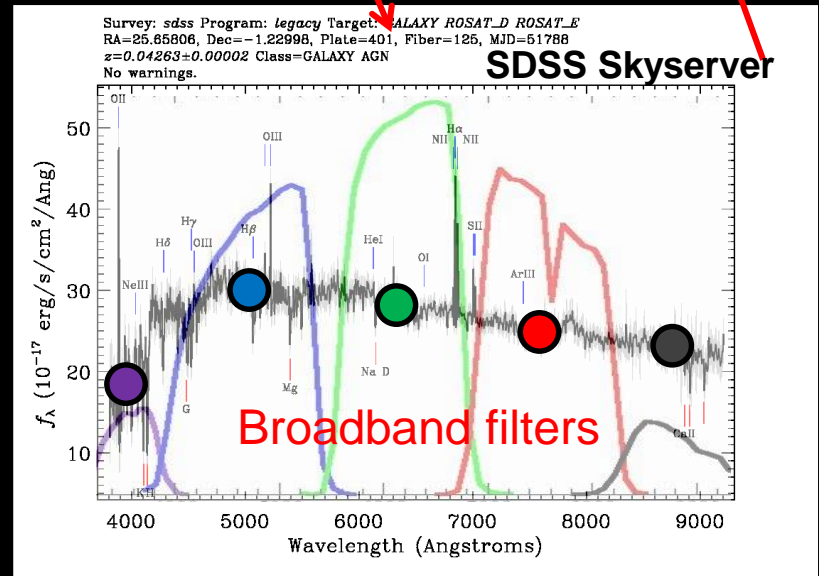
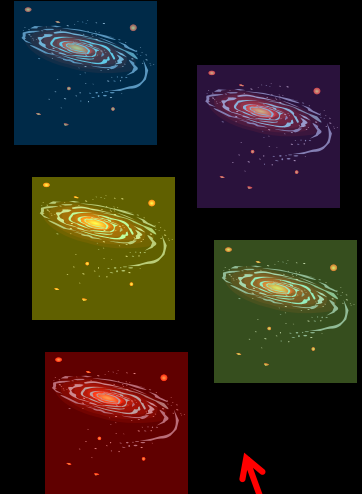
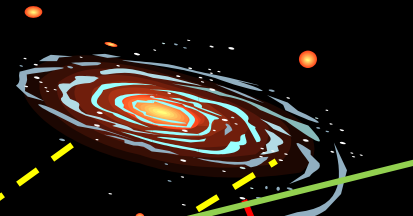


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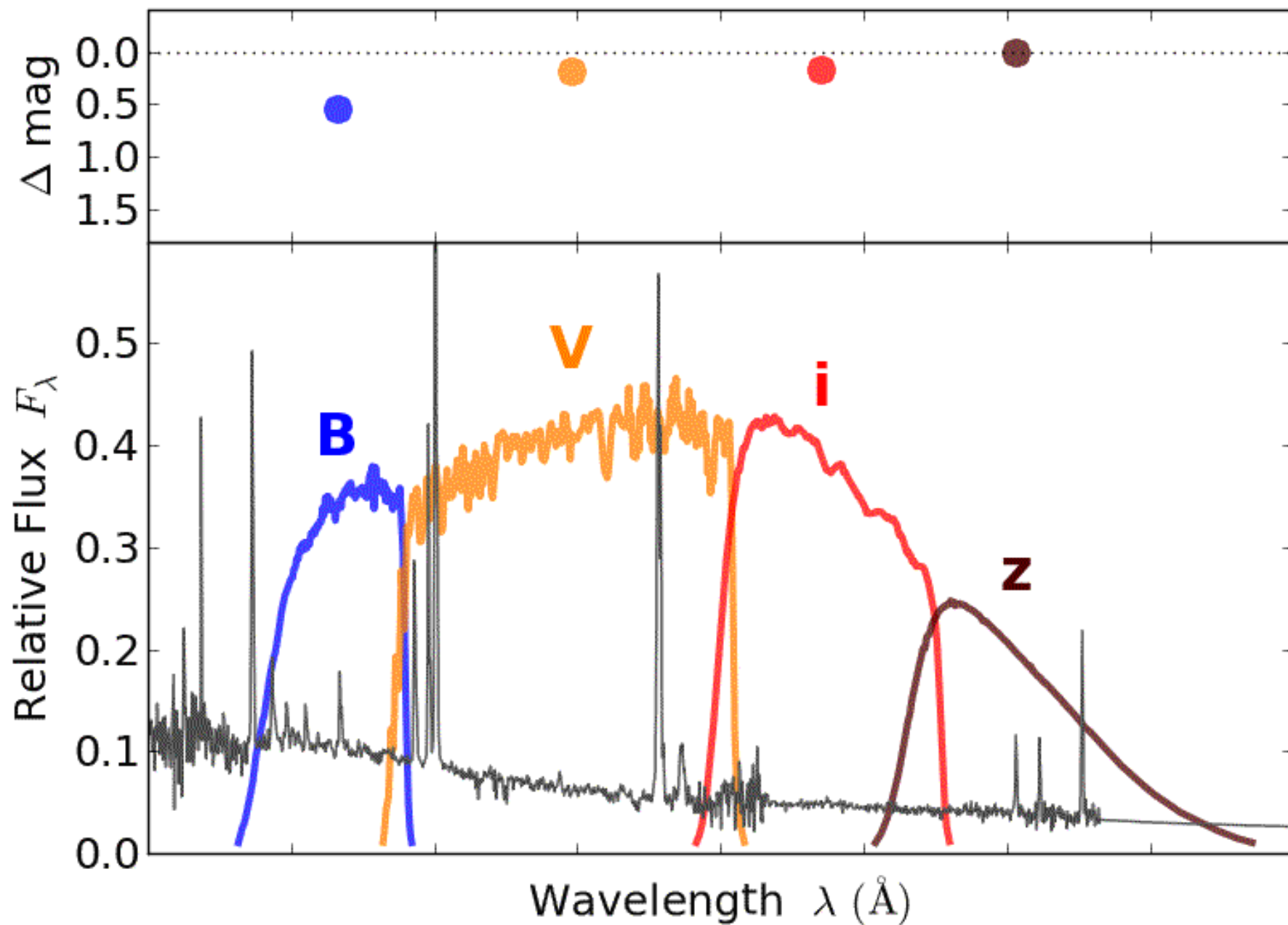
Spectral Energy Distribution (SED)



Photo-Z



$z = 0.00$



Why do we care?

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- **Because we have to.**

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  - Wide-field imaging surveys **much** cheaper and faster than spectroscopic surveys. Also can see fainter objects.

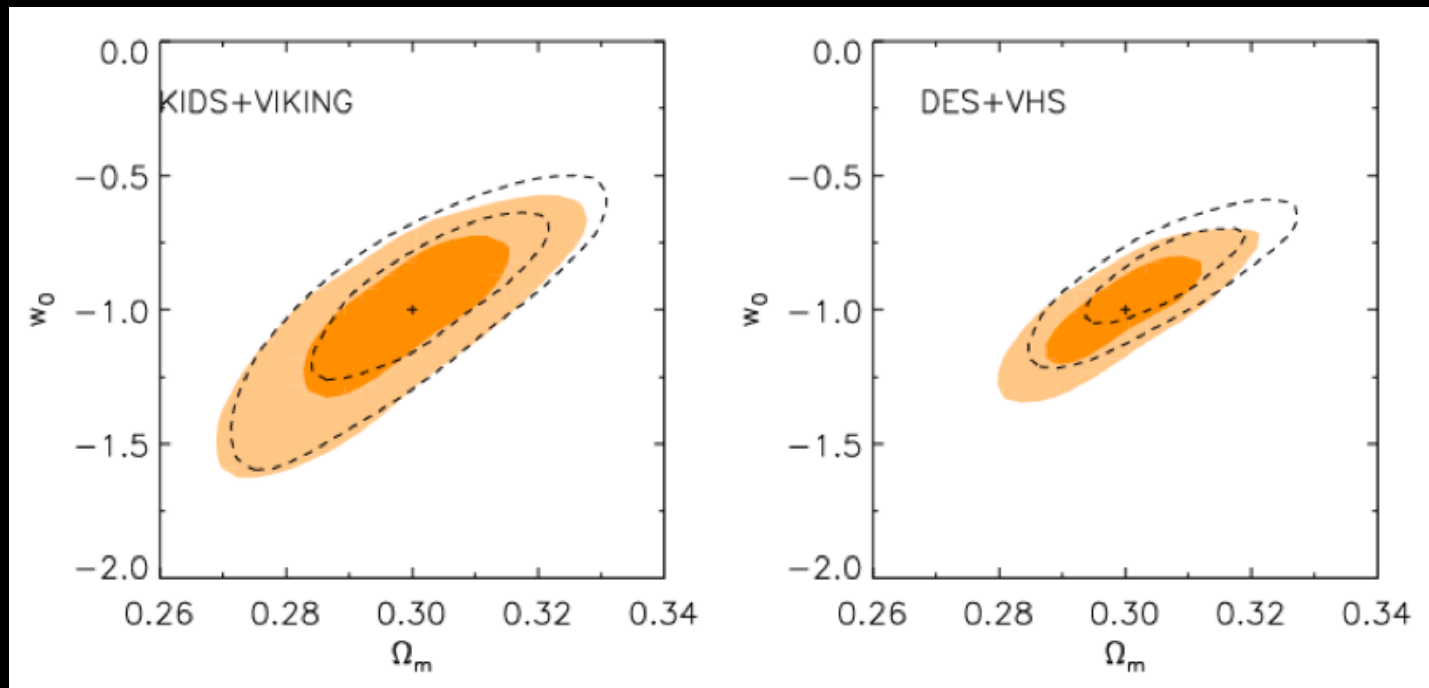
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  - Many questions now require large samples of galaxies to answer – now entering the “**Big Data**” era of astronomy.
  - Wide-field imaging surveys **much** cheaper and faster than spectroscopic surveys. Also can see fainter objects.
  - ~100x increase in sample size, diversity makes up for photo-z uncertainties. (Detailed studies can rely on ~1% spectroscopic subsample.)

# Science Case

## Precision cosmology

- Using large samples of galaxies to pin down the dark energy equation of state, growth of large-scale structure, etc.



# Computing Photo-z's

# Photo-z's: Statistically Speaking

Star formation rate

Star formation history

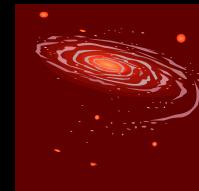
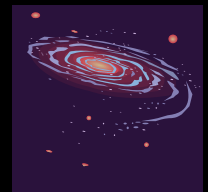
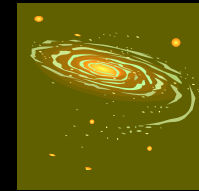
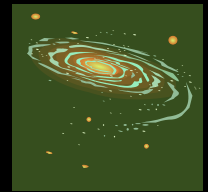
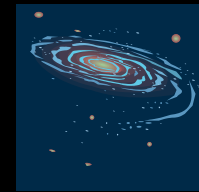
**Redshift**

Stellar mass

Dust content

Metallicity

AGN activity



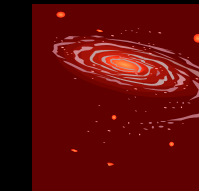
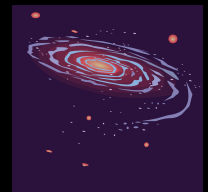
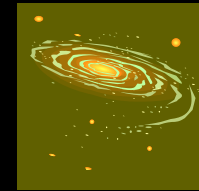
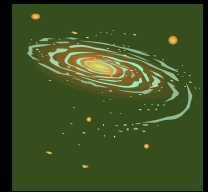
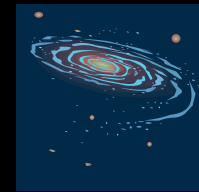
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- A **forward modeling** problem: can we construct a model from parameters we care about that matches the observed SED?

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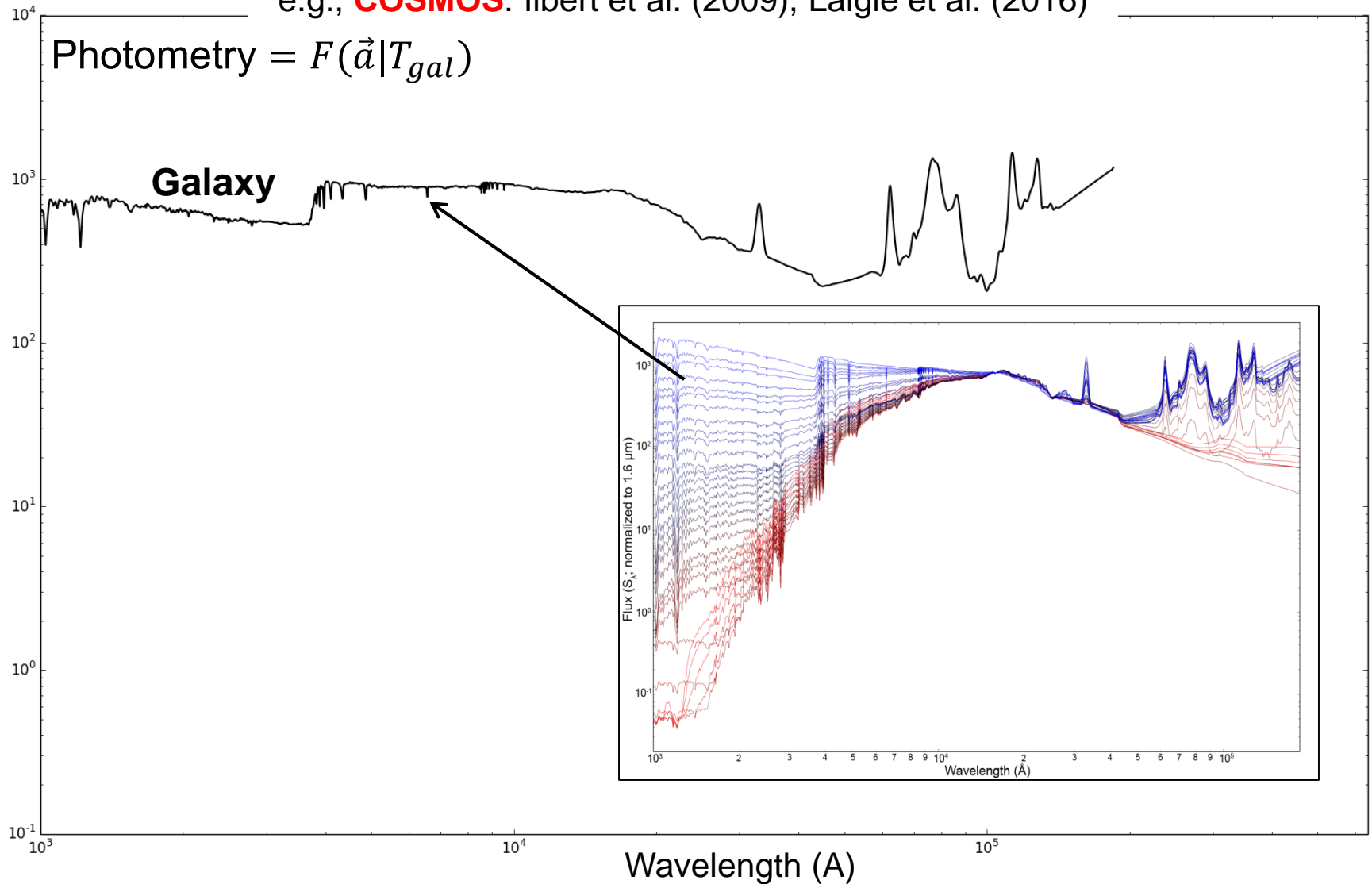
# Traditional Approach

e.g., **COSMOS**: Ilbert et al. (2009), Laigle et al. (2016)

$$\text{Photometry} = F(\vec{a} | T_{gal})$$

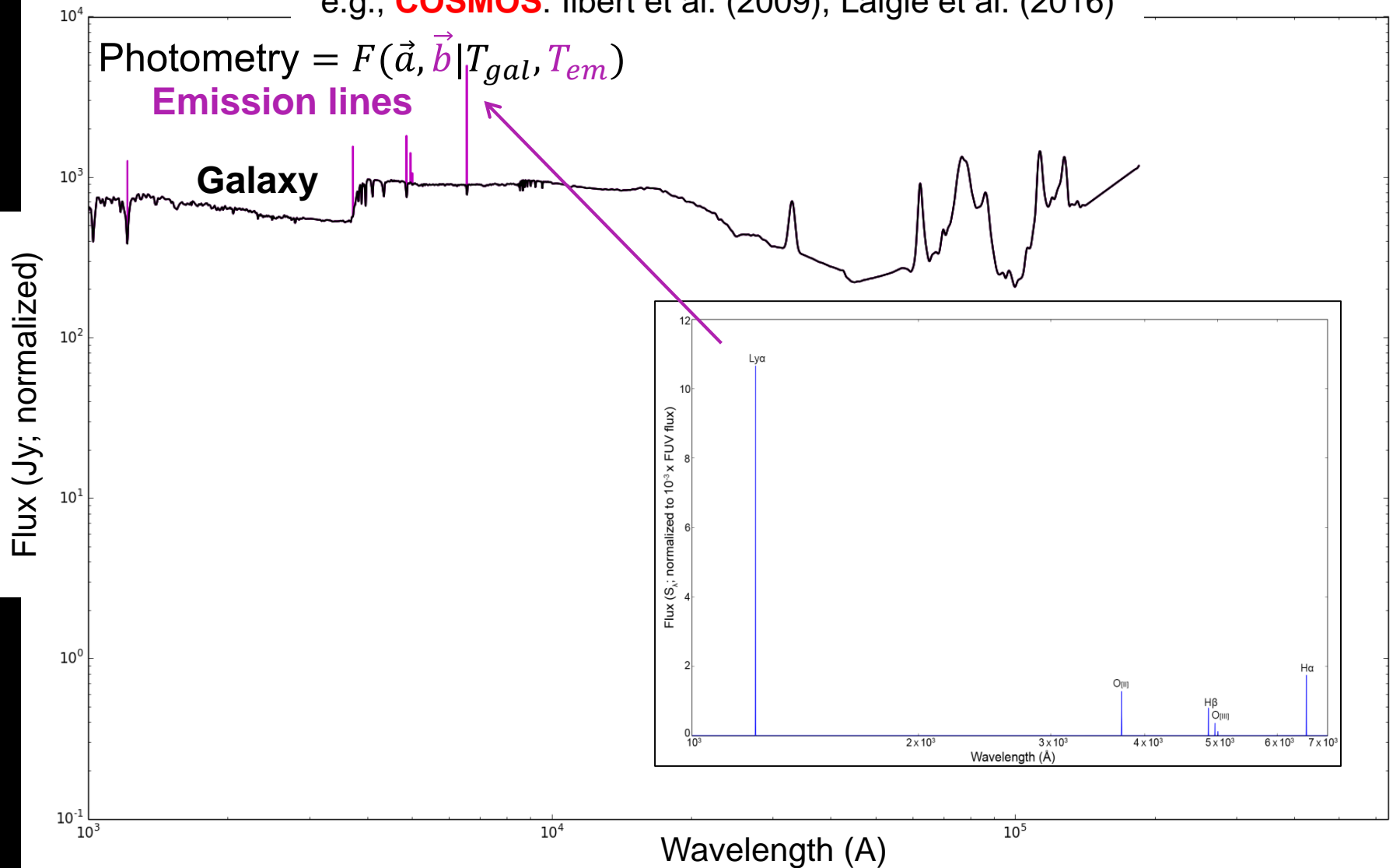
**Galaxy**

Flux (Jy; normalized)



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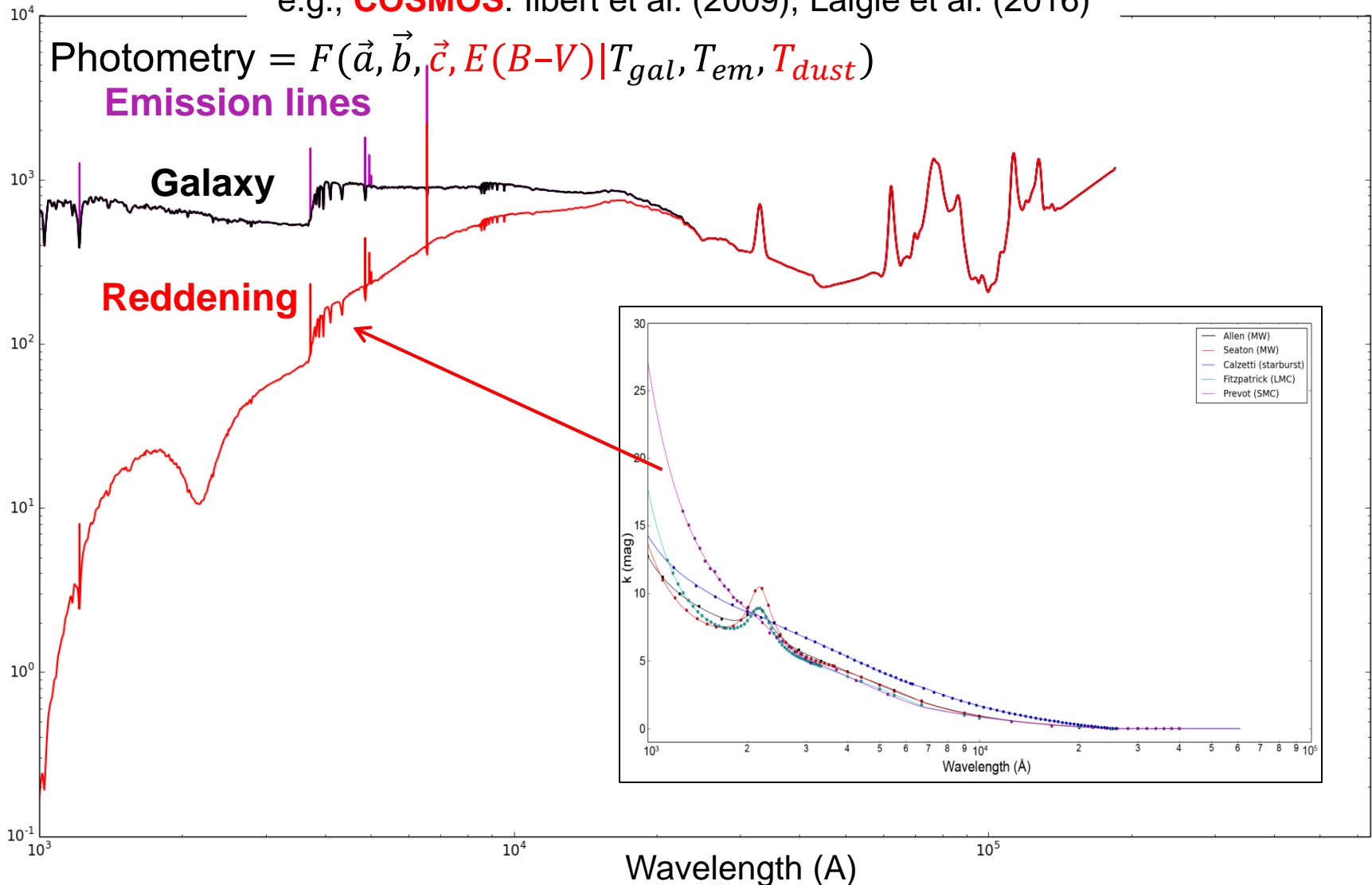
$$\text{Photometry} = F(\vec{a}, \vec{b}, \vec{c}, E(B-V) | T_{gal}, T_{em}, T_{dust})$$

Emission lines

Galaxy

Reddening

Flux (Jy; normalized)



# Traditional Approach

e.g., **COSMOS**: Ilbert et al. (2009), Laigle et al. (2016)

$$\text{Photometry} = F(\vec{a}, \vec{b}, \vec{c}, E(B-V), z | T_{gal}, T_{em}, T_{dust})$$

Emission lines

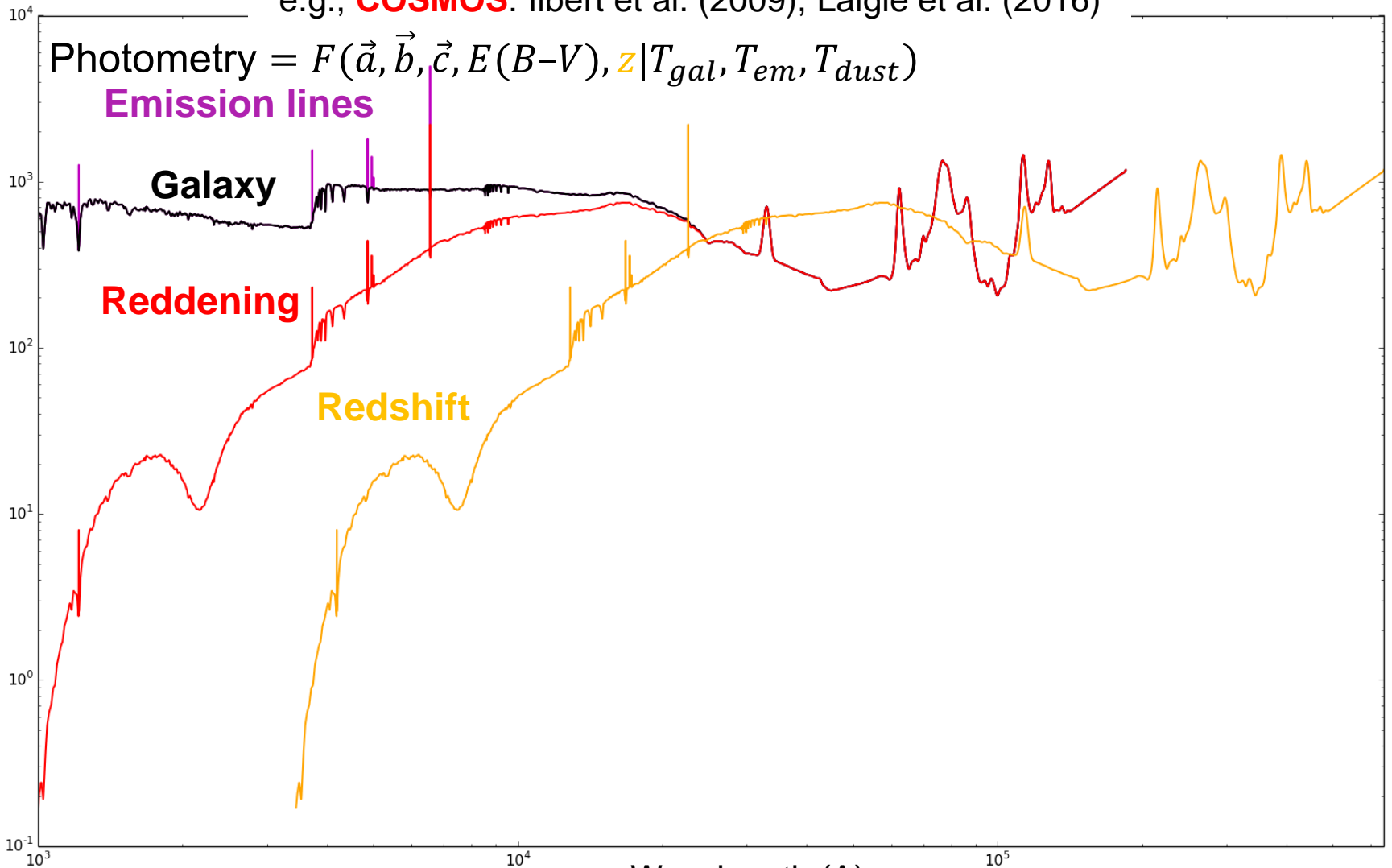
Galaxy

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Redshift

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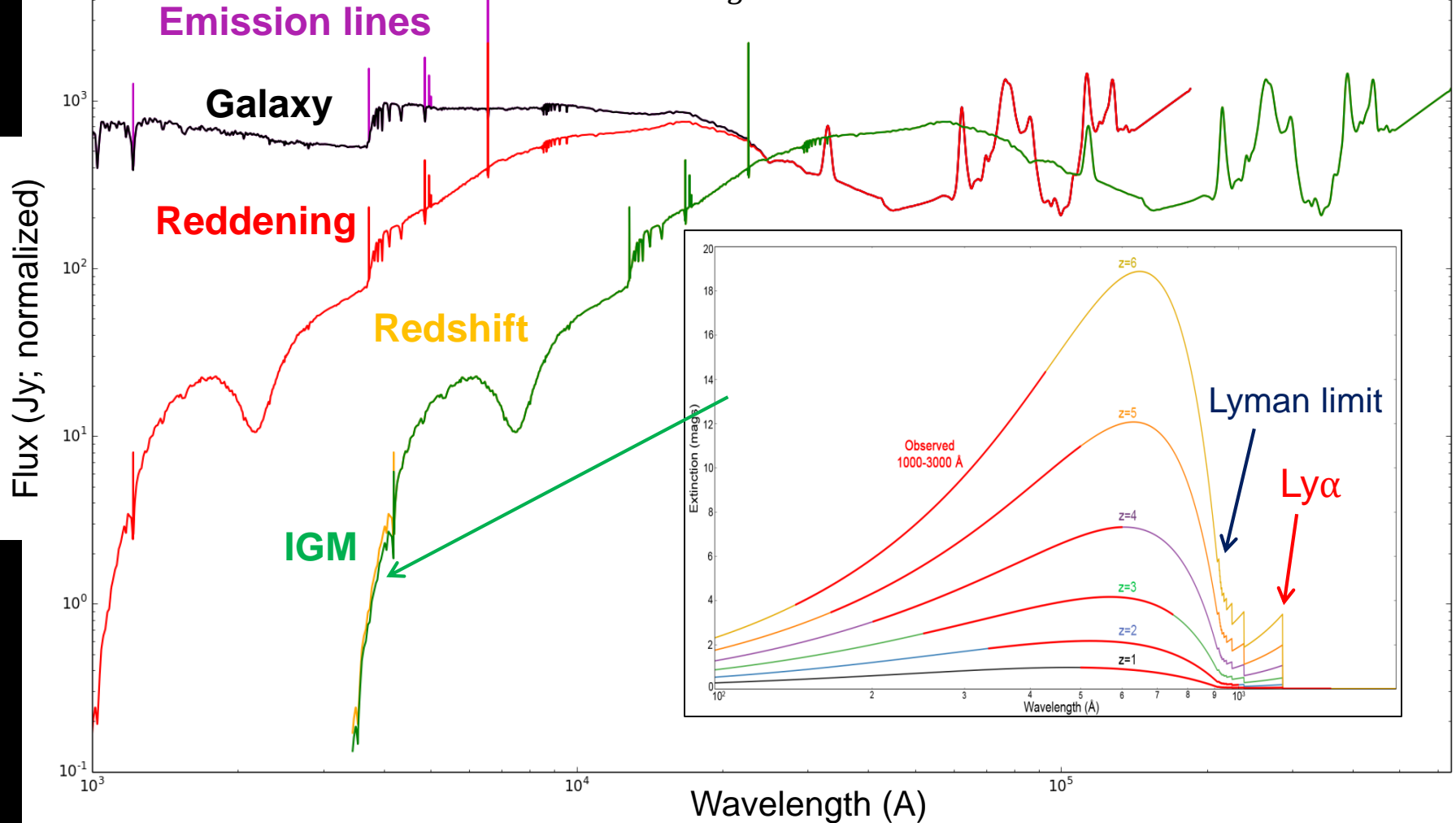
Wavelength (Å)



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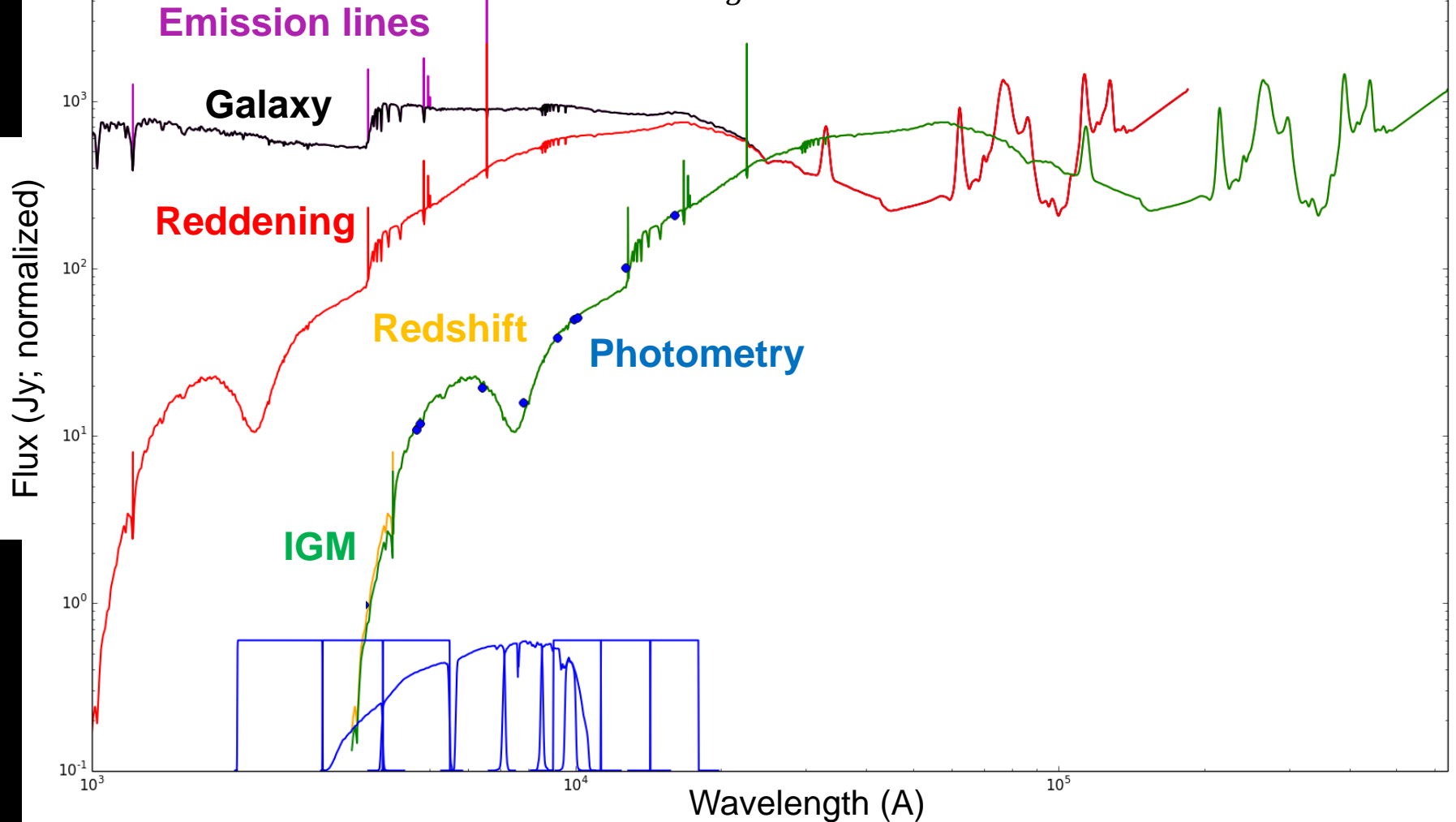
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Photometry =  $F(\vec{a}, \vec{b}, \vec{c}, E(B-V), z | T_{gal}, T_{em}, T_{dust}, T_{IGM}, \text{filters})$

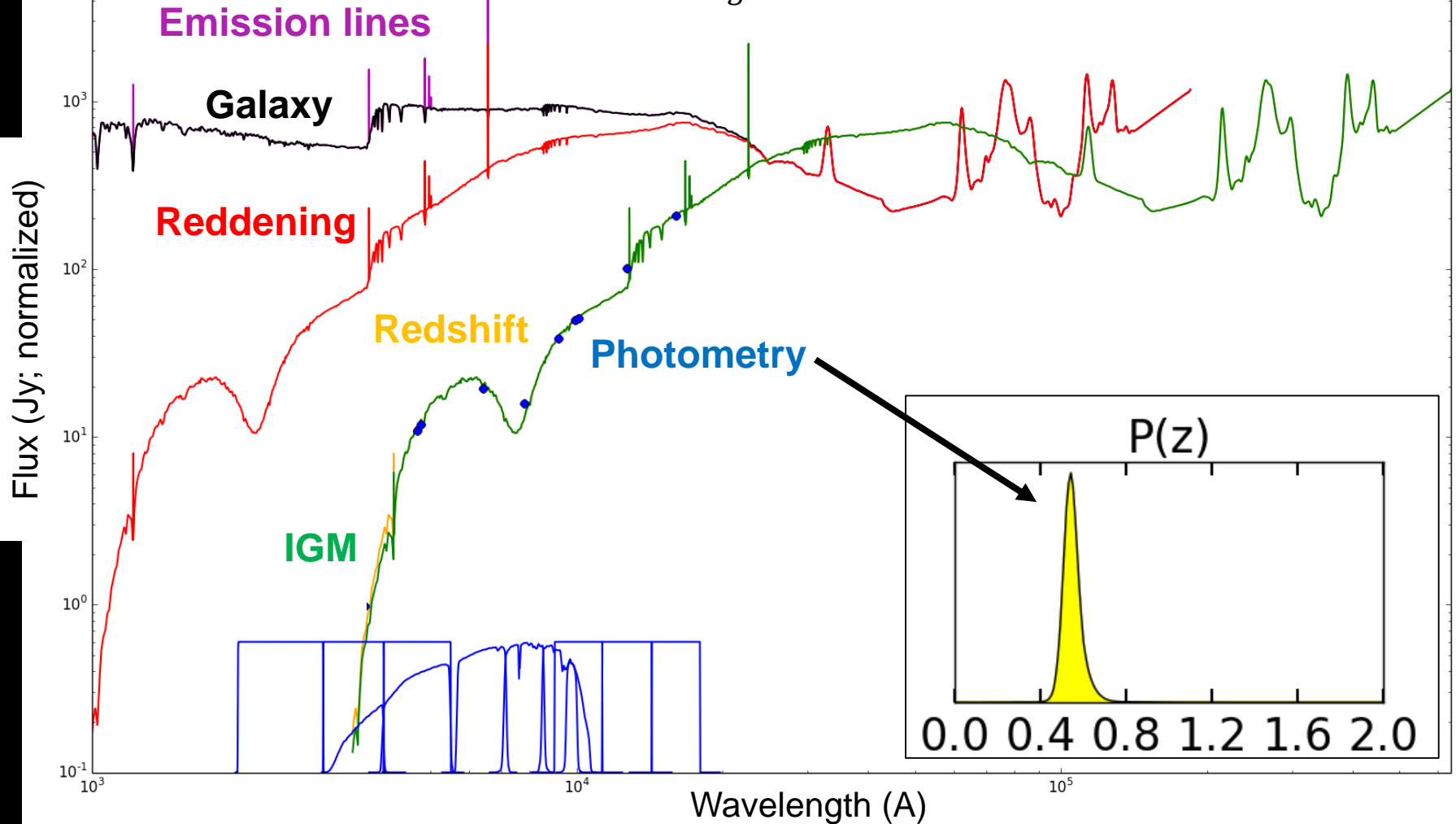




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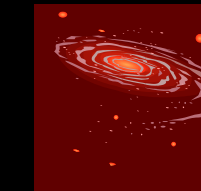
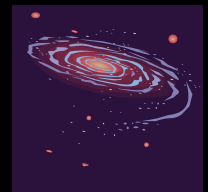
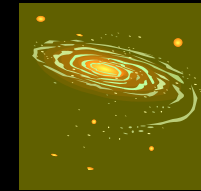
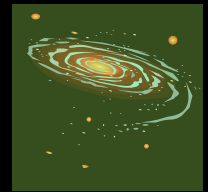
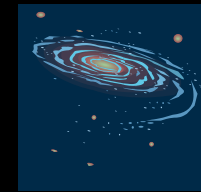
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- A **forward modeling** problem: can we construct a model from parameters we care about that matches the observed SED?

Star formation rate

Star formation history

**Redshift**



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Metallicity

Stellar mass

AGN activity

# Photo-z's: Statistically Speaking

- An **inverse mapping** problem: can we use **machine learning** to construct a mapping from color to redshift?

Star formation rate

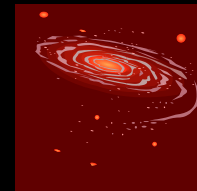
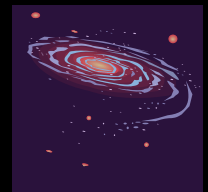
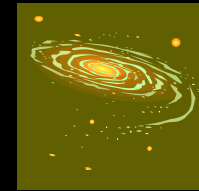
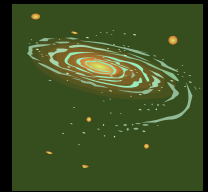
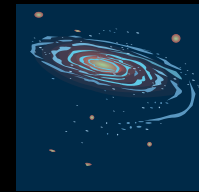
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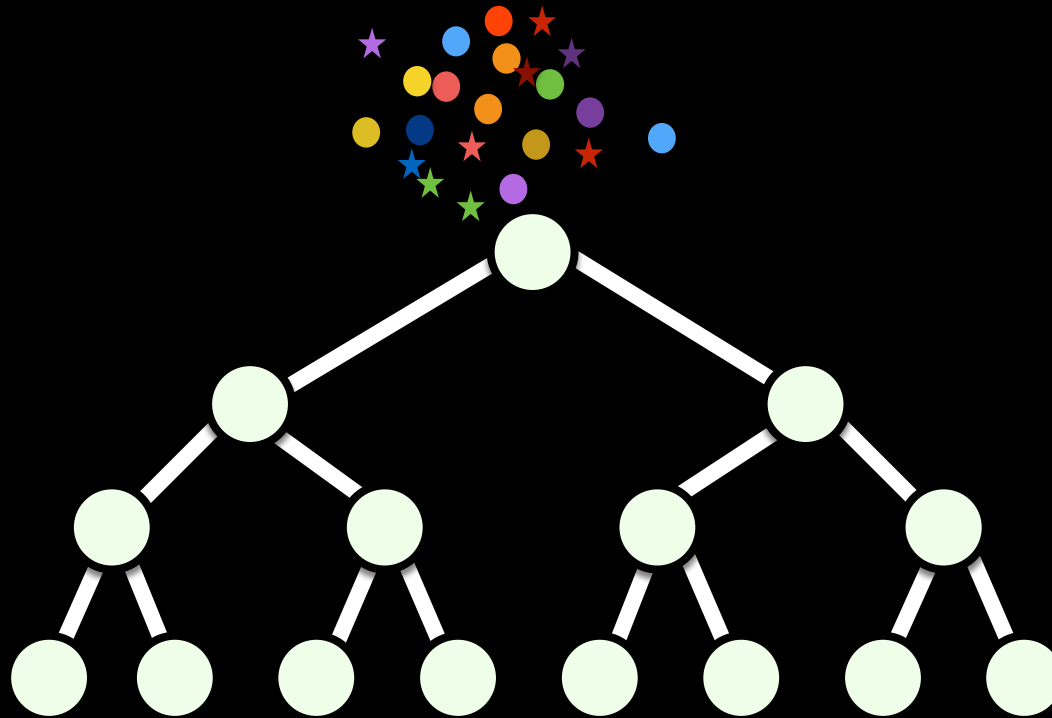


Stellar mass

# Machine Learning

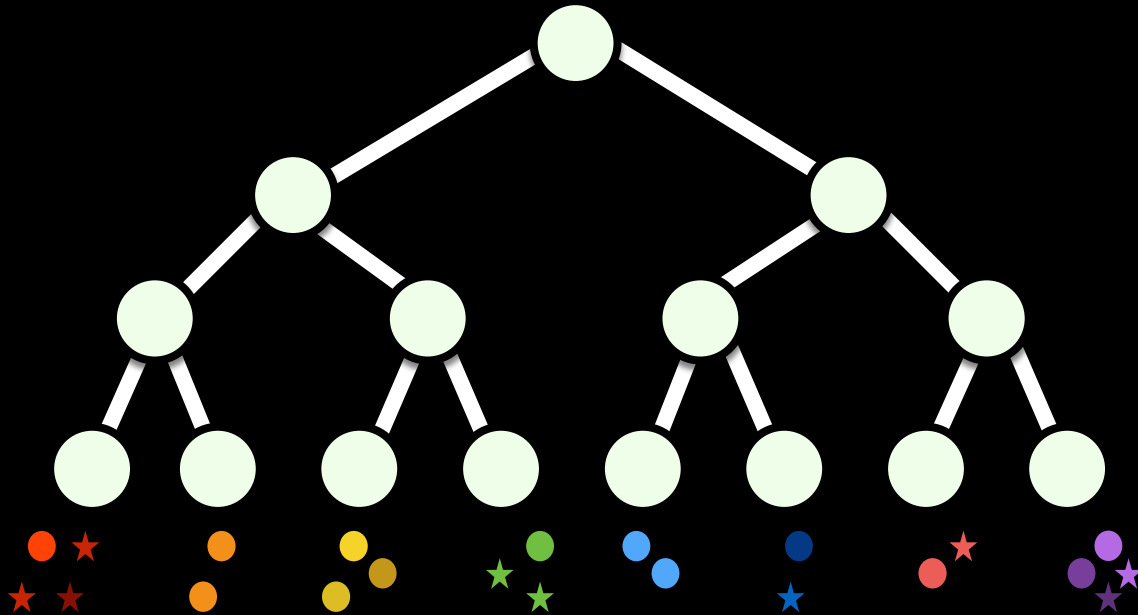


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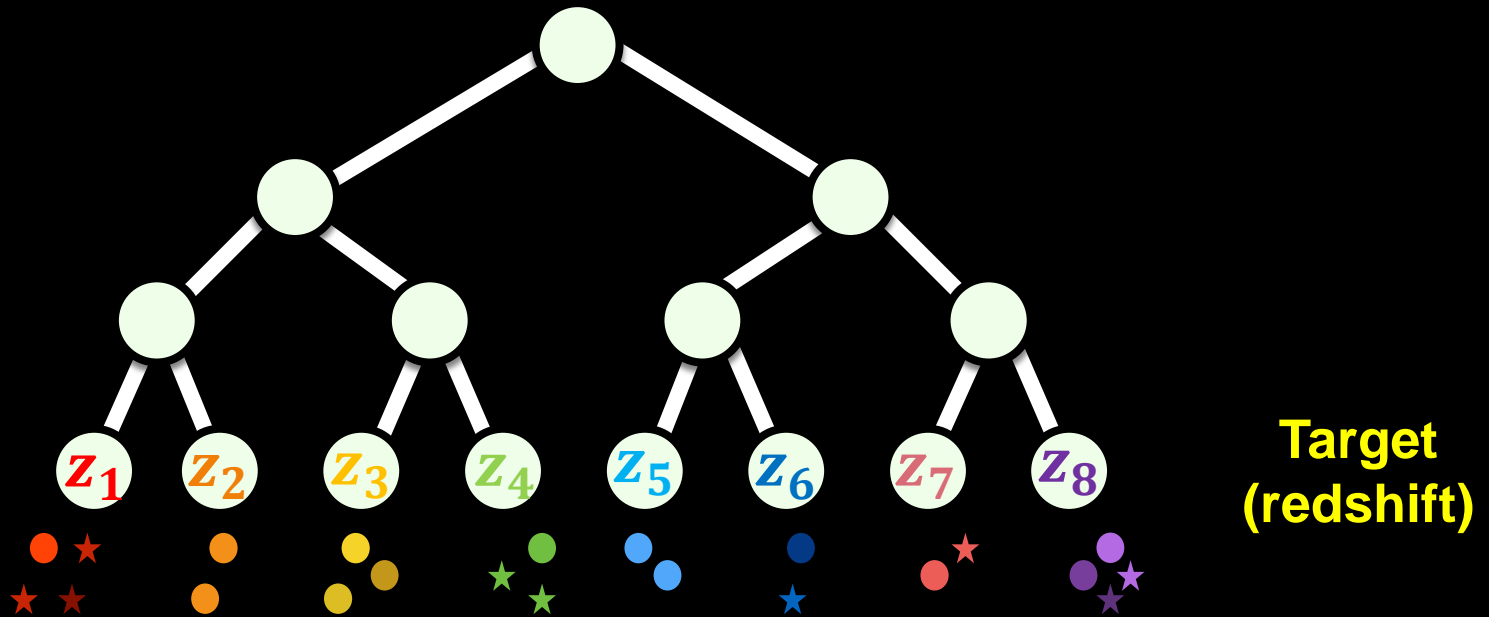


Decision  
Tree

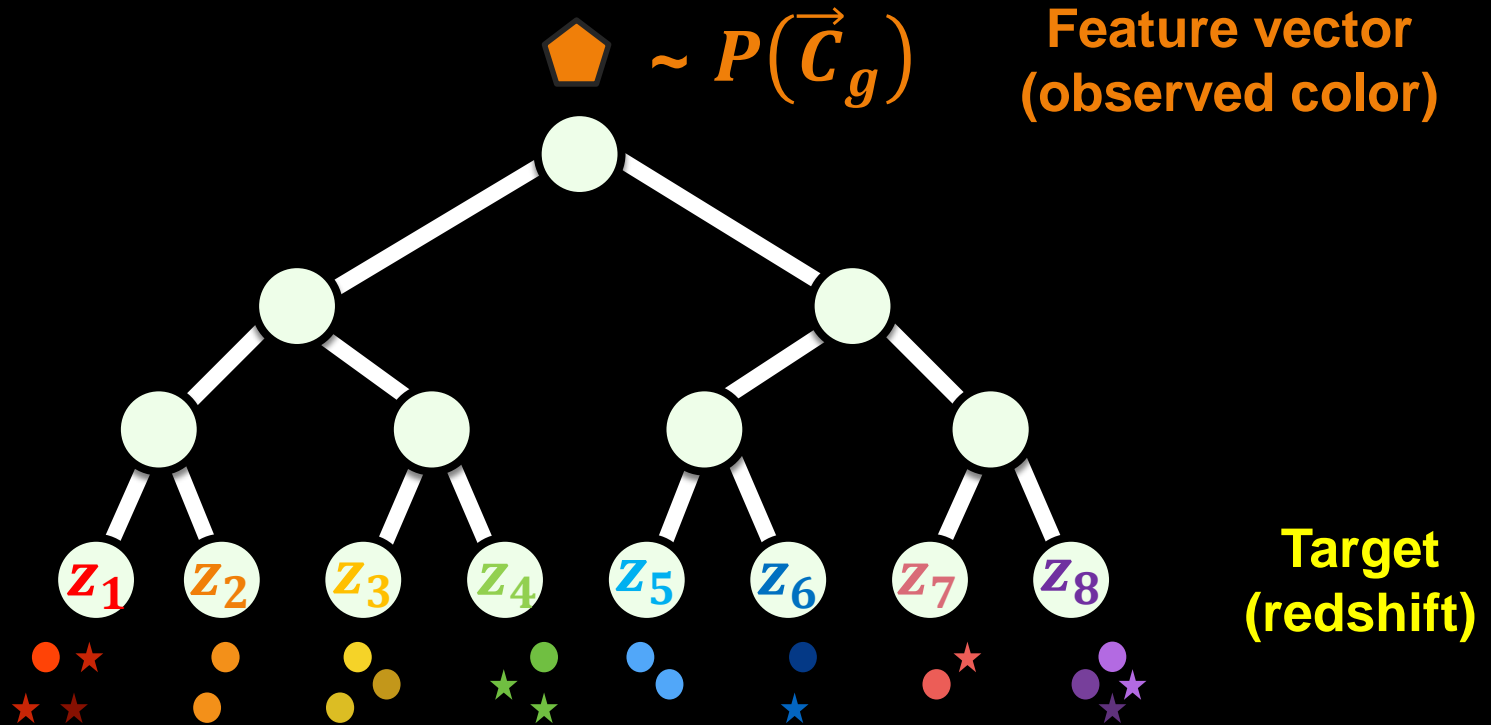
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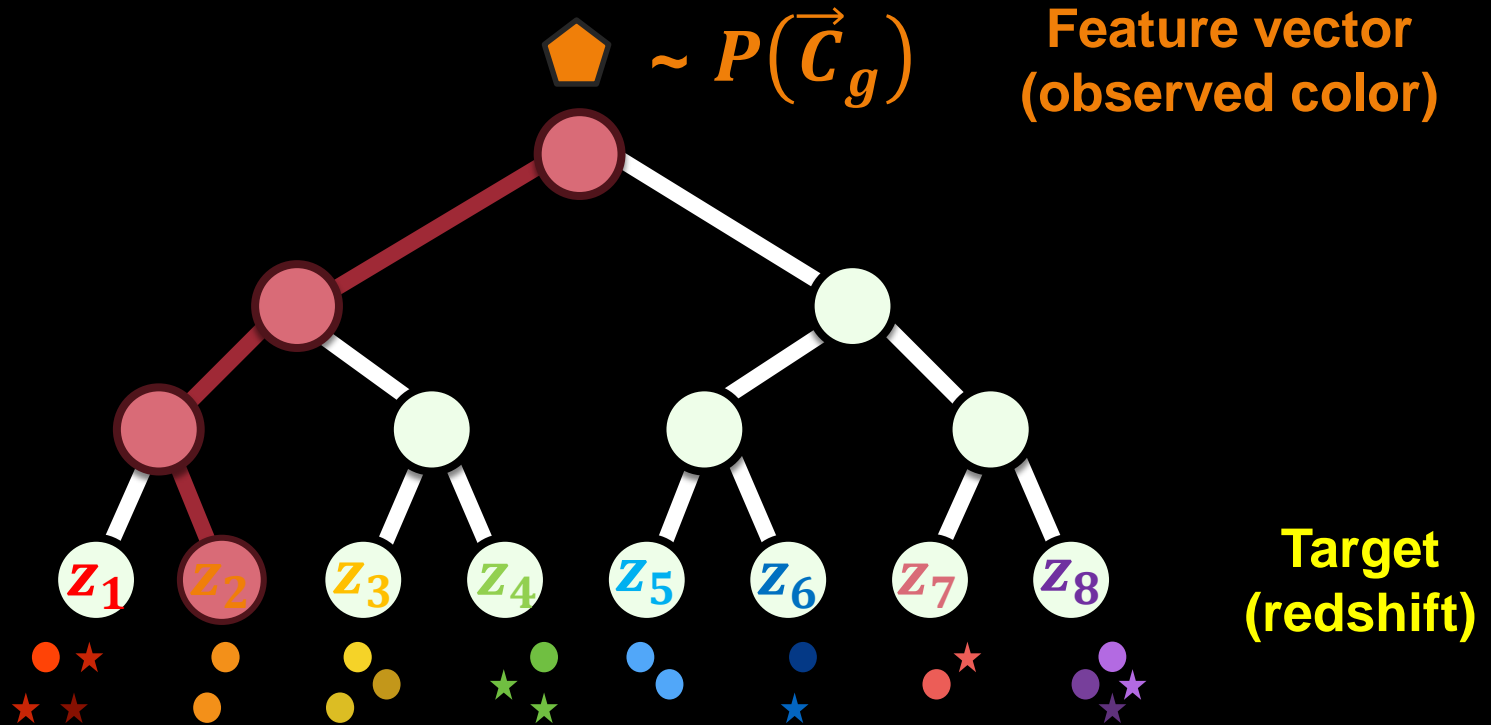


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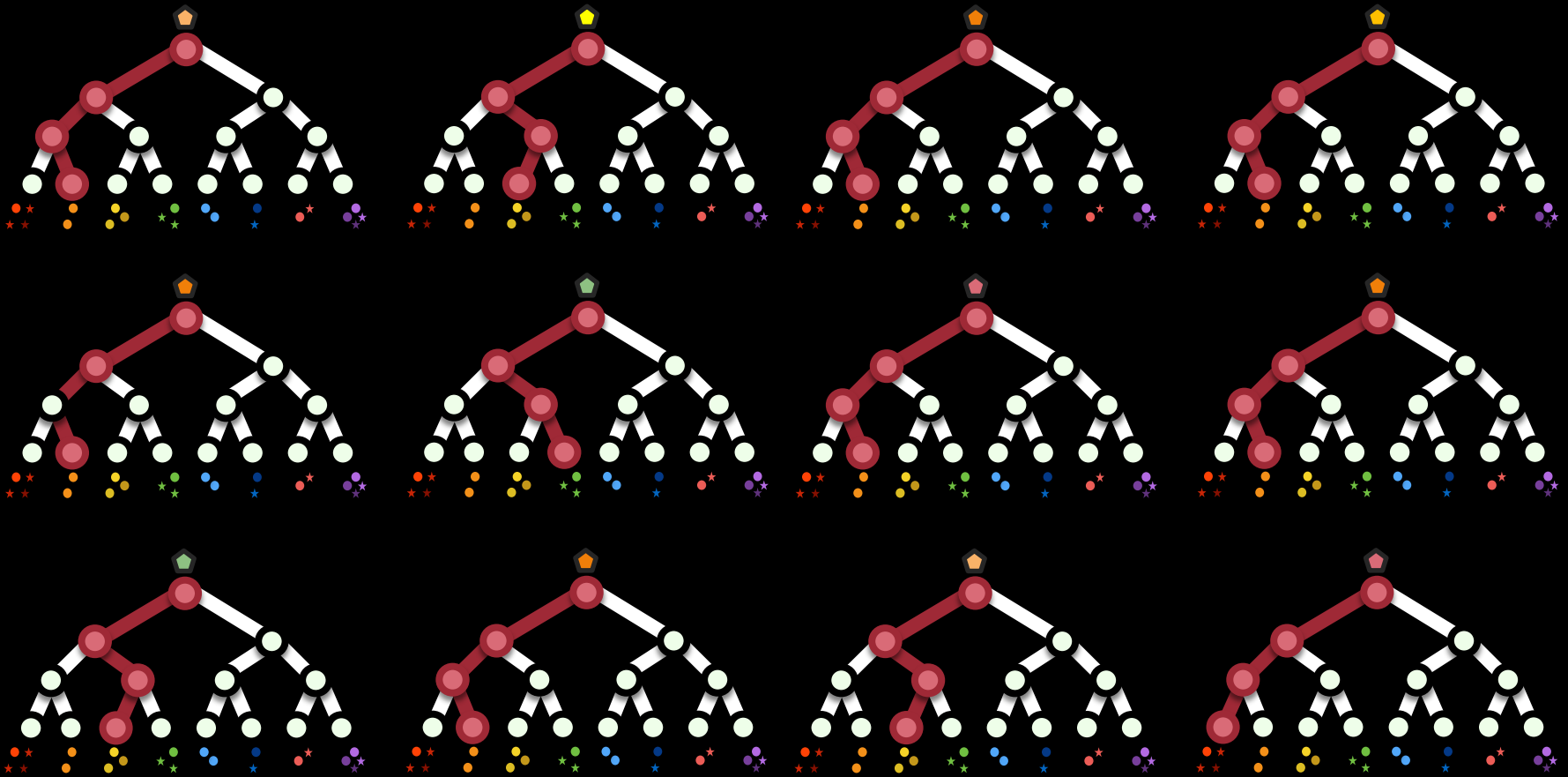




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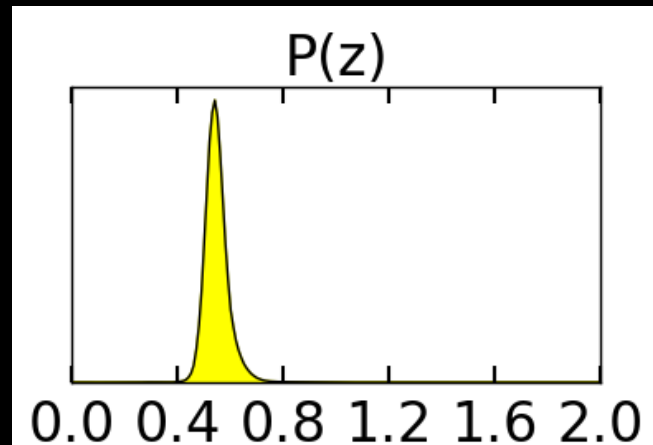
# Machine Learning



# Machine Learning

$z'_1$	$z'_2$	$z'_3$	$z'_4$	$z'_5$	$z'_6$	$z'_7$	$z'_8$	Target
1	7	3	1	0	0	0	0	Weight

Kernel Density Estimation



$P(z|g)$

# Two Communities

Model-fitting  
approaches  
(color-redshift  
relation assumed)

Machine-learning  
approaches  
(feature-redshift  
relation derived)

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# Two Communities

Model-fitting  
approaches  
(color-redshift  
relation assumed)

- Probabilistic
- Interpretable
- Sensitive to systematics
- Generally **slow**

Machine-learning  
approaches  
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# Two Communities

Model-fitting approaches  
(color-redshift relation assumed)

- Probabilistic
- Interpretable
- Sensitive to systematics
- Generally **slow**

- Flexible, data-driven
- More robust to systematics
- Generally **fast**
- Difficult to interpret
- Difficult to derive PDFs

Machine-learning approaches  
(feature-redshift relation derived)

What are we doing?



# Splitting Photo-z's into Two Parts

- Mapping from features to redshift.
  - Can be done through **model fitting** and/or **machine learning**.

$$P(z|F) \text{ or } P(F|z, \eta)$$

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$$P(z|\mathbf{F}) \text{ or } P(\mathbf{F}|z, \boldsymbol{\eta})$$

- Propagating uncertainties in features.

$$P(\mathbf{F}|\hat{\mathbf{F}}, \hat{\mathbf{C}})$$

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$$\{P(z|\hat{\mathbf{F}}_h, \hat{\mathbf{C}}_h)\}$$

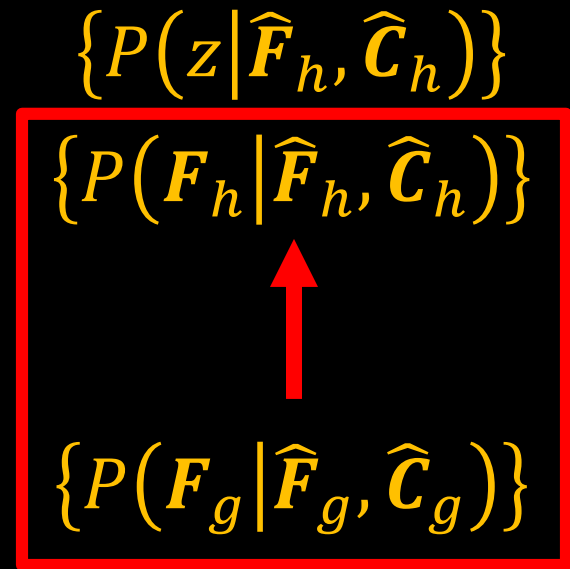
$$\{P(\mathbf{F}_h|\hat{\mathbf{F}}_h, \hat{\mathbf{C}}_h)\}$$

- Propagating uncertainties in features.

$$\{P(\mathbf{F}_g|\hat{\mathbf{F}}_g, \hat{\mathbf{C}}_g)\}$$

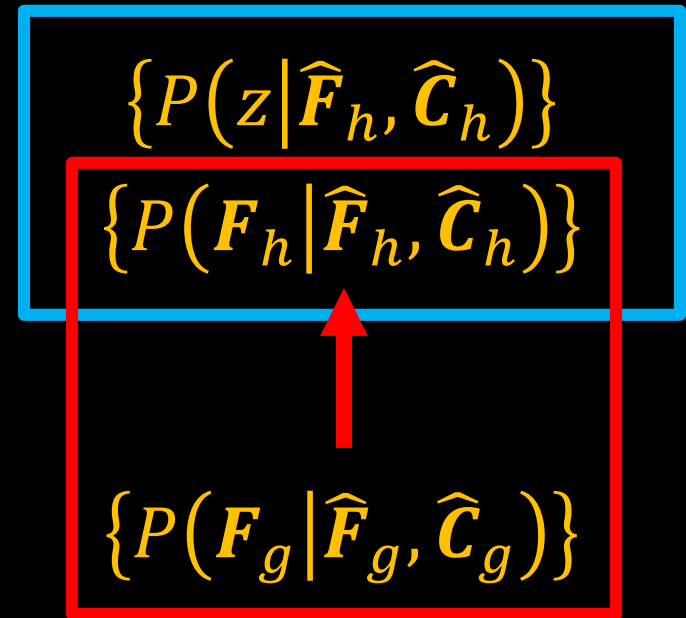
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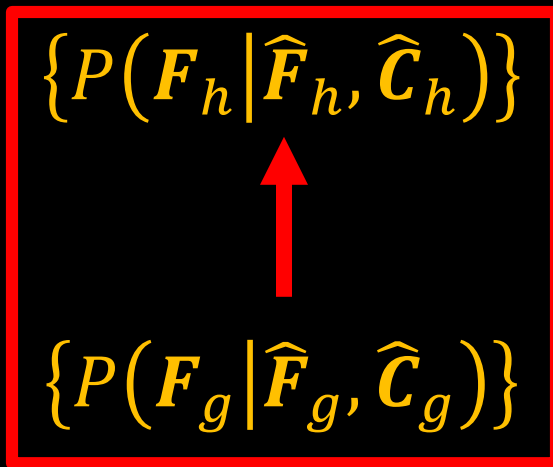


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# Feature Projection



# The “Big Data” Assumption

$$P(z|g) = \sum_h P(z|h)P(h|g)$$

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redshift  
↓  
target galaxy “g”

redshift PDF

photometric posterior

training galaxy “h”



# The “Big Data” Assumption

$$P(z|g) = \sum_h P(z|h)P(h|g)$$

$$= \sum_h P(z|h) \frac{P(g|h)P(h)}{P(g)}$$

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2. How do we compute it?

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$$P(z|g) = \sum_h P(z|h)P(h|g)$$

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band mask

1. What is this likelihood?
2. How do we compute it?
3. How do we deal with missing data?

# The “Big Data” Assumption

$$P(z|g) = \sum_h P(z|h) P(h|g, s_g = 1, \mathcal{S}_g)$$

selection effects

galaxy is  
observed

$$\stackrel{?}{=} \sum_h P(z|h) \frac{P(g|h, \mathbf{b})P(h)}{P(g)}$$

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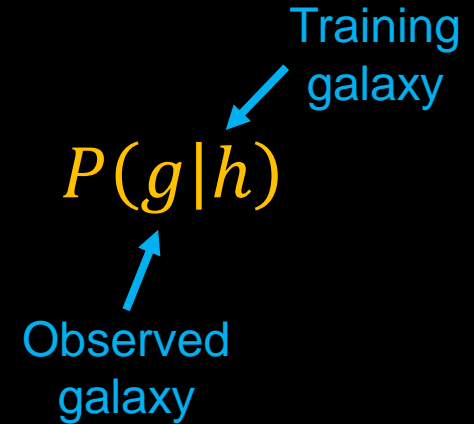
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# Likelihood / Distance Metric

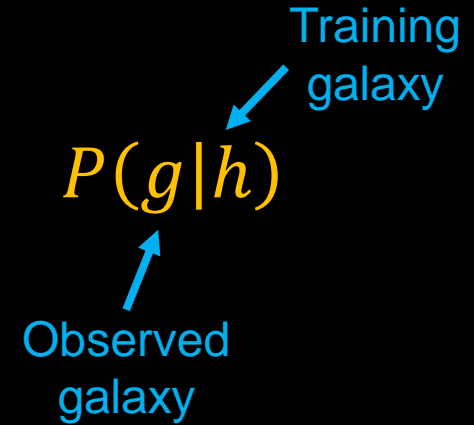
- What metric(s) to use?





# Likelihood / Distance Metric

- What metric(s) to use?



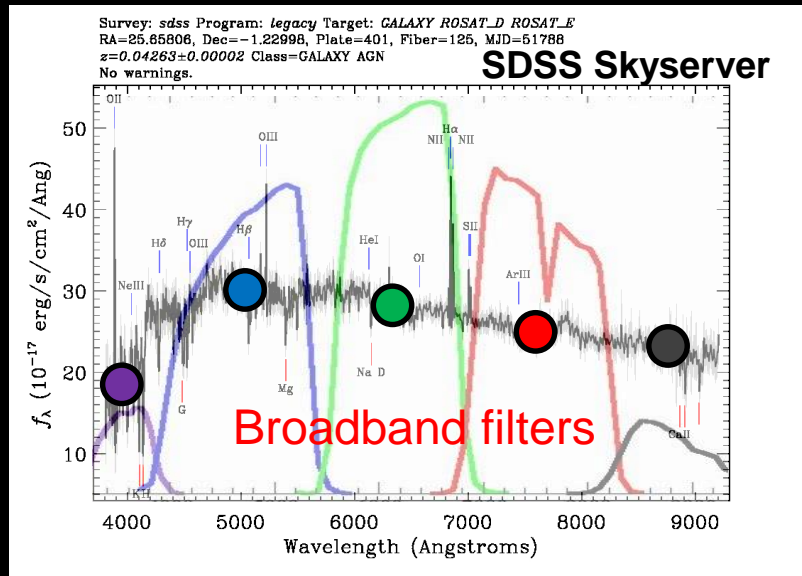
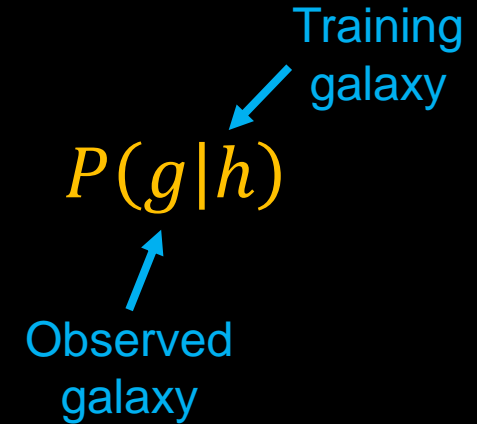
NGC 4414



NGC 5457

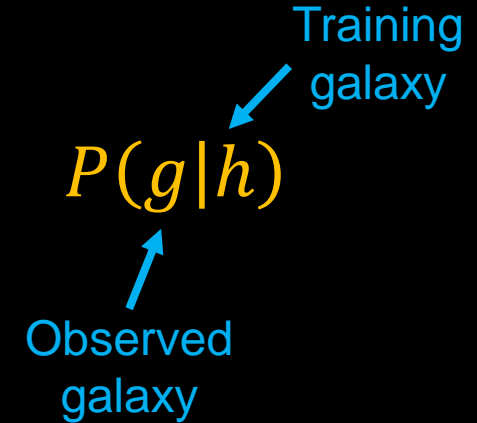
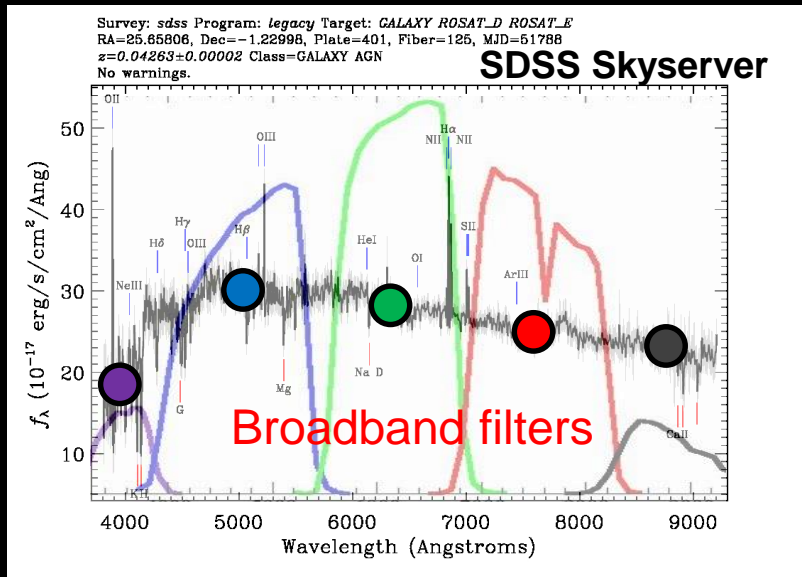
# Likelihood / Distance Metric

- What metric(s) to use?



# Likelihood / Distance Metric

- What metric(s) to use?



Assume data is normally distributed.

$$P(F_g | \hat{F}_g, \hat{C}_g) \sim N(F_g | \hat{F}_g, \hat{C}_g)$$

# Likelihood / Distance Metric

- What metric(s) to use?

$$P(g|h)$$

Color space (traditional)

$$\chi^2 = \sum_i \frac{(\hat{F}_{g,i} - s\hat{F}_{h,i})^2}{\hat{\sigma}_{g,i}^2 + s^2\hat{\sigma}_{h,i}^2}$$

# Likelihood / Distance Metric

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Magnitude space (“new”)

$$\chi^2 = \sum_i \frac{(\hat{F}_{g,i} - \hat{F}_{h,i})^2}{\hat{\sigma}_{g,i}^2 + \hat{\sigma}_{h,i}^2}$$

# Likelihood / Distance Metric

- What metric(s) to use?

$$P(g|h)$$

## Color space (traditional)

Requires magnitude priors to account for galaxy evolution.

“Scale-free”

$$\chi^2 = \sum_i \frac{(\hat{F}_{g,i} - s\hat{F}_{h,i})^2}{\hat{\sigma}_{g,i}^2 + s^2\hat{\sigma}_{h,i}^2}$$

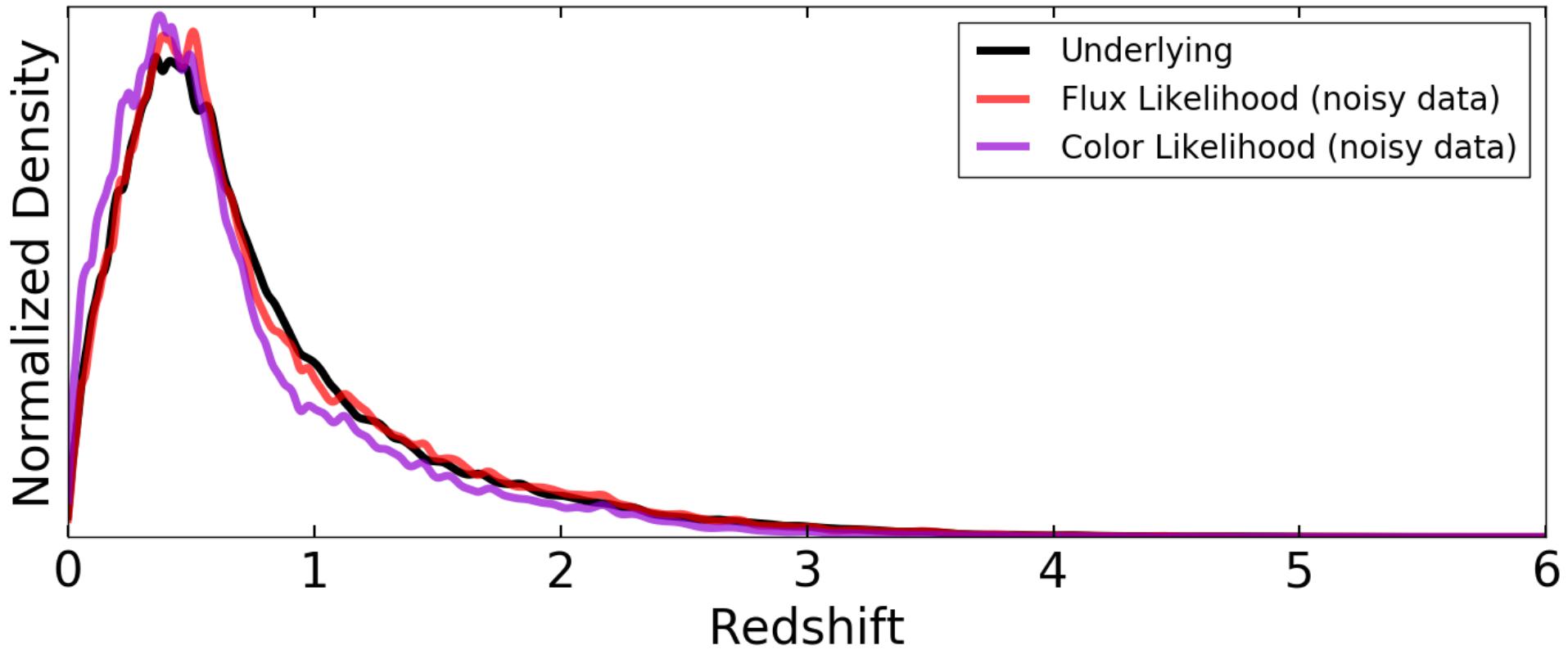
## Magnitude space (“new”)

Requires good sampling in full magnitude space.

“Scale-dependent”

$$\chi^2 = \sum_i \frac{(\hat{F}_{g,i} - \hat{F}_{h,i})^2}{\hat{\sigma}_{g,i}^2 + \hat{\sigma}_{h,i}^2}$$

# Population: Mag v Color





# The “Big Data” Assumption

$$P(z|g) = \sum_h P(z|h)P(h|g, s_g = 1, \mathcal{S}_g)$$

$$\stackrel{?}{=} \sum_h P(z|h) \frac{P(g|h, \mathbf{b})P(h)}{P(g)}$$

1. What is this likelihood?
2. How do we compute it?
3. How do we deal with missing data?
4. How do we incorporate selection effects?
5. What is our prior?

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$$P(z|g) = \sum_h P(z|h)P(h|g, s_g = 1, \mathcal{S}_g)$$

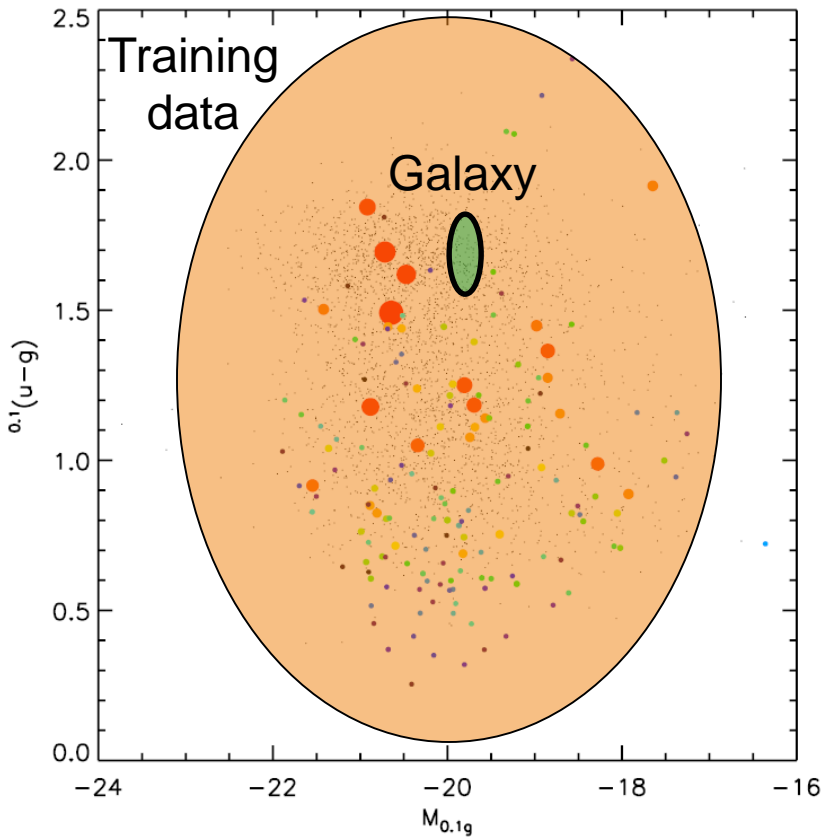
$$\stackrel{?}{=} \sum_h P(z|h) \frac{P(g|h, \mathbf{b})P(h)}{P(g)}$$

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# The Problem

Likelihood

$$\{P(h|g)\}$$



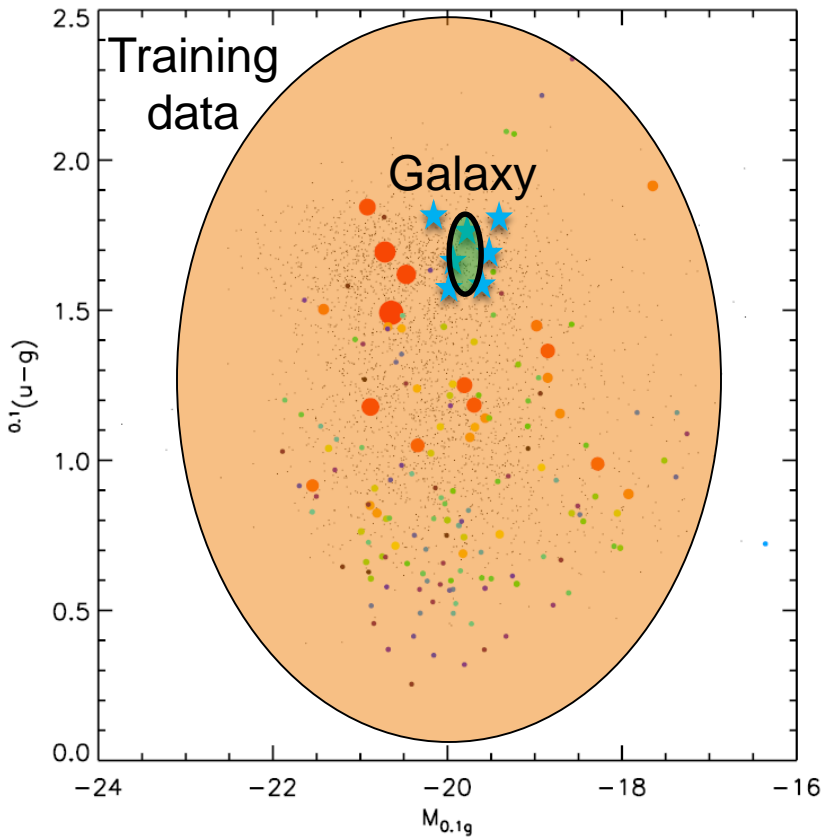
Cool et al. (2007)



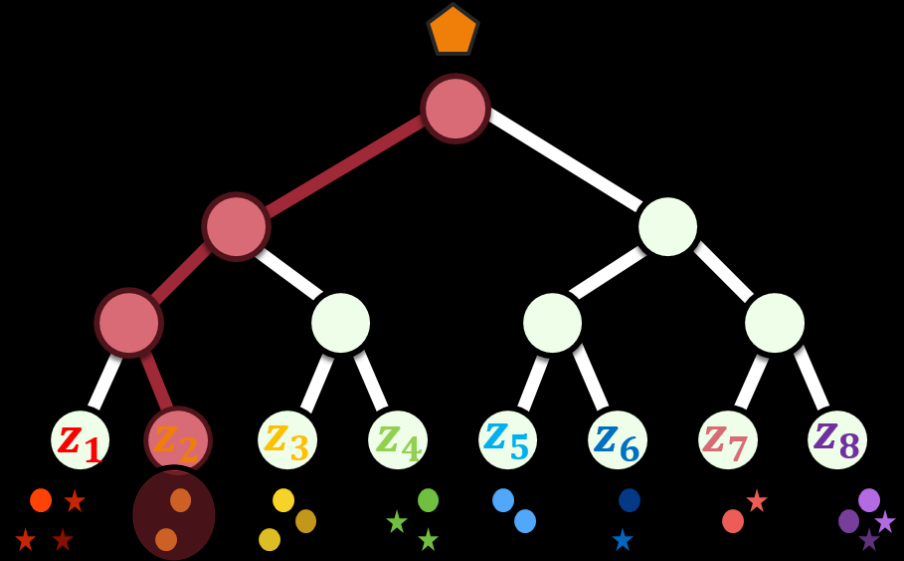
# Machine Learning Approximation

Likelihood

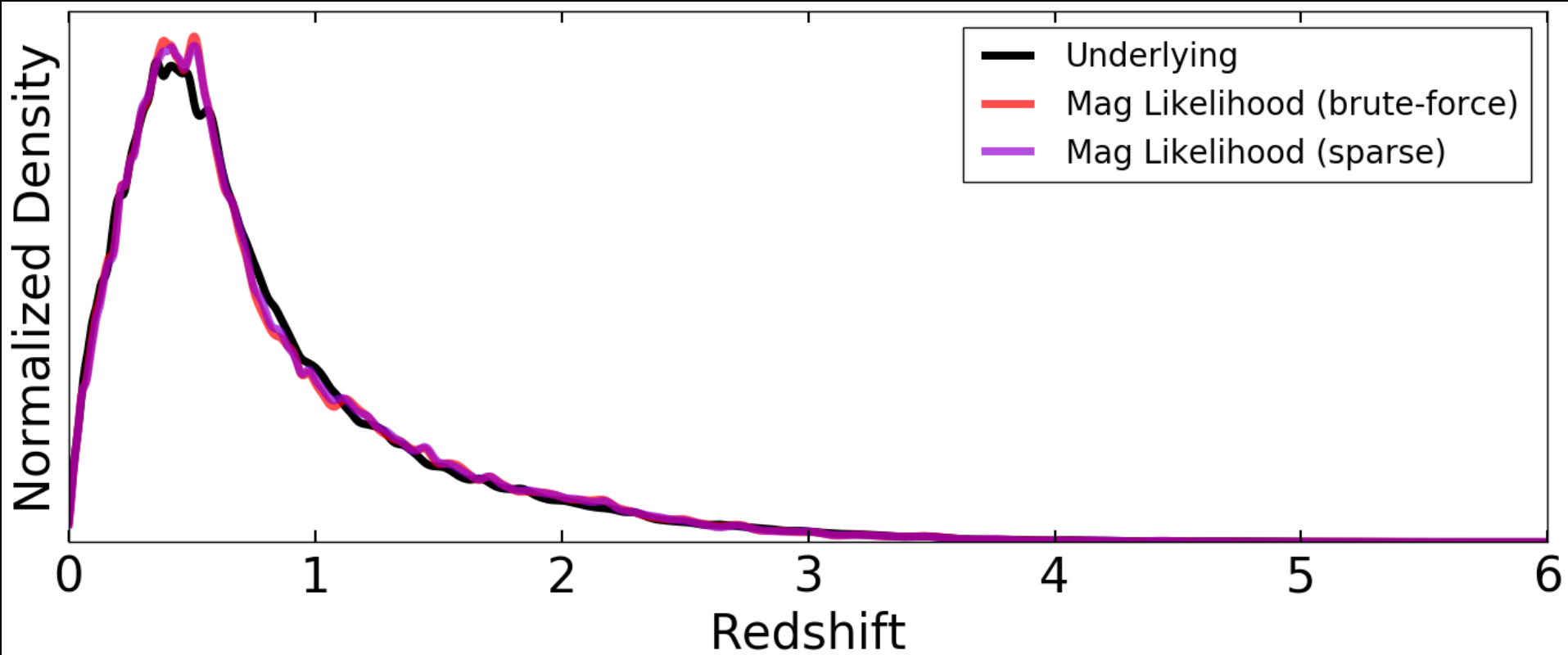
$$\{\hat{P}(h|g)\}$$



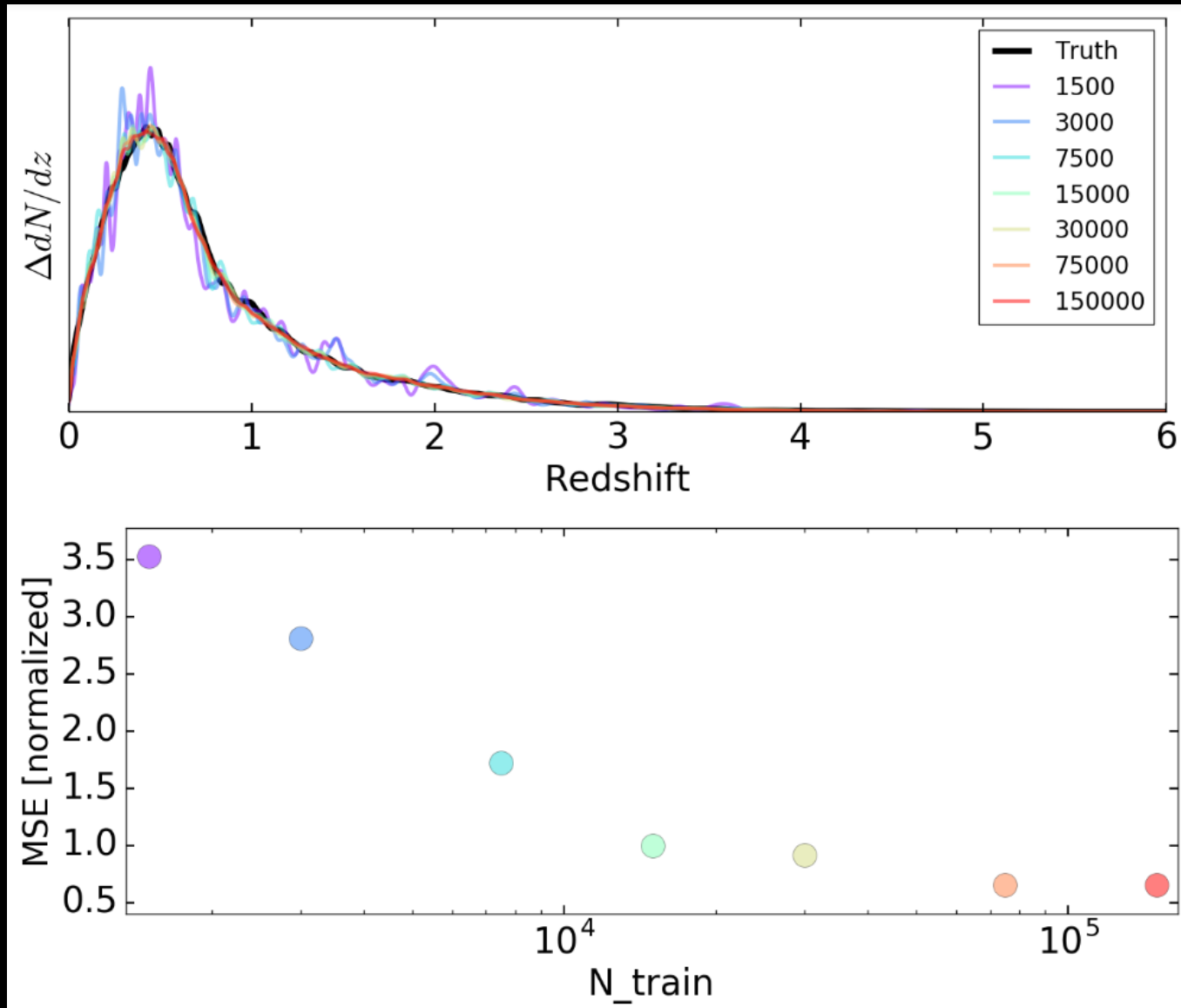
Cool et al. (2007)



# Population: FRANKEN-Z



# How Valid is Our Approximation?



# The “Big Data” Assumption

$$P(z|g) = \sum_h P(z|h)P(h|g, s_g = 1, \mathcal{S}_g)$$

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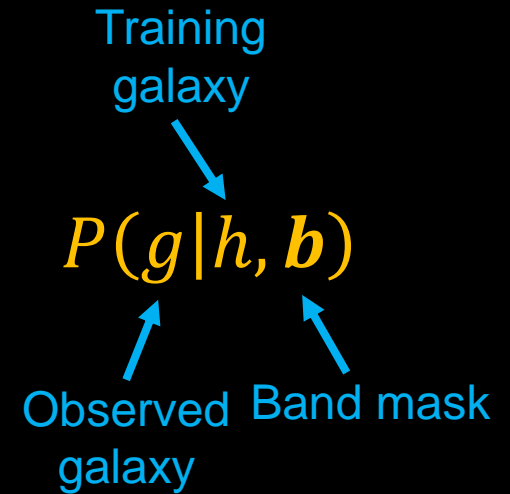
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# Missing Data

- How to deal with missing data?



# Now What?

- How to deal with missing data?

$$P(g|h, \mathbf{b})$$

$$-2 \ln L = ???$$

# Naïve Likelihood: Multivariate Normal

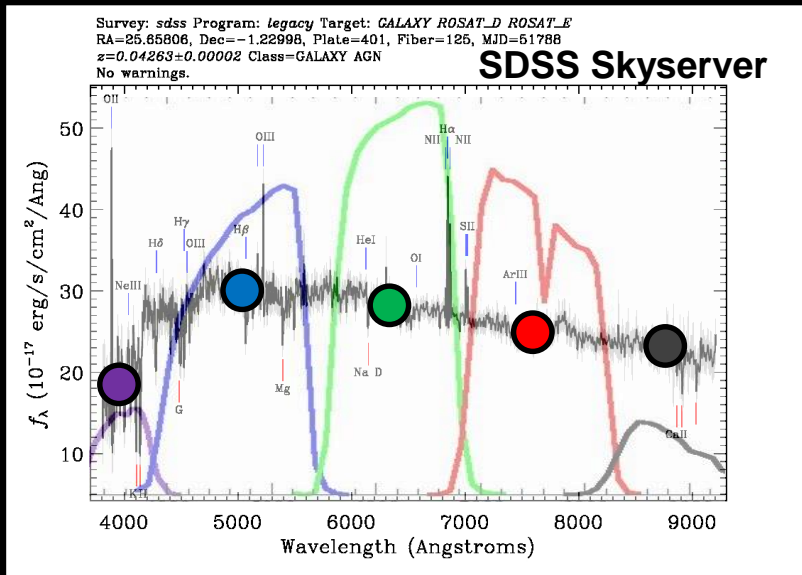
- How to deal with missing data?  $P(g|h, \mathbf{b})$

$$-2 \ln L_n \sim \chi_n^2(\delta_n) + n \ln 2\pi + \ln |\hat{C}_g + \hat{C}_h|$$

# Implications

- How to deal with missing data?

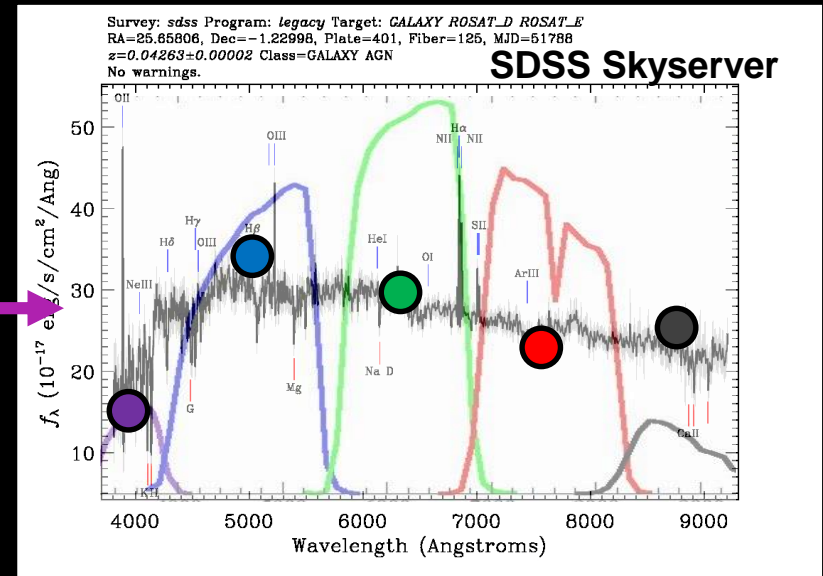
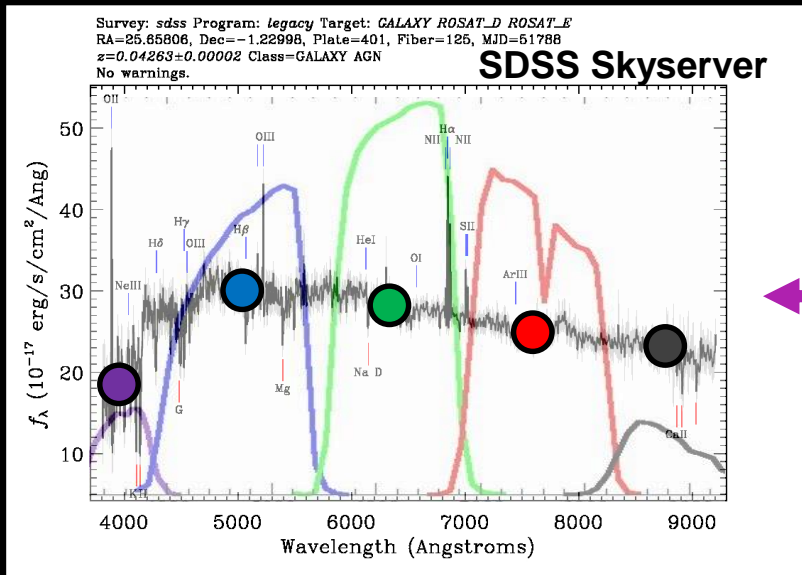
$$P(g|h, \mathbf{b})$$



# Implications

- How to deal with missing data?

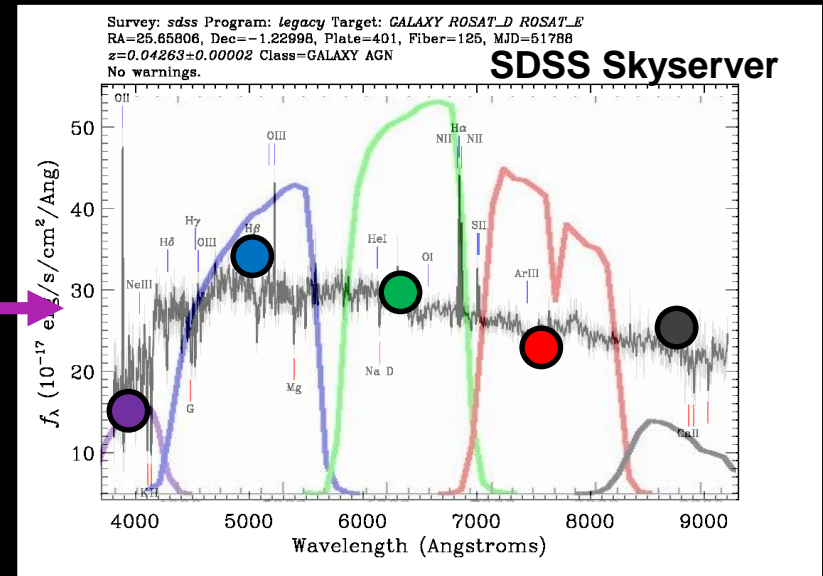
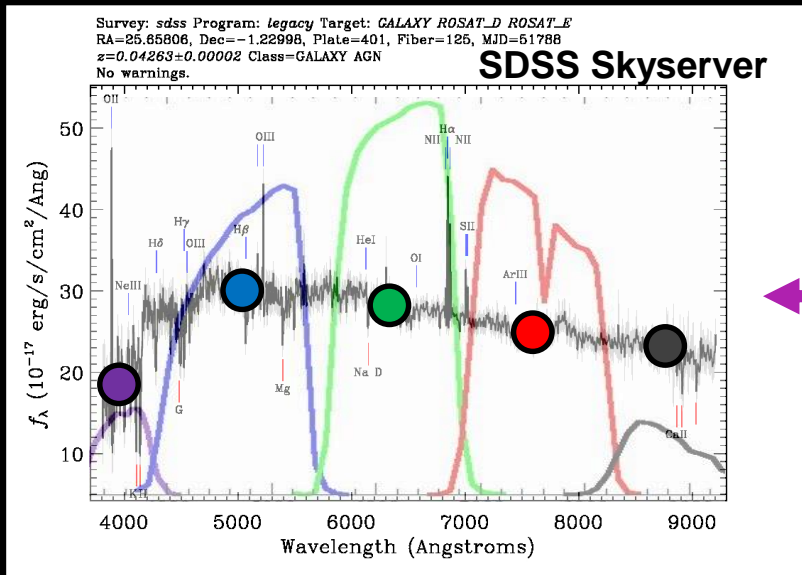
$$P(g|h, b)$$



# Implications

- How to deal with missing data?

$$P(g|h, \mathbf{b})$$

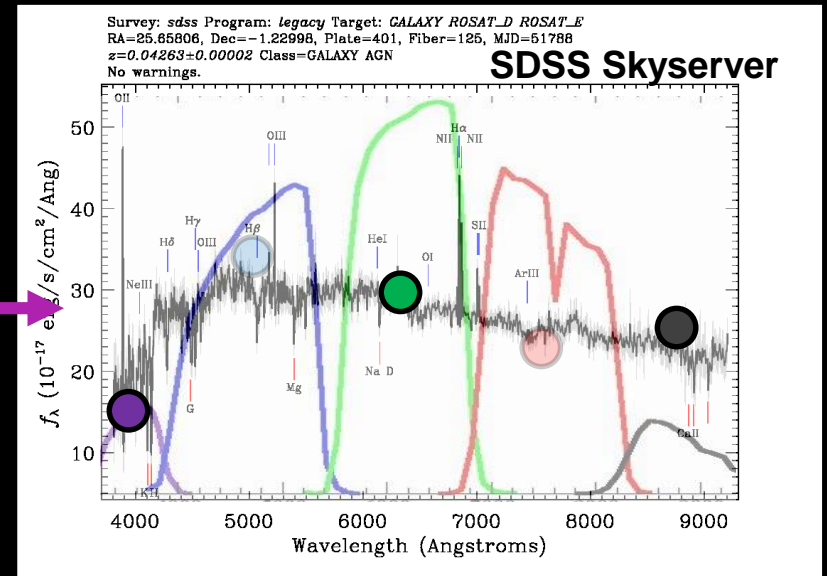
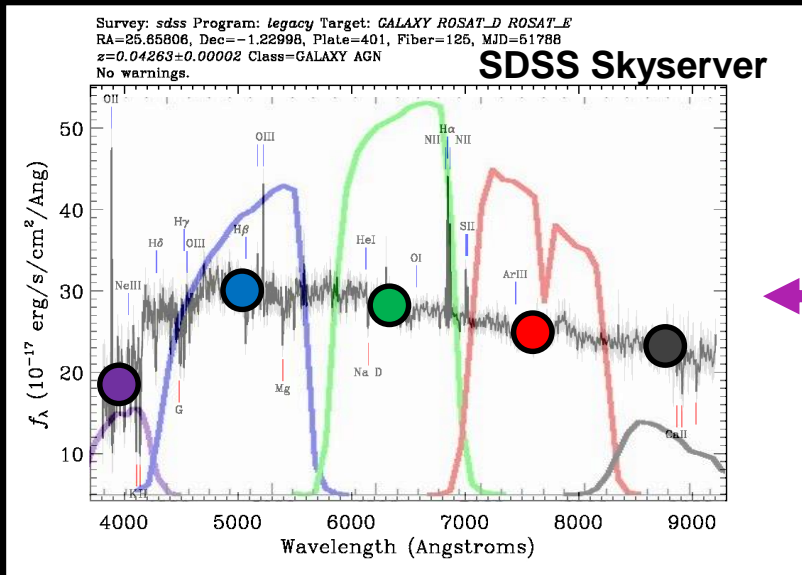


$$-2 \ln L_5 \sim \chi_5^2 + 5 \ln 2\pi + \ln |\hat{C}_g + \hat{C}_h|$$

# Implications

- How to deal with missing data?

$$P(g|h, \mathbf{b})$$

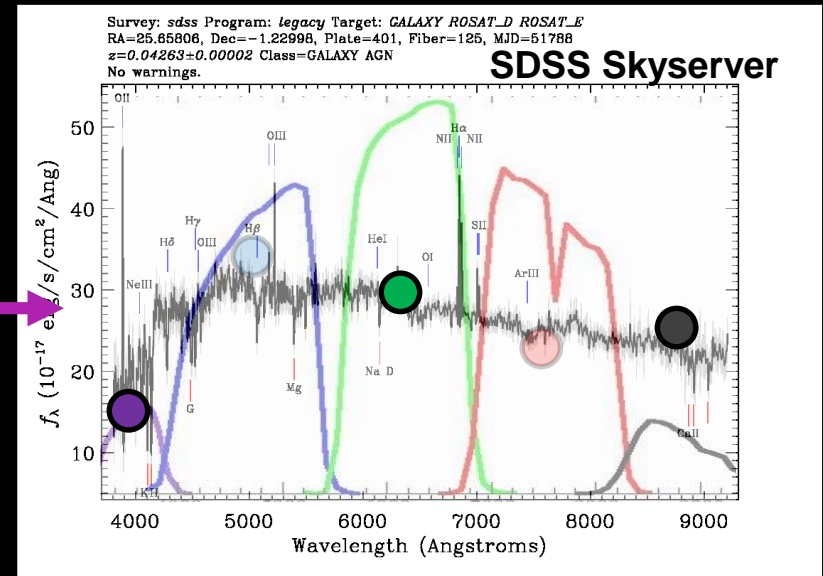
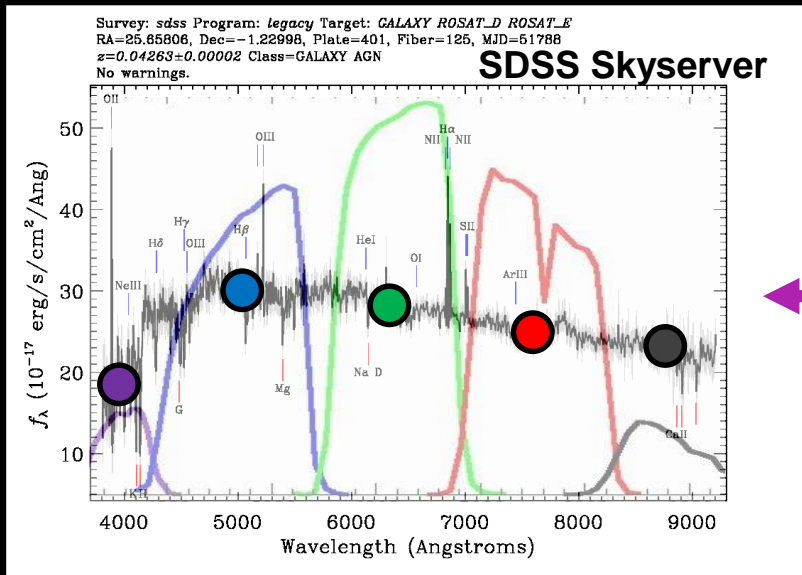


$$-2 \ln L_3 \sim \chi_3^2 + 3 \ln 2\pi + \ln |\hat{C}'_g + \hat{C}'_h|$$

# Solutions

- How to deal with missing data?

$$P(g|h, \mathbf{b})$$



$$-2 \ln L \sim X_n - X'_n, \quad X_n, X'_n \stackrel{\text{i.i.d.}}{\sim} \chi_n^2(\delta_n)$$



# Implementation

- How to deal with missing data?

$$P(g|h, \mathbf{b})$$

$$-2 \ln L = ???$$

some transformation of  
doubly-non-central F-  
distribution

# Implementation

- How to deal with missing data?

$$P(g|h, \mathbf{b})$$

ignore  
non-centrality

$$-2 \ln L = \chi_n^2 - N_b$$

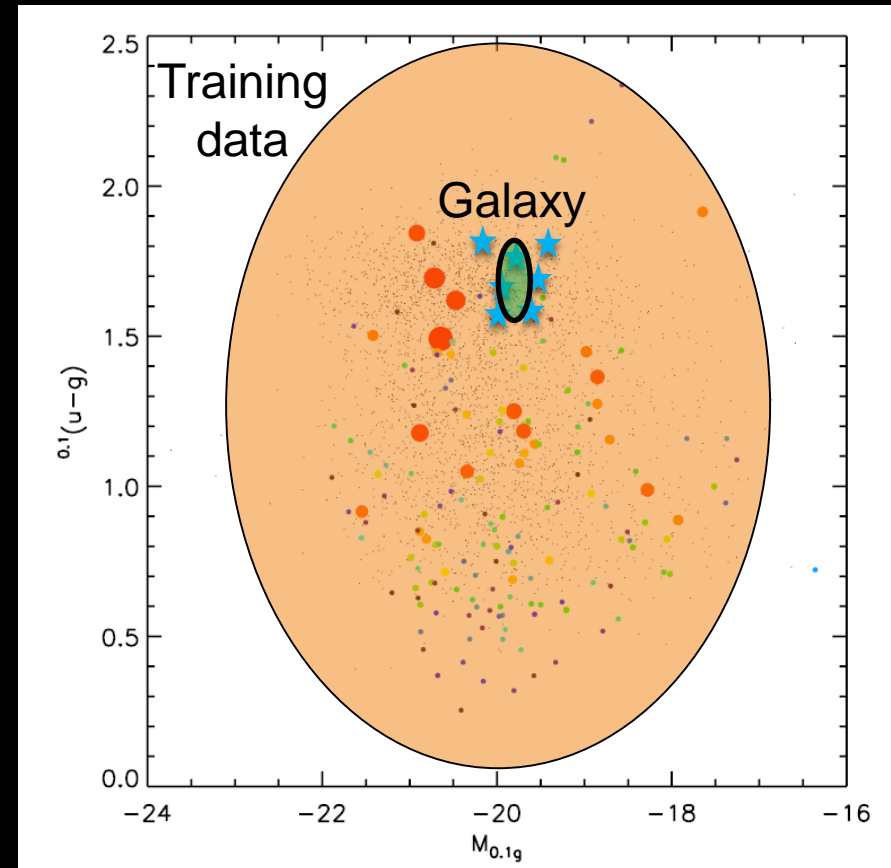
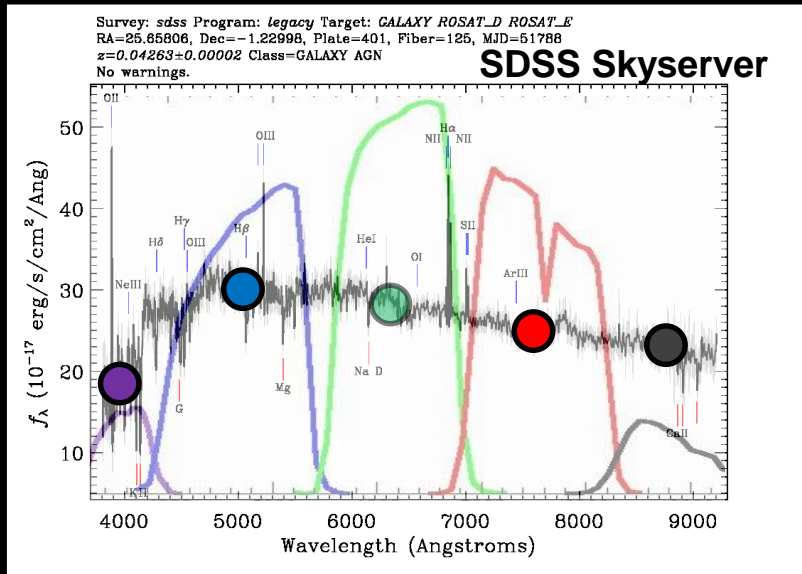
first-order  
correction

$$\chi^2 = \sum_i \frac{(\hat{F}_{g,i} - \hat{F}_{h,i})^2}{\hat{\sigma}_{g,i}^2 + \hat{\sigma}_{h,i}^2}$$

# Missing Data: Searching for Neighbors

- How to deal with missing data?

$$\hat{P}(g|h, b)$$



Cool et al. (2007)

# The “Big Data” Assumption

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# Selection Effects

- How to deal with selection effects?  $P(g|h)$

# Selection Effects

- How to deal with selection effects?  $P(\hat{F}_g | g)$

# Selection Effects

- How to deal with selection effects?  $P(\hat{F}_g | g, s_g = 1, \mathcal{S}_g)$   
Selection effect(s)  
Binary selection flag  
(1=in/0=out)



# Selection Effects

- How to deal with selection effects?  $P(\hat{F}_g | g, s_g = 1, \mathbf{S}_g)$ 

Selection effect(s) ↓

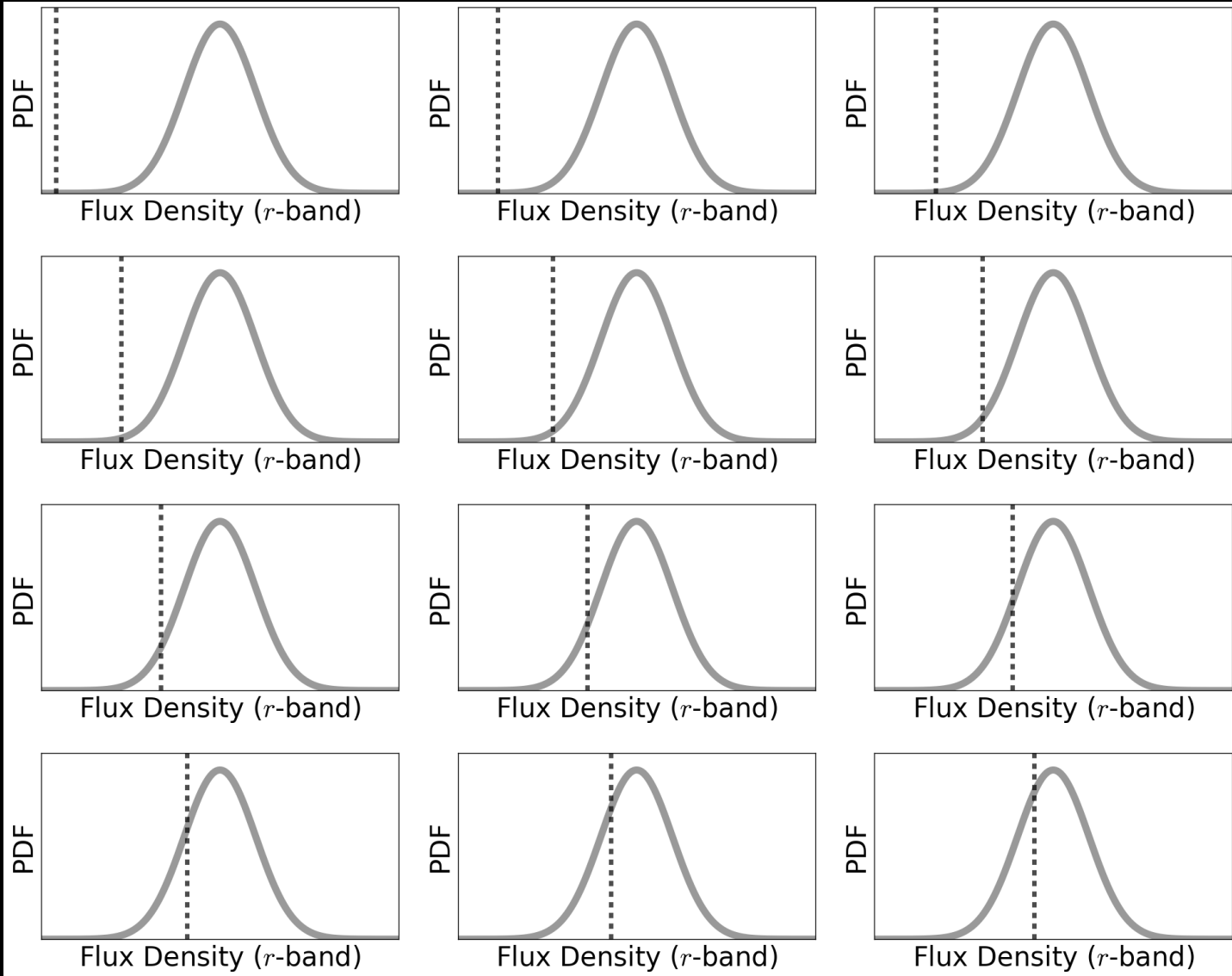
↑

Binary selection flag  
(1=in/0=out)

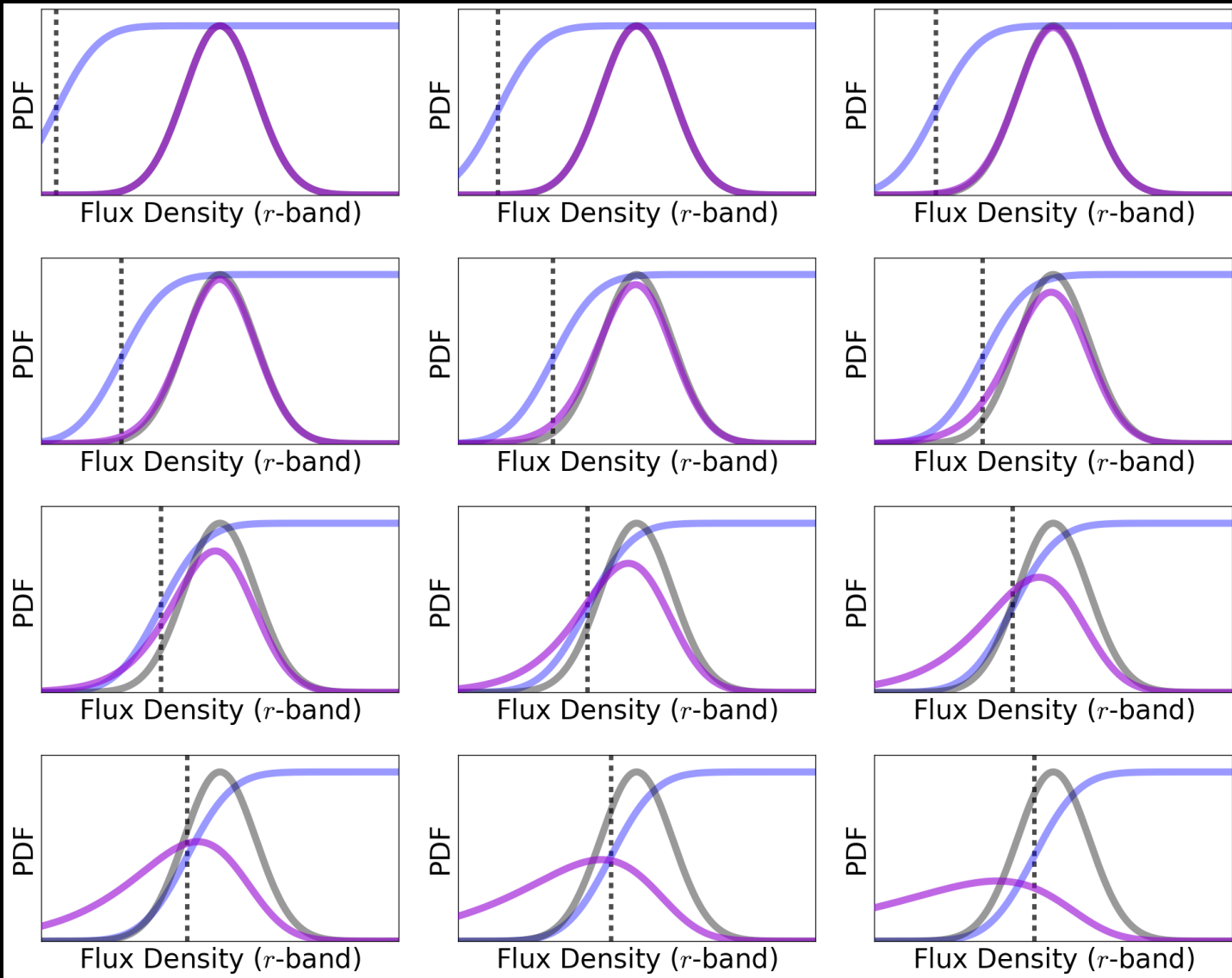
$$\frac{P(s_g = 1 | \hat{F}_g, \mathbf{S}_g) P(\hat{F}_g | g)}{P(s_g = 1 | g, \mathbf{S}_g)}$$

Marginalized  
Selection Probability

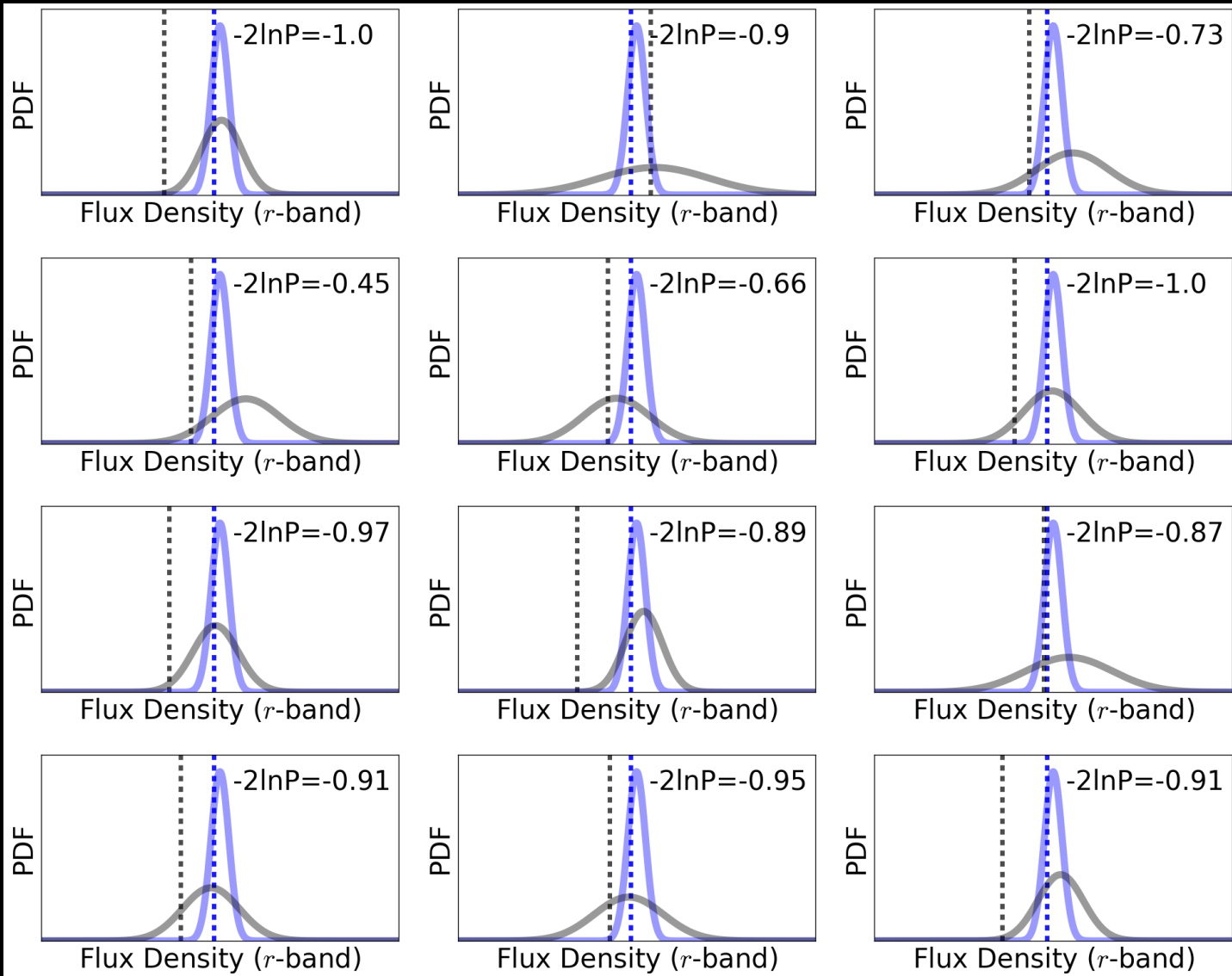
# Application: Signal-to-Noise Cut



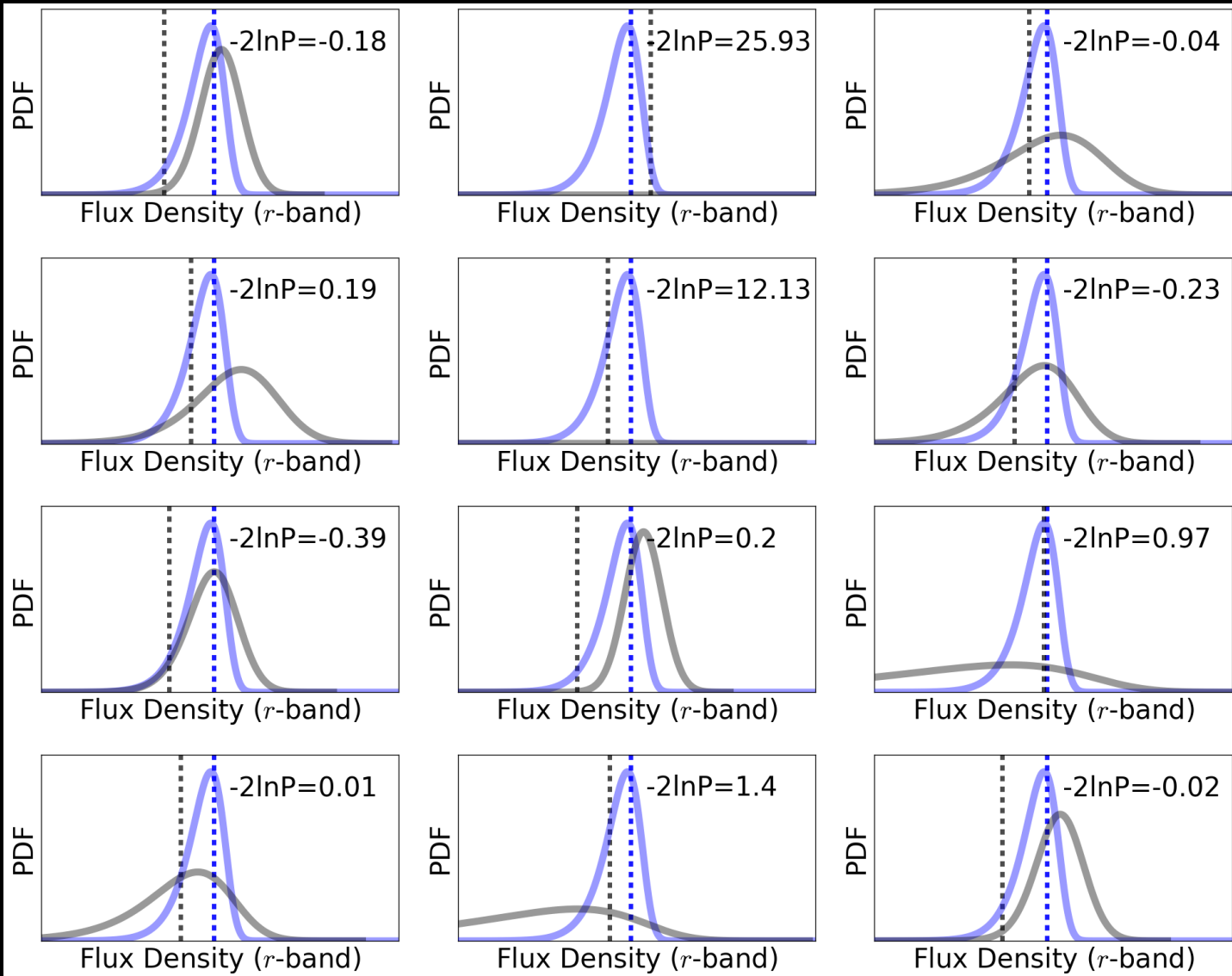
# Application: Signal-to-Noise Cut



# Application: Signal-to-Noise Cut



# Application: Signal-to-Noise Cut



# The “Big Data” Assumption

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# Mixing and Matching Galaxies

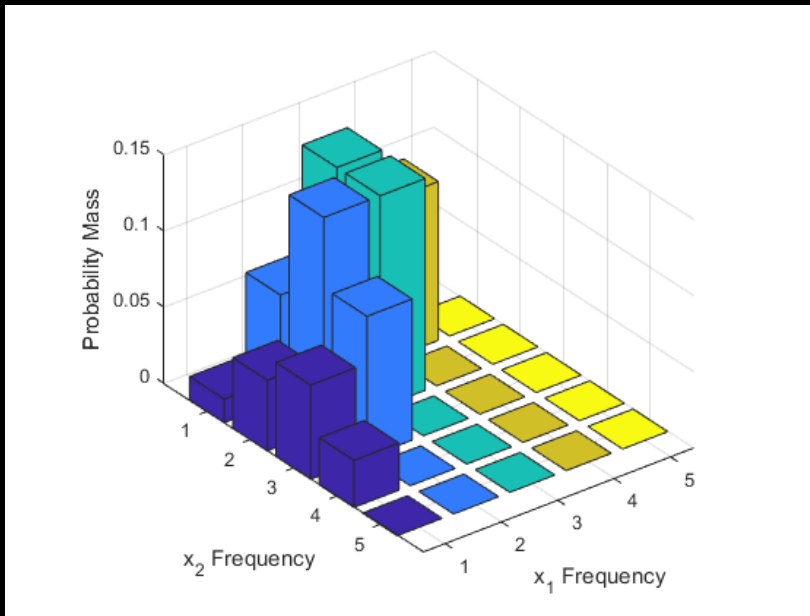
- How to deal with population mismatch?



# Mixing and Matching Galaxies

- How to deal with population mismatch?

$$\mathbf{p}'_g \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g)$$



Trinomial distribution from [Mathworks](#).

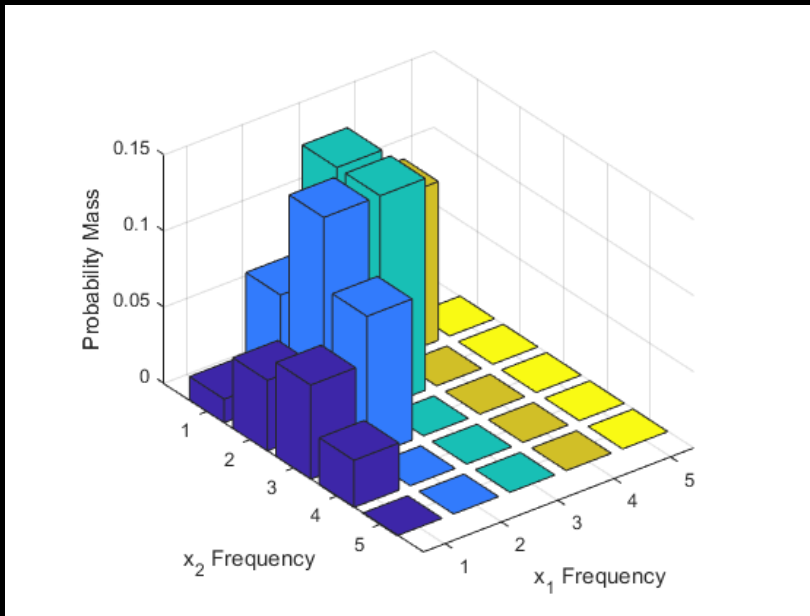
$N_h$  categories with  
probability vector

$$\mathbf{p}_g = \{P(h|g)\}$$

# Mixing and Matching Galaxies

- How to deal with population mismatch?

$$\mathbf{p}'_g \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g)$$



Trinomial distribution from [Mathworks](#).

$N_h$  categories with probability vector

$$\mathbf{p}_g = \{P(h|g)\}$$

$$\mathbf{h} = \{0,1,2\}$$

$$\mathbf{p}'_g = \{0,0,1\} \rightarrow h'_g = 2$$

# Mixing and Matching Galaxies

- How to deal with population mismatch?

$$\mathbf{p}'_g \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g)$$

$$P(\mathbf{h}) \stackrel{?}{=} \mathbf{n} \sim \sum_{g \in \mathcal{g}} \mathbf{p}'_g$$

# Mixing and Matching Galaxies

- How to deal with population mismatch?

$$\mathbf{p}'_g \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g)$$

$$\mathbf{n} \sim \sum_{g \in \mathcal{g}} \mathbf{p}'_g$$

$$\mathbf{P}(\mathbf{h}) \sim \text{Dir}(\mathbf{w} | \boldsymbol{\alpha} = \mathbf{n} + \mathbf{1})$$

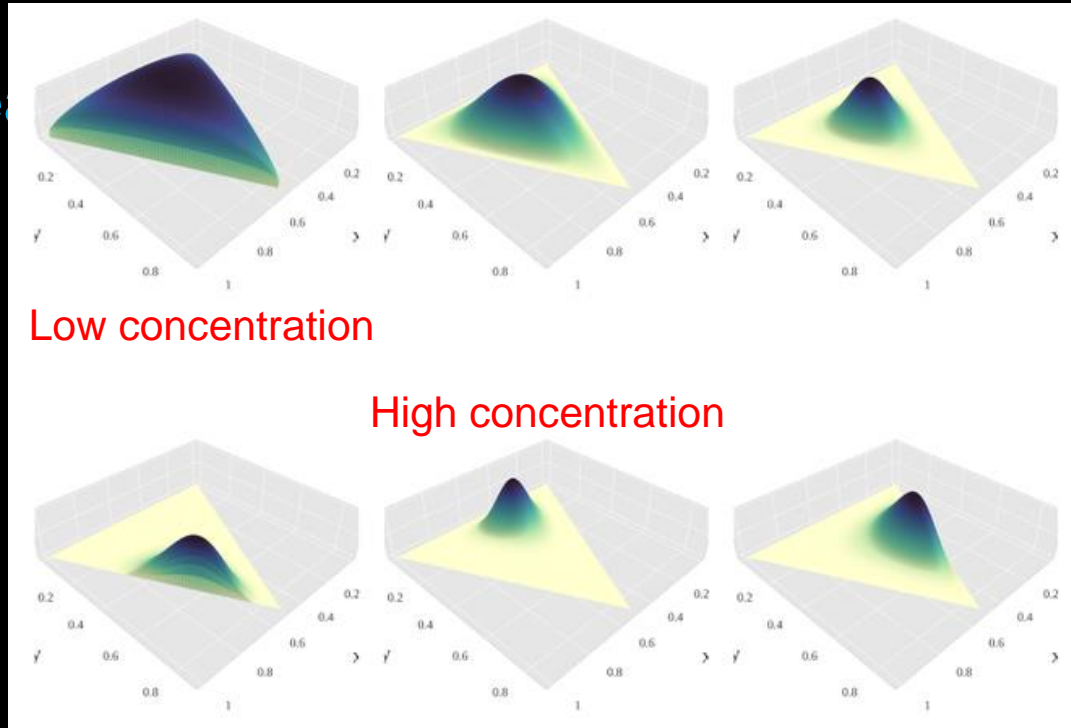
Concentration

Population weights                      Counts

# Mixing and Matching Galaxies

Courtesy of [Wikipedia](#).

- How to de



Low concentration

High concentration

Concentration

$$P(\mathbf{h}) \sim \text{Dir}(\mathbf{w} | \boldsymbol{\alpha} = \mathbf{n} + 1)$$

Population  
weights

Counts

Based on Leistedt, Peiris, & Mortlock (2016)

# Hierarchical Modeling

- How to deal with population mismatch?  $P(\mathbf{w}, \{\mathbf{p}_g\} | \mathbf{D}, \mathbf{S})$
- 
- The diagram illustrates the relationship between population weights and hierarchical posteriors in a hierarchical model. The equation  $P(\mathbf{w}, \{\mathbf{p}_g\} | \mathbf{D}, \mathbf{S})$  is shown. A green arrow points from the text "Population weights (training set)" to the  $\mathbf{w}$  parameter. A blue arrow points from the text "Hierarchical posteriors" to the  $\{\mathbf{p}_g\}$  parameter.

# Hierarchical Modeling

- How to deal with population mismatch?

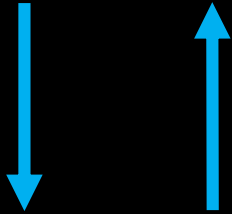
$$P(\mathbf{w}, \{\mathbf{p}_g\} | \mathbf{D}, \mathbf{S})$$

Hierarchical posteriors

Population weights  
(training set)

Gibbs sampling

$$P(\{\mathbf{p}_g\} | \mathbf{w}, \mathbf{S})$$



$$P(\mathbf{w} | \{\mathbf{p}_g\}, \mathbf{S})$$

# Hierarchical Modeling

Hierarchical posteriors

- How to deal with population mismatch?  $P(\mathbf{w}, \{\mathbf{p}_g\} | \mathbf{D}, \mathbf{S})$

Population weights  
(training set)

Gibbs sampling

$$P(\{\mathbf{p}_g\} | \mathbf{w}, \mathbf{S}) \quad 1. \text{ Sample hierarchical posteriors:}$$
$$\mathbf{p}_g^{(i)} \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g \mathbf{w}^{(i-1)})$$

$$P(\mathbf{w} | \{\mathbf{p}_g\}, \mathbf{S})$$



# Hierarchical Modeling

Hierarchical posteriors

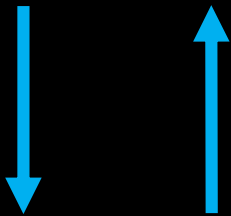
- How to deal with population mismatch?

$$P(\mathbf{w}, \{\mathbf{p}_g\} | \mathbf{D}, \mathbf{S})$$

Population weights  
(training set)

Gibbs sampling

$$P(\{\mathbf{p}_g\} | \mathbf{w}, \mathbf{S})$$



$$P(\mathbf{w} | \{\mathbf{p}_g\}, \mathbf{S})$$

1. Sample hierarchical posteriors:

$$\mathbf{p}_g^{(i)} \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g \mathbf{w}^{(i-1)})$$

2. Compute counts:  $\mathbf{n}^{(i)} \sim \sum_{g \in \mathcal{G}} \mathbf{p}_g^{(i)}$

# Hierarchical Modeling

Hierarchical posteriors

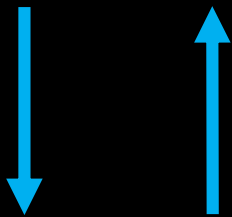
- How to deal with population mismatch?

$$P(\mathbf{w}, \{\mathbf{p}_g\} | \mathbf{D}, \mathbf{S})$$

Population weights  
(training set)

Gibbs sampling

$$P(\{\mathbf{p}_g\} | \mathbf{w}, \mathbf{S})$$



$$P(\mathbf{w} | \{\mathbf{p}_g\}, \mathbf{S})$$

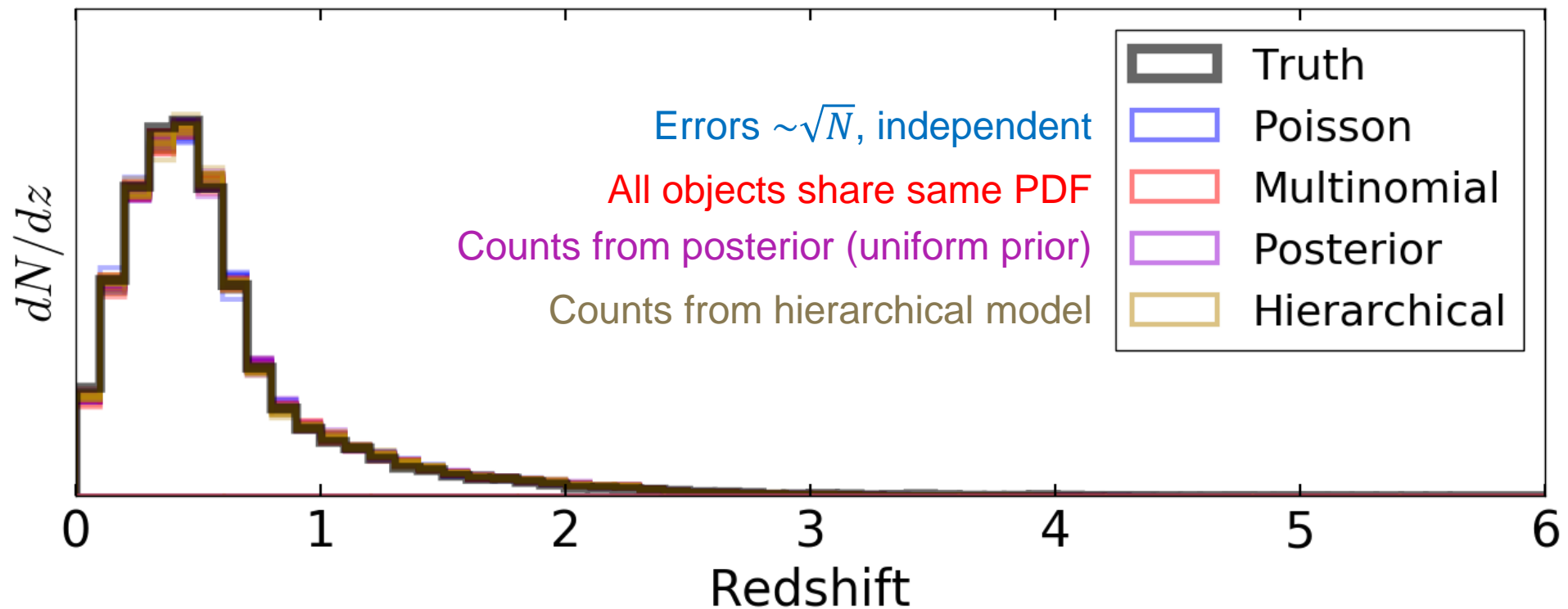
1. Sample hierarchical posteriors:

$$\mathbf{p}_g^{(i)} \sim \text{Mult}(n = 1, \mathbf{p} = \mathbf{p}_g \mathbf{w}^{(i-1)})$$

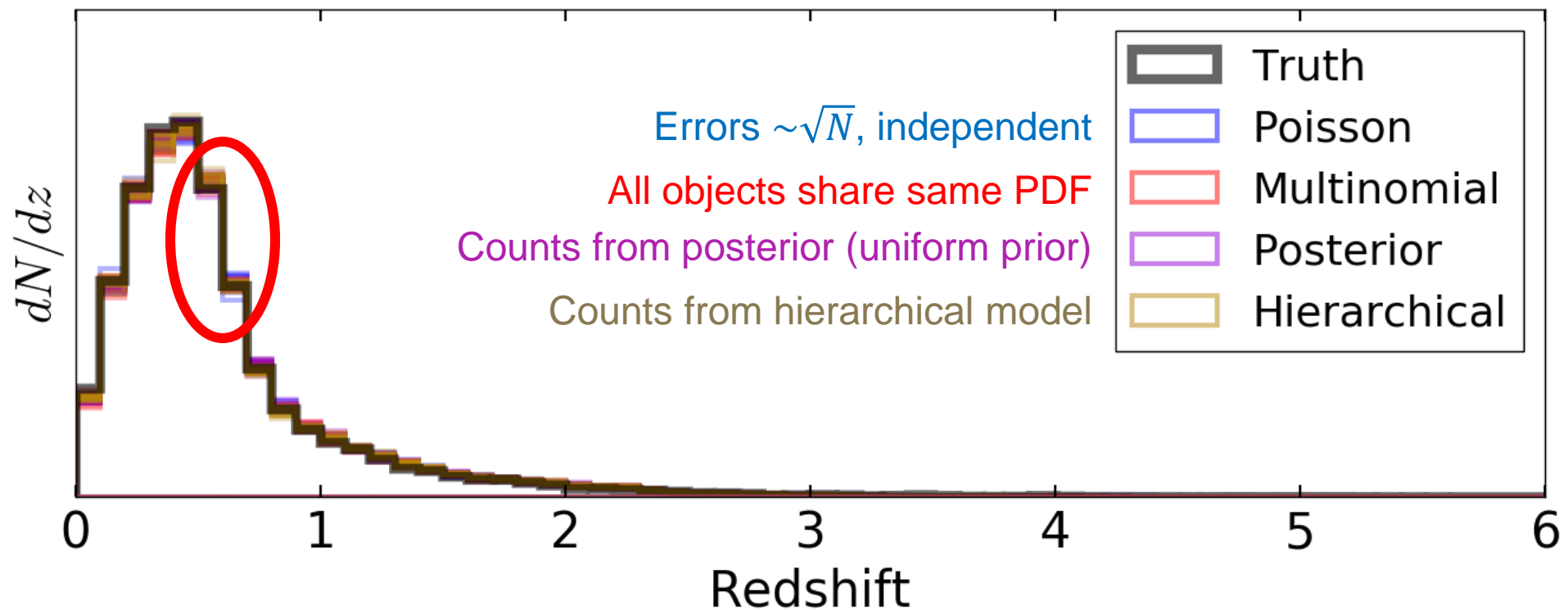
2. Compute counts:  $\mathbf{n}^{(i)} \sim \sum_{g \in \mathcal{G}} \mathbf{p}_g^{(i)}$

3. Sample weights:  $\mathbf{w}^{(i)} \sim \text{Dir}(\mathbf{w} | \mathbf{n}^{(i)} + 1)$

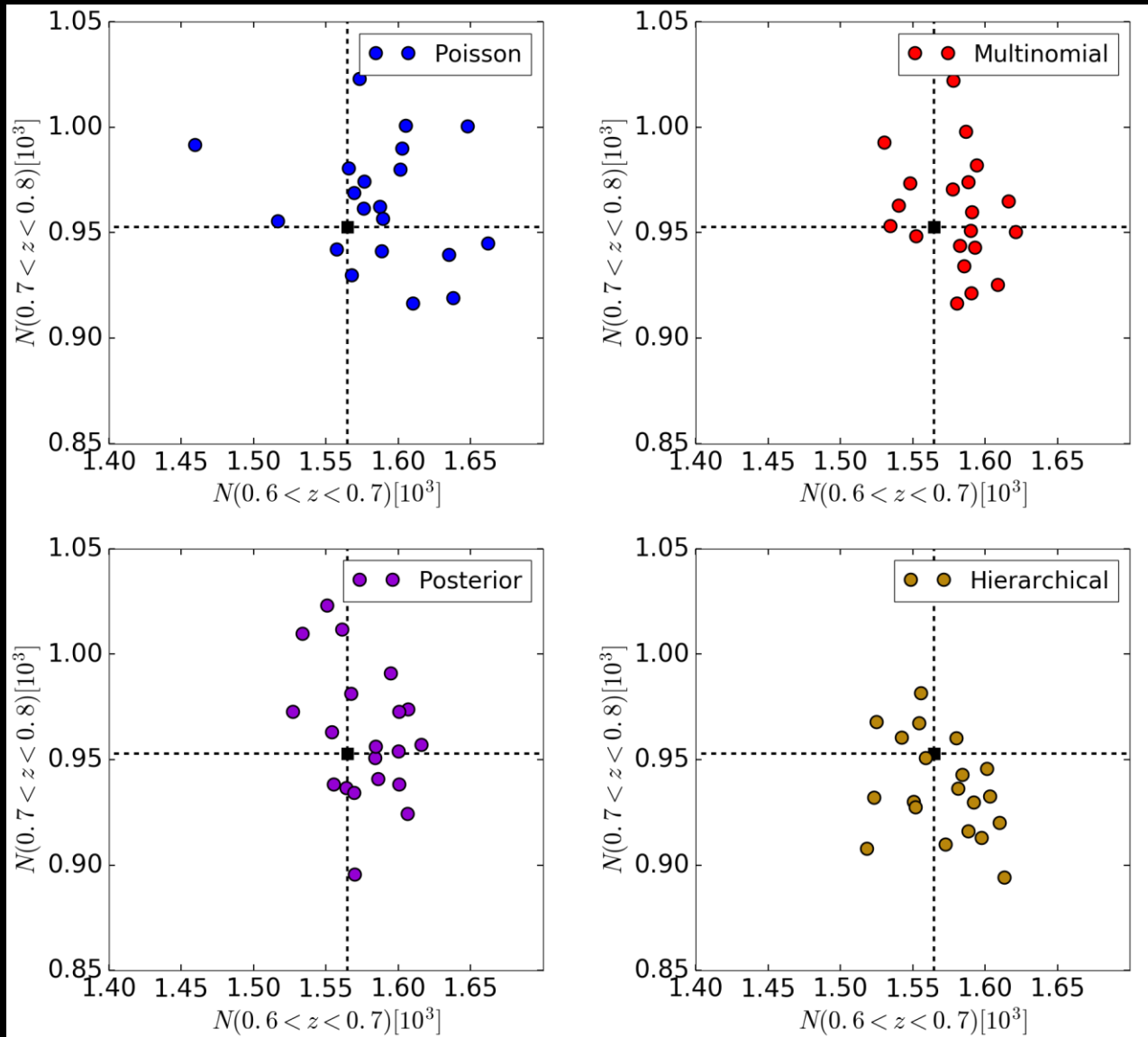
# Application to Mock Data



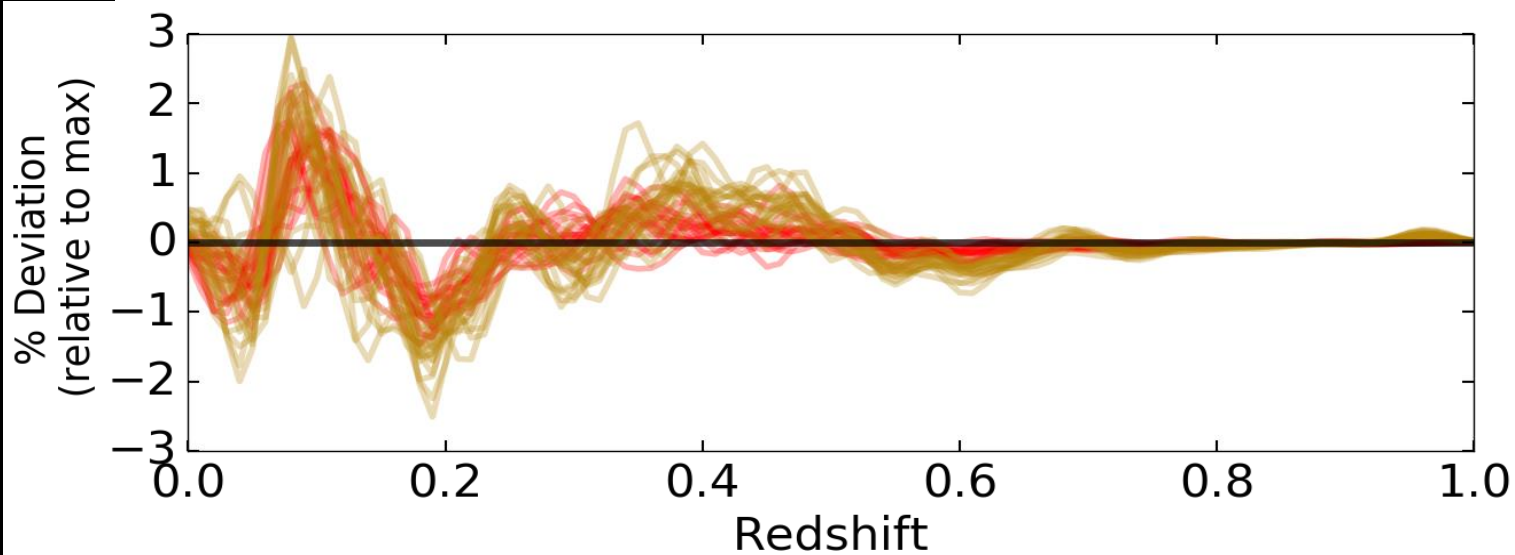
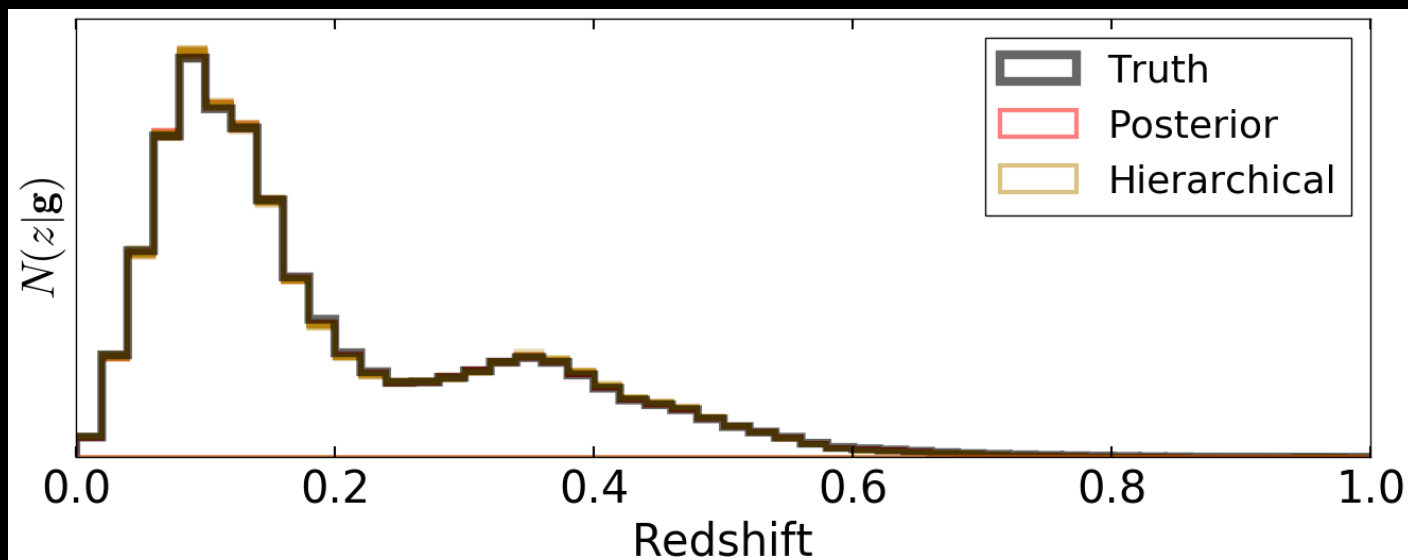
# Application to Mock Data



# Application to Mock Data



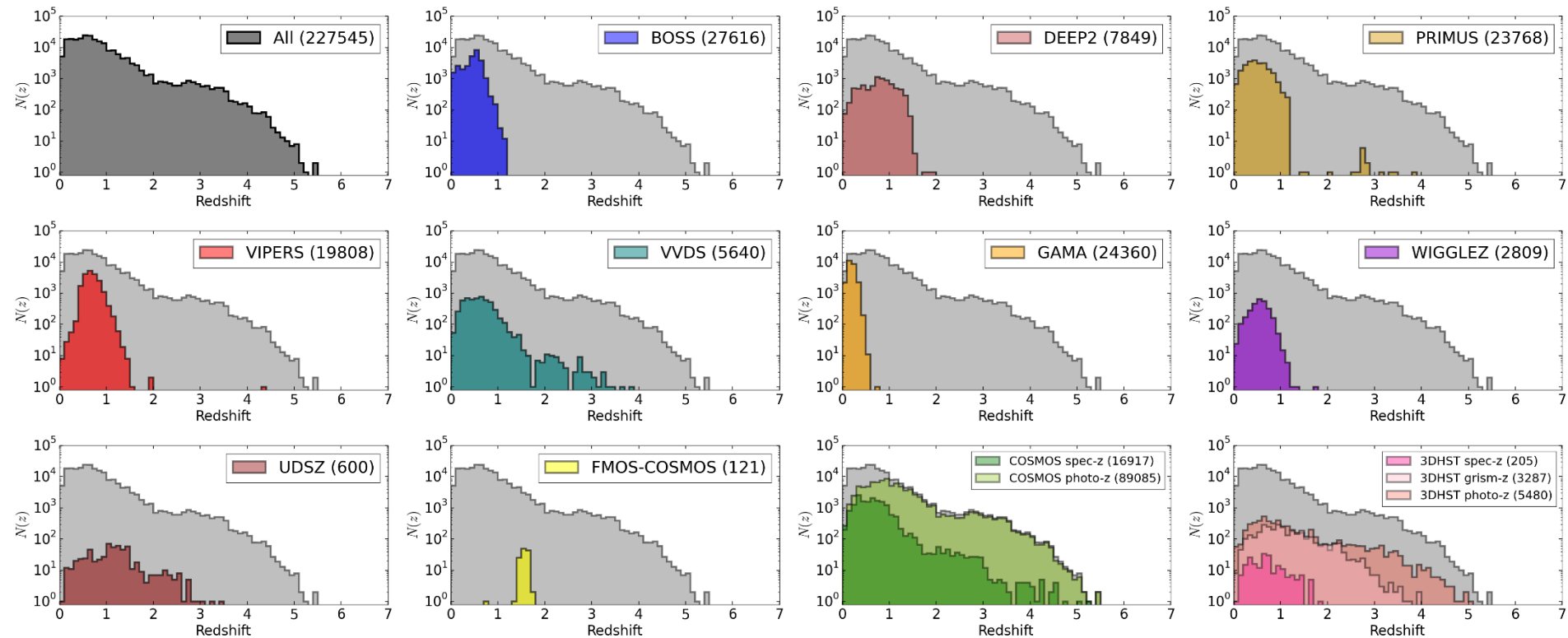
# Tests on ~100k SDSS Galaxies



# Next Steps

# Robustness of Training Data/Priors

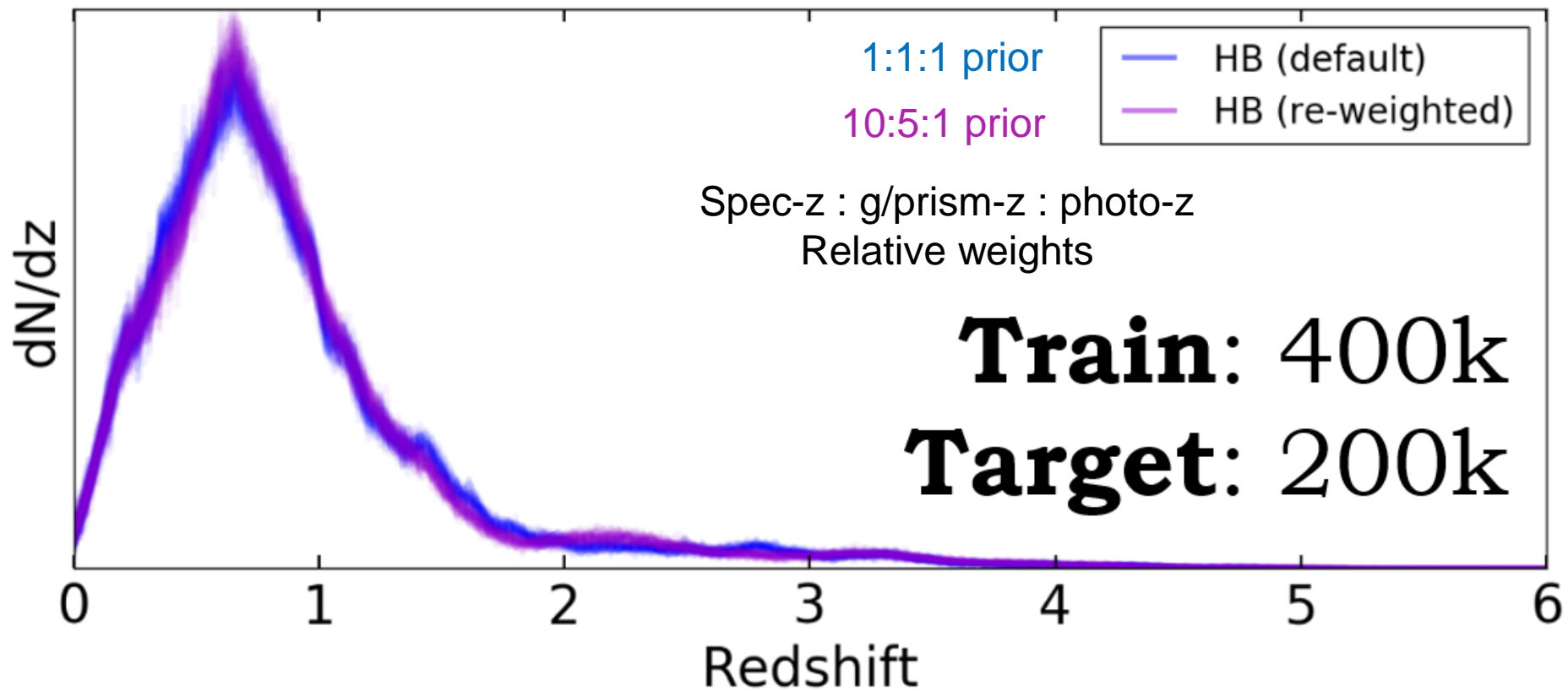
- Hyper Suprime-Cam (HSC) SSP has ~380k objects taken from 11 surveys.
- Wide variety of selection criteria, data quality/reliability.



Note: old plot from early internal data release.



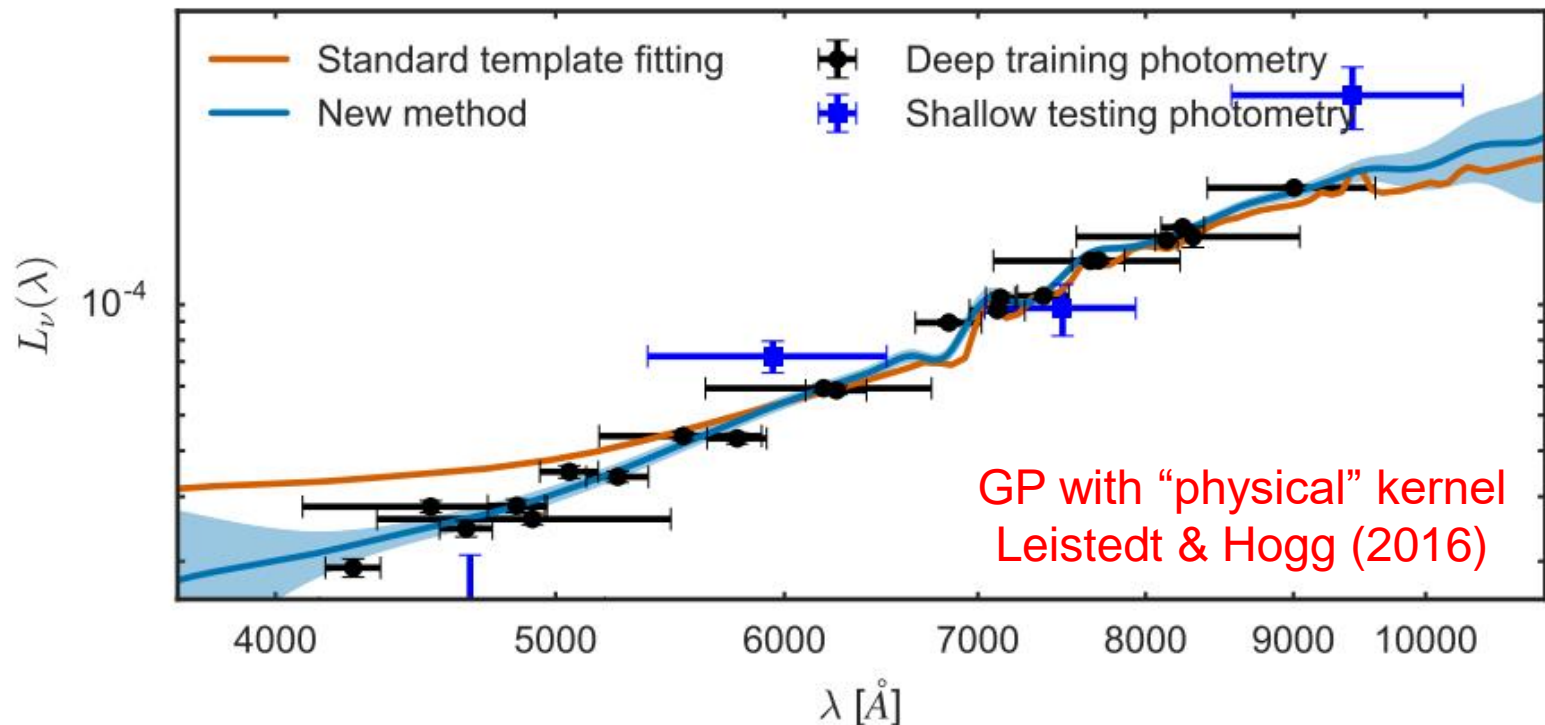
# Robustness of Training Data/Priors



**Preliminary**

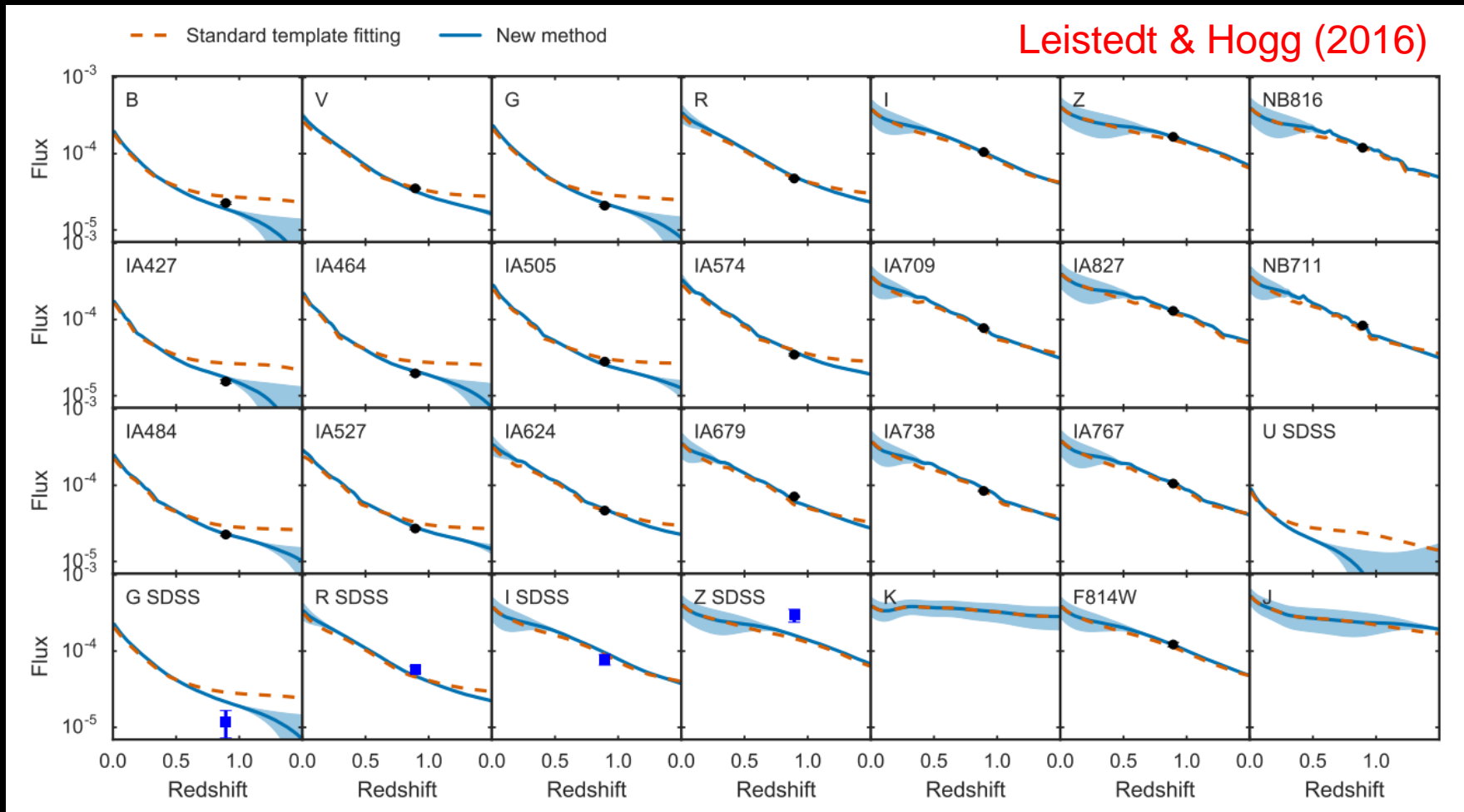
# Incorporating “Physical” Priors

- Moving a galaxy from one redshift to another is a smooth, physical process that is well-understood.
- Want to incorporate this into our priors/predictions.



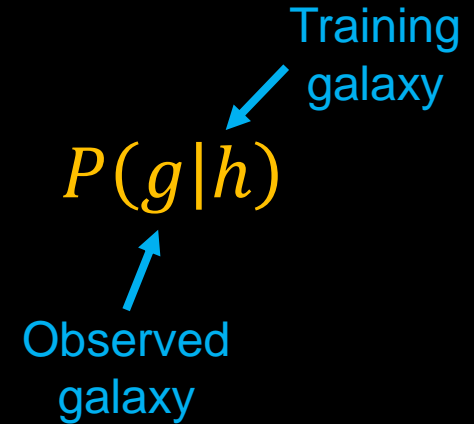
# Incorporating “Physical” Priors

- Can use to augment training data.
- Straightforward to “impute” missing values.



# Likelihood / Distance Metric

- What metric(s) to use?
- More sophisticated machine learning methods could be used to compute posterior samples (or possibly likelihoods) over complex domains.



NGC 4414



NGC 5457

# Summary

- Photometric redshifts (photo-z's) are an integral part of modern “big data” extragalactic science.
- Large training datasets gives new opportunities to develop Bayesian, data-driven photo-z's.
- Taking advantage of these datasets requires dealing with real-world problems (e.g., biased training data) using a variety of statistical methods (e.g., hierarchical Bayes).
- Early results look promising!

# Code is available!

Although still under active development, code, tutorials, and rough draft of a paper are online at:

[github.com/joshspeagle/frankenz](https://github.com/joshspeagle/frankenz)