

Scaling **Gaussian Processes** and the search for **exoplanets**

Dan Foreman-Mackey

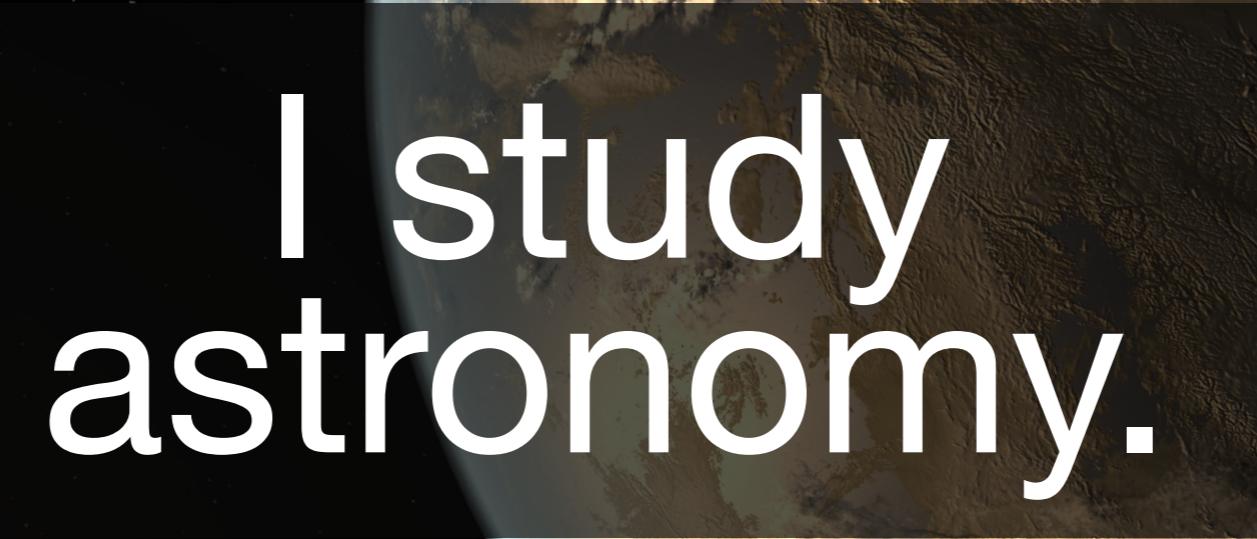
Sagan Fellow, University of Washington

github.com/dfm // [@exoplaneteer](https://twitter.com/exoplaneteer) // dfm.io



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I study
astronomy.



this isn't what
my data look like



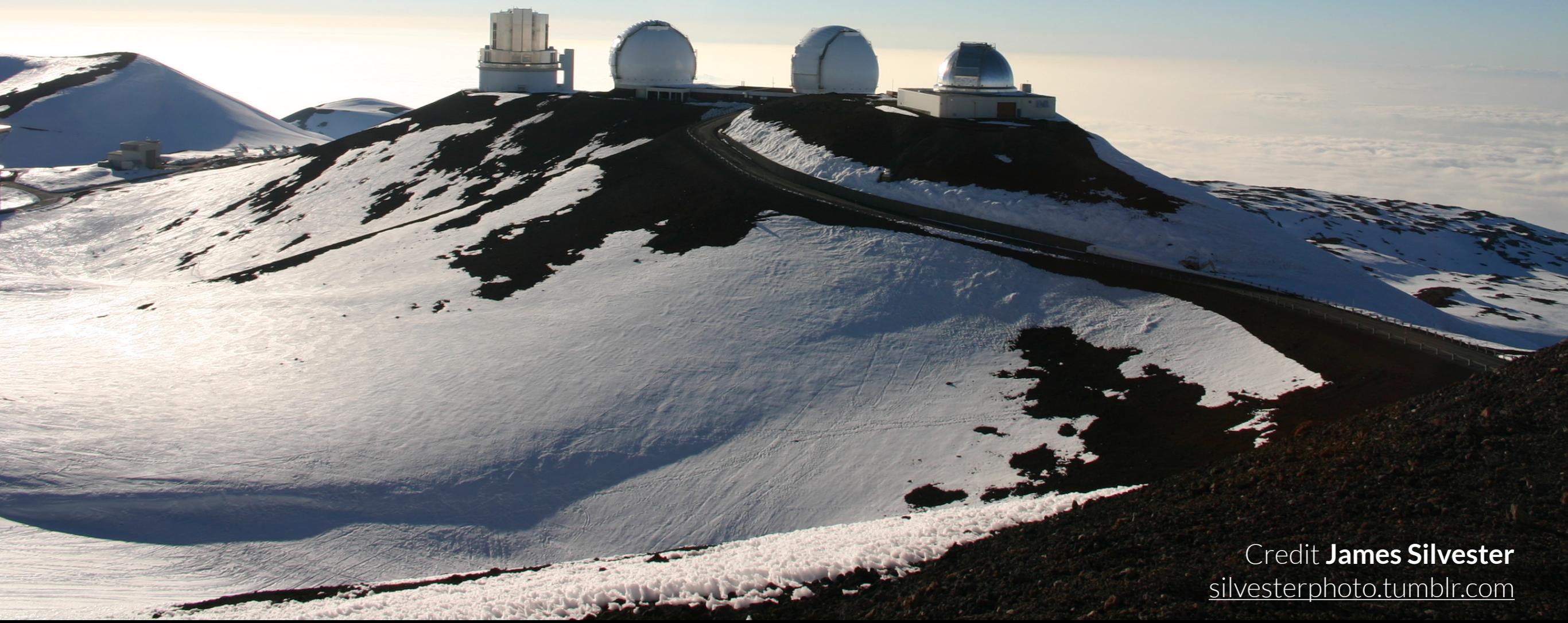
I study
astronomy.



I do data science...

(don't we all?)

this is **not** what my data science looks like.



Credit James Silvester
silvesterphoto.tumblr.com

CATERING PREP

Kitchen

that's more like it...



Flickr user Marcin Wichary

this is what my data science looks like.

$$P(\omega) = \begin{cases} \exp(\theta_i), & \omega \in \Delta_i \\ \vdots \\ \exp(\theta_n), & \omega \in \Delta_n \end{cases}$$
$$\ln P(\{\omega\} | \theta) = \sum_{n,k} \theta_n \mathbf{1}_{[\omega_k \in \Delta_n]} - \sum_i e^{\theta_i} \Delta_i$$
$$f(\omega) \nearrow \text{f(y_1, y_2, ..., y_n)}$$

my

GOALS

for today's talk

convince you that

exoplanets are cool

quals

for today's talk

convince you that

exoplanets are cool

demonstrate some

sick Python code

for today's talk

Why Astronomy?

simple but interesting physical models

precise open-access data

observational only

Why Astronomy?

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precise open-access data

observational only

no chance of financial gain ever

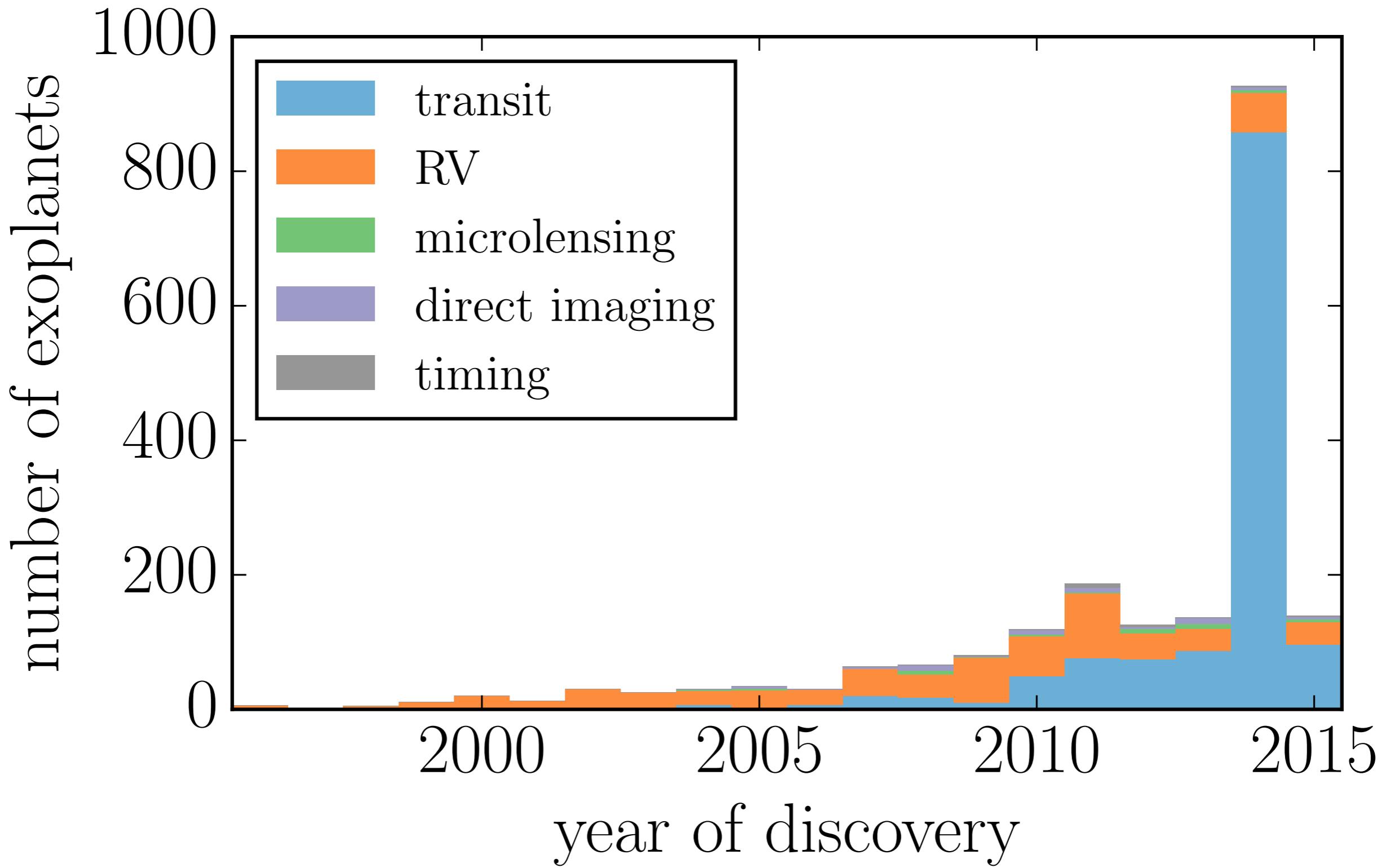
ex·o·plan·et

'eksō,planət/

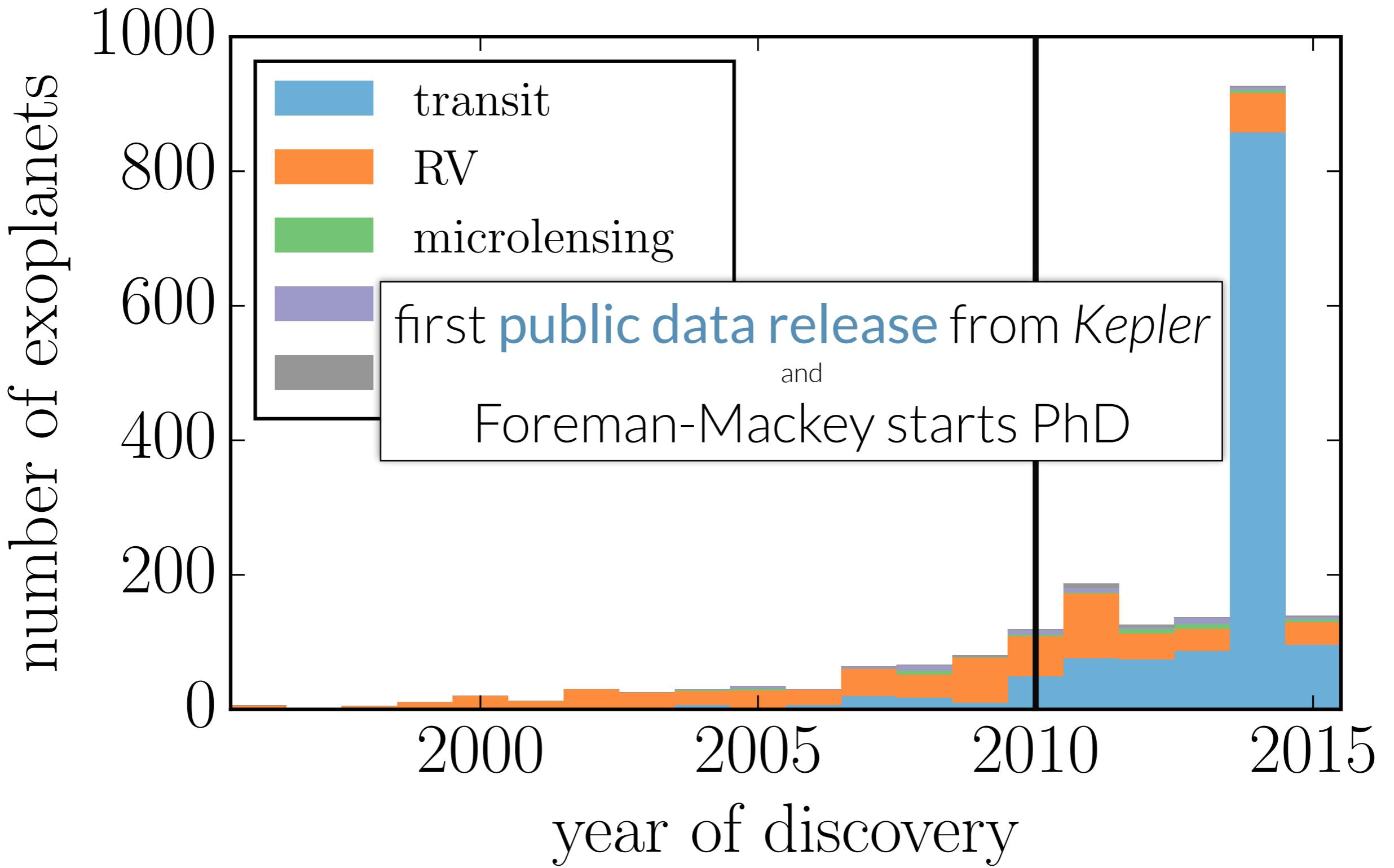
noun. a planet that orbits a star outside the solar system.

How do we **find & study** exoplanets?

- 1307 transit
- 644 radial velocity
- 48 direct imaging
- 37 microlensing
- 24 timing
- 0 astrometry

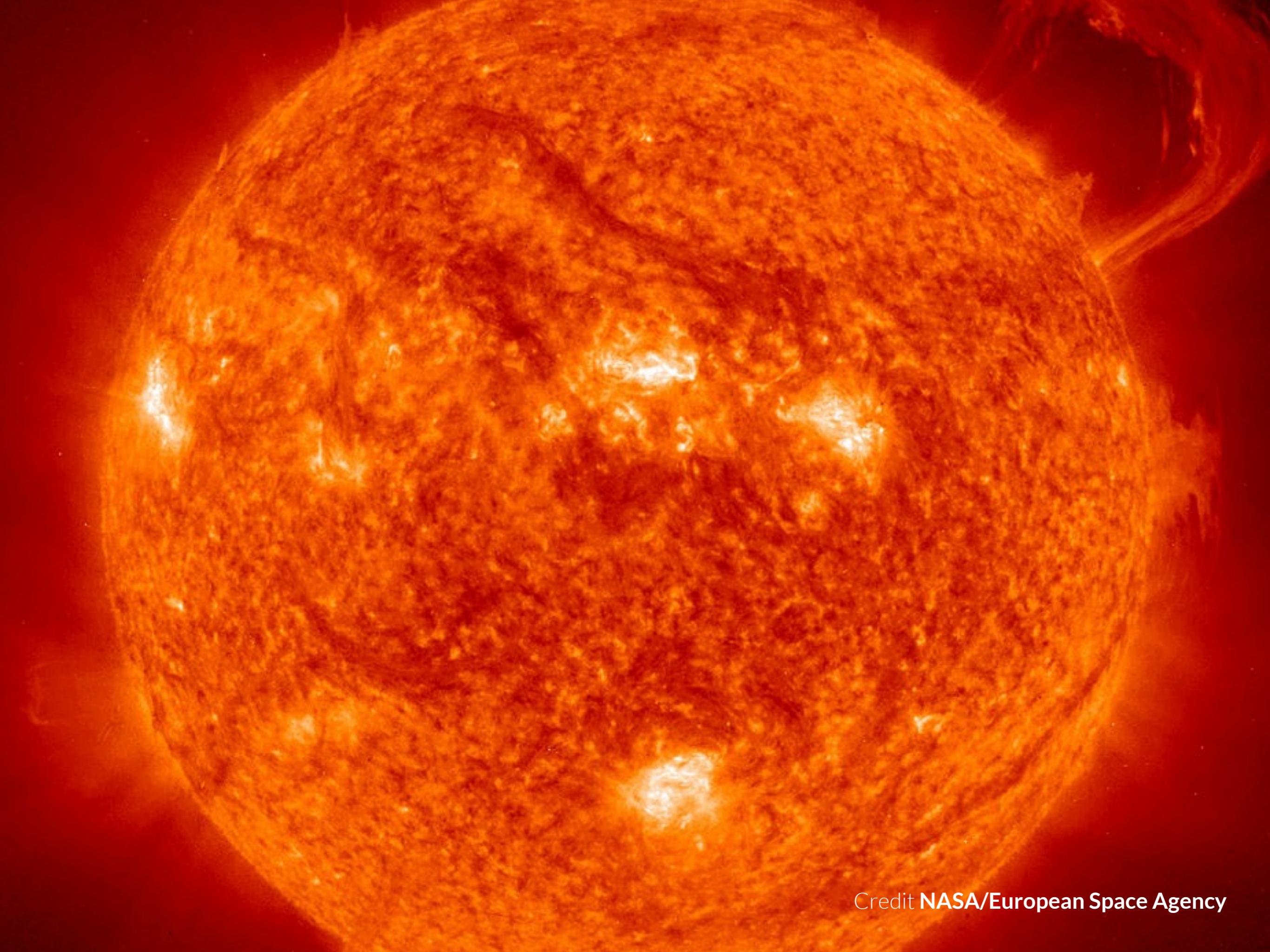


Data from **Open Exoplanet Catalogue** (2015-10-28)

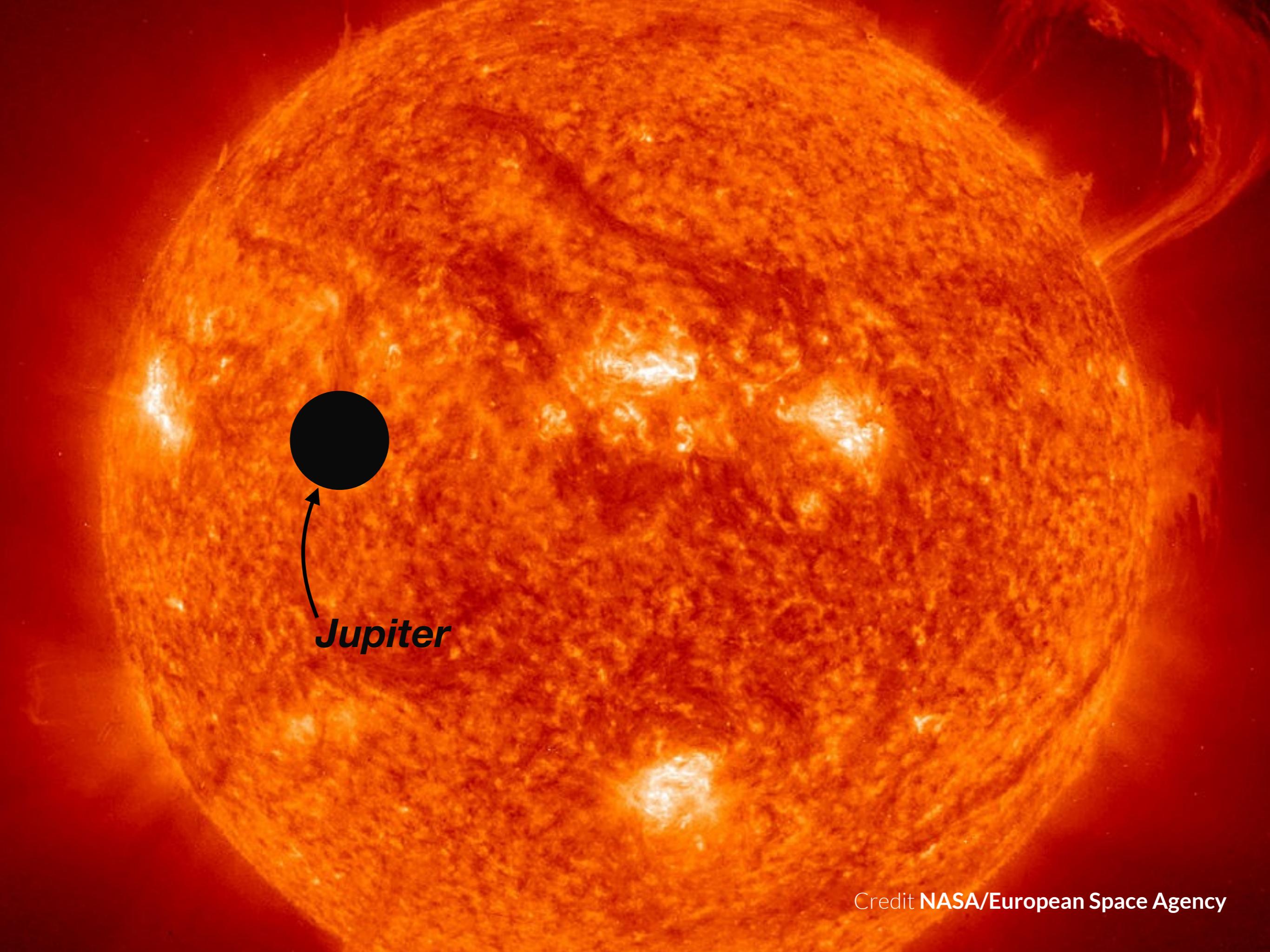


Data from **Open Exoplanet Catalogue** (2015-10-28)

*the **transit** method*

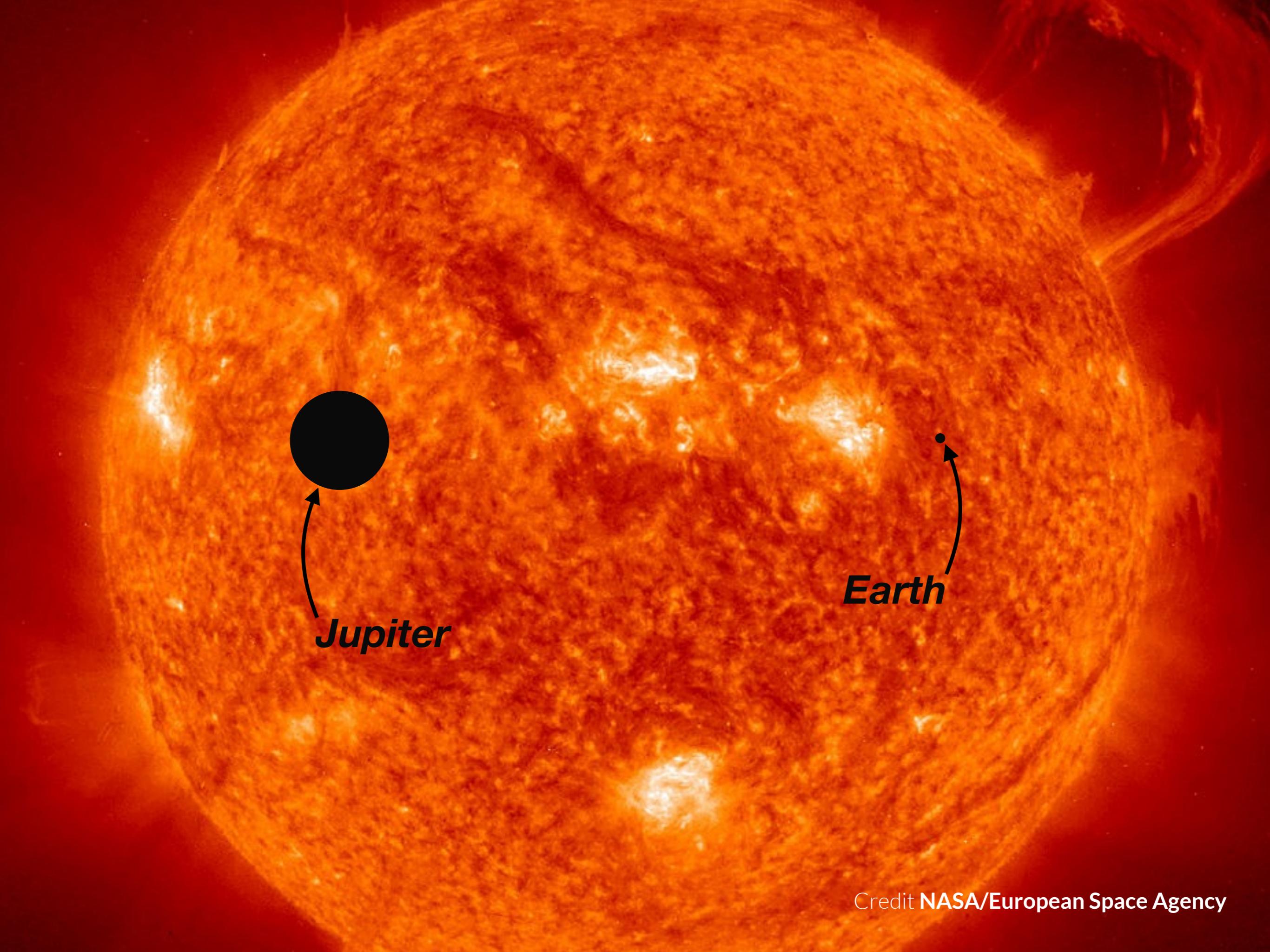


Credit NASA/European Space Agency



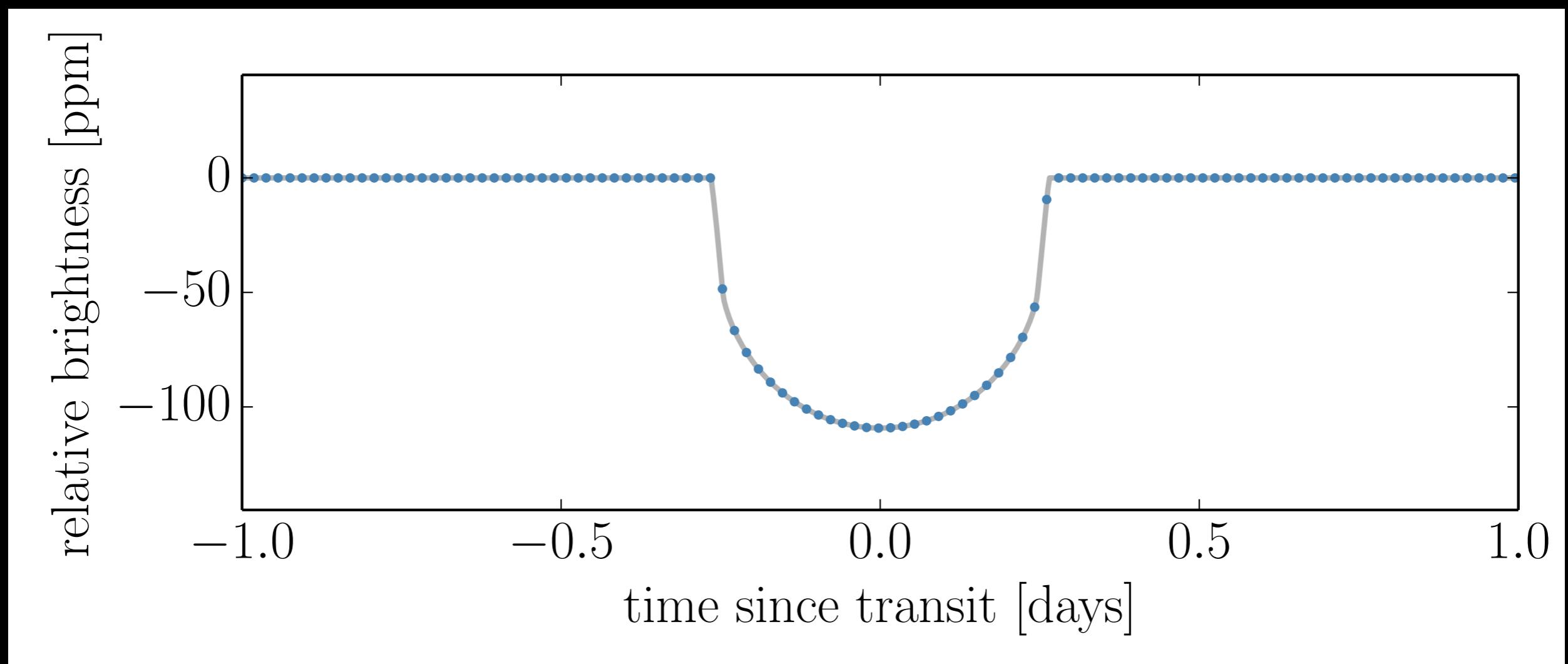
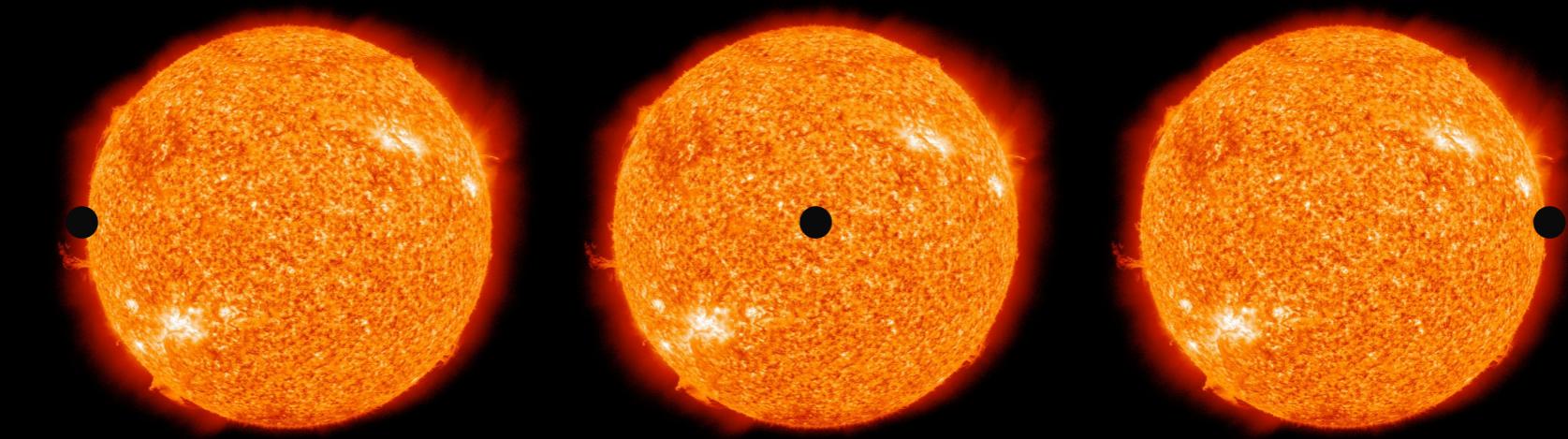
Jupiter

Credit NASA/European Space Agency

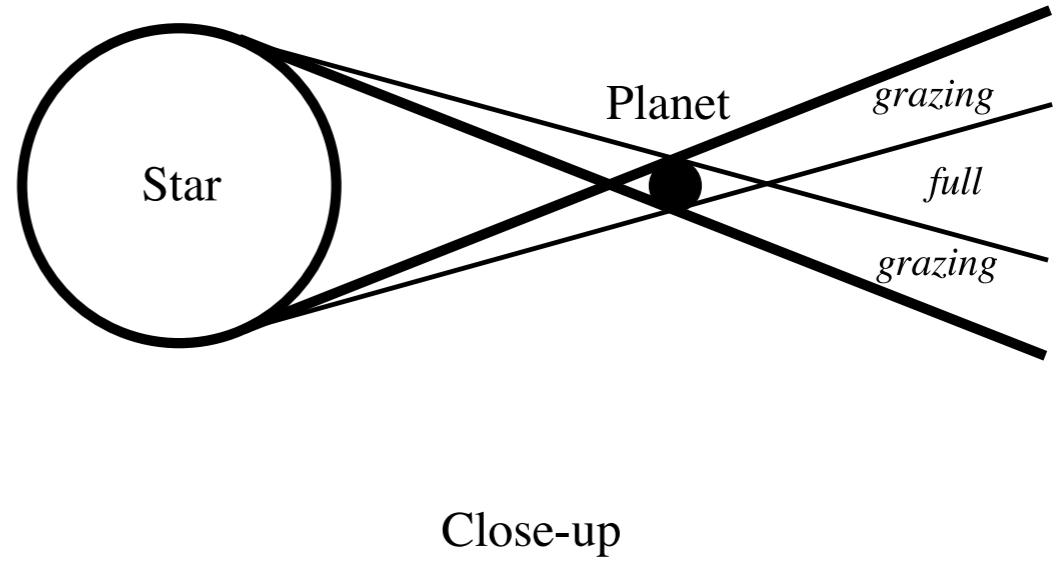
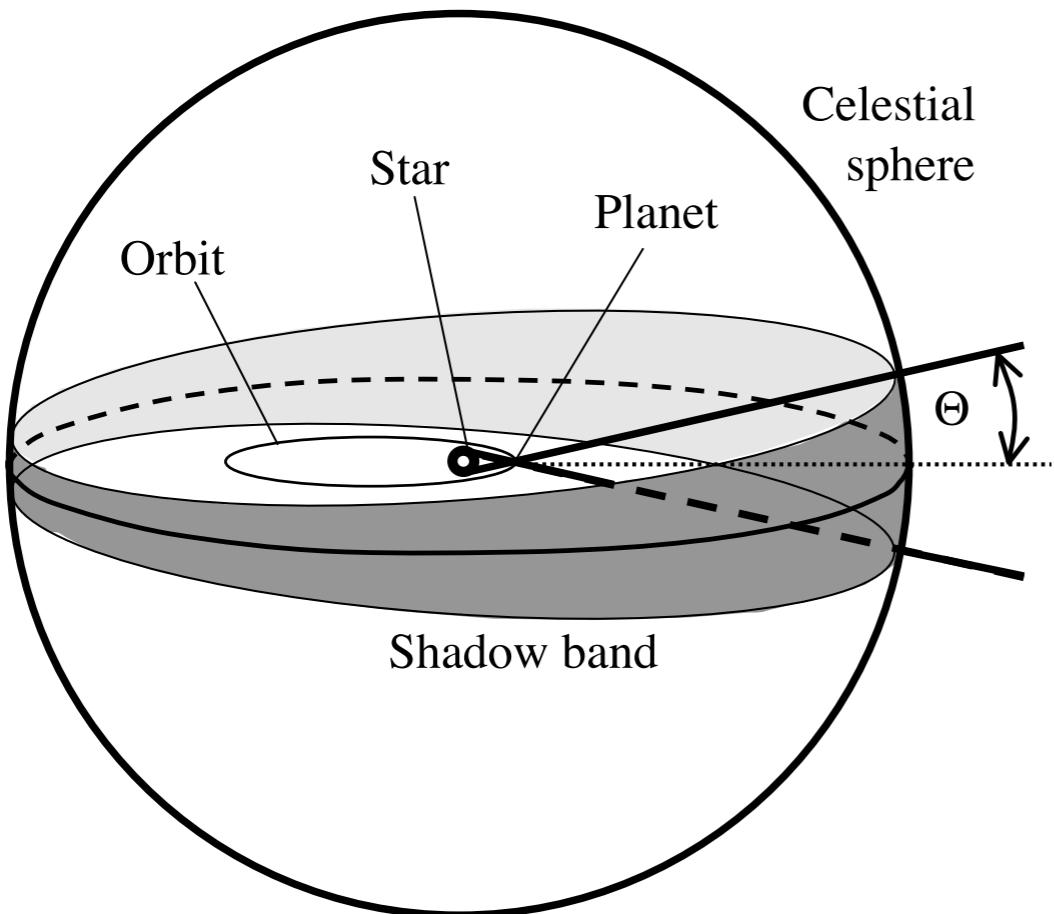


Credit NASA/European Space Agency

that's not what most stars look like!



everything is against us!

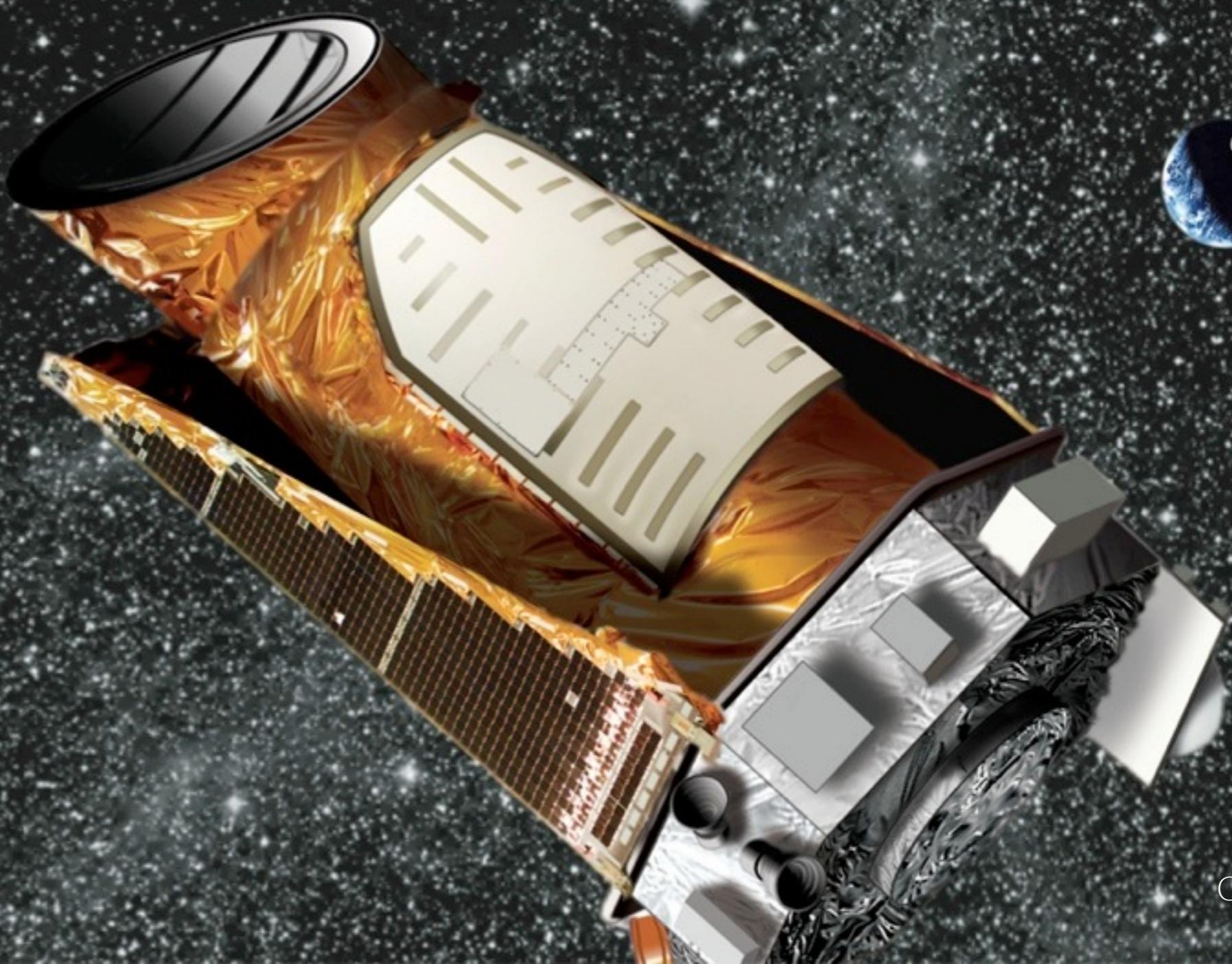


Credit **Winn (2010)**
arXiv:1001.2010

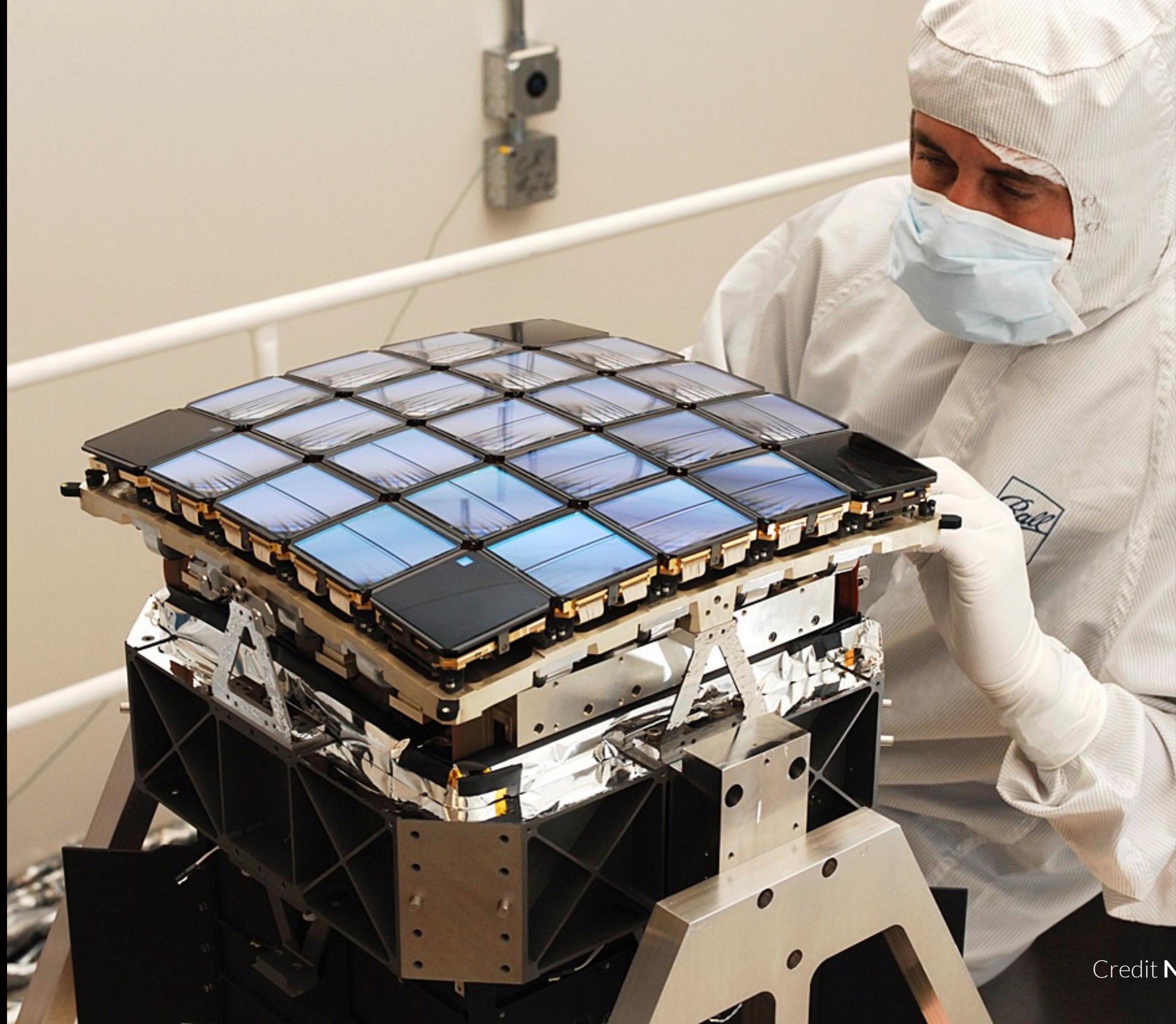
need to look at **the right place**
at **the right time**

and measure
extremely precise
photometry

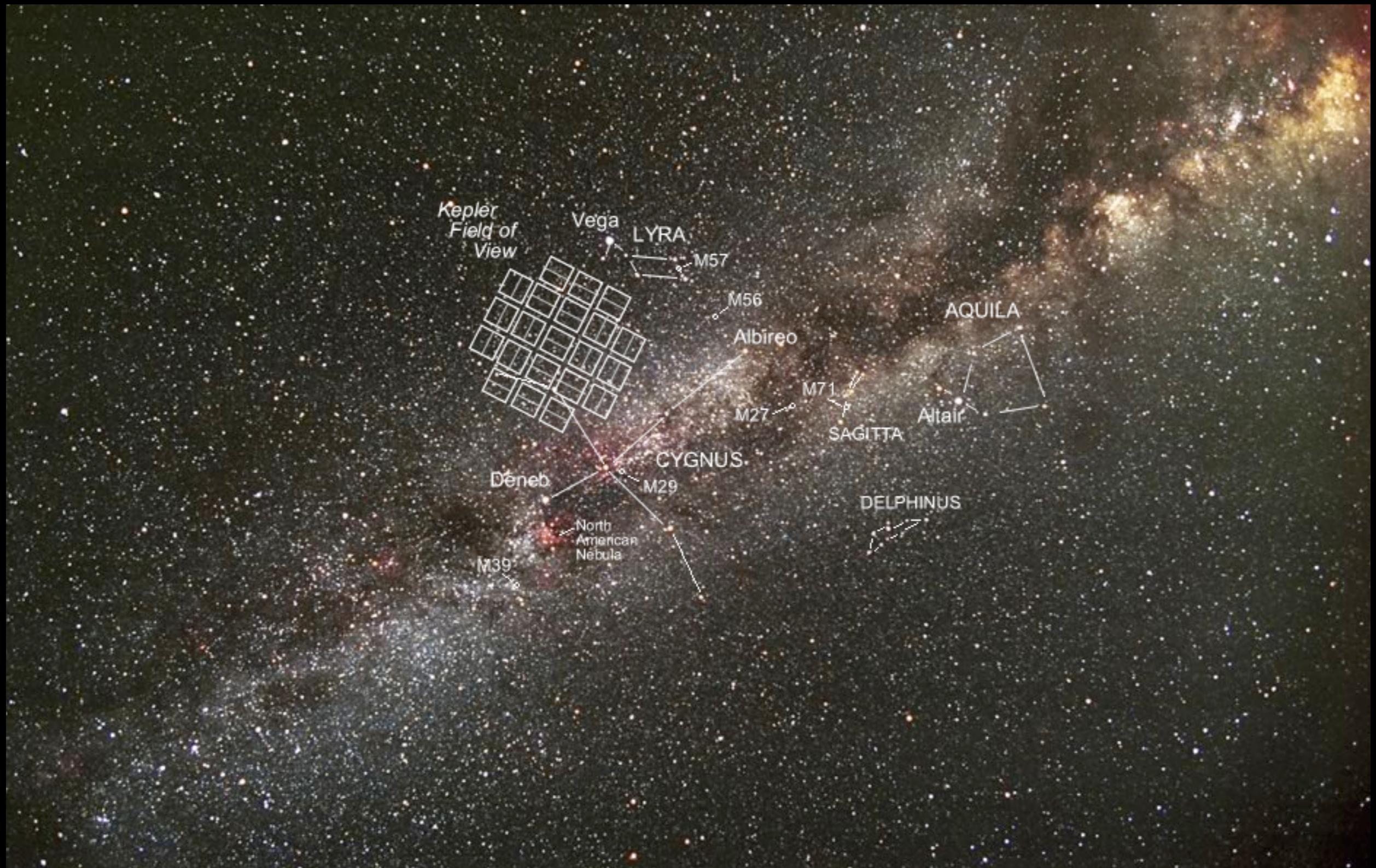
Kepler



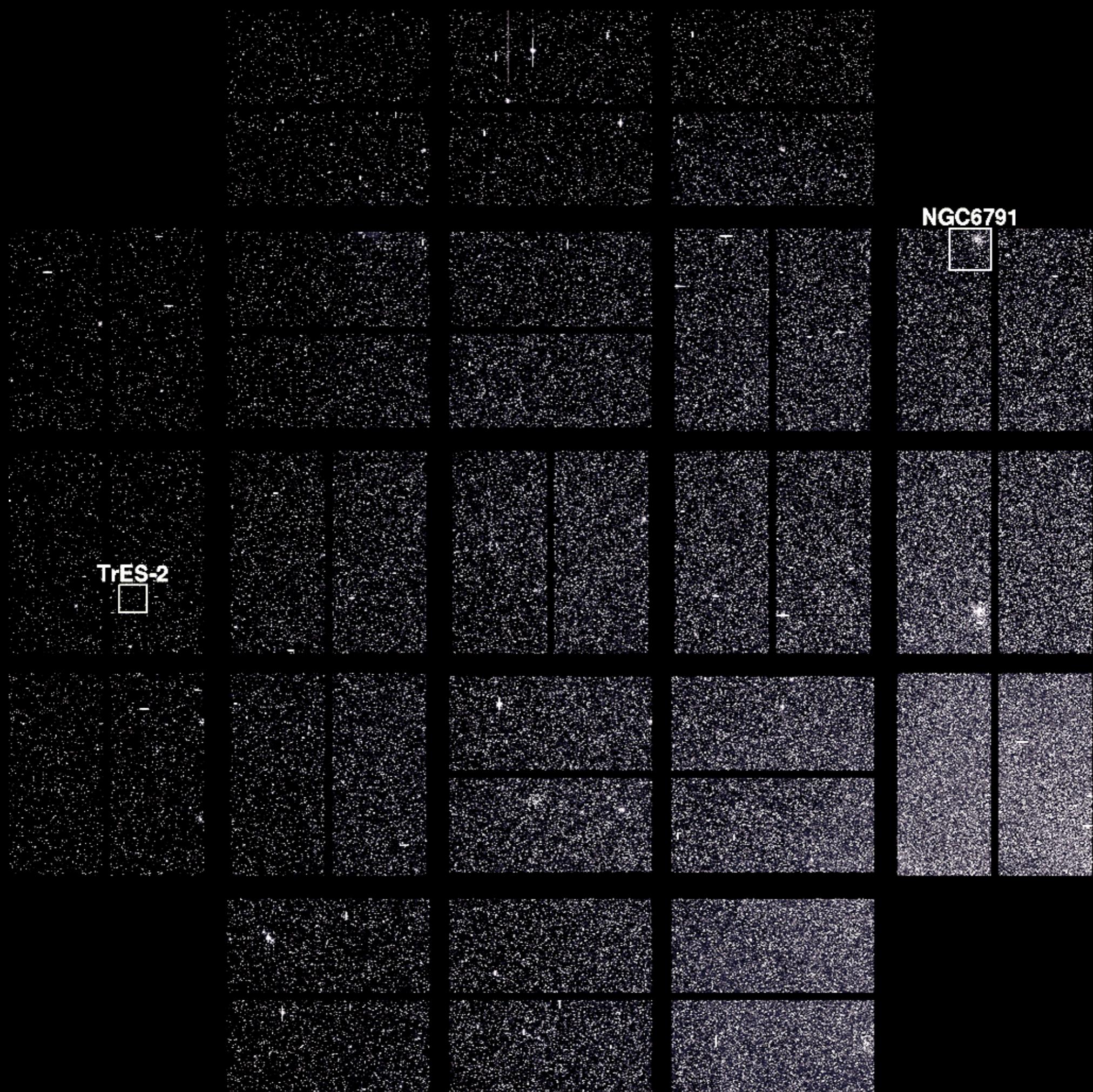
Credit NASA



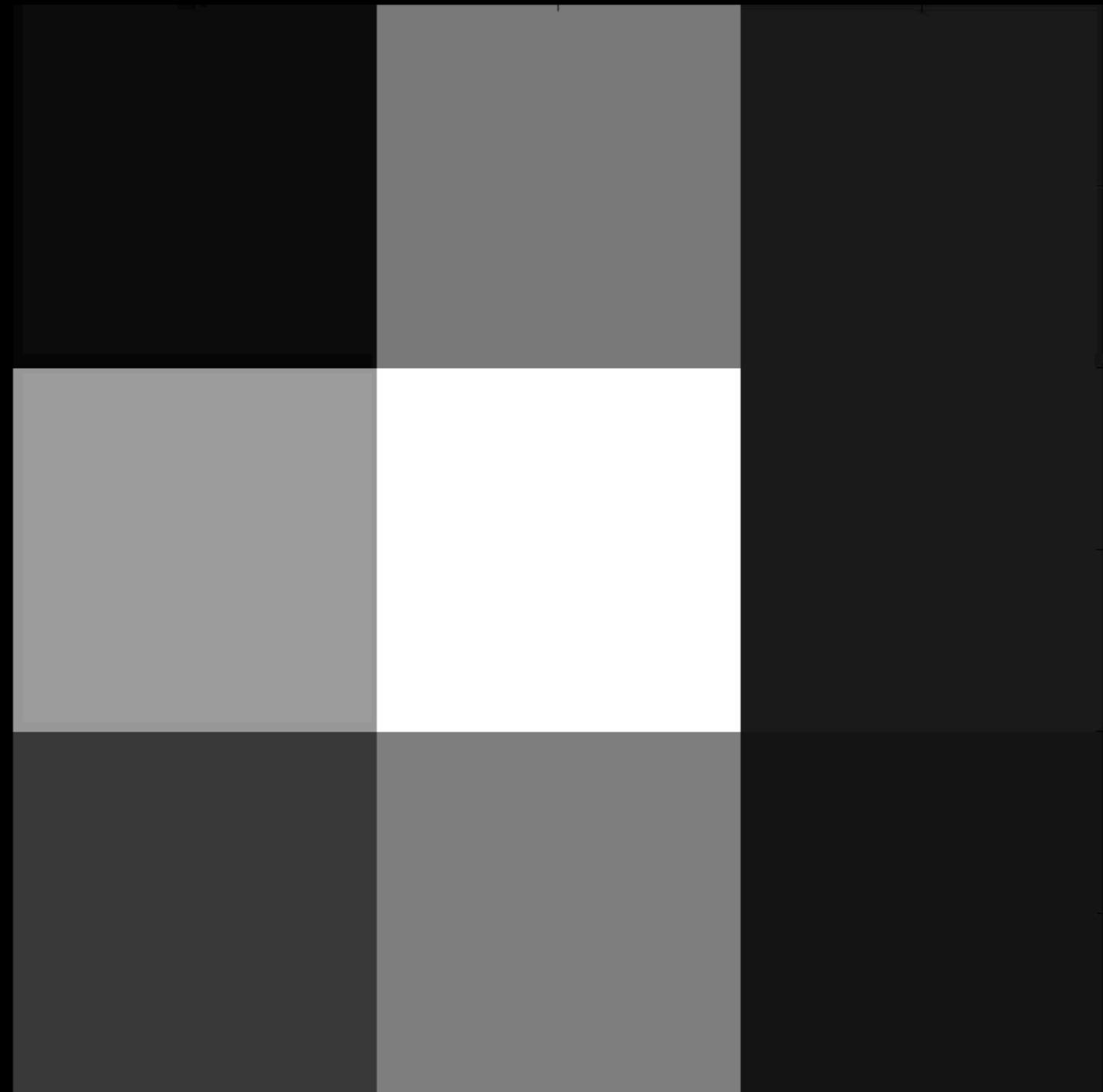
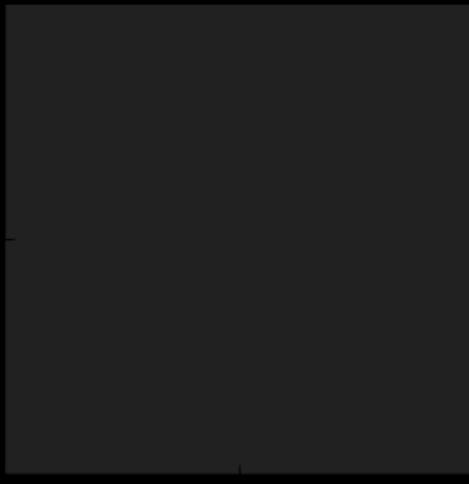
Credit NASA



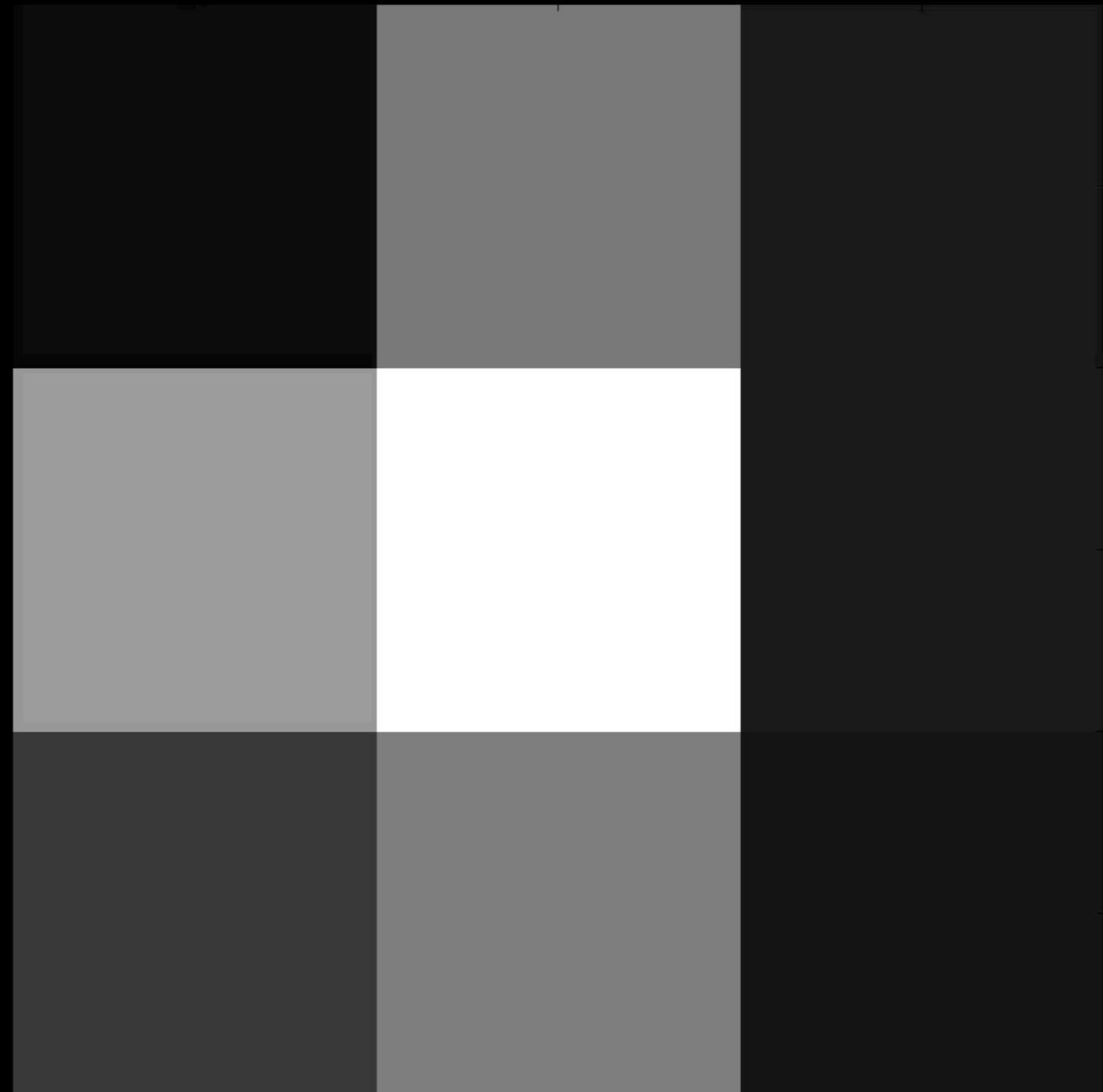
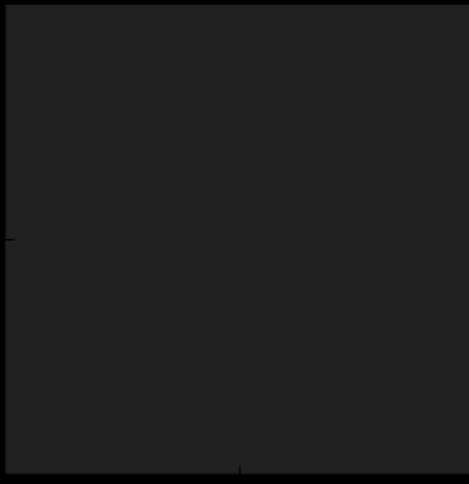
Credit Carter Roberts



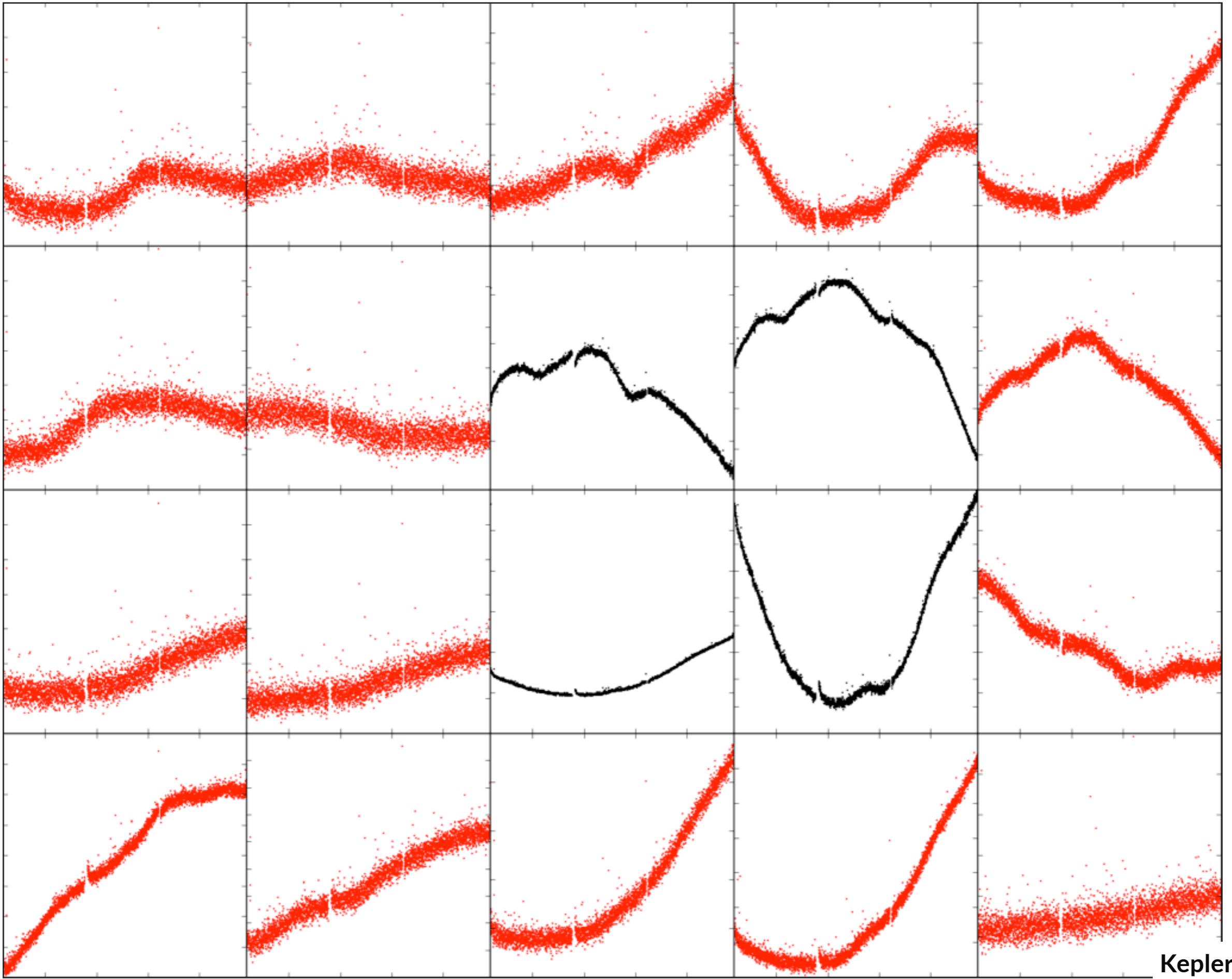
Credit NASA



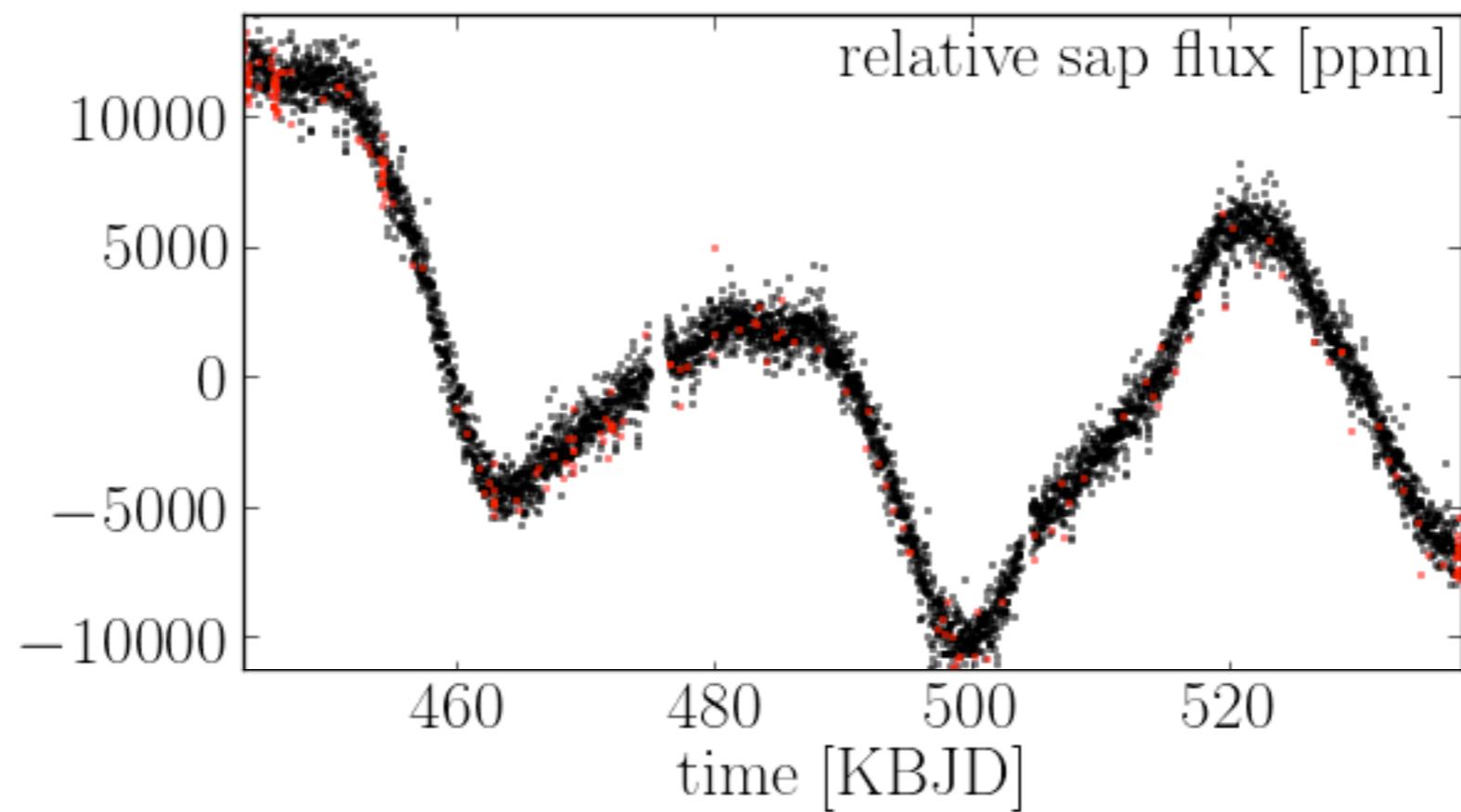
Kepler-32

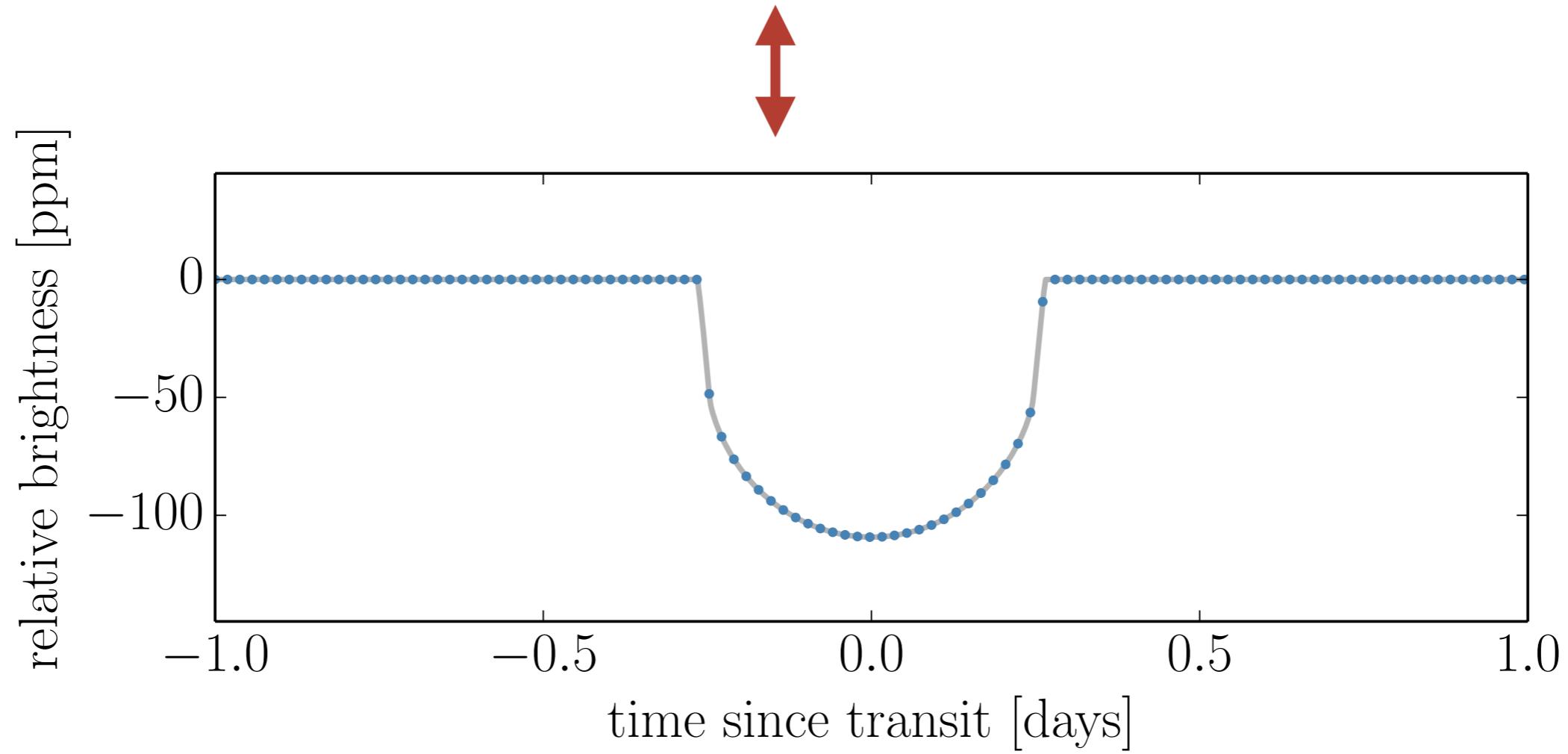
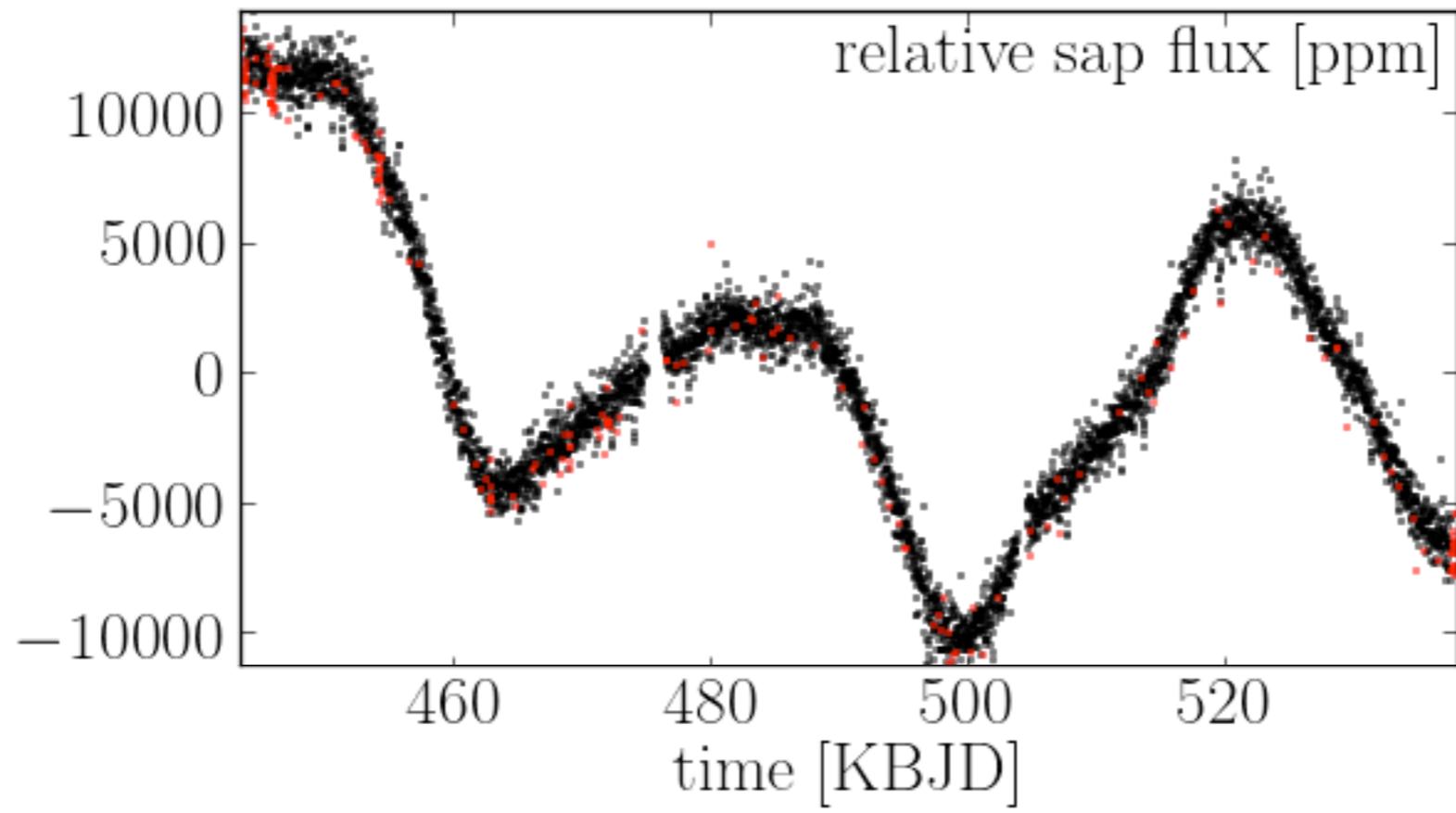


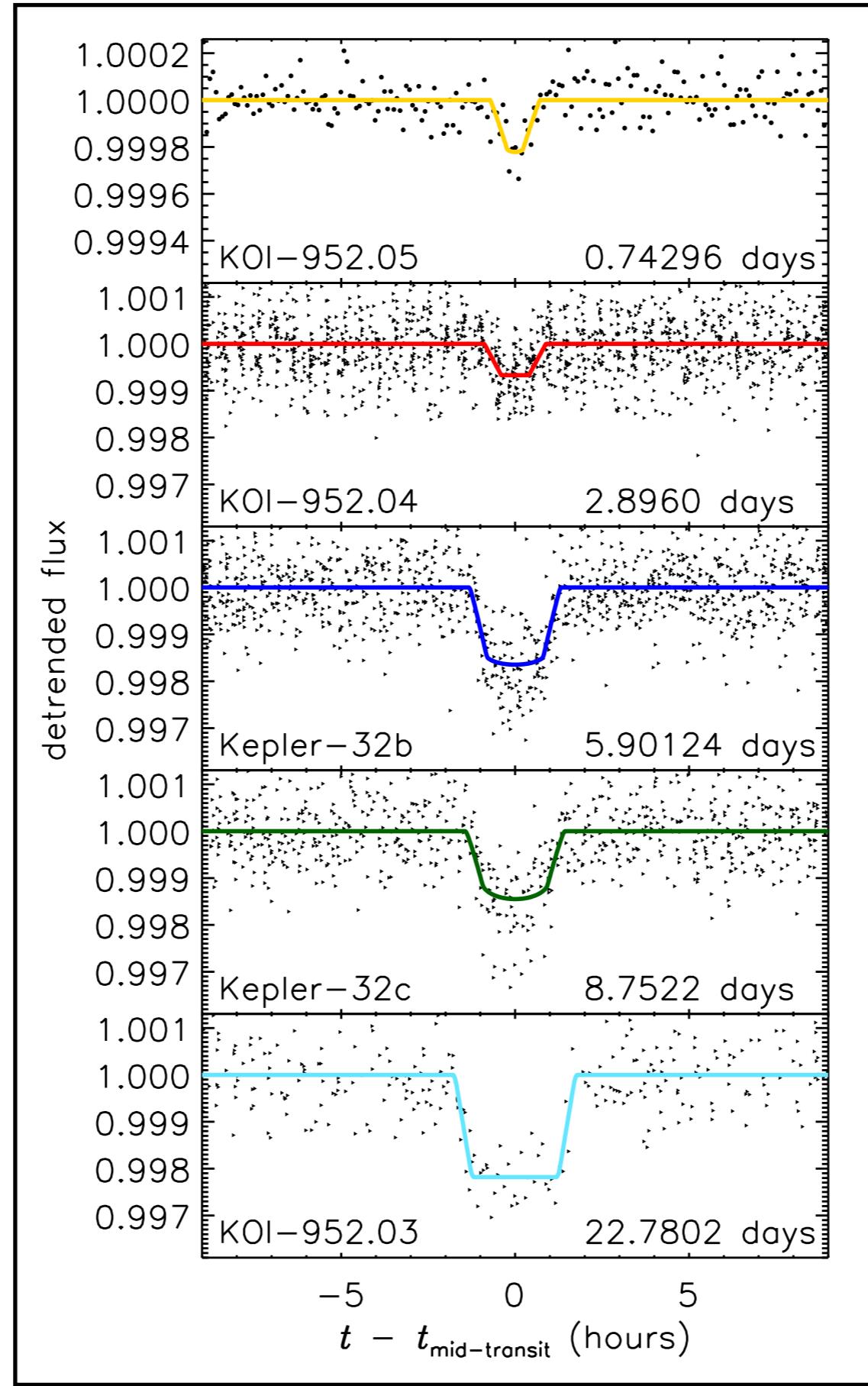
Kepler-32



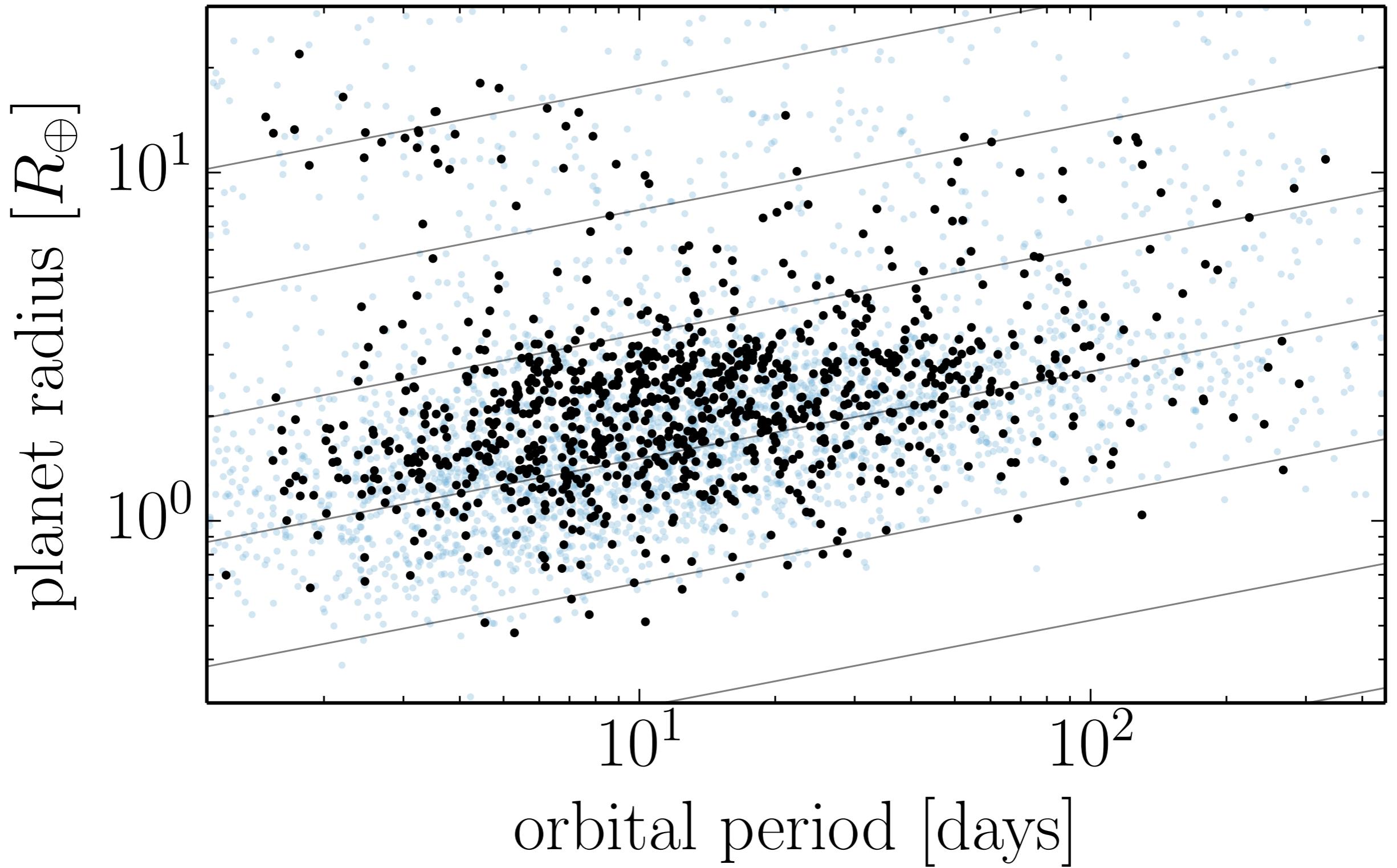
Kepler-32





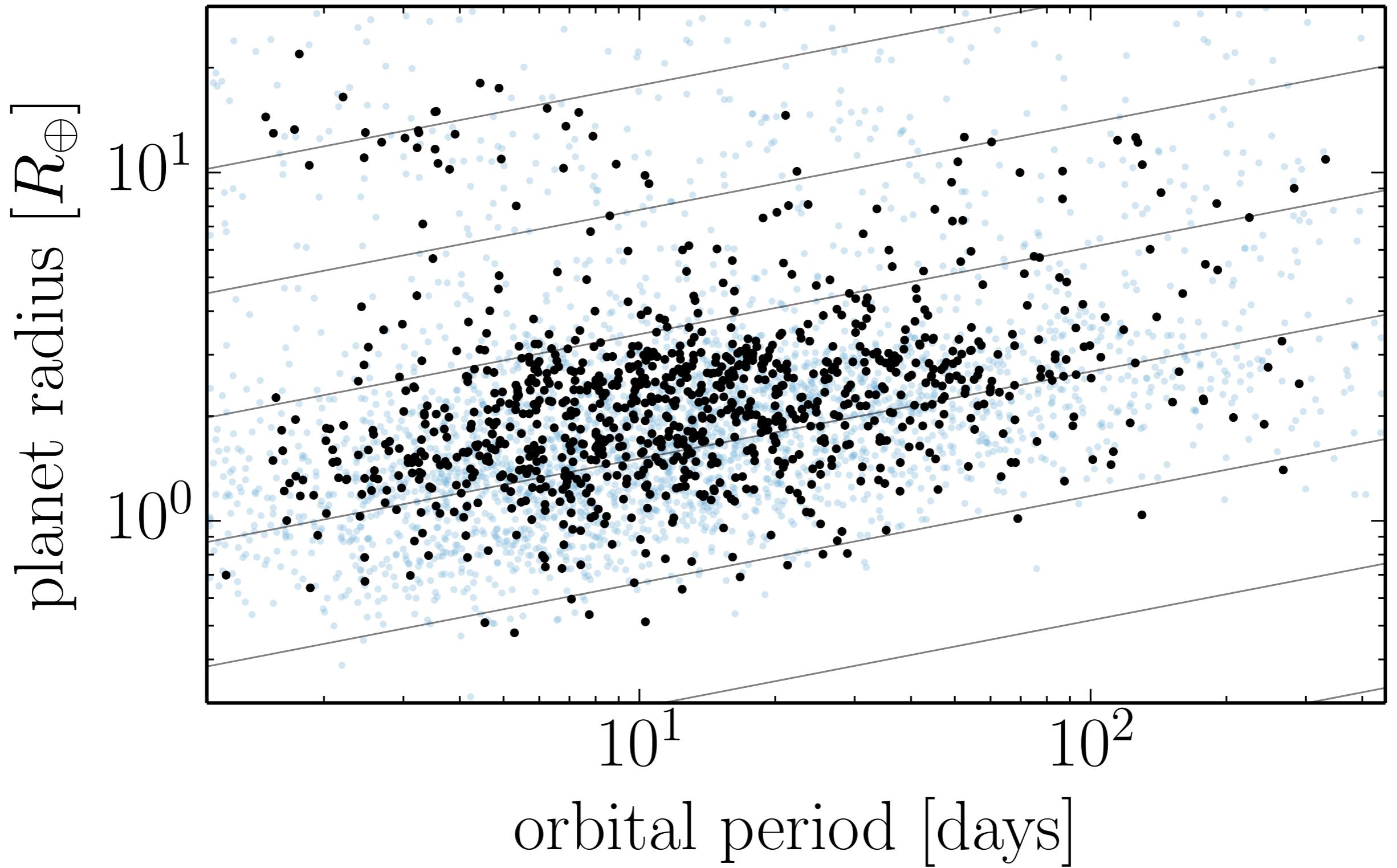


Credit **Fabrycky et al. (2012)**

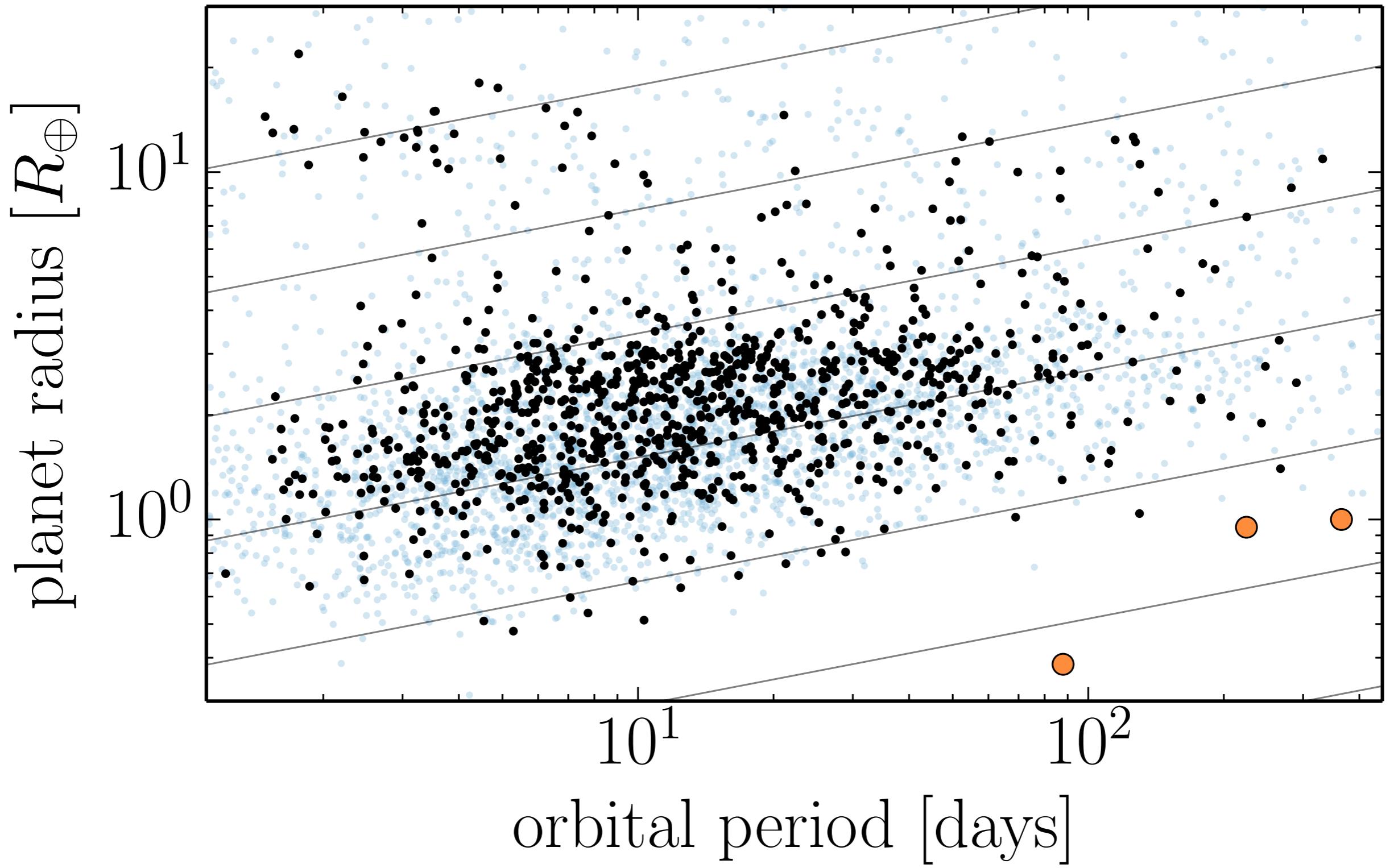


Data from **NASA Exoplanet Archive**

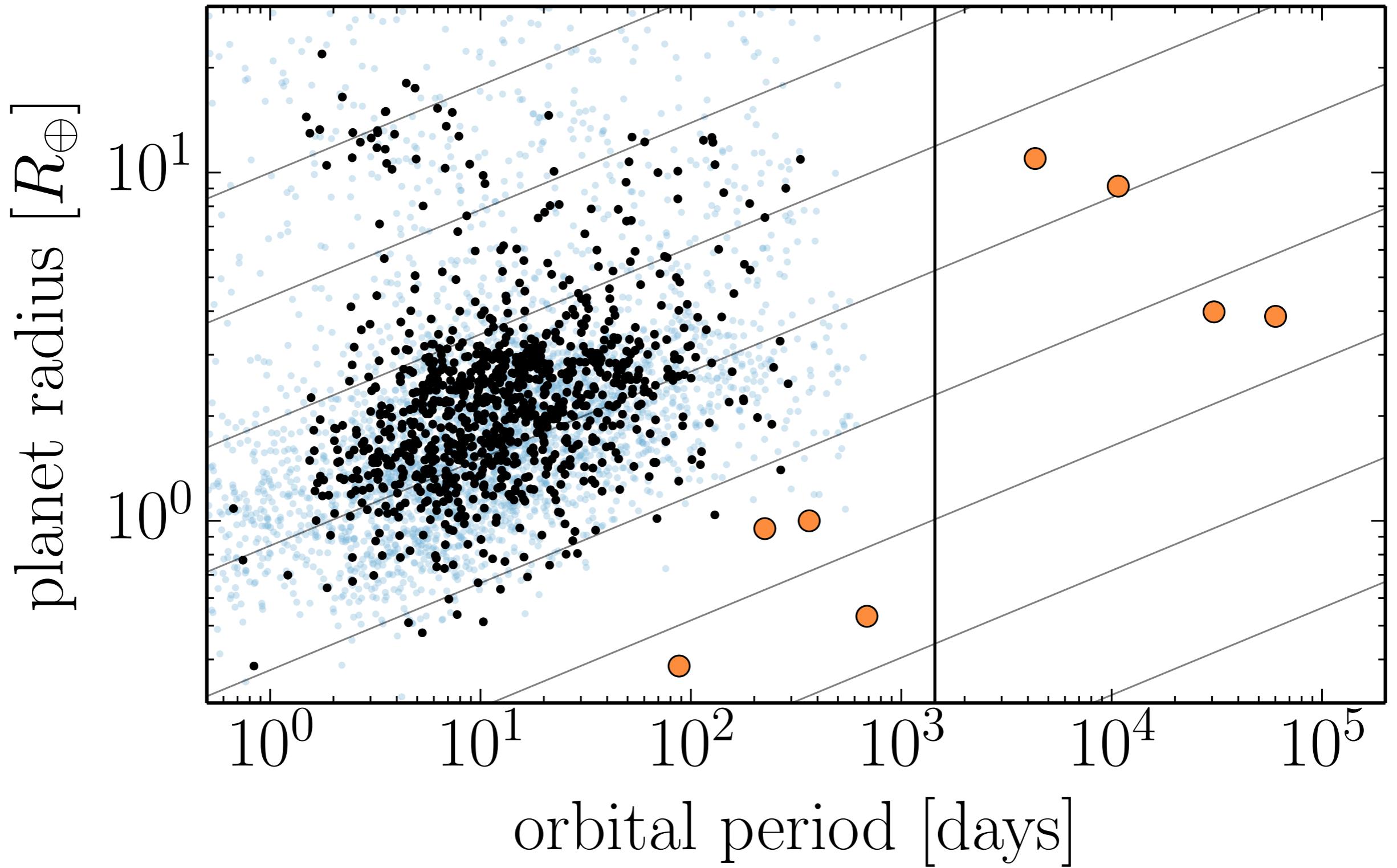
that looks pretty good...



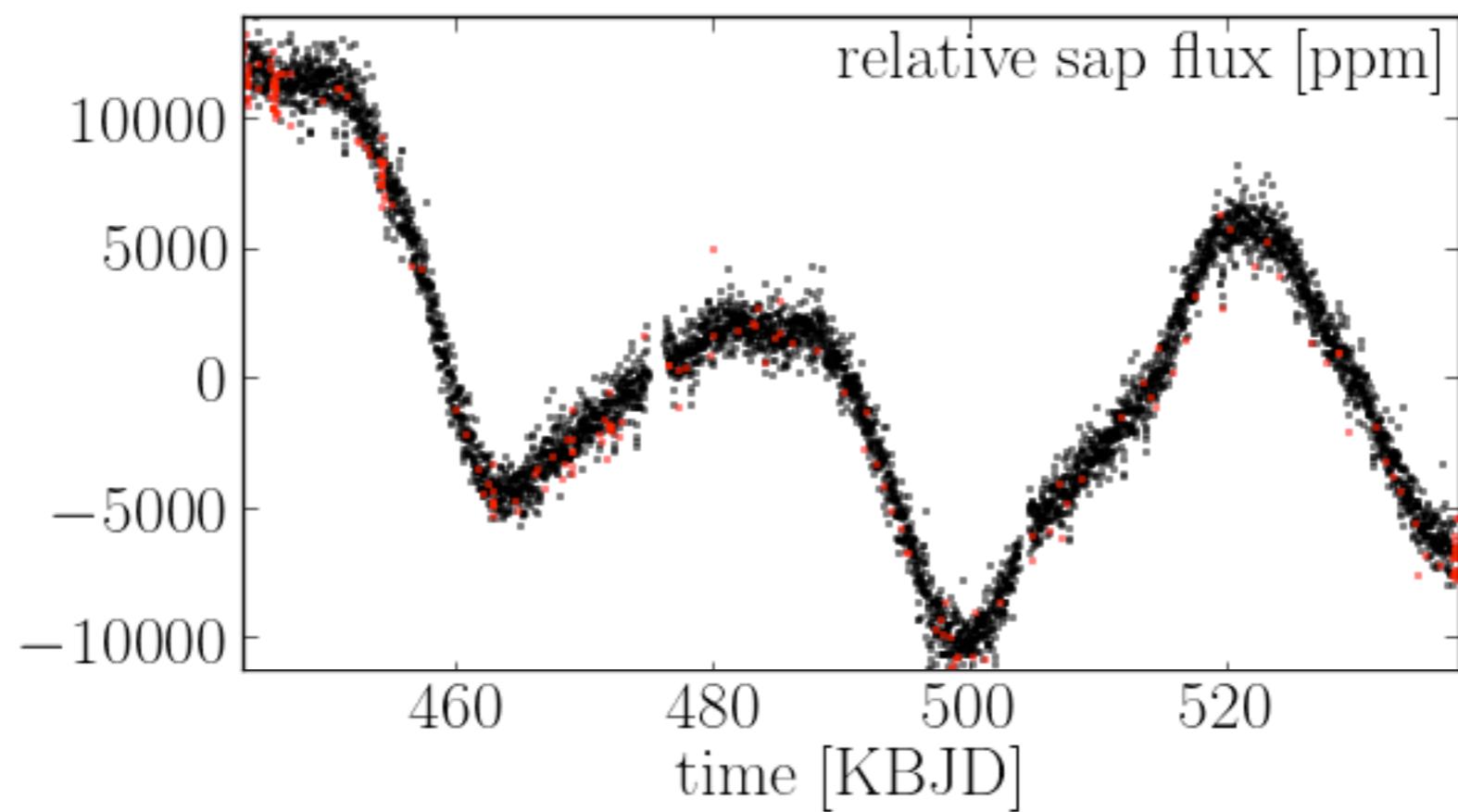
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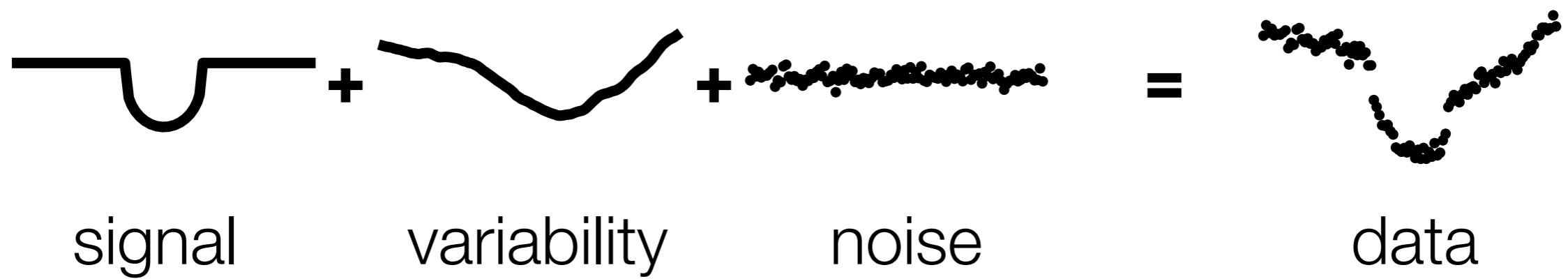
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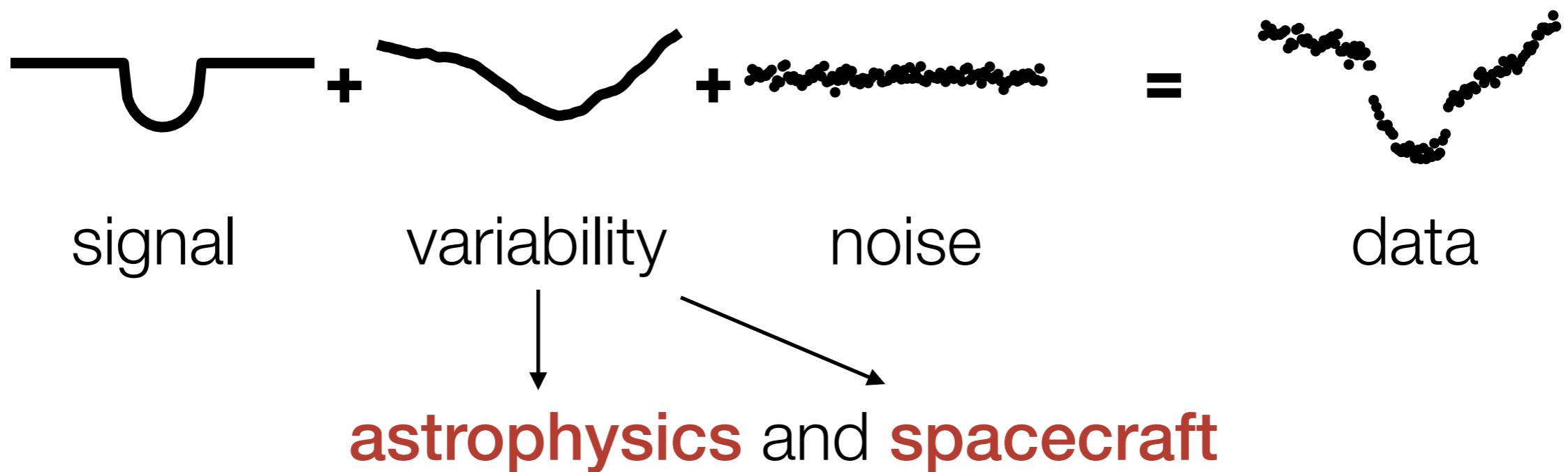
Data from **NASA Exoplanet Archive**



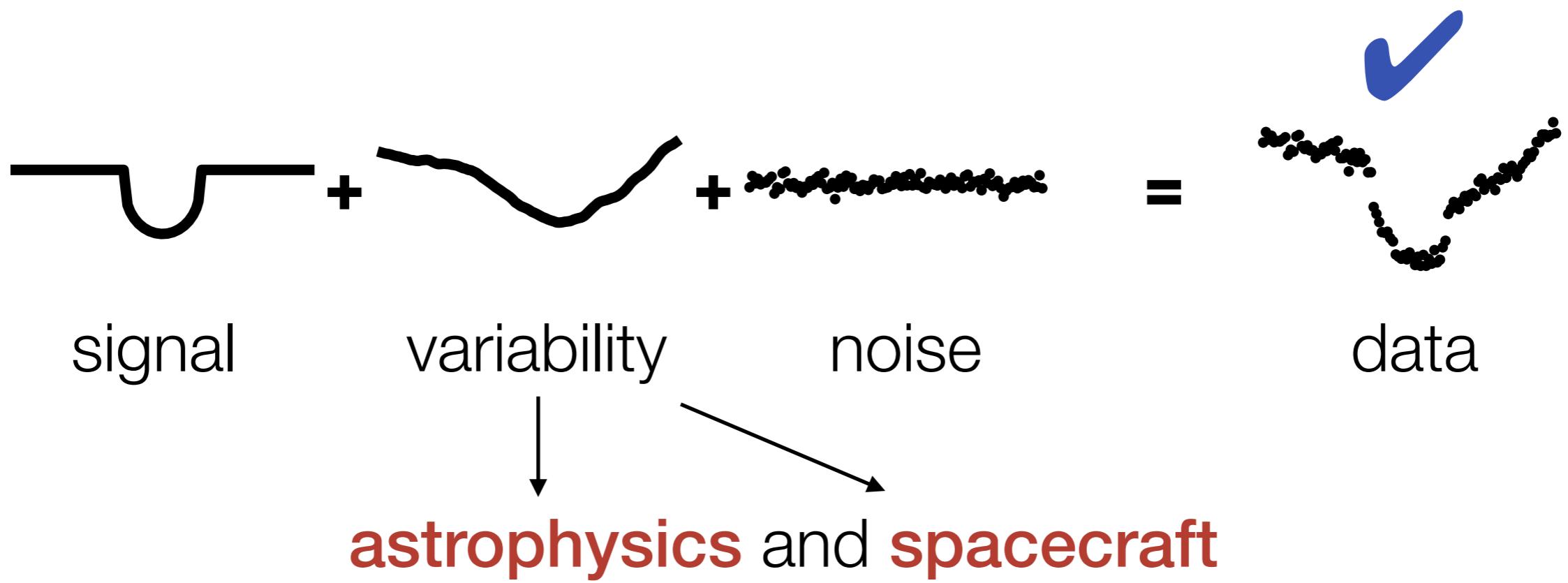
The **anatomy** of a **transit** observation



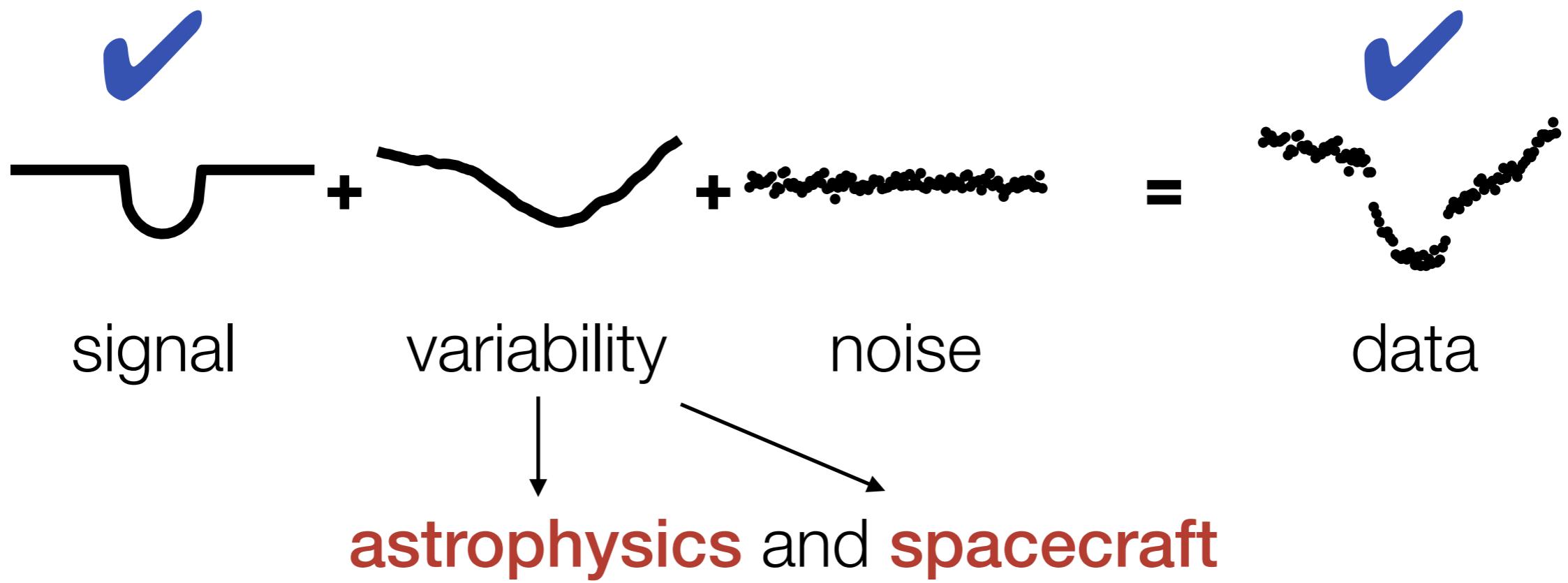
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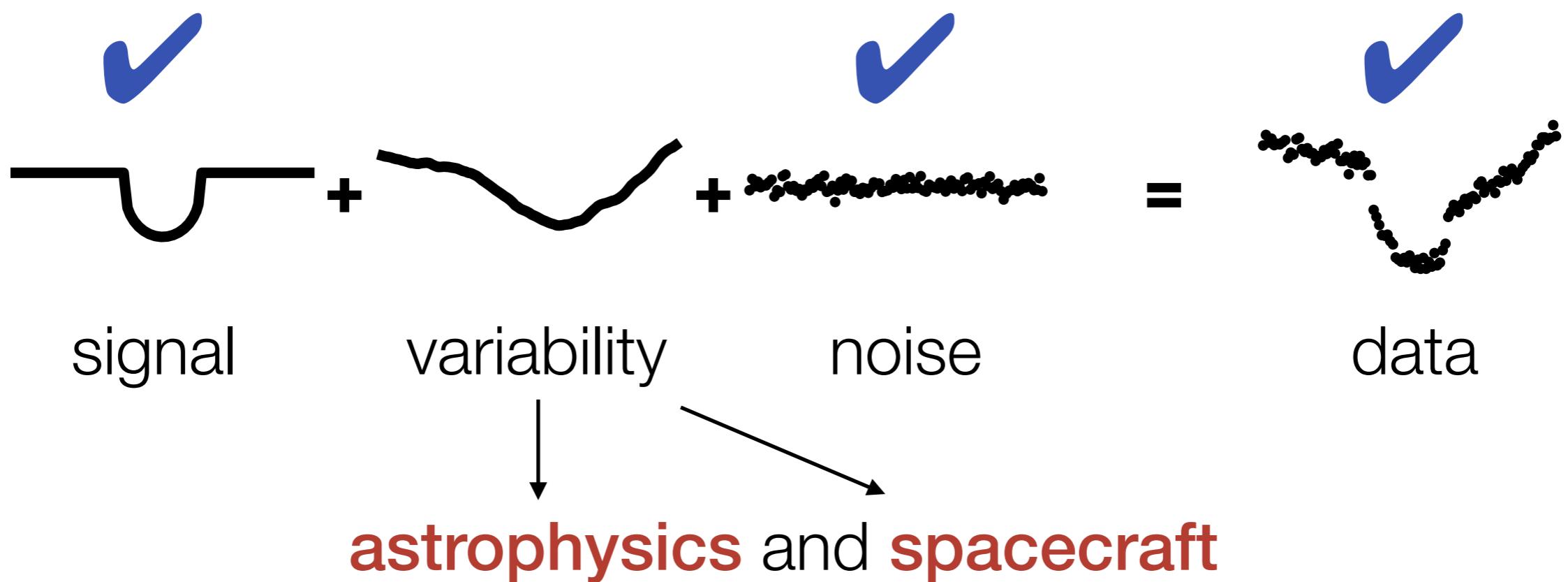
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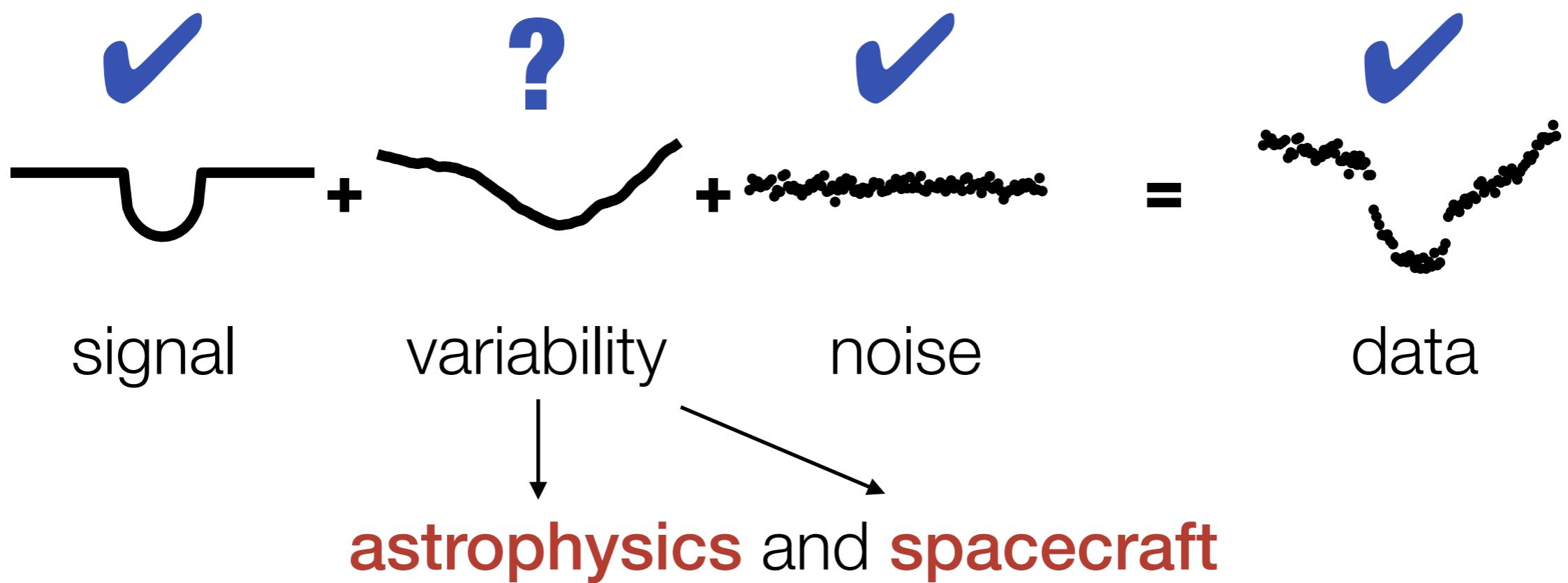
The **anatomy** of a **transit** observation



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The **anatomy** of a **transit** observation



CATERING PREP

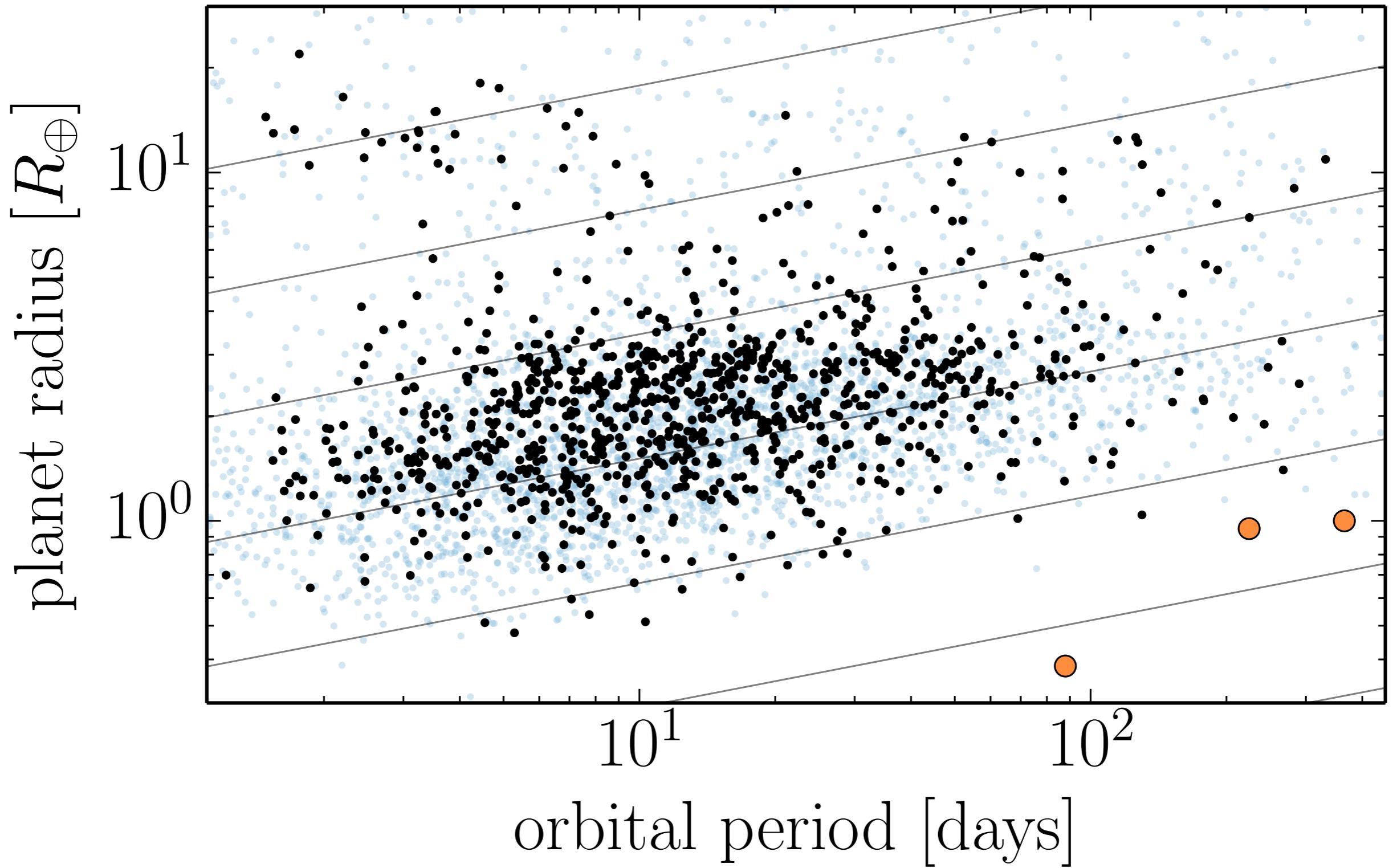
Kitchen

how do we clean up this mess?



Flickr user Marcin Wichary

Standard practice: **Filtering**



Data from **NASA Exoplanet Archive**

Exoplanets are **hard** to find

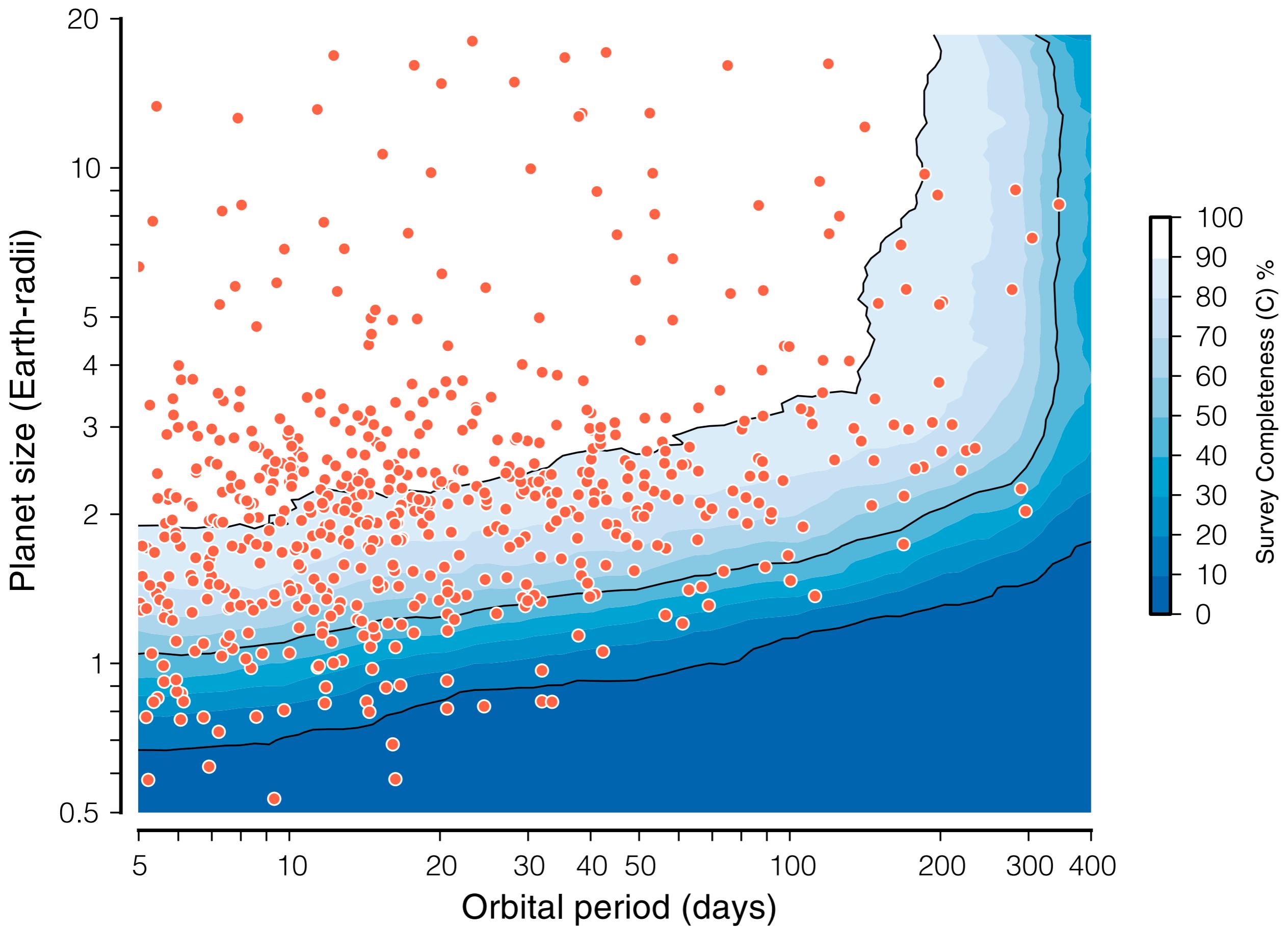


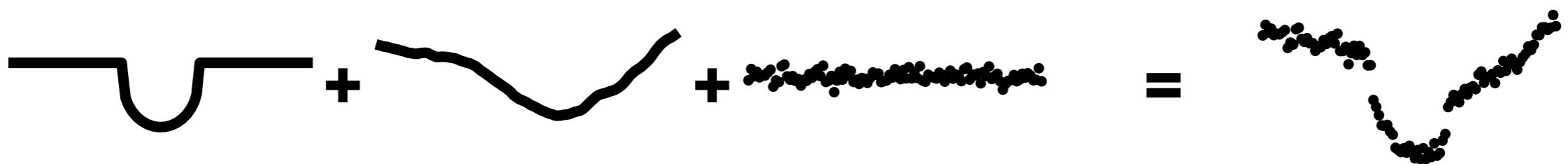
Figure credit: Petigura, Howard & Marcy (2013)

What about Gaussian Processes?

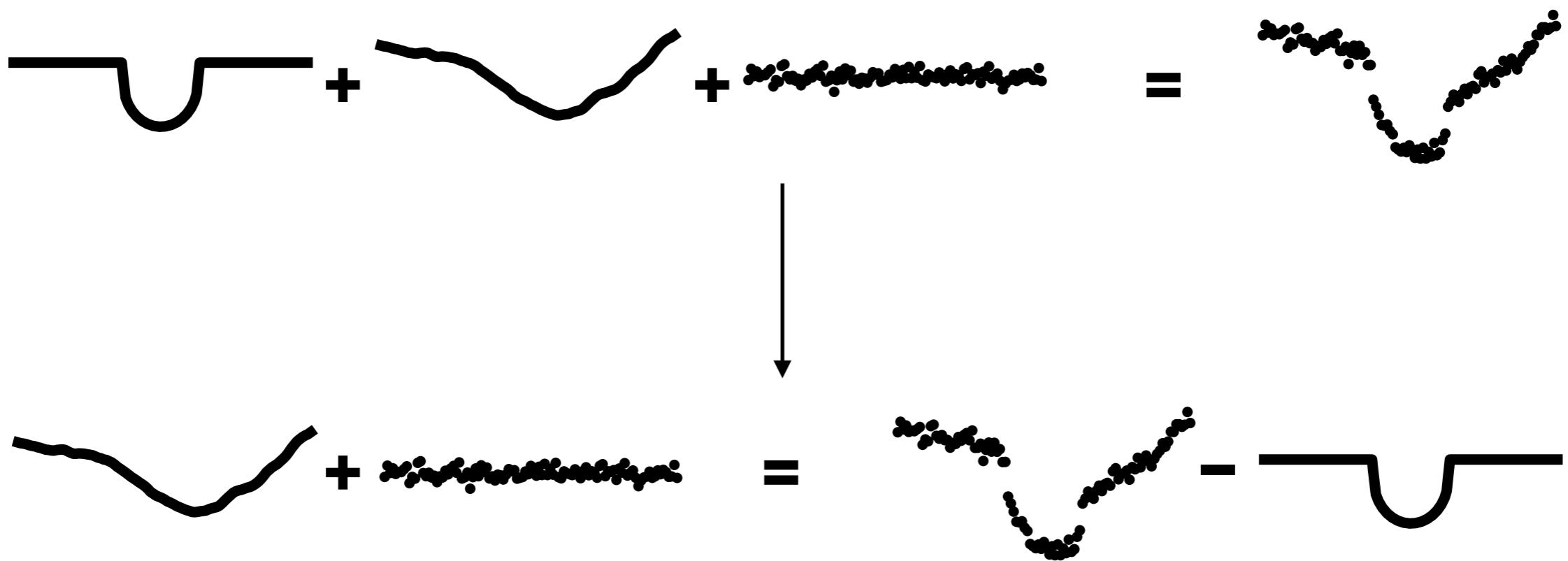
gaussianprocess.org/gpml

Rasmussen & Williams

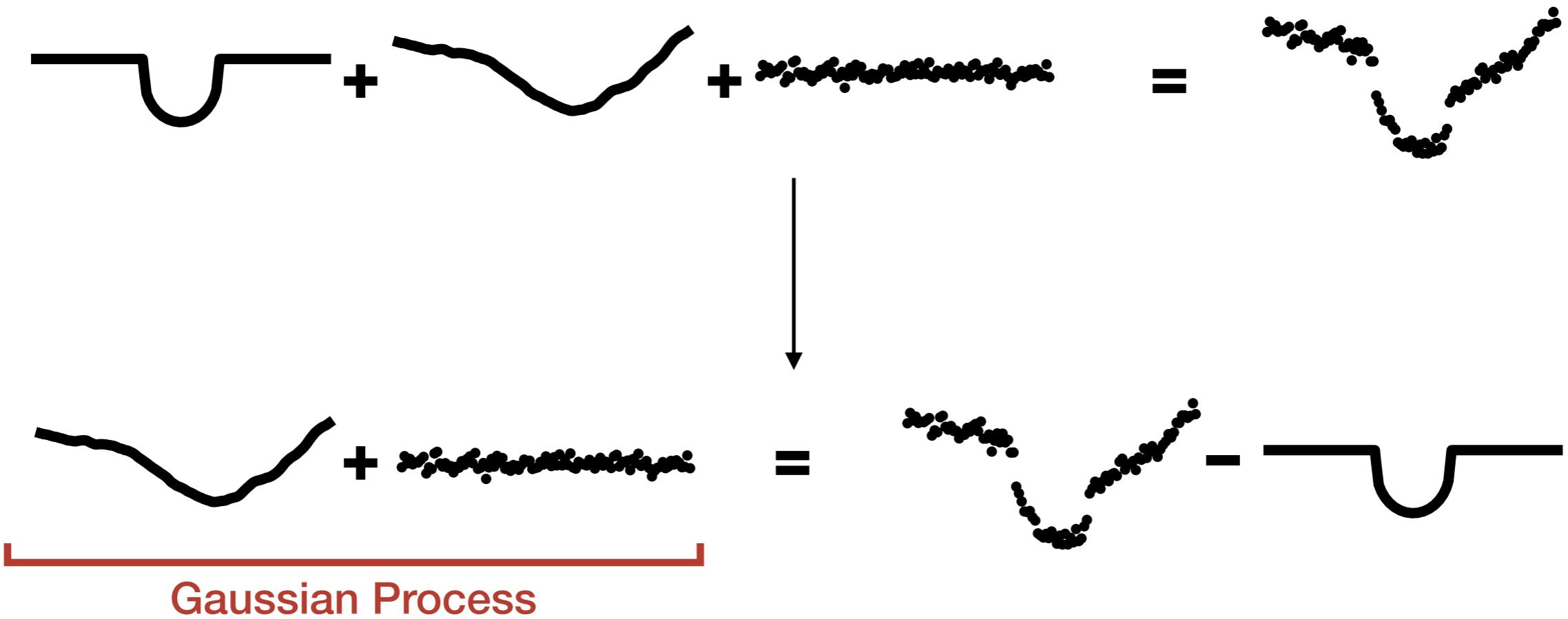
Modeling a **light curve** using a **Gaussian Processes**



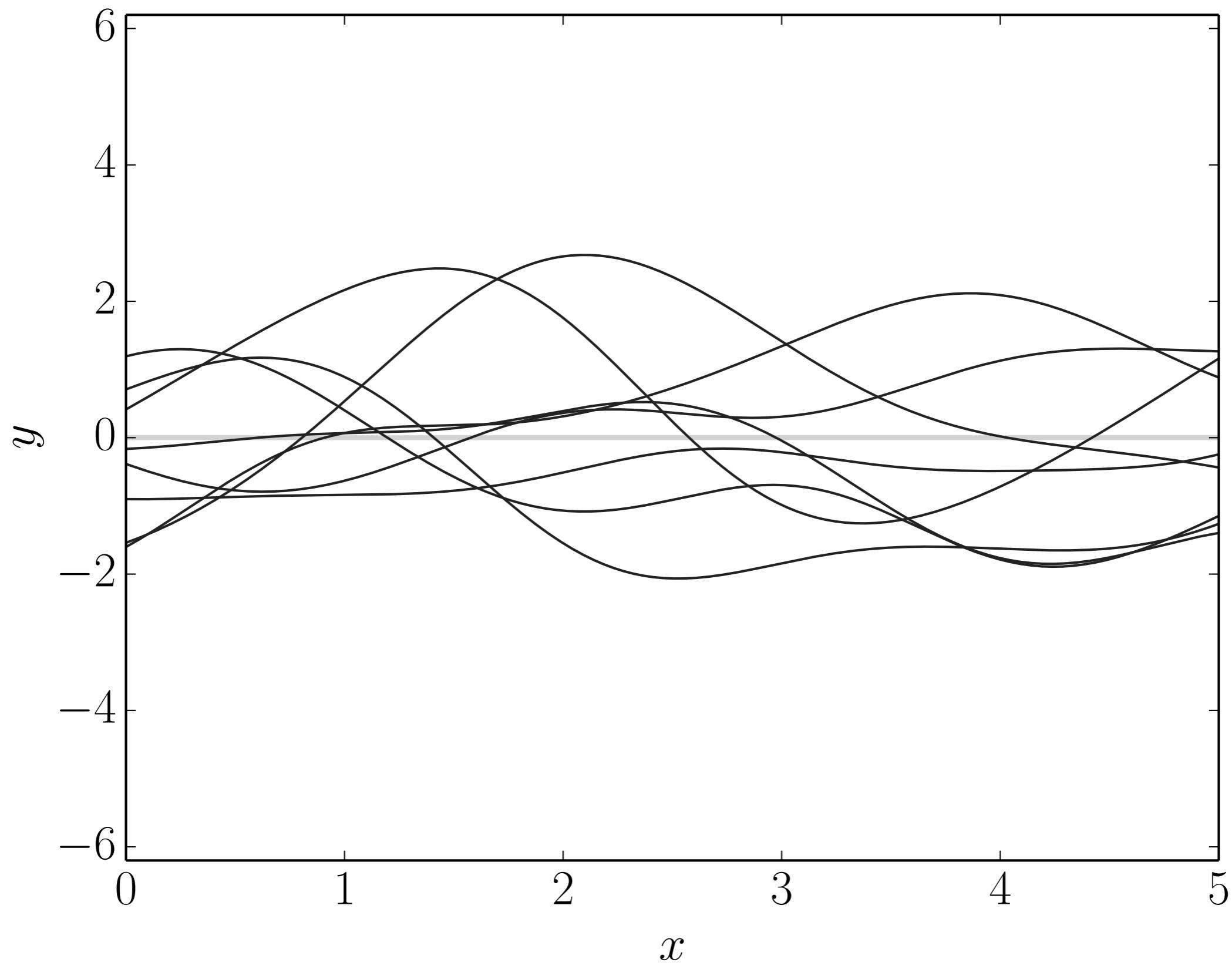
Modeling a **light curve** using a **Gaussian Processes**

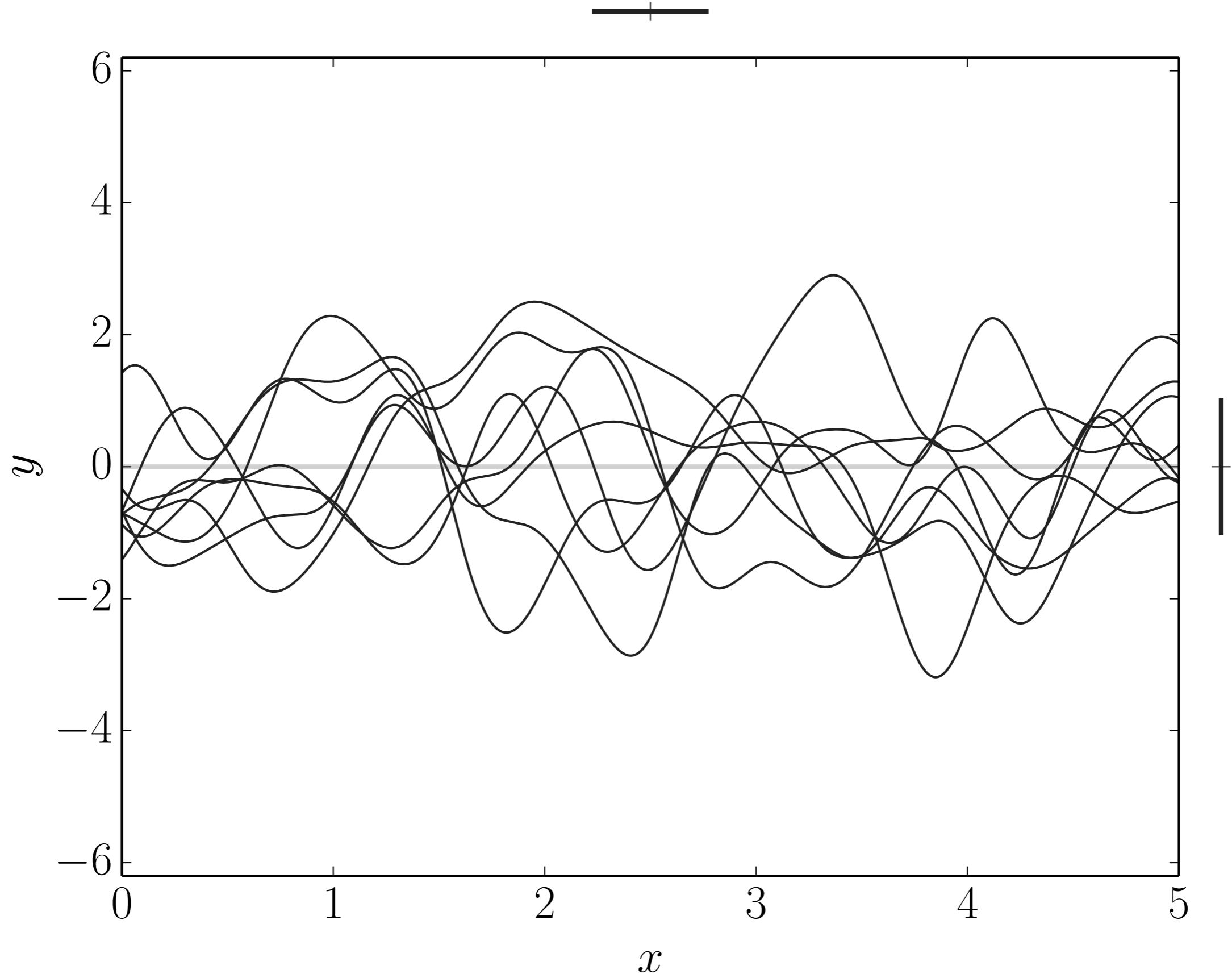


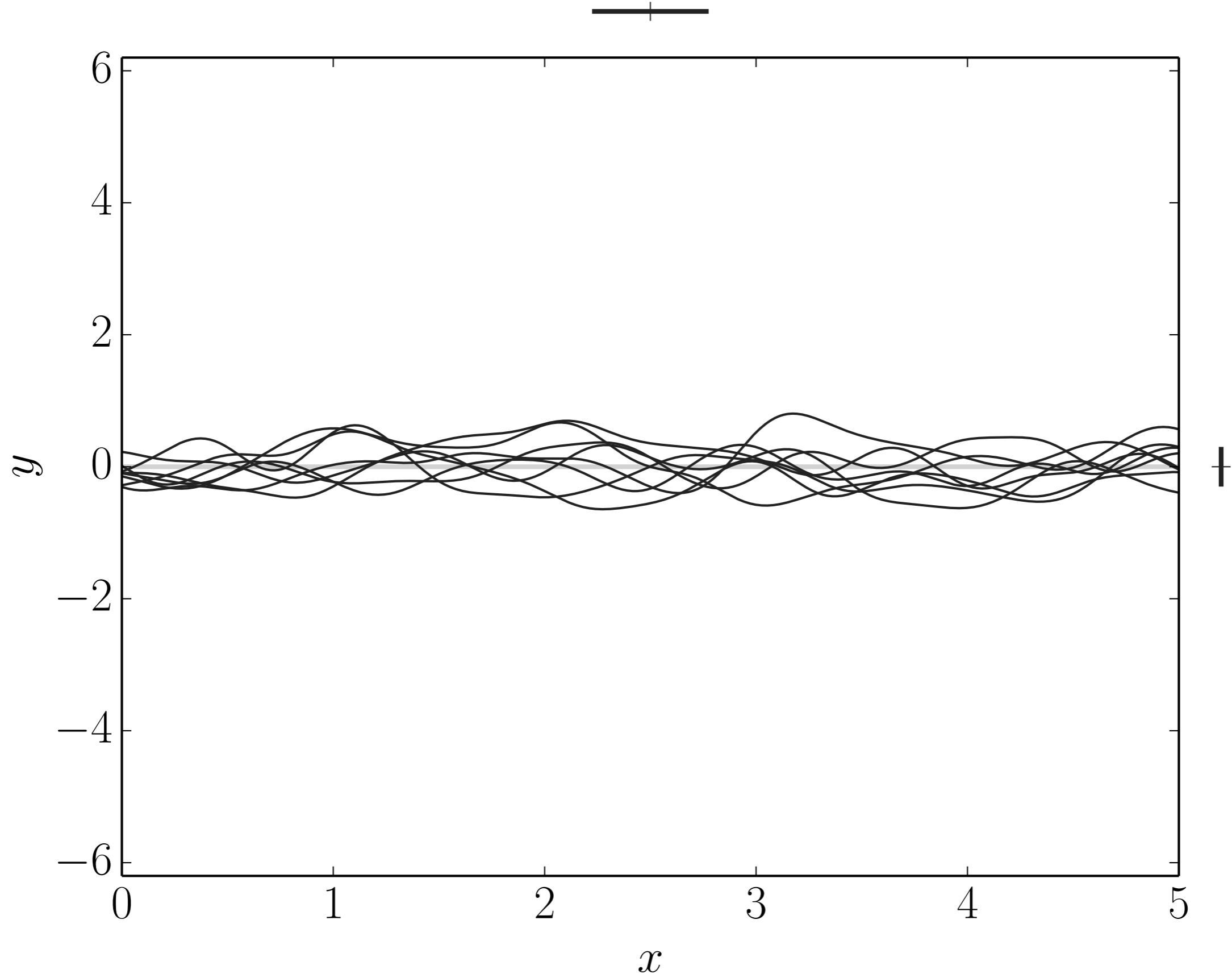
Modeling a light curve using a Gaussian Processes

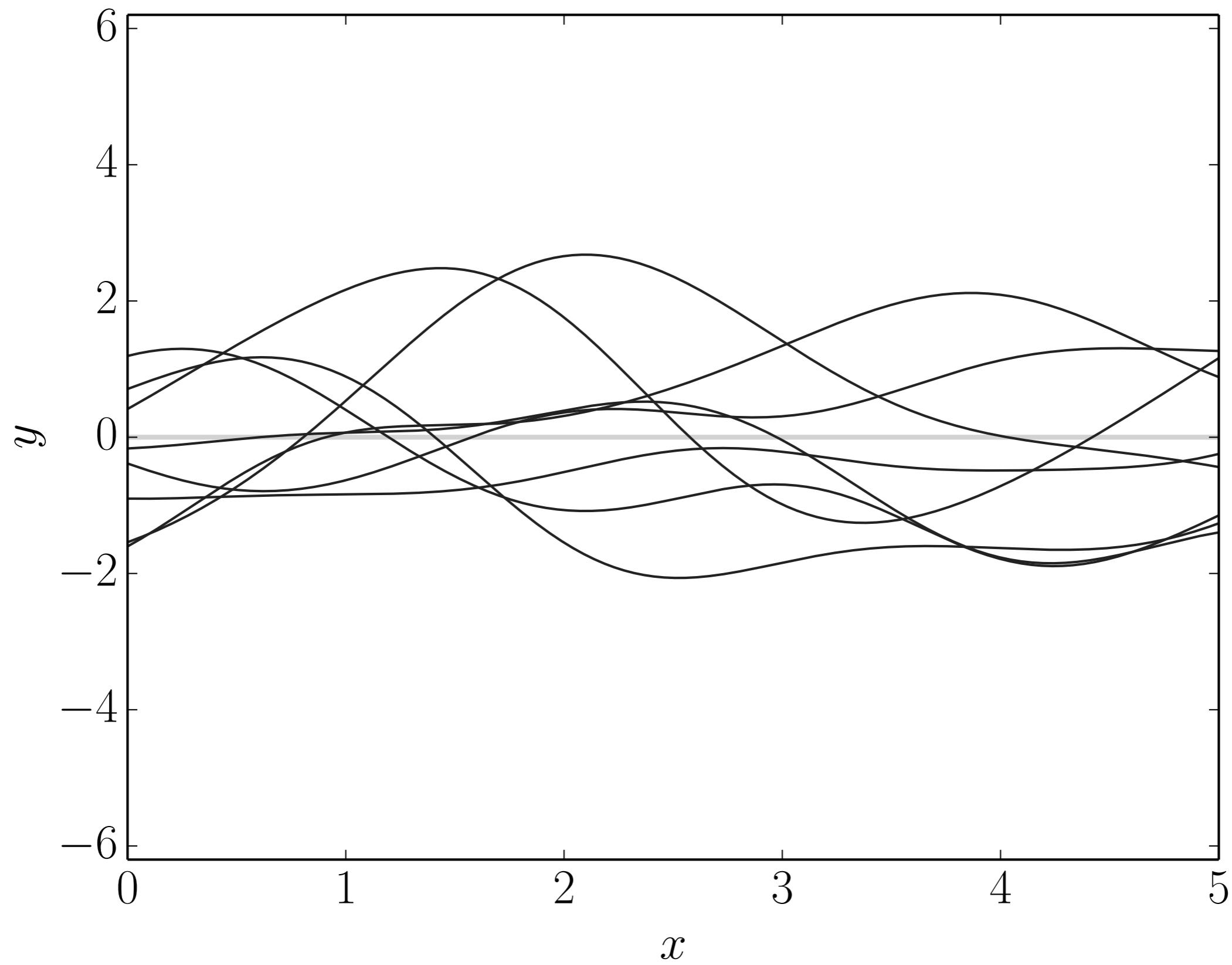


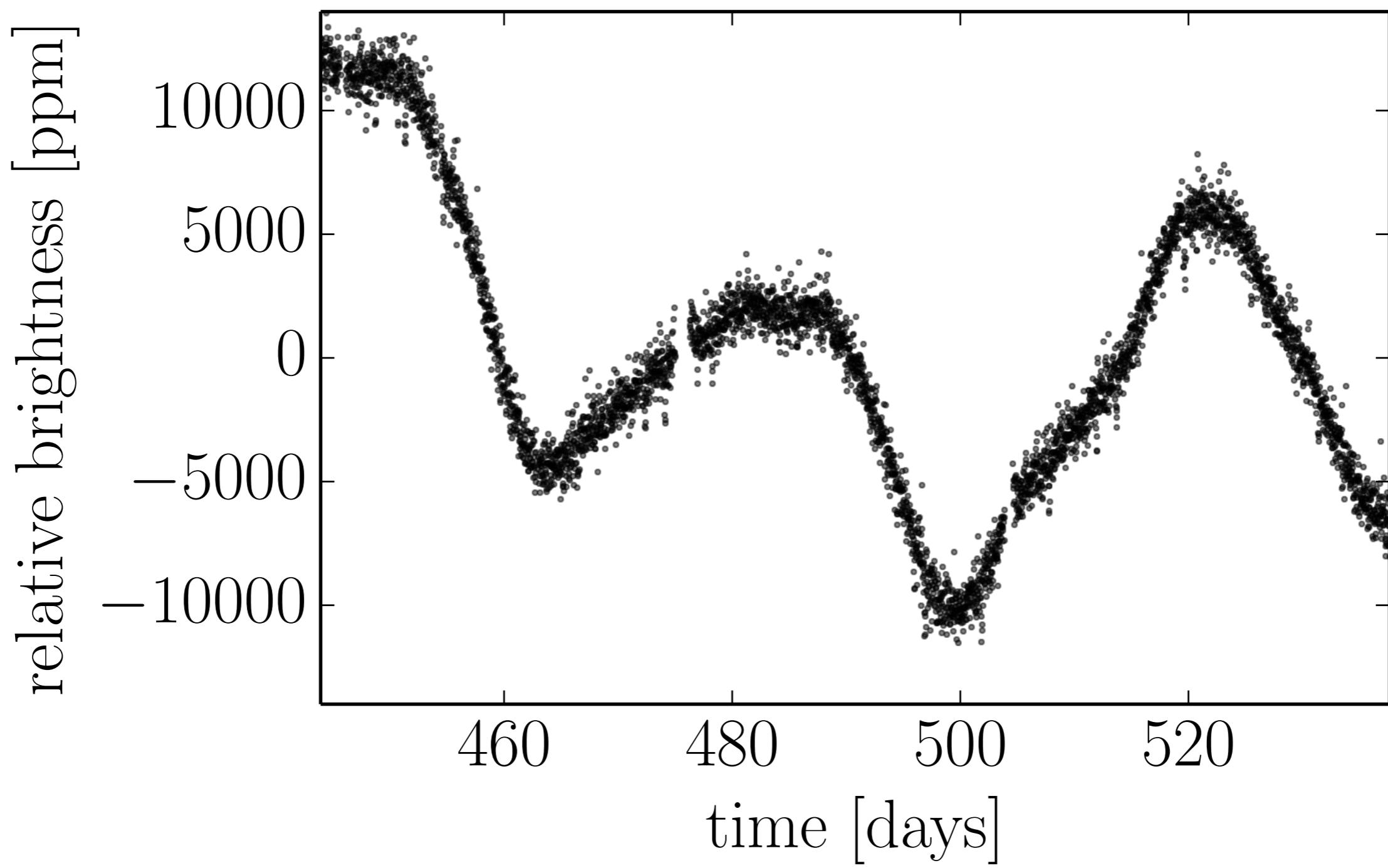
What is a Gaussian Process?

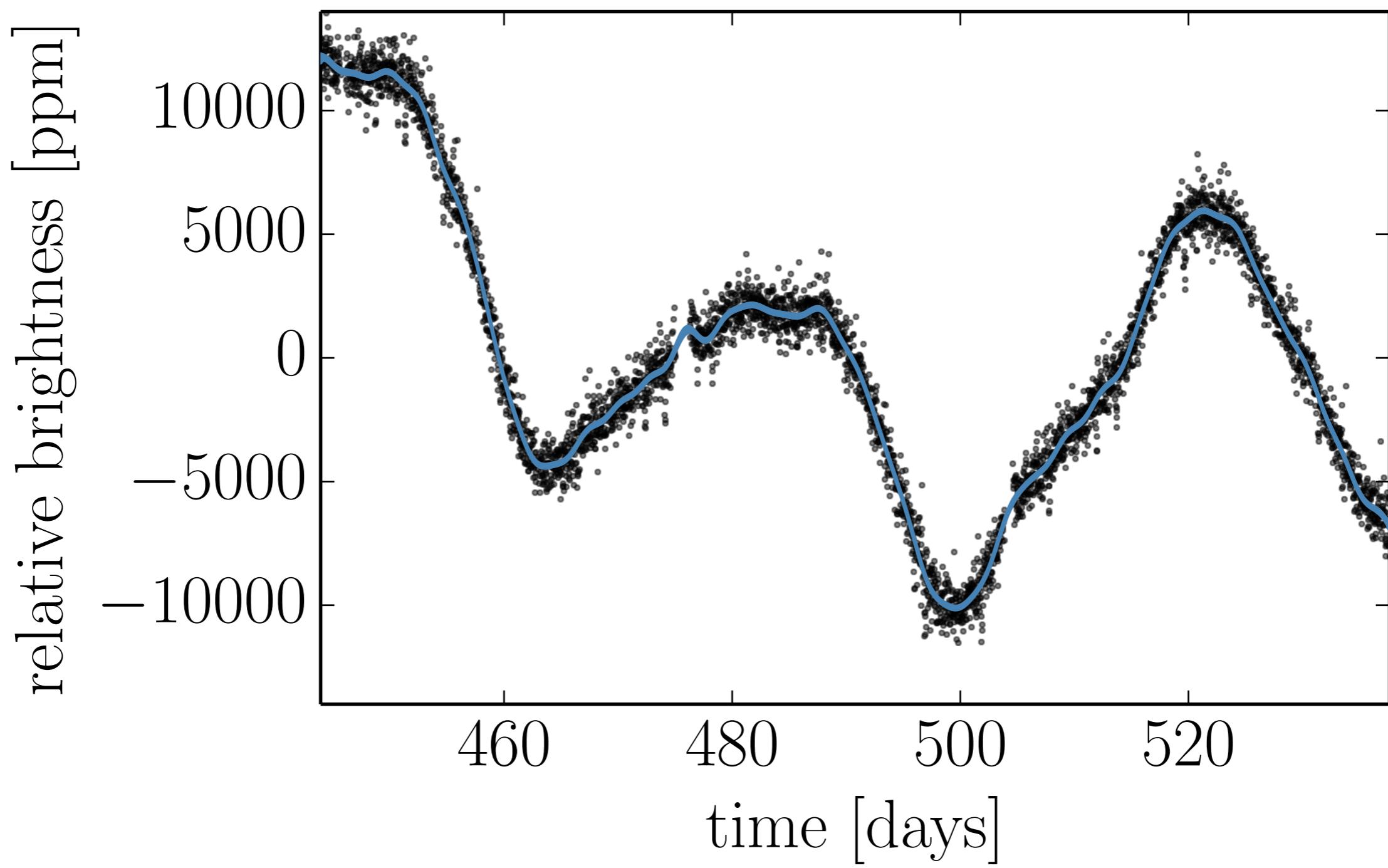












the data are drawn from one

Huge Gaussian

* the dimension is the number of data points.

The mathematical model

$$y \sim \mathcal{N}(f_{\theta}(x), K_{\alpha}(x, \sigma))$$

where

$$[K_{\alpha}(x, \sigma)]_{ij} = \sigma_i^2 \delta_{ij} + k_{\alpha}(x_i, x_j)$$

The mathematical model

$$\begin{aligned}\log p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\sigma}, \boldsymbol{\theta}, \boldsymbol{\alpha}) = & -\frac{1}{2} [\mathbf{y} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})]^T K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma})^{-1} [\mathbf{y} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})] \\ & -\frac{1}{2} \log \det K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma}) - \frac{N}{2} \log 2 \pi\end{aligned}$$

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The mathematical model

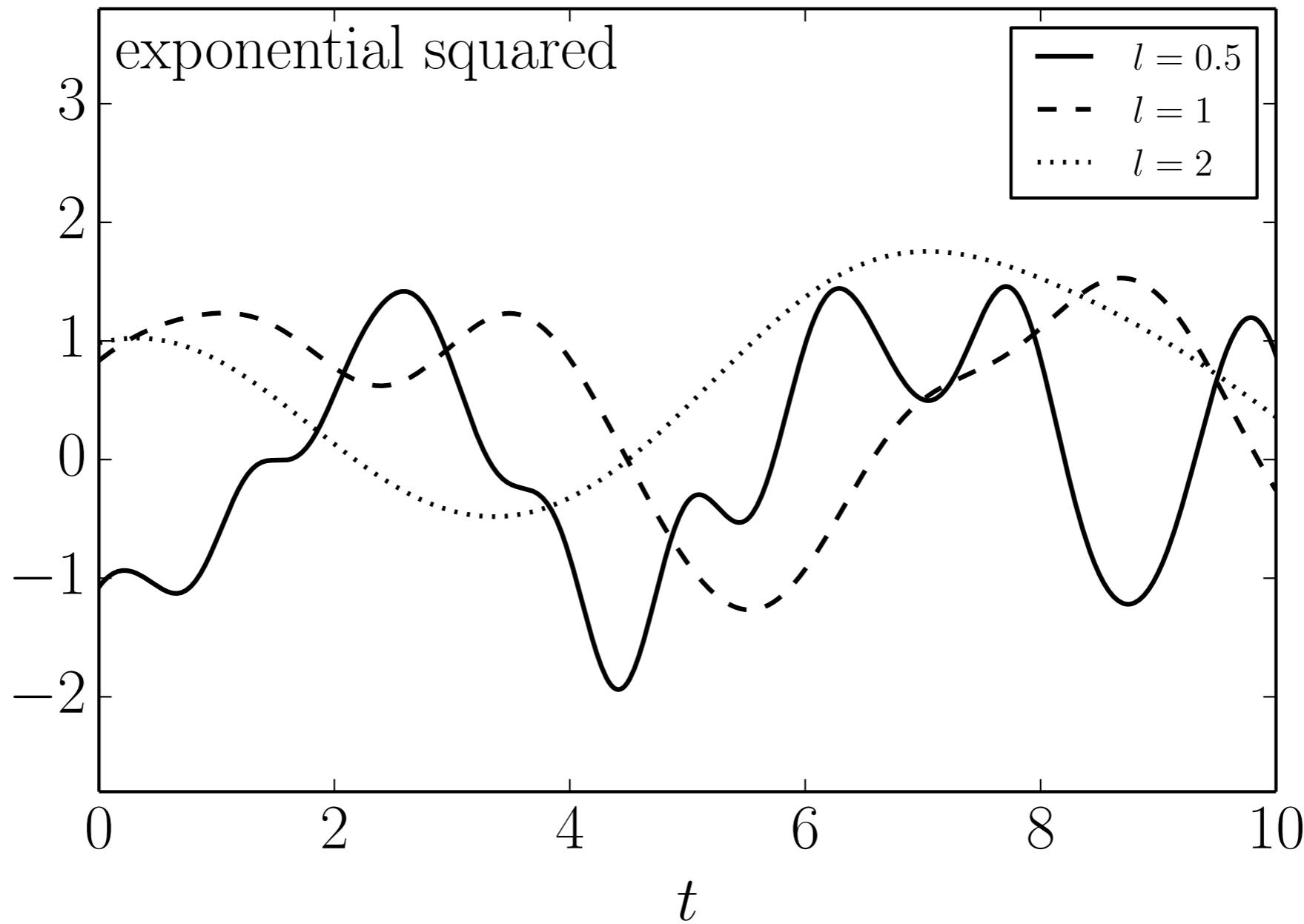
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where

$$[K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma})]_{ij} = \sigma_i^2 \delta_{ij} + \underbrace{k_{\boldsymbol{\alpha}}(x_i, x_j)}_{\text{kernel function}} \quad (where \, the \, magic \, happens)$$

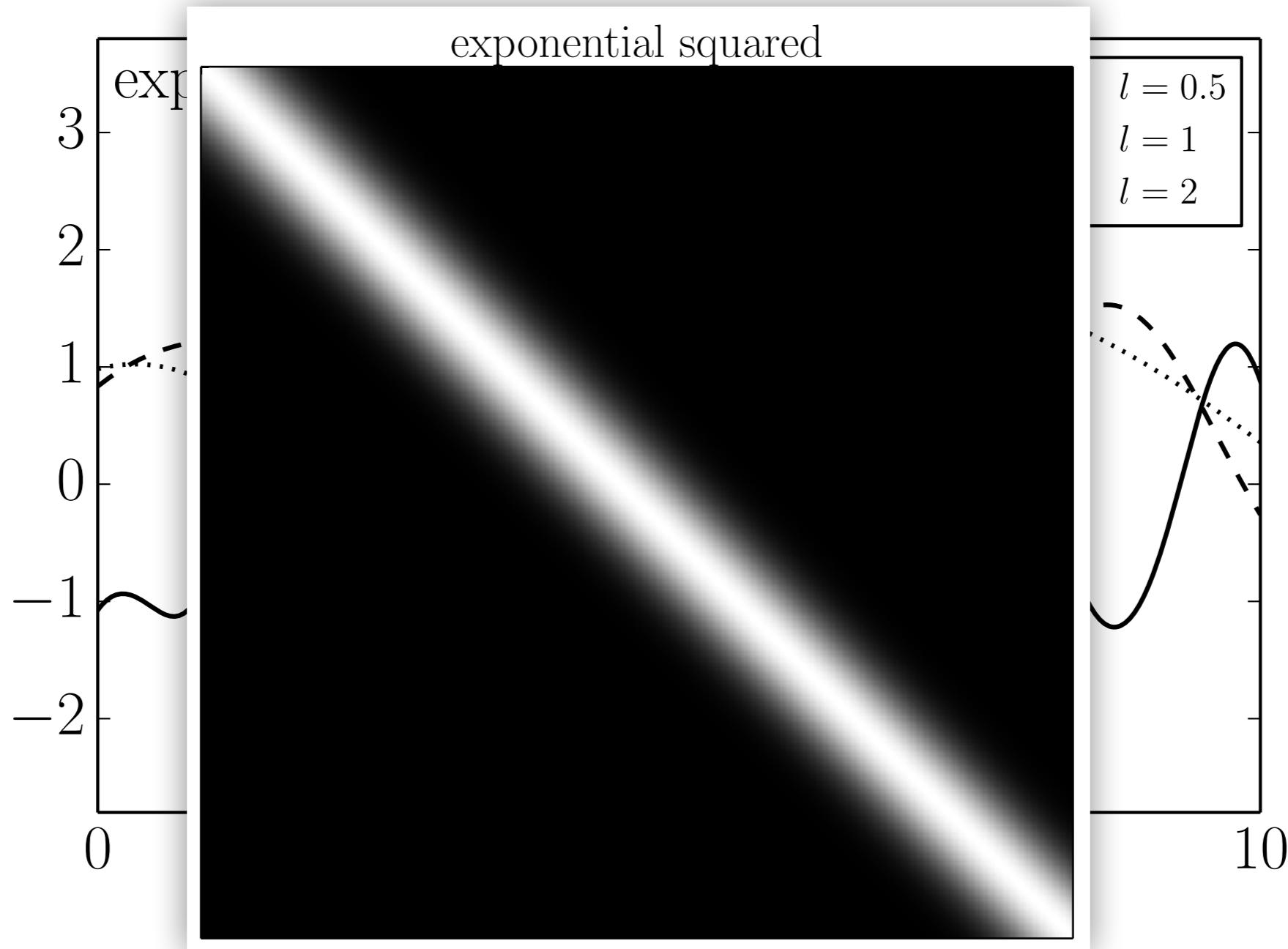
The choice of **kernel**

$$k_{\alpha}(x_i, x_j) = \exp\left(-\frac{[x_i - x_j]^2}{2\ell^2}\right)$$



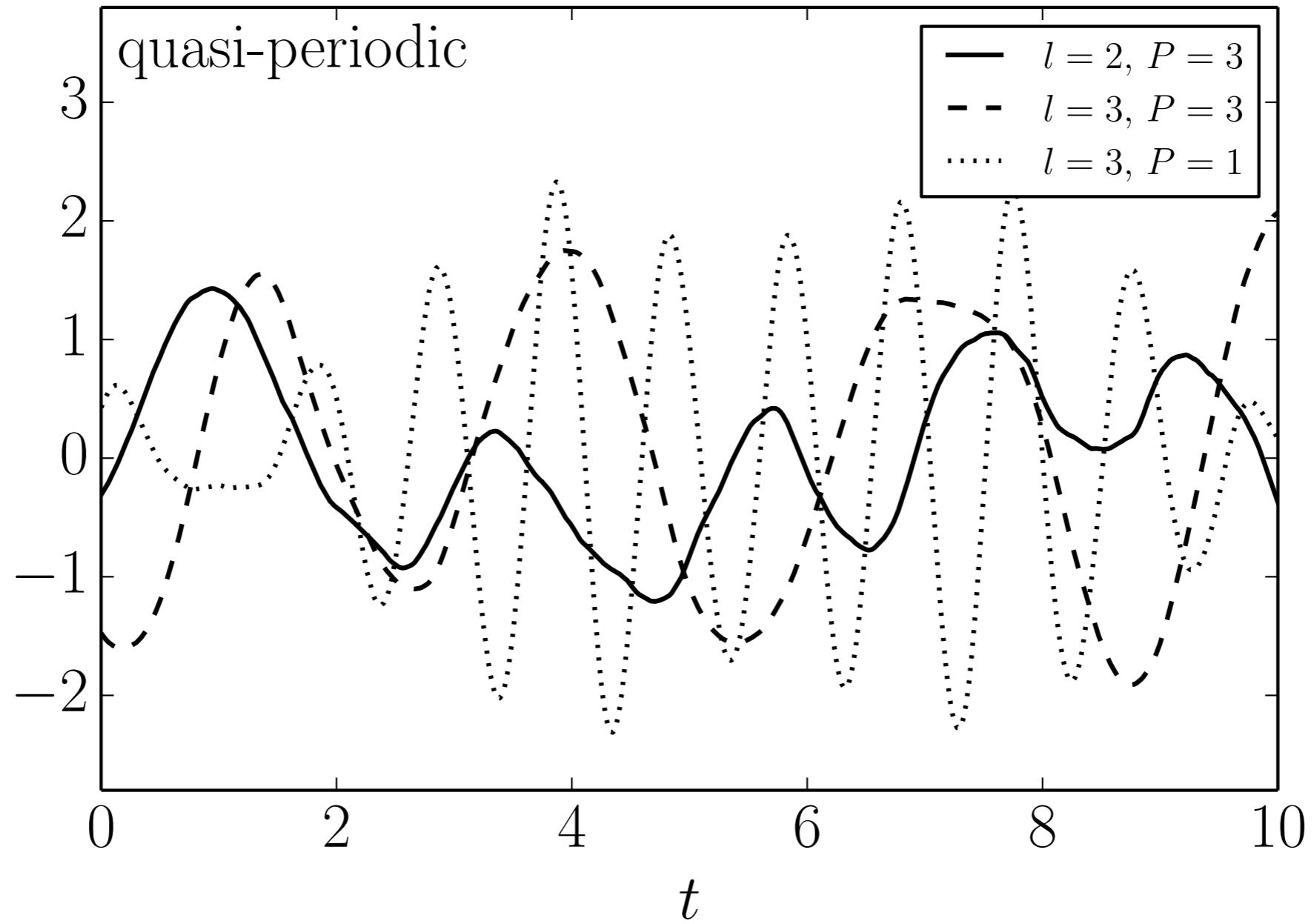
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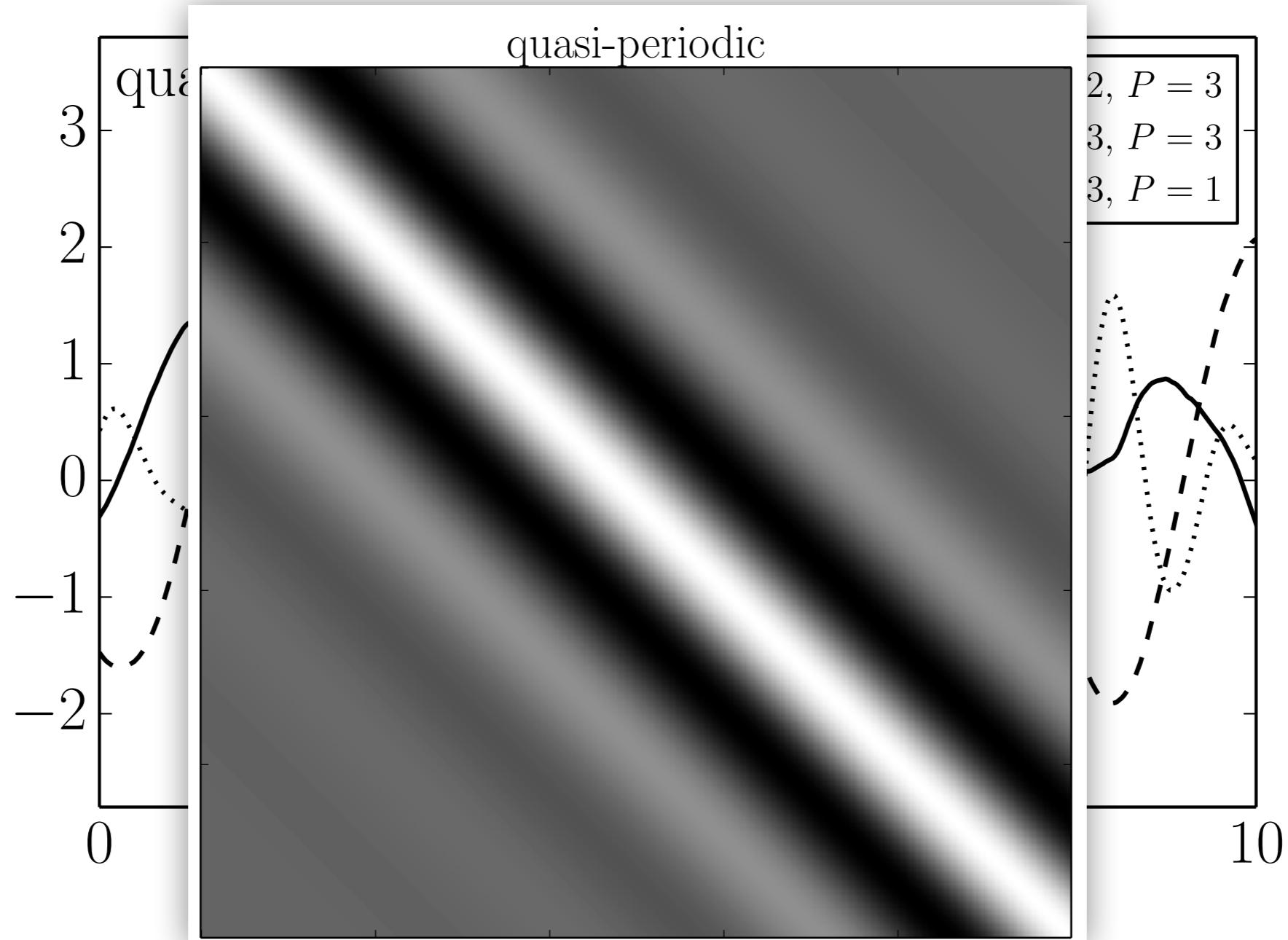
The choice of **kernel**

$$k_{\alpha}(x_i, x_j) = \left[1 + \frac{\sqrt{3} |x_i - x_j|}{\ell} \right] \exp \left(-\frac{|x_i - x_j|}{\ell} \right) \cos \left(\frac{2 \pi |x_i - x_j|}{P} \right)$$

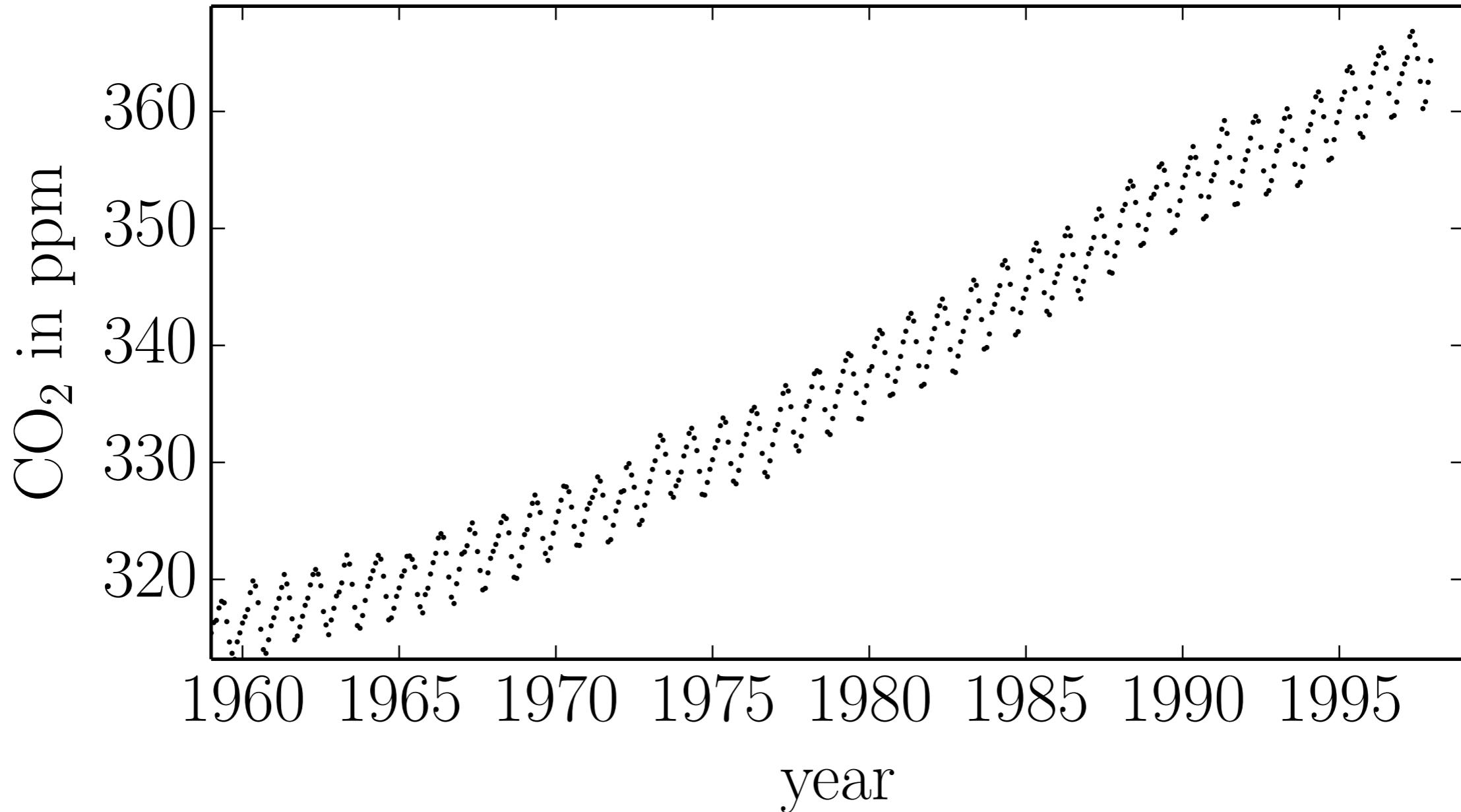


The choice of **kernel**

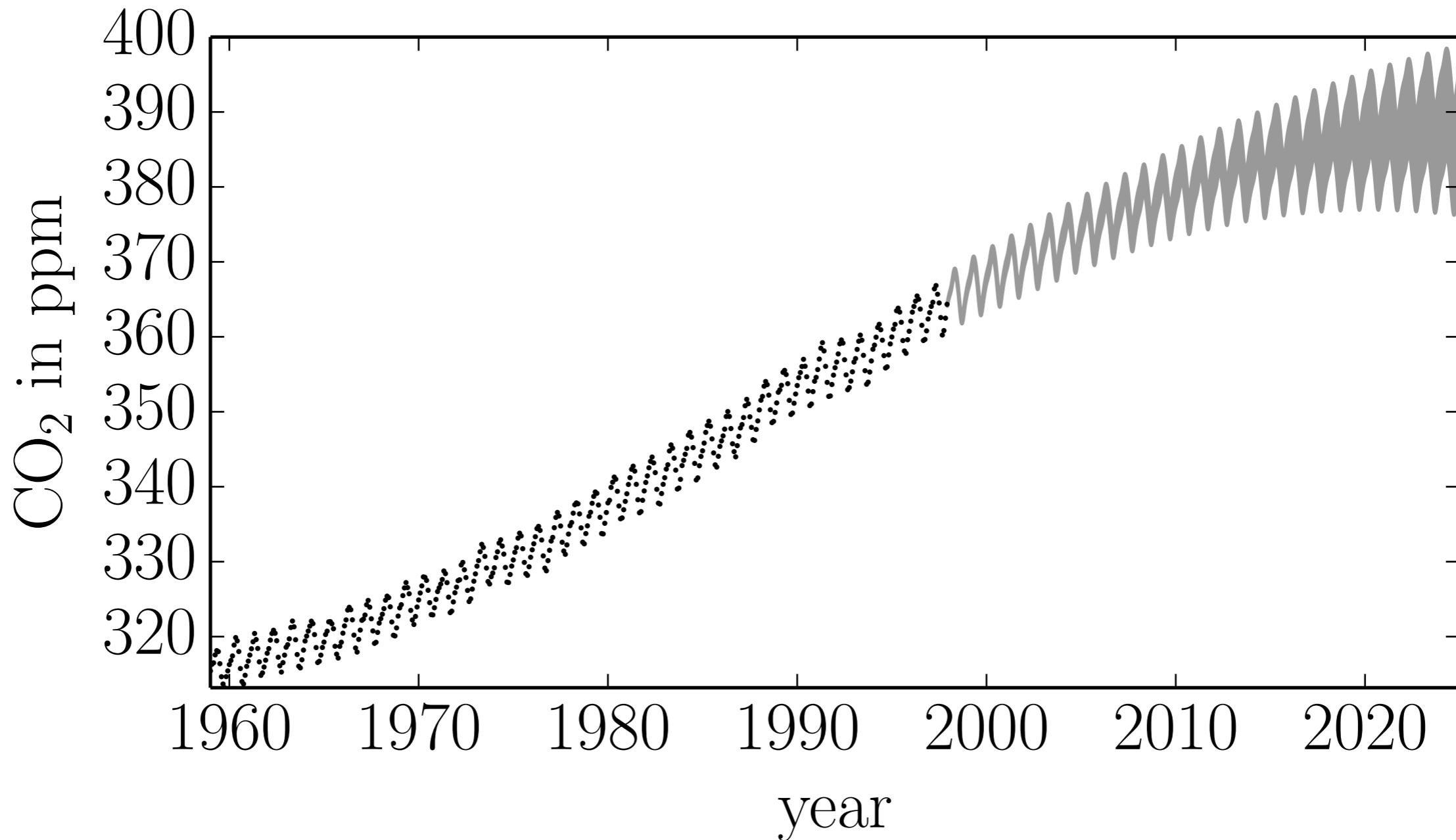
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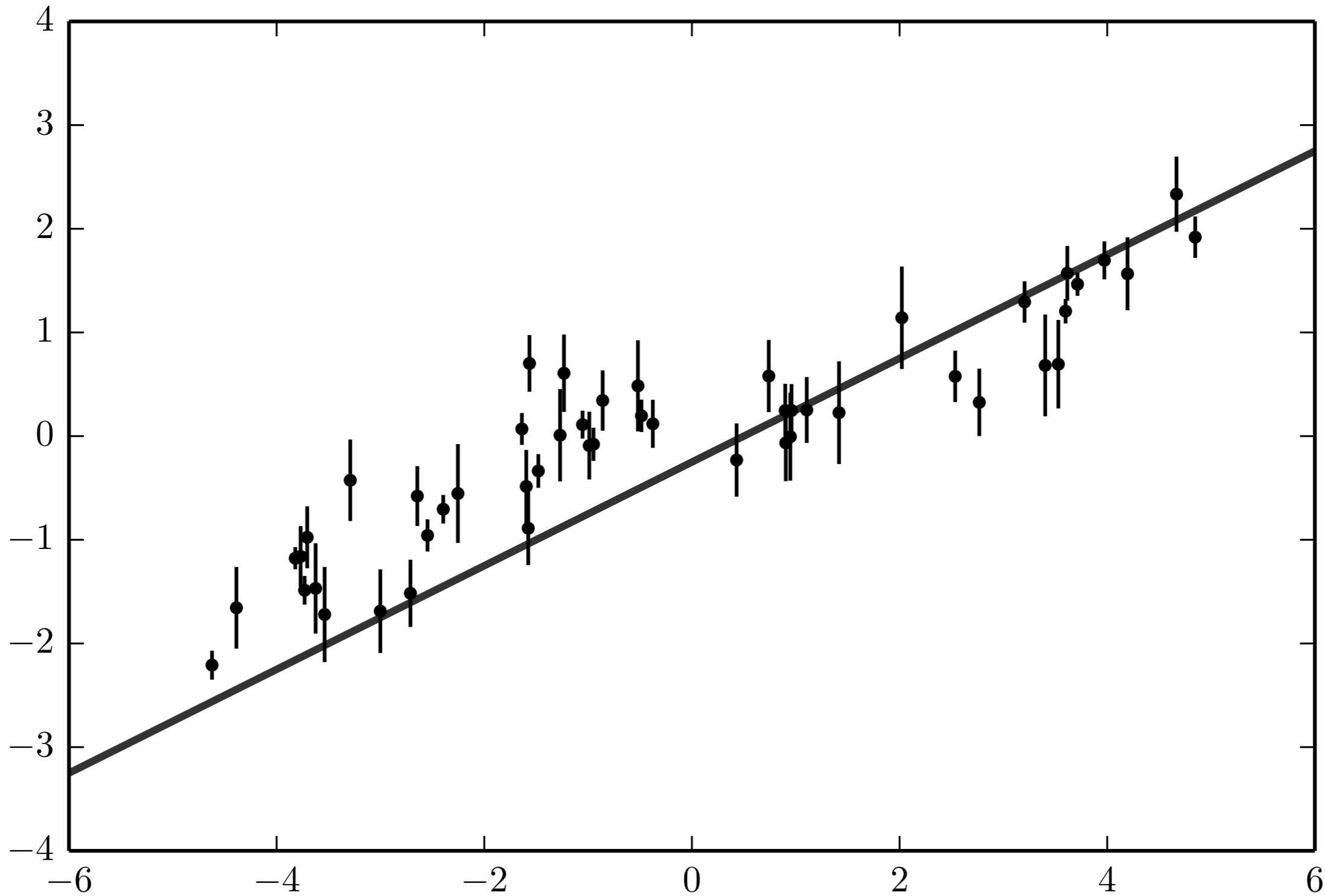
The choice of kernel

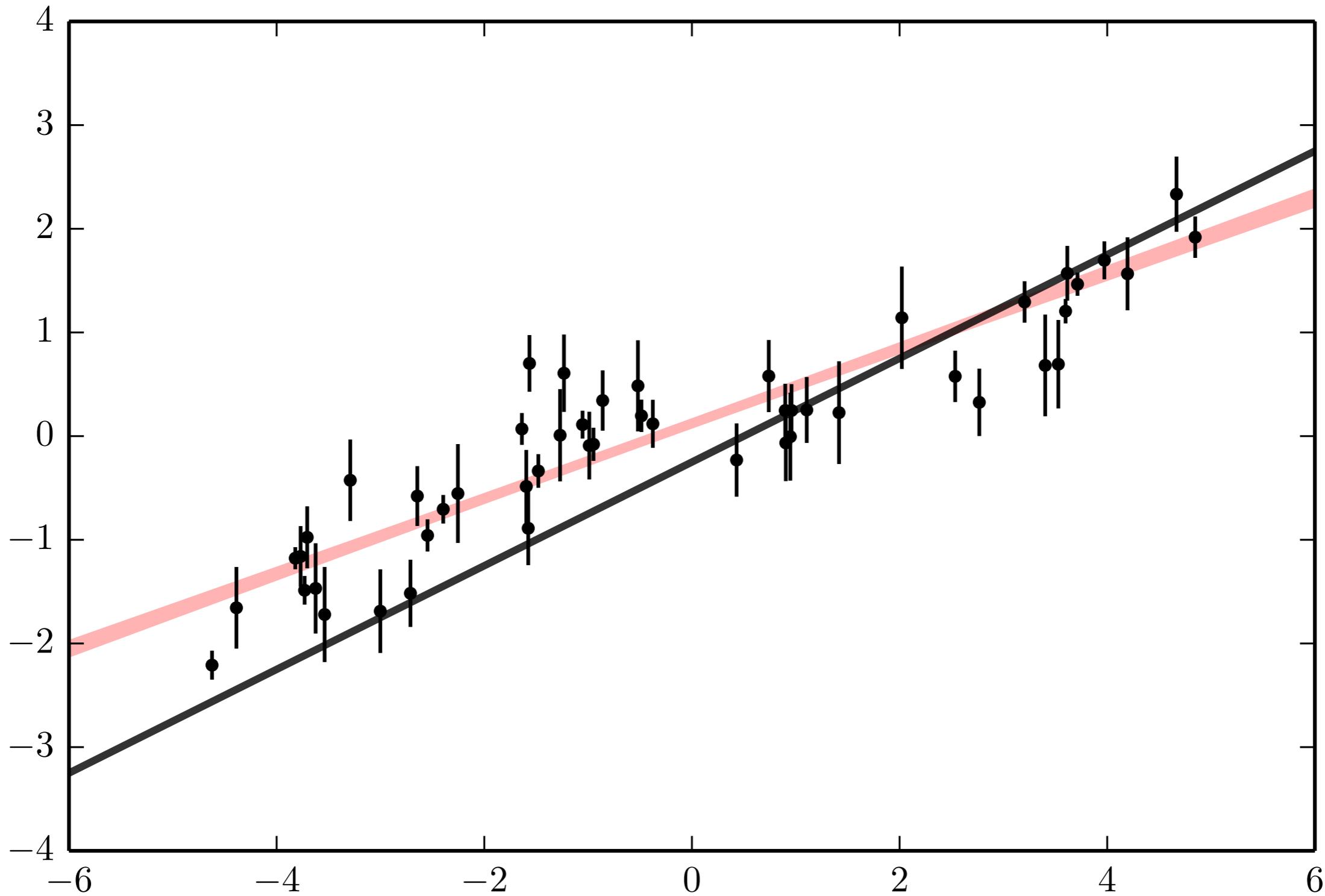


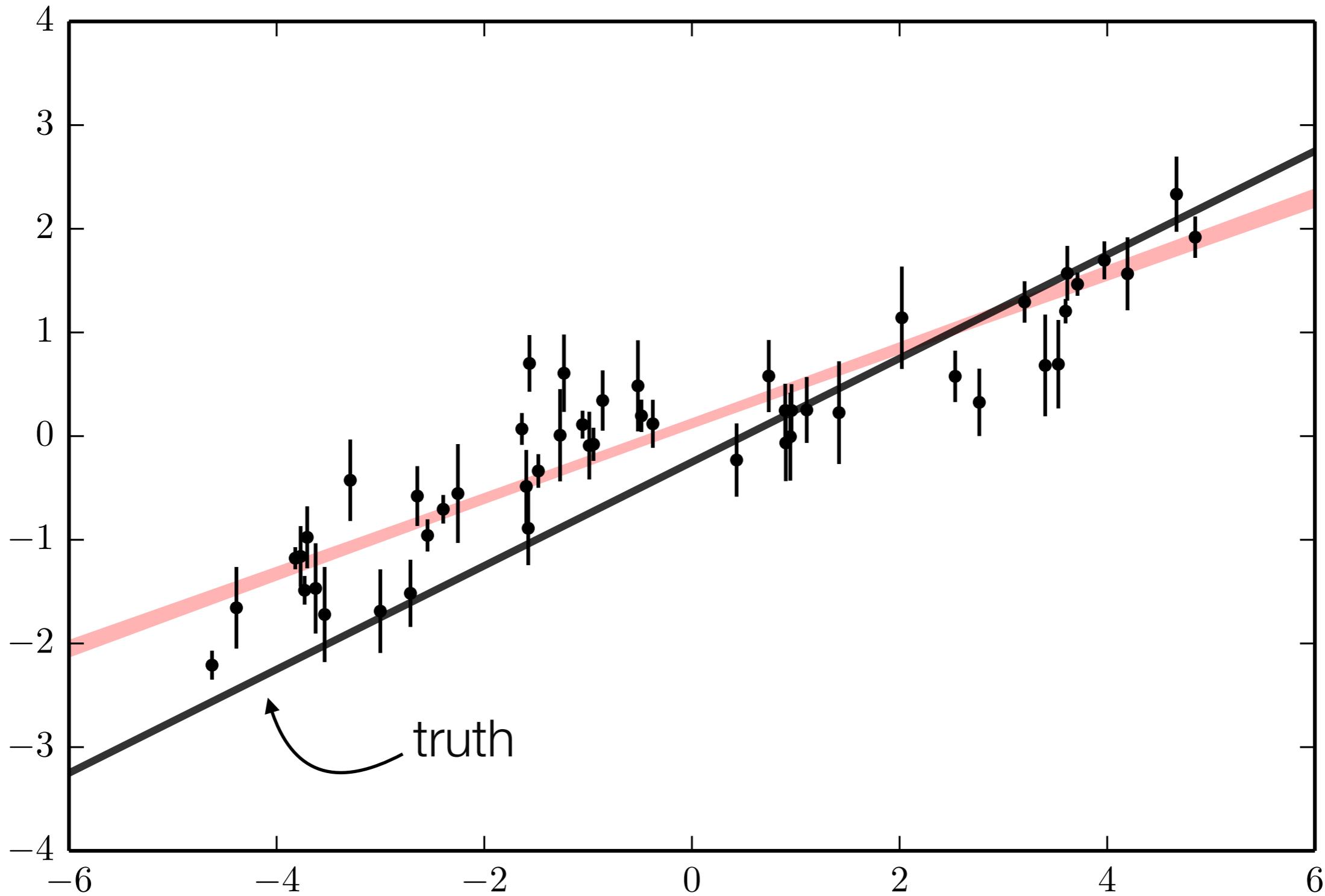
The choice of **kernel**

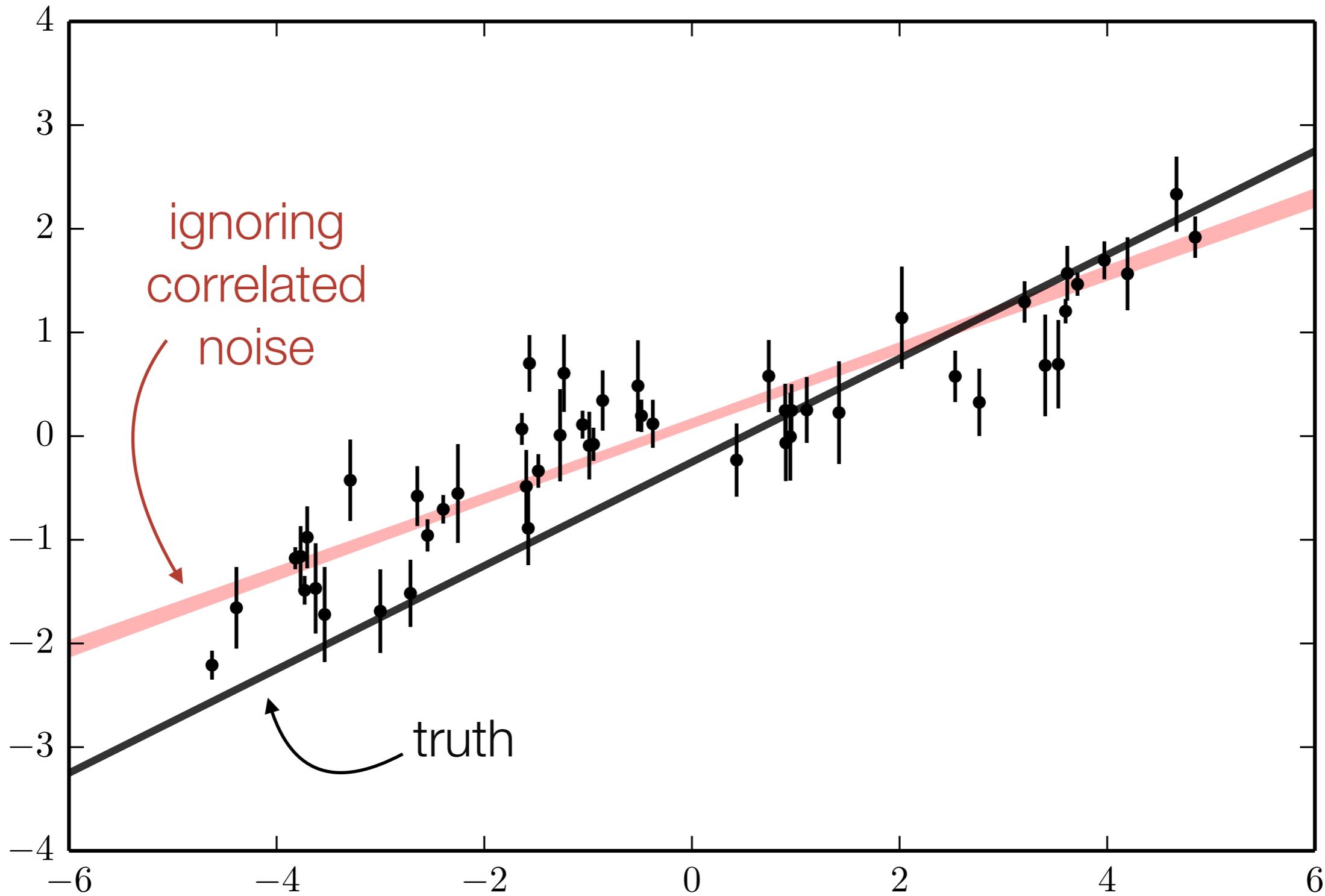


Does this **matter**?

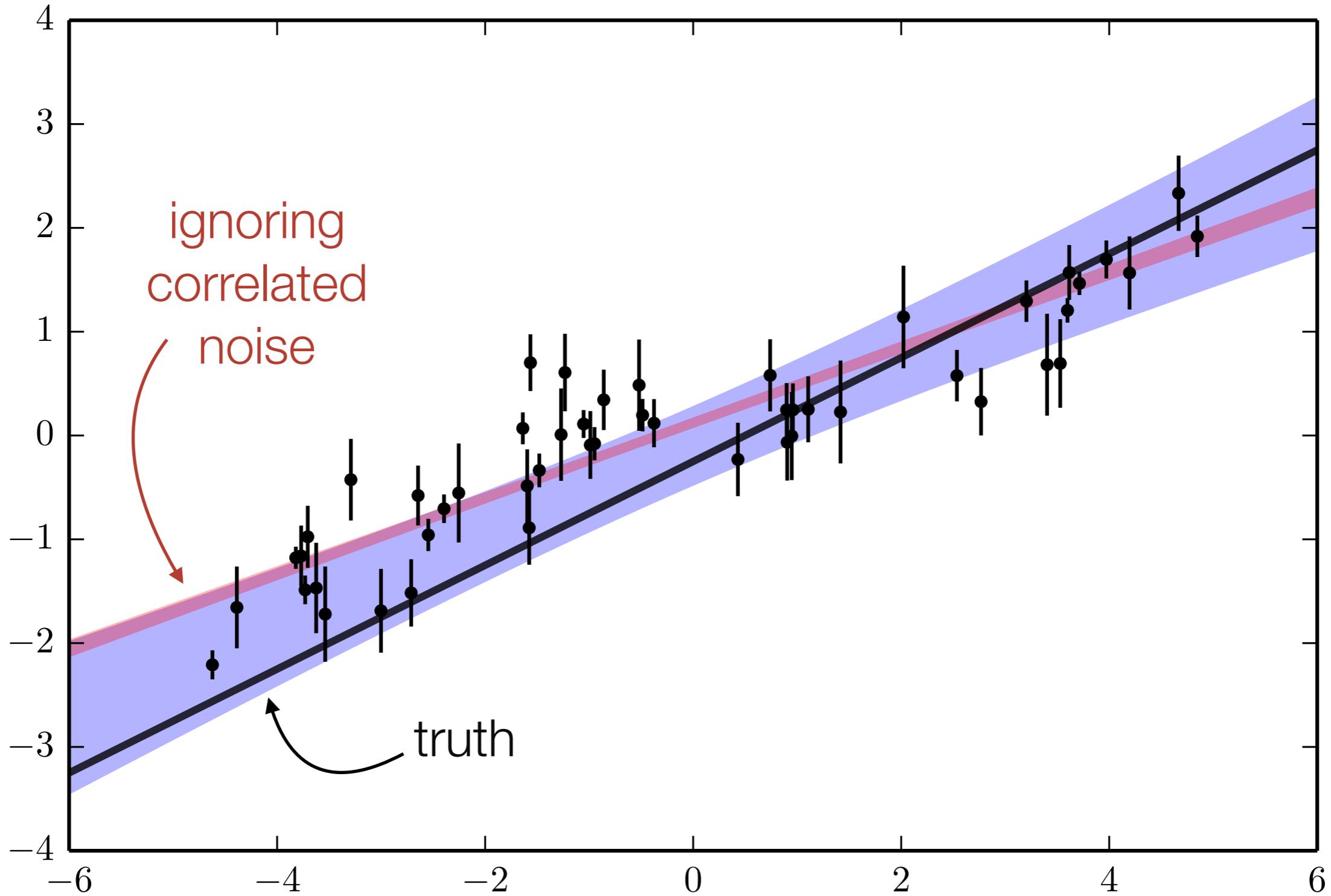




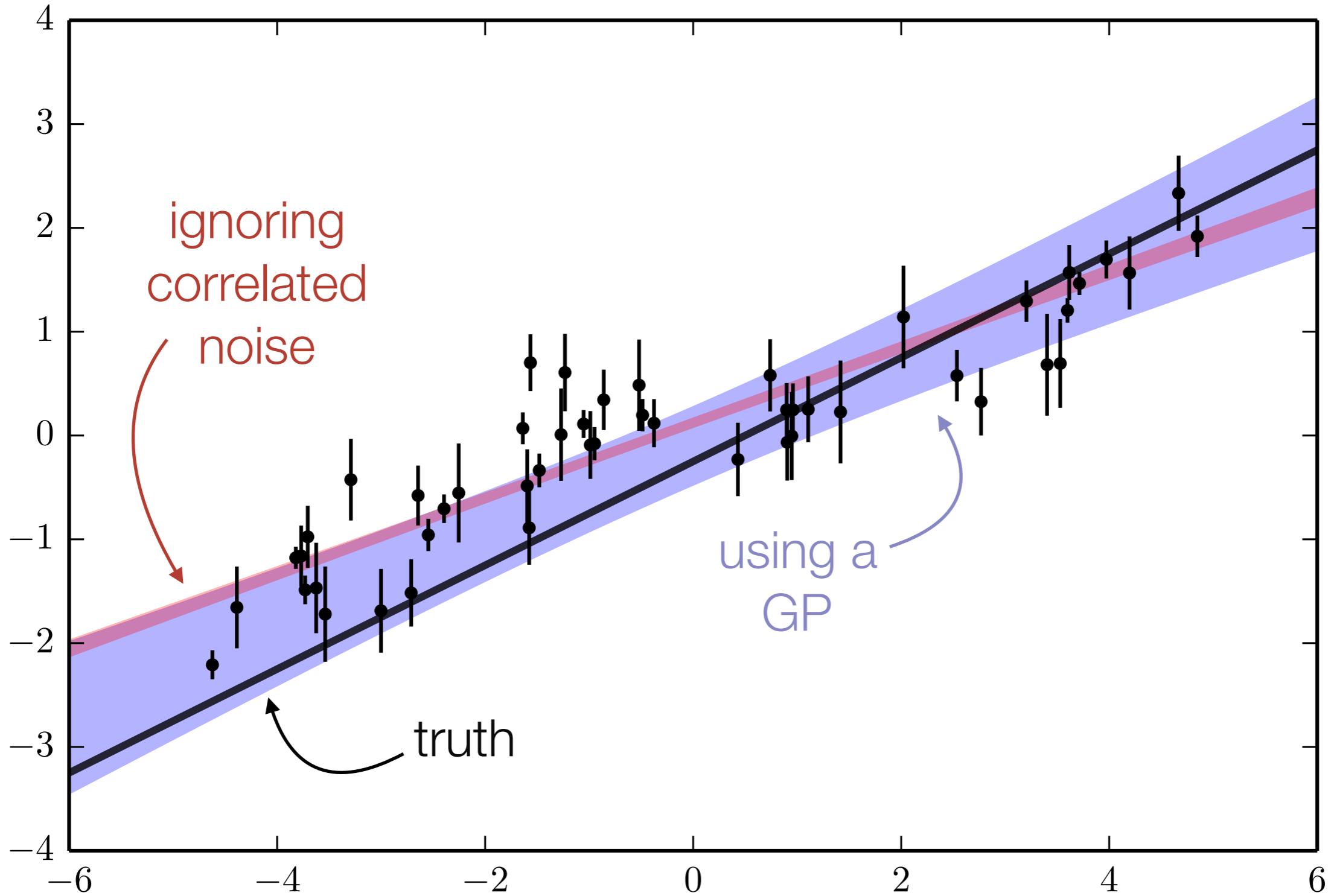




After.



After.



How to use Gaussian Processes?

The mathematical model

$$\begin{aligned}\log p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\sigma}, \boldsymbol{\theta}, \boldsymbol{\alpha}) = & -\frac{1}{2} [\mathbf{y} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})]^T K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma})^{-1} [\mathbf{y} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})] \\ & -\frac{1}{2} \log \det K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma}) - \frac{N}{2} \log 2 \pi\end{aligned}$$

where

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A simple & efficient Python implementation

```
import numpy as np
from scipy.linalg import cho_factor, cho_solve

def kernel(x1, x2):
    # ...

def gp_lnlike(x, y, yerr):
    C = kernel(x[:, None], x[None, :])
    C[np.diag_indices_from(C)] += yerr ** 2
    factor, flag = cho_factor(C)
    logdet = 2*np.sum(np.log(np.diag(factor)))
    return -0.5 * (np.dot(y, cho_solve((factor, flag), y))
                  + logdet + len(x)*np.log(2*np.pi))
```

Using **George**

```
import george
import numpy as np

# kernel = george.kernels...

def george_lnlike(x, y, yerr):
    gp = george.GP(kernel)
    gp.compute(x, yerr)
    return gp.lnlikelihood(y)
```

What's the **catch**?

What's the **catch**?

My Problem

=

Big Data

(by some definition)

Note: I hate myself for this slide too...

Computational complexity.

$$\begin{aligned}\log p(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\sigma}, \boldsymbol{\theta}, \boldsymbol{\alpha}) = & -\frac{1}{2} [\mathbf{y} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})]^T K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma})^{-1} [\mathbf{y} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})] \\ & -\frac{1}{2} \log \det K_{\boldsymbol{\alpha}}(\mathbf{x}, \boldsymbol{\sigma}) - \frac{N}{2} \log 2 \pi\end{aligned}$$

compute **factorization** // evaluate **log-det** // apply **inverse**

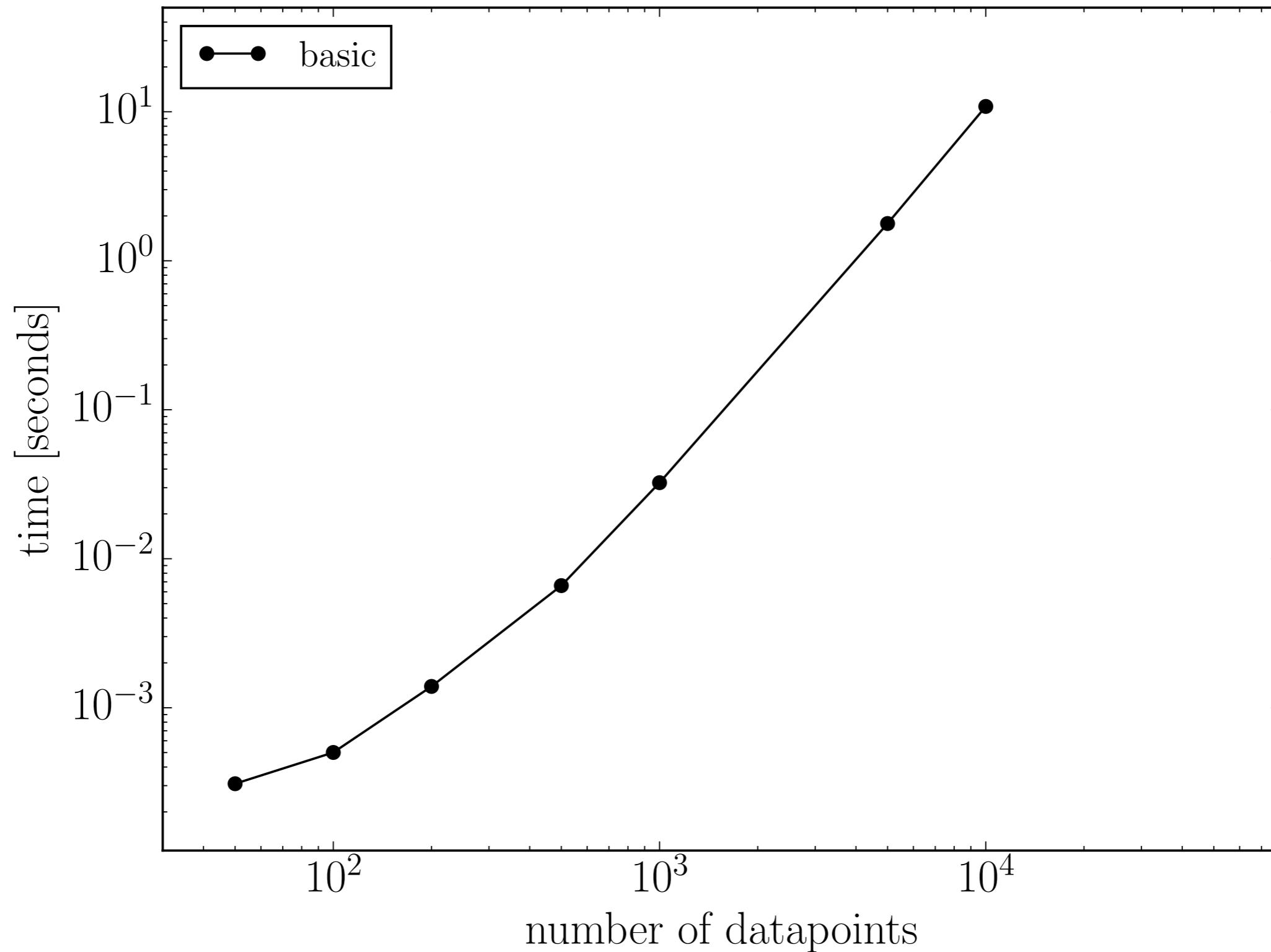
naïvely: $\mathcal{O}(N^3)$

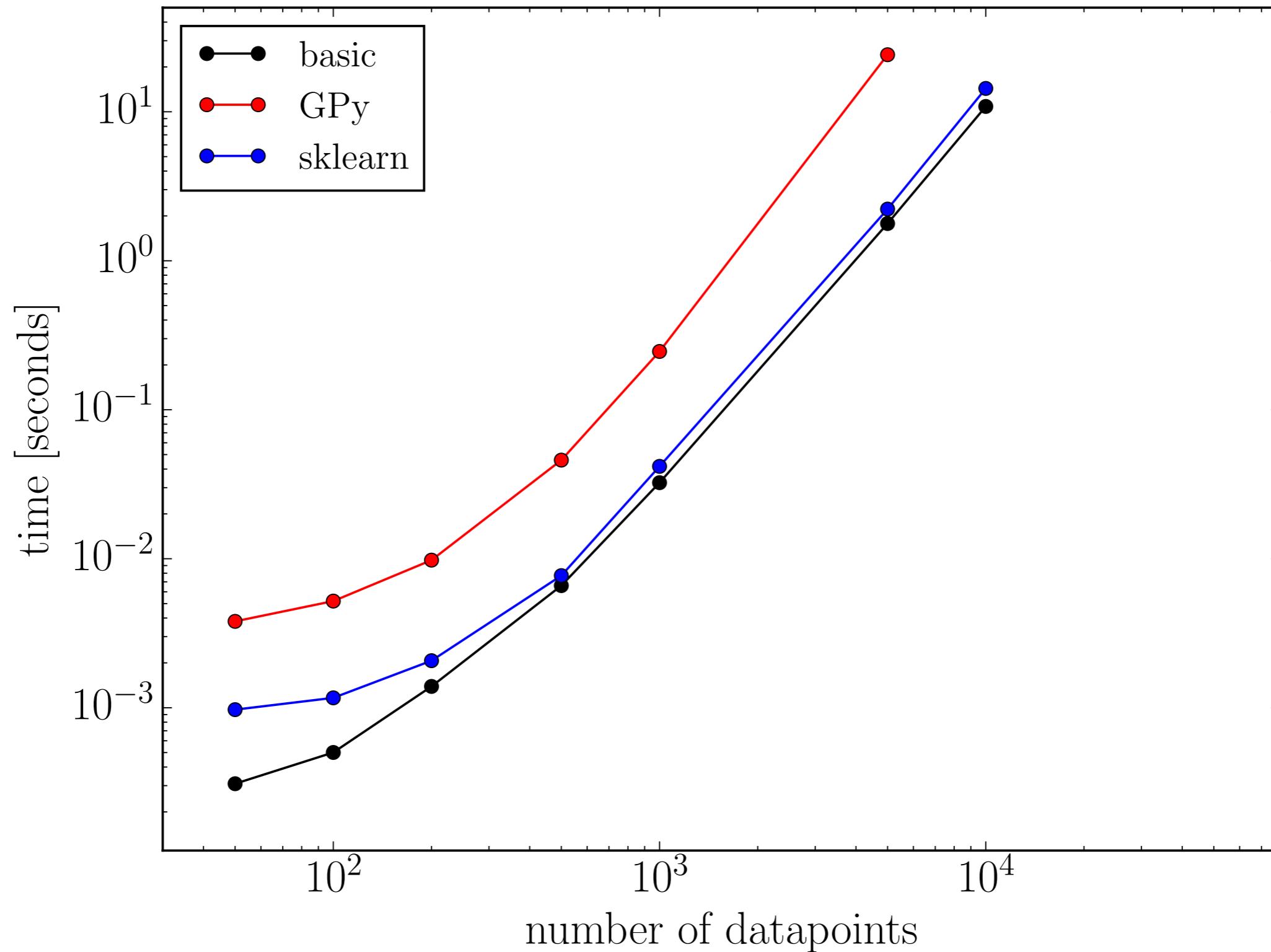
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```





How can we **scale**?

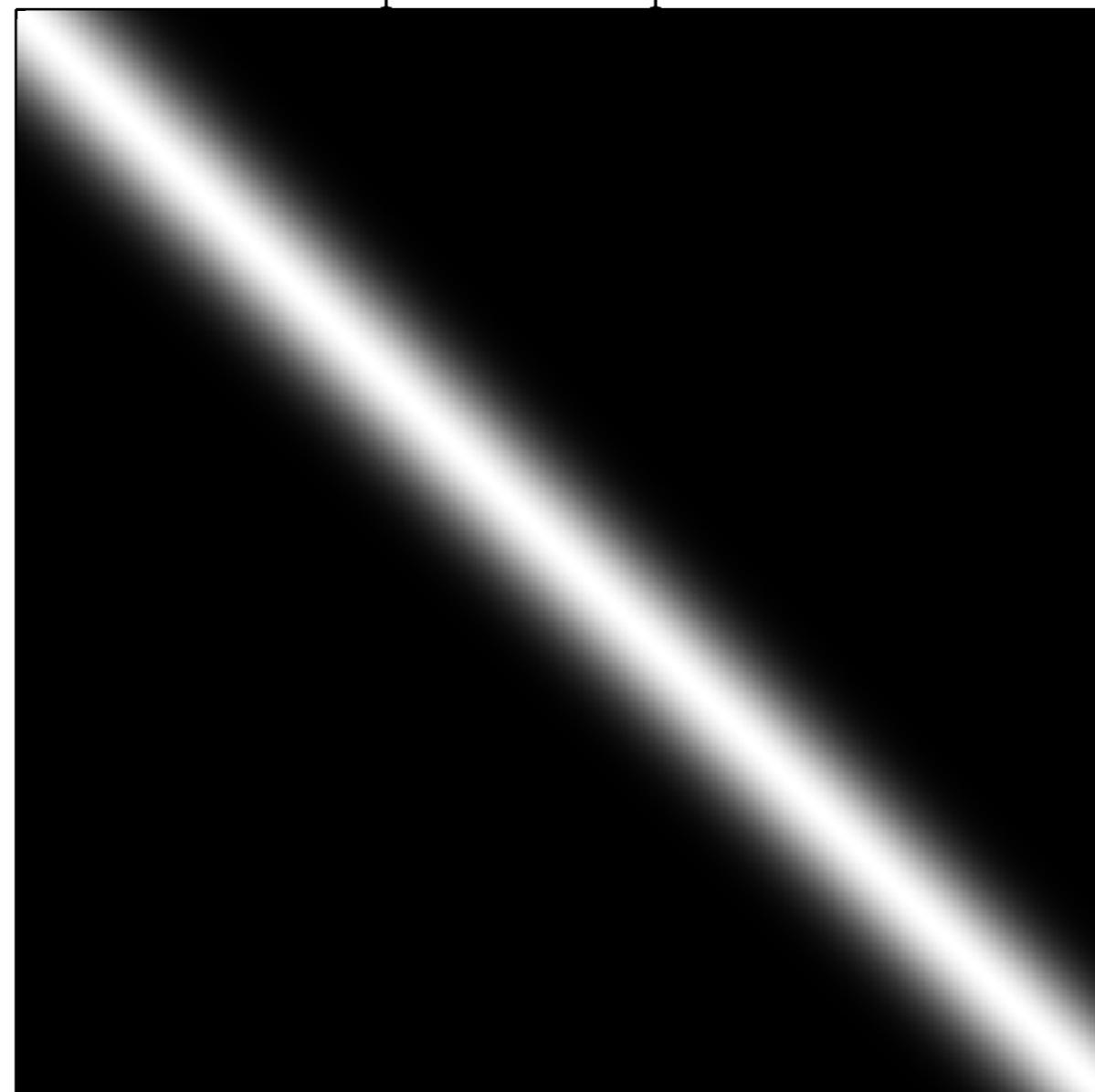
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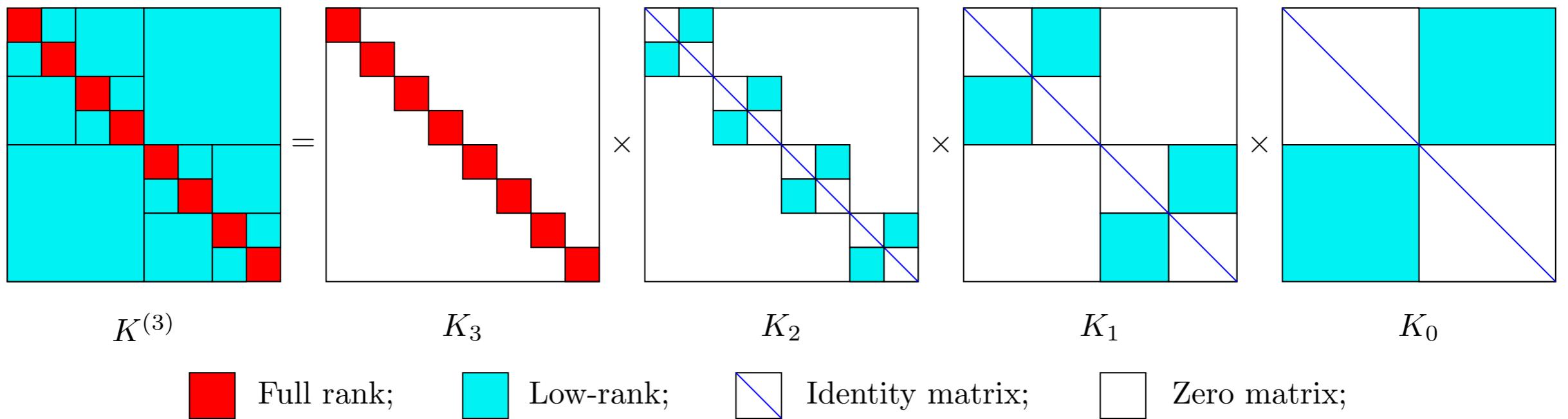
“

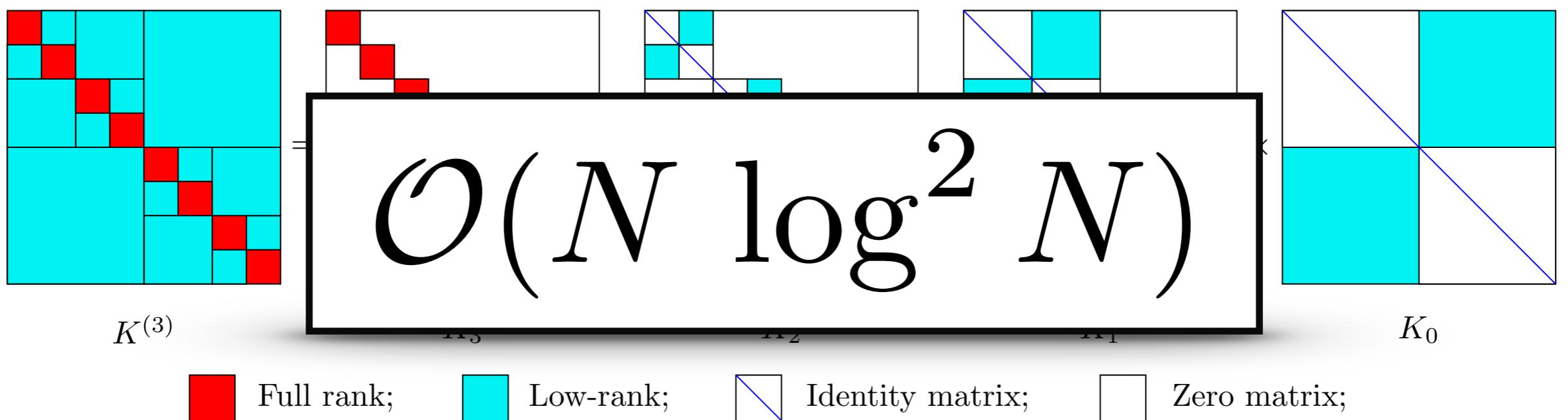
Aren't kernel matrices **Hierarchical Off-Diagonal Low-Rank?**

— not me

exponential squared







github.com/sivaramambikasaran/HODLR

2. dfm@moka | tmux ne...:header (tmux)

```
164 >     >     >     temp.block(nRank[0], 0, nRank[1] , n) => Vinverse[0]*matrix.block(start, 0 , child
165 >
166 >     >     > //> Computes tempSolve => Kinverse\temp-
167 >
168 >     >     > MatrixXd tempSolve => Kinverse.solve(temp);-
169 >
170 >     >     > //> Computes matrix => matrix-Uinverse*tempSolve-
171 >
172 >     >     > matrix.block(start, 0, child[0]->nSize, n) => matrix.block(start, 0, child
173 >     >     > matrix.block(start + child[0]->nSize, 0, child[1]->nSize, n) => matrix.block(sta
174 >     >     }-
175 >     };-
176 >
177 /*!-
178     Computes the determinant of the matrix.-*
179 */
180 > void compute_Determinant() {-
181     if (Kinverse.rows()>0) {           // Check needed when the matrix is predomin
182         MatrixXd LU      = Kinverse.matrixLU();-
183         determinant    = log(fabs(LU(0,0)));-
184         for (int k=1; k<Kinverse.rows(); ++k) {-
185             determinant+=log(fabs(LU(k,k)));-
186         }-
187         // Previous version which had some underflow.-*
188         // determinant=> log(fabs(K.determinant()));-
189     }-
190 }-
HODLR_Node.hpp [cpp]
```

george 1:Vim ✘ 0 ✓ 0 17 Nov 19:22

The HODLR solver from **George**

```
import george
import numpy as np

# kernel = george.kernels...

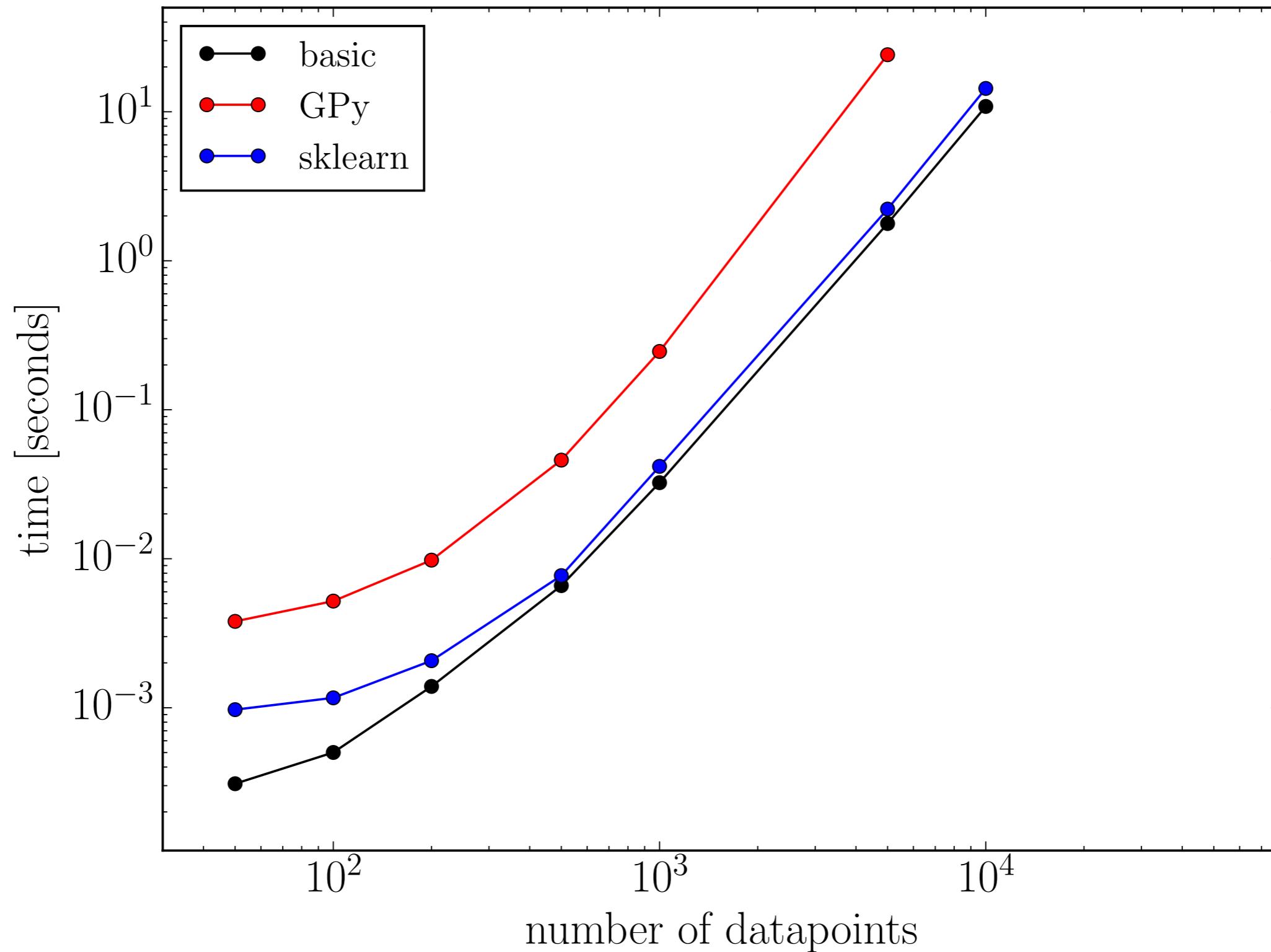
def george_lnlike(x, y, yerr):
    gp = george.GP(kernel)
    gp.compute(x, yerr)
    return gp.lnlikelihood(y)
```

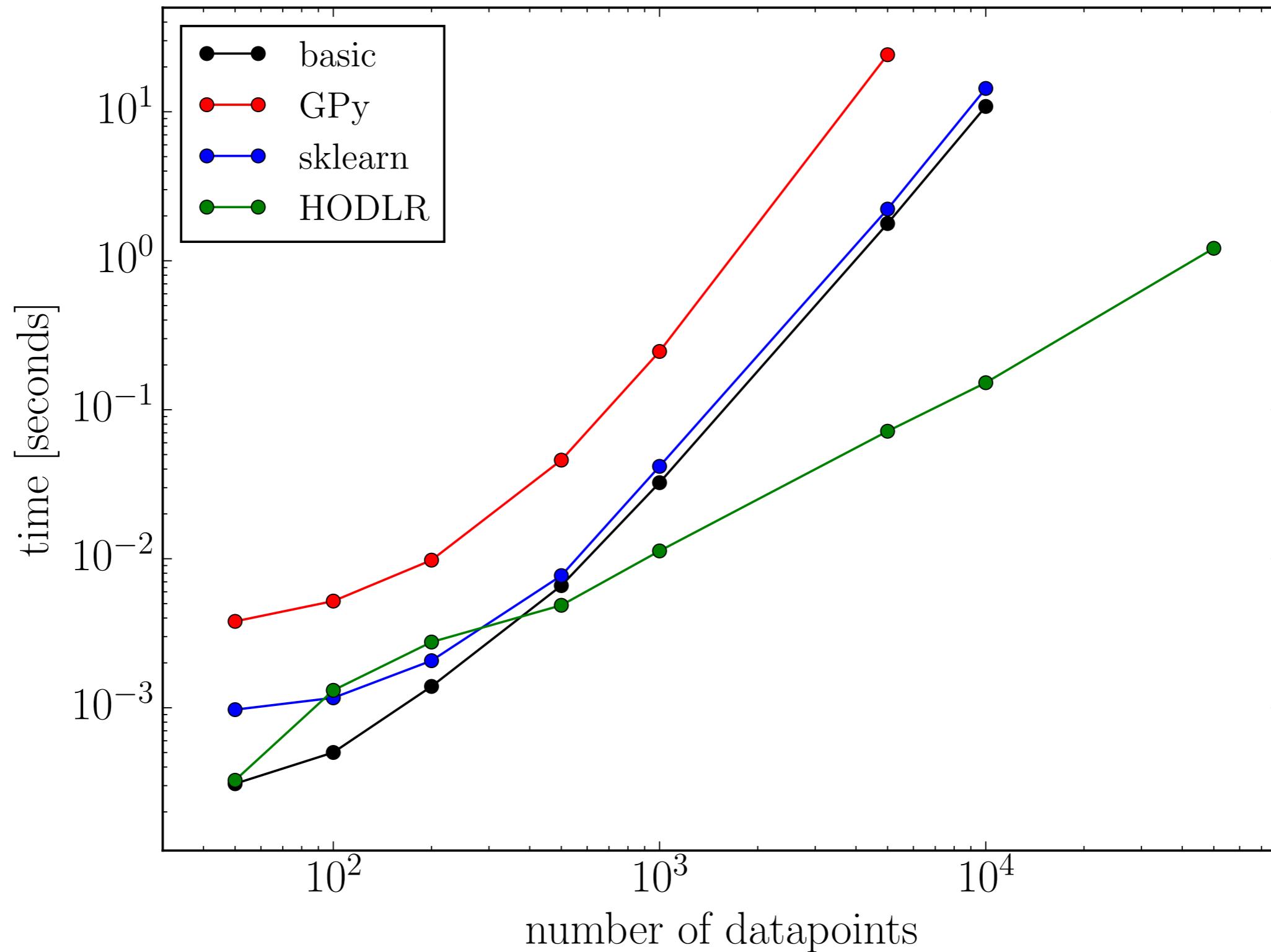
The HODLR solver from George

```
import george
import numpy as np

# kernel = george.kernels...

def george_lnlike(x, y, yerr):
    gp = george.GP(kernel, solver=george.HODLRSolver)
    gp.compute(x, yerr)
    return gp.lnlikelihood(y)
```





Does this **work**?

Yes.

K2 Campaign 1 exoplanet discoveries

21,703 stars

80 days of data

36 planet candidates

18 confirmed planets

Published:

Foreman-Mackey, Montet, Hogg, *et al.* (arXiv:1502.04715)

Montet, Morton, Foreman-Mackey, *et al.* (arXiv:1503.07866)

Schölkopf, Hogg, Wang, Foreman-Mackey, *et al.* (arXiv:1505.03036)



NASA HAS ANNOUNCED THE DISCOVERY
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I SUGGEST WE NAME THIS PLANET "PLUTO,"
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WHILE WE WAIT TO HEAR FROM THE IAU,
HERE'S A REVISED AND UPDATED LIST OF
PLANET NAME SUGGESTIONS (SEE XKCD.COM/1253)
NEW OR UPDATED ENTRIES IN RED

STAR PLANET ↓ SUGGESTED NAME

GLIESE 667C	b	SPACE PLANET
	c	PILF
	d	A STAR
	e	e'); DROP TABLE PLANETS;--
	f	BLOGOSPHERE
	g	BLOGODROME
	h	EARTH
TAU CETI	b	SID MEIER'S TAU CETI B
	c	GIANT DOG PLANET
	d	TINY DOG PLANET
	e	PHIL PLAINET
	f	UNICODE SNOWMAN
GLIESE 832	b	ASSHOLE JUPITER
	c	LAWLESS STARRING KEVIN COSTNER
GLIESE 581	b	WAIST-DEEP CATS
	c	PLANET #14
	d	BALDERRAAN
	e	ETERNIA PRIME
	f	TAUPE MARS
	g	JELLY-FILLED PLANET
EPSILON ERIDANI	b	SKYDOT
	c	LASER NOISES
GLIESE 176	b	PANDORA
	c	PANTERA
KEPLER-61	b	GOLDENPALACE.COM
GROOMBRIDGE 34A	b	HOT MESS
KEPLER-442	b	SEAS OF TOOTHPASTE
GLIESE-422	b	THIS ONE WEIRD PLANET
EPIC-201367065	b	SULAWESI
	c	HUGE SOCCER BALL
	d	GEODUDE
KEPLER-296	b	KERBAL SPACE PLANET
	c	A\$APLANET
	d	JURASSIC WORLD
	e	THIS LAND
	f	SPRINGFIELD
HR 7722	b	BETELGEUSE
	c	BEETLEJUICE
EPIC 201912552	b	NETHERLANDS VII
GLIESE 3293	b	ANTISPIT
	c	GOOGLE EARTH
	d	PLANET OF THE APES (DISAMBIGUATION)
KEPLER-283	b	'Juárenas
	c	jú'reinas
UPSILON ANDROMEDAE	b	FOURTHMEAL
	c	STAMPY
	d	MOONCHILD
	e	HAM SPHERE
HD 20794	b	COSMIC SANDS
	c	LEGOLAND
	d	PLANET WITH ARMS
HD 85512	b	LAX MORALITY
	b	GOOD PLANET
	c	PROBLEMLAND
	d	SLICKLE
	e	SPARE PARTS
	f	NEW JERSEY VI
	g	HOW DO I JOIN THE IAU
GLIESE 163	b	NEIL TYSON'S MUSTACHE
	c	HELP@GMAIL.COM
	d	HAIR-COVERED PLANET
PI MENAE	b	MOON HOLDER
HD 189733	b	PERMADEATH
KEPLER-22	b	BLUE IVY
KOI-2474	b	STORE-BRAND EARTH
KEPLER-437	b	UNICORN THRESHER
KOI-2418	b	SPHERICAL DISCWorld
KEPLER-438	b	EMERGENCY BACKUP EARTH
KOI-3010	b	FEEEOOOOOOOOP
KEPLER-442	b	LIZ
82 ERIDANI	b	HORSEMEAT SURFACE
	c	THE MOON
	d	CONSTANT SAXOPHONES
HD 102365	b	LITTLE BIG PLANET
GLIESE 180	b	DUNE
FOMALHAUT	b	ARRAKIS
KEPLER-62	b	SWARM OF BEES
	c	SPORTY
	c	BABY
	d	SCARY
HD 69830	e	GINGER
	f	POSH
	b	PLANET.XXX
	c	NOVELLA
GLIESE 682	d	SEXOPLANET
	b	VERDANT HELLSCAPE
	c	UNSUBSCRIBE
KEPLER-452	b	PLUTO



KEPLER-452b

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HR 7722

EPIC 201912552

b BETELGEUSE

C BEETLEJUICE

b ANTISPLIT

C GOOGLE EARTH



dfm/george at 1.0-dev Dan

GitHub, Inc. [US] https://github.com/dfm/george/tree/1.0-dev

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dfm / george Unwatch 14 Star 98 Fork 35

Fast Gaussian Processes for regression <http://dan.iel.fm/george> — Edit

430 commits 3 branches 1 release 5 contributors

Branch: 1.0-dev george / +

This branch is 79 commits ahead, 2 commits behind master.

	Pull request	Compare
dfm fixing general metric bug and multi-d constant kernel scaling	Latest commit 2e32ce3 19 days ago	
docs py3 xrange in kernels		2 months ago
document A few words for the paper		10 months ago
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hodlr @ 2213b25 updating hodlr for symmetric assembly		a year ago
kernels building bounded kernels		2 months ago
templates fixing general metric bug and multi-d constant kernel scaling		19 days ago
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.gitmodules Starting C++ and HODLR version		2 years ago
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<> Code

Issues 15

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github.com/dfm/george

dfm.io/george

Foreman-Mackey, Montet, Hogg, et al. (arXiv:1502.04715)
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Schölkopf, Hogg, Wang, Foreman-Mackey, et al. (arXiv:1505.03036)

extra

