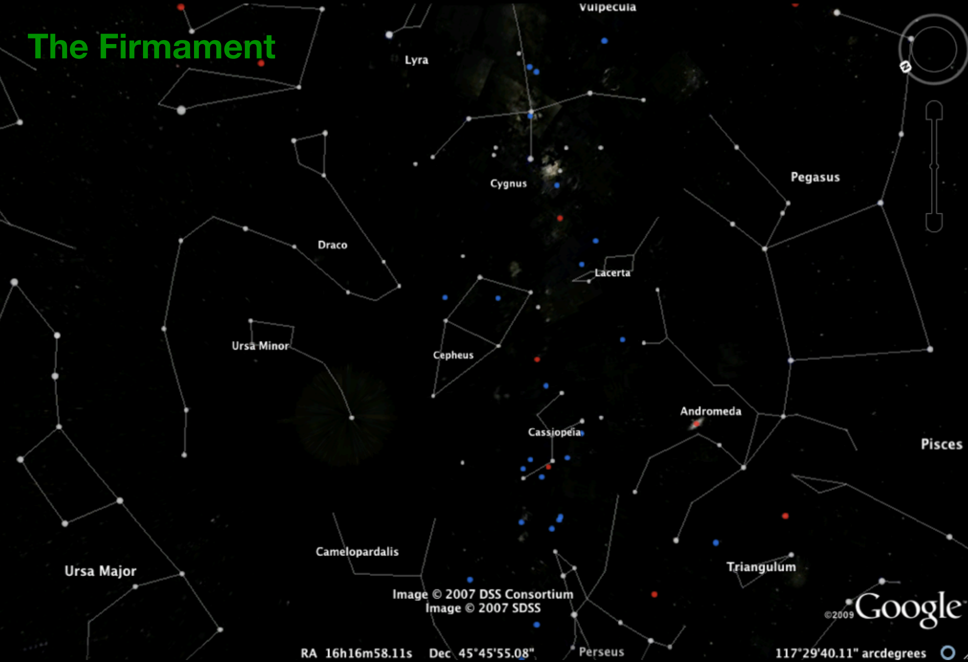
Welcome!

17th HEAD Meeting Special Session

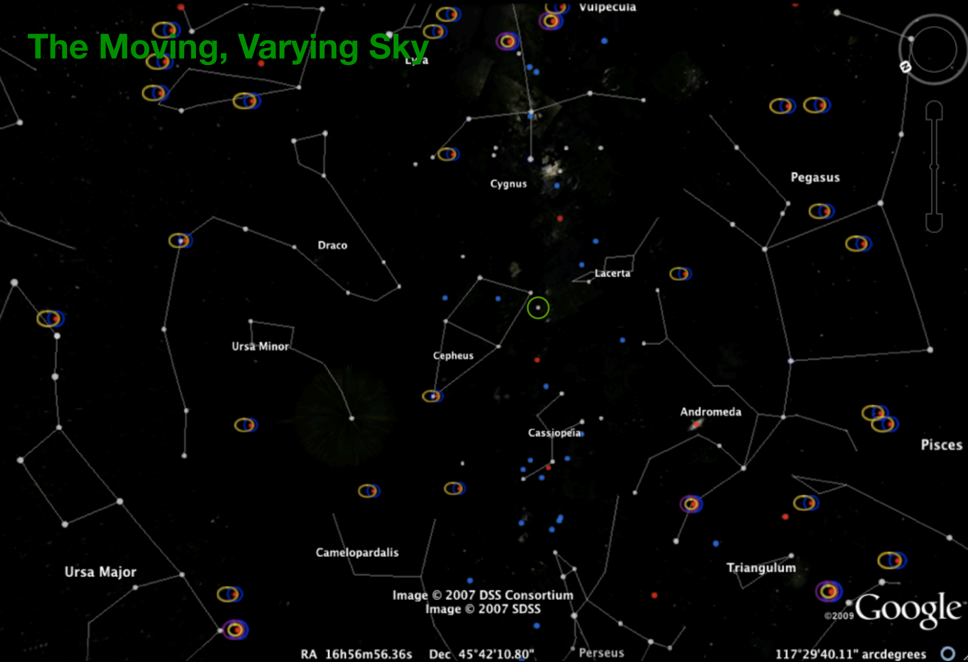
Exploring time series data in high energy astrophysics

Session material public GitHub repo:
`https://github.com/tloredo/HEAD2019-TSE`

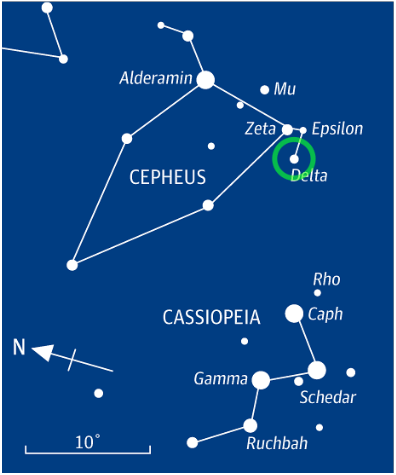
The Firmament



The Moving, Varying Sky



Delta Cephei — Variability!



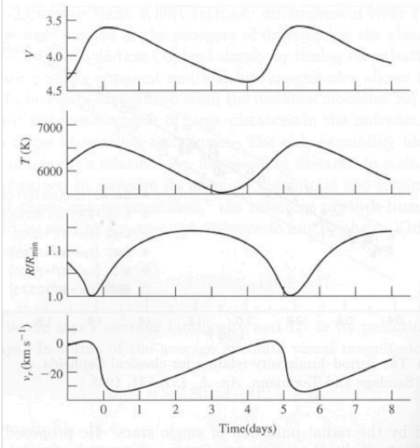
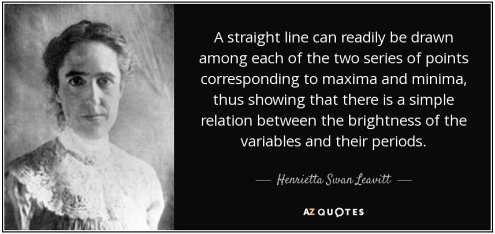


Figure 14.5 Observed pulsation properties of δ Cephei.

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



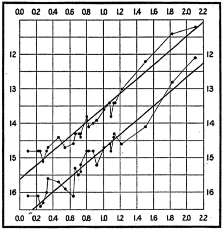


Fig. 2.

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

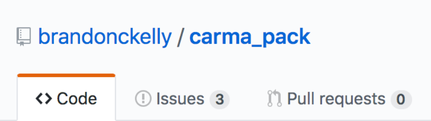
CRAN packages

- 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: lsp 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

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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

Wikipedia

"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!"

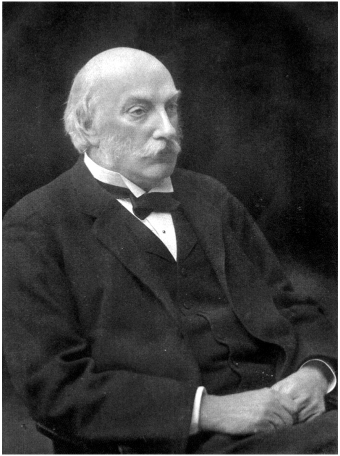
— *John Tukey*

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

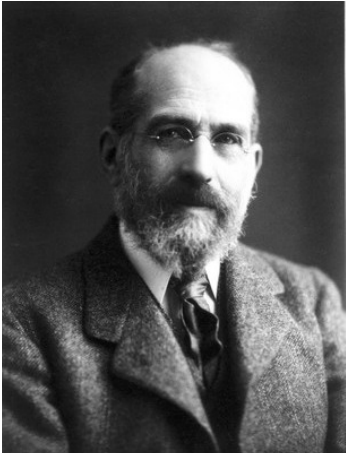
Lord Rayleigh
(John William Strutt)
1842–1919



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

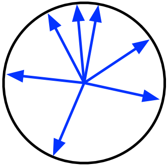
Schuster (& Rayleigh) inventing periodograms

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 δ-function in the *signal's* power spectrum
- $\Rightarrow$ Devise an *estimator* for the signal's power spectrum and look for δ-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)

$\Rightarrow$ *focus on Fourier frequencies*

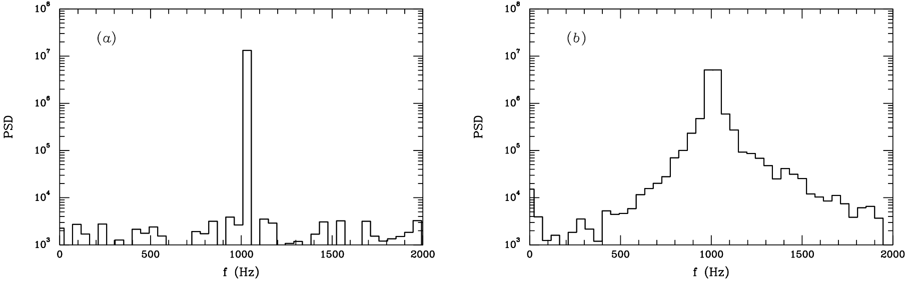
- Variability: The number of spectrum estimates (at Fourier frequencies) grows with $N \to$ periodogram value is an *inconsistent* estimate of the signal power spectrum
- Bias: The window function (finite duration, discrete sampling) biases the expectation value of the periodogram away from the true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

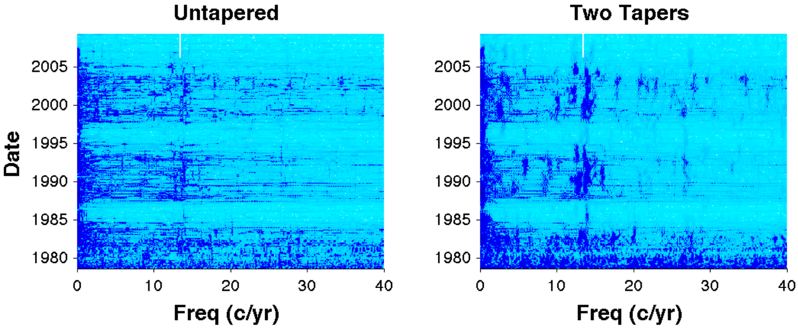


Bias reduction techniques: Periodogram smoothing, data tapering

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 δ-function spectrum!):

$$\begin{aligned} f(t) &= A\cos(\omega t - \phi) && \text{parameters } \omega, A, \phi \\ &= A_1 \cos\omega t + A_2 \sin\omega t && \text{parameters } \omega, A_1, A_2 \end{aligned}$$

$$d_i = f(t_i) + e_i \qquad \text{Gaussian error } \textit{pdf}\text{s; rms} = \sigma$$

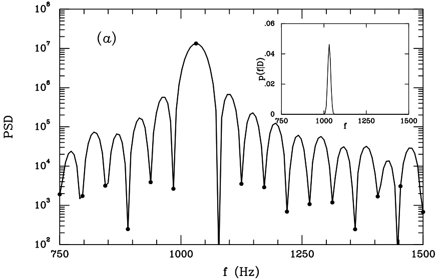
Estimate ω via profile likelihood, or Bayes (*Jaynes-Bretthorst alg.*):

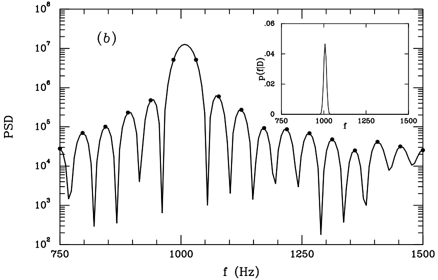
$$\begin{aligned} p(\omega|D) &\propto \int dA_1 \int dA_2 \, p(\omega, A_1, A_2)\mathcal{L}(\omega, A_1, A_2) \\ &\propto p(\omega)J(\omega)\exp\left[\frac{S(\omega)}{\sigma^2}\right] \end{aligned}$$

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

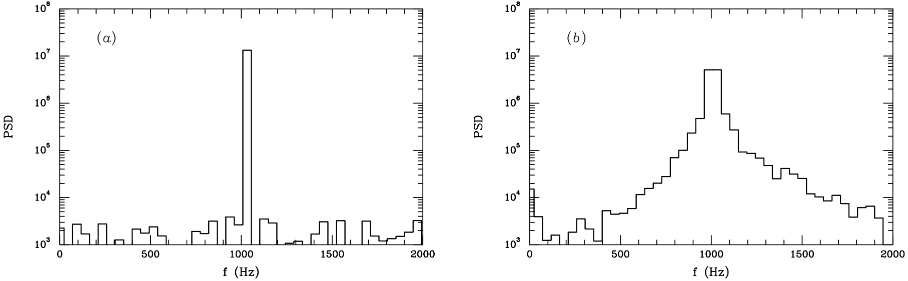
The posterior dist'n for ω is related to a *continuous* version of the periodogram/power spectrum

1024 samples at 48 kHz sampling rate
$S/N = 5$
$f = 1031.25$ Hz (Fourier frequency) and $f = 1008$ 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 ω
- 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*:

$$\mathcal{L}(signal) \approx \exp\left[\frac{P_{\rm max}}{\sigma^2}\right] \times \frac{\text{peak width}}{\text{prior search range}}$$

  Handles multiple testing issues via marginalization

- Conventional periodograms optimal only for *single sinusoids*

Two Sinusoids

Adopt a model with two sinusoids at distinct frequencies:

$$
\begin{aligned}
f(t) &= A\cos(\omega_1 t - \phi_1) + B\cos(\omega_2 t - \phi_2) \\
&= A_1 \cos\omega_1 t + A_2 \sin\omega_1 t \\
&\quad + A_3 \cos\omega_2 t + A_4 \sin\omega_2 t
\end{aligned}
$$

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

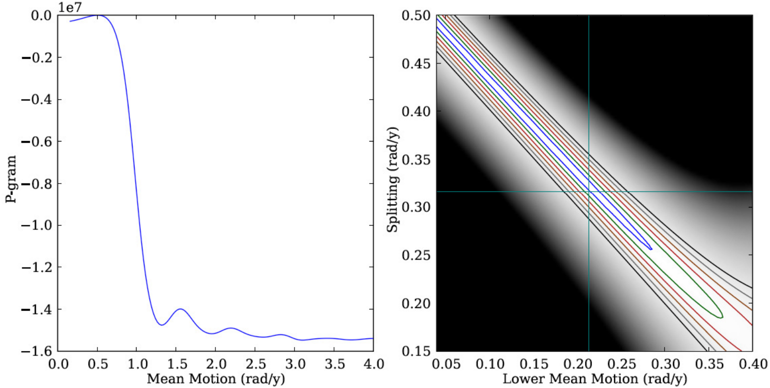
$$
p(\omega_1, \omega_2|D) \propto p(\omega_1, \omega_2) J(\omega_1, \omega_2) \exp\left[\frac{P(\omega_1)}{\sigma^2}\right] \exp\left[\frac{P(\omega_2)}{\sigma^2}\right]
$$

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 $\approx 45^\circ$ inclination. The data span 10 y, with 0.86 μas 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 θ:

$$C(u;\theta) = \mathrm{E}[f(t)f(t-u)] \qquad \text{(zero-mean case)}$$

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 θ may be approximately calculated using the periodogram (*Whittle likelihood*, $O(N \log N)$ i/o $O(N^2)$; see Simon Vaughan's work):

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

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

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

Using periodograms w/o losing your life

Tailor manipulations to goals:

- Nonparametrically estimate a spectrum (data spectrum $\neq$ signal spectrum):
  - Raw power null distribution $\propto e^{-S(\omega_i)/\sigma^2}$
  - Raw periodogram is inconsistent and biased (window, leakage) $\rightarrow$ 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 δ-function):
  - Single sinusoid: $\mathcal{L}_m(\omega) \propto e^{S(\omega)/\sigma^2}$
  - Multiple sinusoids (harmonics?) $\rightarrow$ *multiplet periodograms*
  - TSE provides tools for building generalized periodograms via Jaynes-Bretthorst algorithm
- Whittle likelihood for semiparametric stationary GPs