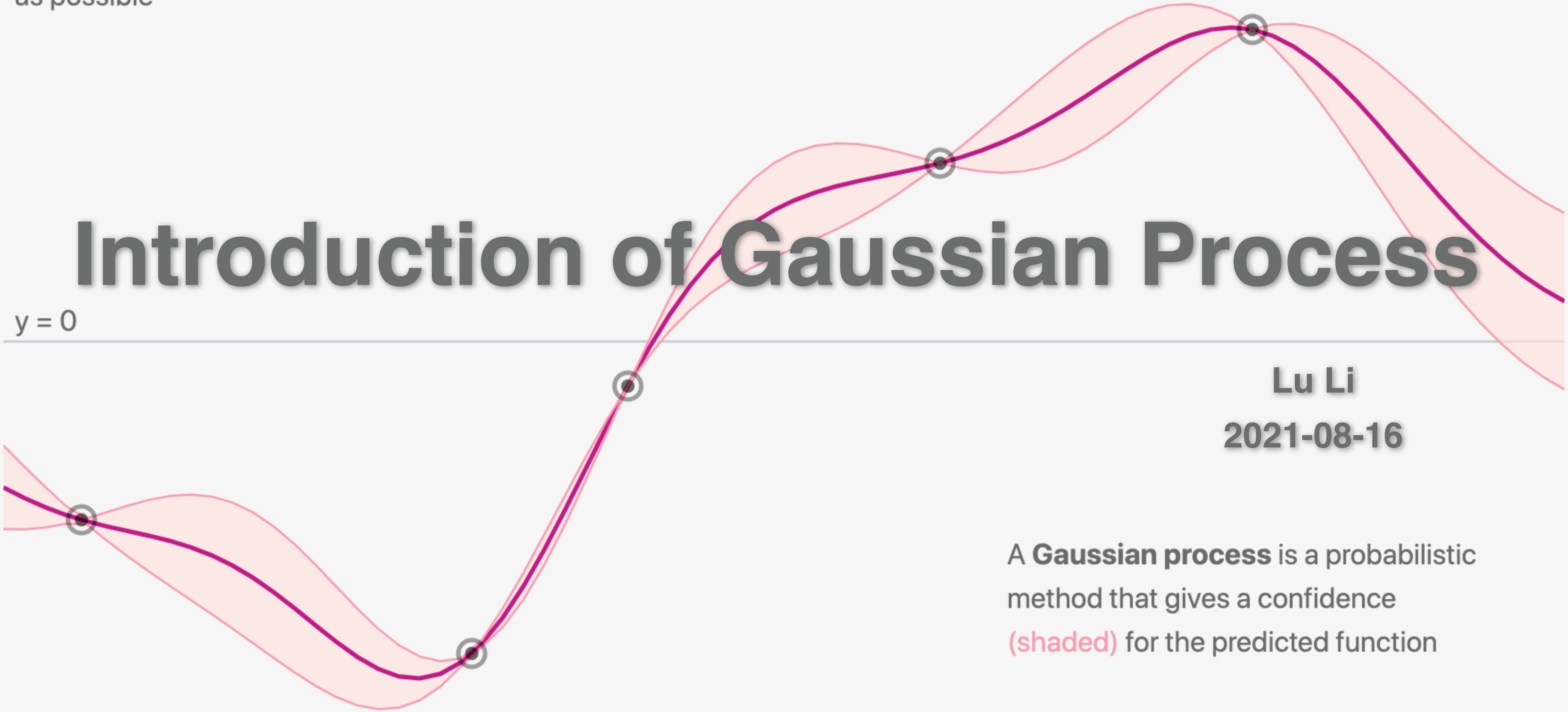
Regression is used to find a function (line) that represents a set of data points as closely as possible

Introduction of Gaussian Process



Lu Li

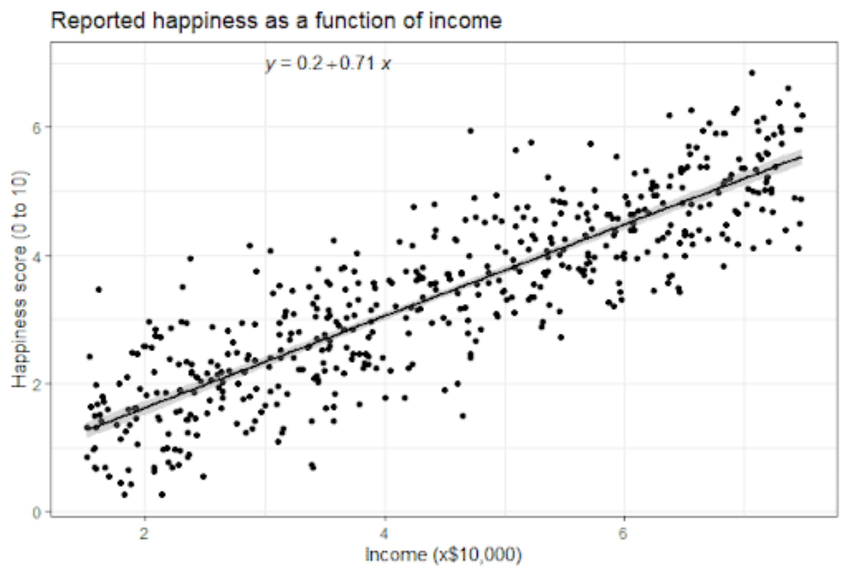
2021-08-16

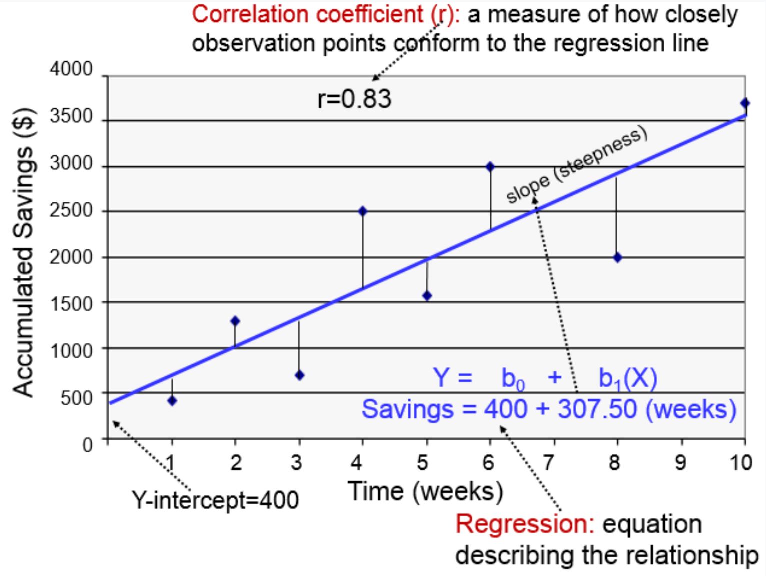
A **Gaussian process** is a probabilistic method that gives a confidence (shaded) for the predicted function

Regression

Definition (wiki)

Regression analysis is a set of statistical processes for estimating the relationships between a dependent variable (often called the 'outcome' or 'response' variable. 因变量，y.) and one or more independent variables (often called 'predictors', 'covariates', 'explanatory variables' or ‘features’. 自变量，x).
Then you can do prediction: a y for a new x.



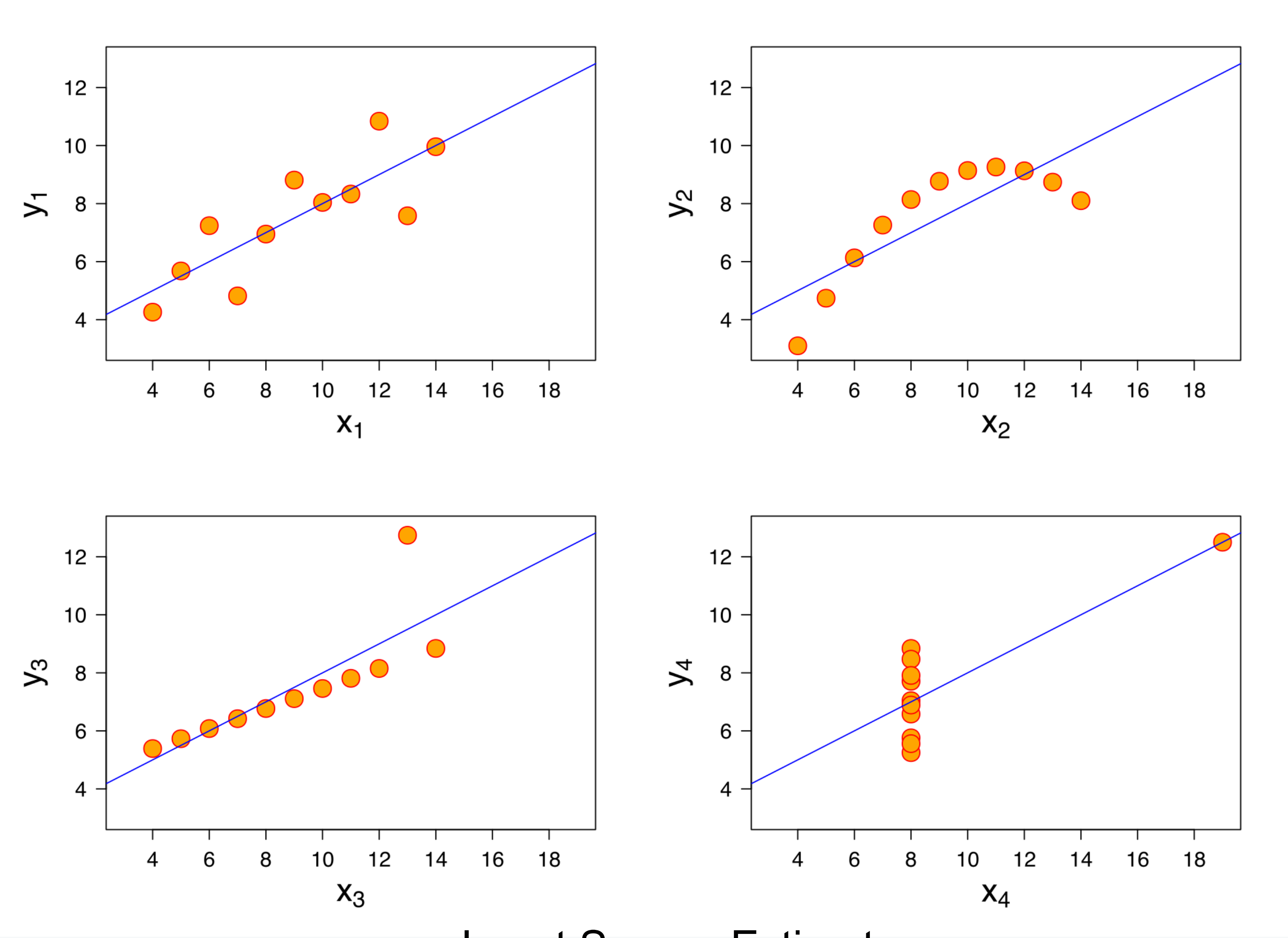


Simple Linear Regression

the same linear regression line, but are graphically very different.

This illustrates the pitfalls of relying solely on a fitted model to understand the relationship between variables.

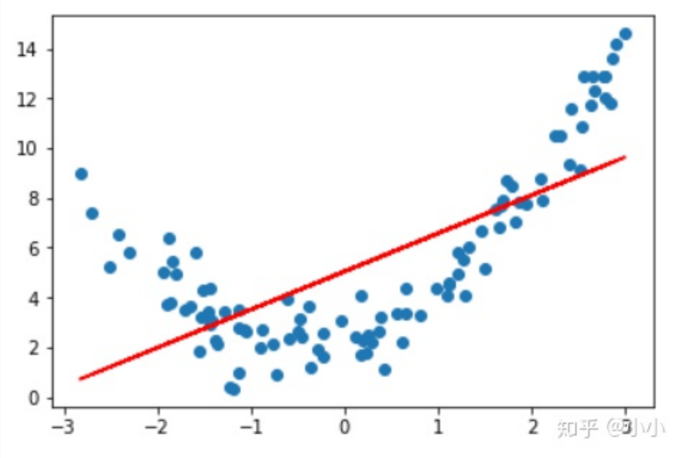
不同的数据得到同样的结果：线性回归，模型依赖的缺陷。

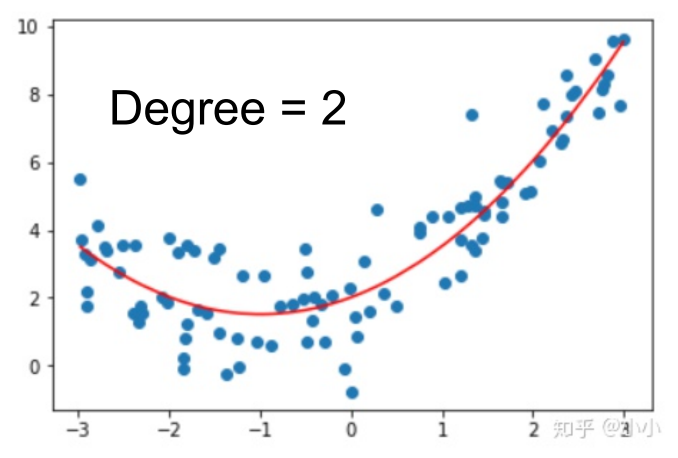


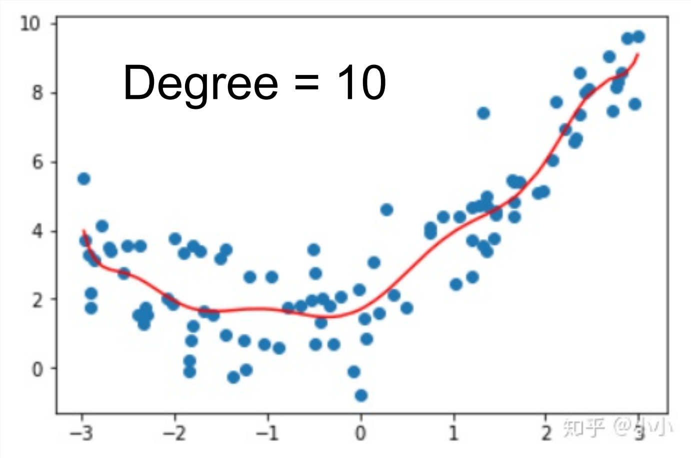
Least Square Estimates

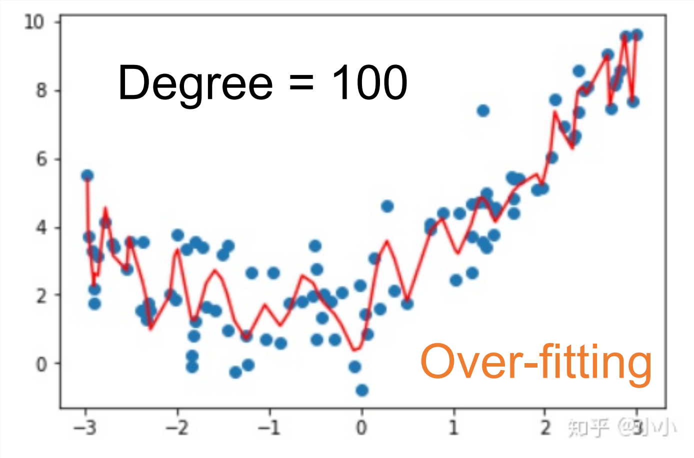
Wikipedia

Polynomial Regression 多项式回归







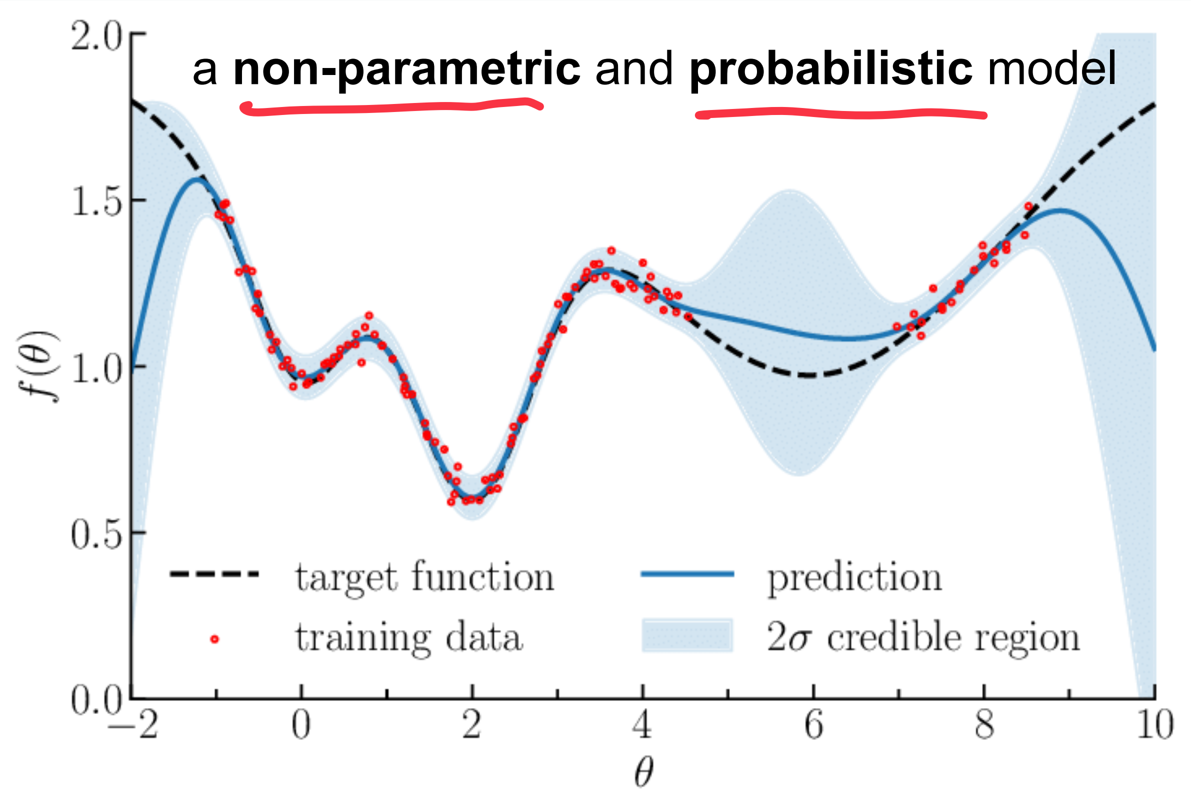


Polynomial regression is a form of regression analysis in which the relationship between the independent variable *x* and the dependent variable *y* is modelled as an *n*th degree polynomial in *x*.

多项式回归是回归分析的一种形式，其中自变量 x 和因变量 y 之间的关系被建模为关于 x 的 n 次多项式

- Parametric, model dependent.
- Can not obtain the confidence level of the “line”.

Gaussian Process (GP)



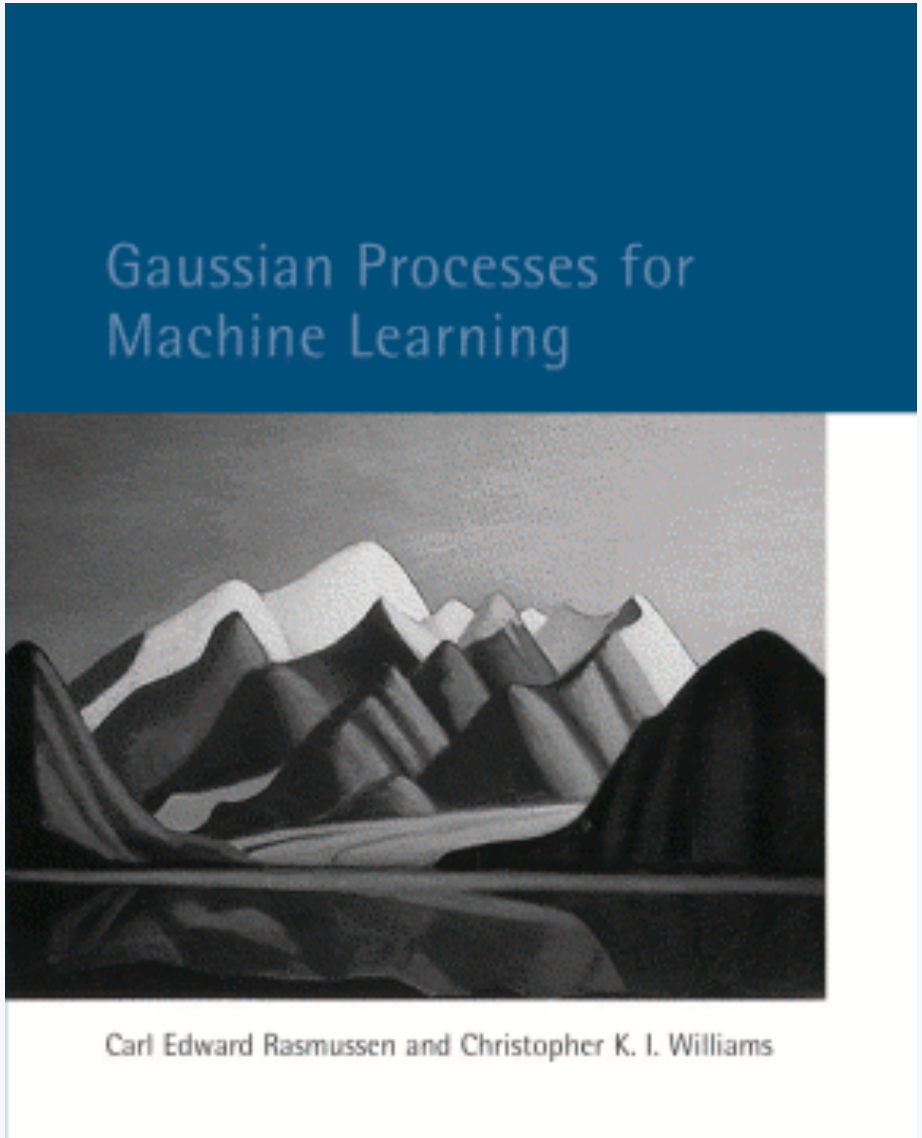
The posterior mean and the uncertainty.

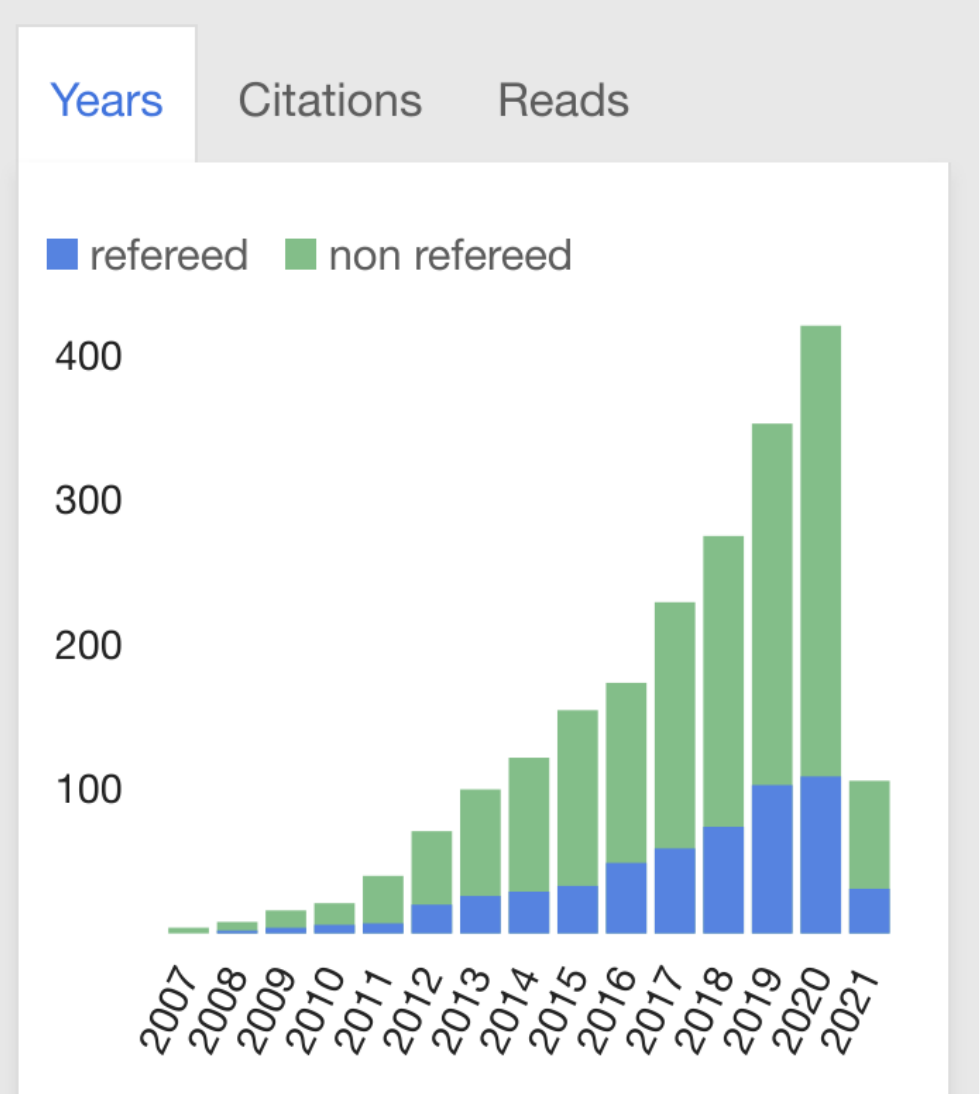
Definition (wiki)

A Gaussian process is a stochastic process (a collection of random variables indexed by time or space), such that every finite collection of those random variables has a multivariate normal distribution.

因变量 y_i 服从 multivariate normal distribution

- Data-driven
- Bayesian frame


Gaussian Processes for
Machine Learning
Carl Edward Rasmussen and Christopher K. I. Williams


Years
Citations
Reads
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400
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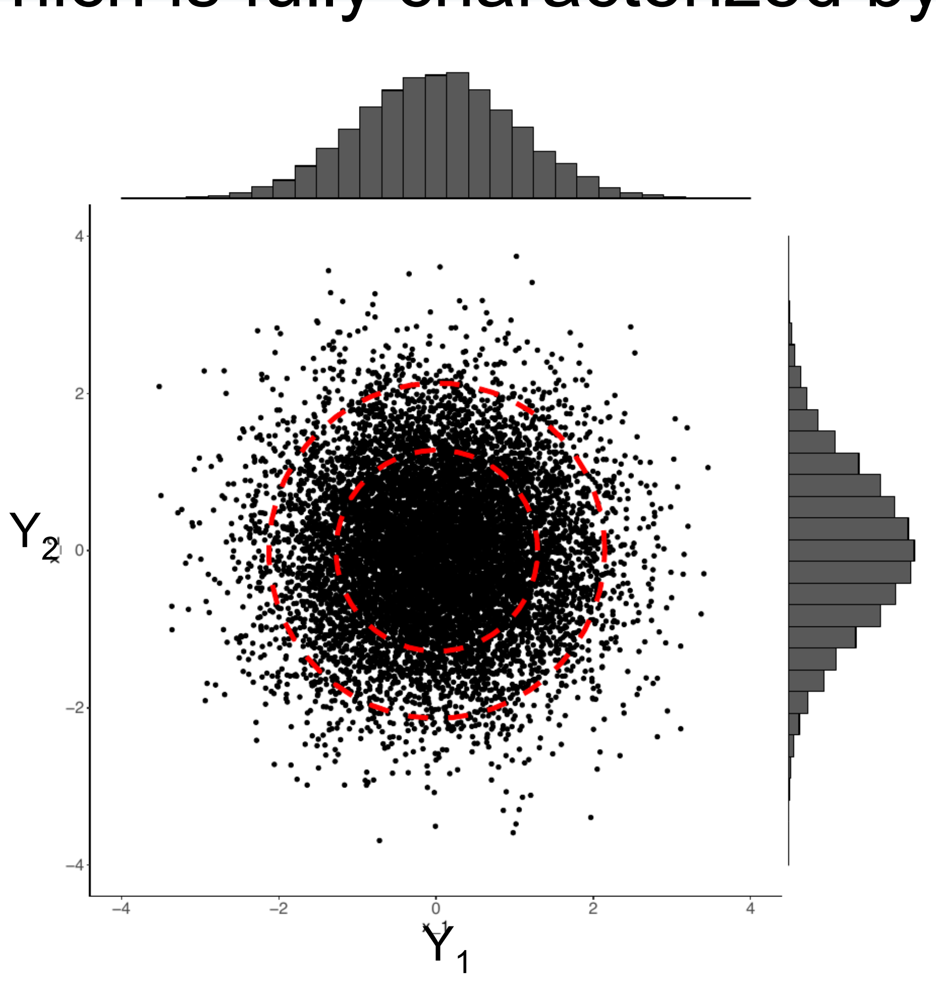
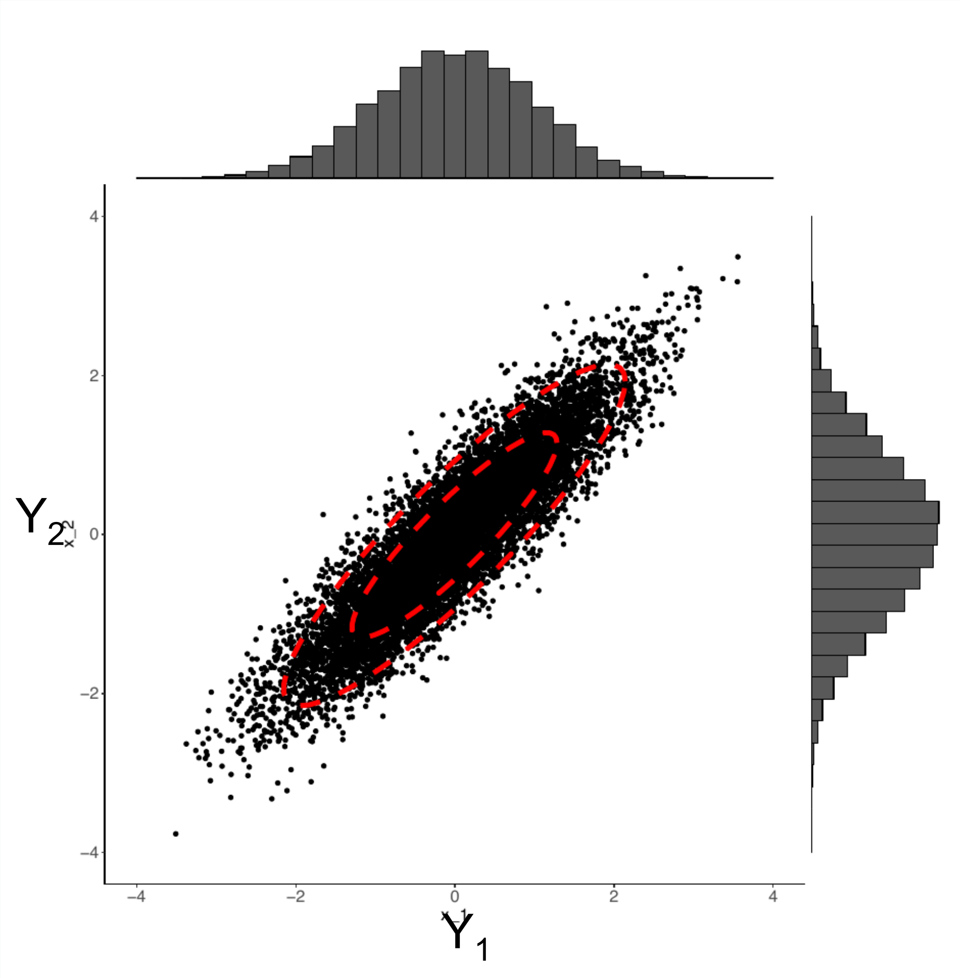
Multivariate Gaussian distribution

which is fully characterized by mean and covariance matrix



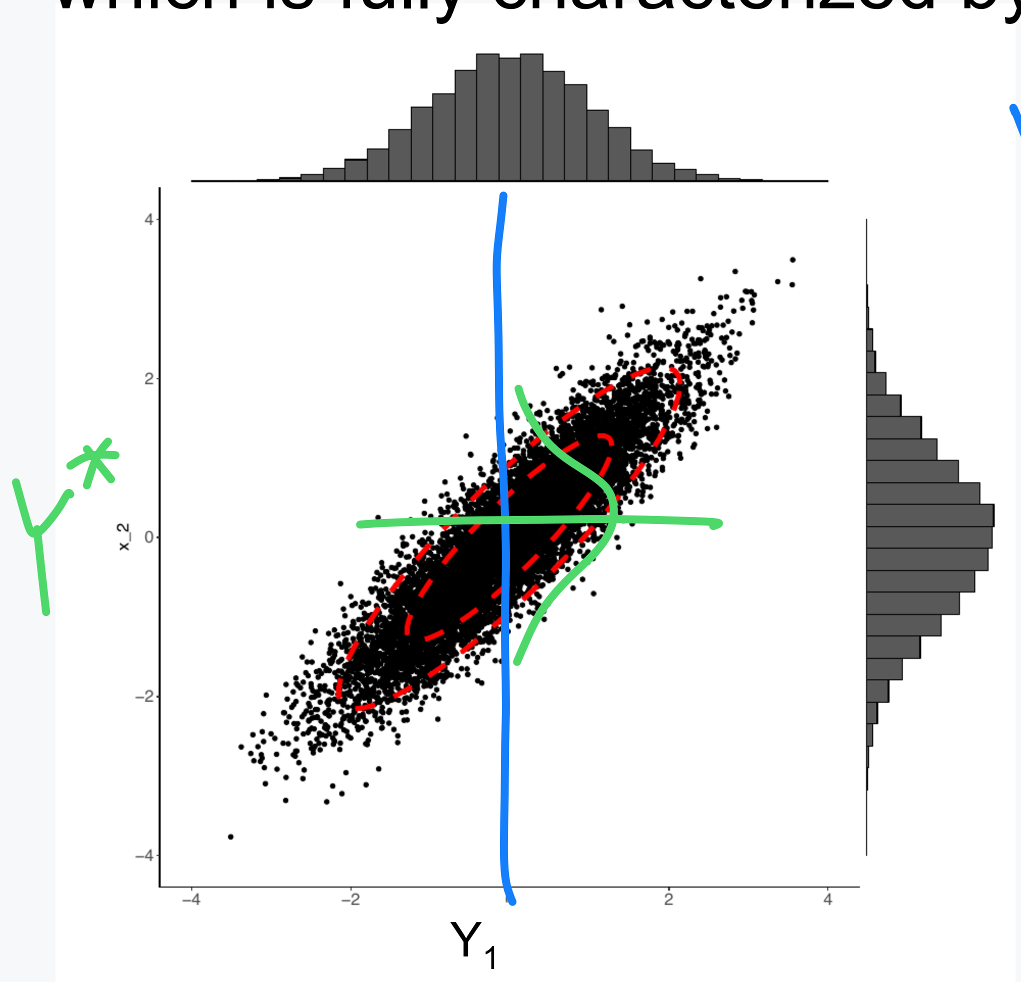


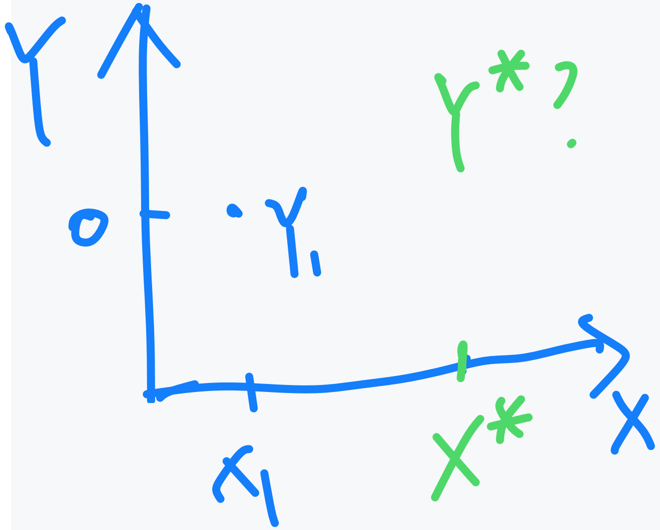
If Y_1 is known, then Y_2 is constrained as $p(Y_2 \mid Y_1)$

Multivariate Gaussian distribution

kernel

which is fully characterized by mean and covariance matrix





obs data $\{Y_i\}$

$$P(Y^*, \{Y_i\}) = P(Y^* | \{Y_i\}) \cdot P(\{Y_i\})$$

$$P(Y^* | \{Y_i\}) = \frac{P(Y^*, \{Y_i\})}{P(\{Y_i\})}$$

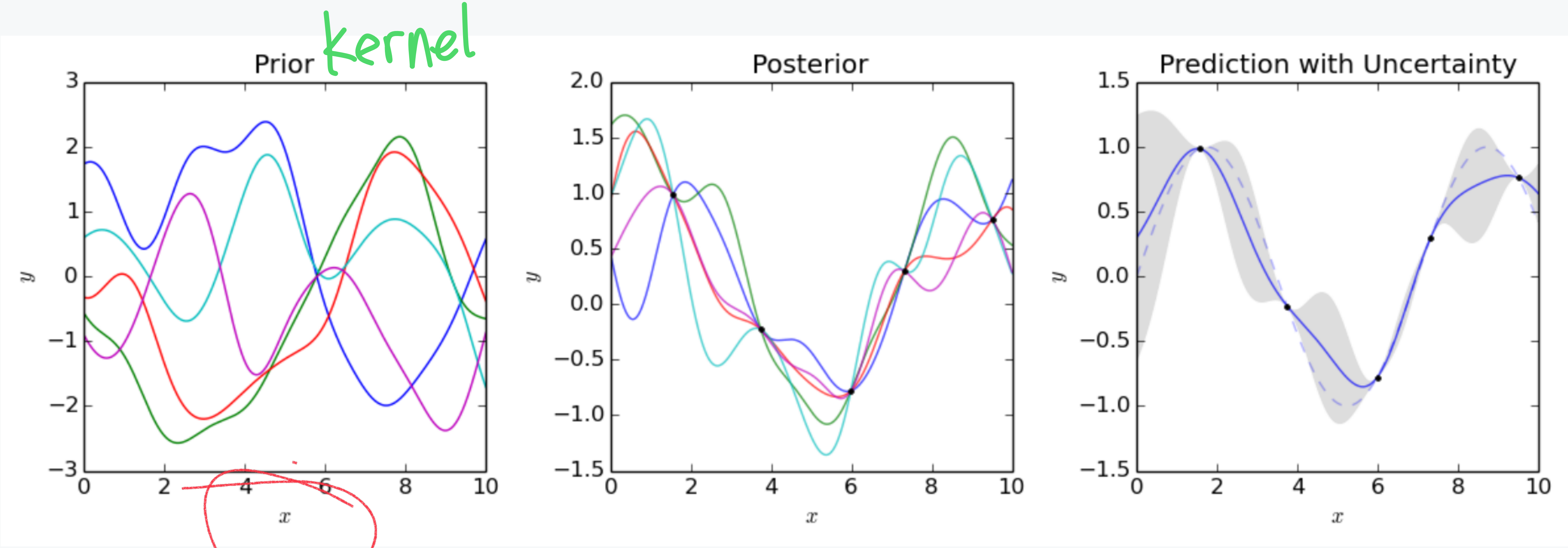
→ Prior

= constant

P(obs data)

If Y_1 is known, then Y^* is constrained as $p(Y^* | Y_1)$

Gaussian Process (GP)



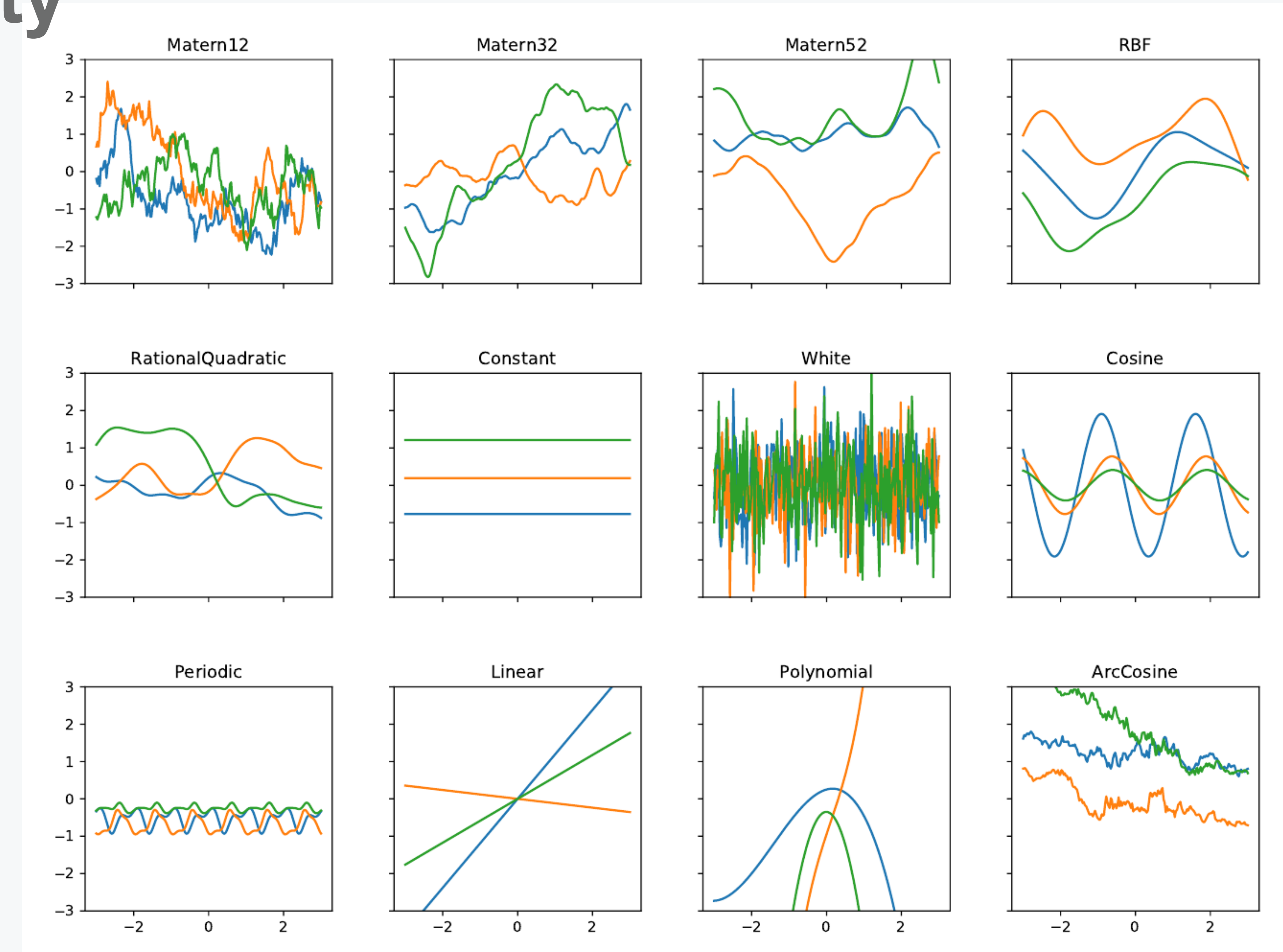
When we know
the mean function m(x)
and the covariance $cov(y_i, y_j)$
between any x_i, x_j
=> A family of functions!

When we further know the y value
at several positions $\{y_i\}$
=> we can predict y at new x*:
$p(y^* \mid \{y_i\})$

The posterior mean and the
uncertainty

Flexibility

Kernel



However, GP is not robust to outliers

$$y = f(\boldsymbol{x}) + \epsilon,$$

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Full length article

Robust Gaussian process regression based on iterative trimming

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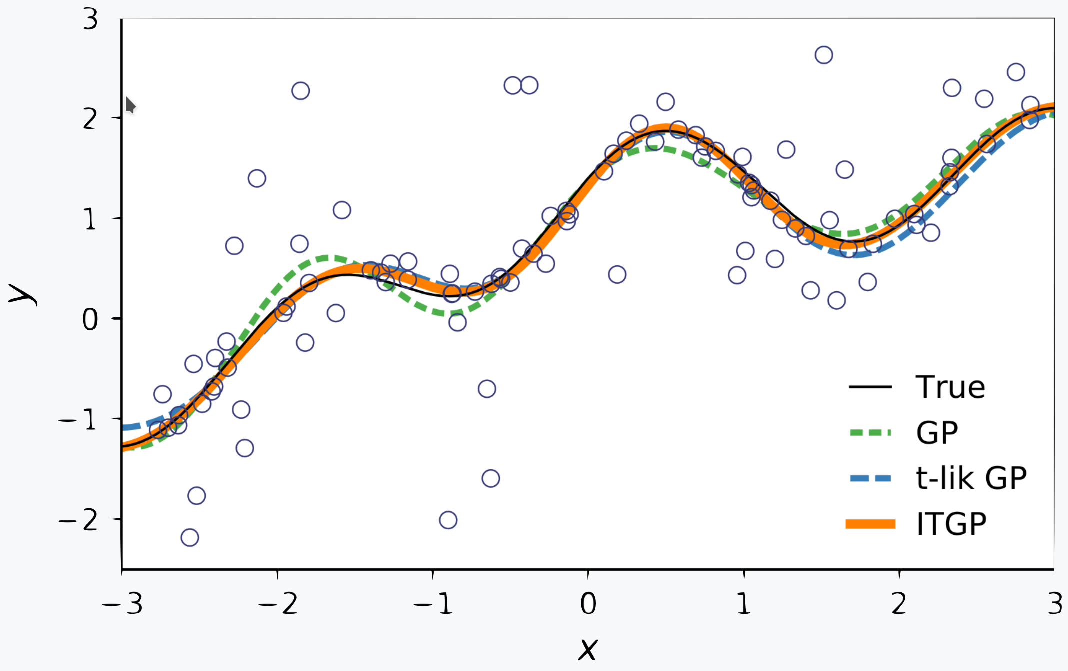
[d] Key Lab for Astrophysics, Shanghai 200234, China

Two solutions:

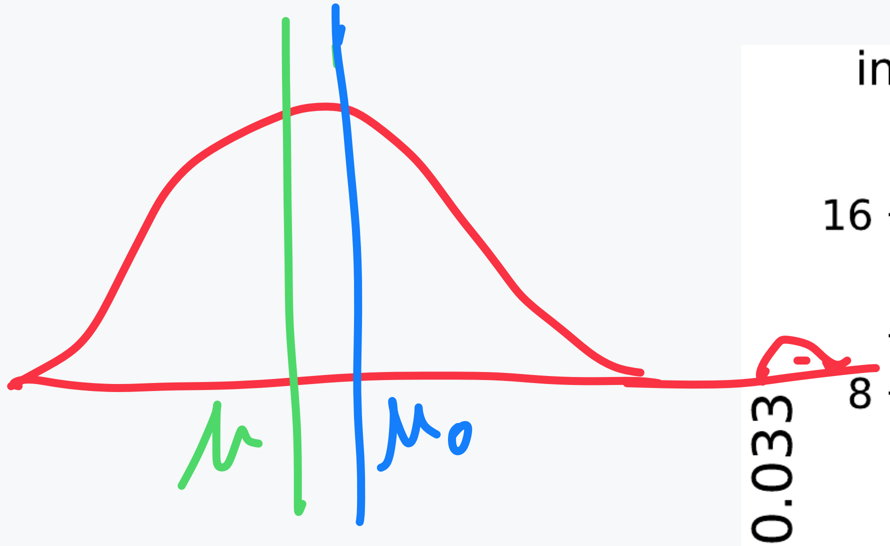
a) lower the significance of poits with large deviation, e.g., using a Students' t distribution for observation model (instead of Gaussian)

b) discard such points
... but in a iterative way

=> Iterative Triming Gaussian Process (ITGP)



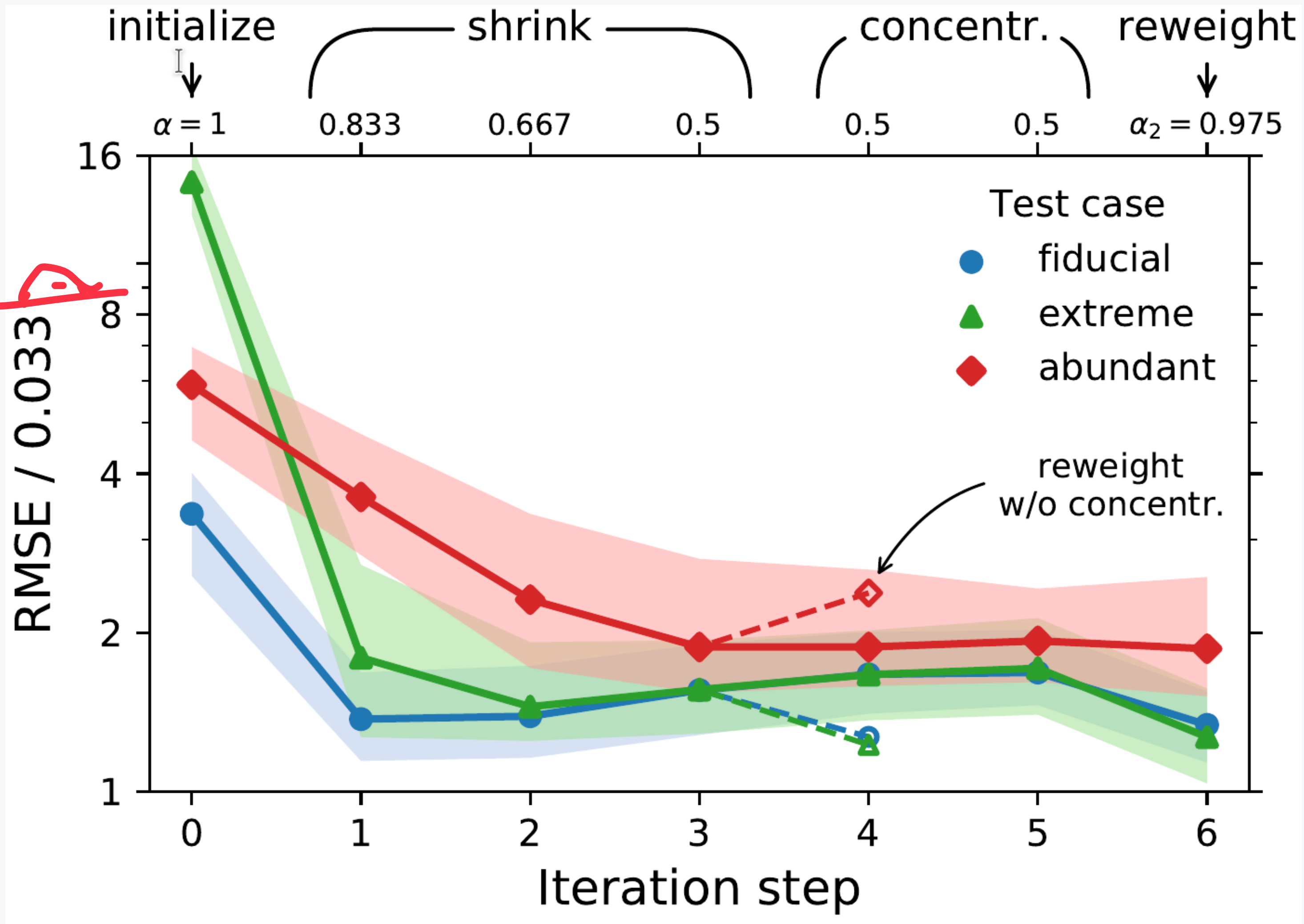
Iterative Trimming Gaussian Process (ITGP)



step 1. trim $3\sigma_0 \to \mu_1, \sigma_1$

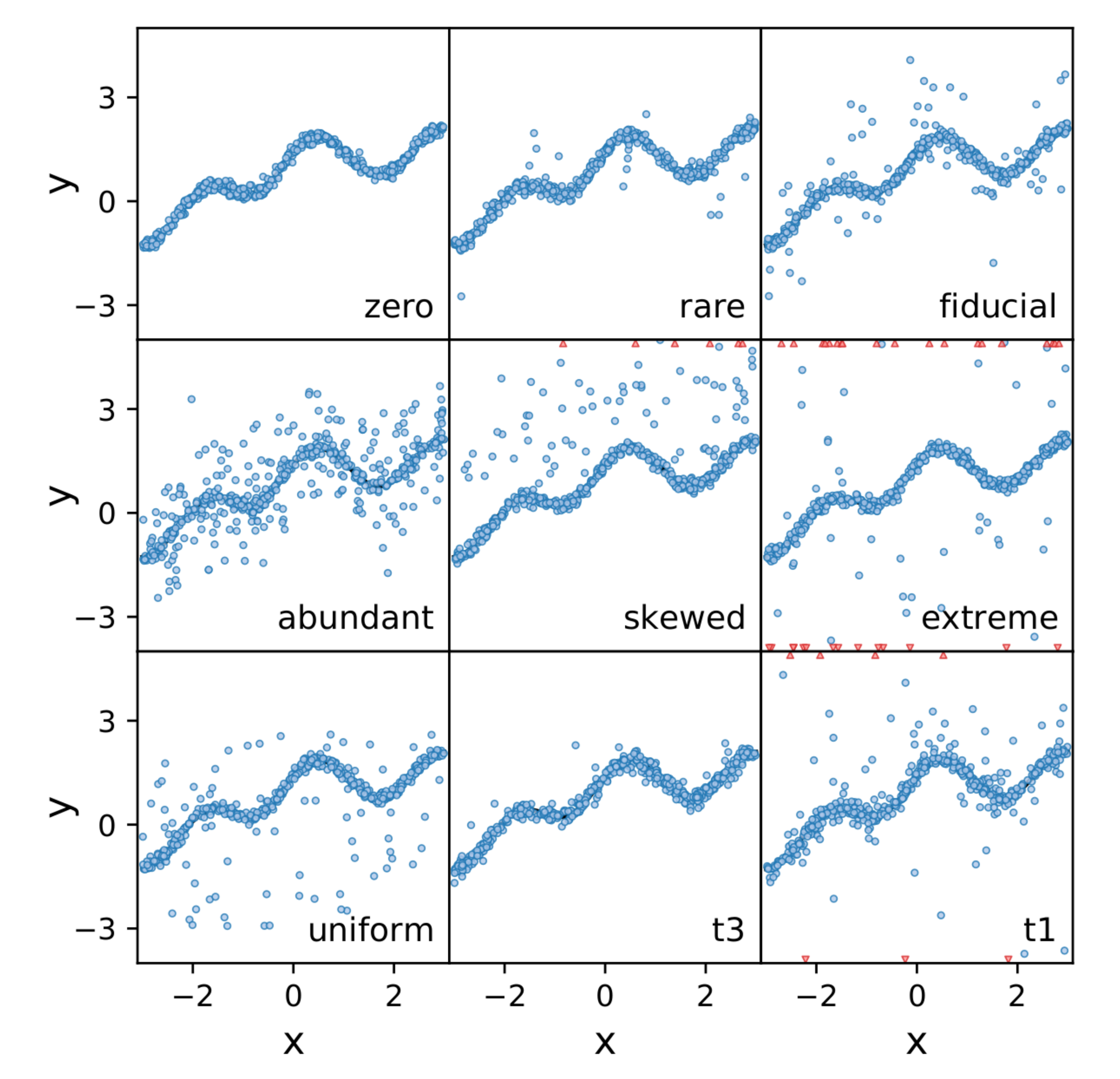
step 2. trim $3\sigma_1 \to \mu_1, \sigma_2$

⋮

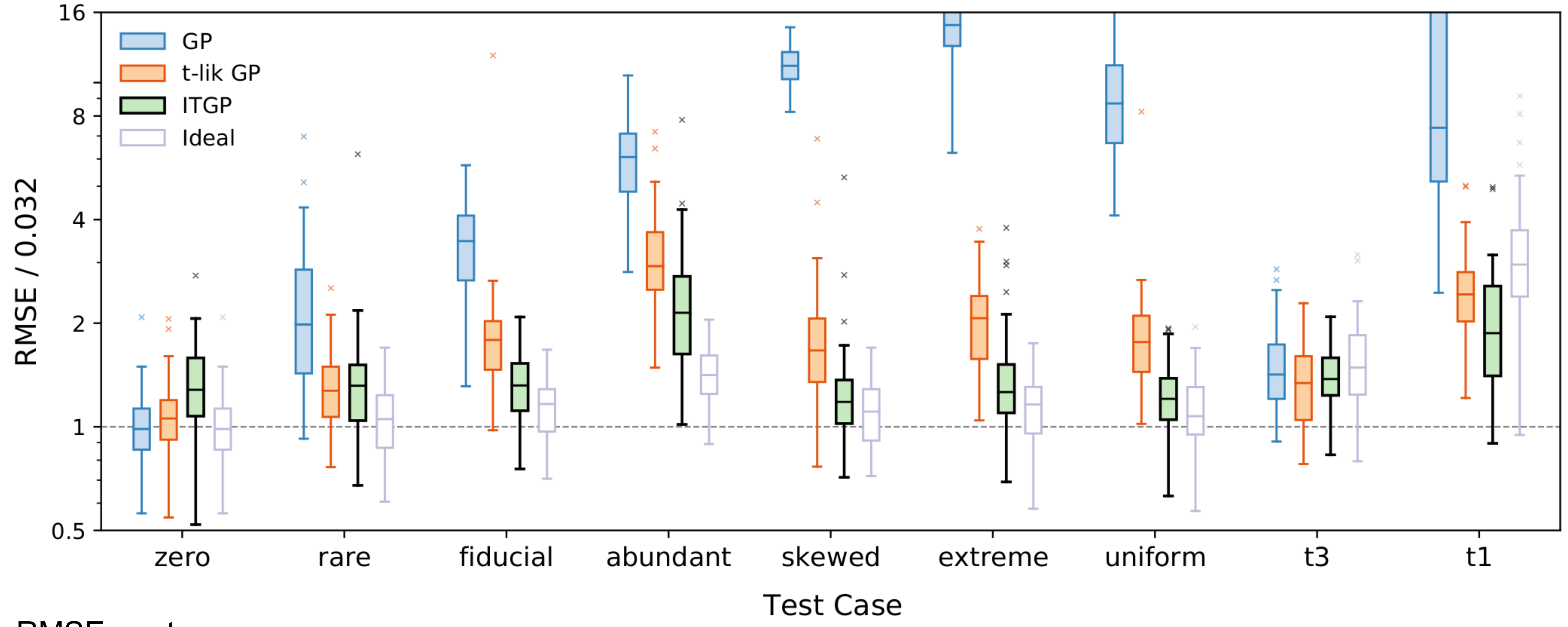


We trim the outliers in an iterative way (ITGP)

Benchmark: test cases

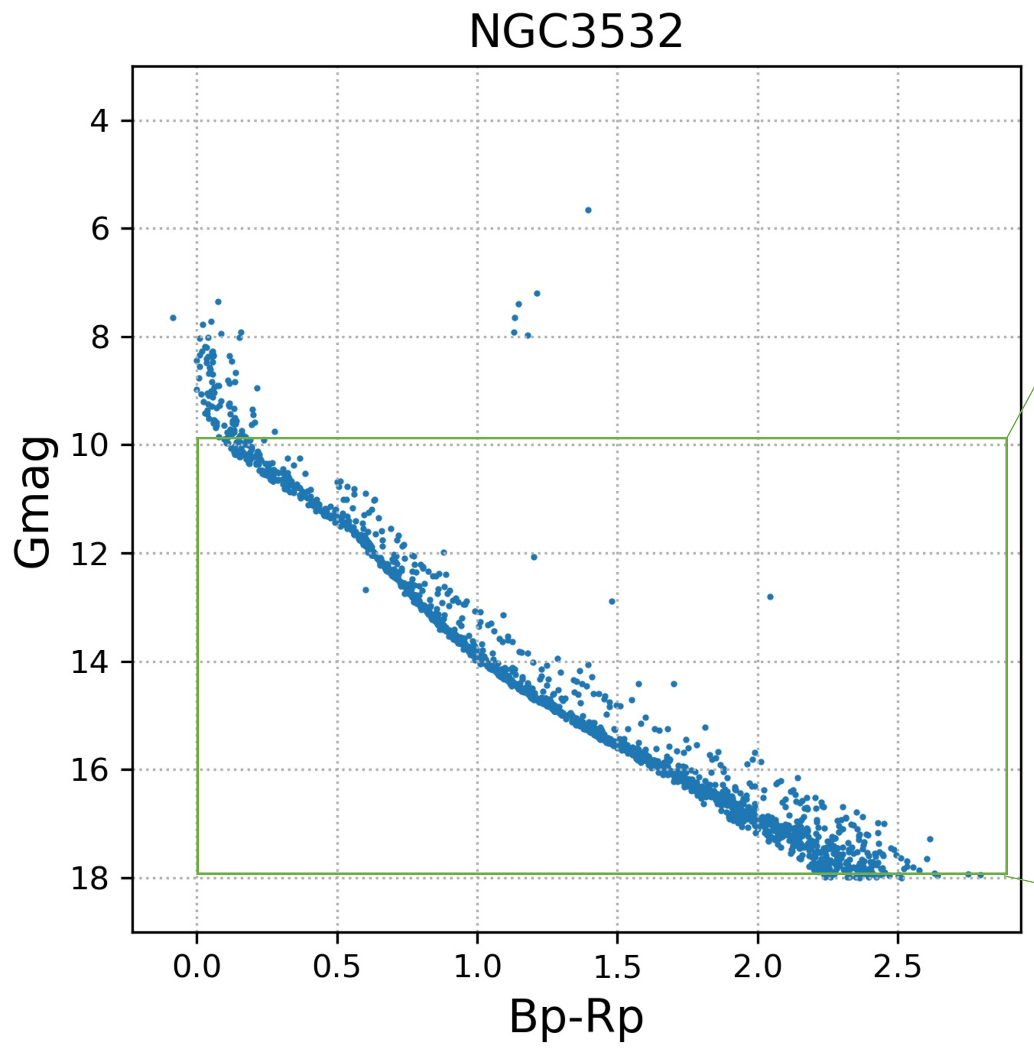


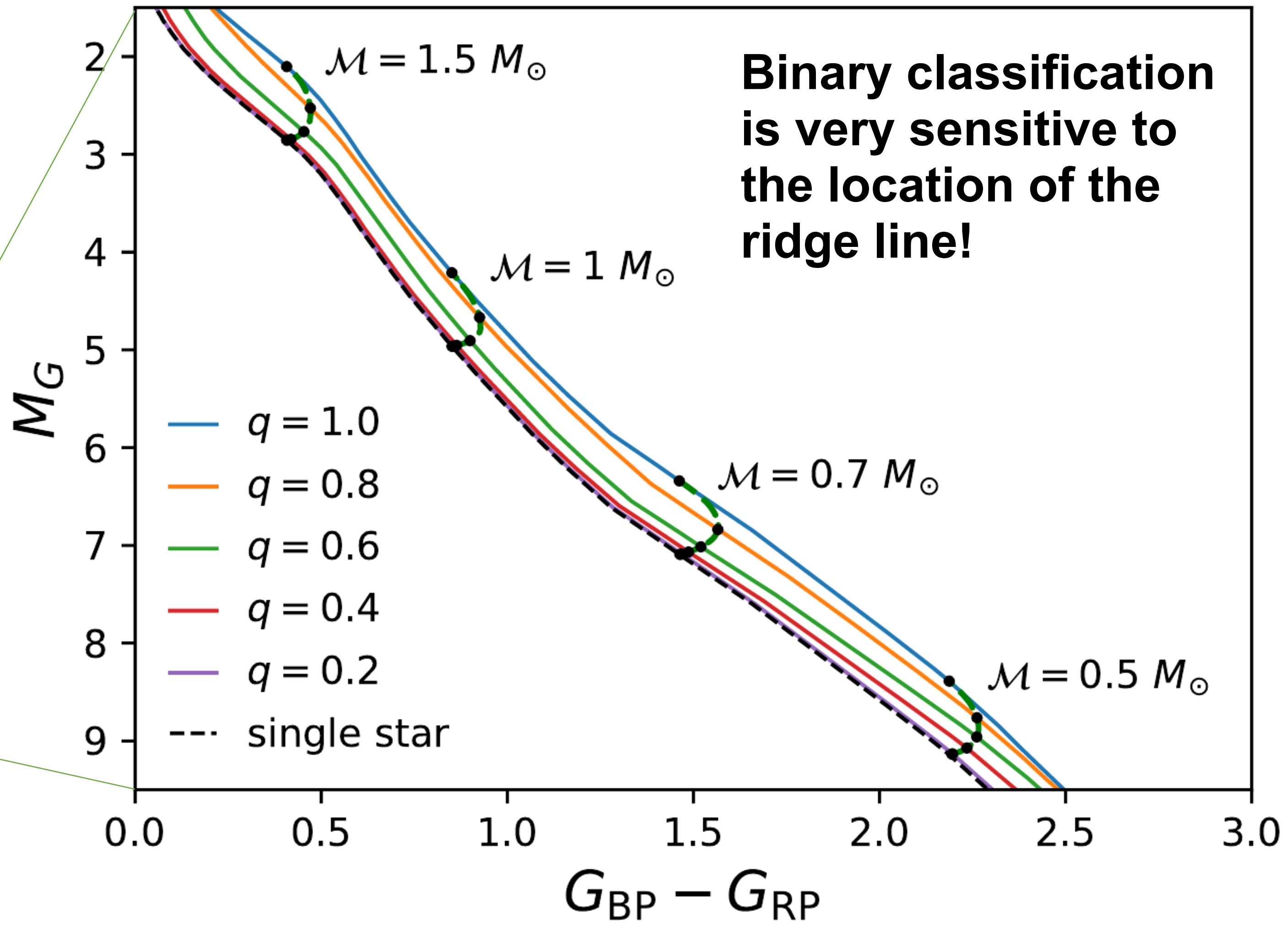
Benchmark



RMSE: root-mean-square error
<(y_pred - y_true)^2>^0.5

Main-sequence ridge line in CMD

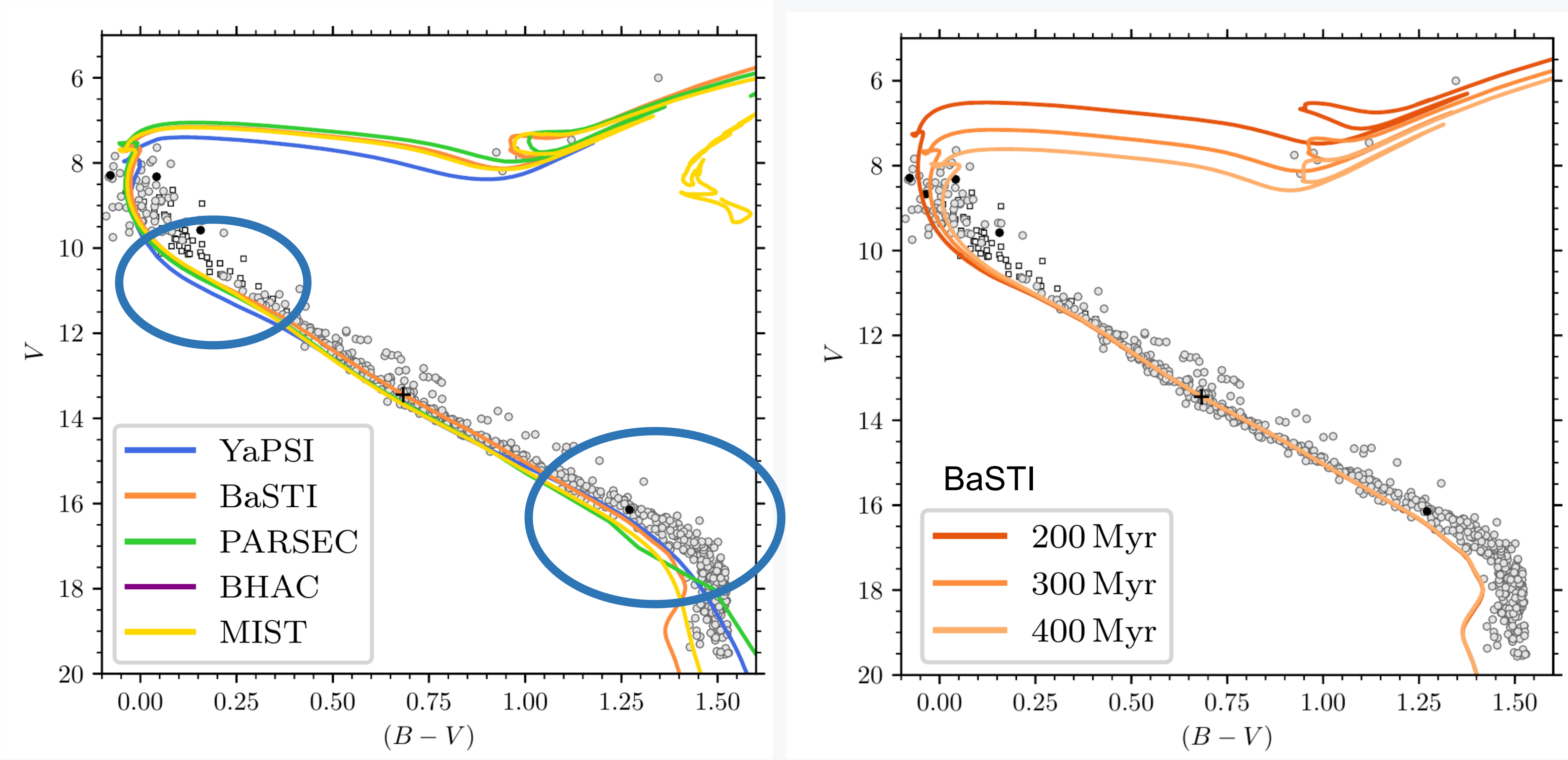




Binary classification is very sensitive to the location of the ridge line!

Lu Li+ 2020

Stellar models are not perfect for observation



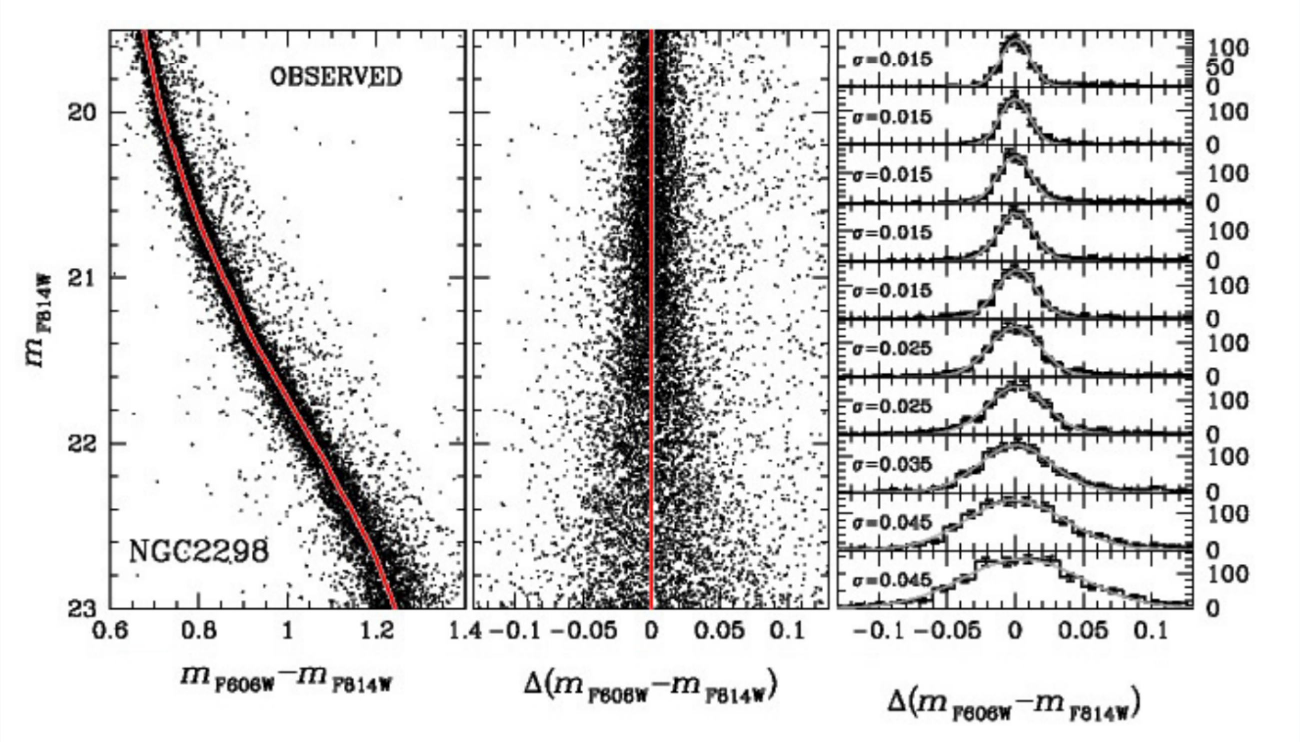
Fritzewski+ 2019

Observed ridge lines of clusters can be used to calibrate stellar models

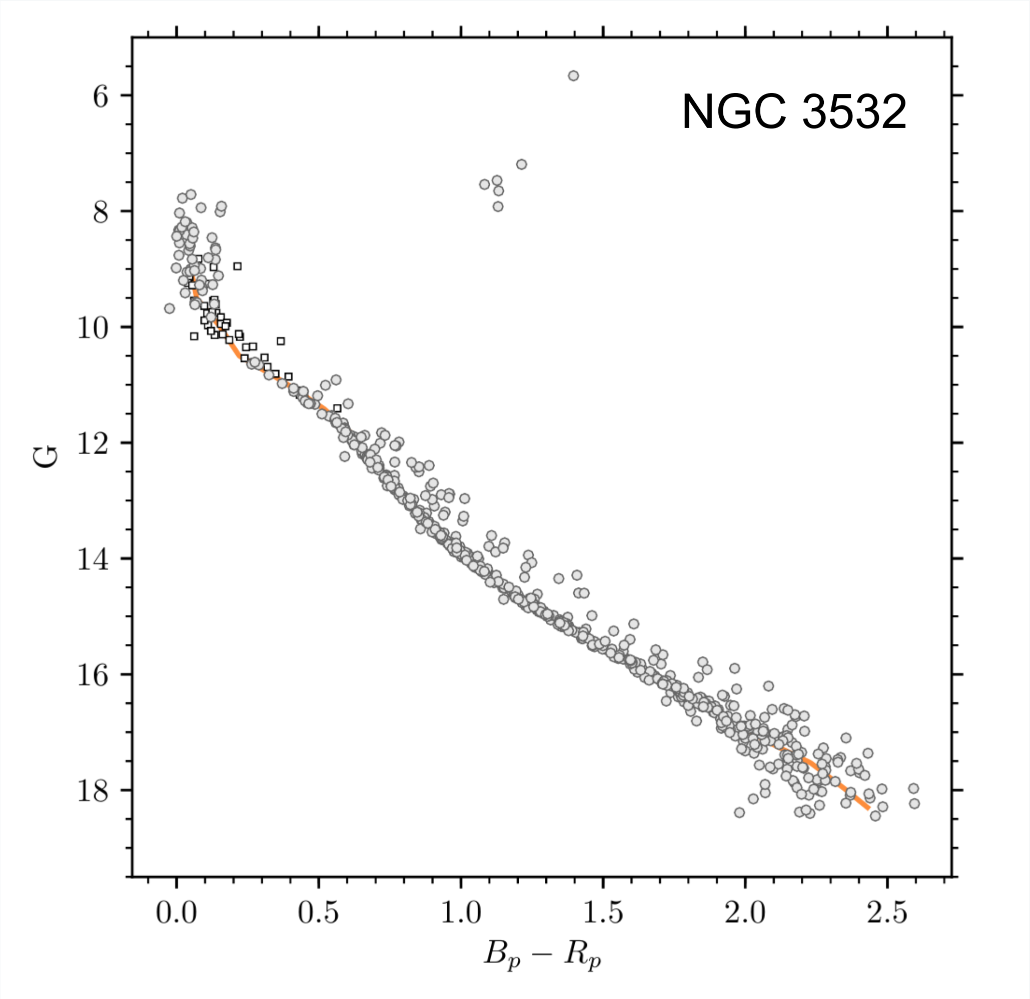
How to let the data itself talk?

Draw the line manually
➢ Arbitrary, lack of reproducibility
➢ Not practical when you have thousands of clusters

Use the peak of histogram of color
➢ Requiring many many member stars (e.g., globular clusters)
➢ Not applicable to open clusters



Milone et al. 2012

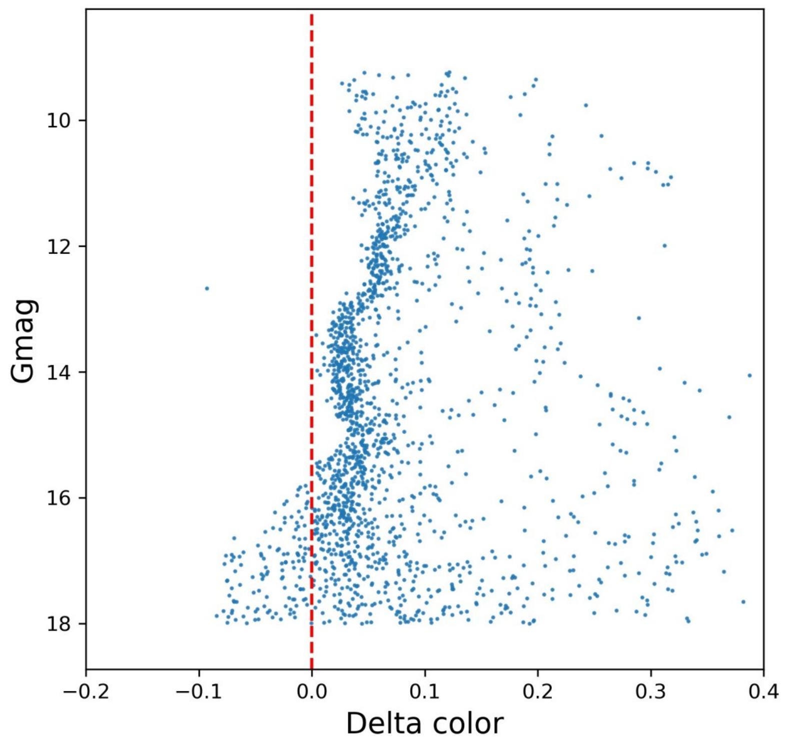


Fritzewski et al. 2019

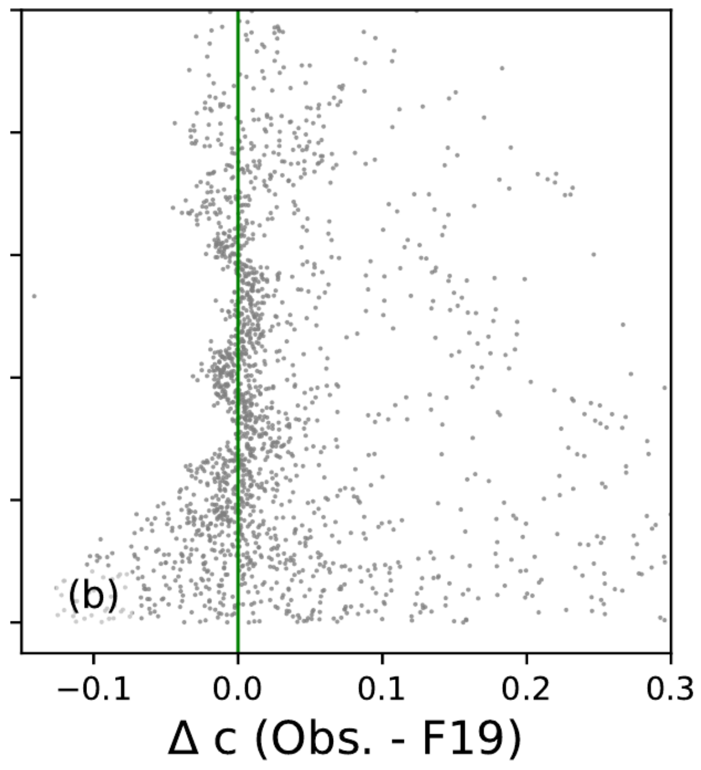
Better solution: Robust GP

Residual color of NGC 3532:

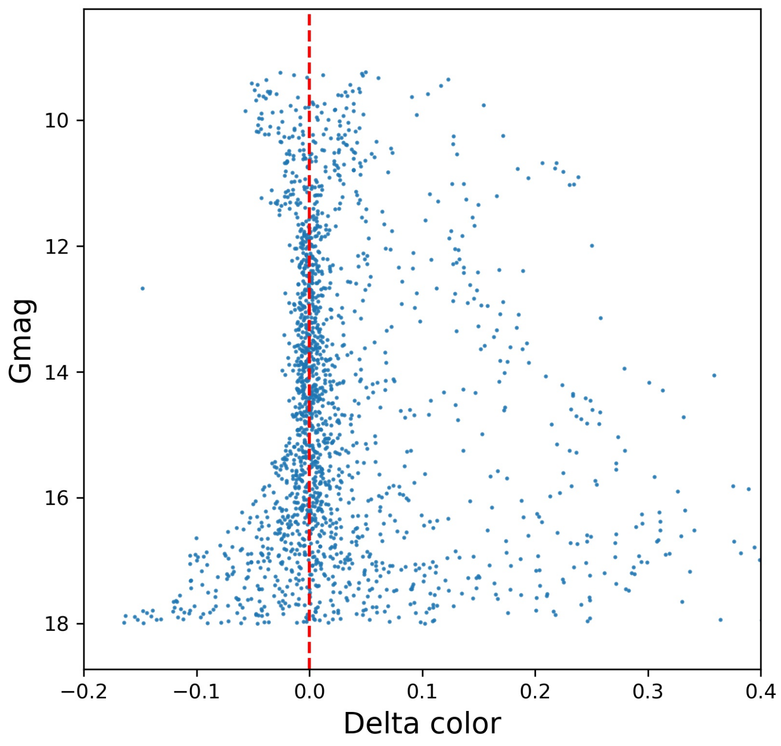
PARSEC (stellar model)



By hand (Fritzewski 19)



Our method (robust GP)



Summery

Gaussian process (GP):

a **non-parametric** and **probabilistic** method

- a non-parametric method, completely data-driven and does not assume any explicit functional form between variables, which is particularly attractive in the big data era.
- provides a Bayesian framework with a natural way of characterizing prior and posterior distributions over functions.
- can naturally handle the noises that are assumed to follow normal distributions.

We can make GP robust by **iterative trimming (ITGP)** outliers

with a practical example in star cluster study

Some sources:

Classic book: Gaussian Processes for Machine Learning, by Rasmussen and Williams 2006

GP tutorial: http://gpss.cc

Python implementation:

for beginner: GPy, scikit-learn

for speed: pytorch, GPflow, celerite

application: 2008.04684

method: 2011.11057

code: https://github.com/syrte/robustgp/