## data-driven discovery in the astronomical time domain

#### dan foreman-mackey cca@flatiron dfm.io github.com/dfm @exoplaneteer

## noise models, algorithm development, and open source scientific software

dan foreman-mackey cca@flatiron dfm.io github.com/dfm @exoplaneteer

# my goals for today

Discuss the role of open source software in astrophysics

Demonstrate the impact of interdisciplinary collaboration, good documentation, and open development on this research.

# motivated by the study of time domain astronomical surveys.

## **time domain astronomy** Measure [something] as a function of time.

## time domain astronomy Measure [something] as a function of time.

where **[something]** = position brightness color

 $\bullet \bullet \bullet$ 

## exoplanets One of the recent time domain success stories.



source: The Open Exoplanet Catalogue





so what?

## kepler was designed as a statistical mission.



data: NASA Exoplanet Archive



data: NASA Exoplanet Archive



data: NASA Exoplanet Archive

## state-of-the-art discovery requires pushing the technical boundaries

when you push the boundaries you won't have a good training set

## the transit method





## Jupiter



### Jupiter













of many stars

## we need to precisely measure the brightness at high cadence for a long time



# kepler 190k targets

30 min cadence 4 year baseline 5,000 planet candidates

\*note: all numbers are approximate















star spacecraft detector



=

#### observation

## auxiliary science





time



time







#### source: Huber+ (2013)



# it's not stopping anytime soon



## tess

3.2M / 500k targets 30 min / 2 min cadence 30 day baseline 15,000 planet candidates

\*note: all numbers are **predictions** 



## what do we do with al these data?


# $p(\text{physics} \mid \text{data})$



p(data | physics)





### Efficient computation of the likelihood 2



## Markov chain Monte Carlo (MCMC)

## 2 Gaussian processes (GPs)

## Markov chain Monte Carlo





 $\int f(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \boldsymbol{D}) \, \mathrm{d}\boldsymbol{\theta}$ 























samples from







samples from







## in astronomy, we use MCMC





## **MCMC is brittle** Either: **algorithm requires tuning** or **model must be simplified**.





PUBLICATIONS OF THE ASTRONOMICAL SOCIETY OF THE PACIFIC, 125:306–312, 2013 March

### emcee: The MCMC Hammer

DANIEL FOREMAN-MACKEY,<sup>1</sup> DAVID W. HOGG,<sup>1,2</sup> DUSTIN LANG,<sup>3,4</sup> AND JONATHAN GOODMAN<sup>5</sup> Received 2013 January 09; accepted 2013 January 30; published 2013 February 25





Algorithm 3 The parallel stretch move update step 1: for  $i \in \{0, 1\}$  do 2: **for** k = 1, ..., K/2 **do** // This loop can now be done in parallel for all k3: 4:  $X_k \leftarrow S_k^{(i)}$ 5: 6:  $z \leftarrow Z \sim g(z)$ , Equation (10) 7:  $Y \leftarrow X_j + z \left[ X_k(t) - X_j \right]$ 8:  $q \leftarrow z^{n-1} p(Y) / p(X_k(t))$ 9:  $r \leftarrow R \sim [0, 1]$ if  $r \leq q$ , Equation (9) then 10:  $X_k(t+\frac{1}{2}) \leftarrow Y$ 11: else 12:  $X_k(t+\frac{1}{2}) \leftarrow X_k(t)$ 13: end if 14: 15: **end for** 16:  $t \leftarrow t + \frac{1}{2}$ 17: **end for** 

from: DFM, Hogg, Lang, Goodman (2013)

Draw a walker  $X_j$  at random from the complementary ensemble  $S^{(\sim i)}(t)$ 





## this project has been quite DODUCIT.











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GitHub, Inc. [US] https://github.com/dfm/emcee			
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tests	fixing py2 bug in tests		5 months ago
.appveyor.yml	no progress bars		6 months ago
.coveragerc	better coverage tracking		5 months ago
.gitattributes	Create .gitattributes to fix language	statistics	a year ago
.gitignore	CI: Drop 3.2. Ignore coverage outpu	ıt	2 years ago
.rtd-environment.yml	adding rtd config		a year ago
.travis.yml	travis install		7 months ago
AUTHORS.rst	adding incremental tutorial		7 months ago
CODE_OF_CONDUCT.md	Create CODE_OF_CONDUCT.md		6 months ago
CONTRIBUTING.md	Typos		a year ago
E HISTORY ret	adding contributors		7 months ago



MCMC



### 🖈 🕼 🎽 🝖 :



emcee is an MIT licensed pure-Python implementation of Goodman & Weare's Affine Invariant Markov chain Monte Carlo (MCMC) Ensemble sampler and these pages will show you how to use

This documentation won't teach you too much about MCMC but there are a lot of resources available for that (try this one). We also published a paper explaining the emcee algorithm and imple-

emcee has been used in quite a few projects in the astrophysical literature and it is being actively de-

If you wanted to draw samples from a 10 dimensional Gaussian, you would do something like:

```
return -0.5 * np.sum(ivar * x ** 2)
p0 = [np.random.rand(ndim) for i in range(nwalkers)]
sampler = emcee.EnsembleSampler(nwalkers, ndim, lnprob, args=[ivar])
```

A more complete example is available in the <u>quickstart documentation</u>.





MCMC

## imitations

emcee does not scale well with the number of dimensions.











## what to co?

1. Compute derivatives by hand or using autodiff. 2. Use an emulator or surrogate model.





### transit light curve





### derivative w.r.t.









• From Source

next | modules | index

☆ 층 :

license MIT build passing docs passing DOI 10.5281/zenodo.2536576 powered by starry powered by celerite powered by PyMC3 powered by AstroPy

exoplanet is a toolkit for probabilistic modeling of transit and/or radial velocity observations of exoplanets and other astronomical time series using PyMC3. PyMC3 is a flexible and high-performance model building language and inference engine that scales well to problems with a large number of parameters. exoplanet extends PyMC3's language to support many of the custom functions and distributions required when fitting exoplanet datasets. These features

• A fast and robust solver for Kepler's equation.

- Scalable Gaussian Processes using celerite.
- Fast and accurate limb darkened light curves using starry.
- Common reparameterizations for limb darkening parameters, and planet radius and im-

All of these functions and distributions include methods for efficiently calculating their gradients so that they can be used with gradient-based inference methods like Hamiltonian Monte Carlo, No U-Turns Sampling, and variational inference. These methods tend to be more robust than the methods more commonly used in astronomy (like ensemble samplers and nested sampling) especially when the model has more than a few parameters. For many exoplanet applications, exoplanet (the code) can improve the typical performance by orders of magnitude.

exoplanet is being actively developed in a public repository on GitHub so if you have any trou-





MCMC



## Markov chain Monte Carlo (MCMC)

## 2 Gaussian processes (GPs)

## Gaussian processes





**GPs** 



star spacecraft detector



=

### observation





+ MMMMM + conversion

spacecraft detector



### observation





### a Gaussian Process (incl. physics)

## spacecraft detector



### observation












































### There's a problem!



# $\log \mathcal{L}_{\rm GP} = -\frac{1}{2} r^{\rm T} K^{-1} r - \frac{1}{2} \log \det K - \frac{N}{2} \log 2\pi$



# $\log \mathcal{L}_{\rm GP} = -\frac{1}{2} \boldsymbol{r}^{\rm T} \boldsymbol{K}^{-1} \boldsymbol{r} - \frac{1}{2} \log \det K - \frac{N}{2} \log 2\pi$













**kepler** 190k targets 70k obs./target





### tess

### 500k targets 20k obs./target







## my first try: hodir Hierarchical Off-Diagonal Low Rank approximations. In collaboration: Sivaram Ambikasaran (NYU $\rightarrow$ IIT)



IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. 38, NO. 2, 2015

### Fast Direct Methods for Gaussian Processes

Sivaram Ambikasaran, Daniel Foreman-Mackey, Leslie Greengard, Member, IEEE, David W. Hogg, and Michael O'Neil, Member, IEEE

reference: arXiv:1403.6015



Ifm/george: Fast and flexible &			
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Fast and flexible Gaussian Processpythongaussian-processestime-	series cpp c-plus-plus Manage topics	edocs.io	Edit
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<b>dfm</b> updating history			Latest commit 7f4d301 on Jan 8
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docs	trying to fix docs build [ci skip]		4 months ago
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paper	a few words		4 months ago
templates	updating tutorials version and bumping version	number	4 months ago
tests	working x gradients		4 months ago
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.coveragerc	cleaning up coverage		10 months ago
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### That's still not fast enough!



# my second try: célérité Semi-separable matrices.

In collaboration: Sivaram Ambikasaran (IIT)



THE ASTRONOMICAL JOURNAL, 154:220 (21pp), 2017 December

### Fast and Scalable Gaussian Process Modeling with Applications to **Astronomical Time Series**

Daniel Foreman-Mackey<sup>1,2,6</sup>, Eric Agol<sup>1,7</sup>, Sivaram Ambikasaran<sup>3</sup>, and Ruth Angus<sup>4,5</sup>, Astronomy Department, University of Washington, Seattle, WA, USA <sup>2</sup> Center for Computational Astrophysics, Flatiron Institute, 162 5th Avenue, 6th Floor, New York, NY 10010, USA <sup>3</sup> Department of Computational and Data Sciences, Indian Institute of Science, Bangalore, India <sup>4</sup> Department of Astronomy, Columbia University, 550 W 120th Street, New York, NY 10027, USA Received 2017 March 27; revised 2017 October 9; accepted 2017 October 10; published 2017 November 9

### reference: arXiv:1703.09710

C ss k





reference: DFM+ (2017), arXiv:1703.09710



![](_page_92_Figure_0.jpeg)

reference: DFM+ (2017), arXiv:1703.09710

![](_page_92_Picture_3.jpeg)

function celerite\_factor(U, P, d, W) # Initially d = a and W = V $S \leftarrow \operatorname{zeros}(J, J)$  $w_1 \leftarrow w_1/d_1$ for  $n = 2, \dots, N$ :  $S \leftarrow \operatorname{diag}(p_{n-1}) [S + d_{n-1} w_{n-1}]$  $d_n \leftarrow d_n - u_n S u_n^T$  $w_n \leftarrow [w_n - u_n S] / d_n$ return d, W, S

reference: DFM (2018), arXiv:1801.10156

$$S + d_{n-1} \boldsymbol{w}_{n-1}^{\mathrm{T}} \boldsymbol{w}_{n-1}] \operatorname{diag}(\boldsymbol{p}_{n-1})$$

$$\prod_{n} [J/d_{n}] / d_{n}$$

![](_page_93_Picture_3.jpeg)

![](_page_94_Figure_1.jpeg)

reference: DFM (2018), arXiv:1801.10156

## $\mathcal{O}(NJ^2)$

![](_page_94_Picture_4.jpeg)

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☐ dfm / celerite <> Code ① Issues ⑧	Pull requests 2 Projects 0 Insights	Owner     Watch     12     ★ Star     112     % Fork     28
Scalable 1D Gaussian Pro python gaussian-processe	cesses in C++, Python, and Julia http://celerite.rtfd.io s astronomy time-series stars exoplanets julia cpp	c-plus-plus
F 1,008 commits     Branch: master ▼   New pu     Image: State of the state	P 4 branches > 7 releases	Find file Clone or download  Latest commit 846c239 on Nov 28, 2017
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docs	updating zenodo DOI	2 years ago
examples/benchmark	updating benchmark plots	2 years ago
paper	zenodo links	a year ago
tests	noqa annoyingness	2 years ago
.appveyor.yml	Update .appveyor.yml	a year ago
■ .coveragerc	adding coverage and coveralls	2 years ago
.gitattributes	Update .gitattributes	2 years ago
.gitignore	bumping version number to 0.3.0	a year ago
.rtd-environment.yml	Update .rtd-environment.yml	a year ago
🖹 .travis.yml	develop on ci	2 years ago
AUTHORS.rst	working on docs [ci skip]	2 years ago
	bumping version number	2 years ago
HISTORY.rst	bumping version number to 0.3.0	a year ago
	Adding 2017 to license [ci skip]	2 years ago

![](_page_95_Picture_1.jpeg)

![](_page_96_Picture_0.jpeg)

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![](_page_97_Picture_0.jpeg)

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![](_page_97_Picture_2.jpeg)

## imitations

célérité is restricted to semi-separable matrices and (in my

# implementation) this means 1D inputs with a stationary kernel.

![](_page_98_Picture_3.jpeg)

### summery

célérité provides a **scalable** method for evaluating GP likelihoods. This makes GP inference feasible for astronomical surveys.

The class of kernel functions have a **useful physical** interpretation.

![](_page_99_Picture_3.jpeg)

# future cirections

- flexible.
- 2. Extend to multiple dimensions for structured data (e.g. parallel time series).

![](_page_100_Picture_3.jpeg)

# 1. Combine with deep kernel learning to make the kernel more

![](_page_100_Picture_5.jpeg)

# long period transiting planets it all comes together...

![](_page_102_Figure_0.jpeg)

source: NASA Exoplanet Archive

### DFM+ (2016); arXiv:1607.08237

![](_page_103_Figure_1.jpeg)

source: NASA Exoplanet Archive

# these are (mostly) single transits

![](_page_105_Figure_0.jpeg)

star spacecraft detector

![](_page_105_Picture_3.jpeg)

=

### observation

![](_page_106_Figure_0.jpeg)

+ MMMMM + conversion

spacecraft detector

![](_page_106_Picture_3.jpeg)

### observation

![](_page_107_Figure_0.jpeg)

DFM+ (2016); arXiv:1607.08237

![](_page_107_Picture_2.jpeg)
### DFM+ (2016); arXiv:1607.08237



source: NASA Exoplanet Archive

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	document	Merge remote-tracking branch 'upstream/m	aster'	a year ago	
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		readme		2 years ago	
	README.rst	Another link typo		2 years ago	
	environment.yml	adding conda env		2 years ago	
	ms_revised.pdf	added documents, period estimate for e=0		a year ago	
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a deficit of planets inside 10^3 days. Take the 2 R_earth. There are ~9 planets in that bin (and a from 1000 to 2000 days. Given that the longer [3/2] ~ 2.8, this would imply a rise in dN/d ln P	Labels 🔅 None yet			
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### REVISITING THE LONG-PERIOD TRANSITING PLANETS FROM KEPLER

MIRANDA K. HERMAN<sup>1</sup>, WEI ZHU (祝伟)<sup>2</sup>, AND YANQIN WU (武延庆)<sup>1</sup> & Astrophysics, University of Toronto, 50 St. George St., Toronto, ON M5S 3H4, Canada; he

<sup>1</sup>Astronomy & Astrophysics, University of Toronto, 50 St. George St., Toronto, ON M5S 3H4, Canada; herman@astro.utoronto.ca and <sup>2</sup>Canadian Institute for Theoretical Astrophysics, University of Toronto, 60 St. George St., Toronto, ON M5S 3H8, Canada Draft version March 7, 2019

reference: arXiv:1901.01974



### tess

3.2M / 500k targets 30 min / 2 min cadence 30 day baseline 15,000 planet candidates

\*note: all numbers are **predictions** 



Modern astrophysics requires the development (and implementation) of new algorithms.

Modern astrophysics **requires** the development (and <u>implementation</u>) of new algorithms.

This really benefits from interdisciplinary collaboration, good documentation, and open development.

Every project described here is open source software with an associated journal article.

Every project described here is open source software with an associated journal article.

Is this a hack?

## references

dfm/emcee gradient-free MCMC in Python dfm/exoplanet gradient-based inference for time series dfm/george simple Gaussian processes in Python dfm/celerite fast & scalable Gaussian processes dfm/peerless long period transiting exoplanets

> dan foreman-mackey cca@flatiron dfm.io github.com/dfm @exoplaneteer

# fast/accurate light curve models work led by Rodrigo Luger (Flatiron)







### a Gaussian Process (incl. physics)

### spacecraft detector



### observation



























constant

linear

quadratic







constant
linear
quadratic
cubic
quartic
auintic























The real spherical harmonics

















































github.com/rodluger/starry

rodluger.github.io/starry

arxiv.org/abs/1810.06559











test_compare_to_v1.py	E test_high_order_ld.py	test_phasecurves.py
test_evaluation.py	test_light_travel.py	test_rotation.py
test_exposure.py	E test_mcmc.py	test_slices.py
test_flux_ld_gradients.py	E test_memory.py	test_sturm.py









Figure 9. Sample analytic exoplanet system light curves computed with starry. *Top:* a hot Jupiter transiting a Sun-like star. The planet's map is a simple dipole, with the hotspot offset 15° from stellar noon; the offset in the secondary eclipse from the peak of the phase curve is apparent. *Bottom:* a two-planet system with more complex surface maps. In addition to transits and secondary eclipses, a few planet-planet occultations are visible (e.g., the very short events at t = 0.1 and t = 3.4 days).





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1	"""Exoplanet system example."""								
2	from starry.kepler import Primary, Secondary, System								
3	import matplotlib.pyplot as pl								
4	import numpy as np								
5									
7	# Setup								
2	# secup fig as $=$ nl subplots(2 figsize=(12 6))								
q	fig.subplots_adjust(hspace=0.35)								
10	ax[0].set vlabel('Normalized flux', fontsize=16)								
11	ax[0].set xlabel('Time [days]'. fontsize=16)								
12	<pre>ax[1].set vlabel('Normalized flux', fontsize=16)</pre>								
13	<pre>ax[1].set_xlabel('Time [days]', fontsize=16)</pre>								
14	ax[0].set_xlim(0, 20)								
15	ax[1].set_xlim(0, 20)								
16	time = np.linspace(0, 20, 10000)								
17									
18									
19	<pre># System #1: A one-planet system with a hotspot offset</pre>								
20	#								
21									
22	# Instantiate the star								
23	<pre>star = Primary()</pre>								
24									





where  $_{2}F_{1}(a,b;c;x)$  is the generalized Hypergeometric function. These functions can alternatively be expressed as series in  $k^2$  by expanding  $(1 - k^2 w)^{-1/2}$  as a series in  $k^2w$ , and then integrating each term over w, giving

$$\mathcal{I}_{v} = 2k^{1+2v} \sum_{j=0}^{\infty} \frac{(2j-1)!!}{2^{j}j!(2j+2v+1)} (k^{2})^{j},$$
$$\mathcal{J}_{v} = \frac{3\pi}{4} k^{1+2v} \sum_{j=0}^{\infty} \frac{(2j-1)!!(2j+2v-1)!!}{2^{2j+v}j!(j+v+2)!} (k^{2})^{j}.$$



credit: Rodrigo Luger

D42)



