

# ASTROSTATISTICS AND THE PATHWAY TO INTERDISCIPLINARITY

Rafael S.de Souza  
Shanghai Astronomical Observatory  
Chair: Cosmostatistics Initiative  
Vice-President: International  
Astrostatistics Association



# OUTLINE

- Generalized Linear Models
- Statistical Learning
- Discovering stellar clusters



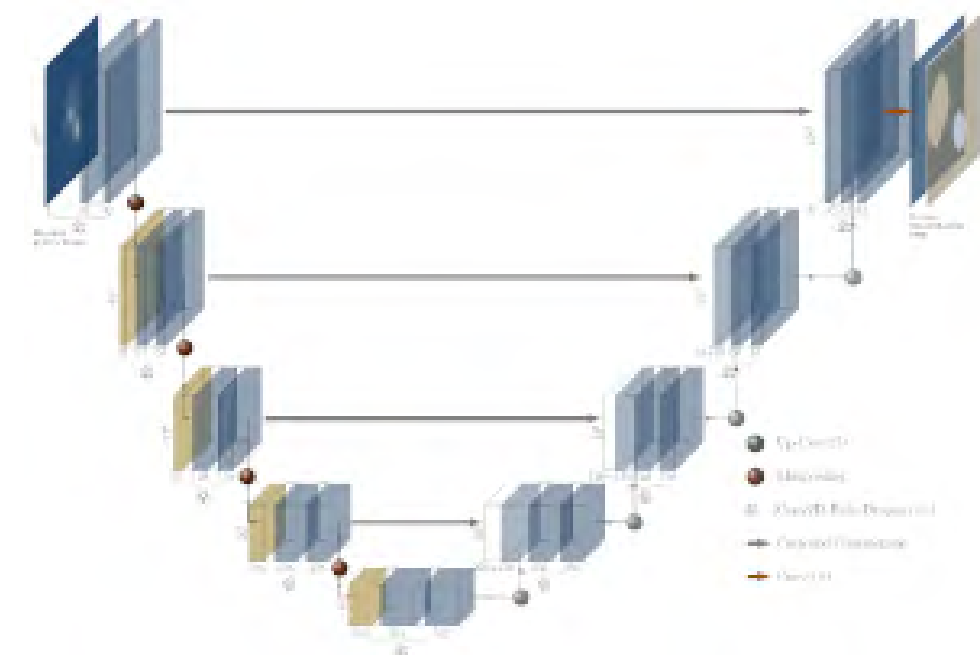
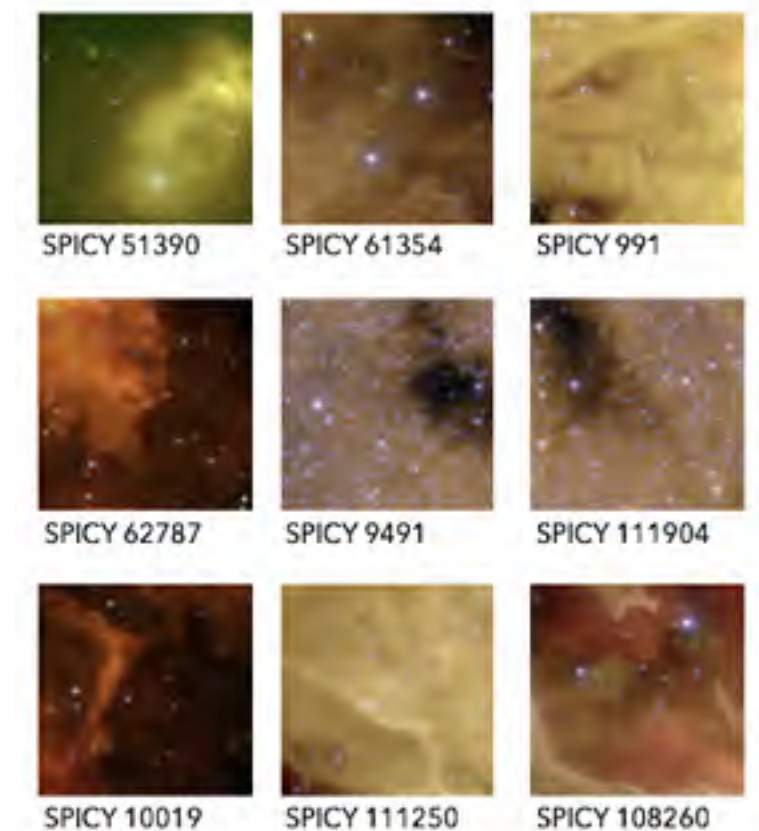
Cosmostatistics Initiative



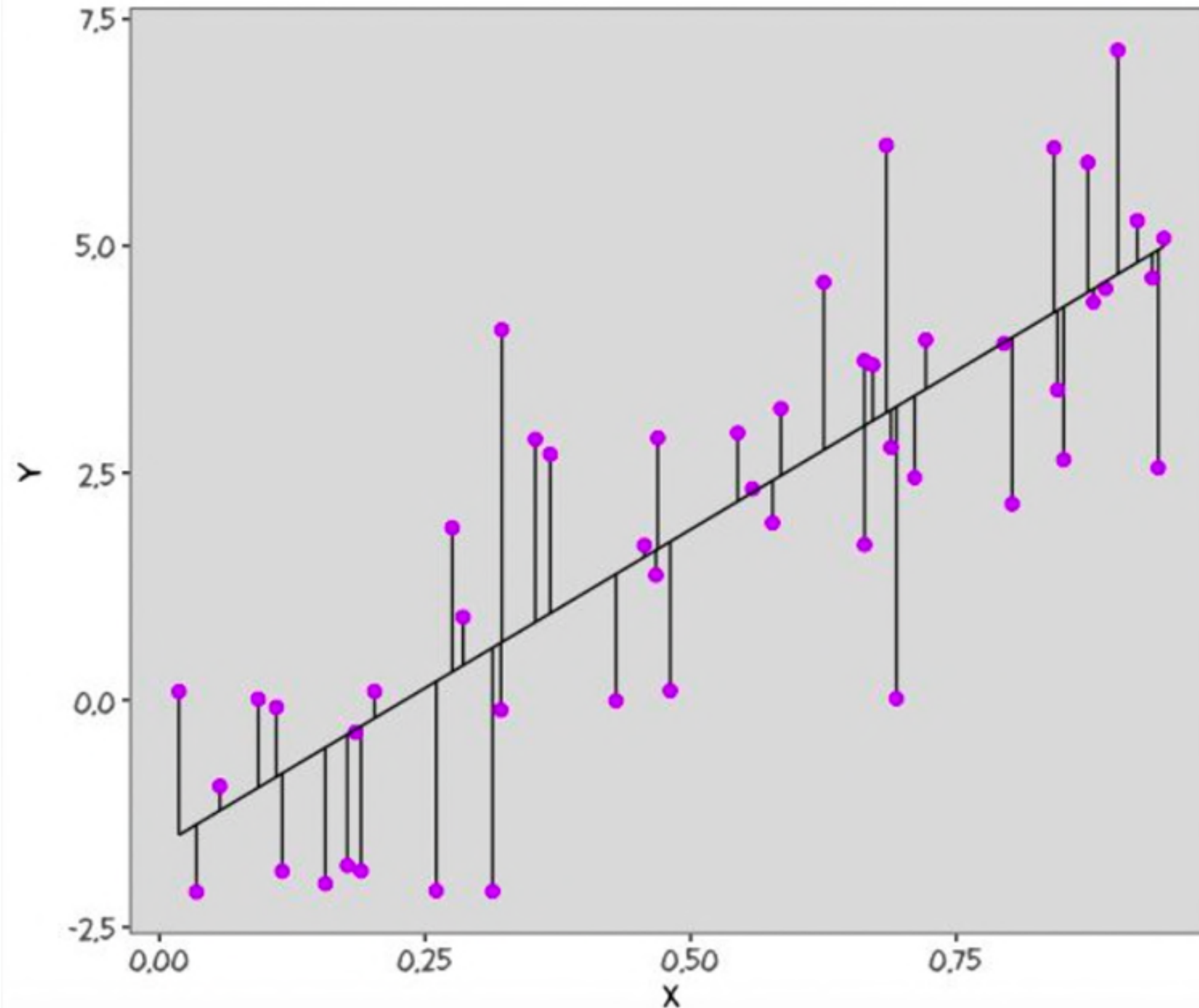
Cosmostatistics Initiative

# Interdisciplinary science development

70 researchers over 25  
Countries



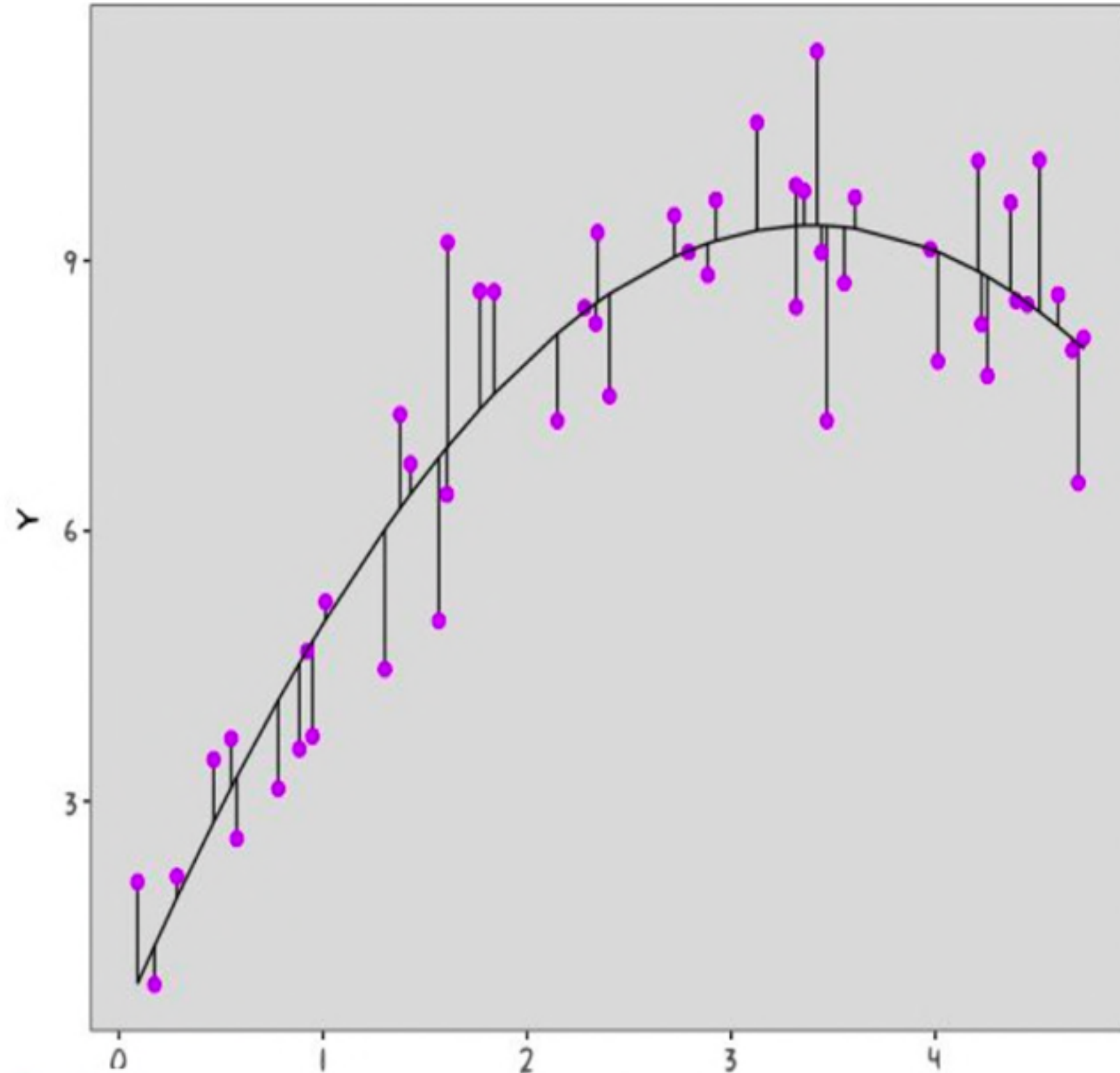
# Normal Linear Models



$$y = ax + b + \varepsilon$$
$$\varepsilon \sim N(0, \sigma^2)$$

Key assumptions:  
y is real and unbounded;  
Homoscedastic variance

# Normal (Gaussian) Linear Models

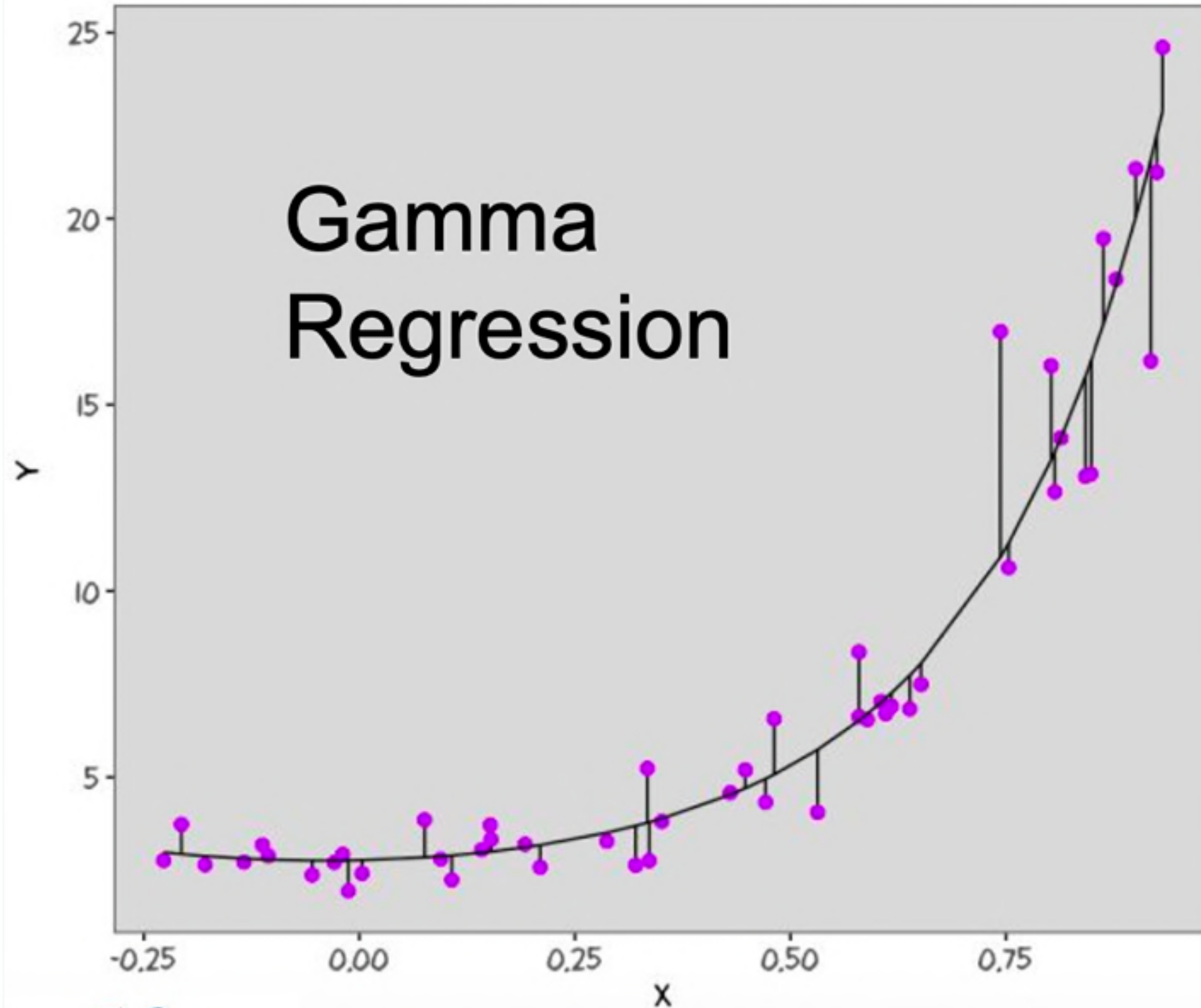


$$Y_i \sim \text{Normal}(\mu_i, \sigma^2)$$
$$\mu_i = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2$$

# Gaussian Models

## Limitations

Gamma  
Regression

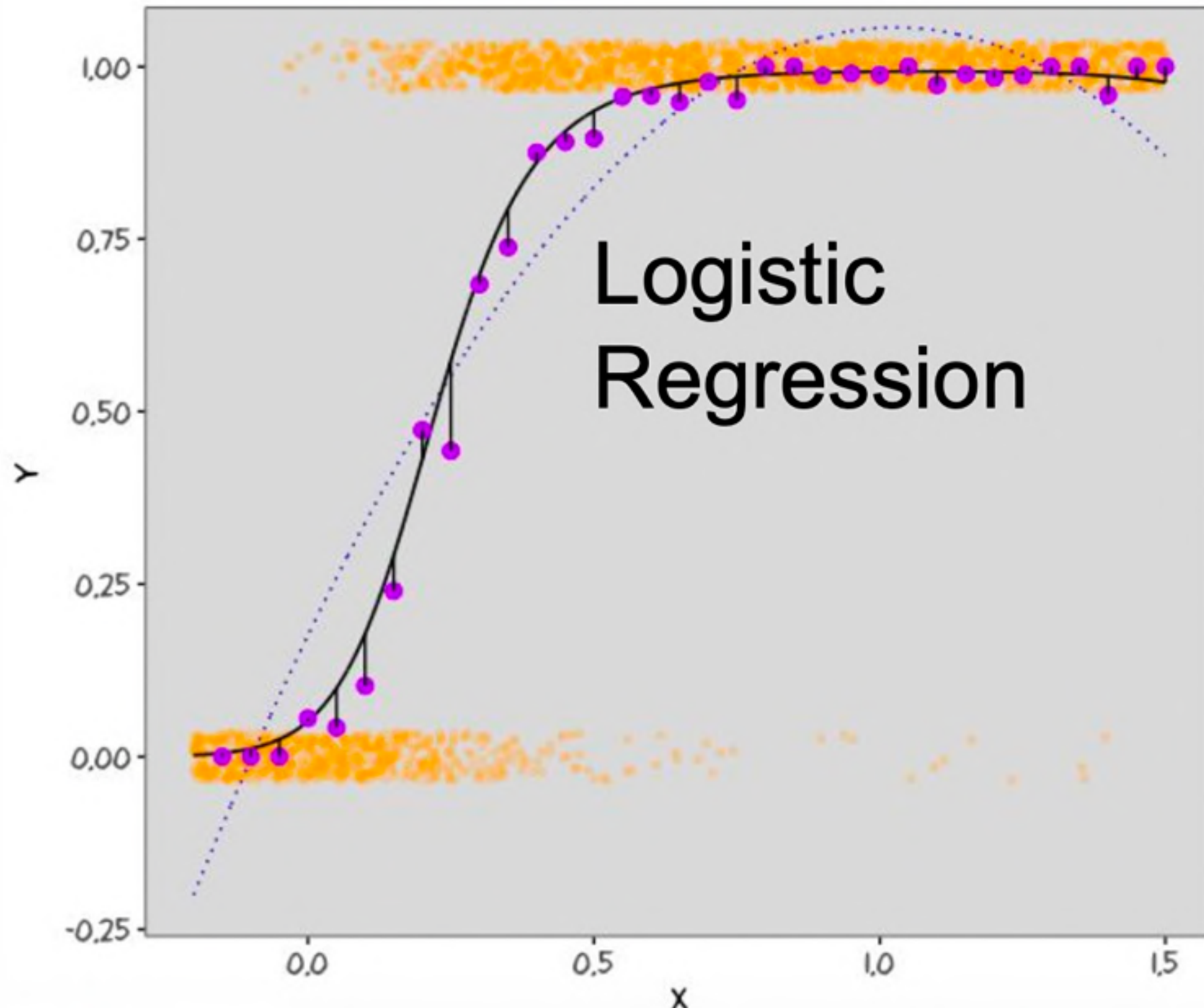


Non-fixed variance,  
aka Heteroscedasticity



# Gaussian Models

## Limitations

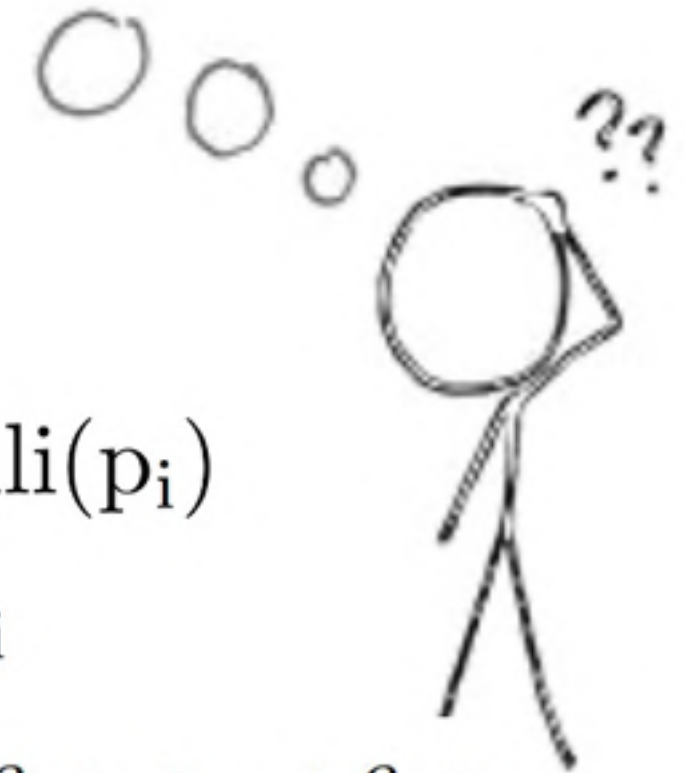


Binary data

$$y_i \sim \text{Bernoulli}(p_i)$$

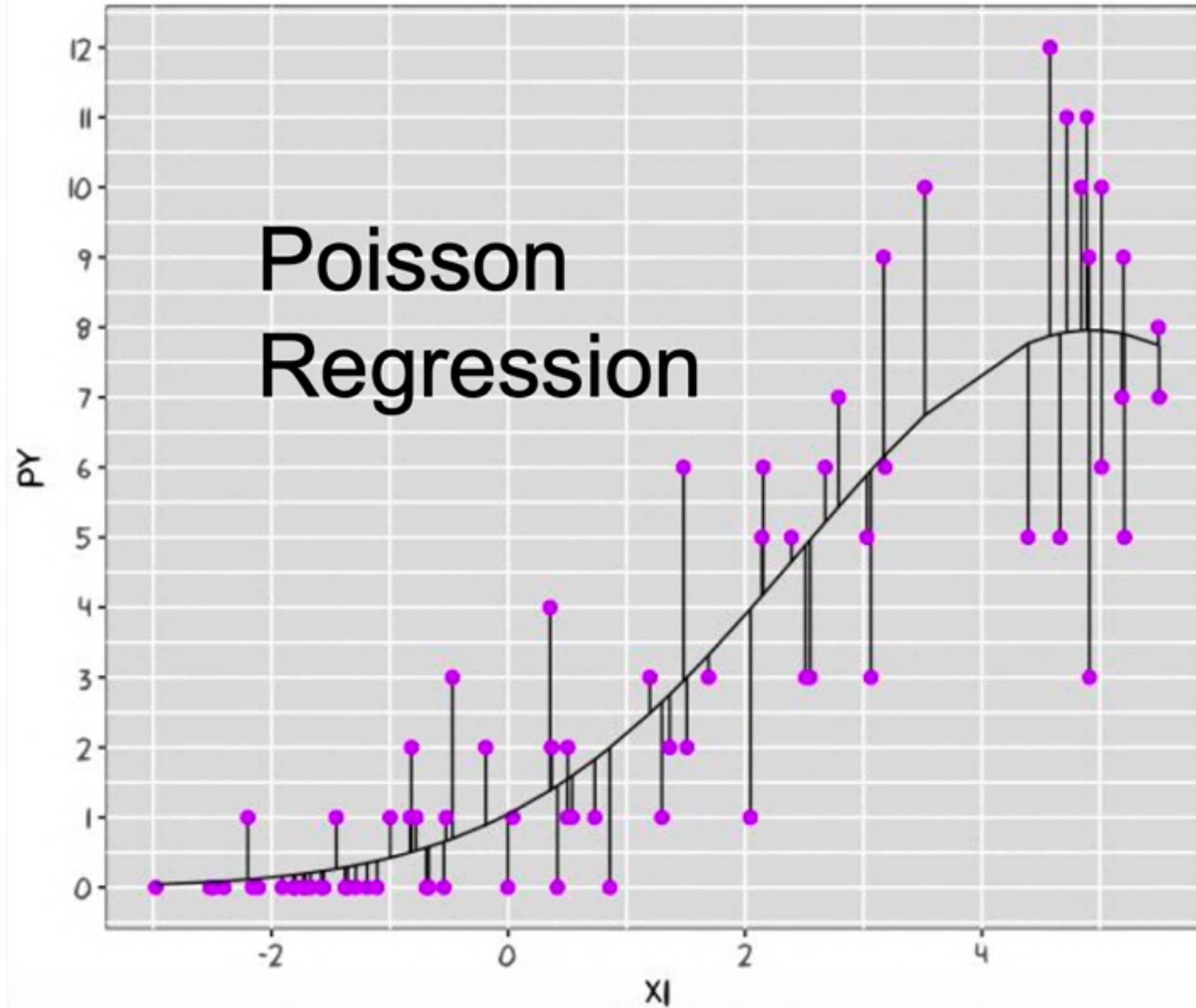
$$\text{logit}(p_i) = \eta_i$$

$$\eta_i \equiv \mathbf{x}_i^T \boldsymbol{\beta} = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$$



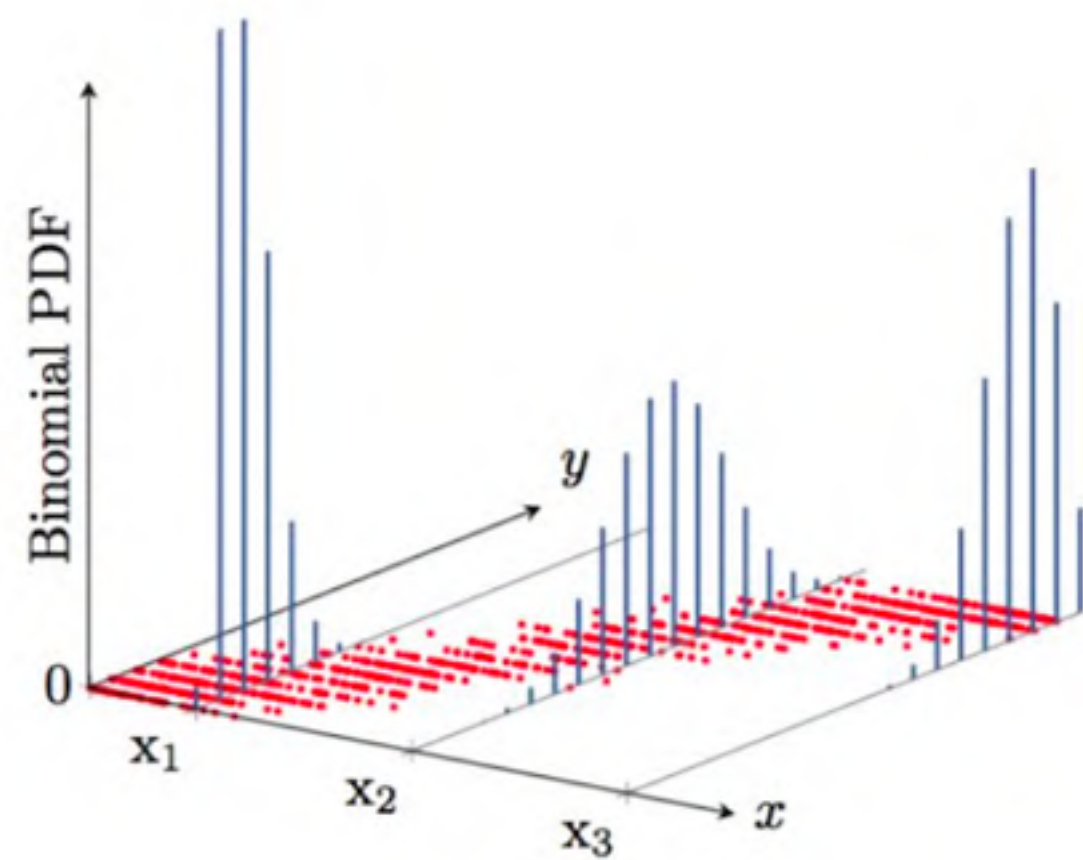
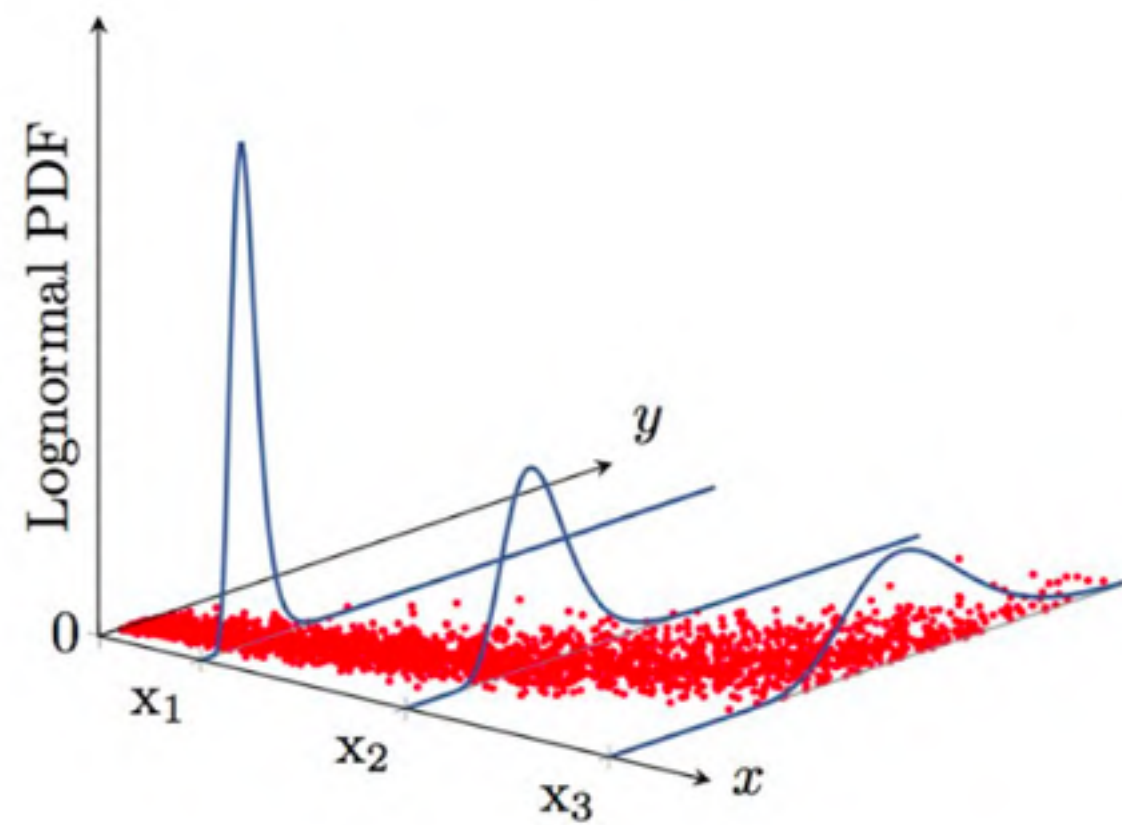
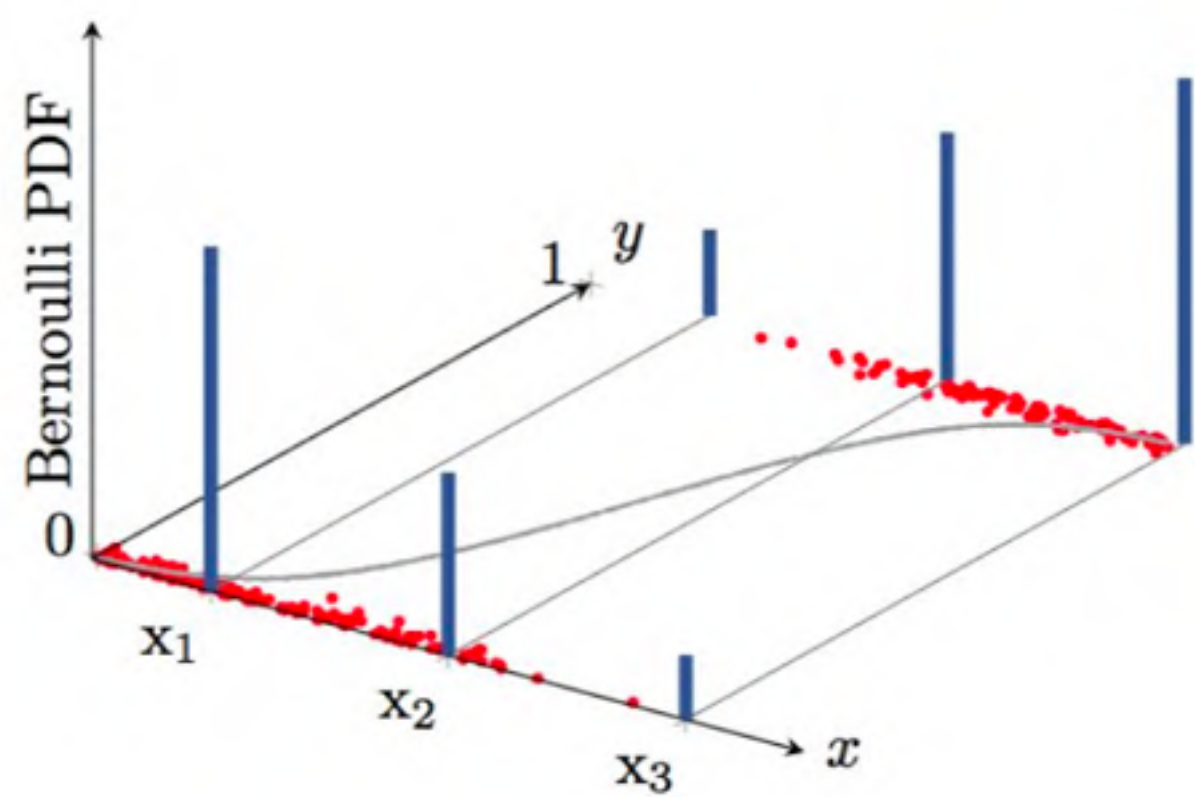
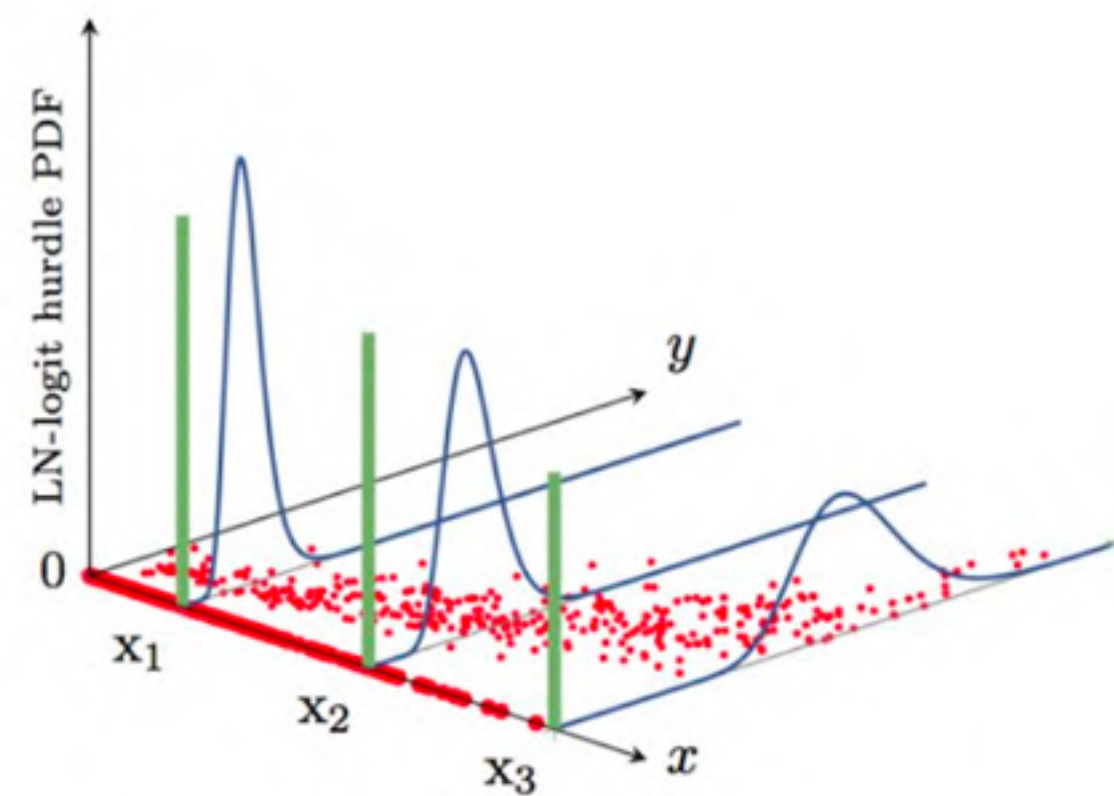
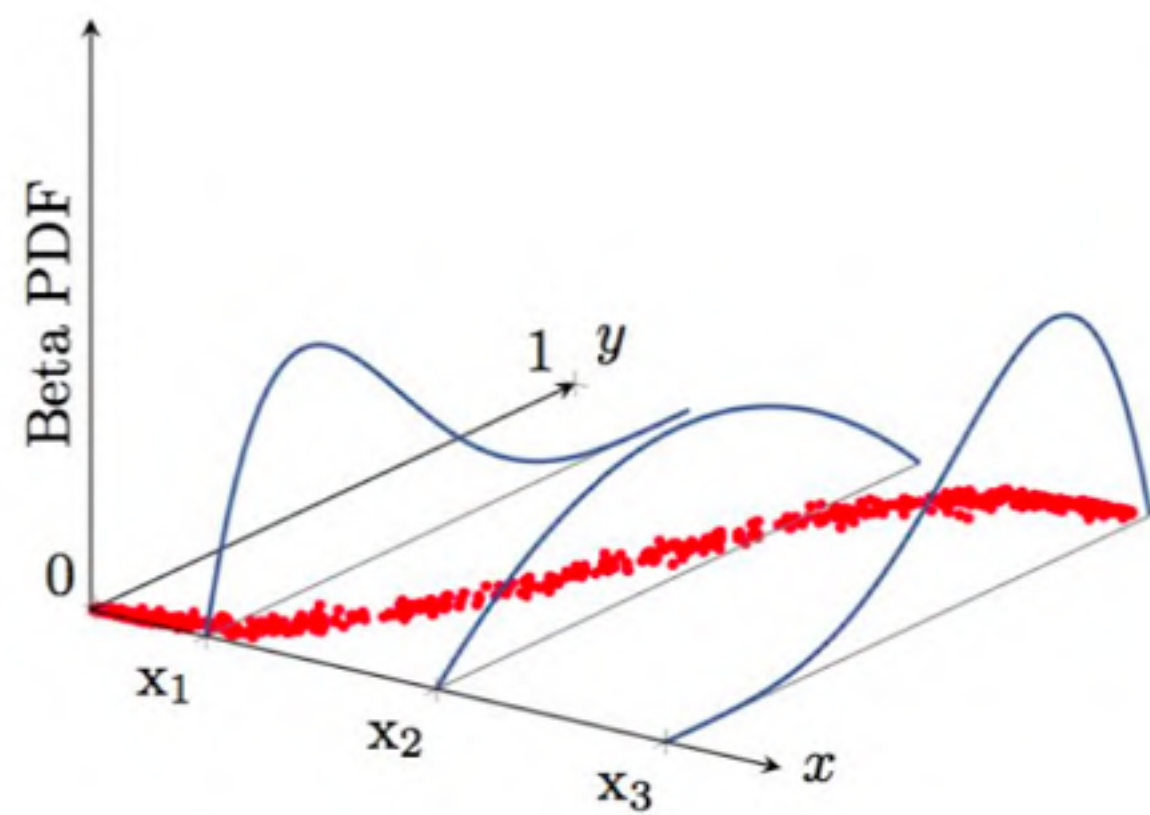
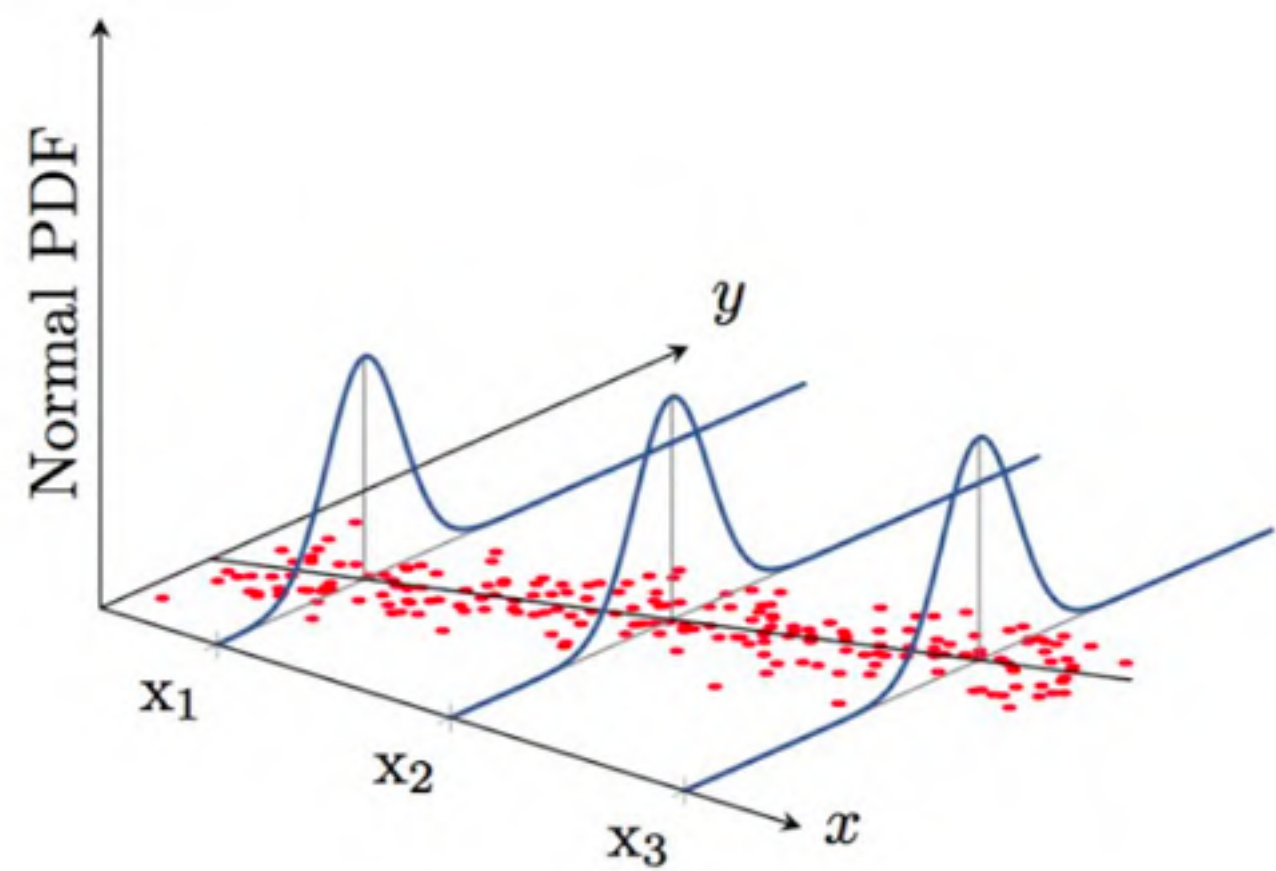
# Gaussian Models

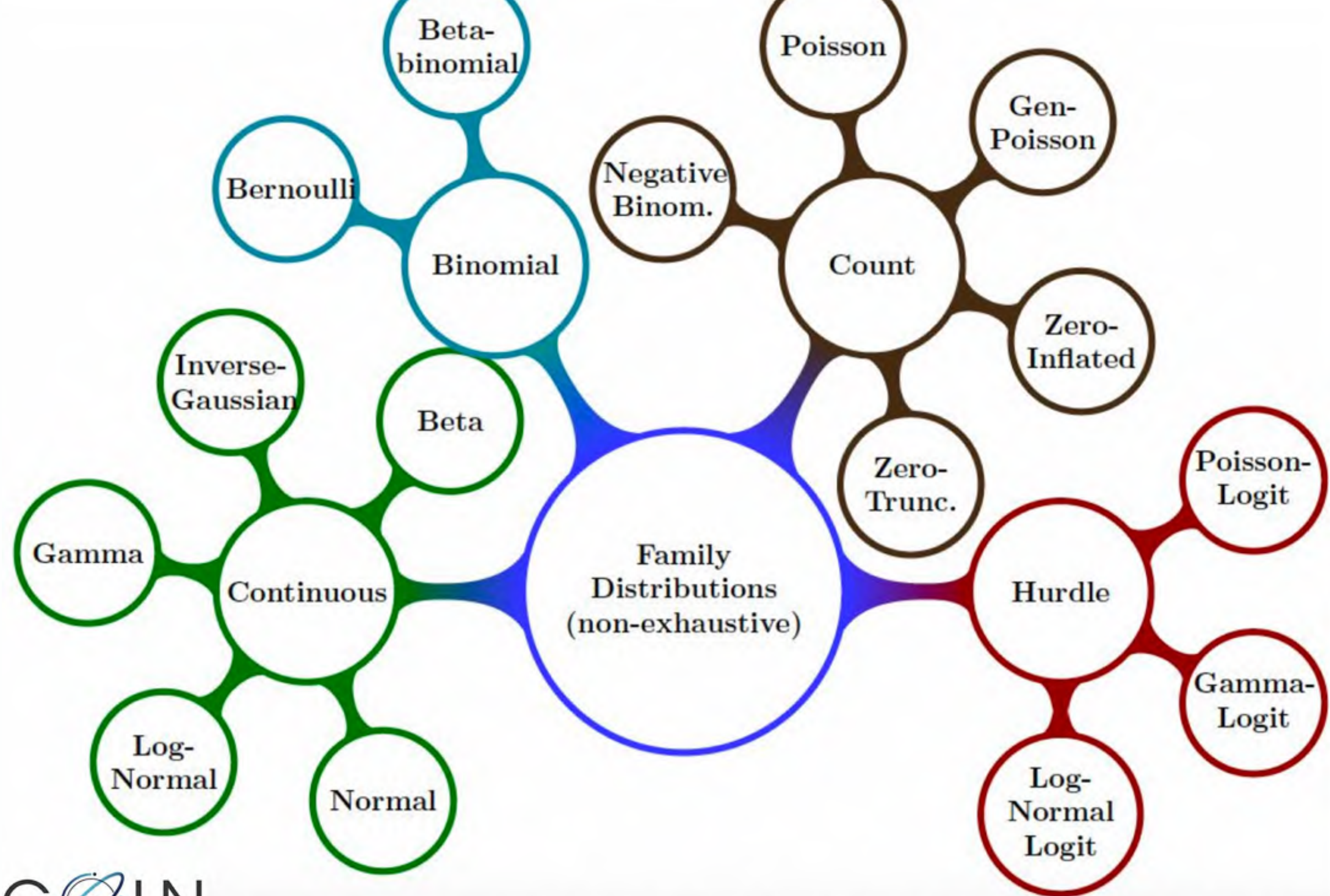
## Limitations



Discrete data







$$Y_i \sim f(\mu_i, a(\phi)V(\mu_i)),$$

$$g(\mu_i) = \eta_i,$$

$$\eta_i \equiv \mathbf{x}_i^T \boldsymbol{\beta} = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p.$$

## Special Cases

### Linear regression

$$Y_i \sim \text{Normal}(\mu_i, \sigma^2),$$

$$\mu_i = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

### Logistic regression

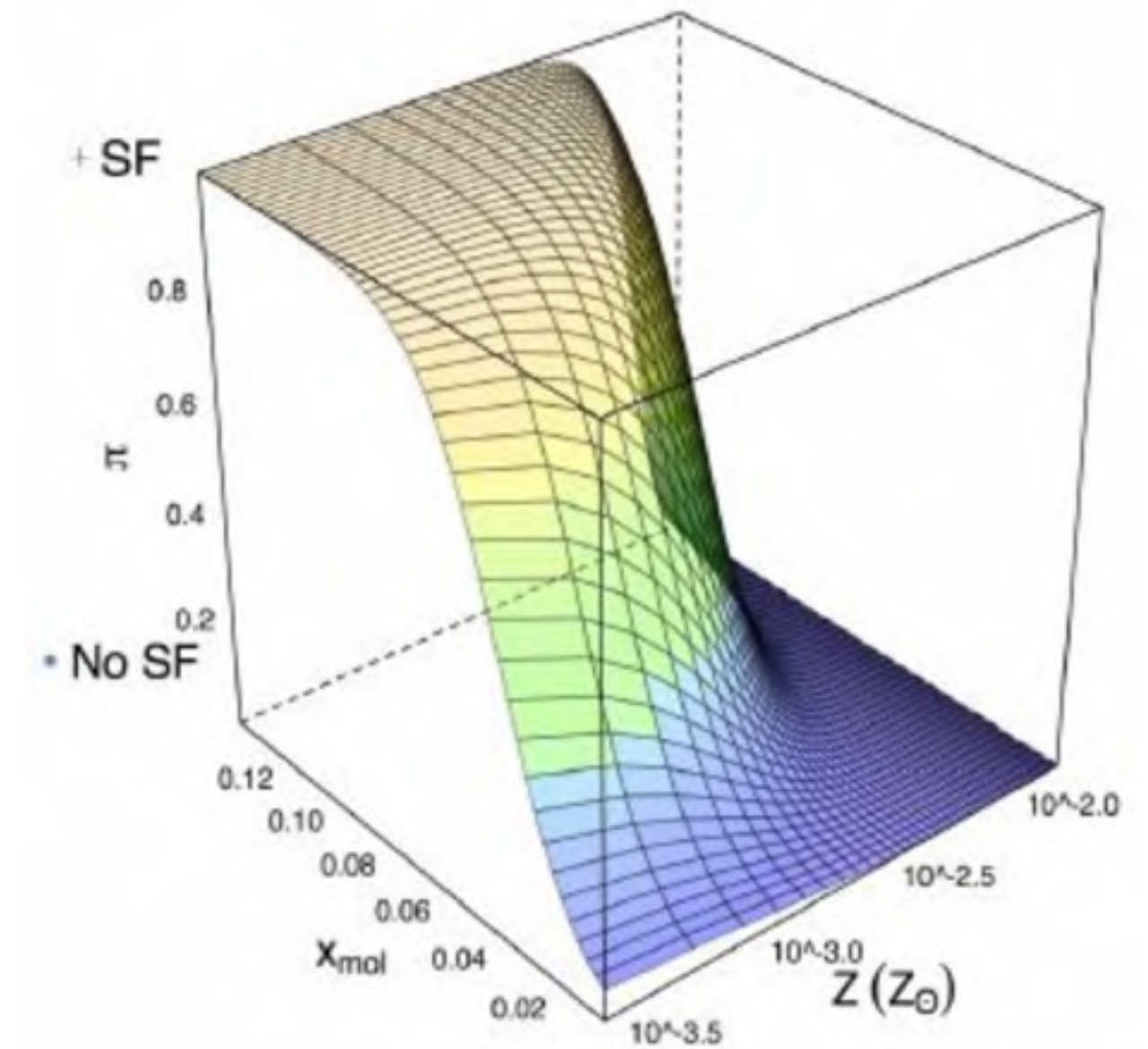
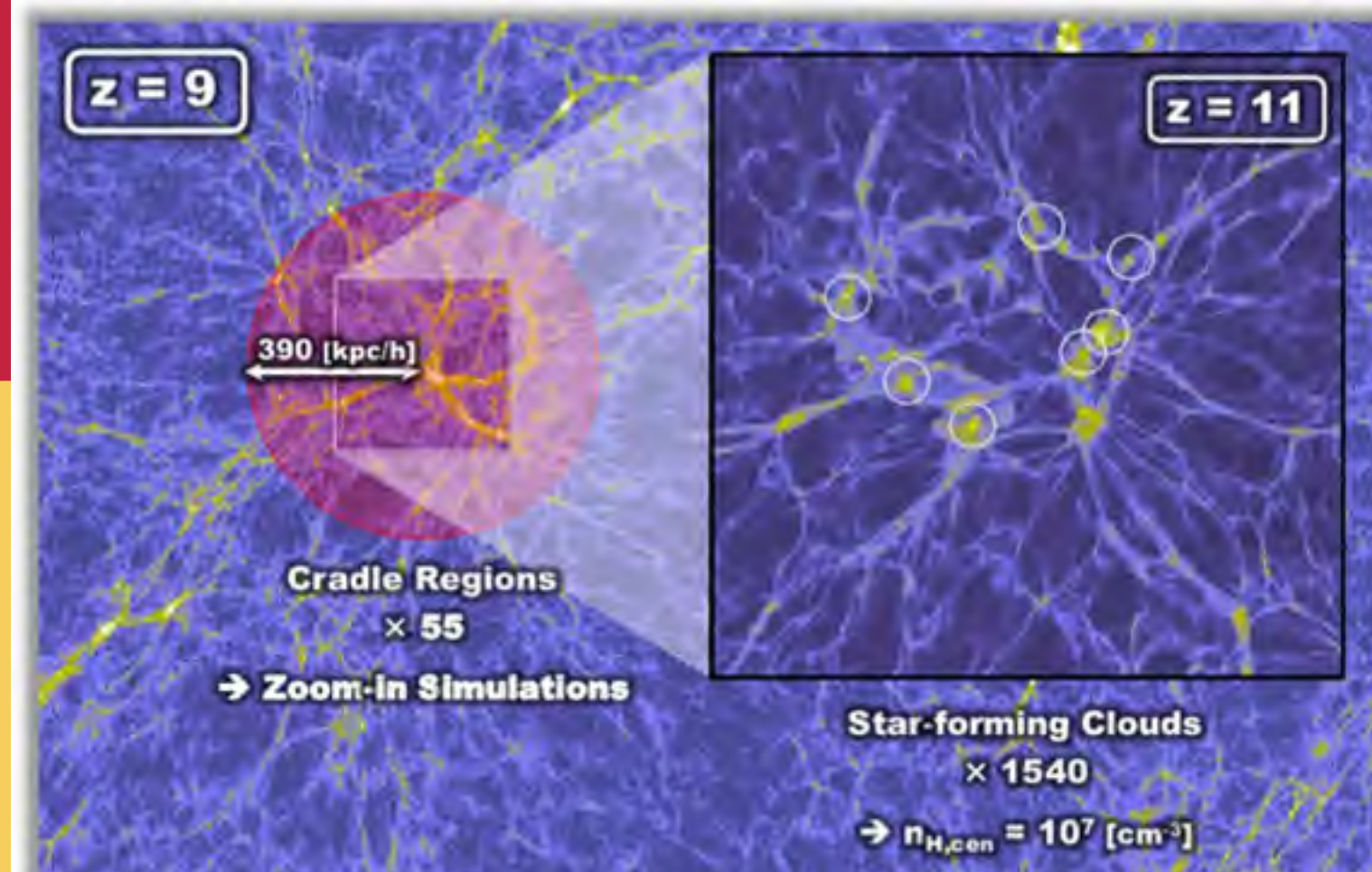
$$y_i \sim \text{Bernoulli}(p_i)$$

$$\text{logit}(p_i) = \eta_i$$

$$\eta_i \equiv \mathbf{x}_i^T \boldsymbol{\beta} = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k$$

# Generalized Linear Models: Logistic regression

Modelling Star Formation activity as a  
function of molecular fraction and  
metallicity in primordial haloes  
simulations

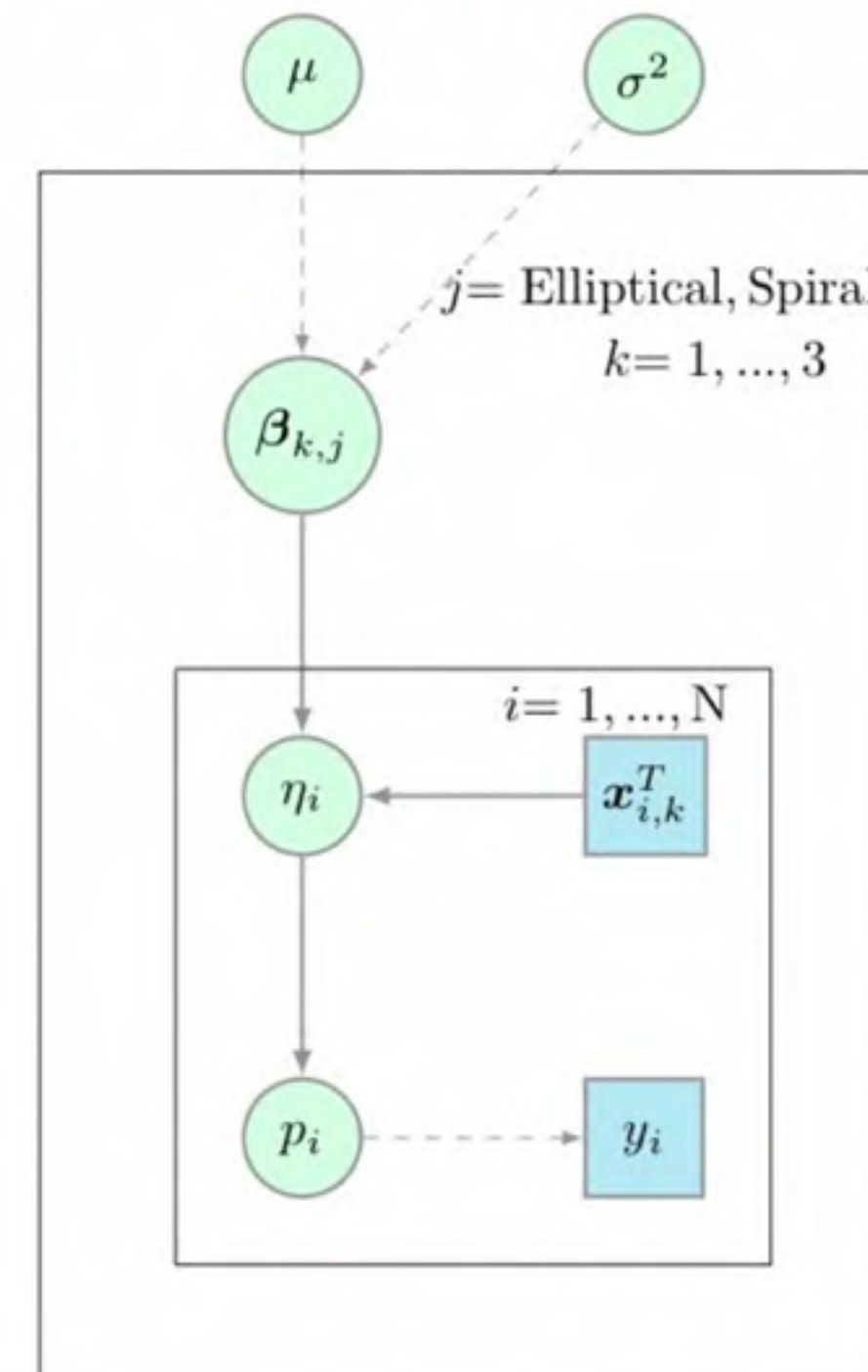
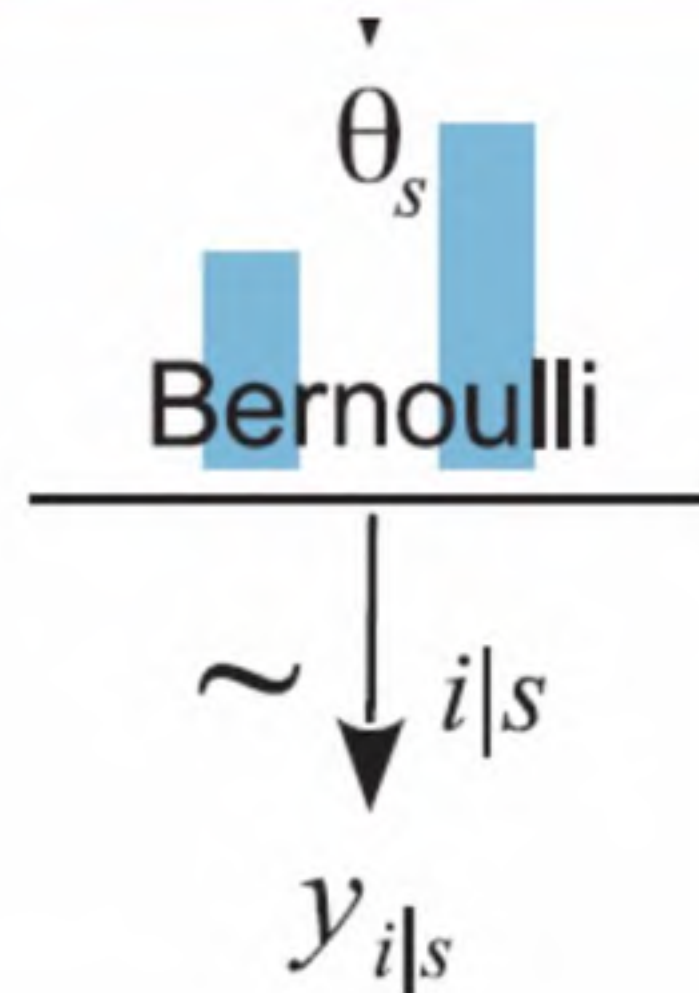


# Is the cluster environment quenching the Seyfert activity in elliptical and spiral galaxies?

R. S. de Souza ✉, M. L. L. Dantas ✉, A. Krone-Martins, E. Cameron, P. Coelho, M. W. Hattab, M. de Val-Borro, J. M. Hilbe, [J. Elliott](#), A. Hagen ... [Show more](#)

*Monthly Notices of the Royal Astronomical Society*, Volume 461, Issue 2, 11 September 2016, Pages 2115–2125, <https://doi.org/10.1093/mnras/stw1459>

## Bayesian Hierarchical Logistic Regression



$$y_i \sim \text{Bernoulli}(p_i)$$

$$\text{logit}(p_i) = \eta_i$$

$$\eta_i = \mathbf{x}_{i,k}^T \beta_{k,j}$$

$$\mathbf{x}_{i,k}^T = \begin{pmatrix} 1 & (\log M_{200})_1 & \left(\frac{r}{r_{200}}\right)_1 \\ \vdots & \vdots & \vdots \\ 1 & (\log M_{200})_N & \left(\frac{r}{r_{200}}\right)_N \end{pmatrix}$$

$$\beta_{k,j} \sim \text{Normal}(\mu, \sigma^2)$$

$$\mu \sim \text{Normal}(0, 10^3)$$

$$\tau \sim \text{Gamma}(10^{-3}, 10^{-3})$$

$$\sigma^2 = 1/\tau$$

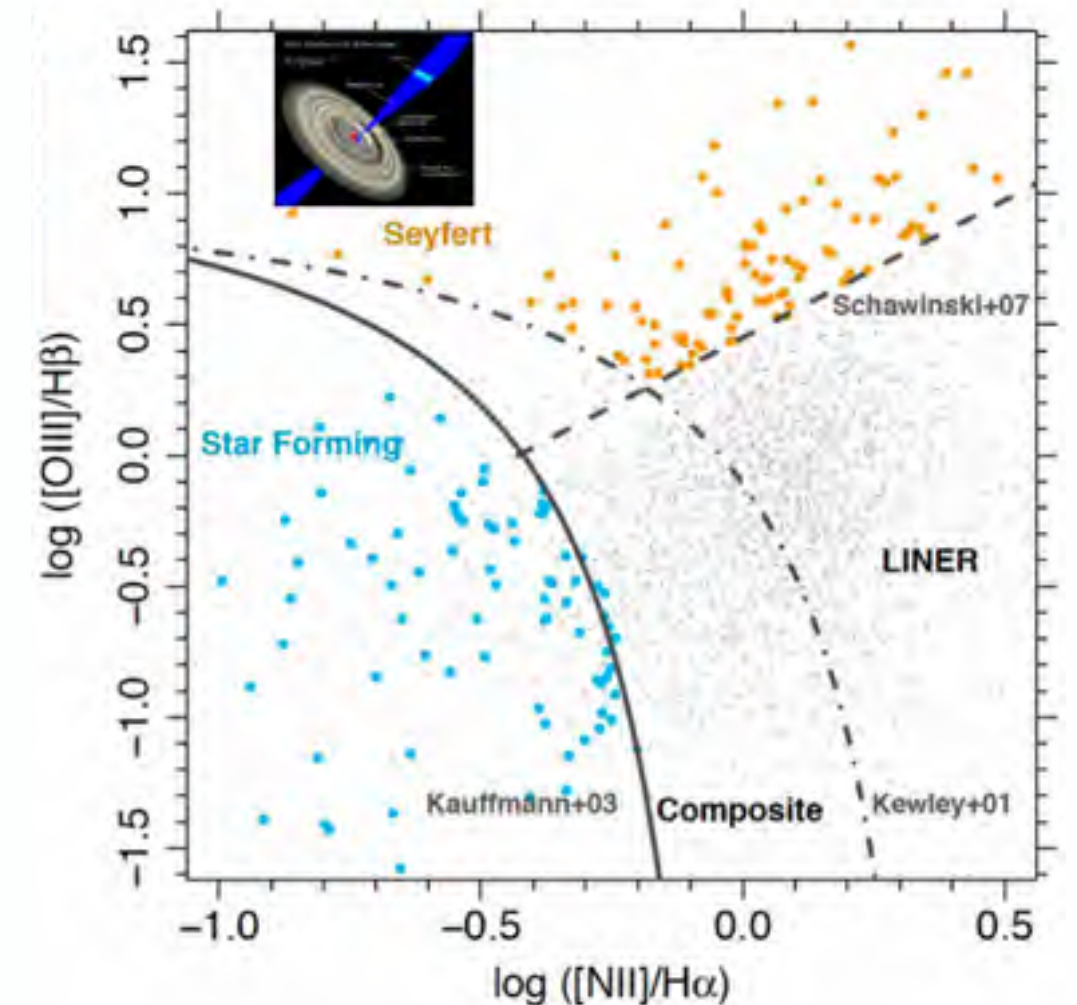
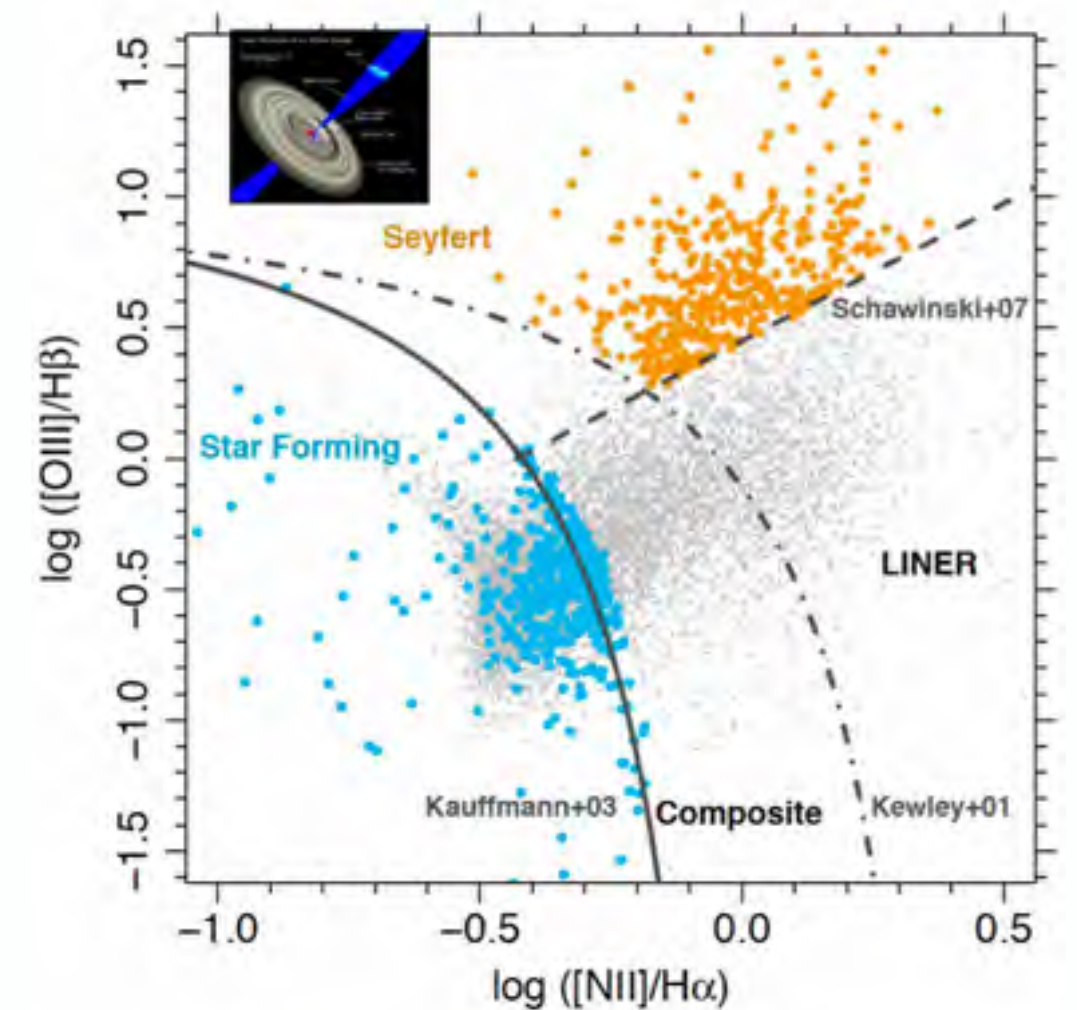
$$j = \text{Elliptical, Spiral}$$

$$k = 1, \dots, 3$$

$$i = 1, \dots, N$$

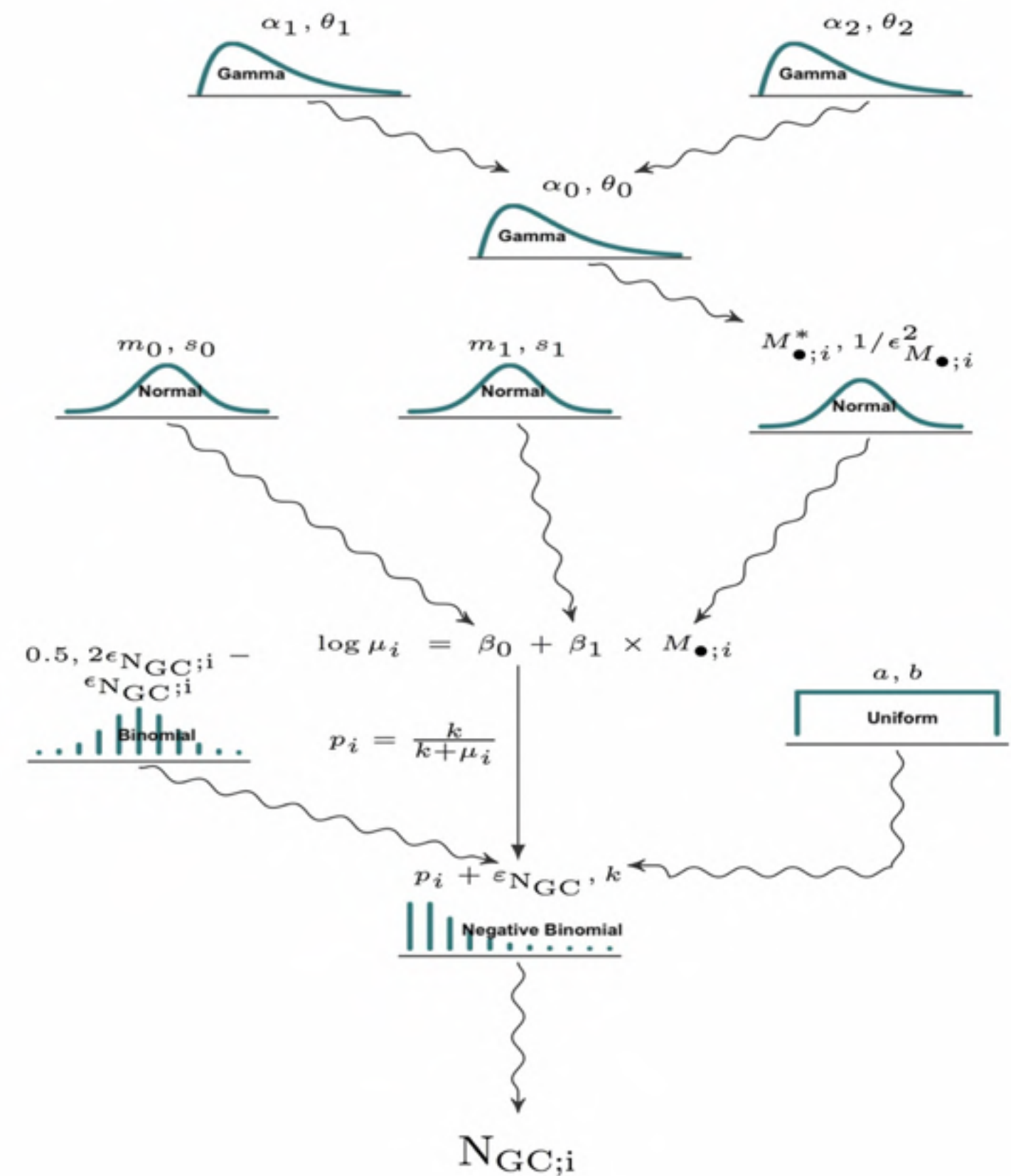
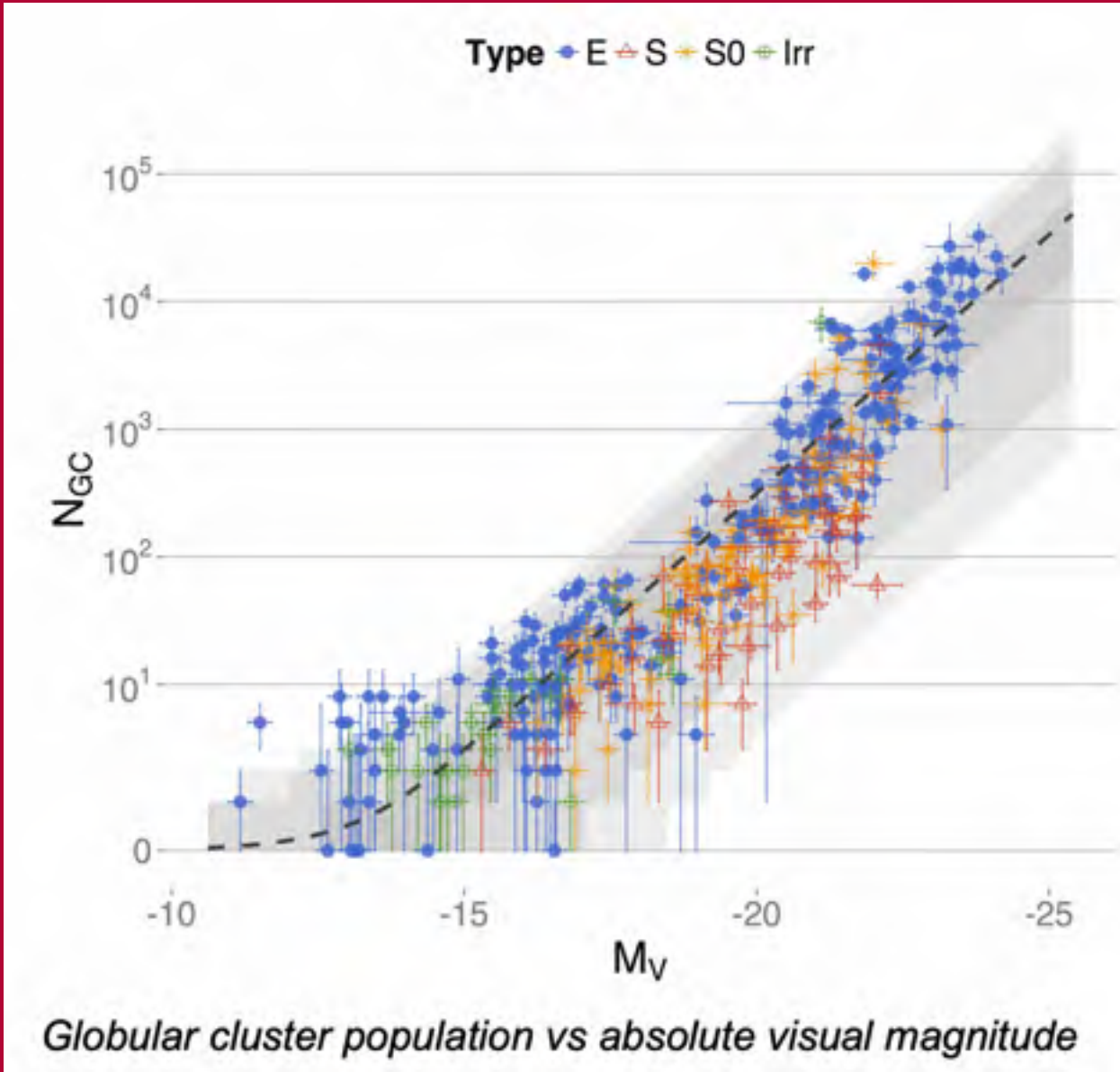
# Generalized Linear Models

Seyfert prevalence as function of  
environment and galaxy  
morphology



# Generalized Linear Models: Negative Binomial Regression

## Globular Cluster Counts as function of galaxy properties



# Generalized Linear Models

$$Y_i \sim f(\mu_i, a(\phi)V(\mu_i)),$$

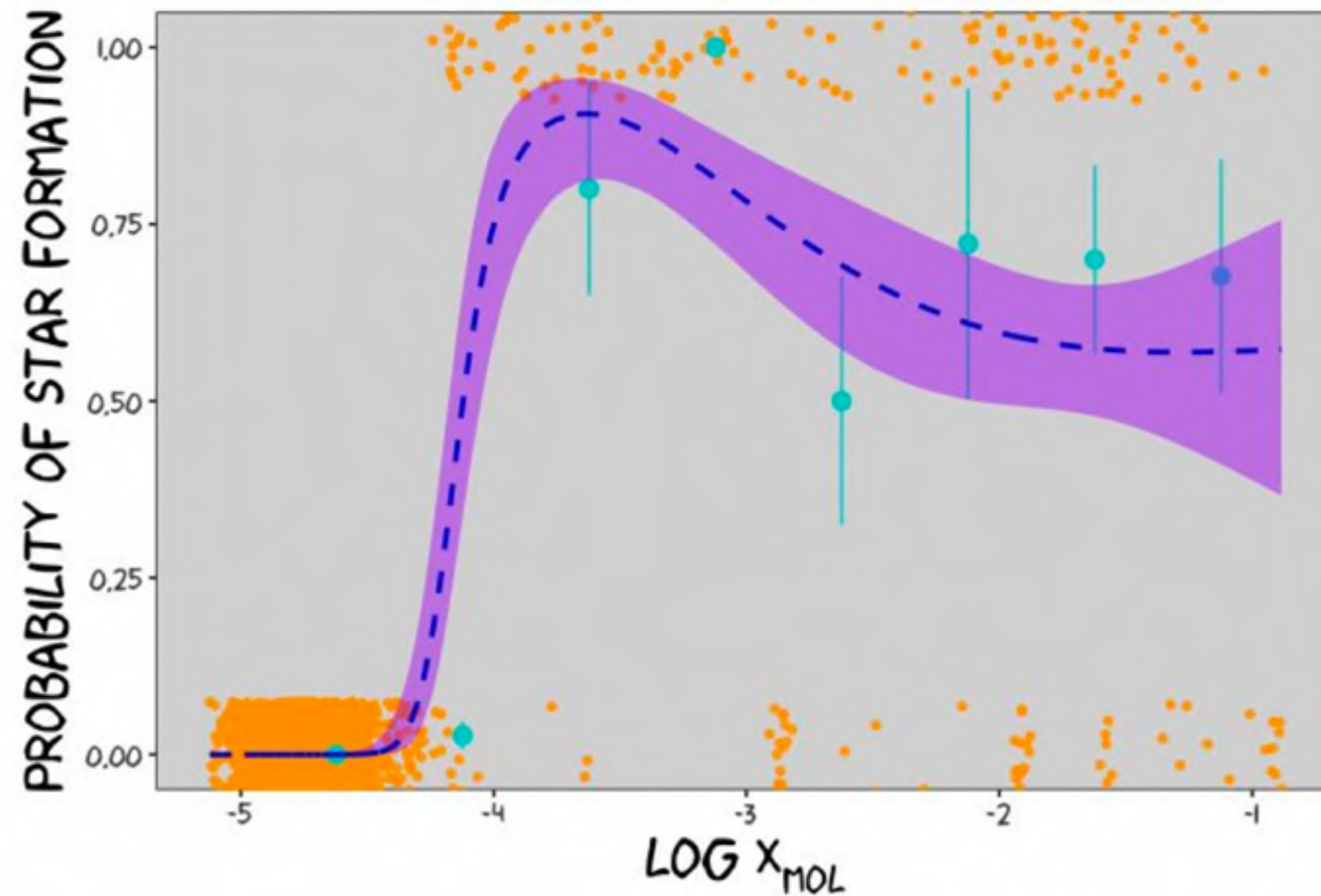
$$g(\mu_i) = \eta_i,$$

$$\eta_i \equiv \mathbf{x}_i^T \boldsymbol{\beta} = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p.$$

# Natural GLM extension

## Generalized Additive Models

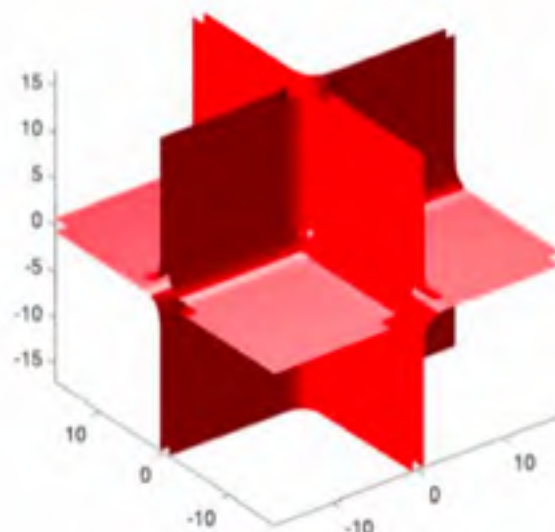
$$g(y) = f(x_1) + f(x_2) + \cdots + f(x_{\underline{D}})$$



# Geometric Interpretation

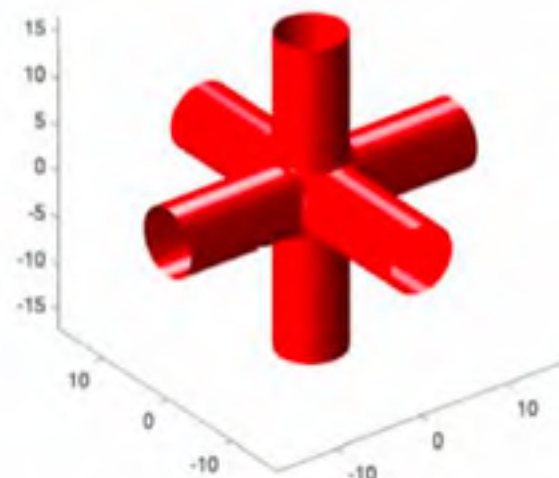
Changes how you perceive the data

Non-local Interactions

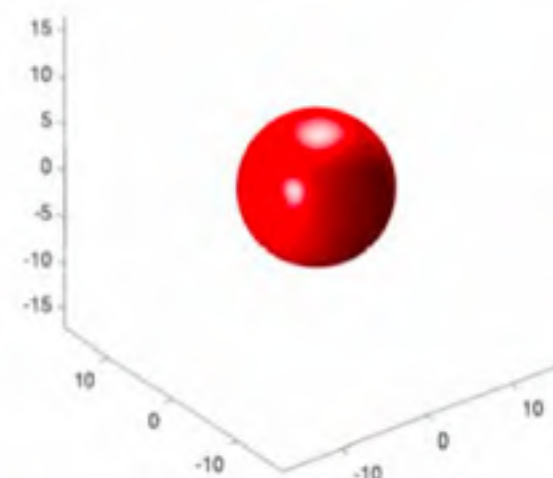


1st order interactions  
 $k_1 + k_2 + k_3$

Local interactions

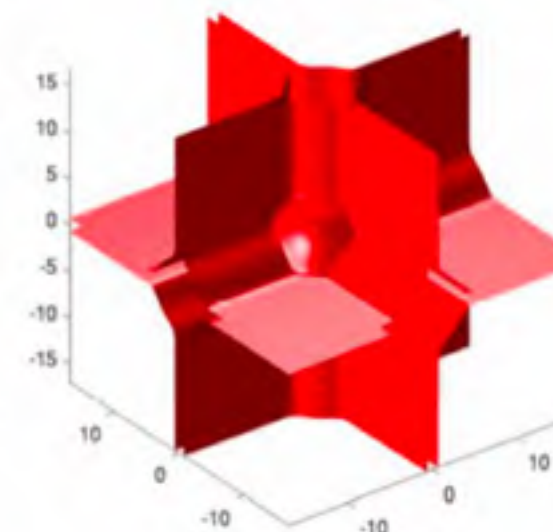


2nd order interactions  
 $k_1k_2 + k_2k_3 + k_1k_3$

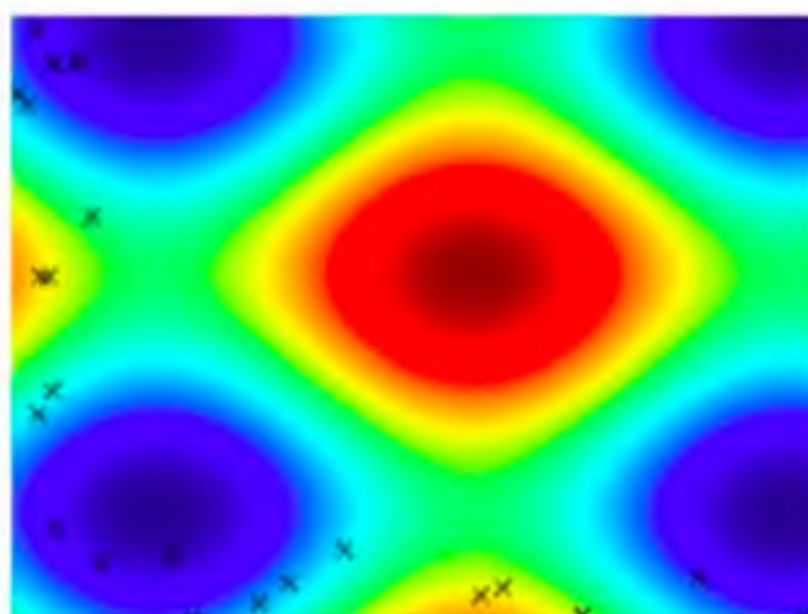


3rd order interactions  
 $k_1k_2k_3$   
(Squared-exp kernel)

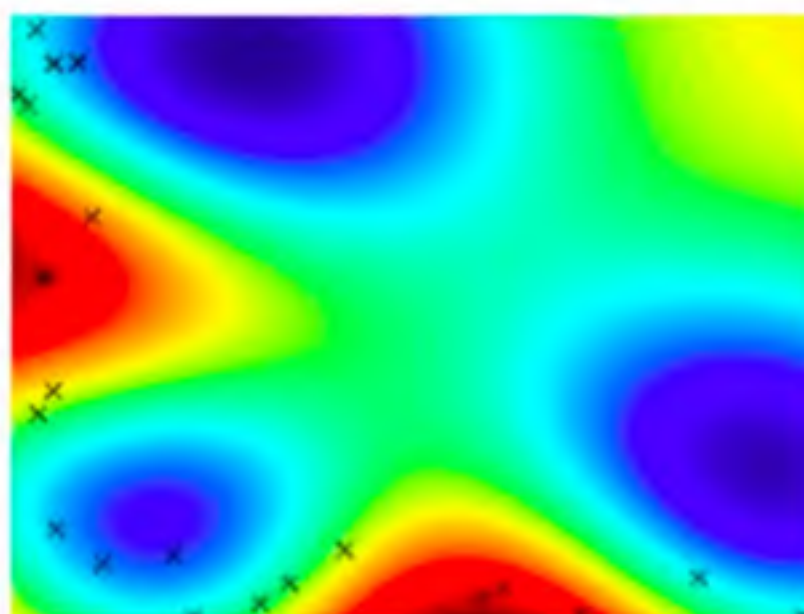
Hybrid



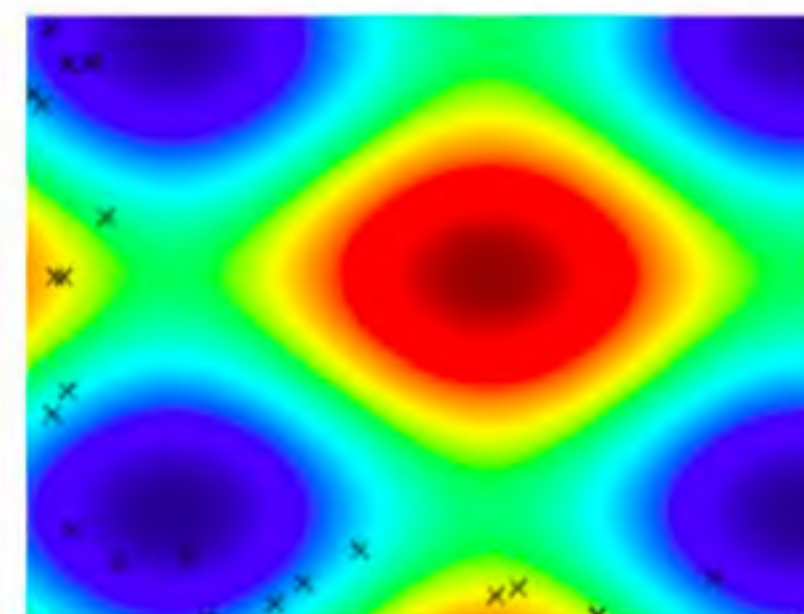
All interactions  
(Additive kernel)



True Function  
& data locations



Squared-exp GP  
posterior mean



Additive GP  
posterior mean

# OUTLINE

- Generalized Linear Models
- Statistical Learning
- Discovering stellar clusters

# Supervised ML model

data	training, target
$\mathcal{X}$	set of all samples, $x$
$\mathcal{Y}$	set of possible labels, $y$
$h_{\text{train}}$	learner: $y_{\text{est};i} = h_{\text{train}}(x_i)$
$L$	Loss function

Hypothesis:  
Training is  
representative  
of target

Data generation model:

$$x_i \sim P_{\mathcal{X}}$$

$f \rightarrow$  true labeling function,  $y_i = f(x_i)$

$$L_{\text{data},f}(h) \equiv P_{x \sim \text{data}}(h_{\text{train}}(x) \neq f(x))$$

# Supervised ML model

data

training, target

$\mathcal{X}$

set of all samples,  $x$

$\mathcal{Y}$

set of possible labels,  $y$

*Machine Learning algorithm*

Hypothesis:  
training is  
representative  
of target

$h_{\text{train}}$

learner:  $y_{\text{est};i} = h_{\text{train}}(x_i)$

$L$

Loss function

Data generation model:

$$x_i \sim P_{\mathcal{X}}$$

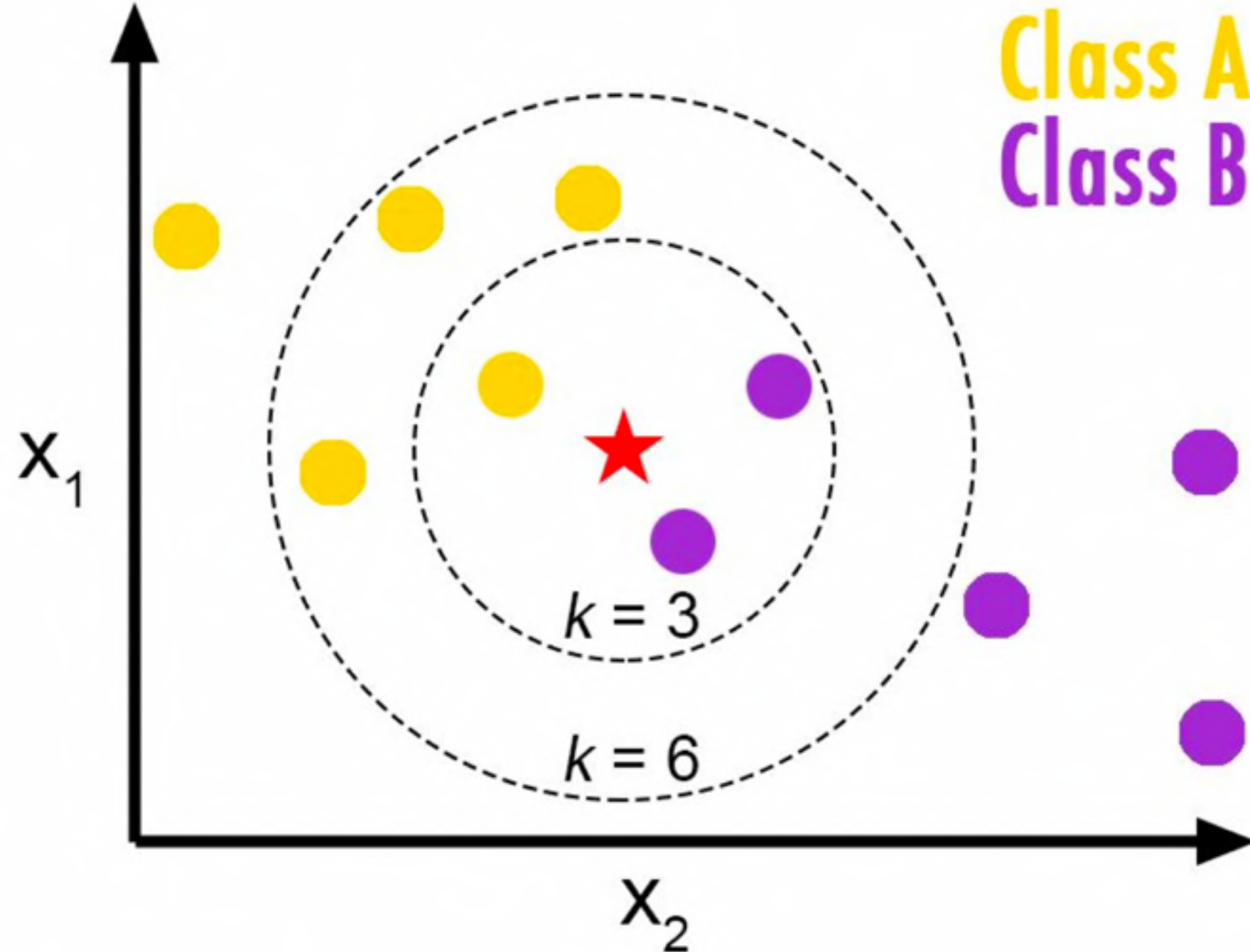
$f \rightarrow$  true labeling function,  $y_i = f(x_i)$

$$L_{\text{data},f}(h) \equiv P_{x \sim \text{data}}(h_{\text{train}}(x) \neq f(x))$$

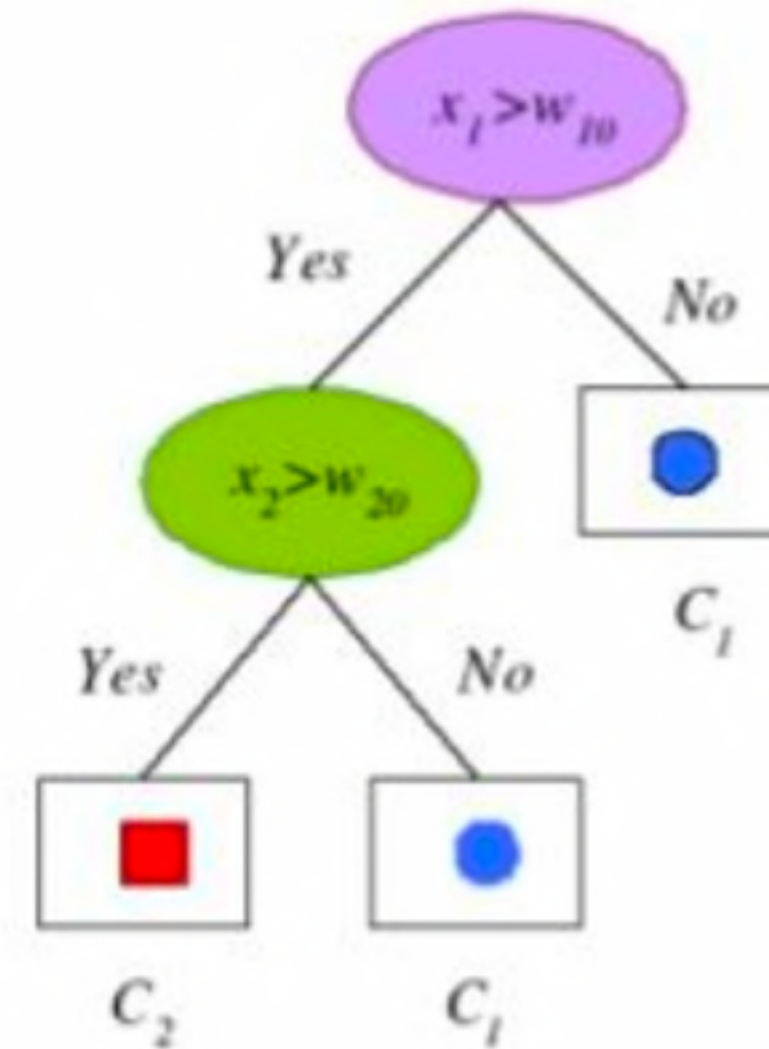
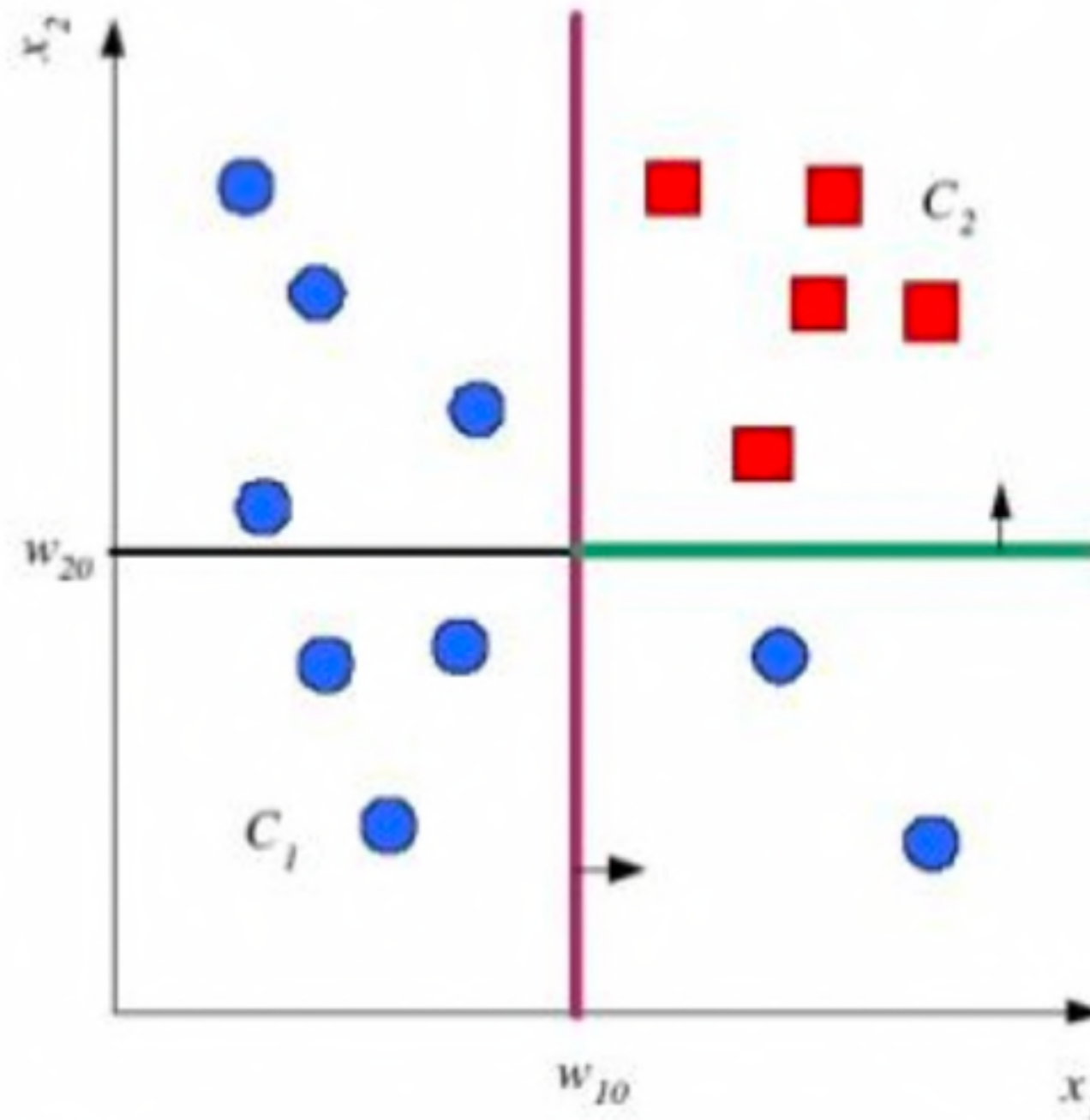
*Example of supervised ML algorithm for classification*

# k-Nearest Neighbor (kNN)

*Distance based*



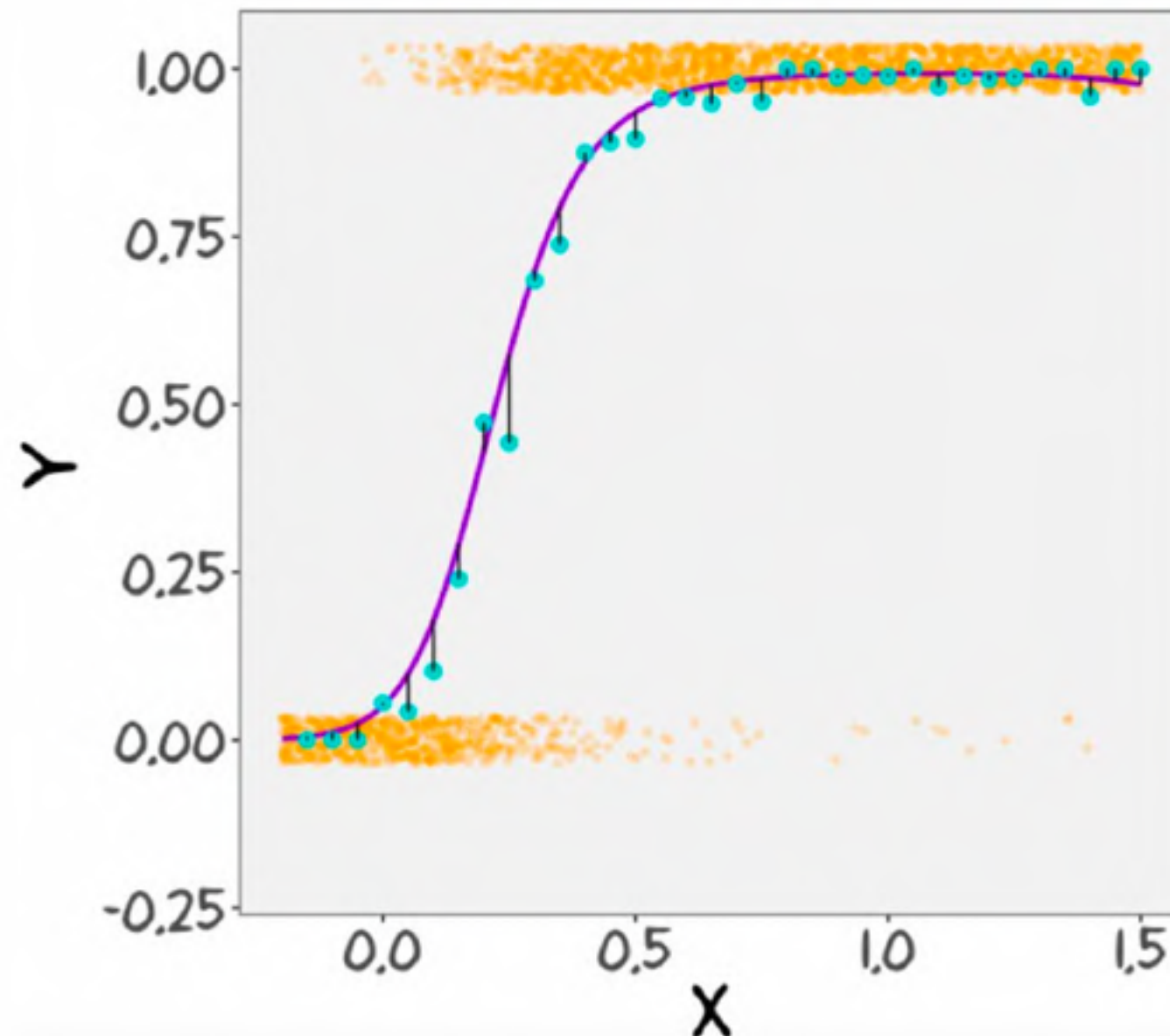
# Decision Trees



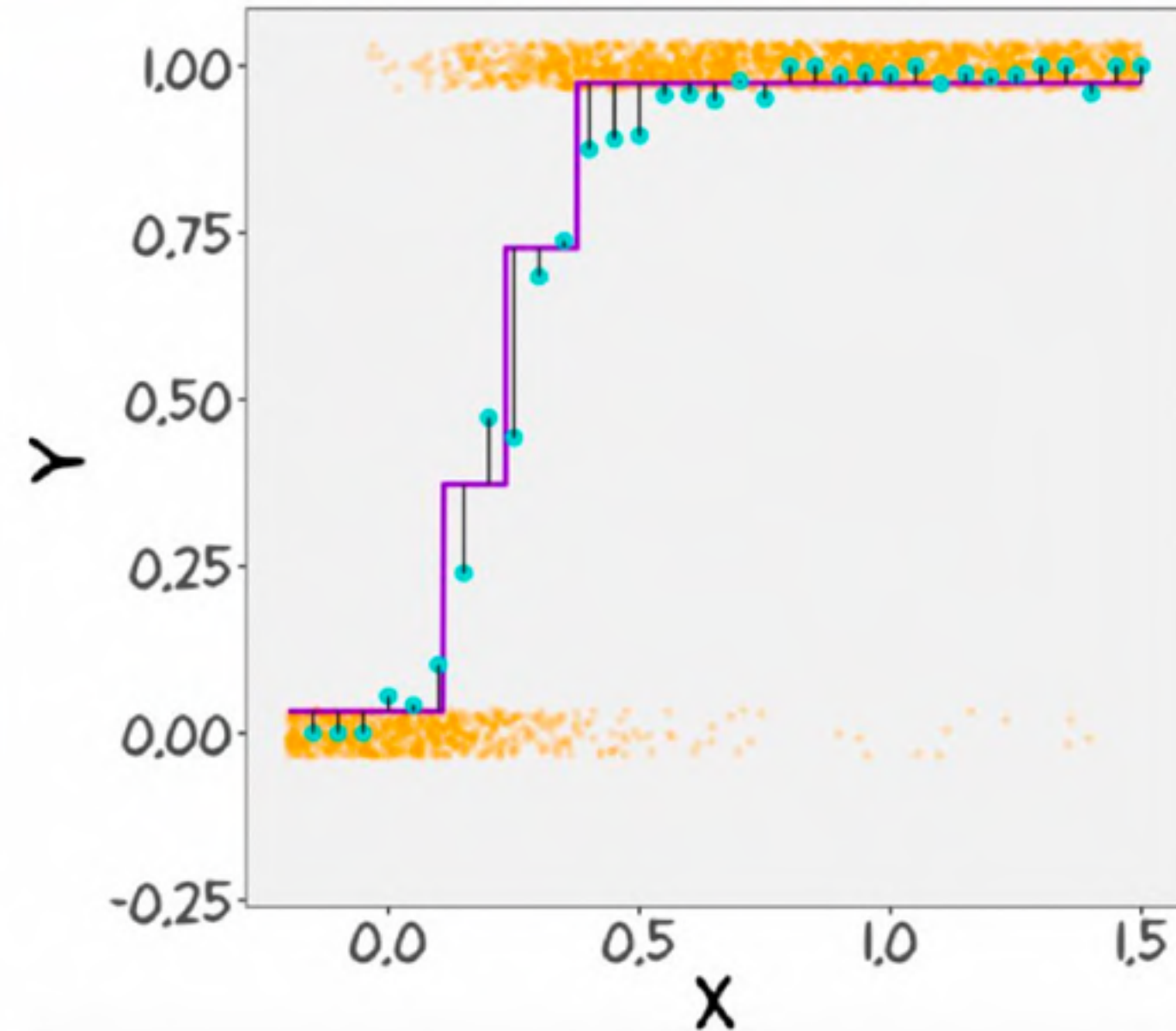
# Logistic regression "vs" Decision Tree

Caveat: You get what you ask for

## Logistic Regression



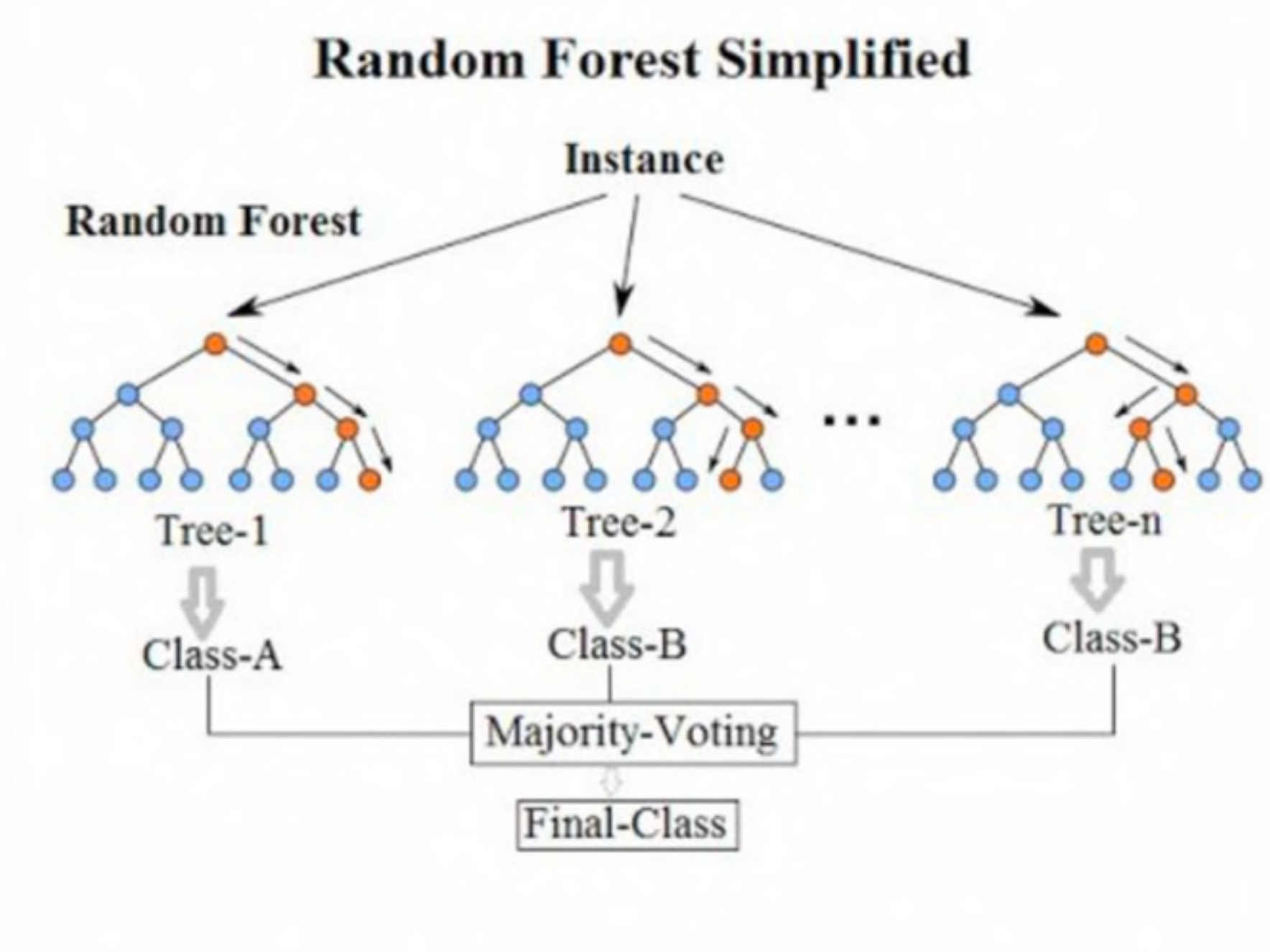
## Decision Tree



*Example of supervised ML algorithm for classification*

# Random Forests

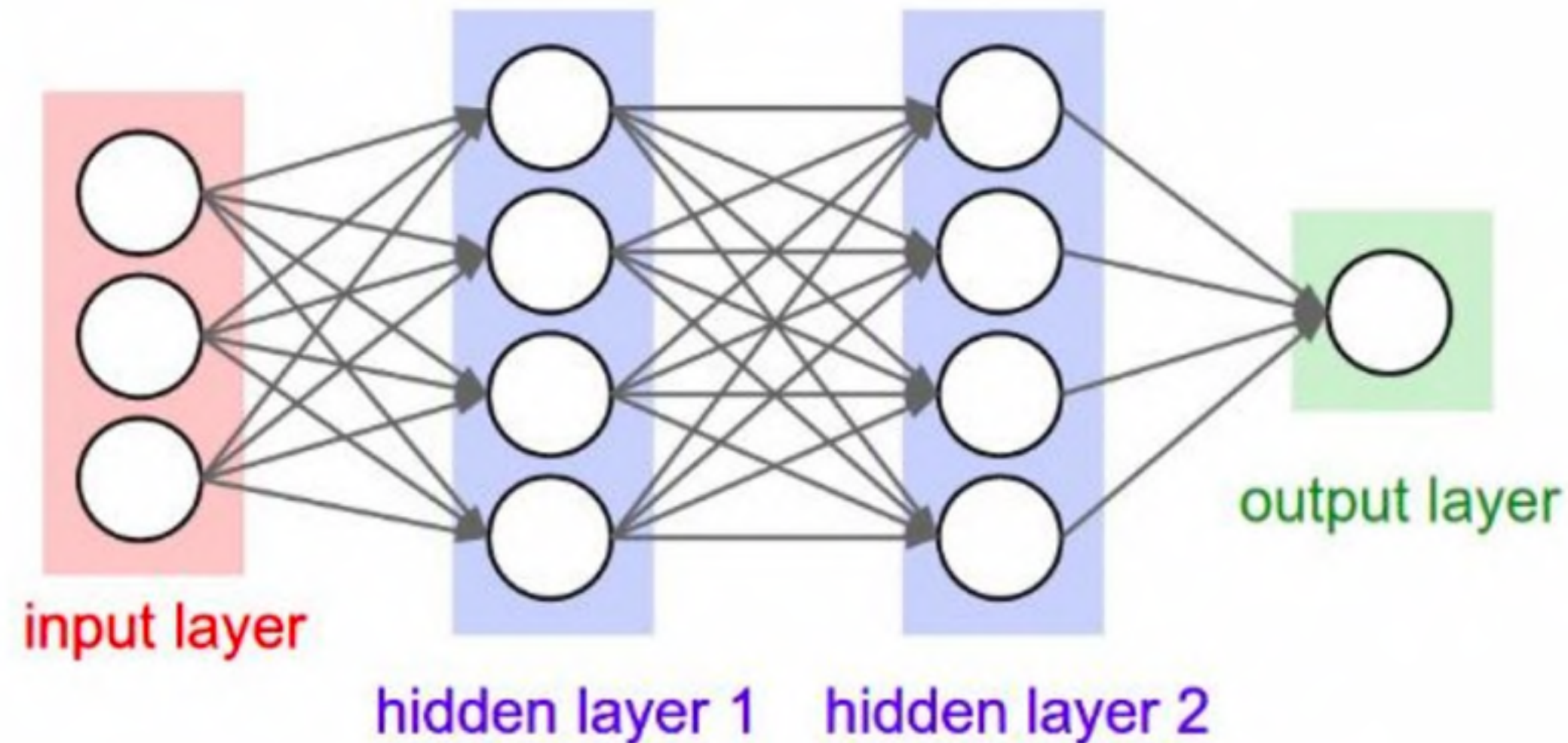
*Ensemble method*



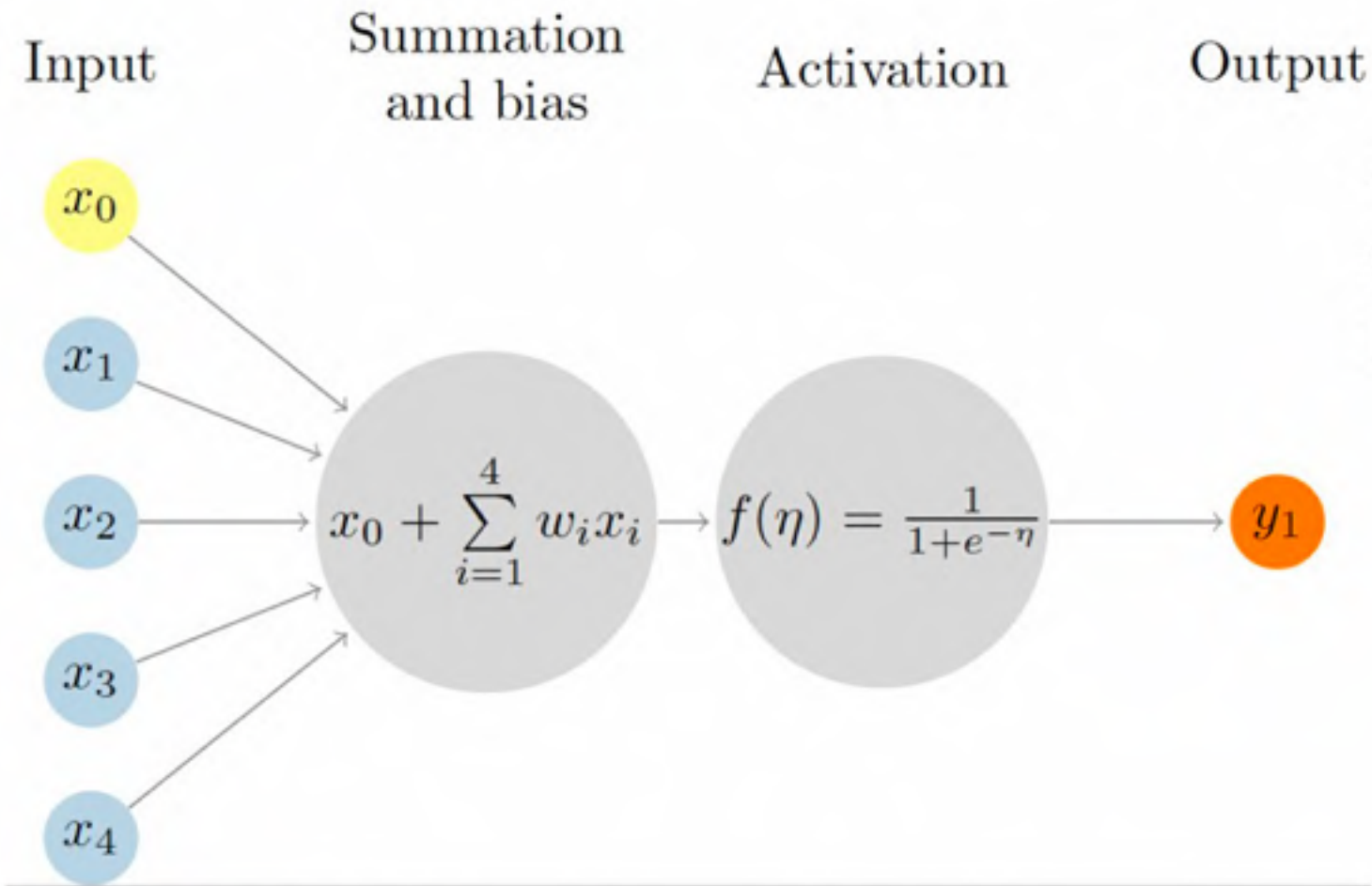
*Example of supervised ML algorithm:*

# Deep Neural Network

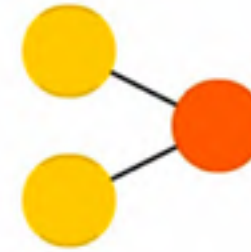
All layers internal to the network (not input or output layer) are considered **hidden layers**.



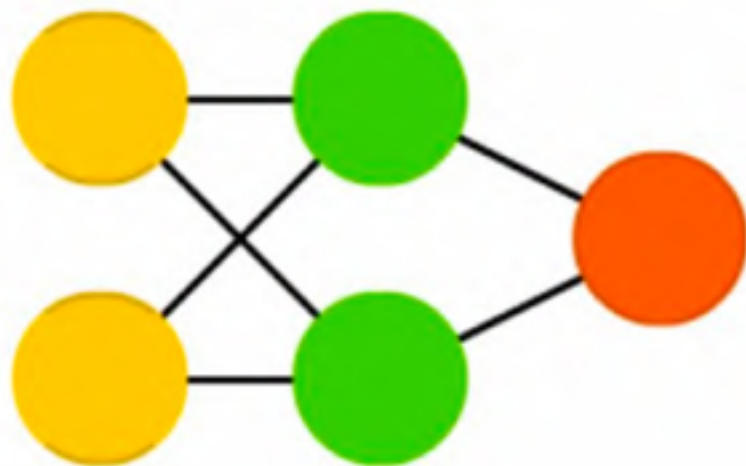
# Single-Layer Perceptron $\equiv$ Logistic Regression



Good old days. Pretty much it, gets data, sums data, transforms data (i.e. sigmoid, logit, ...), outputs data.



## Multi-Layer Perceptron

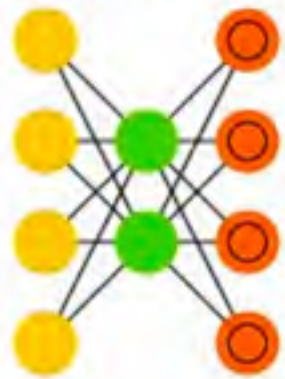


The 50's. Let's add some extra layer between input and output ("hidden layer").

# Neural Networks

## Architecture is the key

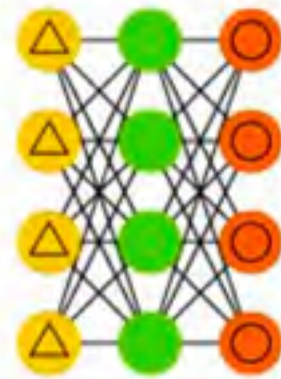
Auto Encoder (AE)



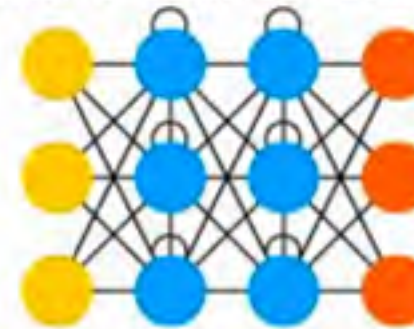
Variational AE (VAE)



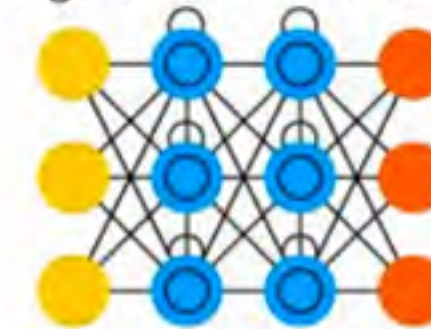
Denoising AE (DAE)



Recurrent Neural Network (RNN)



Long / Short Term Memory (LSTM)



Markov Chain (MC)



Hopfield Network (HN)



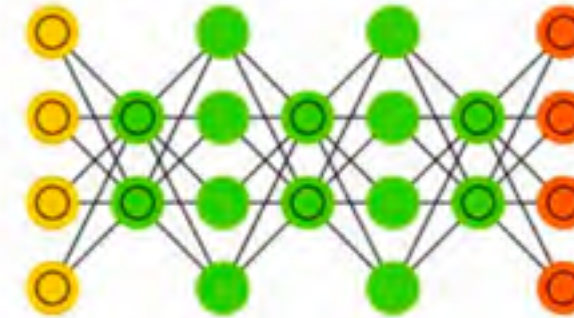
Boltzmann Machine (BM)



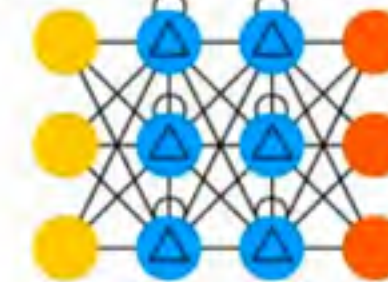
Restricted BM (RBM)



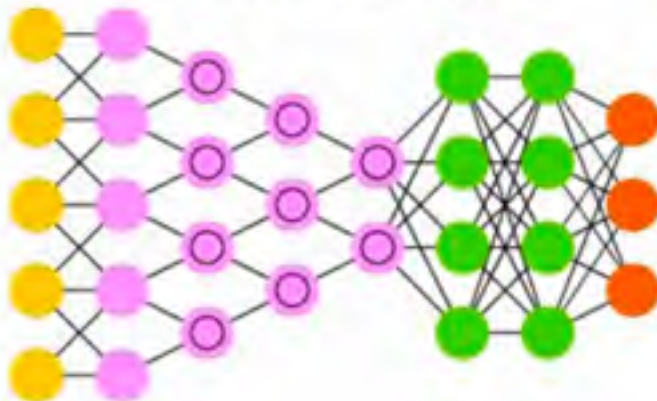
Deep Belief Network (DBN)



Gated Recurrent Unit (GRU)



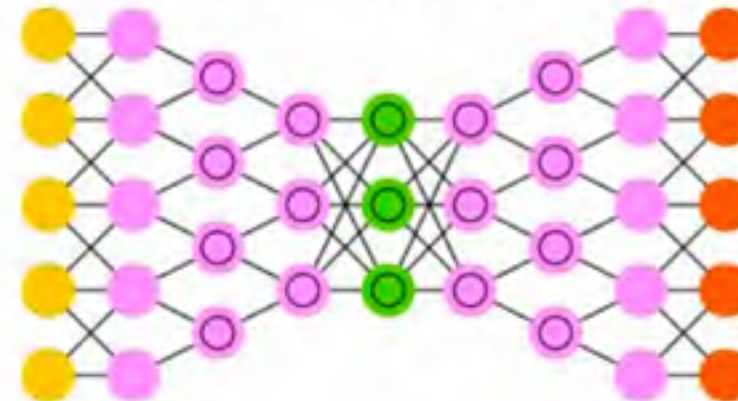
Deep Convolutional Network (DCN)



Deconvolutional Network (DN)

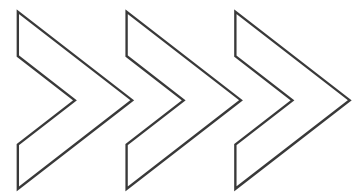


Deep Convolutional Inverse Graphics Network (DCIGN)

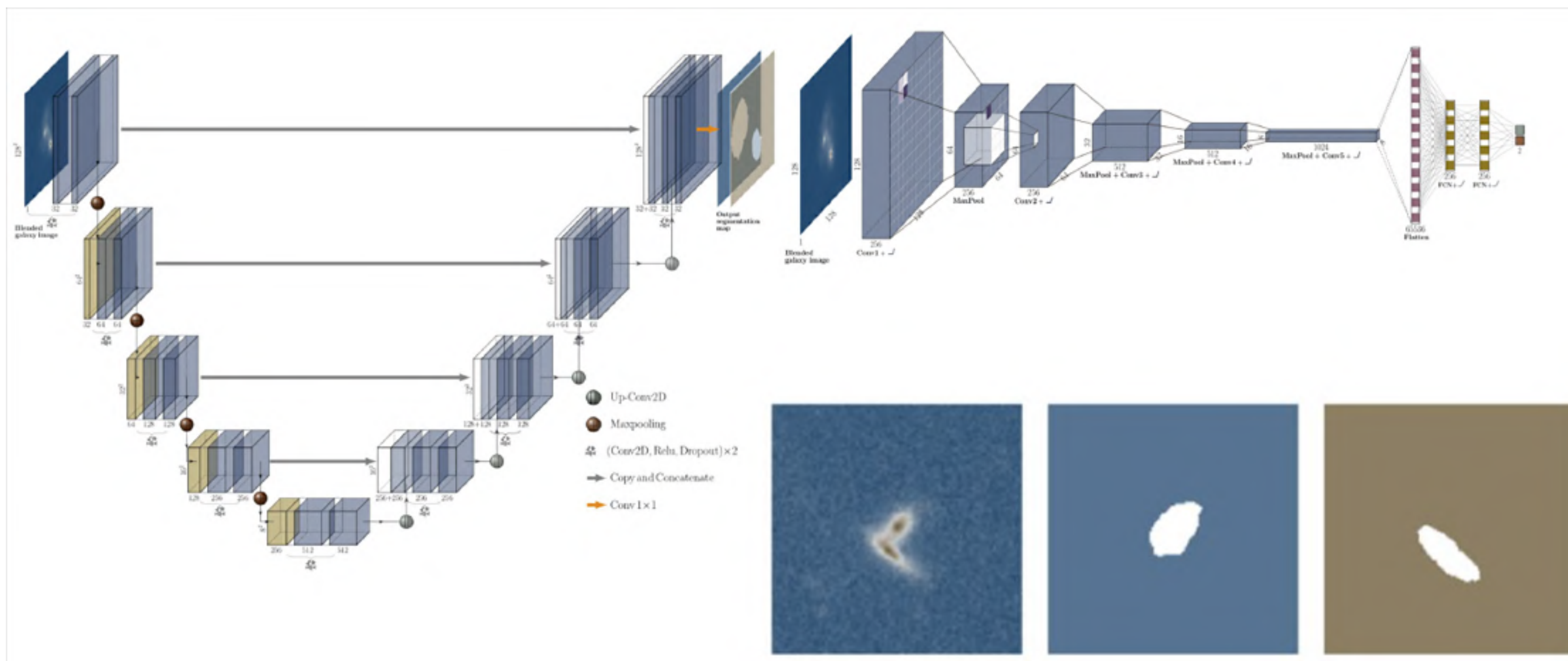


Sparse AE (SAE)





# Galaxy Deblending via Deep Learning



# Supervised ML model

data	training, target
$\mathcal{X}$	set of all samples, $x$
$\mathcal{Y}$	set of possible labels, $y$
$h_{\text{train}}$	learner: $y_{\text{est};i} = h_{\text{train}}(x_i)$
$L$	Loss function

Hypothesis:  
Training is  
representative  
of target

Data generation model:

$$x_i \sim P_{\mathcal{X}}$$

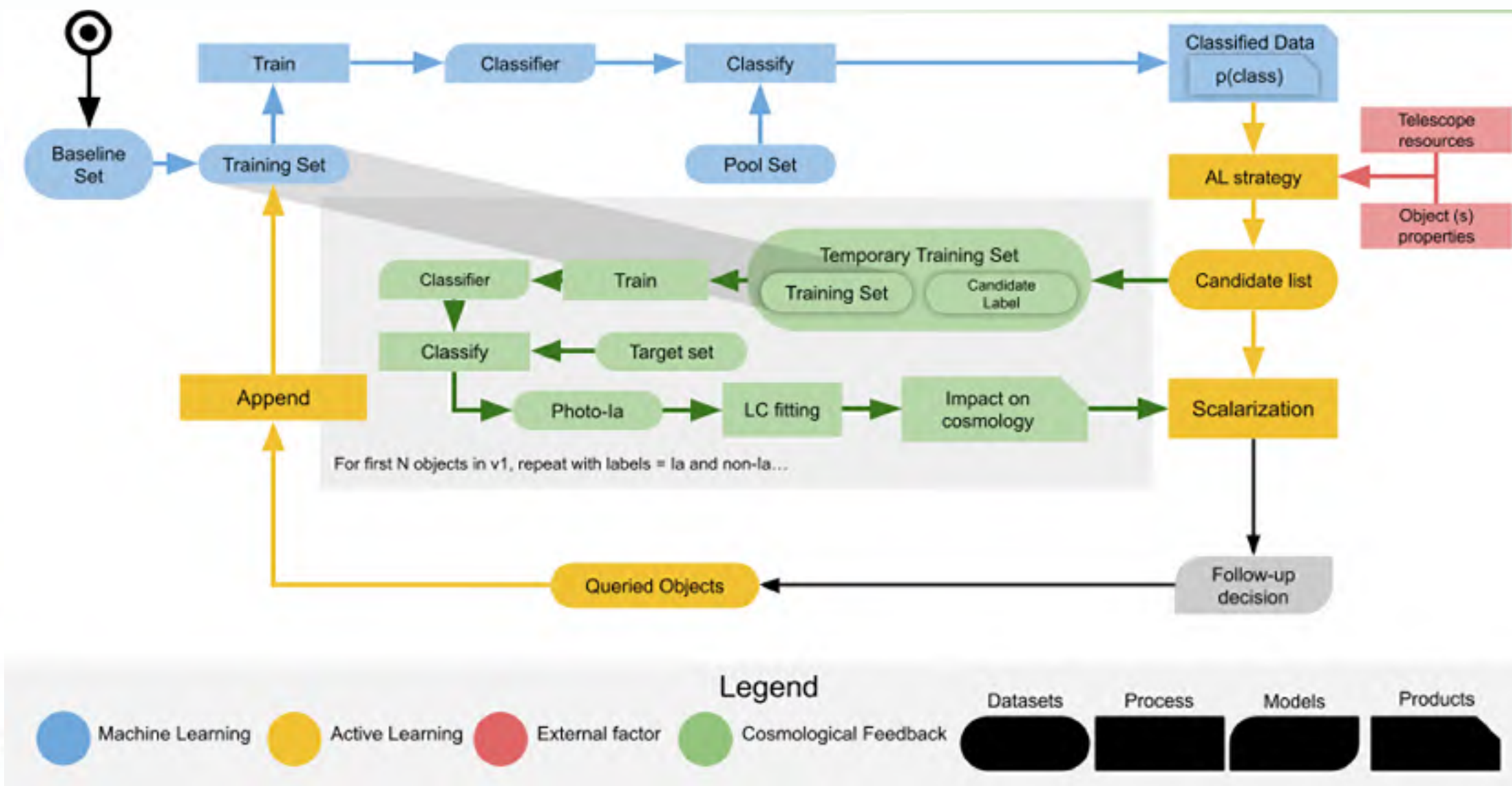
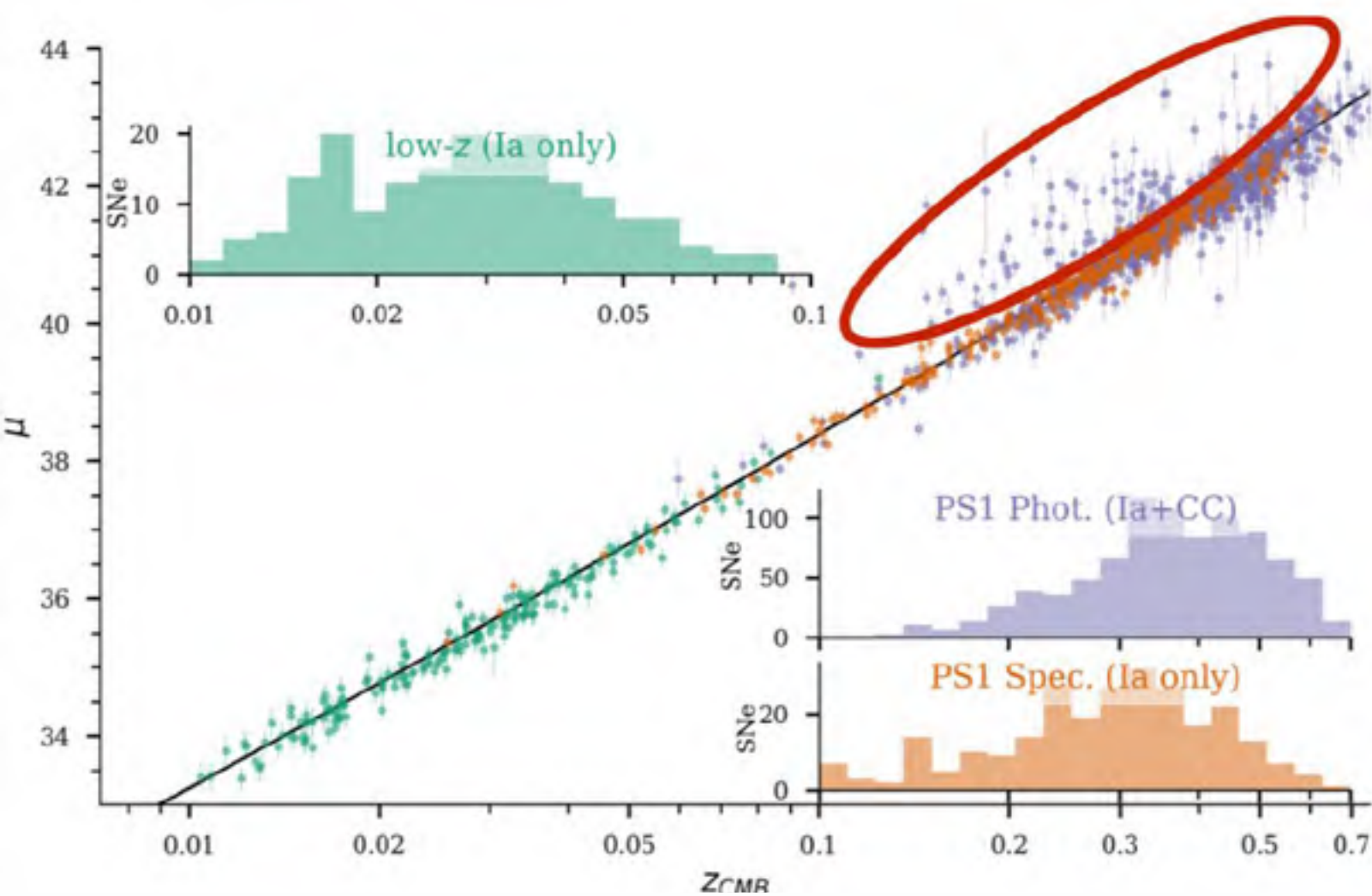
$f \rightarrow$  true labeling function,  $y_i = f(x_i)$

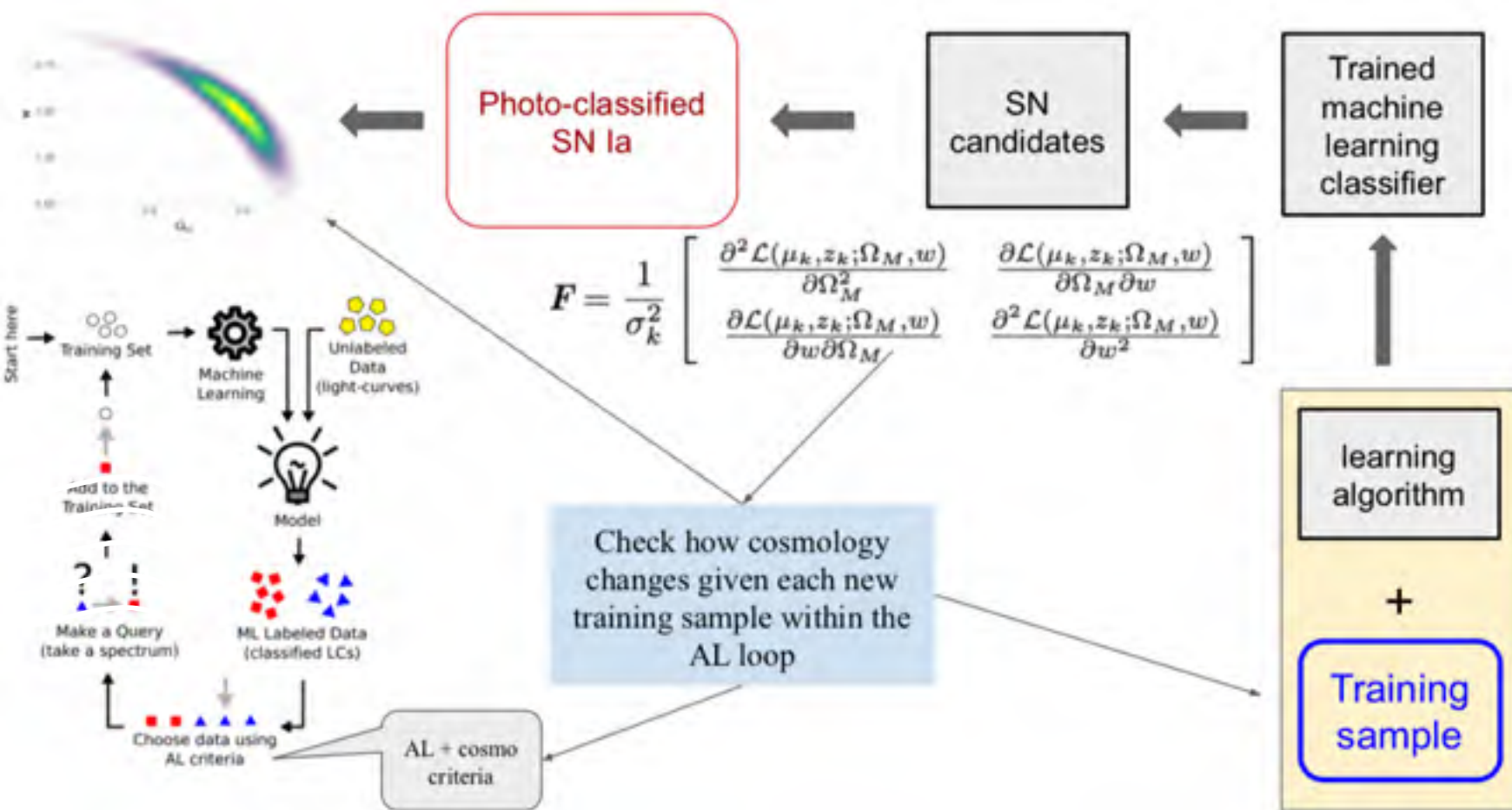
$$L_{\text{data},f}(h) \equiv P_{x \sim \text{data}}(h_{\text{train}}(x) \neq f(x))$$



The REcommendation System for SPECTroscopic follow-up (RESSPECT) is a collaboration between COIN and LSST-DESC which aims to adapt active learning strategies for the construction of optimized training samples for supernova photometric classification in the context of LSST.

# Supernova Cosmology photometric data





# Resource allocation for extragalactic Transients

## Challenges:

- Feature extraction of unevenly, noisy, incomplete multivariate time-series
- Online learning
- Scalable uncertainty quantification
- Domain-specific knapsack constraints, e.g. telescope time allocation, cosmology informed loss function



## The Cosmostatistics Initiative

The Cosmostatistics Initiative (COIN) is an international network which aims to create an interdisciplinary environment where collaborations between astronomers, statisticians and machine learning experts can flourish. The group utilizes a management model which can find parallel in technological start-ups: based on a dynamic, non-hierarchical and people-centric approach.

## The LSST Dark Energy Science Collaboration

The LSST Dark Energy Science Collaboration (DESC) is an international collaboration preparing for a variety of cosmological analyses with the Large Synoptic Survey Telescope (LSST) data. In advance of LSST's first observations, DESC will help prepare for LSST science analysis, make synergistic connections with ongoing cosmological surveys and provide the dark energy community with state of the art analysis tools.



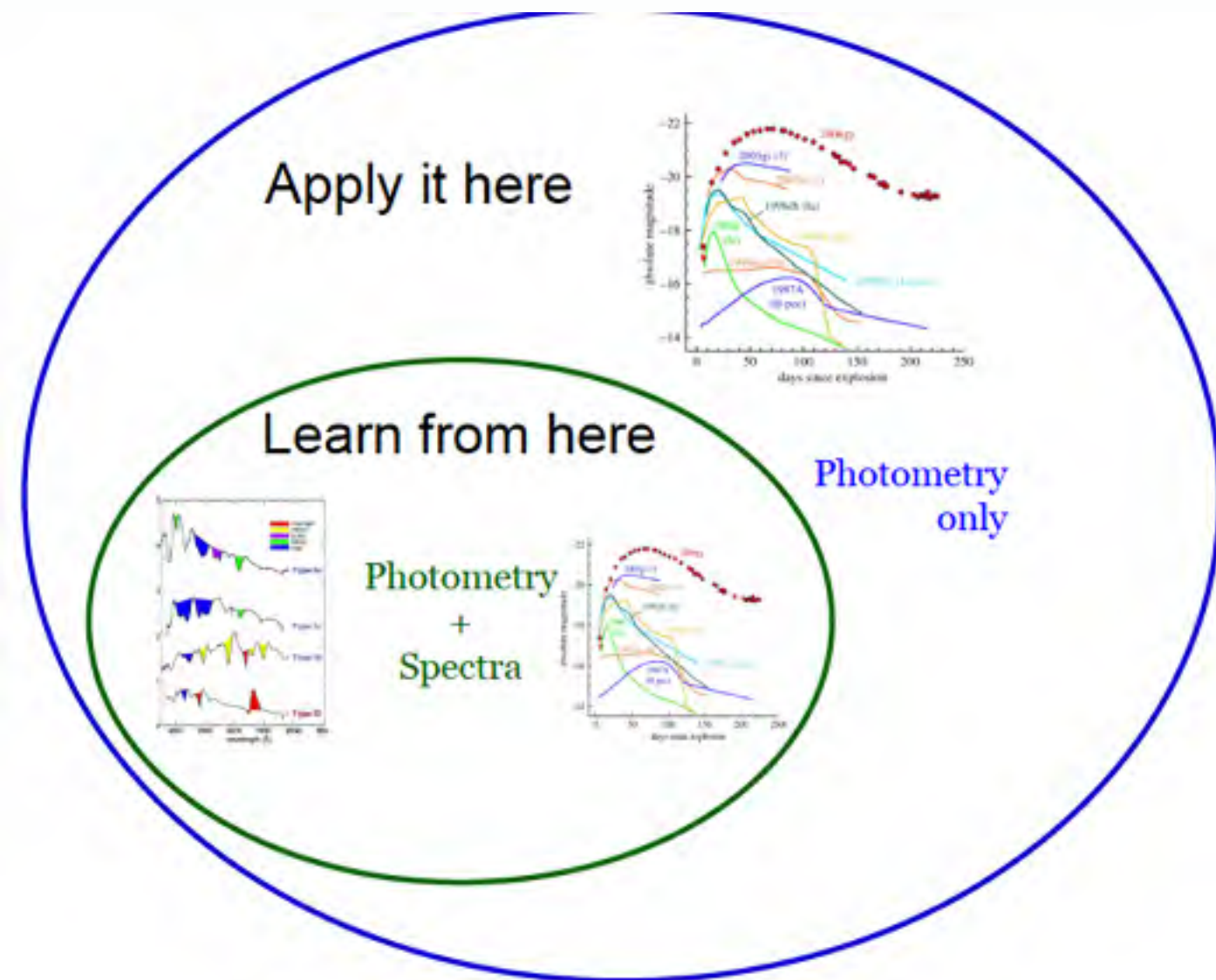
## RESPECT

The REcommendation System for SPECTroscopic follow-up (RESPECT) is a collaboration between COIN and LSST-DESC which aims to adapt active learning strategies for the construction of optimized training samples for supernova photometric classification in the context of LSST.

The team is formed by researchers from both collaborations who are working together in the development of a recommendation system which will enable informed decisions regarding the allocation of spectroscopic follow-up resources and consequent optimized scientific results from purely photometric samples.



# Supernova Cosmology photometric data



~ 3,000 cosmological useful SNe

~ 100,000 cosmological useful SNe

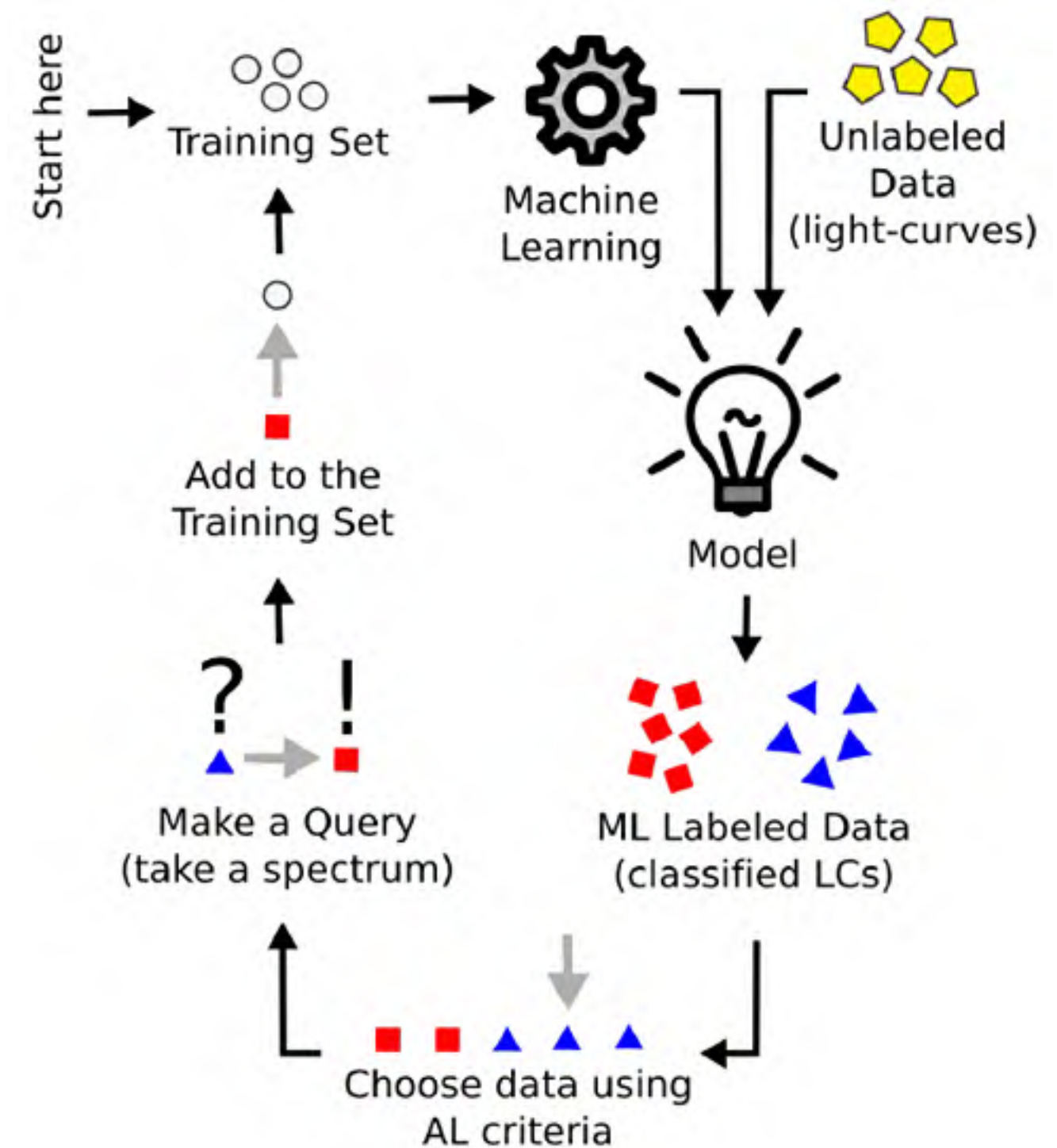


LSST DESC & COIN  
**RESSPECT**  
Recommendation System for Spectroscopic Follow-up

## Challenges:

- Window of Opportunity for Labelling
- Evolving Samples - We must make query decisions before we can observe the full LC
- Multiple Instruments
- Evolving Costs - Observing costs for a given object changes as it evolves.

# Active Learning



# OUTLINE

- Generalized Linear Models
- Statistical Learning
- Discovering stellar clusters

# Star Clusters

The cluster members share common properties, like age, distance from the Sun, and velocity, span ages from  $\sim 1$  Myr to  $> 10$  Gyrs.

Laboratories for Stellar  
Evolution Models!

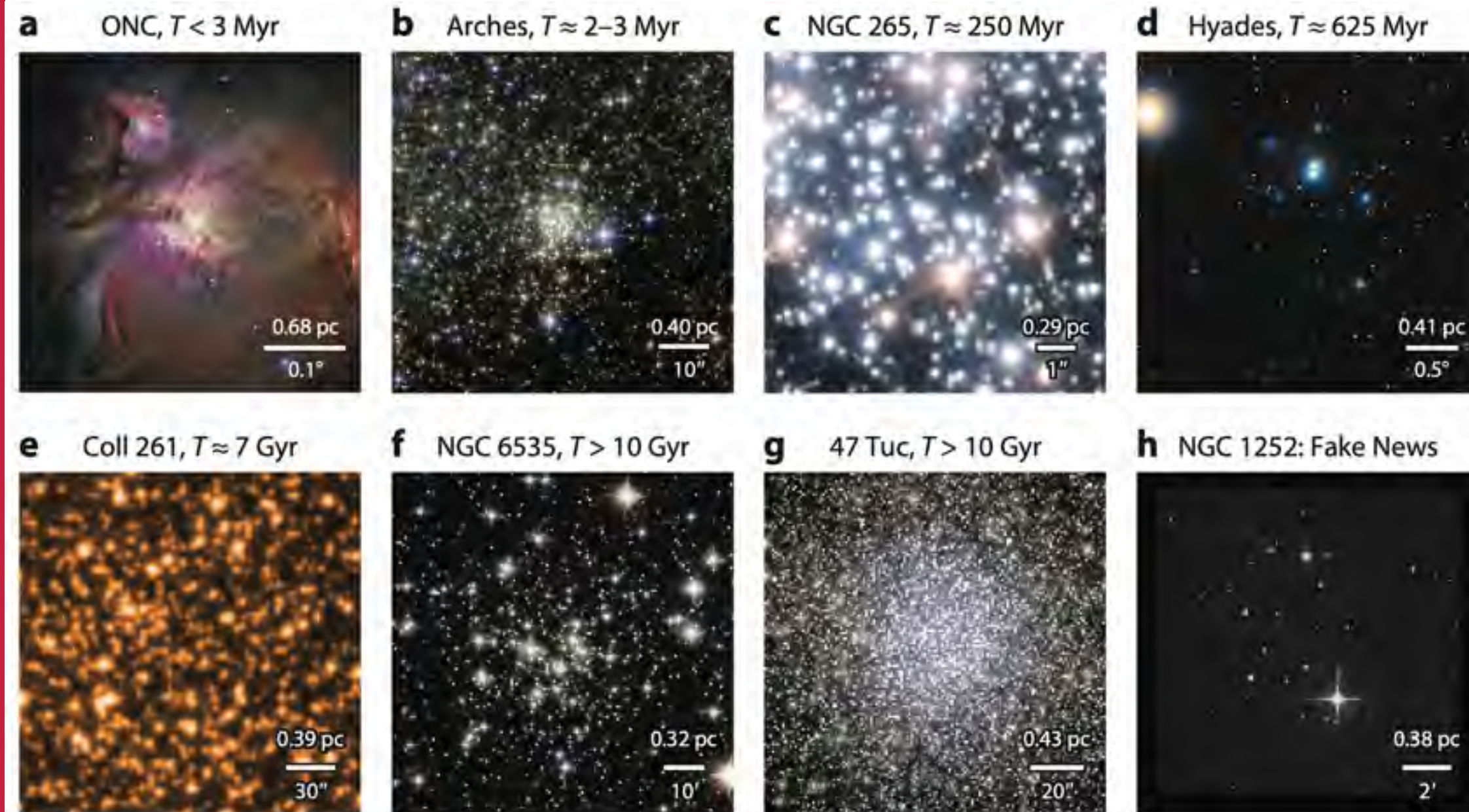
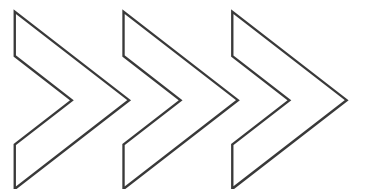
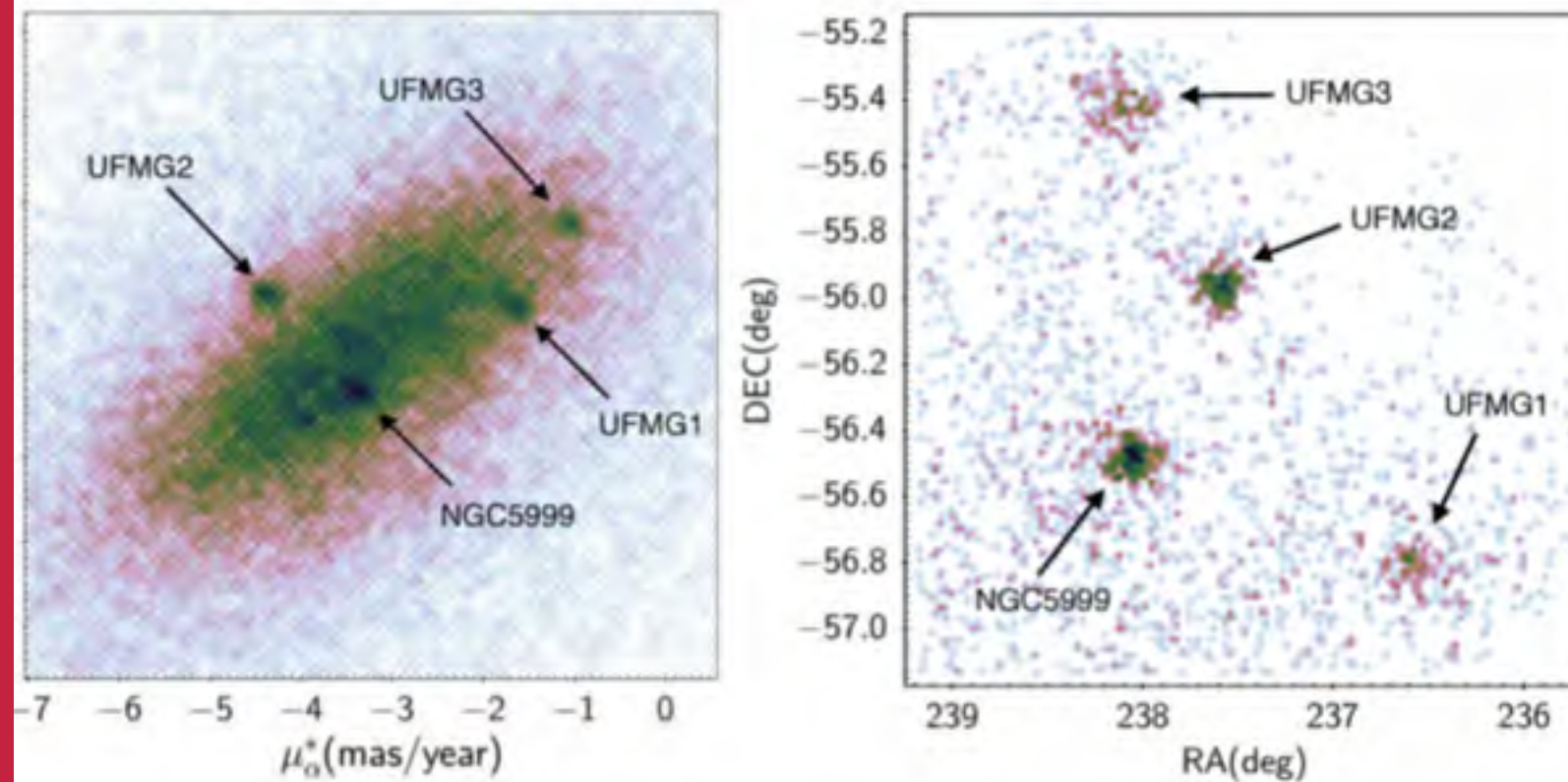


Figure from *Star Clusters Across Cosmic Time*  
M.R. Krumholz, C. F. McKee, J. Bland-Hawthorn  
Annual Review of Astronomy and Astrophysics 2019 57:1, 227-303

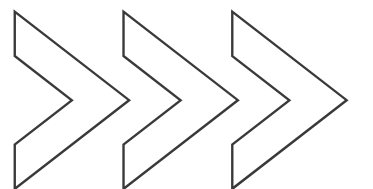


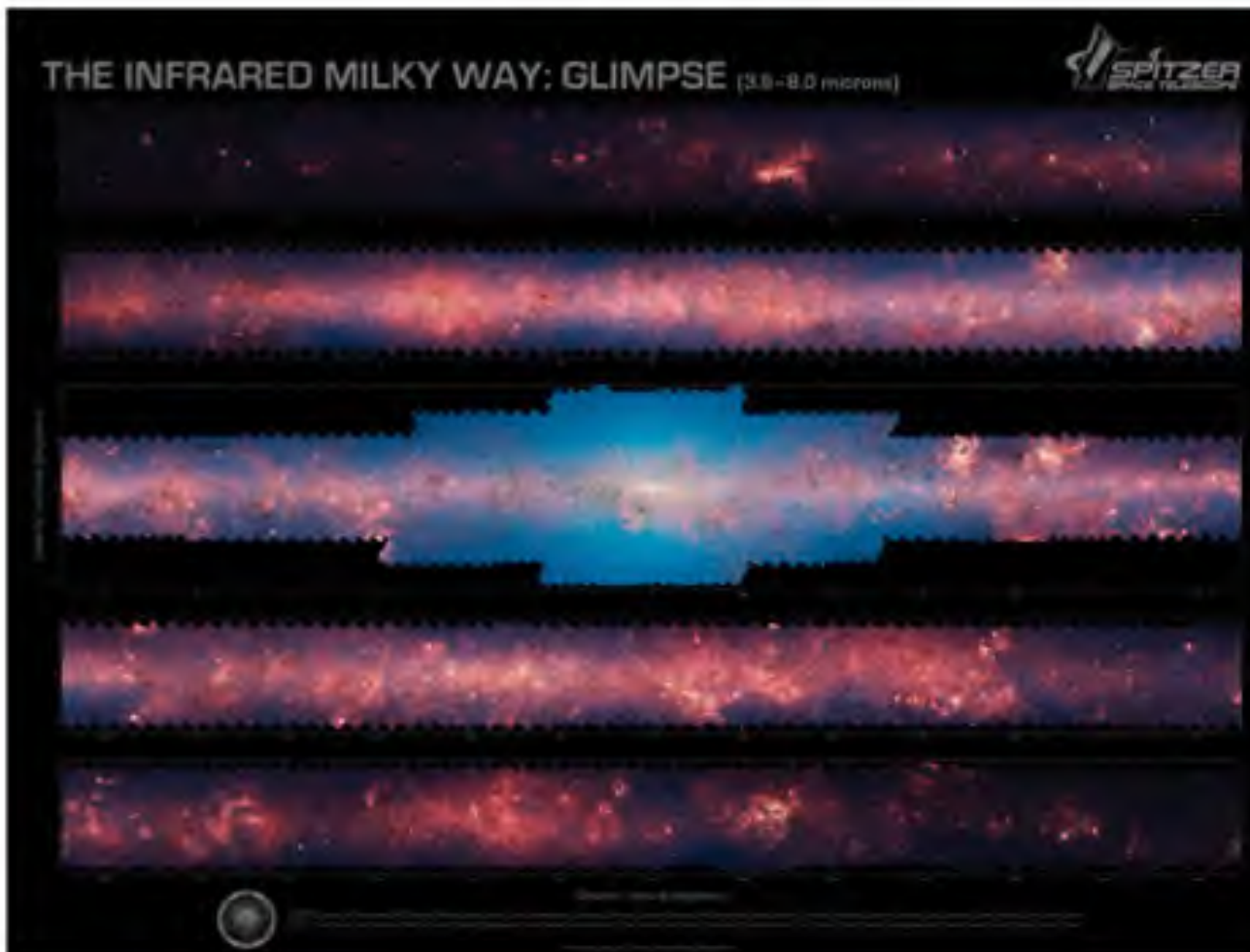
# A needle in a haystack

There are still associations hidden in plain sight



Ferreira, et. al. MNRAS, 2019, 483, 4 p. 5508





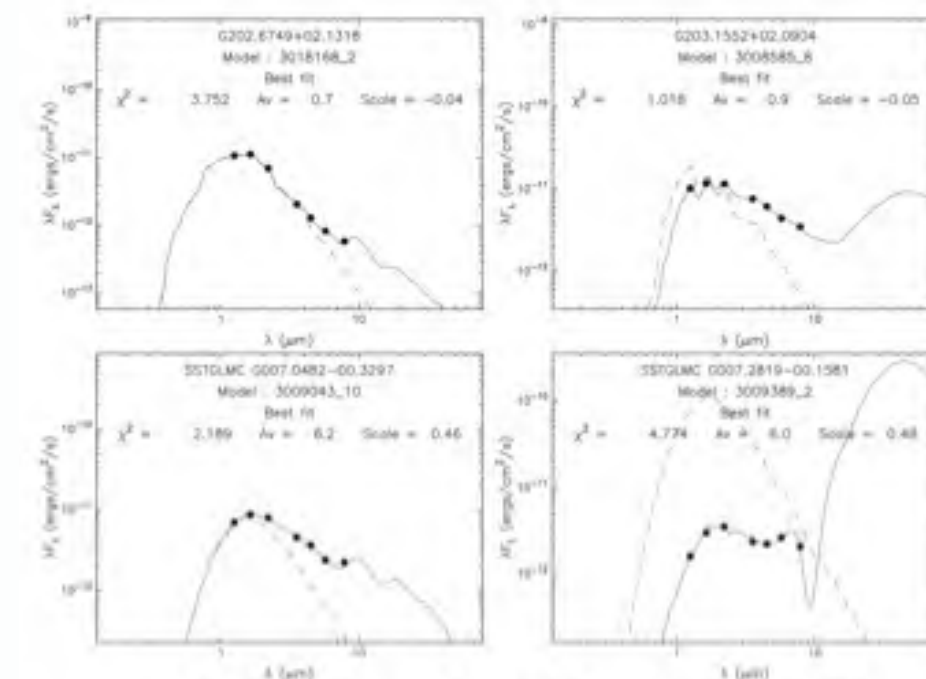
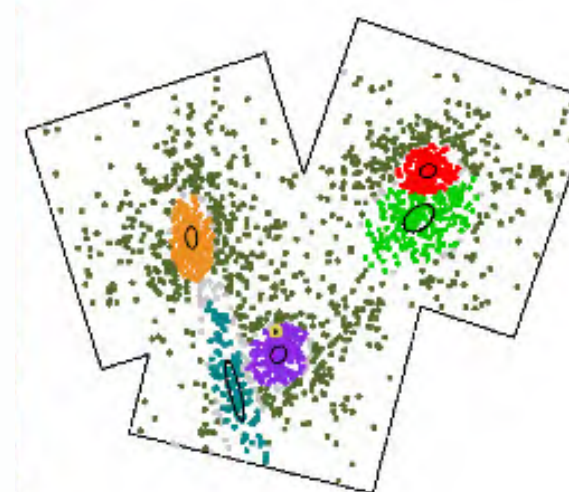
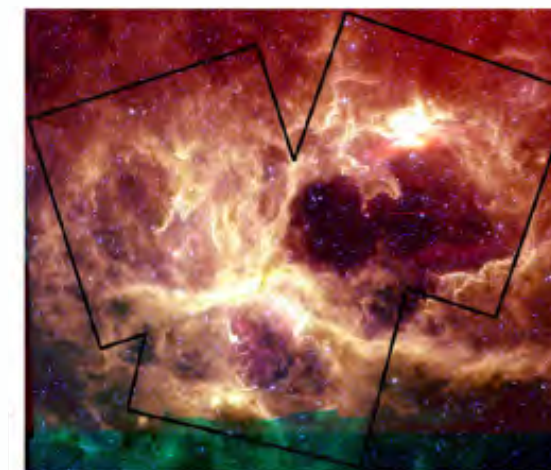
## Spitzer's GLIMPSE survey

$$|b| < 1-2 \text{ deg}$$

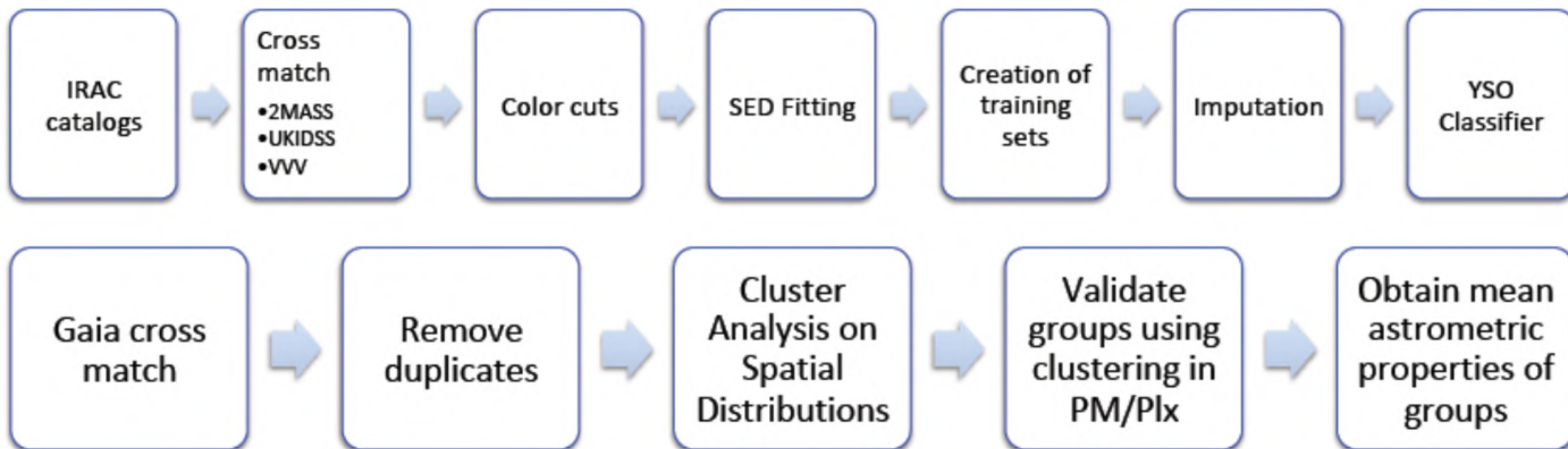
Benjamin+2003  
Churchwell+2009

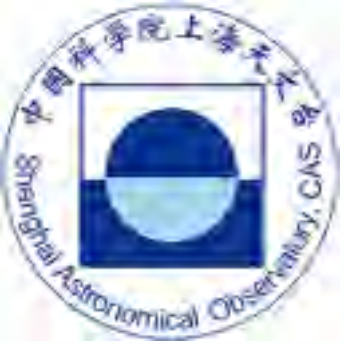
## Massive Young Star-forming Complex Study in IR and X-ray

Feigelson+2013  
Townesley+2014  
Kuhn+2013ab,2014  
Povich+2013  
Broos+2013







SED fitting from Povich+2013





THE ASTROPHYSICAL JOURNAL  
SUPPLEMENT SERIES

SPICY: The Spitzer/IRAC Candidate YSO Catalog for the Inner Galactic Midplane

Michael A. Kuhn<sup>1</sup> , Rafael S. de Souza<sup>2</sup> , Alberto Krone-Martins<sup>3,4</sup> , Alfred Castro-Ginard<sup>5</sup> ,  
Emille E. O. Ishida<sup>6</sup> , Matthew S. Povich<sup>1,7</sup> , Lynne A. Hillenbrand<sup>1</sup>, and  
for the COIN Collaboration

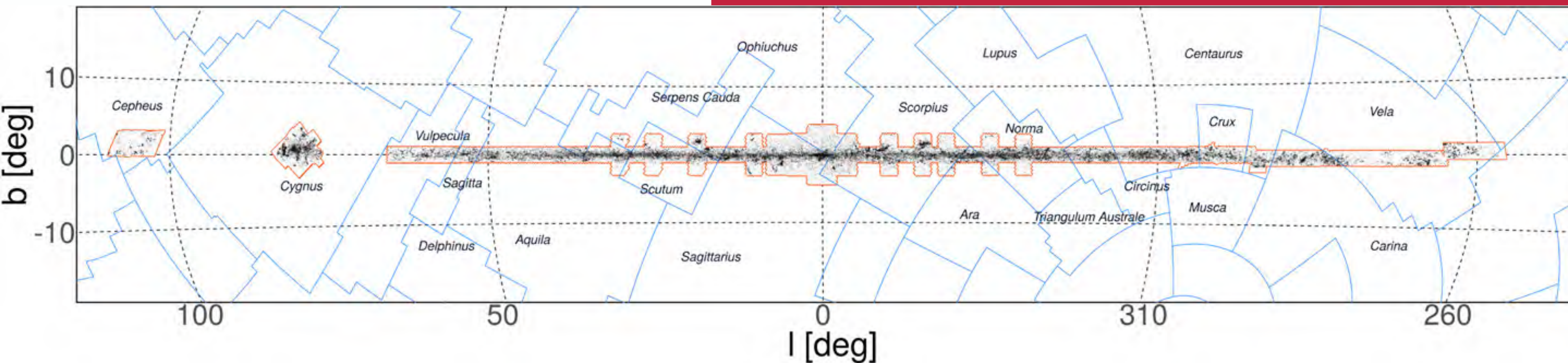
Published 2021 June 2 • © 2021. The American Astronomical Society. All rights reserved.

[The Astrophysical Journal Supplement Series, Volume 254, Number 2](#)

Citation Michael A. Kuhn et al 2021 *ApJS* 254 33

# 120,000 new YSOs

The SPICY catalog is the largest homogeneous sample of YSO candidates available to date for the inner regions of the Milky Way

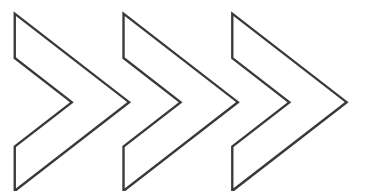
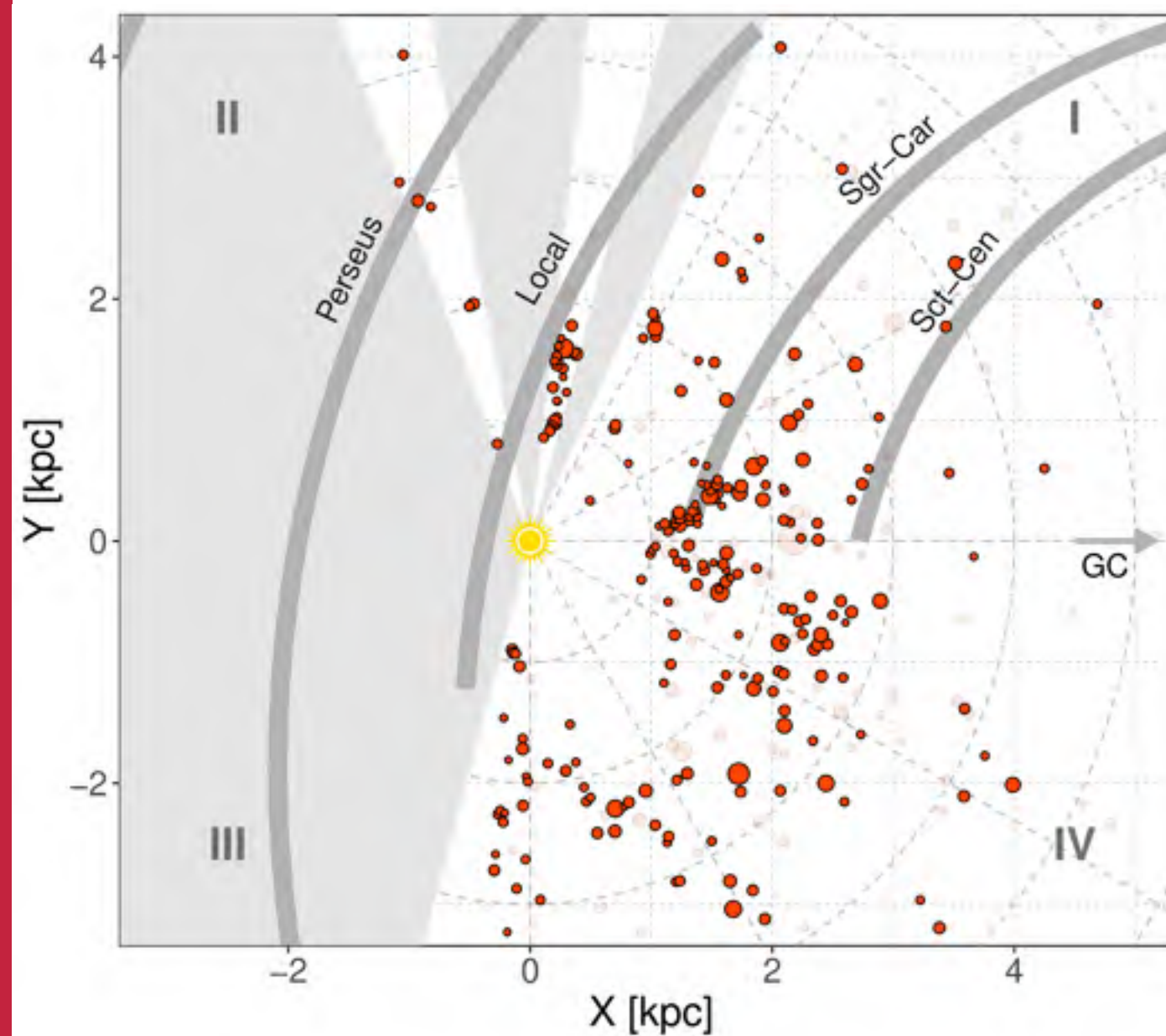


# SPICY - 120,000 YSOs discovered in the Galaxy

ASTRO-AWARE STATISTICAL LEARNING

## Challenges:

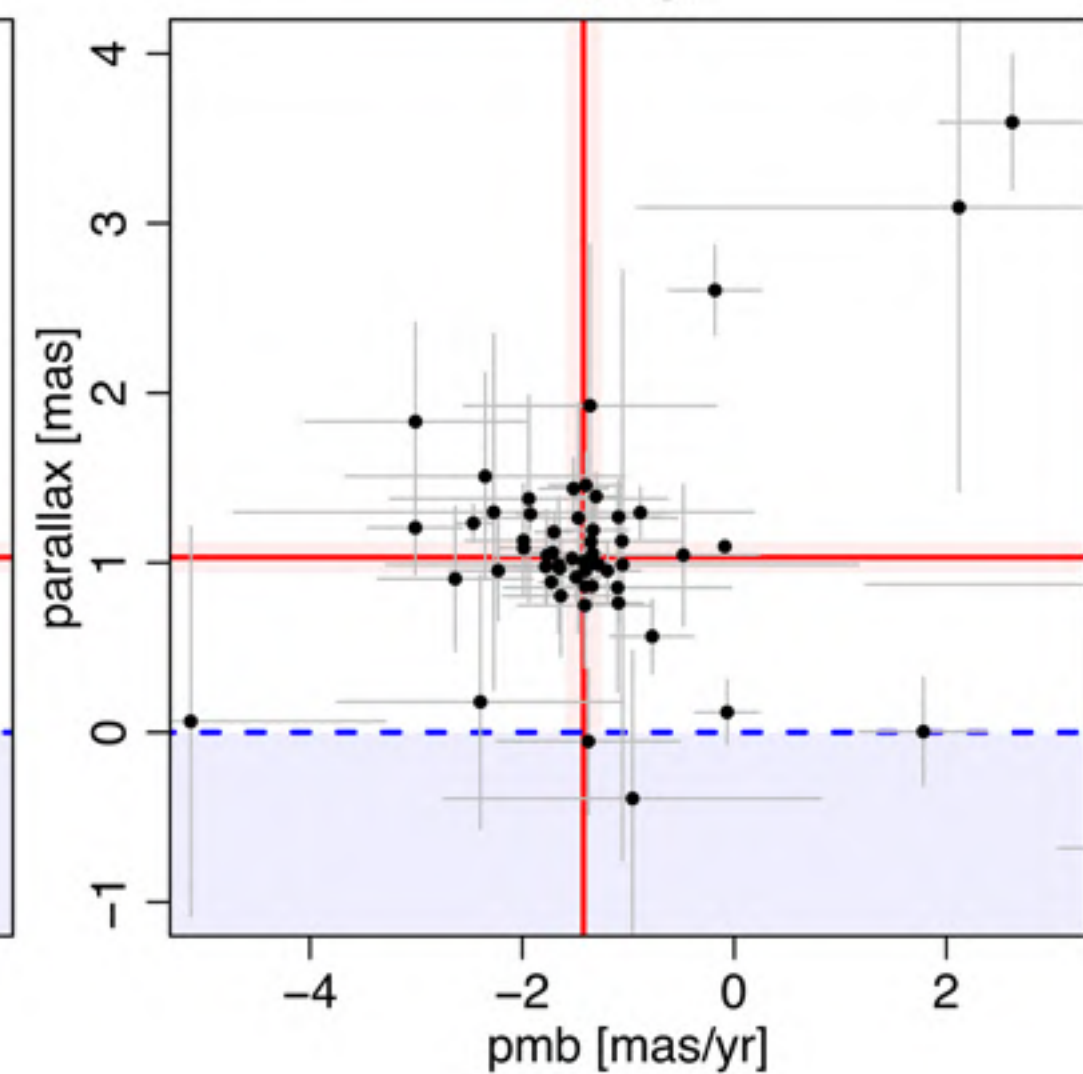
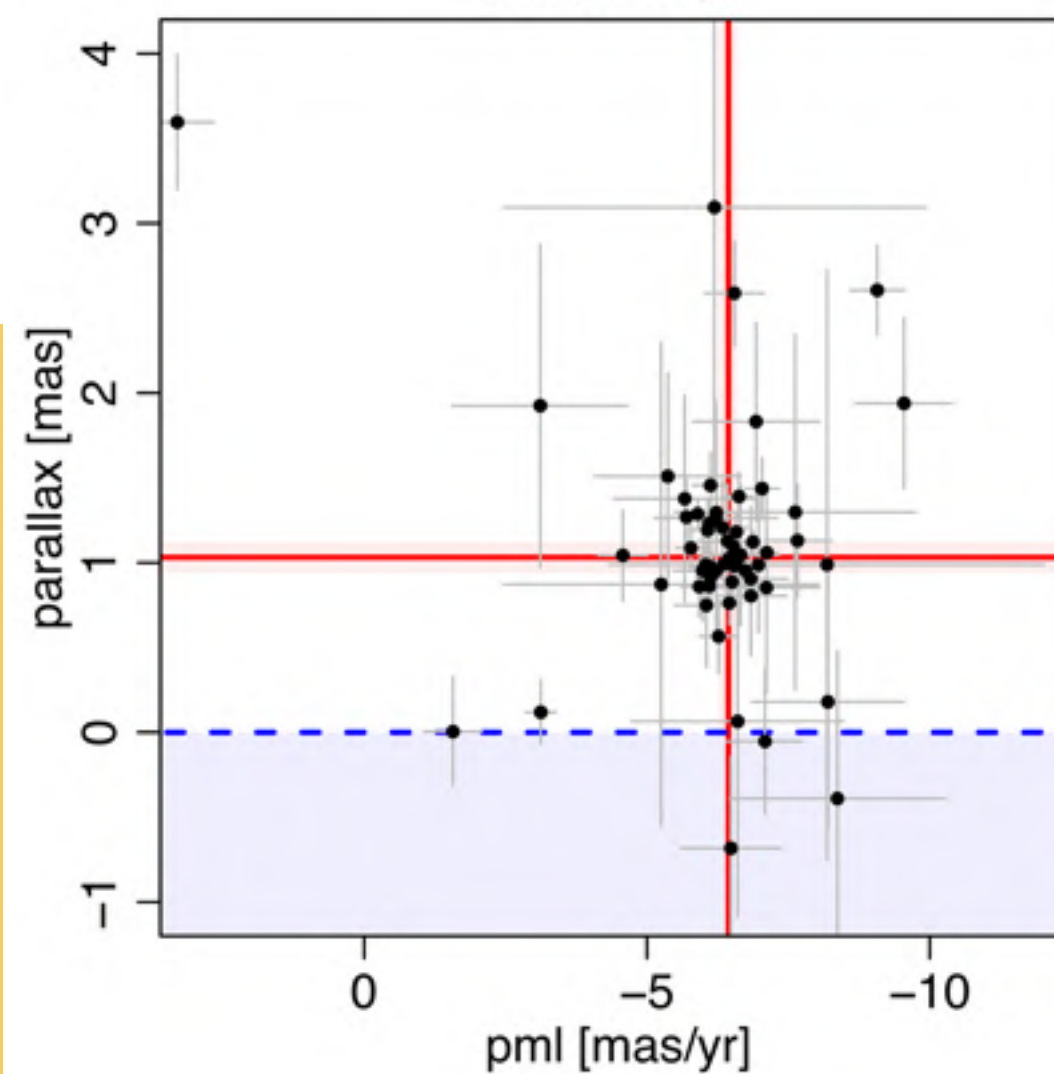
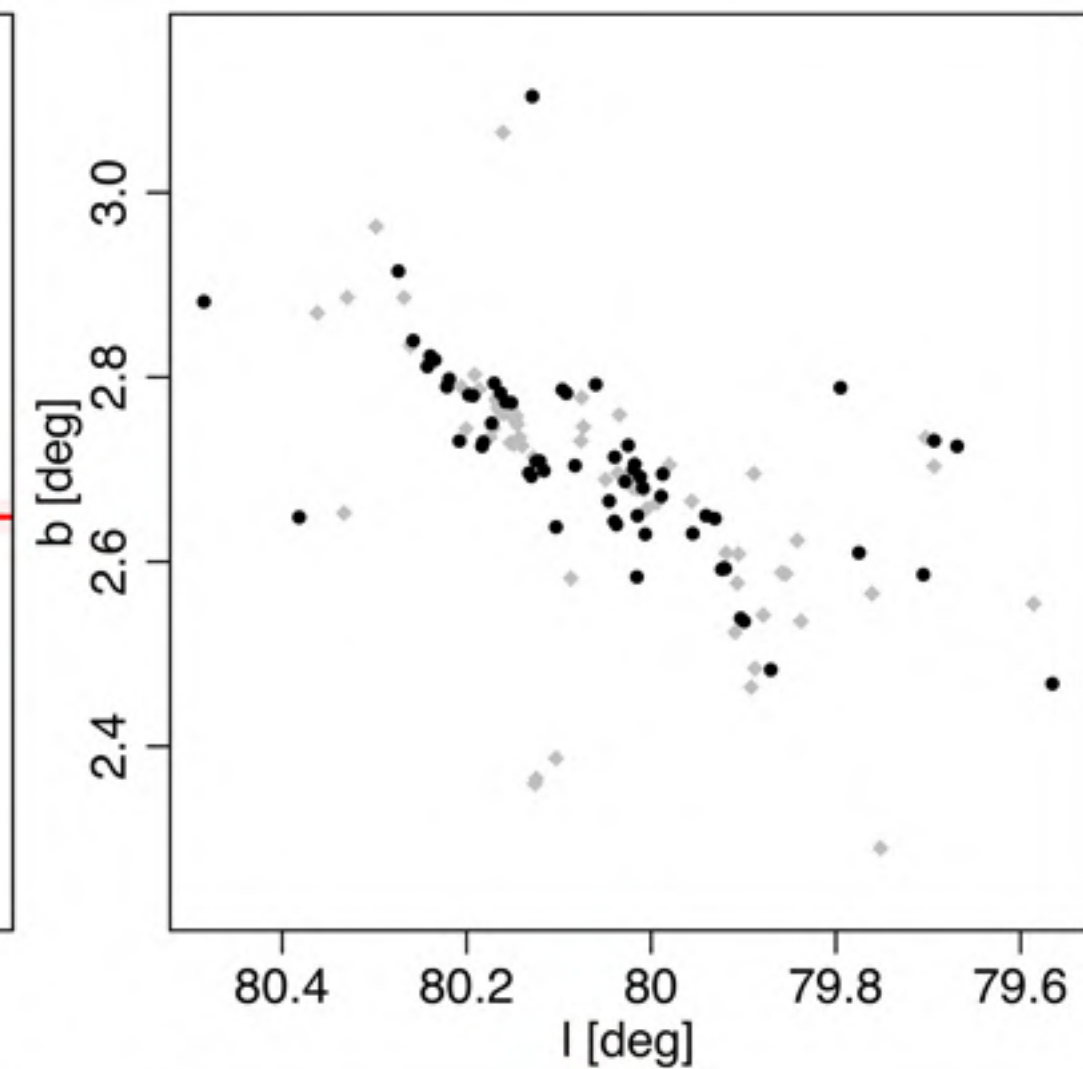
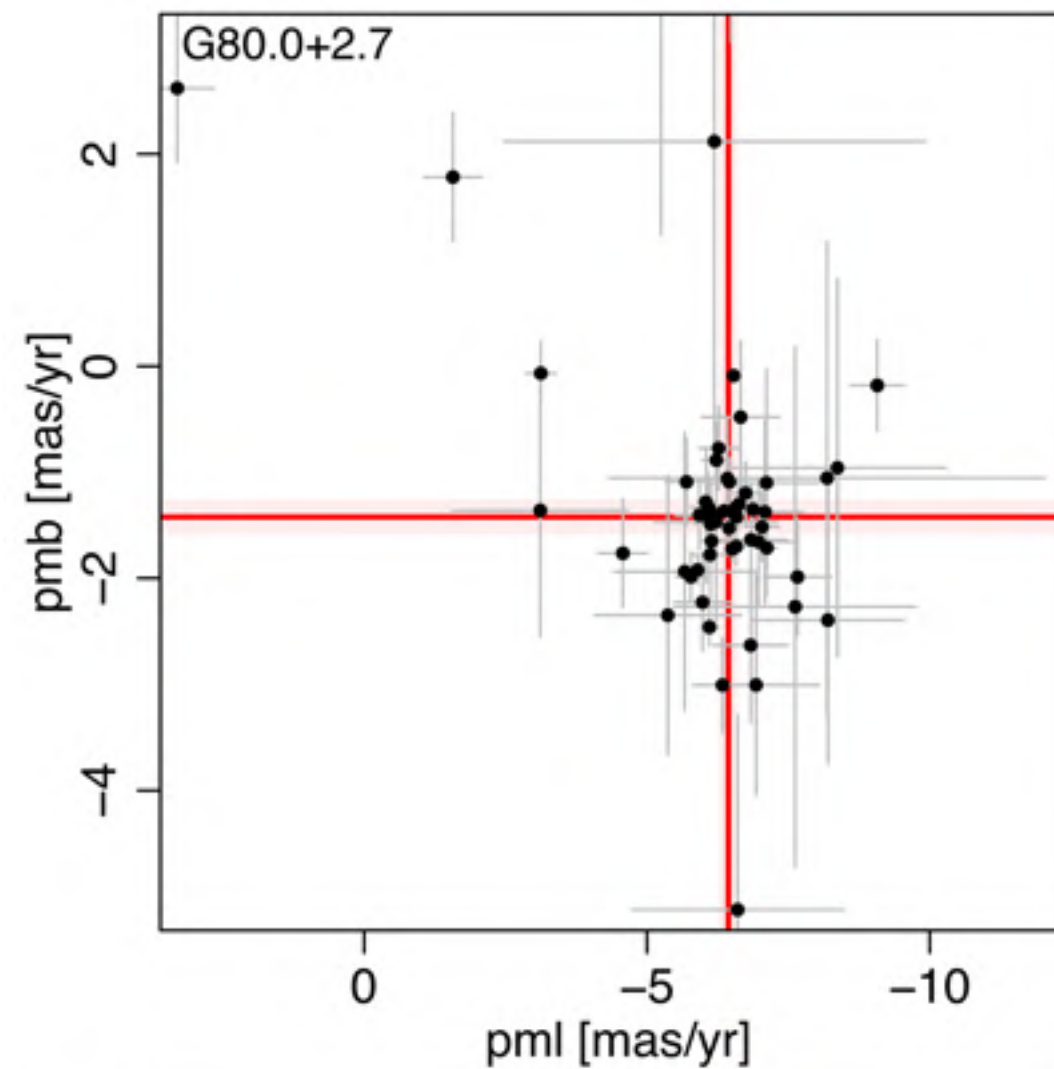
- Domain knowledge regularization - statistical clusters vs Astronomical ones
- Heteroscedastic uncertainties with known variance, covariance
- Selection effects, missing not at random

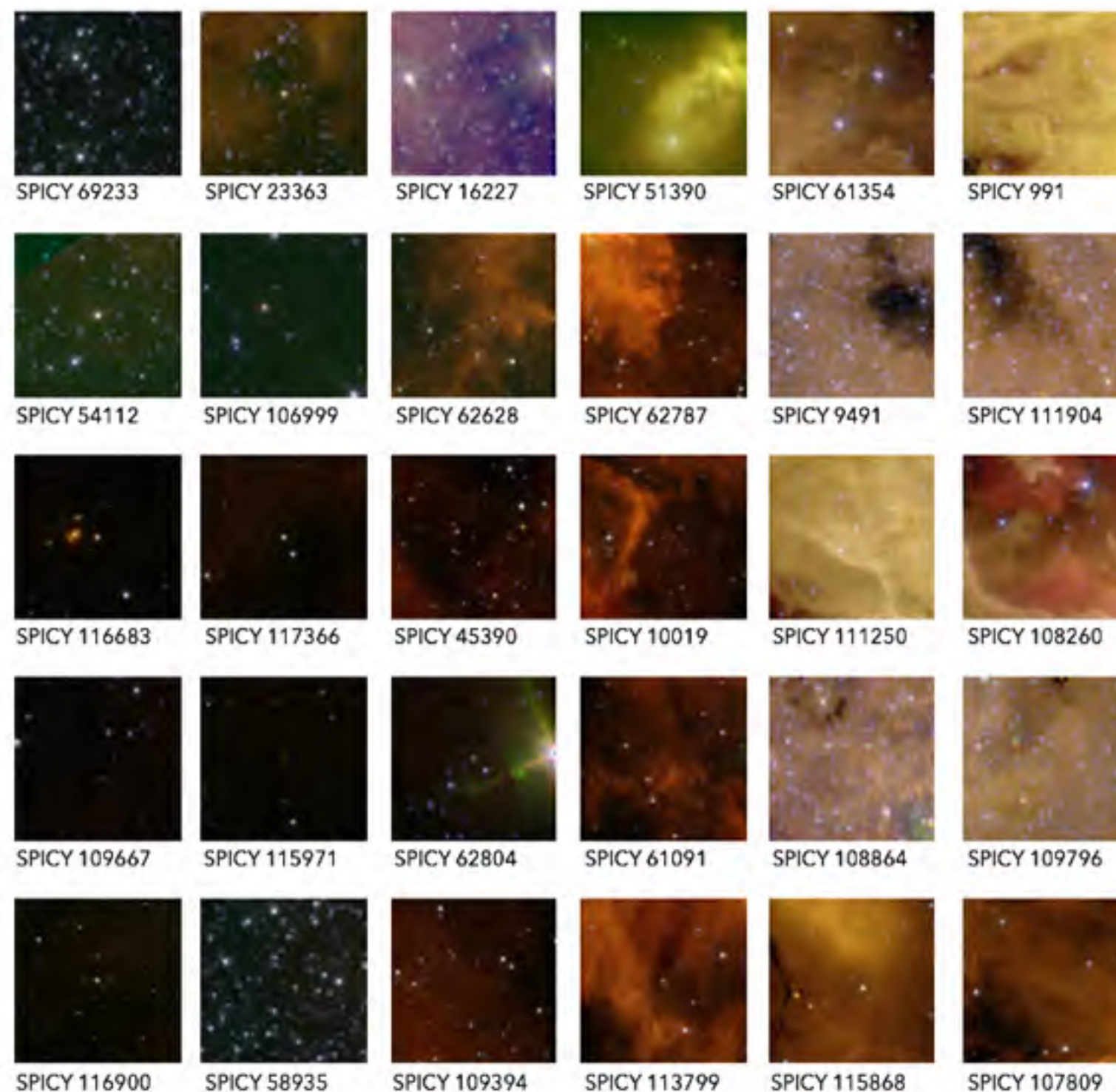
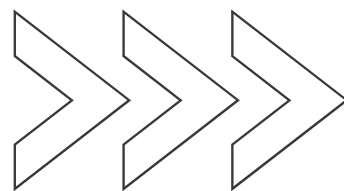


# Hierarchical Bayesian Models

## ASTROMETRIC PROPERTIES OF THE STELLAR GROUPS

- Heteroscedastic measurement errors, outliers, non-normality, etc.
- Principled statistics still needed





# 117,224 PNG stamps

251GB album built via  
PostgreSQL

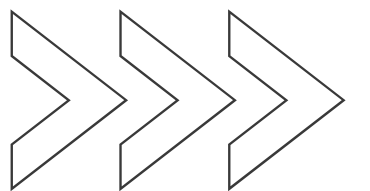
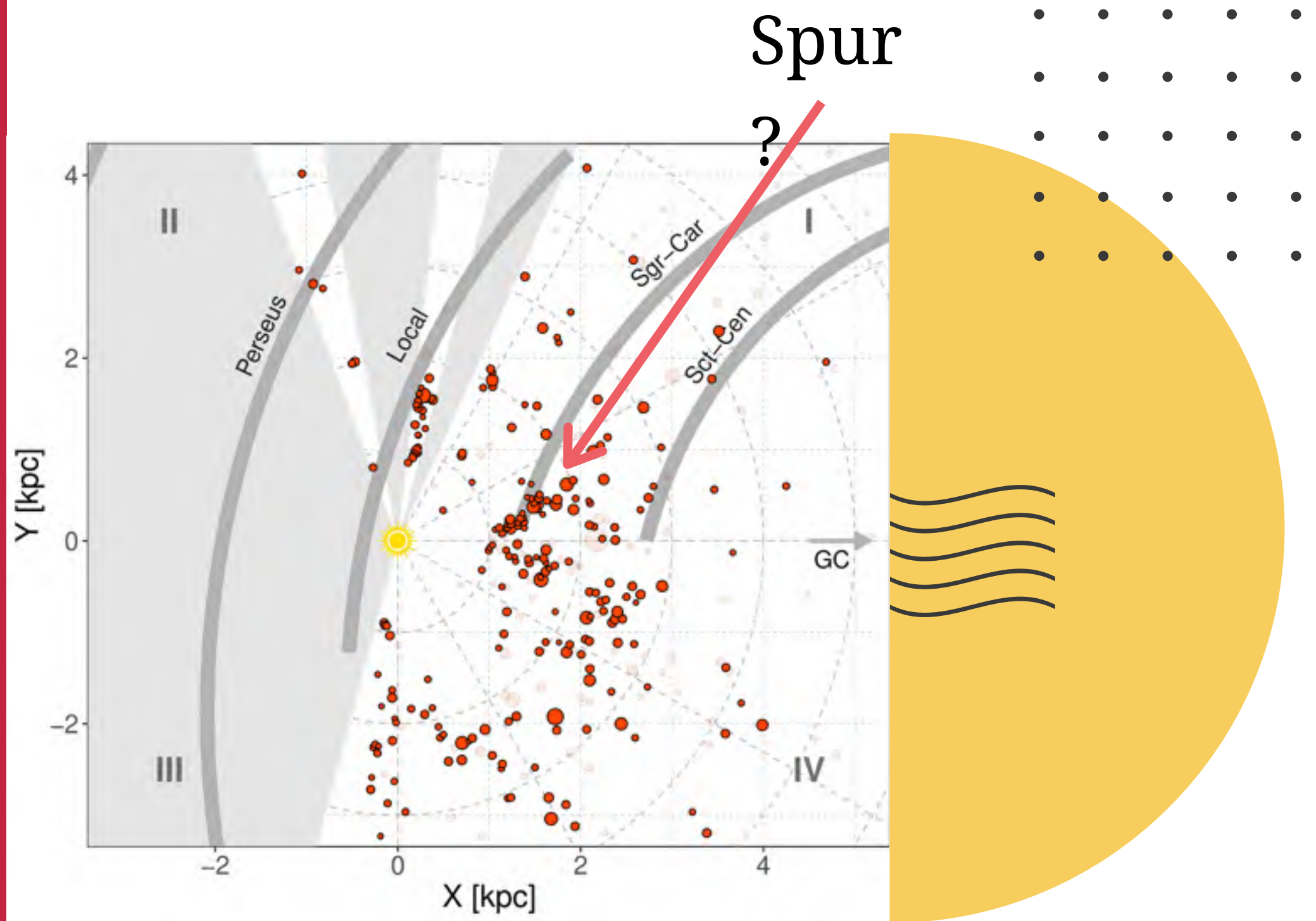
Potential testbed for computer  
vision, texture analysis, novelty  
detection, feature extration, etc.

# Spatial distribution of YSO groups

Good tracers of star forming regions and galactic structure



Independent probe of spiral arms structure

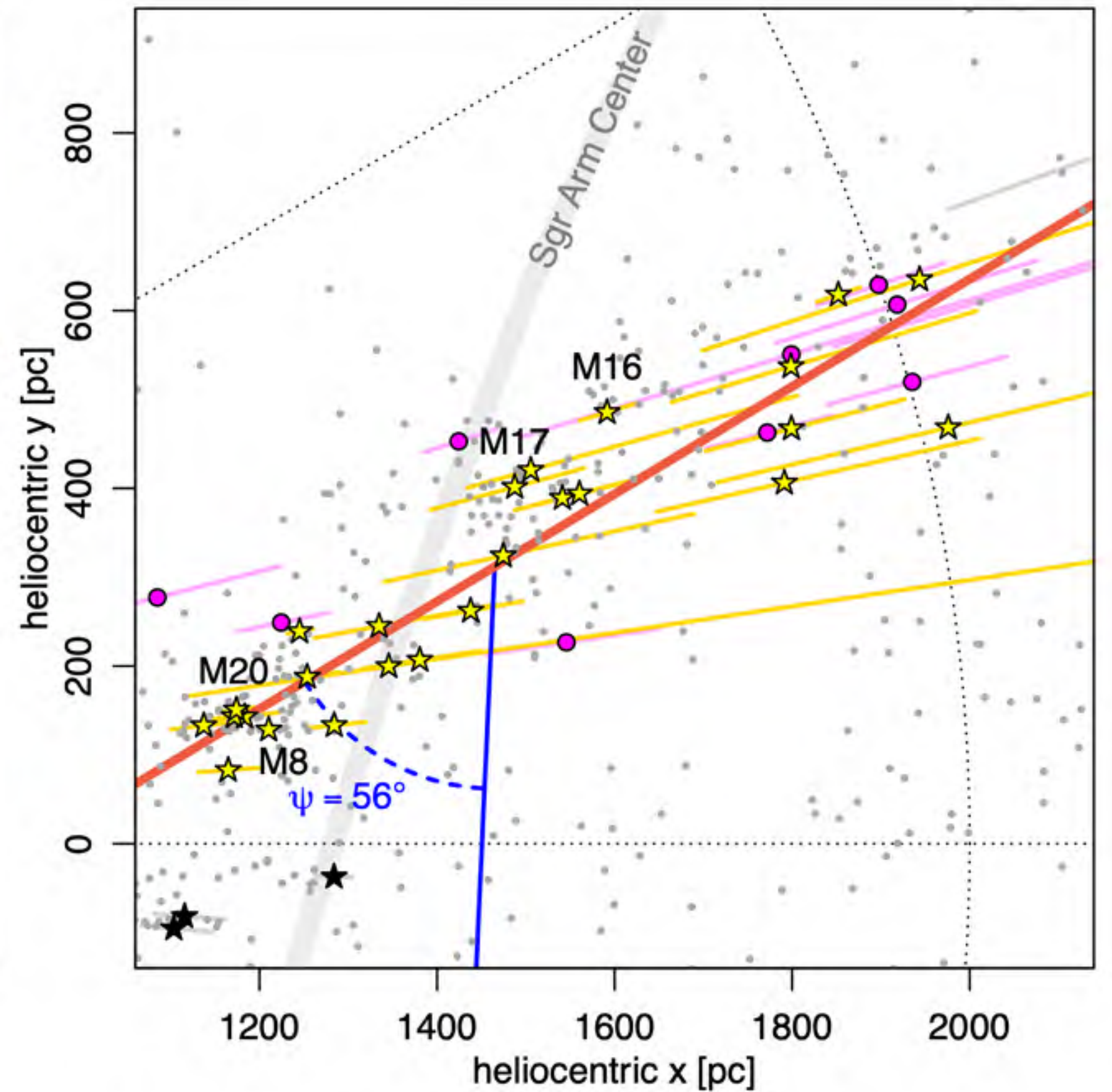
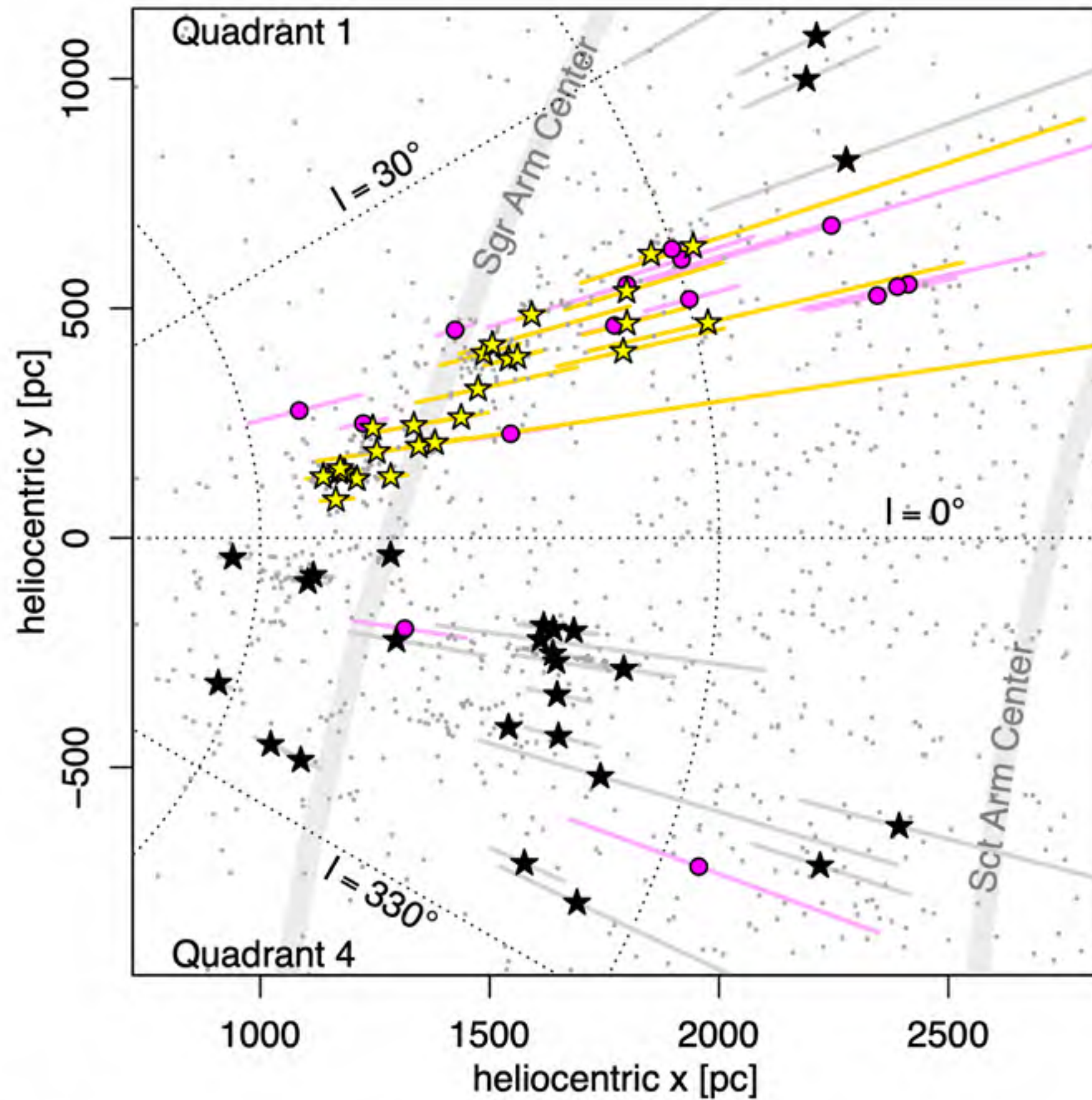


NGC 5236 (Larsen & Richtler 1999)

Spiral arms are not smooth,  
continuous features.

This substructure appears associated  
with  
much of the star formation in the  
arm.





**Fig. 3.** Galactic map of YSO groups (star symbols), masers (magenta circles), and non-clustered SPICY YSO candidates (gray points) in heliocentric  $xy$  coordinates. The right panel shows a zoomed-in view. Groups associated with the structure are color-coded yellow, while others are black. The spiral-arm centers defined by Reid et al. (2019) are indicated by the grey bands. The red line indicates the major axis of the feature identified here with its  $56^\circ$  pitch angle illustrated in blue.

*Sit down before fact as a little  
child, be prepared to give up every  
preconceived notion, follow  
humbly wherever and to whatever  
abysses nature leads...*

Thomas Huxley

