In Defense of Extreme Openness

Jake VanderPlas

Python In Astronomy 2016

I think we all see the benefit of *coding* in the open . . .

Eases Collaboration — Eases Sharing
Heightens Visibility — Encourages Reproducibility
Encourages Extensibility — Encourages Integrity
etc. — etc.

. . . why not do *all research* in the open?

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etc. — etc.

A case study from yours truly . . .

We wrote this paper on GitHub *from day 1*

The Astrophysical Journal, 812:18 (15pp), 2015 October 10 doi:10.1088/0004-637X/812/1/18

PERIODOGRAMS FOR MULTIBAND ASTRONOMICAL TIME SERIES

Jacob T. VanderPlas[1] and Željko Ivezić[2]
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ABSTRACT

This paper introduces the *multiband periodogram*, a general extension of the well-known Lomb–Scargle approach for detecting periodic signals in time-domain data. In addition to advantages of the Lomb–Scargle method such as treatment of non-uniform sampling and heteroscedastic errors, the multiband periodogram significantly improves period finding for randomly sampled multiband light curves (e.g., Pan-STARRS, DES, and LSST). The light curves in each band are modeled as arbitrary truncated Fourier series, with the period and phase shared across all bands. The key aspect is the use of Tikhonov regularization which drives most of the variability into the so-called base model common to all bands, while fits for individual bands describe residuals relative to the base model and typically require lower-order Fourier series. This decrease in the effective model complexity is the main reason for improved performance. After a pedagogical development of the formalism of least-squares spectral analysis, which motivates the essential features of the multiband model, we use simulated light curves and randomly subsampled SDSS Stripe 82 data to demonstrate the superiority of this method compared to other methods from the literature and find that this method will be able to efficiently determine the correct period in the majority of LSST's bright RR Lyrae stars with as little as six months of LSST data, a vast improvement over the years of data reported to be required by previous studies. A Python implementation of this method, along with code to fully reproduce the results reported here, is available on GitHub.

Key words: methods: data analysis – methods: statistical – surveys

https://github.com/jakevdp/multiband_LS/

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Mutiband Lomb-Scargle Periodograms

This repository contains the source for our multiband periodogram paper. It makes use of the gatspy package, which has been developed concurrently. The paper has been submitted to the Astrophysical Journal, and a preprint is available on arXiv. To see a current build of the paper from the master branch of this repository, refer to http://jakevdp.github.io/multiband_LS (powered by gh-publisher).

Feel free to submit comments or feedback via the Issues tab on this repository.

Reproducing the Paper

The LaTeX source of the paper, including all figure pdfs, is in the `writeup` directory. The code to reproduce the analysis and figures in the paper is in the `figures` directory.

To reproduce the figures, first install the following packages (Python 2 or 3):

- Standard Python scientific stack: (IPython, numpy, scipy, matplotlib, scikit-learn, pandas)
- seaborn for plot styles.
- astroML for general astronomy machine learning tools.
- gatspy for astronomical time-series analysis.
- supersmoother for the supersmoother algorithm used by `gatspy`.

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Subject headings: methods: data analysis — methods: statistical

1. INTRODUCTION

Many types of variable stars show periodic flux variability (Eyer & Mowlavi 2008). Periodic variable stars are important both for testing models of stellar evolution and for using such stars as distance indicators (e.g., Cepheids and RR Lyrae stars). One of the first and main goals of the analysis is to detect variability and to estimate the period and its uncertainty. A number of parametric and non-parametric methods have been proposed to estimate the period of an astronomical time series (e.g., Graham et al. 2013, and references therein).

The most popular non-parametric method is the phase dispersion minimization (PDM) introduced by Stellingwerf (1978). Dispersion per bin is computed for binned phased light curves evaluated for a grid of trial periods. The best period minimizes the dispersion per bin. A similar and related non-parametric method that has been recently gaining popularity is the Supersmoother routine (Reimann 1994). It uses a running mean or running linear regression on the data to fit the observations as a function of phase to a range of periods. The best period minimizes a figure-of-merit, adopted as weighted sum of absolute residuals around the running mean. Neither the Supersmoother algorithm nor the PDM method require *a priori* knowledge of the light curve shape.

The most popular parametric method is the Lomb-Scargle periodogram, which is discussed in detail in Section 2. The Lomb-Scargle periodogram is related to the ing model of the LombScargle periodogram is nonlinear in frequency and so the likelihood surface in frequency is non-convex. This non-convexity is readily apparent in the many local maxima of the typical periodogram, which makes it difficult to find the maximum via standard numerical optimization routines. Thus in practice the global maximum of the periodogram is often found by a brute-force grid search (for details see, e.g. Ivezić et al. 2014).

A more general parametric method based on the use of continuous-time autoregressive moving average (CARMA) model was recently introduced by Kelly et al. (2014). CARMA models can also treat non-uniformly sampled time series with heteroscedastic measurement uncertainties, and can handle complex variability patterns.

A weakness of all these standard methods is that they require homogeneous measurements – for astronomy data, this means that successive measurements must be taken through a single photometric bandpass (filter). This has not been a major problem for past surveys because measurements are generally taken through a single photometric filter (e.g. LINEAR, Sesar et al. 2011), or nearly-simultaneously in all bands at each observation (e.g. SDSS, Sesar et al. 2010). For the case of simultaneously taken multiband measurements, Süveges et al. (2012) utilized the principal component method to optimally extract the best period. Their method is essen-

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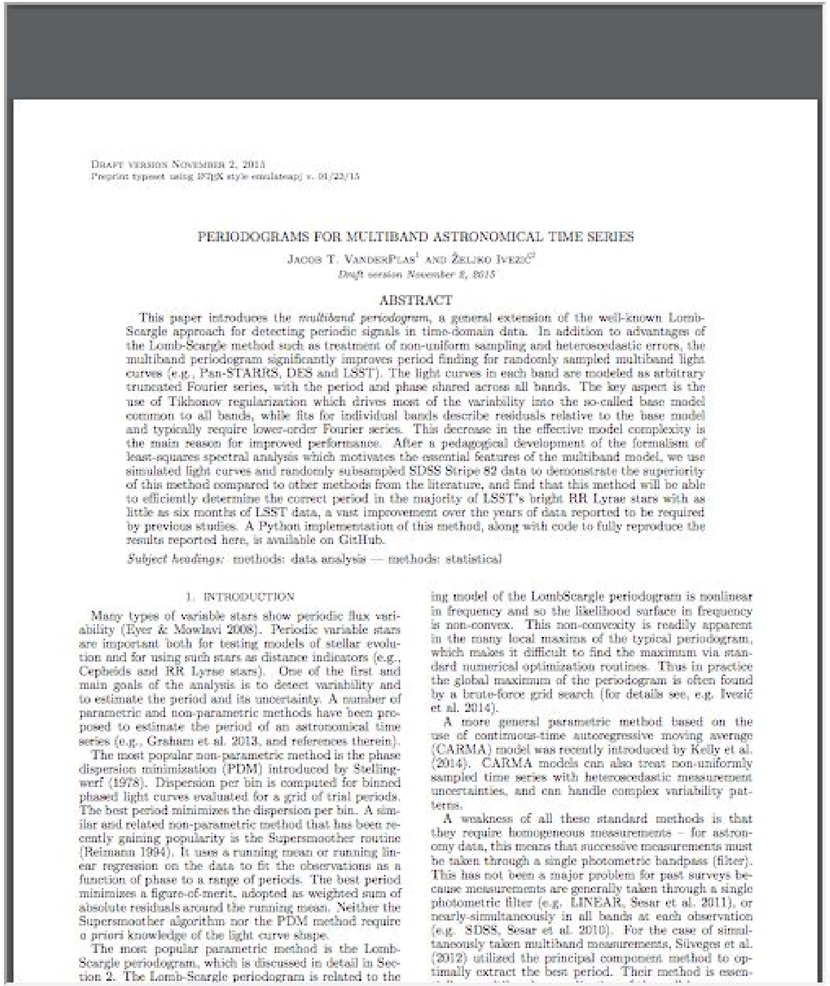

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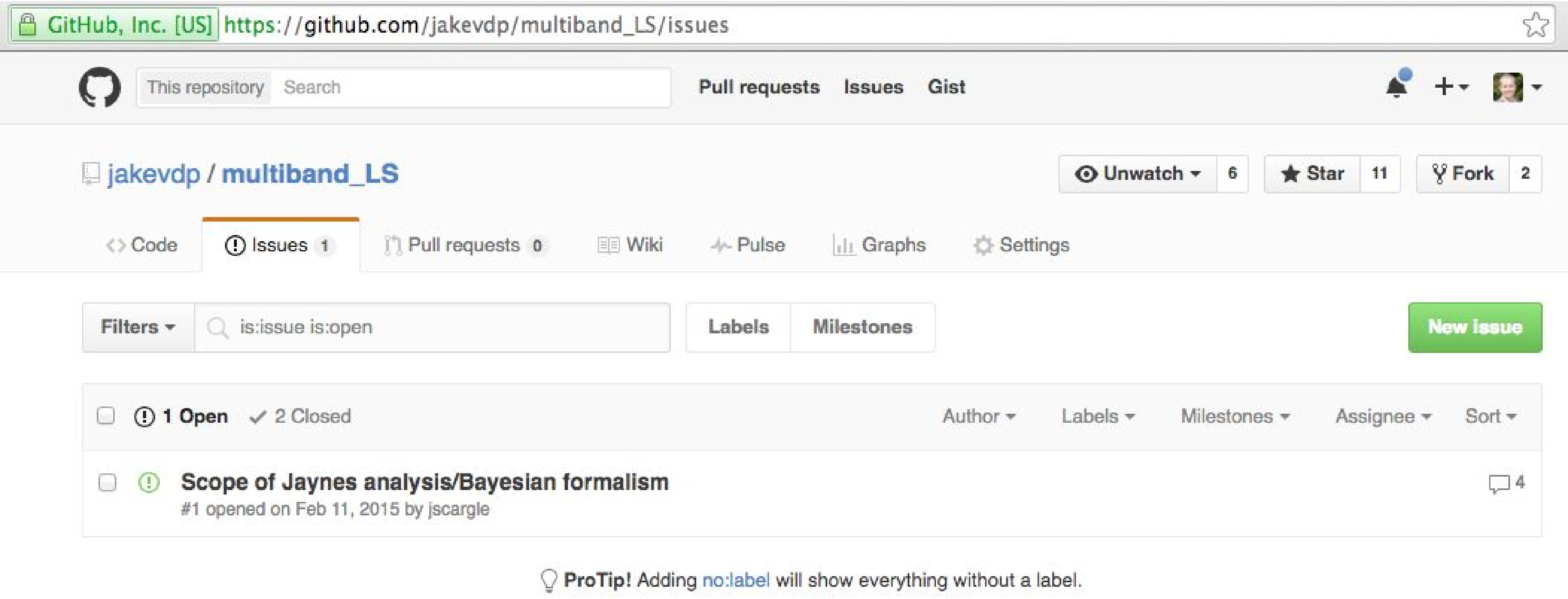
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Scope of Jaynes analysis/Bayesian formalism
#1 opened on Feb 11, 2015 by jscargle
4
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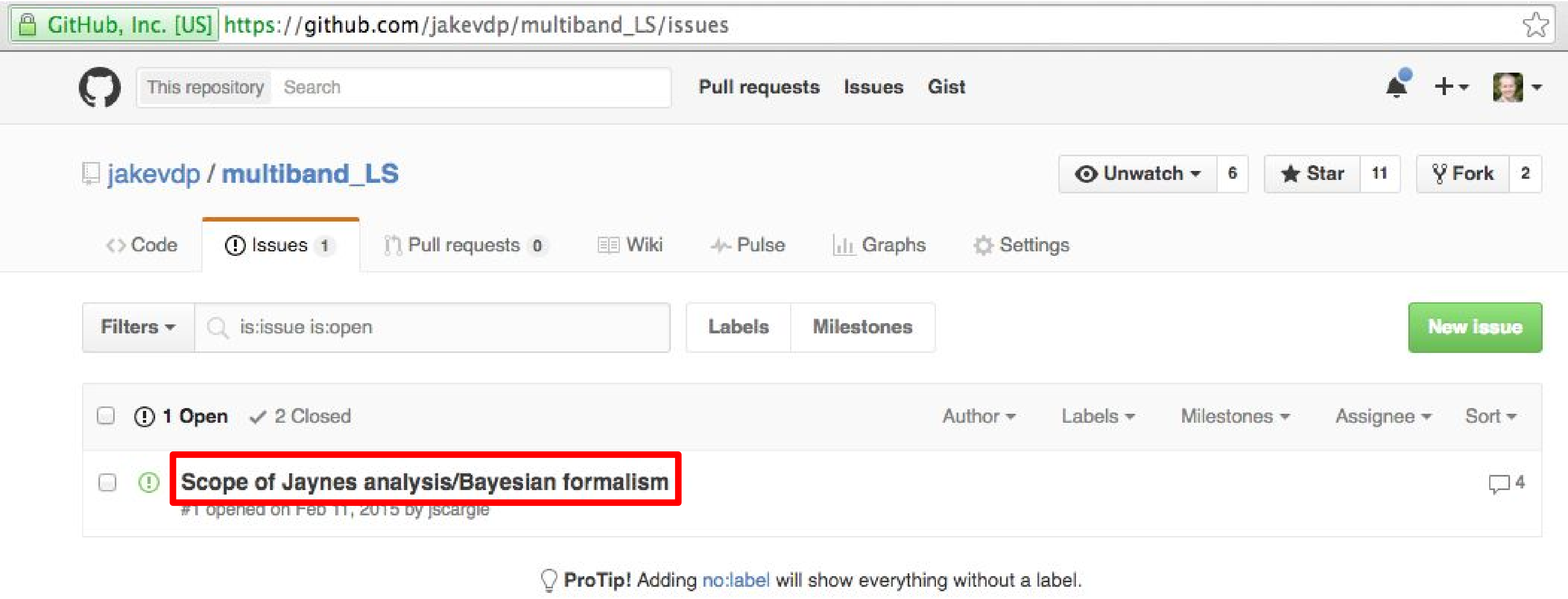
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Scope of Jaynes analysis/Bayesian formalism #1

Open **jscargle** opened this issue on Feb 11, 2015 · 4 comments

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Your reference to Jaynes (1987) implies that he discussed the Lomb-Scargle periodogram. I don't think he knew about this particular algorithm, but was remarking more generally on least-squares fits to sinusoids.

Also, I wonder if you considered and rejected a fully Bayesian formalism for the problem you address in this paper? In http://arxiv.org/abs/math/0111127 I tried to demonstrate a generic link between frequentist statistics such as the periodogram and the Bayesian posterior for a corresponding quantity (in the spirit of Larry Bretthorst's power spectrum analysis: Bretthorst, G. Larry, 1988, Bayesian Spectrum Analysis and Parameter Estimation, Lecture Notes in Statistics, Springer-Verlag, No. 48; http://bayes.wustl.edu/). I don't know how universal it is, but a connection of the form

```
P( a ) ~ exp[ - C(a) / error variance ]
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seems to pop up a lot. C(a) can be an auto- or cross-correlation function; or a power spectrum or a cross-power spectrum, corresponding to a being a time lag or the frequency of a sinusoidal component. Then the expedient of simply multiplying posteriors (for independent quantities) might be useful in the multi band context. If nothing else this might lead to a more rigorous "Occam factor" regularization.

jakevdp commented on Feb 12, 2015 Owner

Thanks @jscargle -- yes, the sentence about the Jaynes paper is a bit misleading. We'll correct that

Scope of Jaynes analysis/Bayesian formalism #1

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Jeff Scargle!!!
— as in "Lomb-*Scargle* Periodogram"!!!!!!!

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Thanks **@jscargle** – yes, the sentence about the Jaynes paper is a bit misleading. We'll correct that.

I'd thought briefly about the Bayesian point-of-view for the multiband method, but I avoided discussing it for a couple reasons:

1. As your paper makes clear, the Bayesian and frequentist results for periodograms are usually related by a simple monotonic function, so going from one to the other is easy.
2. I think a fully-Bayesian treatment of the periodogram would involve marginalization over nuisance parameters in the model, and in some cases you want the nuisance parameter to be the period! Unfortunately, since the posterior is so highly multi-modal with varying period, I don't know of any Bayesian approach which can properly handle the problem in higher than a couple dimensions (perhaps nested sampling, but that's still a long-shot). I thought that rather than doing a half-Bayesian job which amounts to not much more than proposing some improper priors that lead to the exponent of the frequentist result, I'd stick to classical statistics here.

That said, a Bayesian approach to the multiband sinusoid-fitting problem would likely end up with a couple features:

- Priors would probably take the form of some constraint on the deviation of amplitudes and/or phases within each band. Mathematically, the result would be equivalent to a nonlinear regularization of the more satisfying than the statistically motivated (but admittedly still ad hoc) regularization we use.

For a truly Bayesian approach to period finding, I think a CARMA or similar model is a much better avenue (see e.g. Kelly et al 2014)

jscargle commented on Feb 16, 2015

Good comments.

In the restricted context of a single sinusoid don't you think Larry Bretthorst's treatment is pretty compelling? Sure, you have to choose what parameters you take as "nuisance" and there are many possibilities, but Larry treats the most useful case(s) IMHO.

Yes, in this context Bayes and frequentist are related one-to-one in a monotonic fashion. But, if only cosmetically, the exponentiation can emphasize the "correct" mode at the expense of other (smaller) local maxima. More important if you have a good handle on the observational errors the Bayesian expression gives the full posterior probability (as opposed to a single global maximum).

You make excellent points regarding uncertainty in priors making the marginalized distribution ad hoc in much the same way as regularizations. (This is especially clear for regularization via the approximate BIC -- Bayesian Information Criterion. I wonder what the count of regularization schemes is? AIC, BIC, MDL, ...) Alas, well-justified priors are rare; but when then are available the so-called Occam factor in the marginal posterior avoids ad hocery.

jscargle commented on Feb 16, 2015

...on a different topic. In the discussion of Fig. 3 you state:

jscargle commented on Feb 16, 2015

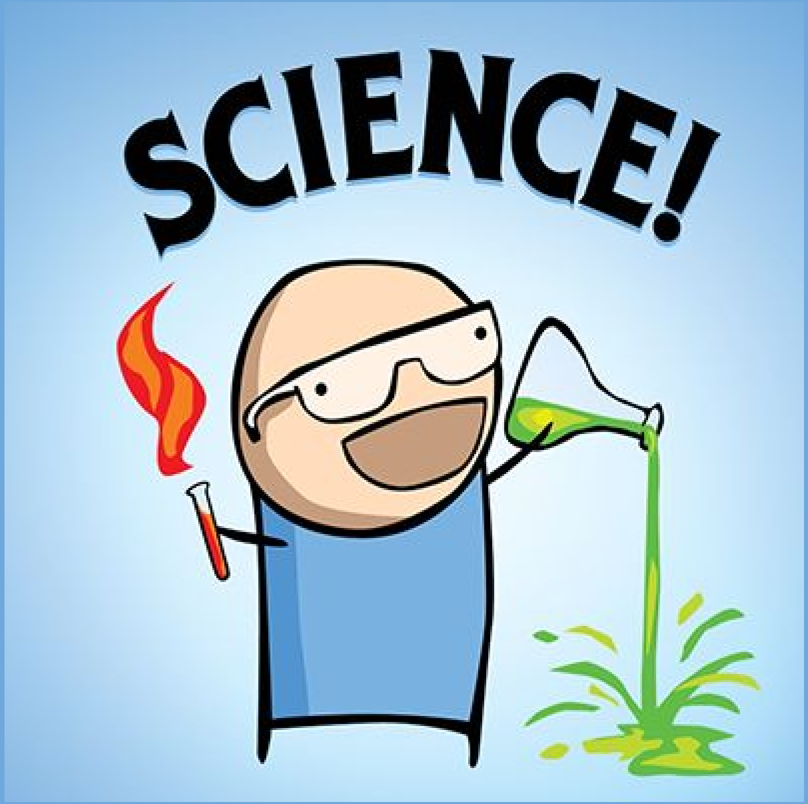
… on a different topic. In the discussion of Fig. 3 you state:
"Second, notice that as the number of terms is increased, the general \background" level
of the periodogram increases. This is due to the fact that the periodogram power is inversely
related to the �chi-squared at each frequency. A more flexible higher-order model can better
fit the data at all periods, not just the true period. Thus in general the observed power
of a higher-order Fourier model will be everywhere higher than the power of a lower-order
Fourier model."
This seems counterintuitive to me. Adding harmonic components to the model in the manner of eq. (14) makes the frequency, omega, represent both omega itself and its harmonics n omega, n > 1. You can see this in the right-hand panels of Fig.3: as n goes from 1 to 2 to 3, the peak power at the true fundamental Po increases -- power from the harmonics is incorporated via eq. (14) into the fundamental. How can one interpret the rise (from total insignificance) of the power at the first harmonic, 2 Po? And why doesn't a better-fitting higher order model move power from the background continuum into the harmonics? -- the reverse of what you state. I am sure you are correct, but I guess I don't understand your "inversely related to … " argument.

jakevdp commented on Feb 16, 2015 Owner

Jeff – thanks for all the comments! I really appreciate your close read of the paper and taking the time to discuss.

A couple responses:

I think you're right that Bretthorst's treatment is compelling in terms of fitting a single sinusoid to data. But the problem is that *P(omega|data, M)* with *M=(a single sinusoid fits our data)* is not exactly what we're


SCIENCE!

“But I might get scooped!”

Merriam-Webster SINCE 1828 MENU

Dictionary publish

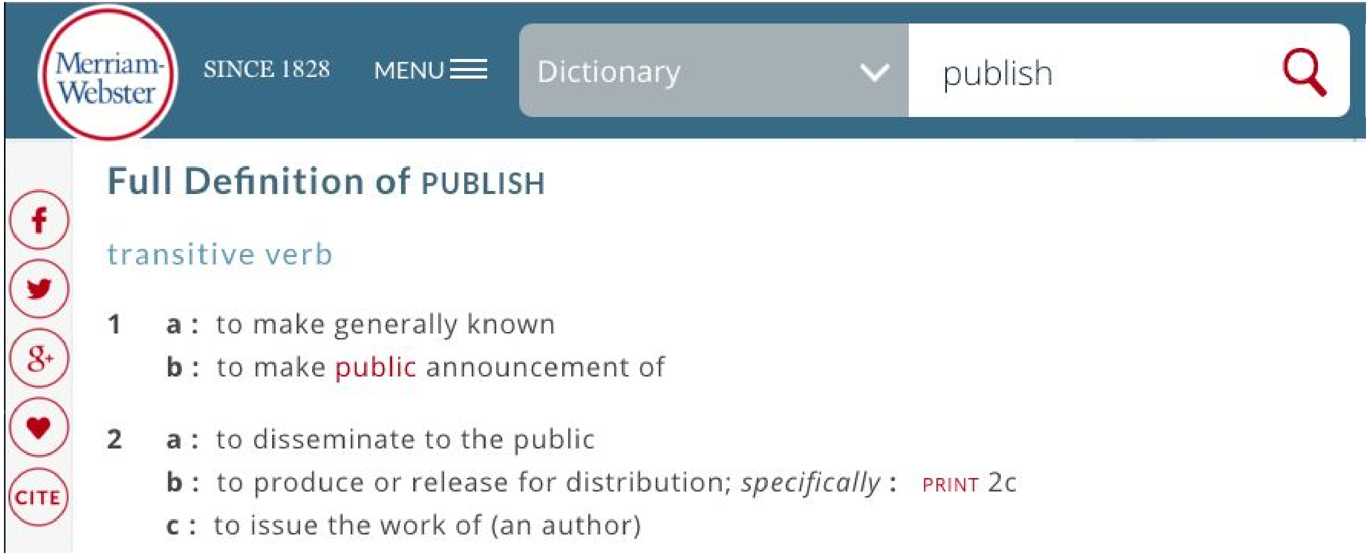
Full Definition of PUBLISH

transitive verb

1 a : to make generally known
  b : to make public announcement of

2 a : to disseminate to the public
  b : to produce or release for distribution; *specifically* : PRINT 2c
  c : to issue the work of (an author)

. . . putting work on Github *is* publication!



. . . putting work on Github
is publication!
~~"Scooping"~~ → "Plagiarism"

“But Jake. . . would you do this if there were any *real* competition?”

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So. . .
how did it turn out?

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(* not that I’m keeping track . . .)

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