A note on spectra ...

https://selipot.github.io



On the inappropriate use of variance-preserving spectra



BY SHANE ELIPOT 💾 JANUARY 20, 2020 ○ 2 COMMENTS

I have been surprised by the continuing use of *variance-preserving spectra* in the oceanographic literature as a tool to diagnose periodicities in time series (this does not seem to happen in the purely climate literature ... we, oceanographers, are often a bit behind). Since I don't think I know much, I often seek out the help of a couple of statistician friends that deal with time series (like all the time). I have casually asked them: "Why do you think people use variance-preserving spectra?". Their answer was revealing: they did not even know what a variance-preserving spectrum was! Once I explained to them (see below), they were even more confused. They also wondered what was wrong with us (oceanographers). On a more serious note, what concerns me is that we collectively spend millions of tax-payer dollars to obtain amazing time series of oceanographic variables (such as oceanic volume transport), and sometimes analyze them with the wrong tools, unfortunately. We need to collectively do better.

So, I have decided to write a little note to demonstrate why variance-preserving spectra should not be used to make conclusive statements about periodicity in a time series, and to suggest alternative methods. I have recently become a research assistant professor, and thus I am trying to get a bit more in the teaching side of things (I do not teach at my





Deriving uncertainties for the Global Drifter Program hourly product Case studies

Shane Elipot, July 16, 2024, OceanUQ Summer School

ROSENSTIEL SCHOOL COOPERATIVE INSTITUTE for MARINE & ATMOSPHERIC STUDIES



Photo Credit: Molly Baringer



Goal is to go over 3 case studies of uncertainty derivations and utilizations

• Elipot et al. (2016), A global surface drifter data set at hourly resolution, JGR: Oceans, with Rick Lumpkin, Renellys C. Perez, Jonathan M. Lilly, Jeffrey J. Early, and Adam Sykulski doi: 10.1002/2016JC011716

-> Examples 1 & 2

with Adam Sykulski, Rick Lumpkin, Luca Centurioni, and Mayra Pazos doi: 10.1038/s41597-022-01670-2

-> Example 3

• Elipot et al. (2022), A dataset of hourly sea surface temperature from drifting buoys, Scientific Data,

Example 1: Characterizing errors and using uncertainty estimates

A global surface drifter data set at hourly resolution Elipot et al. 2016

- <u>Goal</u>: produce time series of drifter positions and velocities estimates, with uncertainty estimates, at regular, hourly intervals.
- **Obstacle:** the observations are uneven in time and **uncertain**.





The Global Drifter Program (GDP)

NOAA/AOML

30°E



https://www.aoml.noaa.gov/phod/gdp/index.php





https://www.aoml.noaa.gov/phod/gdp/index.php

• Funded by the U.S. National Oceanic and Atmospheric Administration (NOAA), the GDP maintains, with international partners, a global array of satellite-tracked drifters to meet the need for an accurate and globally dense set (5°x5°) of in situ observations of near-surface currents, sea surface temperature (SST), and Sea Level Pressure.

The Global Drifter Program (GDP)



Miami FL.

https://www.aoml.noaa.gov/phod/gdp/index.php

• The GDP data are transmitted to operational users via the WMO Global Telecommunication System (GTS) and later distributed to research users in the form of quality-controlled (QC), delayed mode products. The release of QC data products is led by the Data Assembly Center (DAC) of the GDP at the NOAA Atlantic Oceanographic and Meteorological Laboratory (AOML),



What were we trying to do?

Fit a linear model within a sliding window to obtain **estimates** of longitude or latitude at hourly intervals



Obser tim

times

What were we trying to do?

- - $\phi(t; \boldsymbol{\beta}^{\phi}) =$ $\theta(t; \boldsymbol{\beta}^{\theta}) =$
- We seek a set of parameters $\beta =$ likelihood:

$$L(\boldsymbol{\beta}) = \prod_{k=1}^{N} \left\{ p \left[\Phi_k, \Theta_k, \phi(t_k; \boldsymbol{\beta}^{\phi}), \theta(t_k; \boldsymbol{\beta}^{\theta}) \right] \right\}^{w_k}$$

p is the PDF describing whether a location observation (Φ_k, Θ_k)

Mathematical models for longitude and latitude:

$$= \beta_0^{\phi} + \beta_1^{\phi}(t - t_0)$$
$$= \beta_0^{\theta} + \beta_1^{\theta}(t - t_0)$$

$$\left[\boldsymbol{\beta}^{\phi}, \boldsymbol{\beta}^{\theta}\right] = \left[\beta_{0}^{\phi}, \beta_{1}^{\phi}, \beta_{0}^{\theta}, \beta_{1}^{\theta}
ight]$$

that maximizes a weighted probability of the observed data, or weighted

will yield the true location $(\phi(t_k), \theta(t_k))$ \longrightarrow That's the pdf of the errors!





error is observation minus truth

Black dots: GPS positions taken as "truth"

<u>Colored squares:</u> Argos **position estimates** with location **error** characterized by a class, associated with an equivalent radius error r assumed to be representative of **one** standard deviation of the errors:

Class 3: r < 250 m

Class 2: r = 250-500 m

Class 1: r = 500-1500 m

Class 0: r > 1500 m





empirical PDF of errors
Gaussian PDF fits
t location-scale PDF fits



Elipot et al. 2016

Normal PDF —

t location-scale PDF $\longrightarrow p(z|\mu, \sigma, \nu)$ (nonstandardized Student's t PDF)

- μ location parameter
- σ scale parameter
- ν shape parameter

$$p(z|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{z-\mu}{\sigma}\right)^2}$$

$$) = \frac{\Gamma(\frac{\nu+1}{2})}{\sigma\sqrt{\nu\pi}\,\Gamma(\frac{\nu}{2})} \left[1 + \frac{1}{\nu}\left(\frac{z-\mu}{\sigma}\right)^{2}\right]^{-\frac{\nu+1}{2}}$$

$$\Gamma(a) = \int_0^\infty t^{a-1} \exp(-t)$$



4

2

-4

-6

asses PDF

Log -5



@ResearchMark

Class 2 Model quantiles



Observed and fitted distribution



Quantile-quantile plots













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Weighted likelihood: $L(\beta) = \prod^{N} \{p\}$

 $l(oldsymbol{eta}) = \sum_{k=1}^N w_k$ J· log-likelihood:

lat, lon errors $p\left[\Phi_{k},\Theta_{k},\phi\left(t_{k};\boldsymbol{\beta}^{\phi}
ight), heta
ight)$ independent:

and consider that the errors are distributed like t PDFs ...

$$p\left[\Phi_k, \Theta_k, \phi(t_k; \boldsymbol{\beta}^{\phi}), \theta(t_k; \boldsymbol{\beta}^{\theta})\right]\right\}^{w_k}$$

$$\ln p \left[\Phi_k, \Theta_k, \phi \left(t_k; \boldsymbol{\beta}^{\phi} \right), \theta \left(t_k; \boldsymbol{\beta}^{\theta} \right) \right]$$

$$\theta\left(t_{k};\boldsymbol{\beta}^{\theta}\right)\right] = p\left[\Phi_{k},\phi\left(t_{k};\boldsymbol{\beta}^{\phi}\right)\right]p\left[\Theta_{k},\theta\left(t_{k};\boldsymbol{\beta}^{\theta}\right)\right]$$



location, scale, and shape parameters of the t PDF of $\mu_{\Phi_k}, \mu_{\Theta_k}, \sigma_{\Phi_k}, \sigma_{\Theta_k}, \nu_{\Phi_k}, \nu_{\Theta_k}$ longitude or latitude observations with index k.

Log-likelihood expression to maximize $\boldsymbol{\beta} = \left[\boldsymbol{\beta}^{\phi}, \boldsymbol{\beta}^{\theta} \right]$

$$\frac{1}{1-1} - w_k \ln \left[\frac{\sigma_{\Theta_k} \sqrt{\nu_{\Theta_k} \pi} \Gamma\left(\frac{\nu_{\Theta_k}}{2}\right)}{\Gamma\left(\frac{\nu_{\Theta_k}+1}{2}\right)} \right] \right\}$$

$$\frac{1+\frac{1}{\nu_{\Phi_k}} \left(\frac{\Phi_k - \phi(t_k; \boldsymbol{\beta}^{\phi}) - \mu_{\Phi_k}}{\sigma_{\Phi_k}} \right)^2 \right]}{\left. + \frac{1}{\nu_{\Theta_k}} \left(\frac{\Theta_k - \theta(t_k; \boldsymbol{\beta}^{\theta}) - \mu_{\Theta_k}}{\sigma_{\Theta_k}} \right)^2 \right] \right\}$$

$$= [\beta_0^{\phi}, \beta_1^{\phi}, \beta_0^{\theta}, \beta_1^{\theta}] \longrightarrow \begin{cases} \phi(t; \boldsymbol{\beta}^{\phi}) &= \beta_0^{\phi} + \beta_1^{\phi}(t - \theta) \\ \theta(t; \boldsymbol{\beta}^{\theta}) &= \beta_0^{\theta} + \beta_1^{\theta}(t - \theta) \end{cases}$$

Evaluate at $t = t_0$ to obtain fitted/estimated positions ...



Example 2: Deriving uncertainty estimates

Deriving uncertainty estimates of the position estimates Using a bootstrap method



We chose to use N = 4observation points to obtain each $\hat{\boldsymbol{\beta}} = [\hat{\beta}_0^{\phi}, \hat{\beta}_1^{\phi}, \hat{\beta}_0^{\theta}, \hat{\beta}_1^{\theta}]$ at hourly time scale

How to get $Var[\hat{\beta}_i^x]$?

Asymptotic theory:

 $N \to +\infty, \quad \hat{\beta}_j - \beta_j \sim \mathcal{N}(0, \sigma)$

Instead, use a bootstrap method, the jackknife! Re-estimate $\hat{\beta}$ 4 times using three observations out of four to obtain $Var[\beta_i^x]$



Deriving uncertainty estimates of the position estimates Using a bootstrap method

order to obtain $s_j = \operatorname{Var} \left[\hat{\beta}_j \right]$

"t statistic": $t_j = \frac{\widehat{\beta}_j - \beta_j}{s_j/\sqrt{N}}$



$$[\hat{\beta}_j - t_{\alpha/2,N-1} \frac{s_j}{\sqrt{N}}, \hat{\beta}_j + t_{1-\alpha/2,N-1} \frac{s_j}{\sqrt{N}}]$$

$$t_{\alpha/2,N-1} = t_{1-\alpha/2,N-1} = 3.1824 \quad \text{with } \alpha = 0.05$$

Re-calculate estimates 4 times using three observations out of four, in



Validation of uncertainty estimates

100



Elipot et al. 2016

80 60 40 Two-dimensional histograms of the 20 square root of estimated versus 200 observed error variance for each 150 100 different methods of estimation. 50 60

We considered 3366 10-day trajectory 40 segments with 50% overlap in order to 20 calculate the variance of the observed longitude and latitude error time series 60 for each segment, which we compare to the mean of the estimated variances for 20 longitude and latitude



Example 3: Deriving uncertainty estimates

A dataset of hourly sea surface temperature from drifting buoys

Elipot et al. 2022

- <u>Goal</u>: produce time series of drifter SST estimates, with uncertainty estimates, at regular, hourly intervals.
- <u>Obstacle</u>: Many!



Time series of SST observations from drifter ID 55366 [Argos-tracked drifter, SVP type, built by Pacific Gyre]





Time series of temporal intervals (Δt) between consecutive observations:



This drifter sampled every 60 s, averaged every 15 samples, and transmitted every 90 s.

> Argos satellite orbital period (101.47 min)

Uneven sampling



Time series of SST observations from drifter ID 55366

For 85% of drifters, observations are derived from a SST equation:





Quantized observations

a = 0.05 resolution

Causes an added error called quantization error













"Kriging" solution at 6-hour time steps



6-hourly "kriged" estimates @ 00:00, 06:00, 12:00. 18:00 (Hansen and Poulain, 1996):

> ≈ Optimal interpolation method

(using 5 observations before and after estimation times)





Methodology: process model

time t_k .

The goal is to estimate SST at time $t = t_k$ (which is observation time or hourly time steps)



- The noise component, ε_k , is expected to be zero-mean, to have unit variance
- ... locally scaled by σ_k where σ_k^2 is the error variance of the observations around



process model: $s_i = s_m(t_i; t_k) + \sigma_k \varepsilon_k$

model of SST temporal evolution:

$$s_{m}(t_{i};t_{k}) = s_{P}(t_{i};t_{k}) + s_{D}(t_{i};t_{k})$$

$$= \sum_{p=0}^{P} s_{p,k}(t_{i}-t_{k})^{p} + \sum_{n=1}^{N} A_{n,k} \cos[n\omega(t_{i}-t_{k}) + \phi_{n,k}]$$

$$= \sum_{p=0}^{P} s_{p,k}(t_{i}-t_{k})^{p} + \sum_{n=1}^{N} [\alpha_{n,k} \cos n\omega(t_{i}-t_{k}) + \beta_{n,k} \sin n\omega(t_{i}-t_{k})]$$
diurnal evolution, $\omega = 1$ cpe

low-frequency component

Estimate at $t_i = t_k$: $\widehat{s}_{m,k} \equiv s_m(t_k;t_k) =$

D e.g. Gentemann (2003)

$$= s_{0,k} + \sum_{n=1}^{N} \alpha_{n,k}$$



 $s_i = s_m(t_i; t_k) + \sigma_k \varepsilon_k$



 $s_i = s_m(t_i; t_k) + \sigma_k \varepsilon_k$





 $s_m(t_i; t_k) = s_0 + s_1(t_i - t_k)$

 $s_m(t_k; t_k) = s_0$







Methodology: deriving uncertainties $s_m(t_i; t_k) = s_{0,k} + s_{1,k}(t_i - t_k) + \sum_{i=1}^{n} \frac{1}{2} \sum_{i=1}^{n} \frac{1}{$

Method to fit model to observations is adapted from the LOcally WEighted Scatterplot Smoothing estimator (LOWESS), Cleveland (1979); essentially an iterative least squares method

Theoretical formula for the variance of the estimates, i.e squared **standard error** of the estimates:

$$\mathbf{C}_{\boldsymbol{\beta}} \equiv \operatorname{Var}(\widehat{\boldsymbol{\beta}}) = (\mathbf{X}\mathbf{W}^*\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{W}^*\boldsymbol{\Sigma}\mathbf{W}^*\mathbf{X})(\mathbf{X}\mathbf{W}^*\mathbf{X})^{-1}$$

Unknown covariance matrix (~22² terms!) of the observation errors from the process model

How to move forward? See Fan & Gijbels (2018) but ...

$$\sum_{i=1}^{3} \left[\alpha_{n,k} \cos n\omega (t_i - t_k) + \beta_{n,k} \sin n\omega (t_i - t_k) \right]$$

$$s_i = s_m(t_i; t_k) + \sigma_k \varepsilon_k$$



 $\beta =$

Assume homoscedasticity and that the errors are independent

$$\Sigma = \sigma^2(t_k)\mathbf{I} = (\sigma_1^2(t_k) + \sigma_q^2)$$

 Estimate error variance directly from residuals of the fit

$$\widehat{\sigma}_{1}^{2}(t_{k}) = \frac{(\mathbf{s} - \mathbf{X}\widehat{\boldsymbol{\beta}})^{T} \mathbf{W}^{*}(\mathbf{s} - \mathbf{X})^{T}}{\operatorname{tr} \{\mathbf{W}^{*} - \mathbf{W}^{*} \mathbf{X} (\mathbf{X}^{T} \mathbf{W}^{*} \mathbf{X})^{T} \\ = \frac{\sum_{i} \left[s_{i} - \widehat{s}_{m}(t_{i}; t_{k})\right]^{2} \delta_{i} K_{h_{k}}(t_{i})}{\nu}$$

effective number of degrees of freedom for the residuals for weighted least squares

 $\mathbf{C}_{\boldsymbol{\beta}} \equiv \operatorname{Var}(\widehat{\boldsymbol{\beta}}) = (\mathbf{X}\mathbf{W}^*\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{W}^*\boldsymbol{\Sigma}\mathbf{W}^*\mathbf{X})(\mathbf{X}\mathbf{W}^*\mathbf{X})^{-1}$





SST = an + b SST sensor equation

See Chiorboli (2003)

a : resolution distributions



$$\widehat{s}_{m,k} \equiv s_m(t_k; t_k) = s_{0,k} + \sum_{n=1}^{3} \alpha_{n,k}$$



(N+1)² terms extracted from the error covariance matrix with (2N+P)² terms





Estimates at observation times

Estimates at hourly times



Elipot et al. 2022

ad hoc derivation of a quality flag based on estimates and uncertainty estimates



Interpreting uncertainties

process model: $s_i = s_m(t_i; t_k) + \sigma_k \varepsilon_k$

Examine residuals normalized by their estimates of error standard deviations: ε are not normally distributed:

- A least squares method would put too much weight on outliers ...
- A standard error therefore represents an interval encompassing more probable values of the true unknown values of a quantity, thus a more conservative $\frac{1}{2}$ 1.5 confidence interval (78% confidence interval rather than a 68% confidence interval for Normal).
- But 1.96 standard deviation encompasses approximately 94% of the distribution of the residuals, almost like a normal distribution







Interpreting uncertainties

Spatial distribution



$\sqrt{\hat{\sigma}_1^2}$		All	Drogued	Undrogued
Mode	Level-2	0.026	0.020	0.030
	Level-3	0.026	0.020	0.030
50-th percentile	Level-2	0.031	0.025	0.036
	Level-3	0.031	0.025	0.036
$\sqrt{\hat{oldsymbol{\sigma}}^2}$		All	Drogued	Undrogued
Mode	Level-2	0.033	0.031	0.036
	Level-2	0.033	0.031	0.036
50-th percentile	Level-2	0.035	0.030	0.040
	Level-3	0.036	0.030	0.040

Elipot et al. 2022

Drogued vs undrogued







- Example 1: Characterizing and modeling errors for the purpose of conducting parameter estimation
- Example 2: Deriving uncertainty estimates using a bootstrap method
- Example 3: Deriving and interpreting uncertainty estimates

Recap and summary

Thank you! Shane Elipot, <u>selipot@miami.edu</u>



Introduction to afternoon activity

Go to Google slides

- satellite-based product.
- use these estimates to inform the comparisons.
- the statistical and oceanographic aspects of the comparisons

 Goal of the activity is to compare two SST products: The Global Drifter **Program hourly SST product** (*Elipot et al. 2022*) and the **The Multi-scale** Ultra-high Resolution (MUR) SST analysis (Chin et al. 2017), a mostly

Both products provide uncertainty estimates and we would like you to

• A preliminary step of the comparison is "matching" the two datasets in space (and time). This has been prepared for you so that you can focus on

- MUR is available publicly on an AWS S3 bucket but only from 2002 to 2020 (https://registry.opendata.aws/mur/)
- Alternatively, it is is available from NASA PO.DACC from 2002 to present (https://podaac.jpl.nasa.gov/dataset/MUR-JPL-L4-GLOB-v4.1). Datasets for you to play with today were prepared from data downloaded from PODAAC ...
- Global Drifter Data hourly product is available from AWS S3 bucket <u>https://registry.opendata.aws/noaa-oar-hourly-gdp/</u>

- so approximately 1~km scale resolution (at best).
- As stated in Chin et al. (2017), the standard deviation of the formal available.

• MUR is the result of the application of the Multi-Resolution Variational Analysis (MRVA) method. This method fits a basis of wavelet functions to multiple satellite and in situ datasets within multiple spatial and temporal windows.

• The method includes a least square estimation of the coefficients multiplying basis functions, the sum of which leads to an estimate of the SST field T(x,y)which can be evaluated anywhere and continuously on the globe. The MUR product consists of an estimation of T(x,y) on a 0.01 by 0.01 geographical grid,

estimation error is provided at each grid point as an estimate of analysis **uncertainty.** The analysis time is **09:00 UTC.** One global estimate per day is

- To prepare a match-up dataset, we matched drifter and MUR data by doing a nearest neighbor interpolation of MUR data (SST estimates and uncertainty estimates) at the 9:00 am drifter locations.
- Limited ourselves to small region in North Atlantic (60-50W, 30-40N)
- Matched 74,921 9:00am drifter SST estimates from 797 trajectories
- For bonus activity, also matched 1,799,525 hourly drifter SST estimates from 804 trajectories by expanding to nearest neighbor interpolation in time ...



time = 2020-01-01T09:00:00

SST from drifter 18702

Adam S. and Shane E. will be around the classrooms from 1:30pm to 3:30pm

4:00pm we all re-convene in SLAB103 for Science Talk by Mohamed Iskandarani

