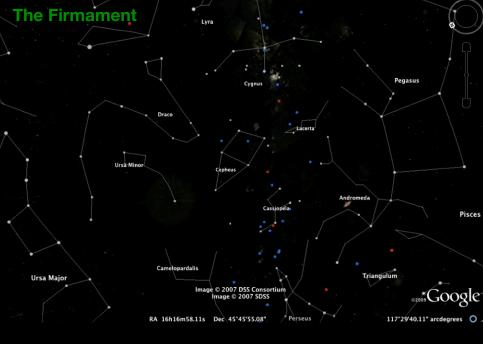
### Welcome!

# 17th HEAD Meeting Special Session

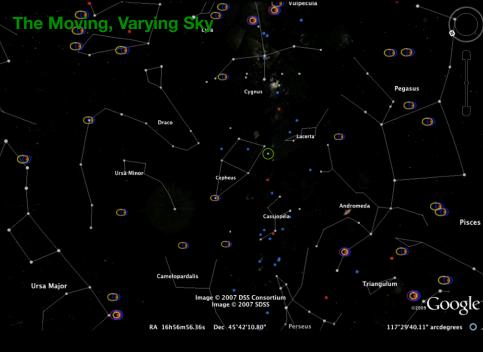
**Exploring time series data** in high energy astrophysics

Session material public GitHub repo:

https://github.com/tloredo/HEAD2019-TSE

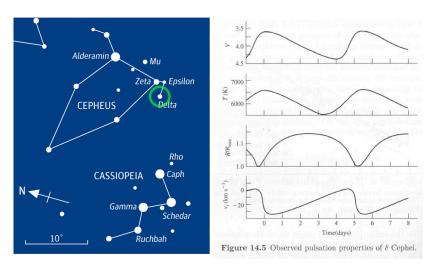


Vuipecuia



Vuipecuia

# Delta Cephei — Variability!



Discovered in 1700s; 5.4 d period, 0.9 mag ampl (Mira & Algol periodic variables discovered in 1600s; "Mira" = "wonderful," "astonishing")

# Leavitt law for Cepheids An early time-domain astronomy triumph



A straight line can readily be drawn among each of the two series of points corresponding to maxima and minima, thus showing that there is a simple relation between the brightness of the variables and their periods.

— Henrietta Swan Leavitt —

AZ QUOTES

# Varied variability in high energy astro

- Periodic (e.g., pulsars)
- Stochastic: (AGN, XRBs; QPOs), transient (XRBs, GRBs, SGRs)
- Spectro-temporal add energy dimension

Talks in this session cover each type

# **Context: Time series software for astronomy**

Packages with generality/breadth/depth (recent/maintained):

- VARTOOLS: Command-line light curve analysis (C)
- SITAR: S-lang/ISIS Timing Analysis Routines
- CULSP: Lomb-Scargle periodograms on GPUs
- LightcurveMC: LC simulation, testing tools in C++, R
- BGLS: Bayesian generalized Lomb-Scargle periodogram
- FATS: Feature analysis for time series
- gatspy: General tools for astro time series (AstroML)
- Spectra: Power spectra for unequally-spaced data
- agatha: Period finding in correlated noise (R)
- Gaussian process packages: George, celerite
- Mission/project-specific tools: Fermi tools, Kepler/TESS lightkurve, Starlink
- Julia: JuliaAstro/LombScargle, cerite, CARMA.jl...
- carma\_pack: Bayesian CARMA modeling via MCMC (C++, Python)
- Stingray: Next-generation spectral-timing software (Python)
- TSE Project: Python and MATLAB packages, e.g., inference, stanfitter, batse5bp...

Documentation, VCS, appealing API are essential for buy-in

# R packages (by statisticians)

# "Best of" list c/o Eric Feigelson

### Base-R functions

- acf-pacf-ccf: correlation functions with significance levels
- arima-prewhiten: autoregressive modeling
- Box.test: test for autocorrelation
- density-spline-loess: kernel & local polynomial interpolations
- fft & convolve : Fast Fourier Transform, convolutions
- fitdistr: maximum likelihood fitting of statistical distributions
- plot: display time series
- runmed-smooth-supsmu: running median-like smoothers
- spec.pgram: Fourier periodogram with tapering & smoothing

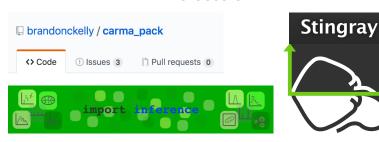
### CRAN packages

- bspec: Bayesian autocorrelation & spectral analysis
- cobs: cobs quantile spline interpolation
- changepoint-Rseg-segmented-strucchange: changepoint detection & segmented regression
- dlm: Bayesian dynamic modeling
- dtw-dtwclust: dynamic time warping & clustering
- dyn-dyn.lm: regression for irregular time series
- forecast: auto.arima-arfima ARIMA modeling with model selection & 1/f-noise
- imputeTS: na.Kalman ARIMA interpolation
- its, xts & zoo: infrastructure for irregular time series
- locfit: locfit local interpolation with bootstrap, weighting & censoring

### CRAN packages

- lomb: Isp Lomb-Scargle periodogram
- meboot: bootstrap for nonstationary time series
- MSBVar: dynamic multivariate autoregressive modeling
- msl.trend: linear, spline, SSA interpolation of gaps for irregular time series
- mvtsplot: visualization of multivariate time series
- nortest: ad.test test for normality
- robfilter: robust treatments of outliers
- RobPer: RobPer robust periodograms: PDM, LSP, etc
- sde: stochastic differential equations
- tseries-TSA: extensive time series analysis & testing
- TSDist-TSClust: distance and clustering ensembles of times series
- wavelets-wavethresh-wmtsa-adlift: wavelet transform, denoising & analysis
- WeightPortTest: tests for autocorrelation with heteroscedastic weights

### This session



- Periodic, power spectra: TSE, inference (Tom & Jeff)
- Stochastic: carma\_pack (Malgosia)
- Spectro-temporal (spectral timing): Stingray (Abbie)

Underlying theme:
Interplay of time-domain and frequency-domain perpectives

# Time series exploration in Python and MATLAB: Bayesian blocks, periodograms, and all that

Tom Loredo\* & Jeff Scargle<sup>†</sup>
\*Cornell Center for Astrophysics and Planetary Science

†NASA Ames Research Center

Funded by NASA ADAP; includes some NSF AAG-funded contributions

17th HEAD Meeting — 18 March 2019

### **TSE:** Time Series Explorer project

- MATLAB (Jeff Scargle, NASA Ames)
  - Exploratory data analysis (graphical)
  - ► Irregularly-spaced data: Global and local power spectra via discrete correlation function (DCF)
  - ▶ Event data: New developments with Bayesian Blocks
- Python (Tom Loredo, CCAPS @ Cornell U.)
  - ▶ Parametric & semiparametric time-domain modeling
  - ► Spectro-temporal pulse decomposition using Lévy processes
  - Python translation of MATLAB algorithms

Documentation: Handbook of Practical Time Series Analysis

Mostly pre-release "alpha" status...

### **Bayesian blocks developments**

### Bayesian blocks

- = locally adaptive histograming of point/event data
- = change point modeling
- Algorithm: Faster O(N) algorithm, usable up to  $N\sim 10^8$
- Diverse regularizers to control binning criteria
- Generalized block shapes (flat, linear...)
- 3-D time-energy-space decomposition

### Online demos (R Shiny translation of MATLAB):

- BB BATSE GRB pulse decomposition
- BB with piecewise-linear blocks

# Probabilistic perspectives on periodograms



"More lives have been lost looking at the raw periodogram than by any other action involving time series!"

— John Tukey

"More lives have been lost looking at the *raw* periodogram than by any other action involving time series!"

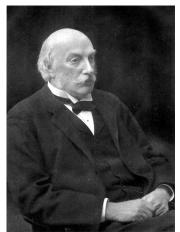
— John Tukey

It's how you *manipulate the periodogram* that makes it useful—for *multiple purposes* 

Literature (vast!) relevant to understanding periodograms:

- Spectral analysis of time series
- Applied harmonic analysis
- Harmonic regression
- Trigonometric regression

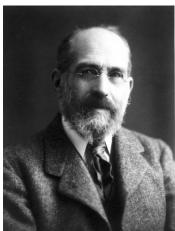
#### Lord Rayleigh (John William Strutt) 1842–1919



Wikipedia

Cavendish Lab, University of Cambridge (succeeded Maxwell); Royal Inst. of Great Britain

# Arthur Schuster 1851–1934



Wikipedia

Cavendish Lab (w. Maxwell, Rayleigh); Owens College, Victoria University; succeeded by Rutherford

# Schuster (& Rayleigh) inventing periodograms

### Motivation

- Find "hidden periodicities" (vs. "obvious periodicities" like tides, sunspot maxima)
- Quantify uncertainty: "[A]pply the theory of probability in such a way that we may be able to assign a definite number for the probability that the effects found by means of the usual methods are real, and not due to accident." [sic! A p-value is NOT a FAP!]

### Name & interpretation

- "Fourier's analysis here serves the same purpose as the prismatic analysis of a luminous disturbance..."
- "It is convenient to have a word for some representation of a variable quantity which shall correspond to the 'spectrum' of a luminous radiation. I propose the word periodogram..."
- Envisioned application to periodic ("lines" from musical instruments), quasiperiodic ("bands" from sunspots) and stochastic ("broad band" from noise) variability



### Two types of periodograms

- "Occurence periodogram" for event times (Rayleigh statistic): Add wrapped/folded unit vectors
- "Magnitude periodogram" for equally-spaced scalar measurements (Schuster periodogram): Add wrapped/folded vectors

### Null distributions (no periodic signal)

- Resultant vector magnitude, R: Rayleigh distribution,  $p(R) \propto Re^{-R^2/\sigma^2}$
- Squared magnitude (power): Exponential distribution,  $p(S) \propto e^{-S/\sigma^2}$

(Use  $\sigma^2 \to N$  for occurence periodograms; beware normalizations!)

# Three uses for periodograms

- Nonparametric spectrum estimation
- Parametric period detection & estimation (least squares, Bayes)
- Semiparametric stochastic process (Gaussian process) modeling

# Periodogram as a spectrum estimator

Underlying idea:

- A periodic signal may be recognized by looking for a  $\delta$ -function in the *signal's* power spectrum
- $\Rightarrow$  Devise an *estimator* for the signal's power spectrum and look for  $\delta$ -function-like peaks in an estimate

Periodogram is the power spectrum of the *data*,  $d_i = f(t_i) + \epsilon_i$ :

$$P(\omega) = \frac{2}{N} \left[ \left( \sum_{i} d_{i} \cos \omega t_{i} \right)^{2} + \left( \sum_{i} d_{i} \sin \omega t_{i} \right)^{2} \right]$$

(Note: Normalization conventions differ!)

- Evenly sampled data: Schuster periodogram
- Unevenly sampled data: Lomb-Scargle periodogram (LSP) (with an optimal choice of phase)

### Bias and variability

Interpret data power spectrum as signal power spectrum corrupted by noise and sampling "window"

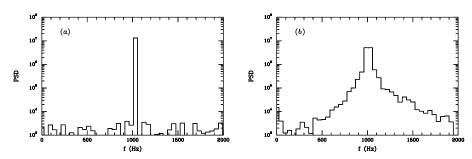
Under no-signal "null" hypotheses, N/2 values at the Fourier frequencies (as returned by the DFT) are statistically independent

(This follows from orthogonality of sines/cosines on a uniform grid; LSP case is more complicated)

- ⇒ focus on Fourier frequencies
  - Variability: The number of spectrum estimates (at Fourier frequencies) grows with N → periodogram value is an inconsistent estimate of the signal power spectrum
  - Bias: The window function (finite duration, discrete sampling) biases the expectation value of the periodogram away from the true signal power

### Spectral Leakage

1024 samples at 48 kHz sampling rate S/N = 5, white noise f = 1031.25 Hz (Fourier frequency) and f = 1008 Hz

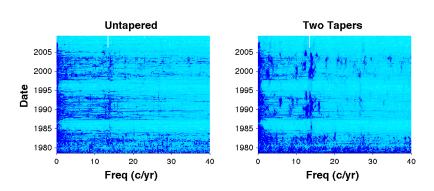


Bias reduction techniques: Periodogram smoothing, data tapering

These are esp. useful for *estimating a continuous spectrum* (vs. period hunting)

### Time-frequency power spectrum via multitapering

MATLAB implementation, applied to 33 y of solar Ca II K line data from Sacramento Peak National Solar Observatory (Keil Worden 1984):



# Periodogram as a period finder

Adopt a sinusoid periodic signal model (a  $\delta$ -function spectrum!):

$$f(t) = A\cos(\omega t - \phi)$$
 parameters  $\omega, A, \phi$   
=  $A_1\cos\omega t + A_2\sin\omega t$  parameters  $\omega, A_1, A_2$ 

$$d_i = f(t_i) + e_i$$
 Gaussian error pdfs; rms=  $\sigma$ 

Estimate  $\omega$  via profile likelihood, or Bayes (*Jaynes-Bretthorst alg.*):

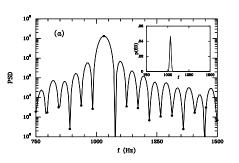
$$p(\omega|D) \propto \int dA_1 \int dA_2 \ p(\omega, A_1, A_2) \mathcal{L}(\omega, A_1, A_2)$$
  
 $\propto p(\omega) J(\omega) \exp \left[\frac{S(\omega)}{\sigma^2}\right]$ 

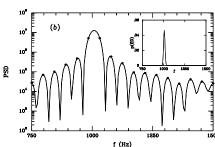
- Equally-spaced samples:  $S(\omega) \to P(\omega)$  for large N (when  $\eta$  is nearly diagonal)
- Unequally-spaced samples:  $S(\omega) \approx \text{Lomb-Scargle}$  periodogram

The posterior dist'n for  $\omega$  is related to a *continuous* version of the periodogram/power spectrum

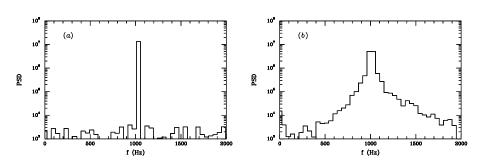
1024 samples at 48 kHz sampling rate S/N = 5

 $f=1031.25~{
m Hz}$  (Fourier frequency) and  $f=1008~{
m Hz}$ 





Same function, evaluated only at Fourier frequencies (whence "leakage" when true frequency  $\neq$  Fourier frequency):



### Contrast with spectrum estimation

- Periodogram here is not a power spectrum estimator, but the logarithm of the marginal pdf for  $\omega$
- No special role for Fourier frequencies
- No "leakage;" log pdf has similar structure for all signal frequencies, but sidelobes get exponentiatally attenuated (no need for smoothing) — sidelobes quantify period uncertainty
- Bayes: Detect signal using signal marginal likelihood:

$$\mathcal{L}(\textit{signal}) ~\approx~ \exp\left[\frac{P_{\mathsf{max}}}{\sigma^2}\right] imes \frac{\mathsf{peak} \; \mathsf{width}}{\mathsf{prior} \; \mathsf{search} \; \mathsf{range}}$$

Handles multiple testing issues via marginalization

Conventional periodograms optimal only for single sinusoids

#### Two Sinusoids

Adopt a model with two sinusoids at distinct frequencies:

$$f(t) = A\cos(\omega_1 t - \phi_1) + B\cos(\omega_2 t - \phi_2)$$
  
=  $A_1\cos\omega_1 t + A_2\sin\omega_1 t$   
 $+A_3\cos\omega_2 t + A_4\sin\omega_2 t$ 

Use JB algorithm to find  $p(\omega_1, \omega_2|D)$  or  $p(\omega_1, \delta\omega|D)$ 

Call log p the doublet periodogram

If the frequencies are well-separated, can show that

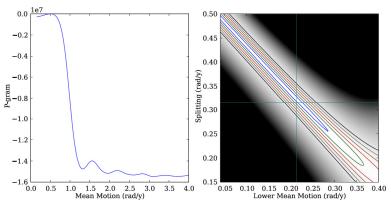
$$p(\omega_1, \omega_2 | D) \propto p(\omega_1, \omega_2) J(\omega_1, \omega_2) \exp\left[\frac{P(\omega_1)}{\sigma^2}\right] \exp\left[\frac{P(\omega_2)}{\sigma^2}\right]$$

a product of two *independent* dist'ns, each determined by the periodogram

If the frequencies are close, there is no such simplification; the real and imaginary parts of the DFT at each frequency (projections!) combine in a more complicated way

### Two-planet example

Singlet periodogram (i.e., single-sinusoid, left) and *doublet periodogram* (right) for simulated *SIM* astrometry data from a Jupiter (11.9 y) + Saturn (29.5 y) system at 10 pc with  $\approx$  45° inclination. The data span 10 y, with 0.86  $\mu$ as errors. The true mean motions (shown by crosshair) are 0.53 and 0.21 rad/y.



# Periodogram as a Gaussian process log likelihood

Model stochastic variability via a stationary Gaussian process with parametric covariance function  $C(u; \theta)$  for lag u and params  $\theta$ :

$$C(u; \theta) = E[f(t)f(t-u)]$$
 (zero-mean case)

This process has power spectrum

$$P(\omega; \theta) = \mathcal{F}\{C(u; \theta)\}$$

Then (under some conditions on C), for equally spaced samples and large N, the likelihood function for  $\theta$  may be approximately calculated using the periodogram (*Whittle likelihood*,  $O(N \log N)$  i/o  $O(N^2)$ ; see Simon Vaughan's work):

$$\mathcal{L}(\theta) \propto \prod_{i=1}^{N/2} \frac{1}{P(\omega_j; \theta)} \exp \left[ -\frac{S(\omega_j)}{P(\omega_j; \theta)} \right]$$

where  $\{\omega_i\}$  are the Fourier frequencies (can be signif. biased)

Intuition: Recall that under the white-noise null, periodogram ordinates at Fourier frequencies follow independent  $\chi^2_2$  (i.e., exponential) distributions

# Using periodograms w/o losing your life

Tailor manipulations to goals:

- Nonparametrically estimate a spectrum (data spectrum ≠ signal spectrum):
  - ▶ Raw power null distribution  $\propto e^{-S(\omega_i)/\sigma^2}$
  - ▶ Raw periodogram is inconsistent and biased (window, leakage)
    → smooth/taper it
  - ➤ TSE provides multitaper methods, including time-frequency and for irregular sampling (currently MATLAB only)
- Detect a periodic signal (spectrum assumed to have  $\delta$ -function):
  - ▶ Single sinusoid:  $\mathcal{L}_m(\omega) \propto e^{S(\omega)/\sigma^2}$
  - ► Multiple sinusoids (harmonics?) → multiplet periodograms
  - ► TSE provides tools for building generalized periodograms via Jaynes-Bretthorst algorithm
- Whittle likelihood for semiparametric stationary GPs