Likelihood-free Inference of Chemical Homogeneity in Open Clusters using Functional Principal Components

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Messier 67
Credit: SDSS, DR14

HOW CHEMICALLY HOMOGENEOUS ARE STAR CLUSTERS?

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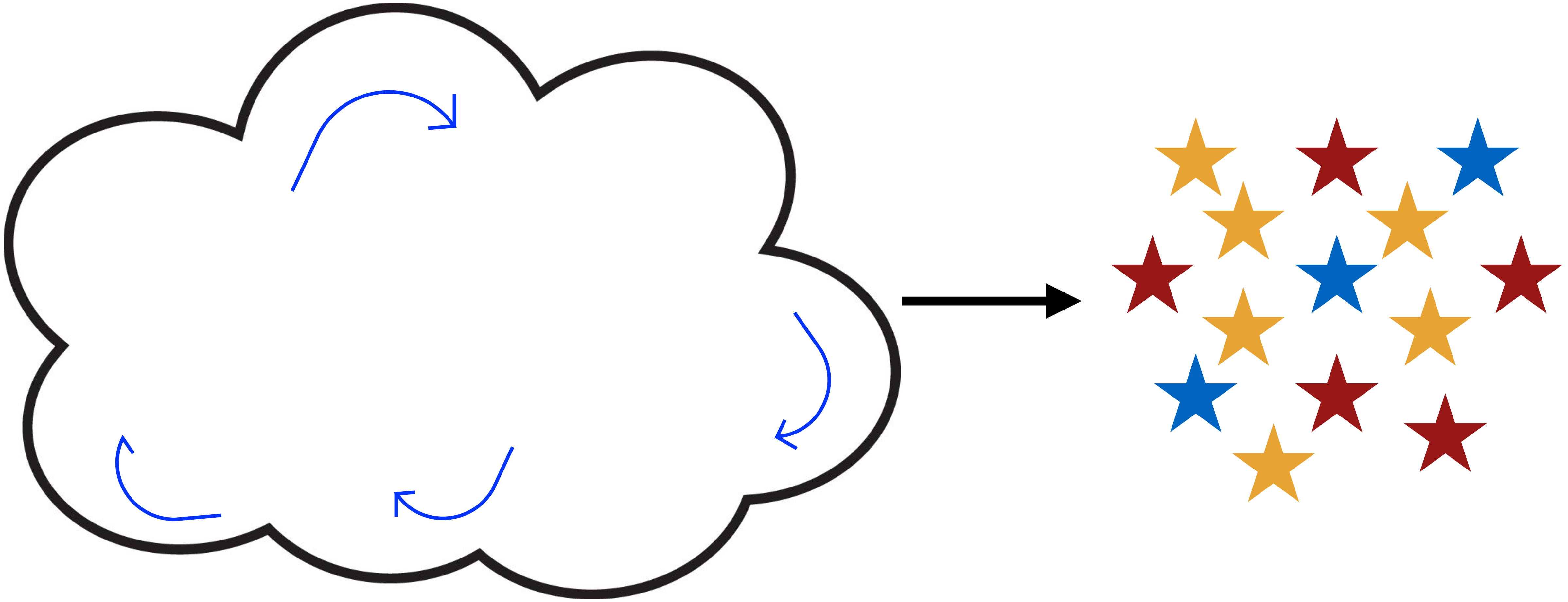
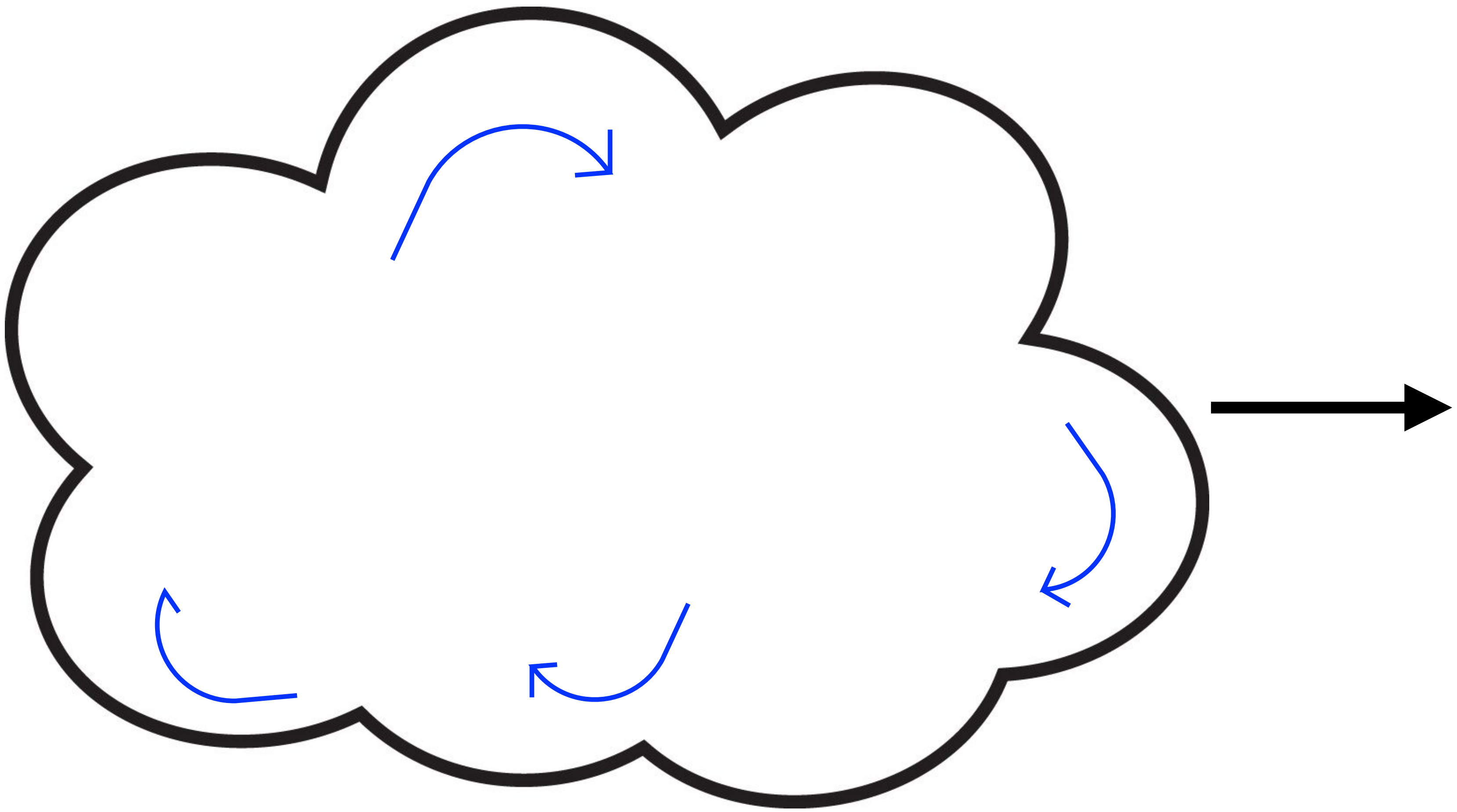
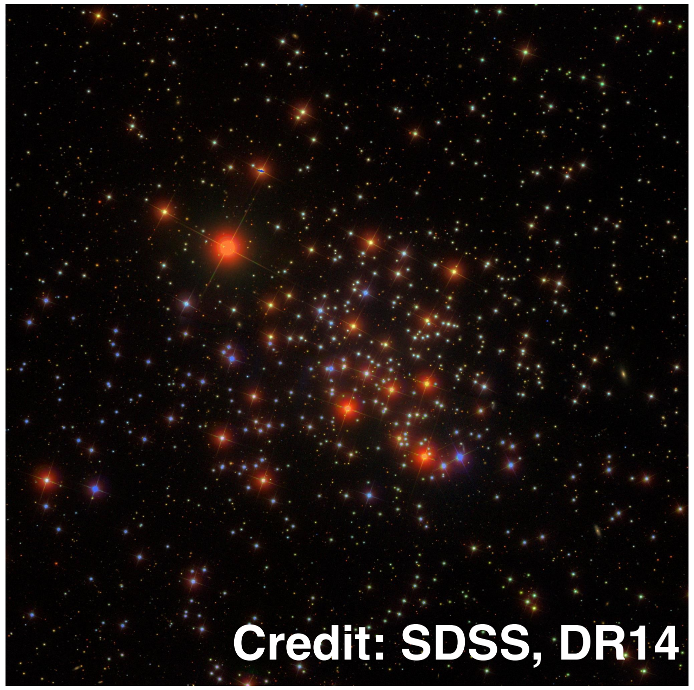


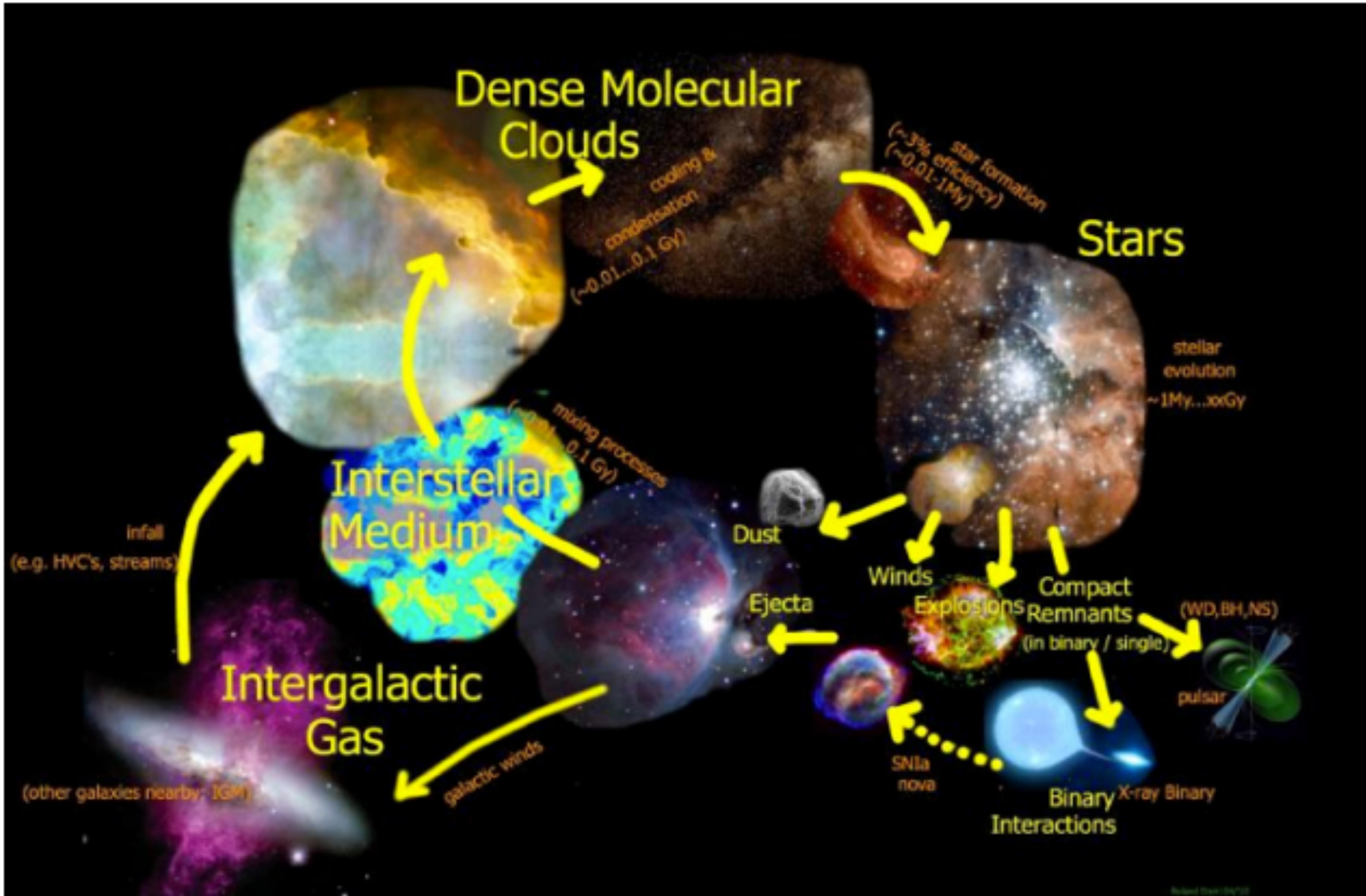
HOW CHEMICALLY HOMOGENEOUS ARE STAR CLUSTERS?

Stars form in groups in molecular clouds.
Stars in a cluster are expected to share the same initial chemical abundances.



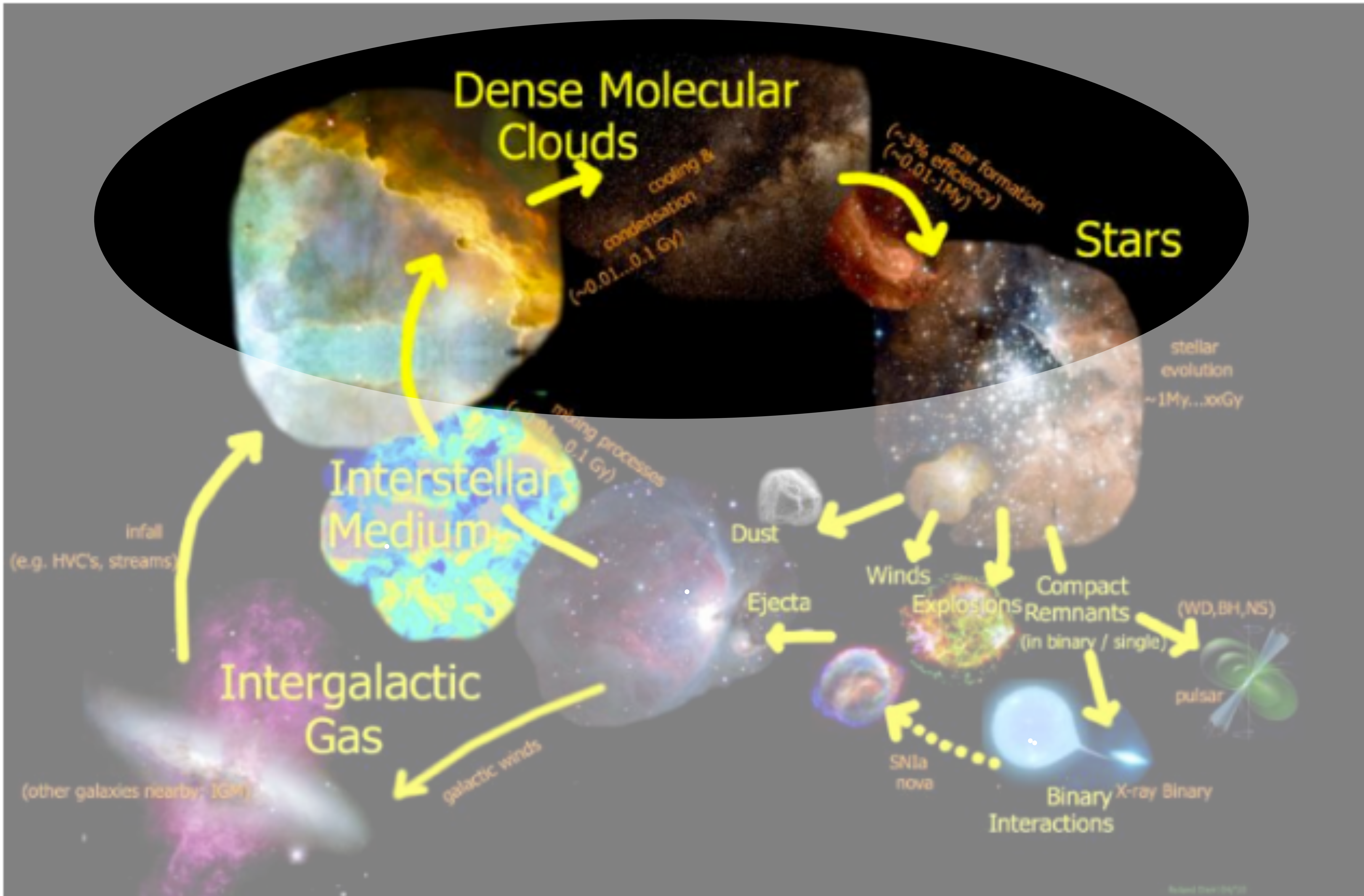


EVOLUTION OF STAR FORMING CLOUDS



Credit: Roland Diehl (MPE, Germany)

EVOLUTION OF STAR FORMING CLOUDS

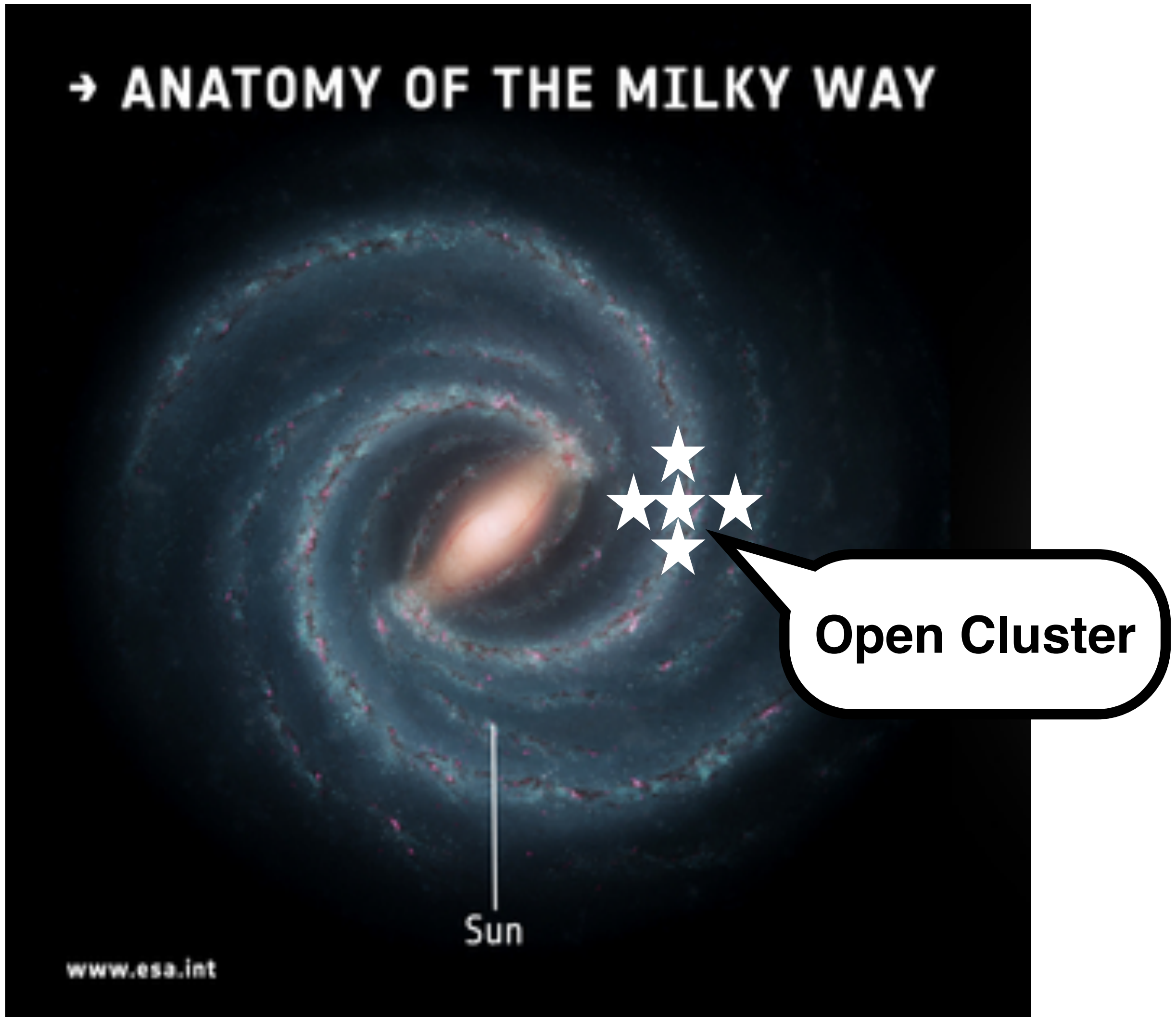


Credit: Roland Diehl (MPE, Germany)

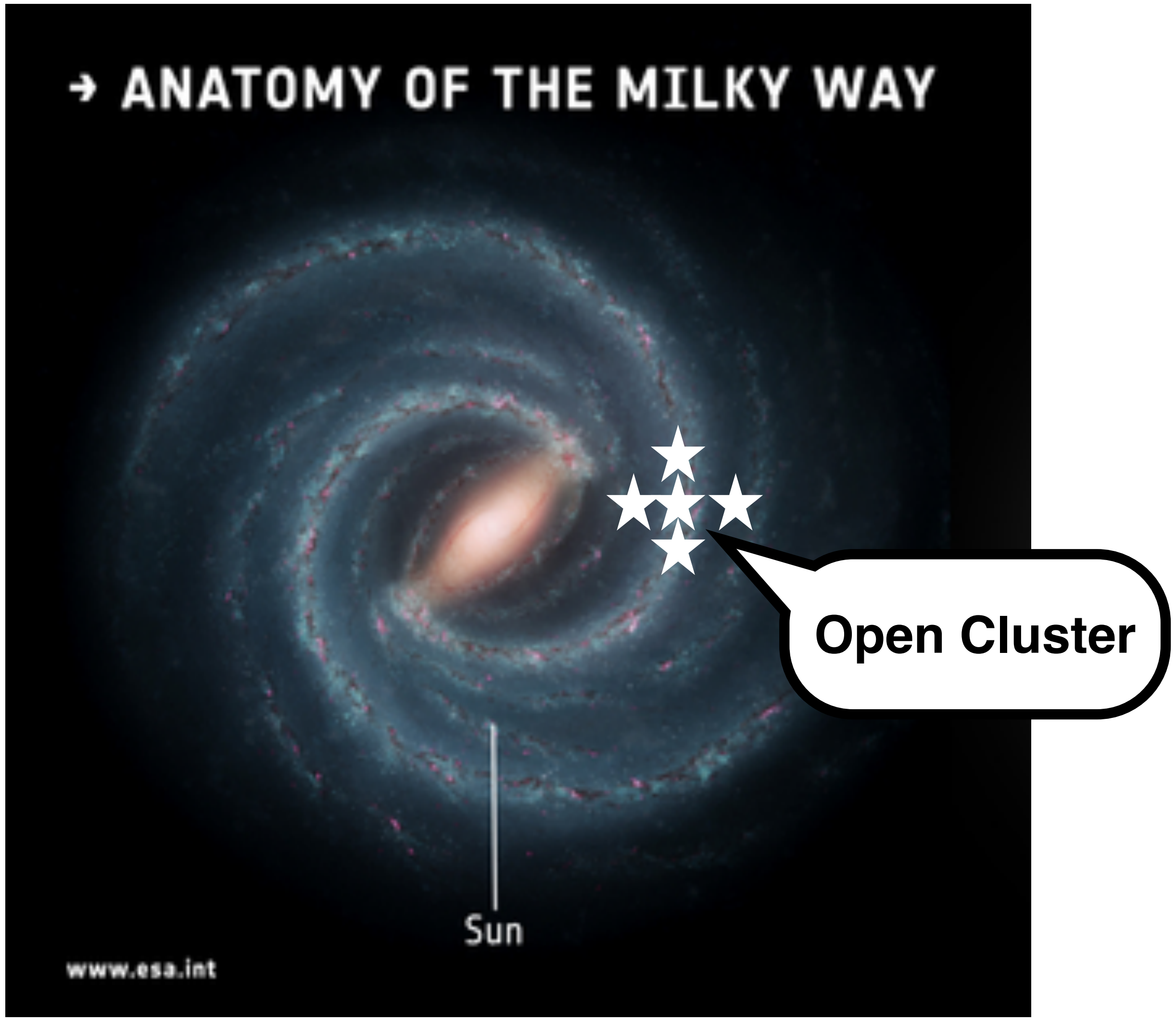
CHEMICAL TAGGING

Reverse trace stars to their birth location using chemical signatures

CHEMICAL TAGGING



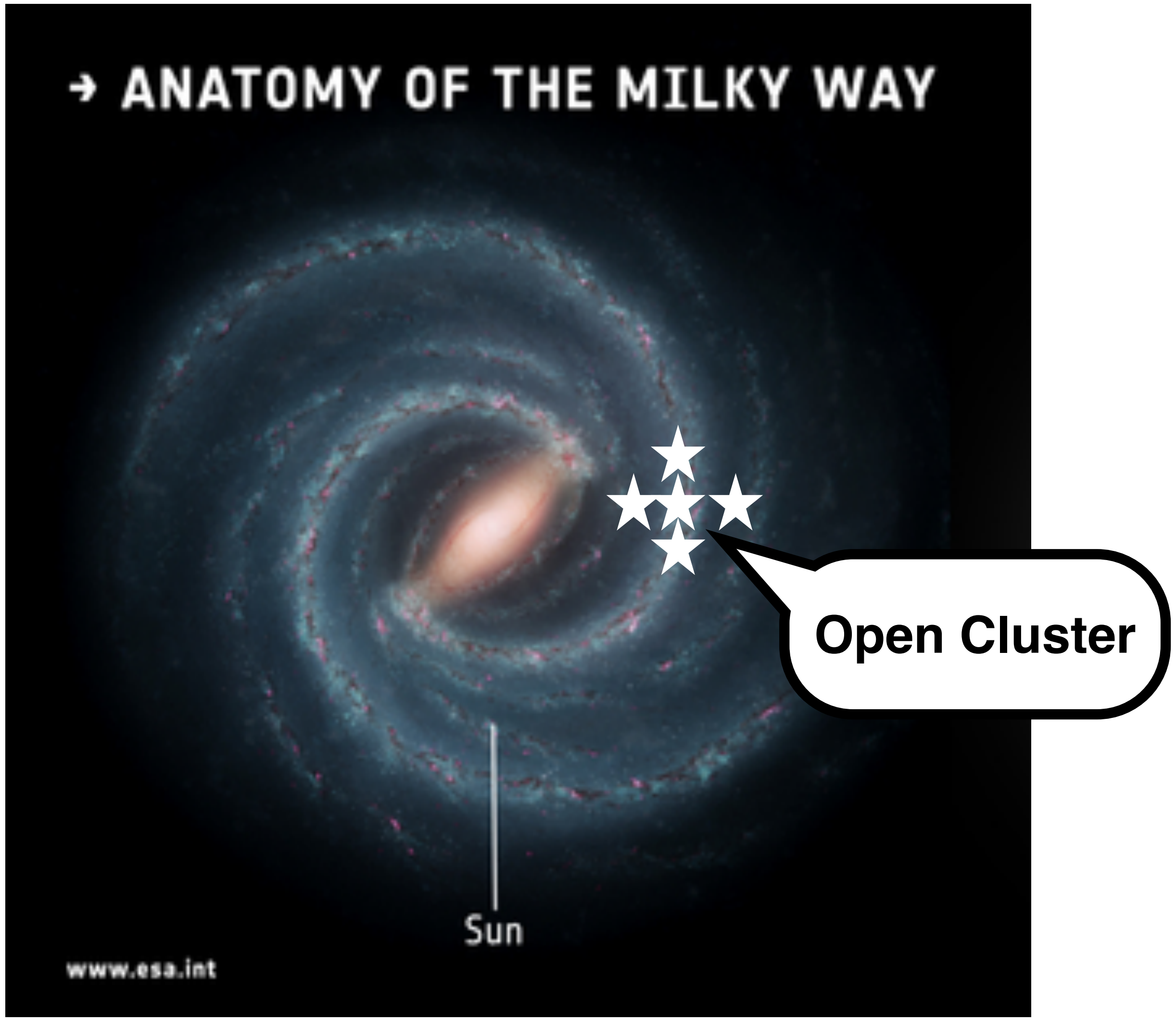
CHEMICAL TAGGING



What is the level of initial abundance spread in star clusters?

Observational uncertainties	Effects of stellar evolution
~0.1 dex (APOGEE Stellar Abundances)	Atomic Diffusion *(Souto et al 2019)*

CHEMICAL TAGGING



What is the level of initial abundance spread in star clusters?

<u>Observational uncertainties</u>

~0.1 dex
(APOGEE Stellar Abundances)

<u>Effects of stellar evolution</u>

Atomic Diffusion
(Souto et al 2019)

Determine chemistry for a large sample of stars to tag individual star-formation events

Statistical Methodology

Constrain abundance of a star

$$p\left(\theta \mid D\right)$$

stellar model (θ)

noisy spectrum (D)

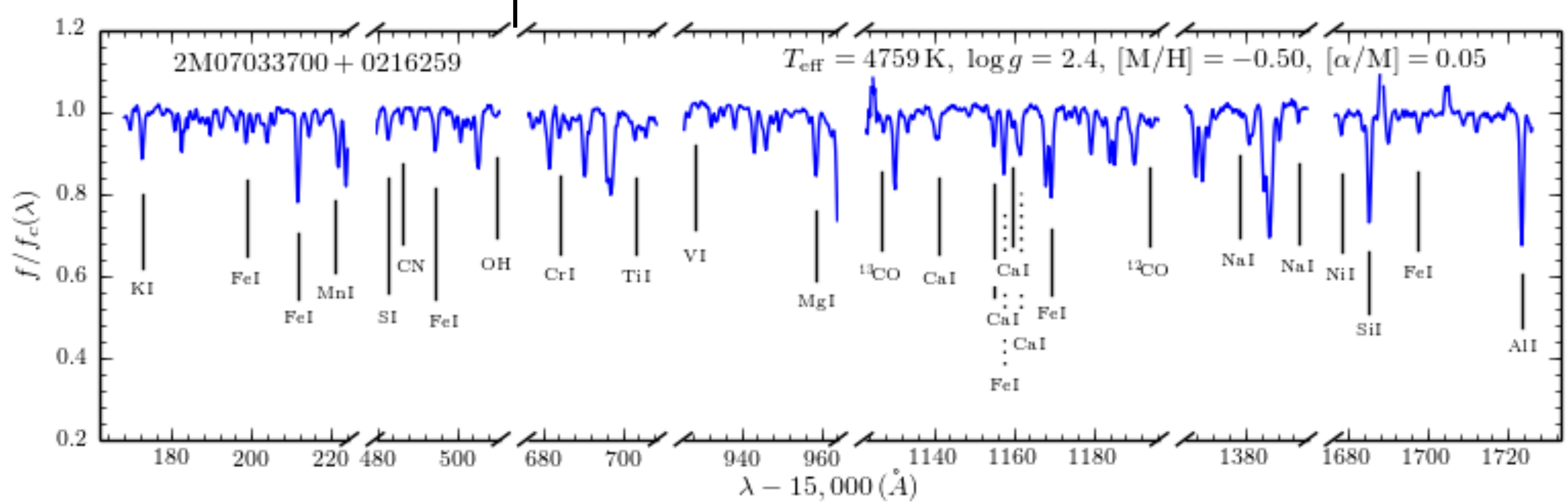
Statistical Methodology

Constrain abundance of a star

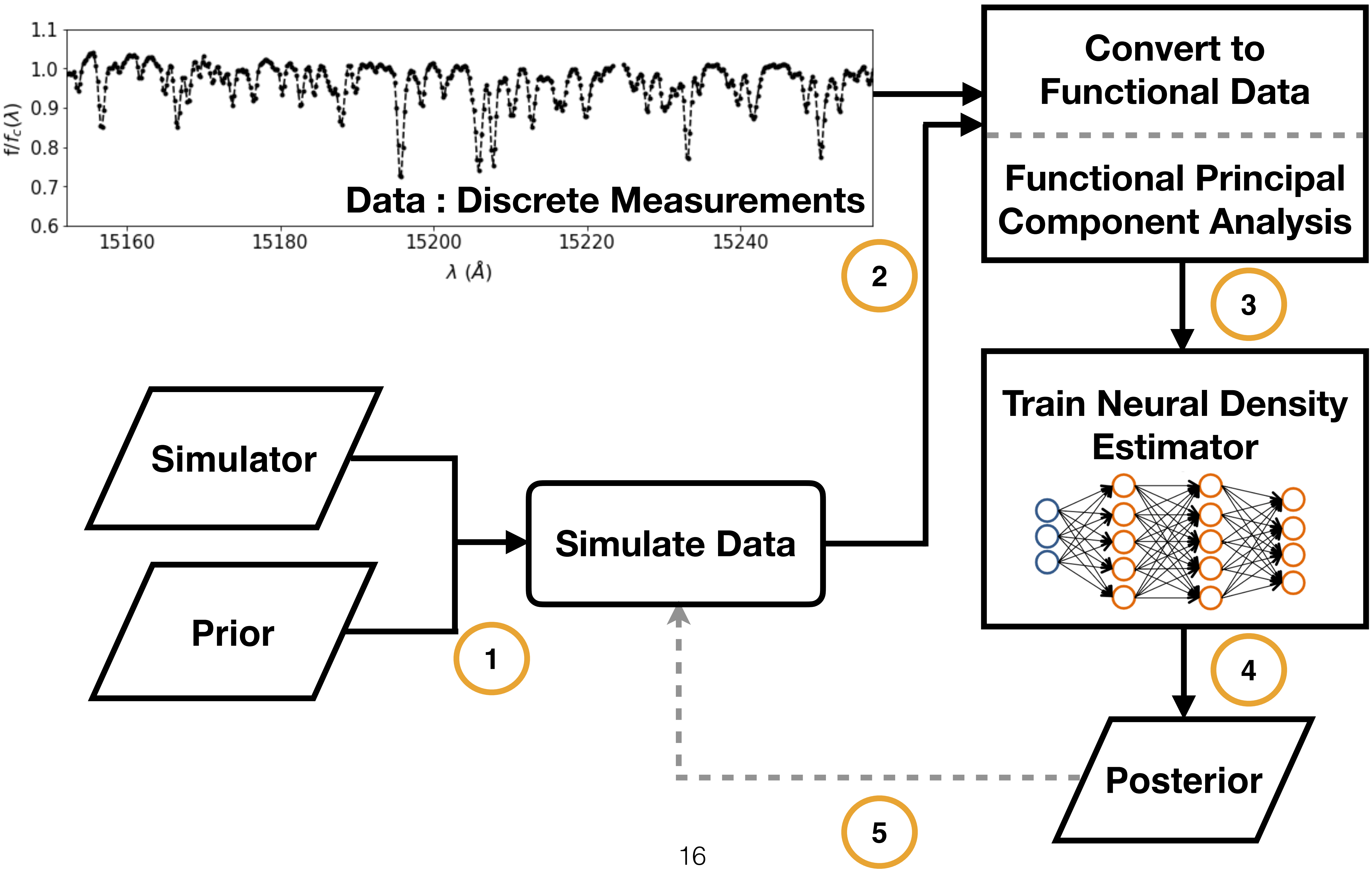
$$p\,(\theta \mid D)$$

each star in cluster → abundance scatter

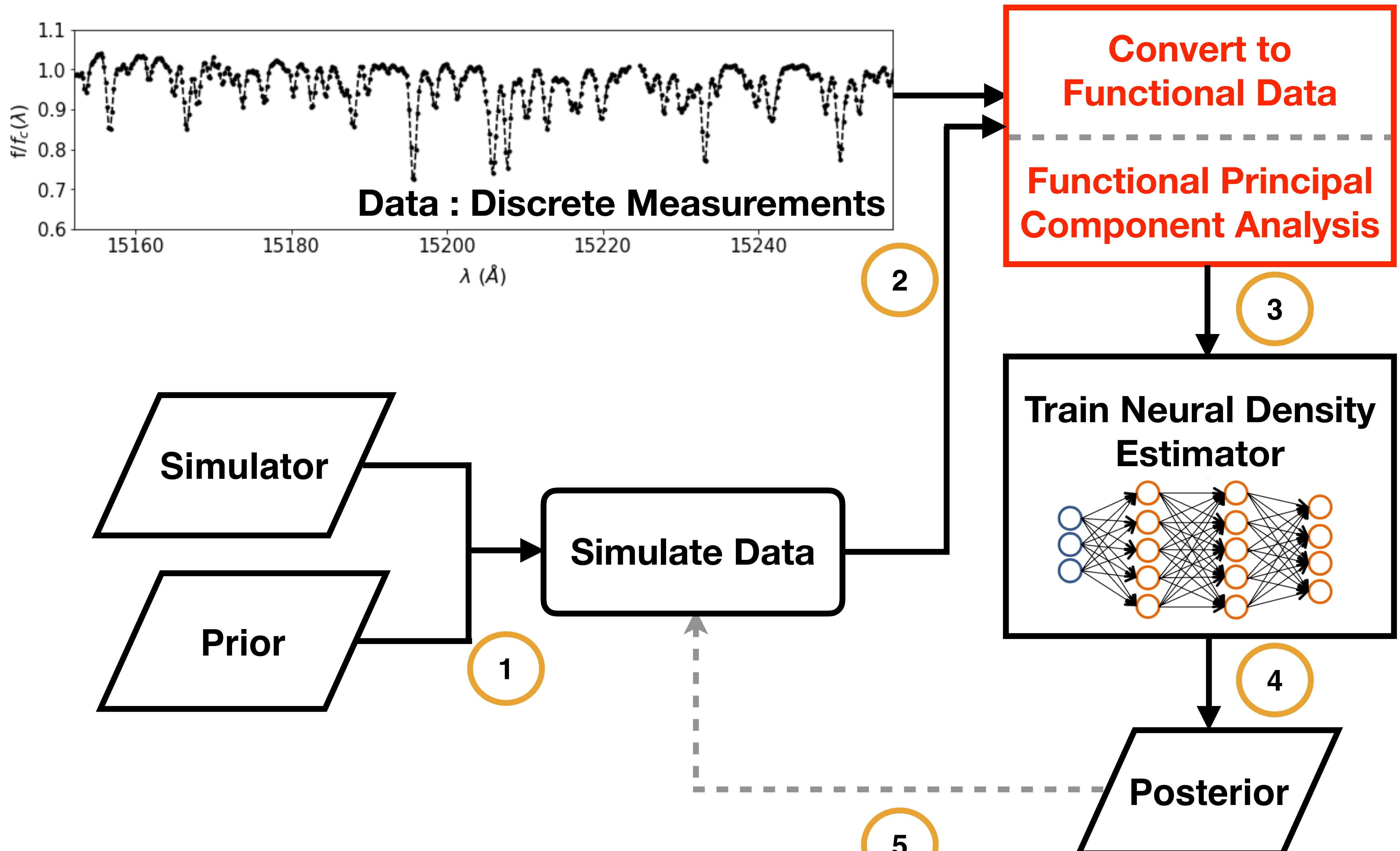
T_{eff}, log g, [X/H]



Statistical Methodology



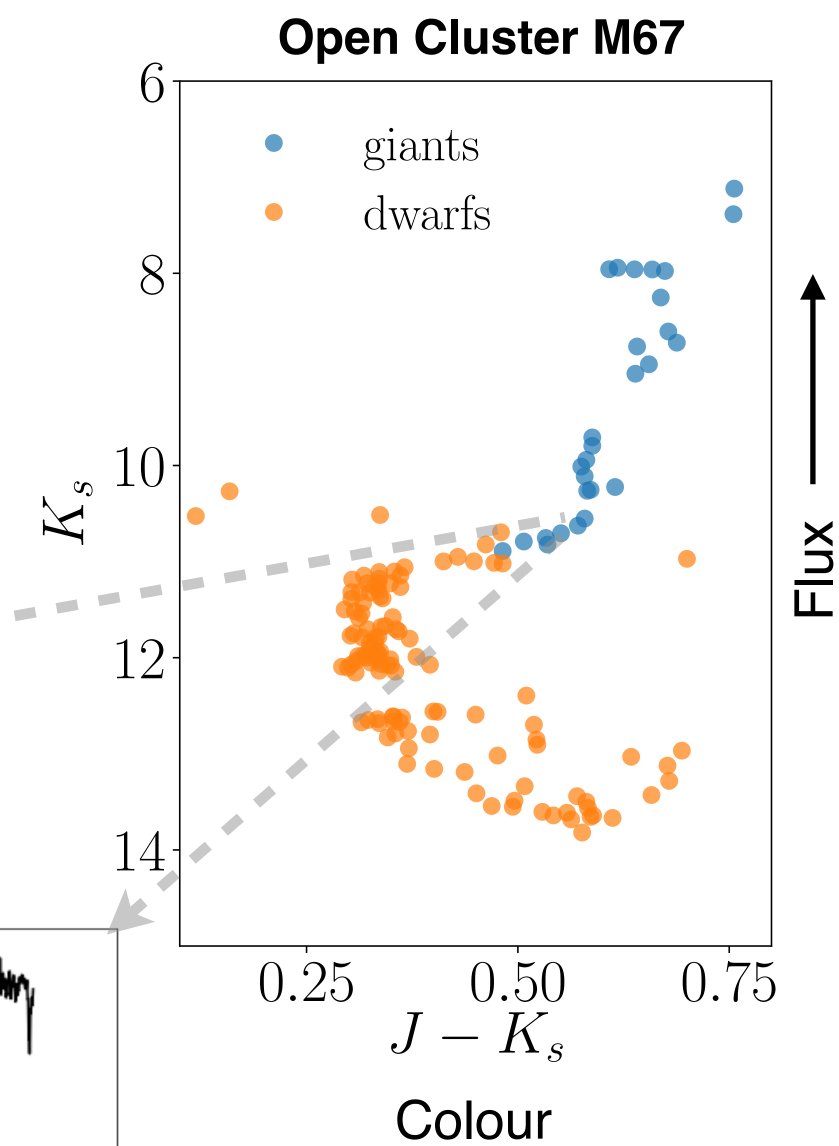
Statistical Methodology

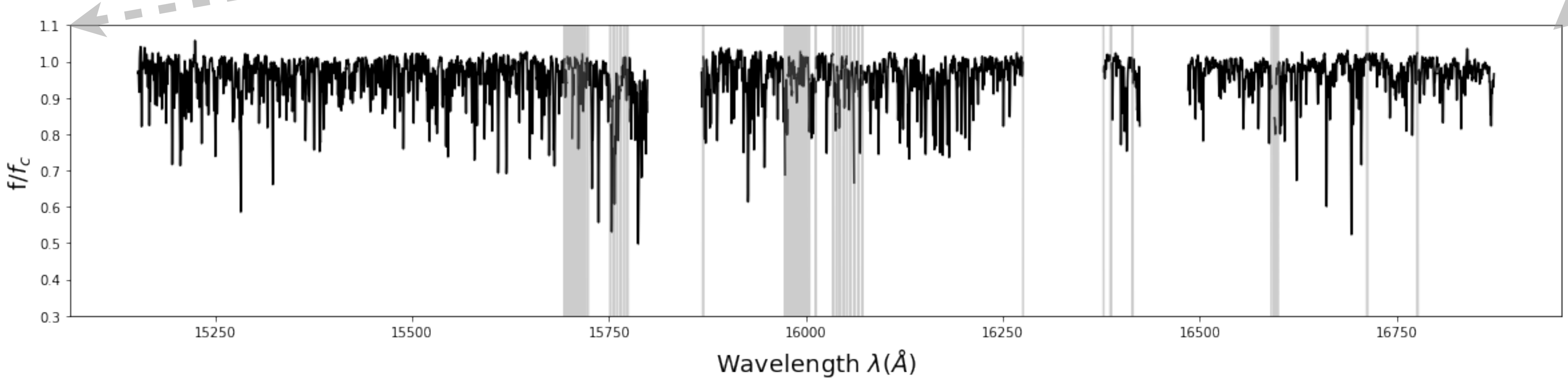


Dimensionality Reduction

Issue Curse of Dimensionality

Solution Low-dimensional intrinsic structure

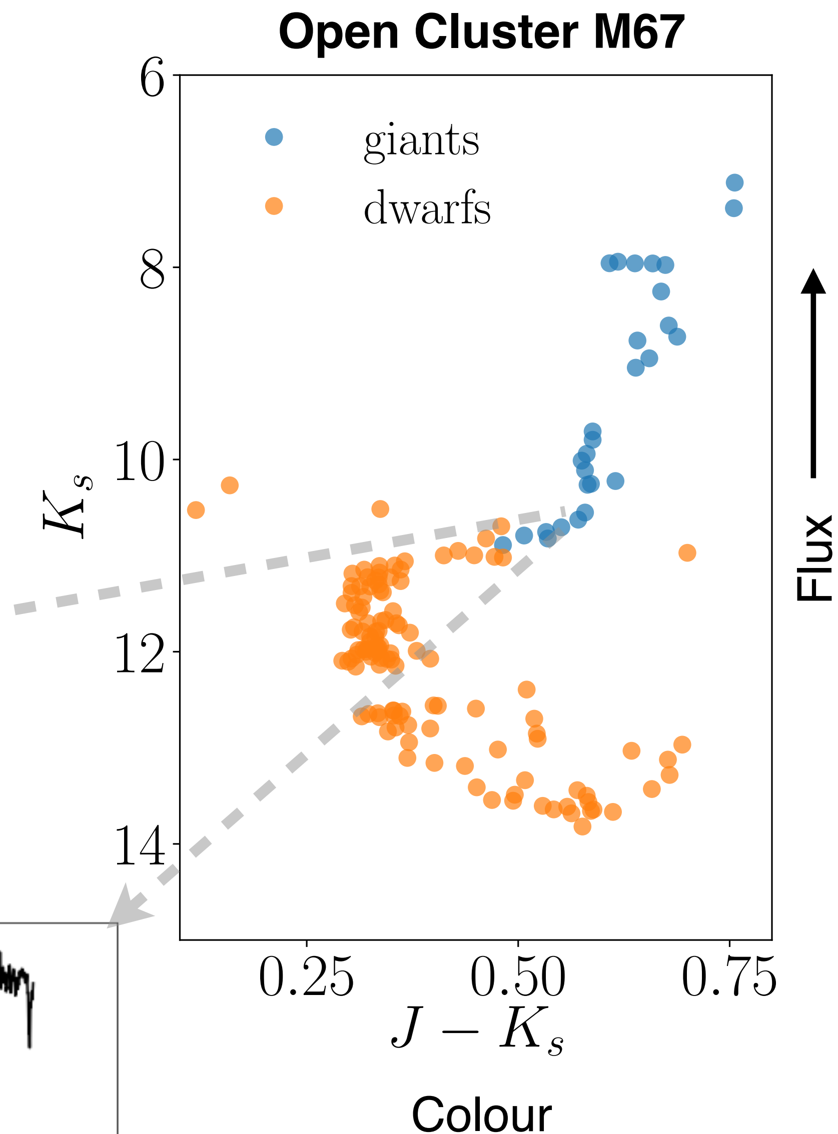


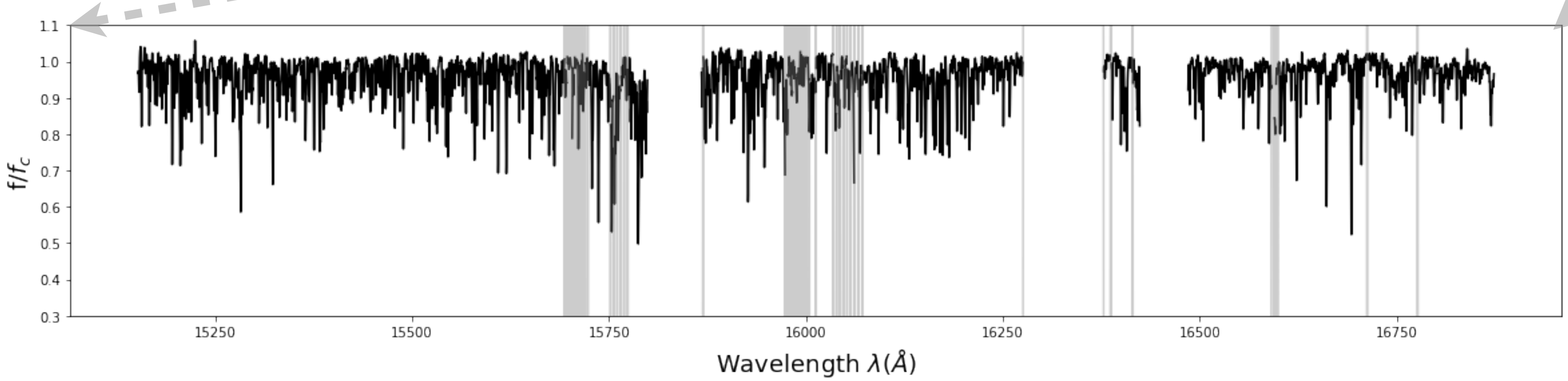


APOGEE spectrum ~10^4 discrete wavelengths

Dimensionality Reduction

Principal Component Analysis





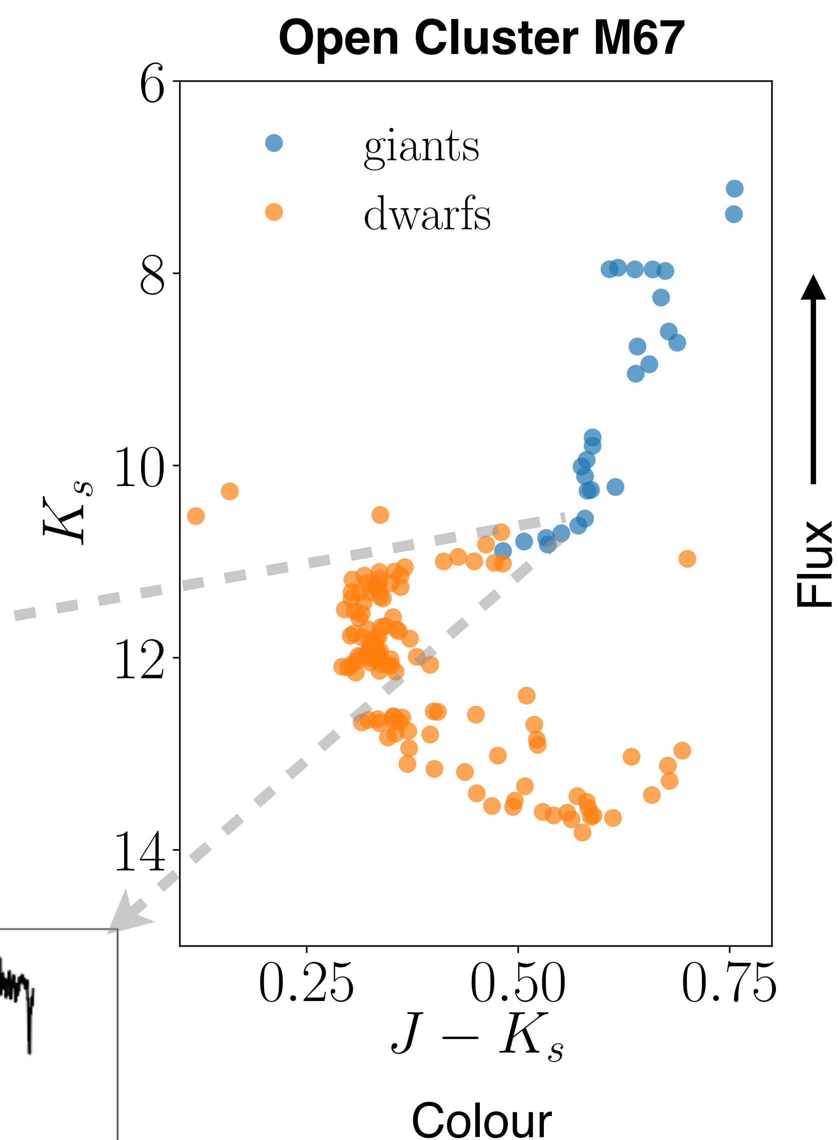
~10^4 discrete wavelengths

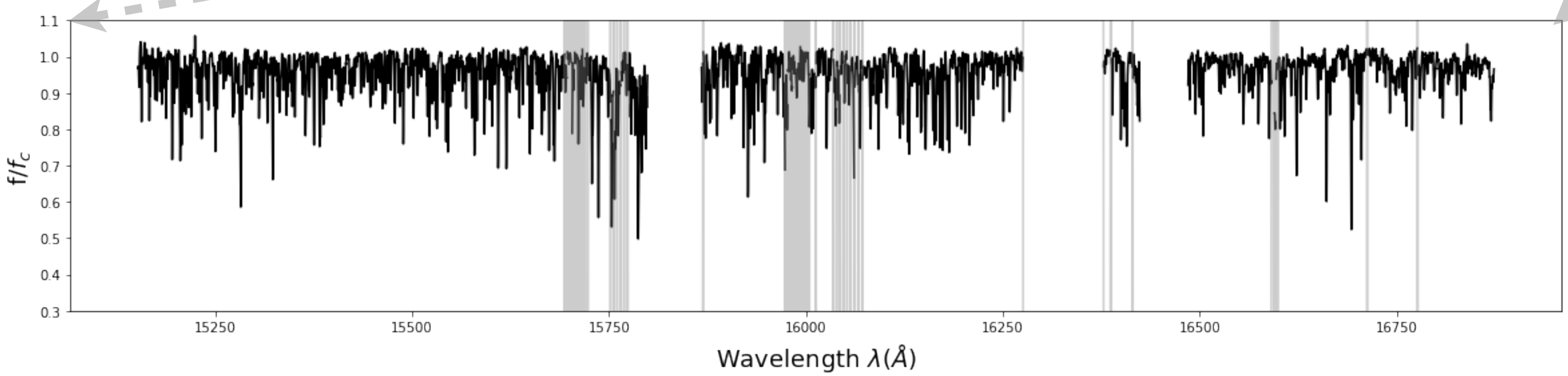
Dimensionality Reduction

Expectation Maximization

Principal Component Analysis

Noisy and missing data

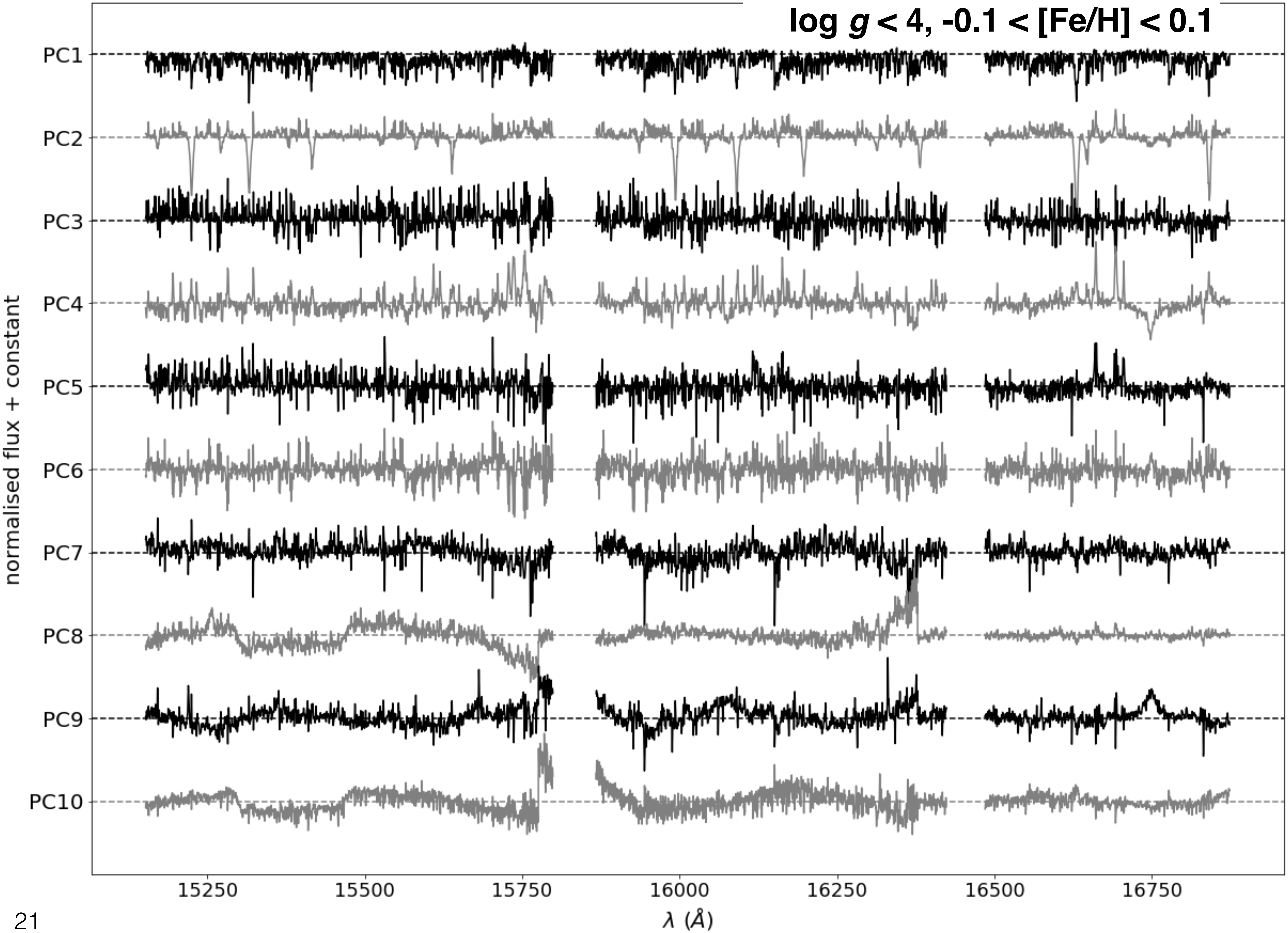




$\sim 10^4$ discrete wavelengths

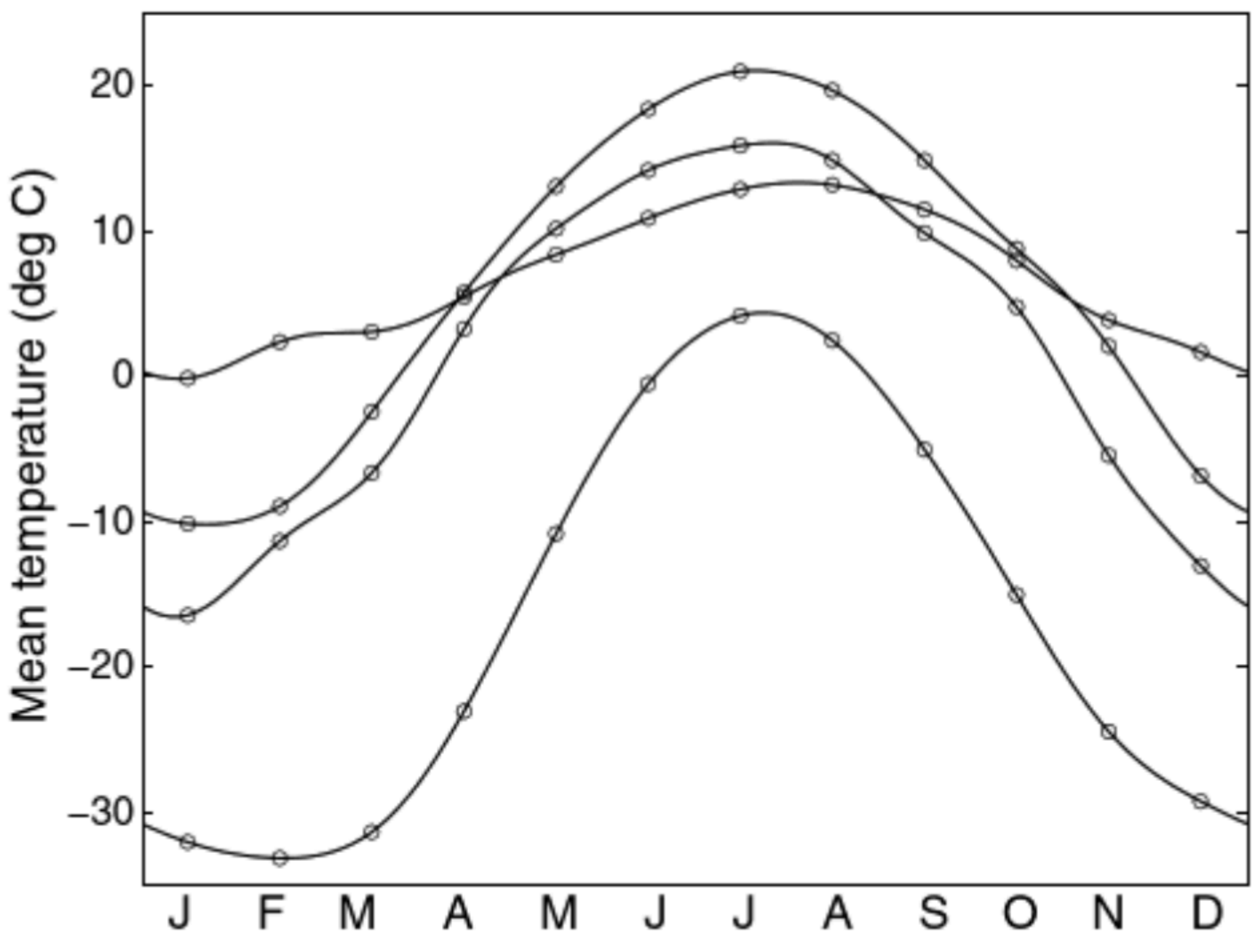
~50,000 APOGEE spectra

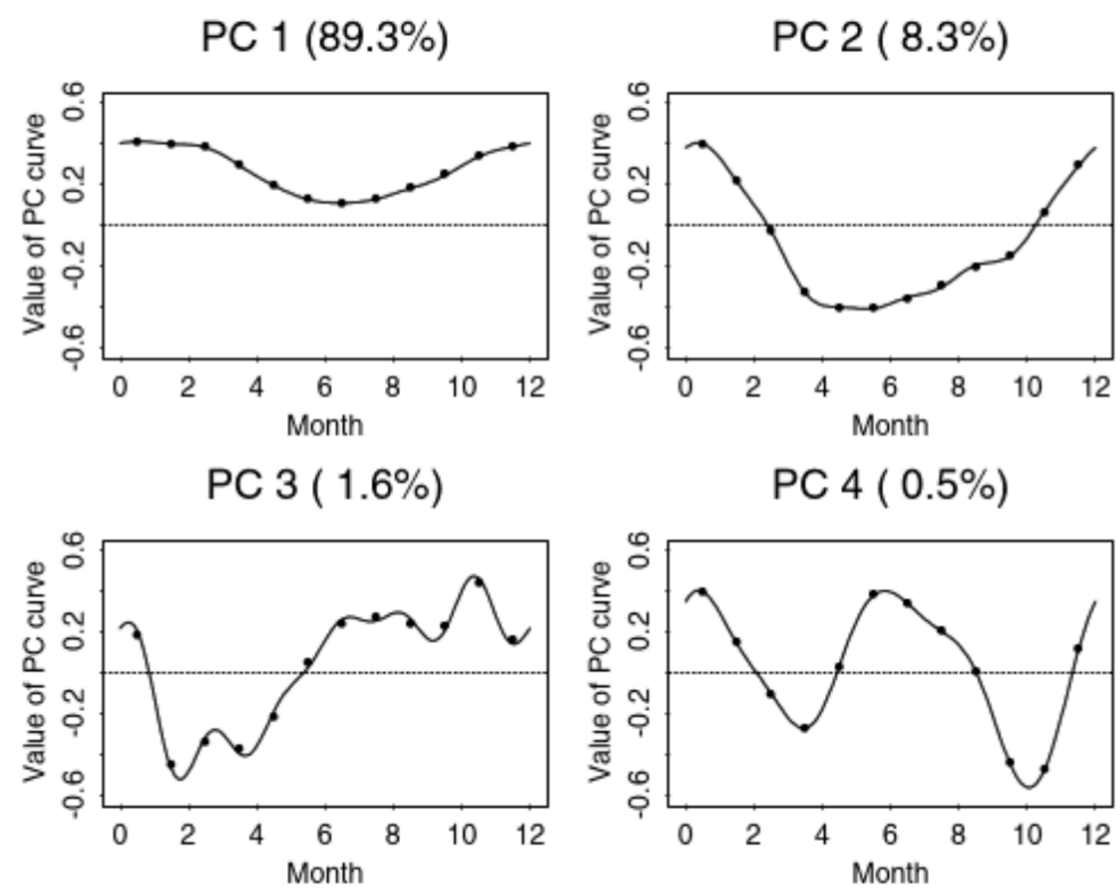
log *g* < 4, -0.1 < [Fe/H] < 0.1



Functional Principal Component Analysis

FPCA The functional version of PCA

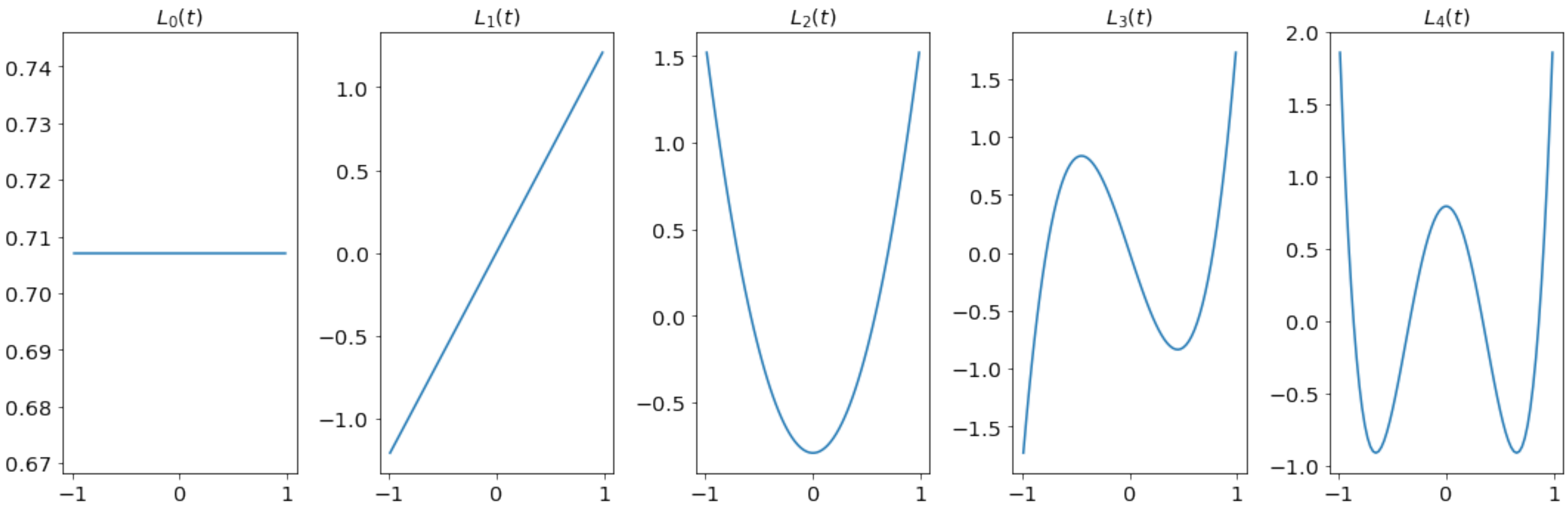




Figures from Functional Data Analysis, Ramsay & Silverman

Functional Principal Component Analysis

FPCA The functional version of PCA



Example Basis Functions: Legendre Polynomials

Functional Principal Component Analysis

FPCA The functional version of PCA

The data is first transformed into functional form:

Raw data $f(x) = \{ f_1(x), \ldots, f_n(x) \}$ *…noisy*

Basis functions $\phi(x) = \{\phi_1(x), \ldots, \phi_K(x)\}$ *…domain knowledge*

Regress the raw data onto the basis functions

$$f_t(x) \approx \sum_{k=1}^{K} \beta_{t,k}\phi_k(x)$$

Functional **P**rincipal **C**omponent **A**nalysis

FPCA The functional version of PCA

The data is first transformed into functional form:

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***Regress the raw data onto the basis* functions**

$$f_t(x) \approx \sum_{k=1}^{K} \beta_{t,k} \phi_k(x)$$

$$\hat{K}(s,t) = \sum_{j=1}^{\infty} \hat{\kappa}_j \, \hat{\psi}_j(s) \, \hat{\psi}_j(t)$$ *...Mercer's theorem*

Functional Principal Component Analysis

FPCA The functional version of PCA

The data is first transformed into functional form:

Raw data $f(x) = \{ f_1(x), \ldots, f_n(x) \}$ *…noisy*

Basis functions $\phi(x) = \{\phi_1(x), \ldots, \phi_K(x)\}$ *…domain knowledge*

Regress the raw data onto the basis functions

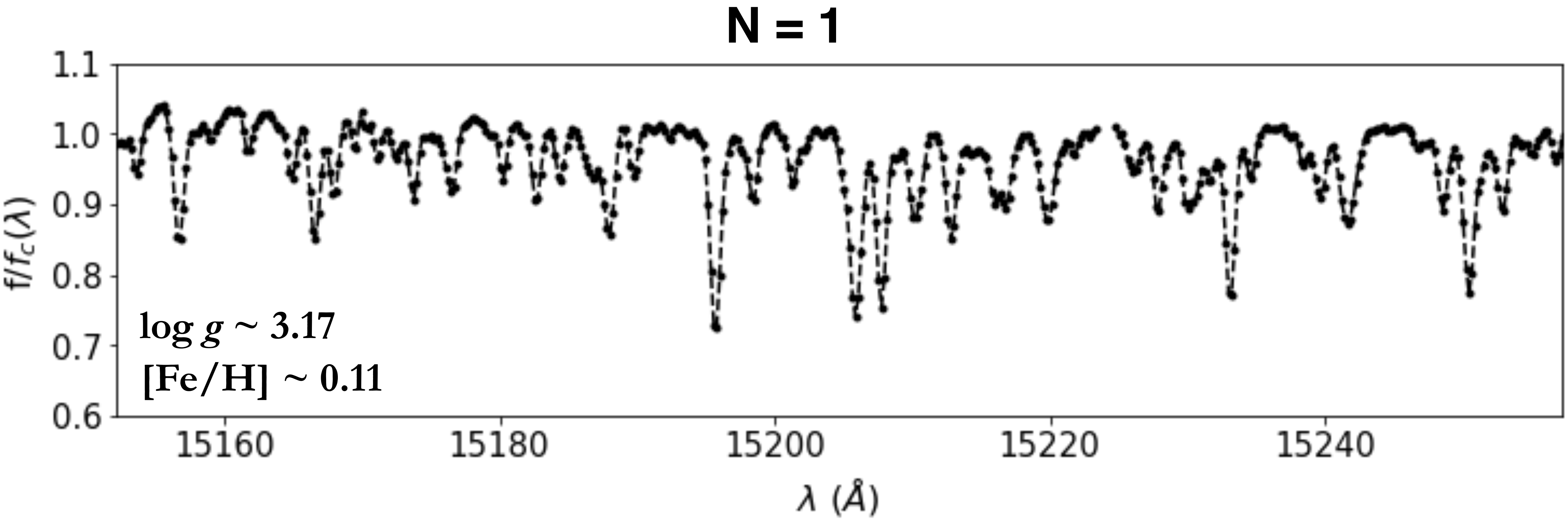
$$f_t(x) \approx \sum_{k=1}^{K} \beta_{t,k} \phi_k(x)$$

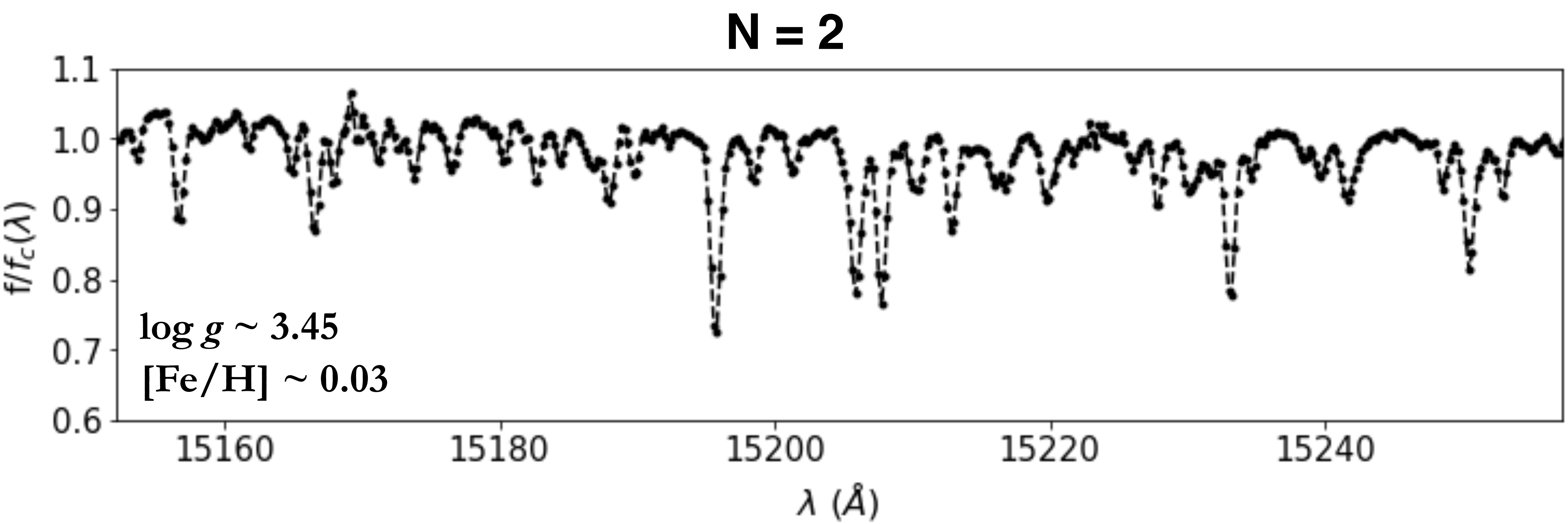
covariance function

$$\hat{K}(s,t) = \sum_{j=1}^{\infty} \hat{\kappa}_j \hat{\psi}_j(s) \hat{\psi}_j(t)$$

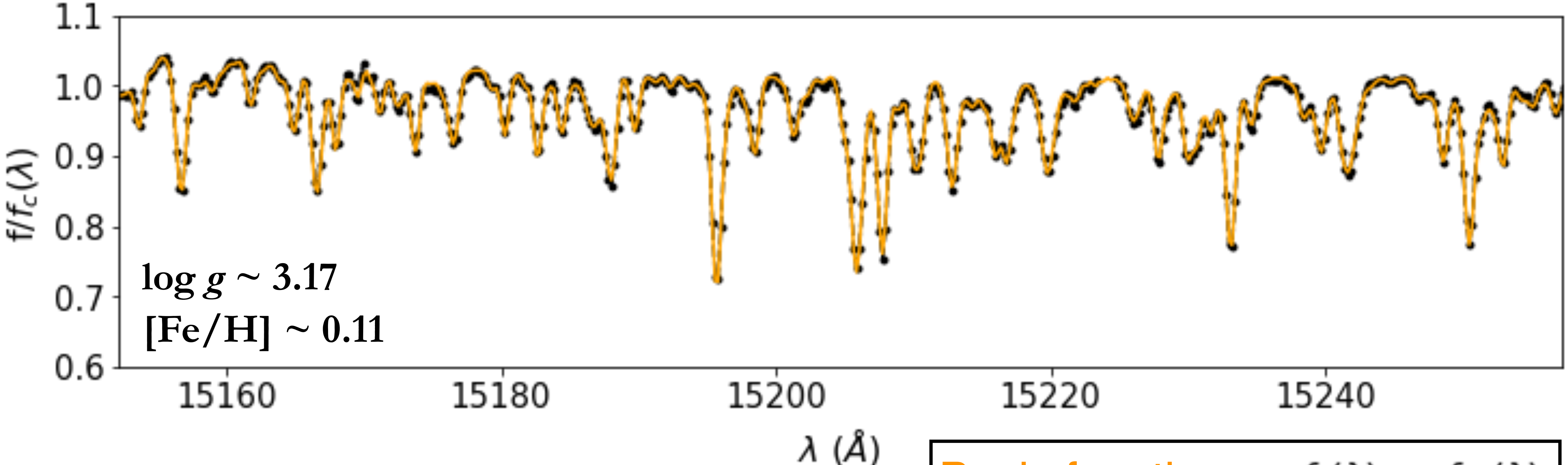
…Mercer's theorem

eigenvalues eigenfunctions


N = 1
1.1
1.0
0.9
0.8
0.7
0.6
$f/f_c(\lambda)$
log g ~ 3.17
[Fe/H] ~ 0.11
15160
15180
15200
15220
15240
λ (Å)

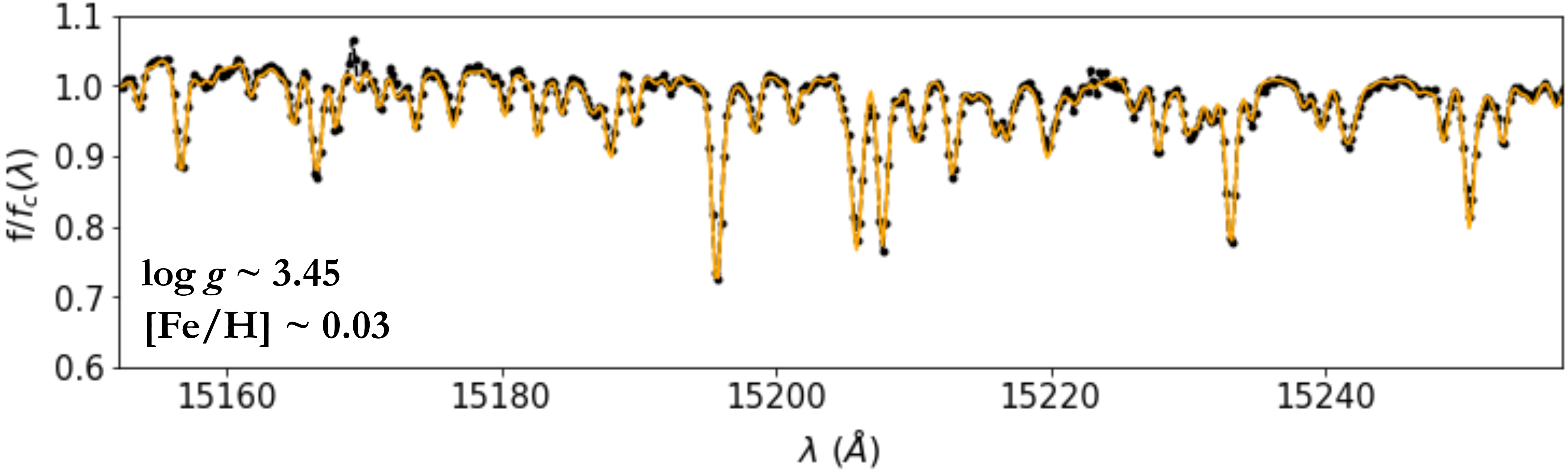

N = 2
1.1
1.0
0.9
0.8
0.7
0.6
$f/f_c(\lambda)$
log g ~ 3.45
[Fe/H] ~ 0.03
15160
15180
15200
15220
15240
λ (Å)

N = 1



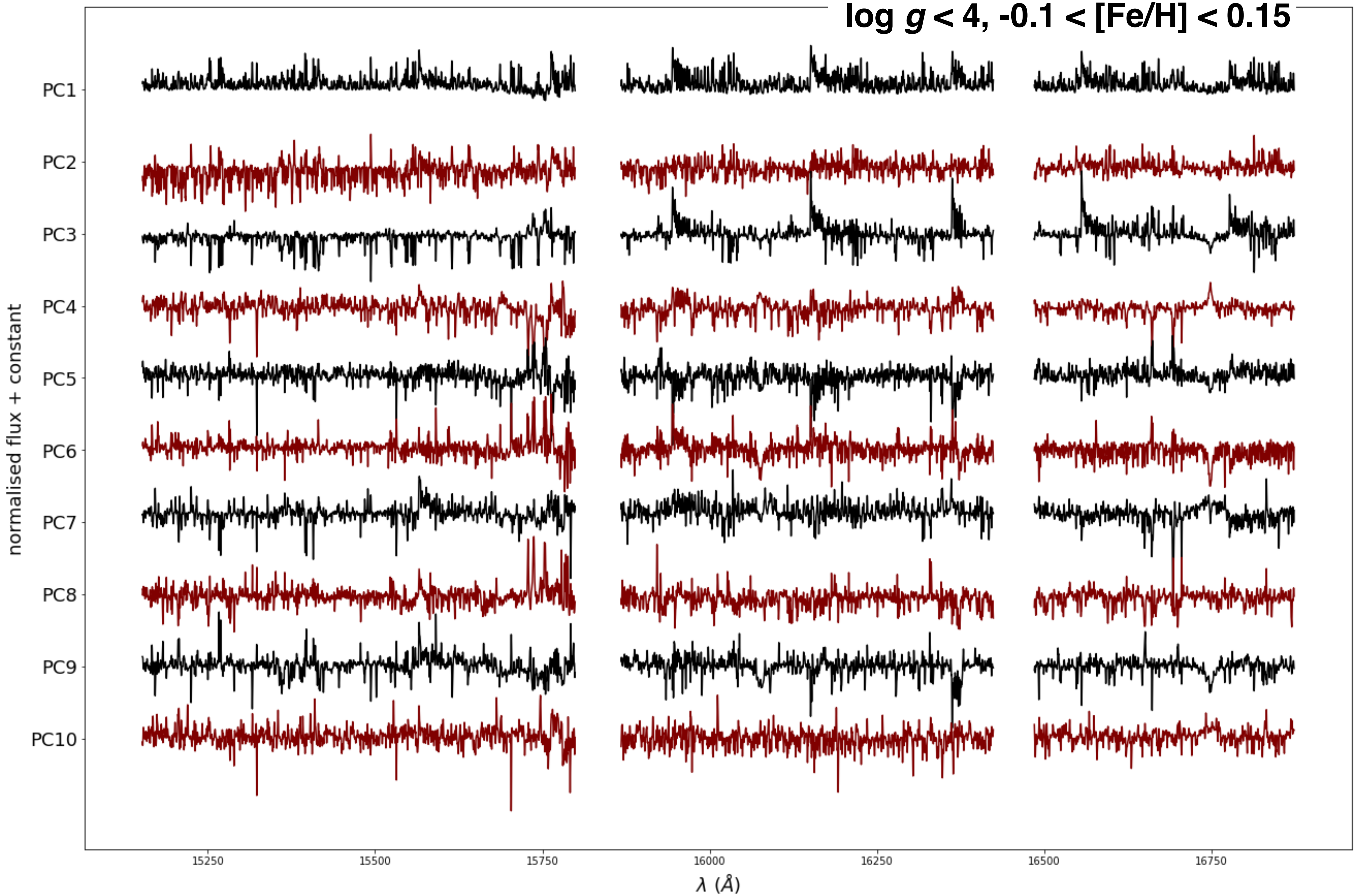
Basis functions: $f_1(\lambda), \ldots, f_{10}(\lambda)$
10 theoretical spectra

N = 2

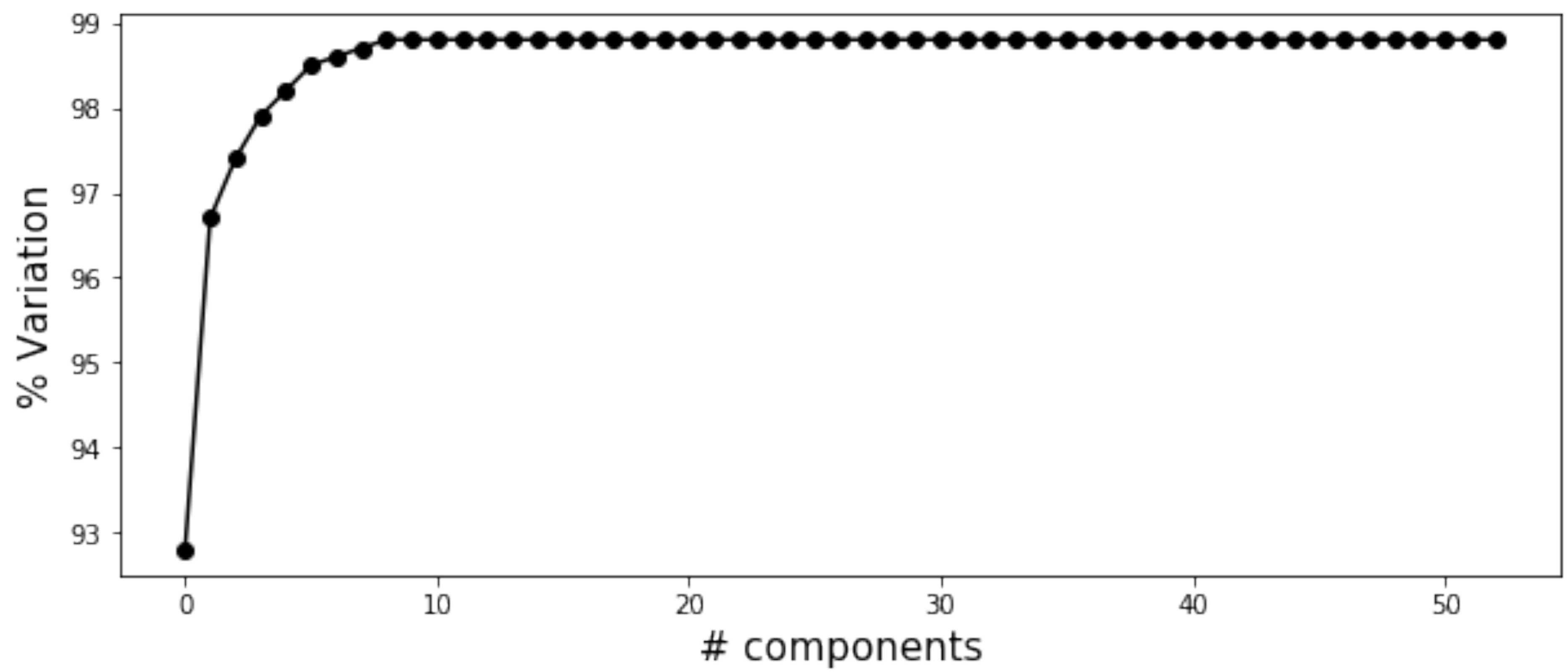


~1,000 APOGEE spectra

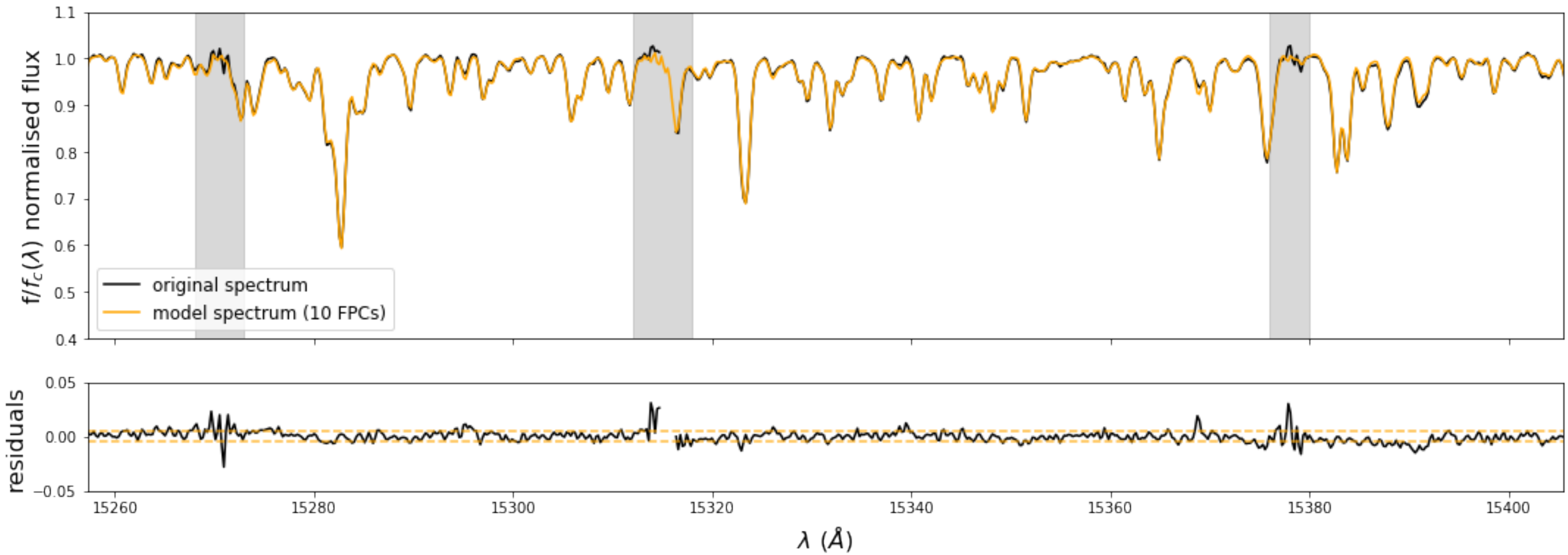
log *g* < 4, -0.1 < [Fe/H] < 0.15



Cumulative explained variance



M67 Red Giant spectrum
FPCA reconstructed spectrum



DENSITY ESTIMATION LIKELIHOOD-FREE INFERENCE

DELFI a new Bayesian Inference method

in simulator models where the likelihood $p(\mathbf{d}\,|\,\theta)$ is intractable.

$$simulator(\theta) = \mathbf{d}$$

parameters → θ

simulated data → $\mathbf{d}$

Papamakarios et al (2017) Alsing et al (2018)

DENSITY ESTIMATION LIKELIHOOD-FREE INFERENCE

DELFI a new Bayesian Inference method

in simulator models where the likelihood $p(\mathbf{d}\,|\,\theta)$ is intractable.

$$\textit{simulator}(\theta) = \mathbf{d}$$

parameters ***simulated data***

Obtain $\{\theta, \mathbf{d}\}$

Fit $p(\mathbf{d}\,|\,\theta; \mathbf{w})$ to $\{\theta, \mathbf{d}\}$

Obtain the (learned) likelihood function $p(\mathbf{d}_o\,|\,\theta; \mathbf{w})$, given data $\mathbf{d}_o$

Papamakarios et al (2017) Alsing et al (2018)

DENSITY ESTIMATION LIKELIHOOD-FREE INFERENCE

DELFI a new Bayesian Inference method

in simulator models where the likelihood $p(\mathbf{d}\,|\,\theta)$ is intractable.

$$\mathit{simulator}(\theta) = \mathbf{d}$$

parameters ***simulated data***

Active learning

Obtain $\{\theta, \mathbf{d}\}$

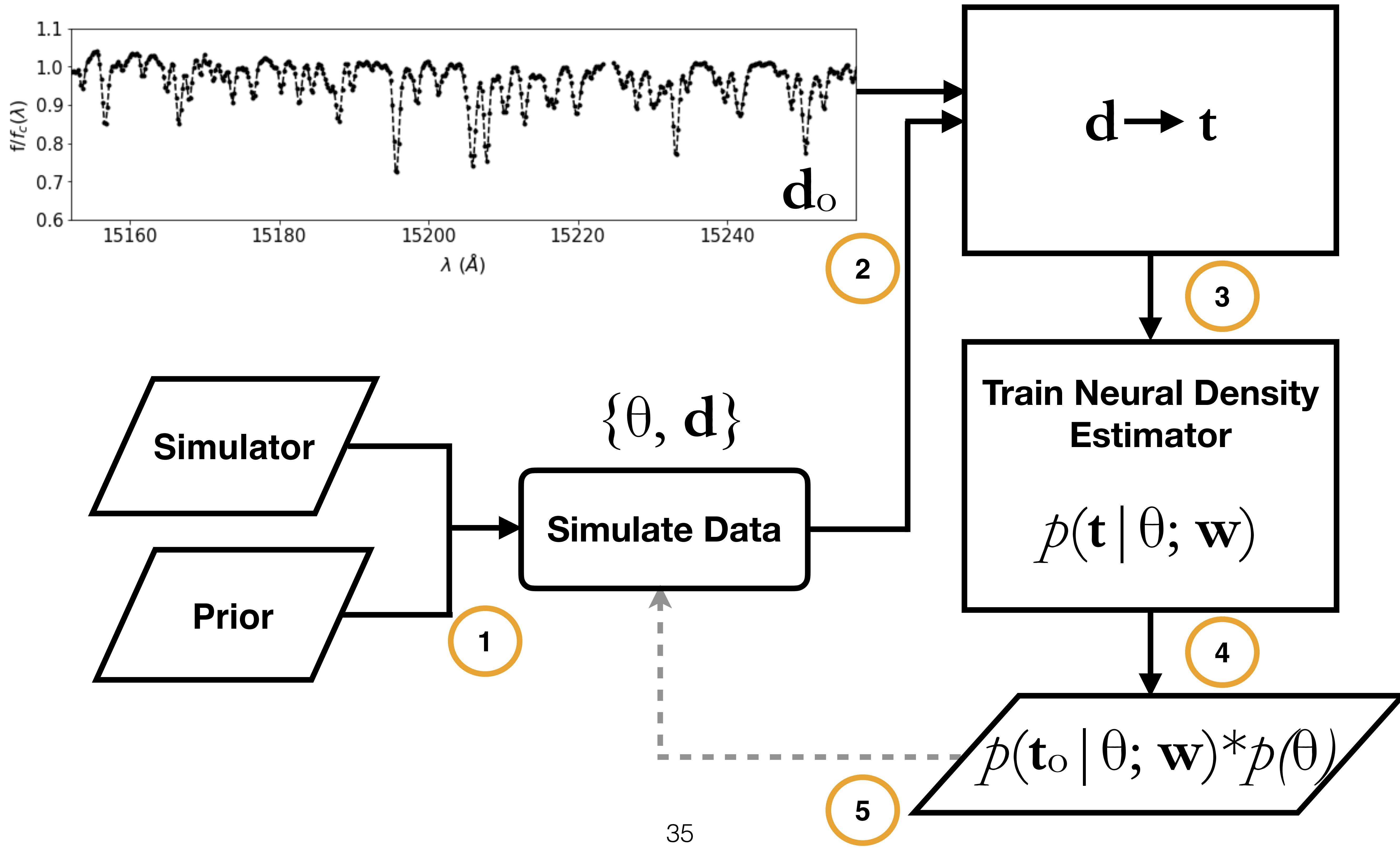
Fit $p(\mathbf{d}\,|\,\theta; \mathbf{w})$ to $\{\theta, \mathbf{d}\}$

Neural Density Estimators

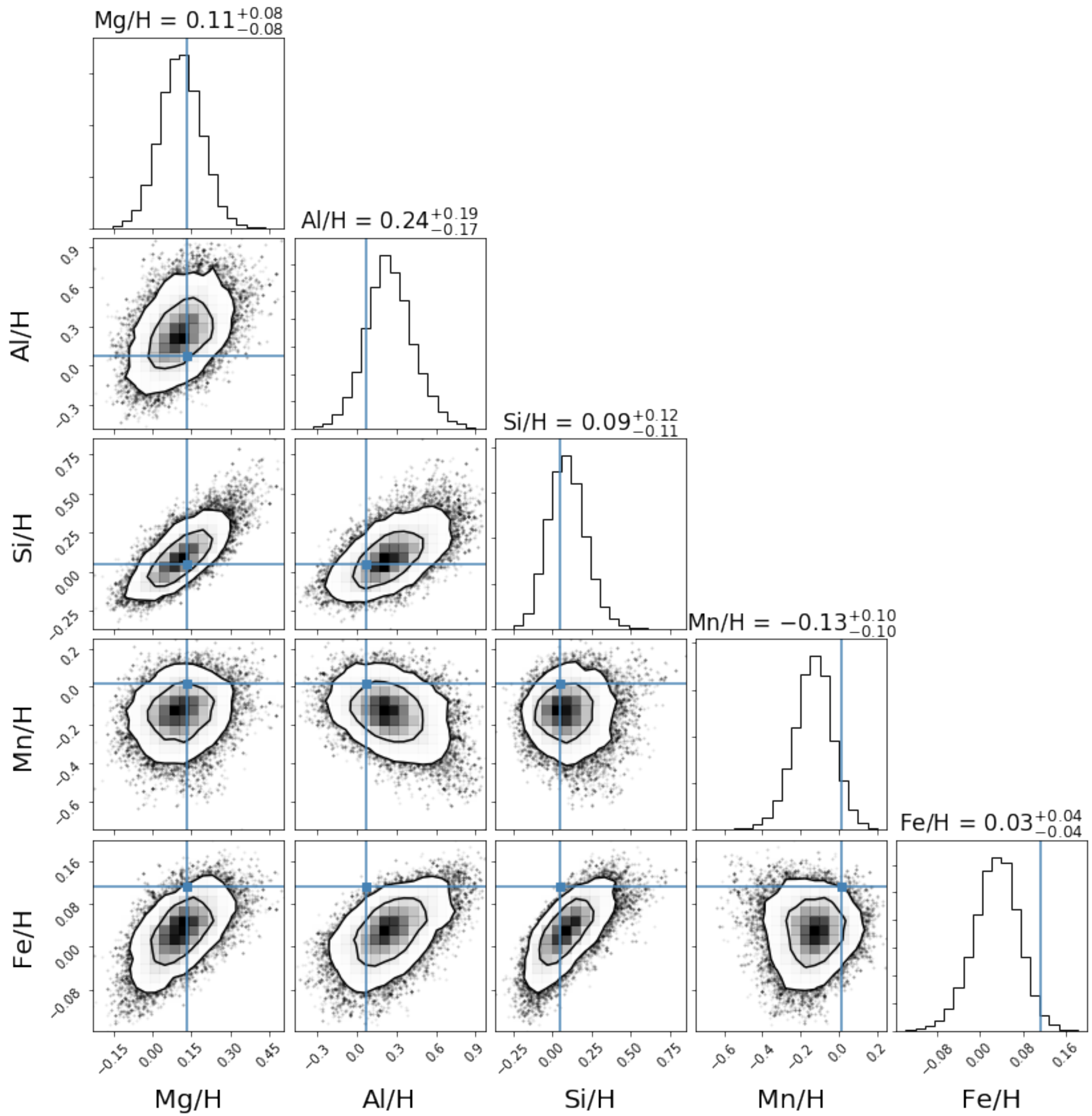
Obtain the (learned) likelihood function $p(\mathbf{d}_o\,|\,\theta; \mathbf{w})$, given data $\mathbf{d}_o$

Papamakarios et al (2017) Alsing et al (2018)

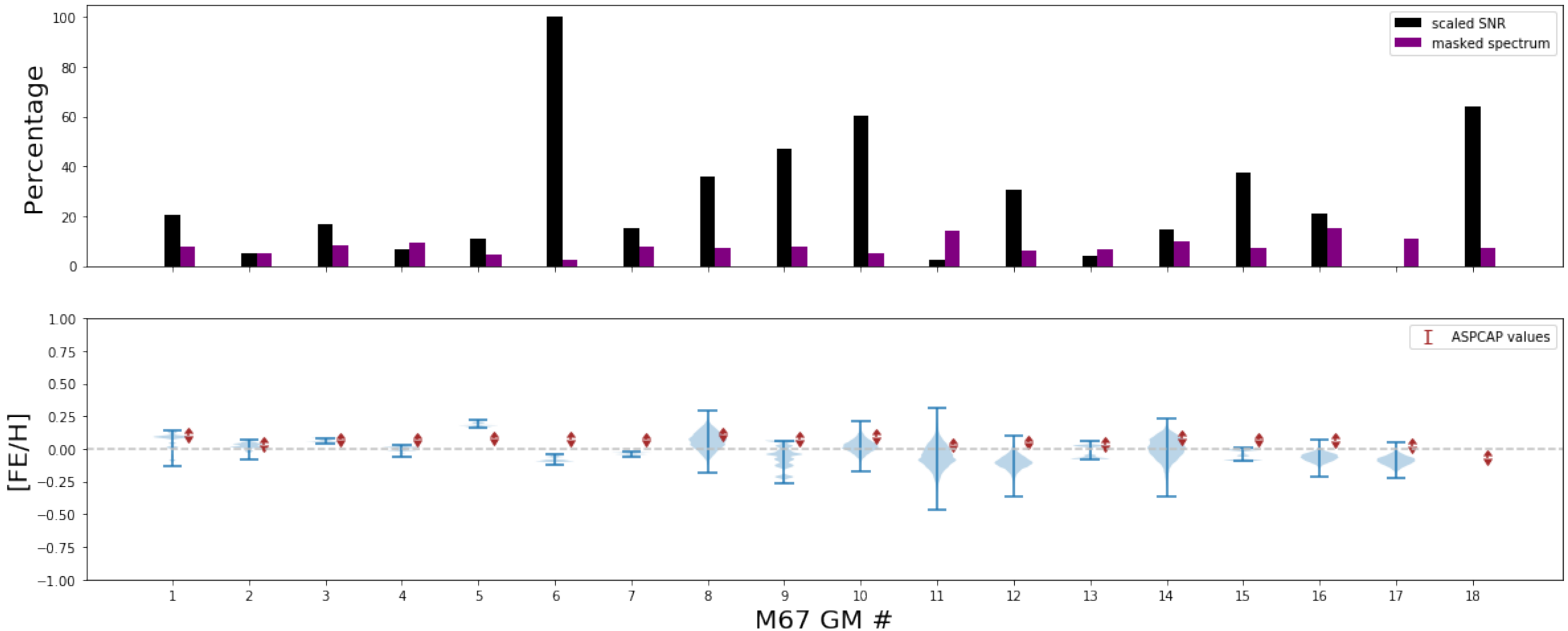
Statistical Methodology



Work in Progress



Work in Progress



Conclusion

- Using FPCA, we have successfully reduced the dimensionality of stellar chemical space.
- FPCA + DELFI shows promising results for fast, accurate and precise inference of abundances.
- We are currently constraining the abundance scatter of M67 open cluster using our inferred abundance values.
- We will then apply our technique to the entire APOGEE DR14 (and latest data releases) to measure abundances and explore chemical tagging.

THANKS!

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