

Spectral Estimation and Iterated Whitening

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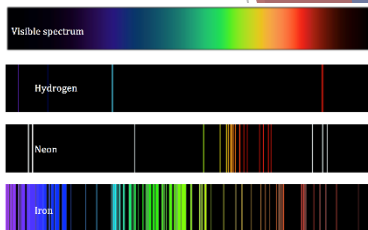
Applied Mathematics
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Power spectrum: “power” or “energy” as function of frequency

Applications

- Time series analysis
- Prediction
- *Data driven model reduction*



Kuramoto-Sivishinsky (KS) equation

- spatiotemporal chaos

$$\begin{cases} u_t + uu_x + u_{xx} + u_{xxxx} = 0 \\ t \in [0, \infty), \quad x \in [0, L] \end{cases}$$

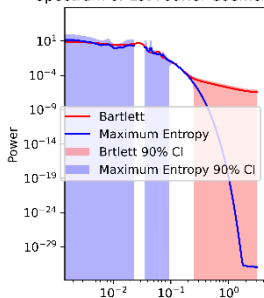
$$u(x, t) = \sum_{k=-\infty}^{\infty} v_k(t) e^{ikt}$$

$$\dot{v}_k = (q_k^2 - q_k^4) v_k - \frac{iq_k}{2} \sum_{j=-\infty}^{\infty} v_j v_{k-j}$$

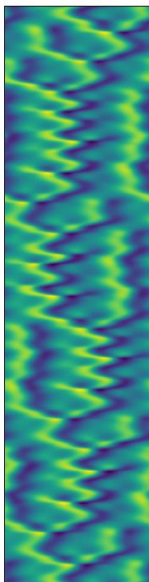
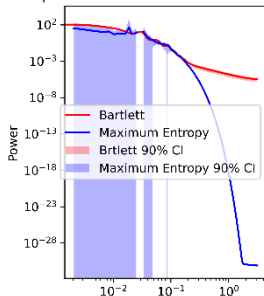
$$q_k = \frac{2\pi}{L} k$$

- Our work requires *accurate spectral estimates*

Spectrum of 1st Fourier Coefficients



Spectrum of 2nd Fourier Coefficients



What is power spectrum?

Terminology and Definition



Given a discrete-time stochastic process (assume all necessary moments exist)

$$X = (\dots, X_{-2}, X_{-1}, X_0, X_1, X_2, \dots)$$

We have

$$\mu_n = \mathbb{E}X_n$$

$$C_X(n, m) = \mathbb{E}(X_n - \mu_n)(X_m - \mu_m)^*$$

X is *wide-sense stationary* (WSS) if

$$\mu_n = \mu \quad (\text{constant})$$

$$C_X(n, m) = C_X(n - m) \quad (\text{depends only on lag})$$

Assume X is WSS and $\mu = 0$ (WLOG)

Def. The *power spectrum* of X is

$$S_X(\omega) = \sum_{n=-\infty}^{\infty} C_X(n) e^{-i\omega n} = \mathcal{F}\{C_X\}(\omega), \quad C_X(n) = \mathbb{E}X_n X_0^*$$

What is power spectrum?

Some intuition



Program in Applied
Mathematics

Spectral representation of time series

$$X_n = \int_{-\pi}^{\pi} e^{in\omega} \sqrt{S_X(\omega)} dW_\omega$$

By inverse Fourier

$$\text{var}(X) = C_X(0) = \frac{1}{2\pi} \int_{-\pi}^{\pi} S_X(\omega) e^{i\omega 0} d\omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} S_X(\omega) d\omega$$

$$S_X(\omega) \approx \frac{1}{N} |\hat{X}(\omega)|^2$$

Filtering: If

$$\ell = (\dots, \ell_{-1}, \ell_0, \ell_1, \dots) \quad \text{and} \quad Y_n = (\ell * X)_n = \sum_{k=-\infty}^{\infty} \ell_k X_{n-k}$$

Then

$$S_Y(\omega) = |L(\omega)|^2 S_X(\omega), \quad L(\omega) = \sum_{k=-\infty}^{\infty} \ell_k e^{-ik\omega}$$

White noise

$$e = (\dots, e_{-1}, e_0, e_1, \dots), \quad e_n \text{ i.i.d. } N(0, \sigma^2)$$

Note: $S_e(\omega) = \sigma^2$

AR(p) process

$$X_n = -a_1 X_{n-1} - \dots - a_p X_{n-p} + e_n, \quad \{e_n\} \text{ is white noise}$$

Note: $e_n = X_n + a_1 X_{n-1} + \dots + a_p X_{n-p} = \sum_{k=0}^p a_k X_{n-k} \quad (a_0 = 1)$

$$S_e(\omega) = S_{a*X}(\omega) = |A(\omega)|^2 S_X(\omega),$$

$$A(\omega) = \sum_{k=0}^p a_k e^{-ik\omega}$$

$$S_X(\omega) = \frac{\sigma^2}{|A(\omega)|^2}$$

Covariance Estimation



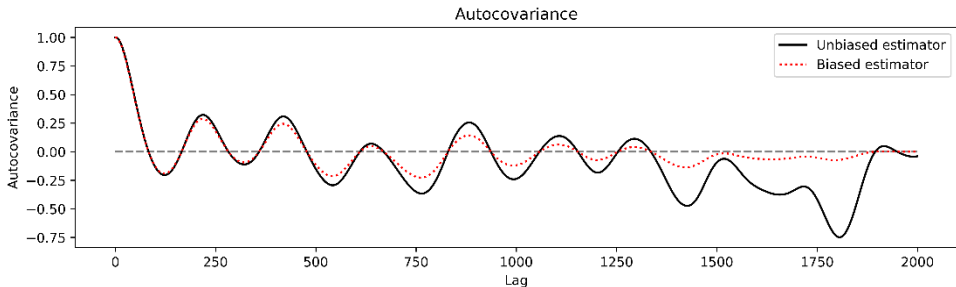
Given $x = (x_n, n = 1, \dots, N)$ (a realization of $(X_n, n = 1, \dots, N)$)

Unbiased Covariance Estimate:

$$R_X(n) = \mathbb{E}[(X_n - \mu)(X_0 - \mu)^*] \approx \frac{1}{N-n} \sum_{j=1}^{N-n} (x_{n+j} - \tilde{\mu})(x_j - \tilde{\mu})^*$$

Biased estimate:

$$R_X(n) \approx \frac{1}{N} \sum_{j=1}^{N-n} (x_{n+j} - \tilde{\mu})(x_j - \tilde{\mu})^* = \tilde{R}_X(n)$$



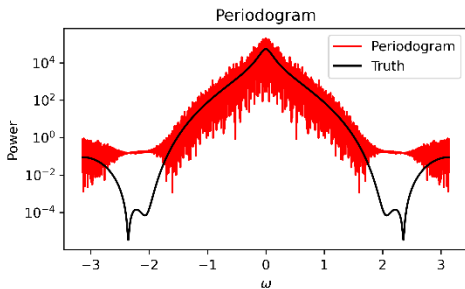
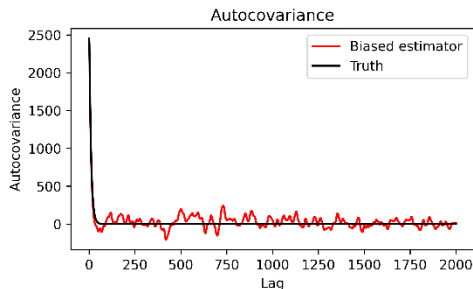
Spectrum Estimation

Windowed Periodogram



Periodogram: (direct approach)

$$\tilde{S}_X^{\text{per}}(\omega) = \sum_n \tilde{R}_X(n) e^{-in\omega} = \dots = \frac{1}{N} |\hat{x}(\omega)|^2 \quad (= \text{abs2}.\text{(fft}(x))/N)$$



Periodogram: asymptotically *unbiased*, but *inconsistent*

Spectrum Estimation

Bartlett



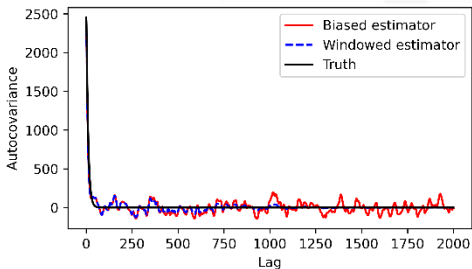
Program in Applied
Mathematics

Bartlett's windowing procedure

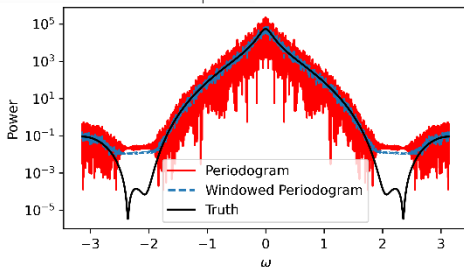
Control *variance* but increase *bias*

$$\tilde{S}_X^{\text{Par}}(\omega) = \sum_{n=-k}^k W^{\text{Par}}(n) \tilde{R}_X(n) e^{-in\omega}$$

Autocovariance



Spectral Estimates



Periodogram: asymptotically *unbiased*, but *inconsistent*

Windowed Periodogram: asymptotically *unbiased*, and *consistent*

Spectrum Estimation

Maximum Entropy Spectral Analysis



Maximize “entropy”

$$E = \int_{-\pi}^{\pi} \log \tilde{S}(\omega) d\omega$$

Subject to:

$$\int_{-\pi}^{\pi} \tilde{S}(\omega) e^{i\omega n} d\omega = \tilde{R}(n) \quad \text{for } n = 0, 1, \dots, p$$

Gives

$$\tilde{S}(\omega) = \frac{\sigma_p^2}{\left| 1 + \sum_{k=1}^p a_k e^{-ik\omega} \right|^2}$$

Here, $\{a_k\}_{k=1}^p$ are the autoregressive coefficients of order p , i.e., they minimize

$$\sum_{n=1}^{N-p} \left| x_{n+1} - \sum_{k=0}^{p-1} a_k x_{n-k} \right|^2$$

Spectrum Estimation

Maximum Entropy Spectral Analysis



AR(p) process:

$$X_n = -a_1 X_{n-1} + \cdots - a_p X_{n-p} + e_n, \quad e_n \text{ i.i.d. } N(0, \sigma_p^2)$$

To fit coefficients:

- Yule-Walker equations: $\{C_X(n)\}_{n=0}^p \Leftrightarrow \{a_n\}_{n=1}^p, \sigma_p^2$

- Levinson-Durbin
- Burg (again)



Recursive: $p = 1, \dots, p_{\max}$

All orders $< p$
Use info criterion to
choose p



a_1^1			σ_1^2
a_1^2	a_2^2		σ_2^2
\vdots	\vdots	\ddots	\vdots
$a_1^{p_{\max}}$	$a_2^{p_{\max}}$	\dots	$\sigma_{p_{\max}}^2$

$$\hat{S}_X^{\text{Burg}} = \frac{\sigma_p^2}{|A(\omega)|^2}, \quad A(\omega) = 1 + \sum_{k=1}^p a_{k,p} e^{-ik\omega}$$

Spectral Factorization and modeling filters



Given

$$S_X(\omega) = \sum_{k=-m}^m C_k e^{-ik\omega}, \quad C_{-k} = C_k^*$$

We can write

$$S_X(\omega) = |L(\omega)|^2$$

for

$$(1) \quad L(\omega) = \sqrt{S_X(\omega)} \approx \sum_{k=-m}^m \ell_k e^{-ik\omega} \quad \text{or} \quad (2) \quad L(\omega) = \sum_{k=0}^m \ell_k e^{-ik\omega}$$

“Spectral factorization”

- Fejér-Riesz theorem
- Levinson-Durbin
- Kalman Filter

If e is white noise with unit variance and $Y = \ell * e$, then

$$(1) \quad S_Y(\omega) = \left| \sum_{k=-m}^m \ell_k e^{-ik\omega} \right|^2 S_e(\omega) \\ \approx |L(\omega)|^2 \cdot 1 = S_X(\omega)$$

$$(2) \quad S_Y(\omega) = |L(\omega)|^2 \\ = S_X(\omega)$$

ℓ is a modeling filter

Spectral Factorization and modeling filters



Given L , define W

$$L^{-1}(\omega) = W(\omega) \approx \sum_{k=0}^m w_k e^{-ik\omega}$$

Observe,

$$|W(\omega)|^2 \approx [S_X(\omega)]^{-1}$$

So,

$$\begin{aligned} S_{w * X}(\omega) &= |W(\omega)|^2 S_X(\omega) \\ &\approx S_X(\omega) / S_X(\omega) = 1 \end{aligned}$$

w is a whitening filter

Conveniently, given Bartlett estimate

$$\tilde{S}_X^{\text{Par}}(\omega) = \sum_{n=-k}^k W^{\text{Par}}(n) \tilde{R}_X(n) e^{-in\omega}$$

can construct approximate *modeling* and *whitening* filters

Motivating Example:

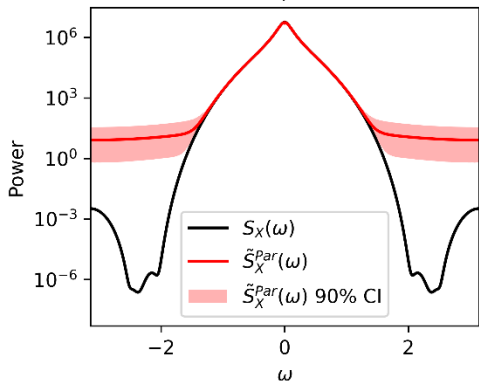
$$X \sim \text{ARMA}(10, 1) \quad N = 10^4,$$

$w_1 =$ causal whitening filter from Parzen estimate $m = 300$

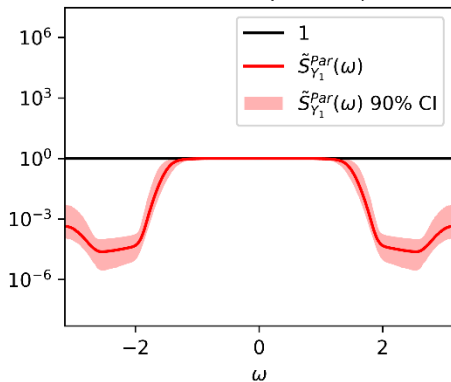
$$Y_1 = w_1 * X$$

Bartlett estimator has a kind of floor

Power spectrum



Iter. 1: 'whitened' power spectrum



Modeling filter Spectral Analysis

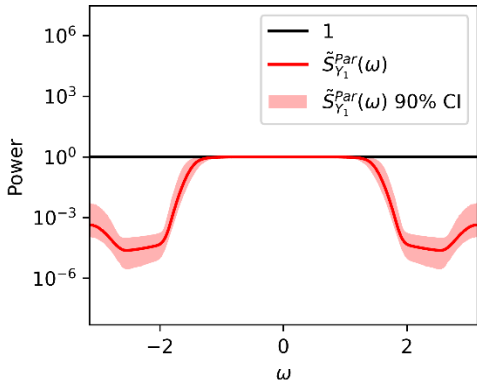


What if we whiten again?

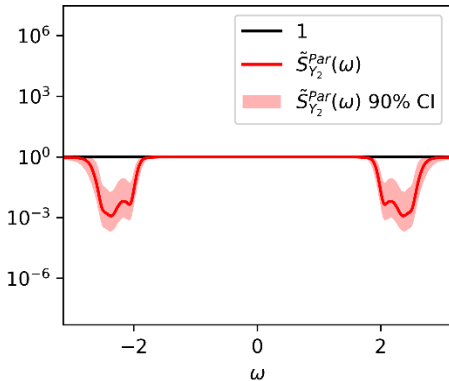
$w_2 =$ causal whitening filter from Parzen estimate of $S_{Y_1}(\omega)$

$Y_2 = w_2 * Y_1 = w_2 * w_1 * X$

Iter. 1: 'whitened' power spectrum



Iter. 2: 'whitened' power spectrum



Modeling filter Spectral Analysis

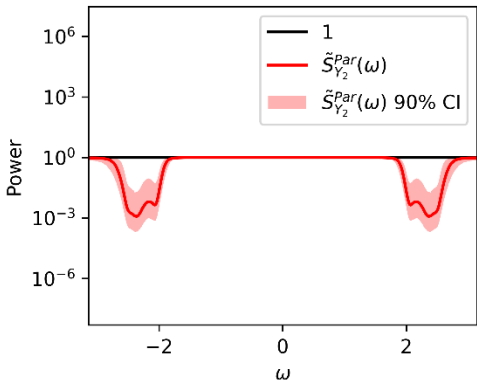


What if we whiten again?

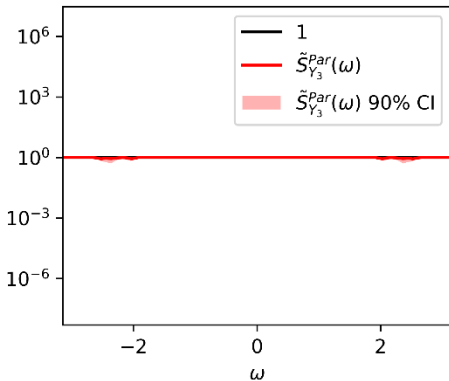
$w_3 =$ causal whitening filter from Parzen estimate of $S_{Y_2}(\omega)$

$Y_3 = w_3 * Y_2 = w_3 * w_2 * w_1 * X$

Iter. 2: 'whitened' power spectrum



Iter. 3: 'whitened' power spectrum



Iterated Whitening Spectral Analysis



Since $1 \approx S_{w_3 * w_2 * w_1 * X}(\omega) \approx |L_3(\omega)|^{-2} |L_2(\omega)|^{-2} |L_1(\omega)|^{-2} S_X(\omega)$

then $S_X(\omega) \approx |L_3(\omega)|^2 |L_2(\omega)|^2 |L_1(\omega)|^2 =: \tilde{S}_X^{IW}(\omega)$

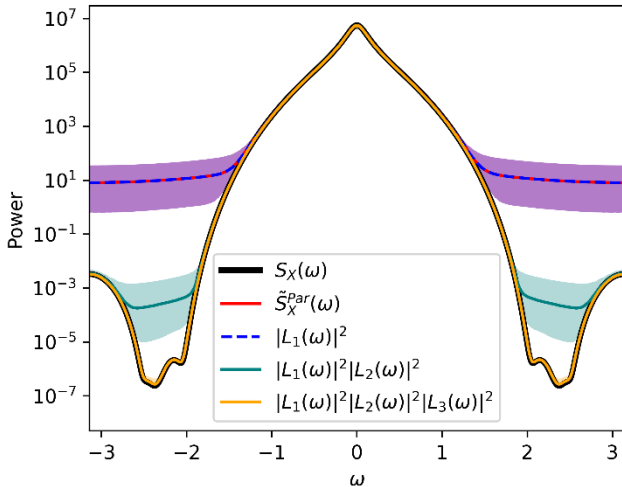
Collect Modeling filters

$\ell^{(1)}$, $\ell^{(2)}$, and $\ell^{(3)}$

here

$$L_j(\omega) = \sum_{k=0}^m \ell_k^{(j)} e^{-ik\omega}$$

IW spectral estimates

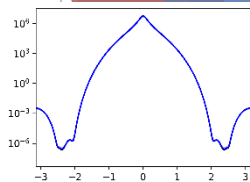
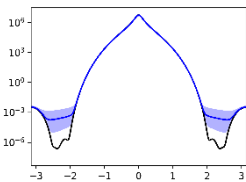
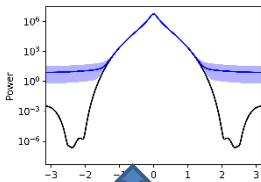


Iteration 1

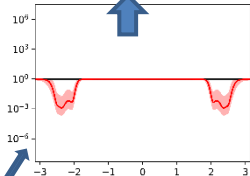
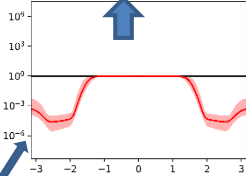
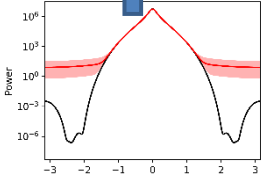
Iteration 2

Iteration 3

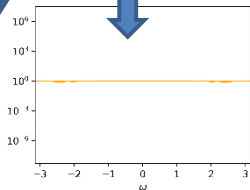
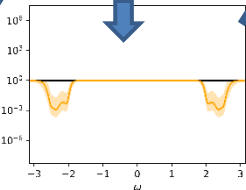
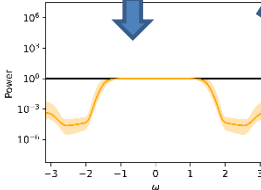
Modeling filter
spectral estimate

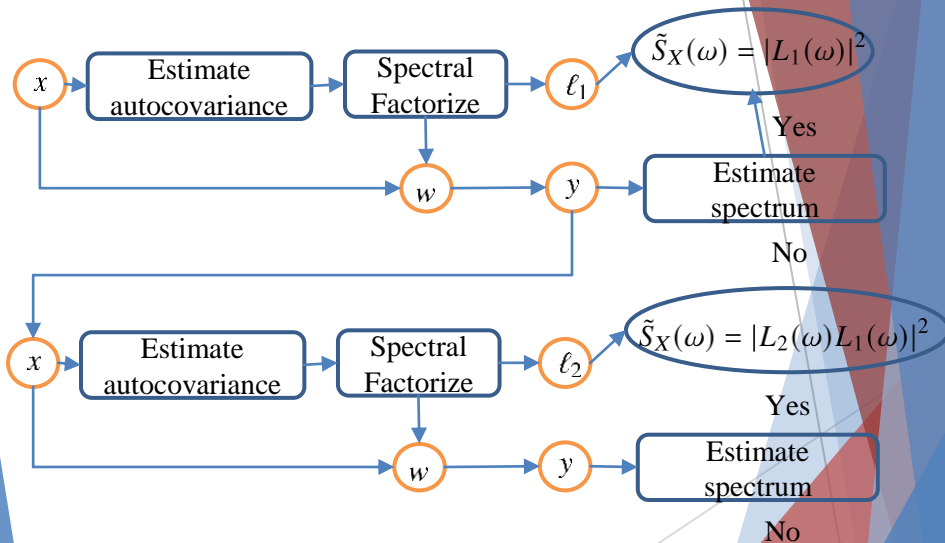


Bartlett
estimate for
current process



Bartlett
estimate of
whitened
process





Iterated whitening converges in finite steps

- Bartlett captures top ~ 6 decades
- Whitening *whitens* accurate frequency range
 - New range is ~ 6 decades less
- Floor goes below 1

$$1 > \tilde{S}_X^{\text{Par}}(\omega) = |L(\omega)|^2 = |W(\omega)|^{-2} \quad \Rightarrow \quad |W(\omega)|^2 > 1$$

$$S_{W * X}(\omega) = |W(\omega)|^2 S_X(\omega) > S_X(\omega)$$

*Whitening raises
low powers*

Emanuel Parzen (1957):

$$\text{var}(\hat{S}_X^{\text{parz}}(\omega)) \sim \frac{151}{280} \frac{L}{N} S_X^2(\omega) \quad (\omega \neq 0, \pm\pi)$$

$$\text{bias}(\hat{S}_X^{\text{parz}}(\omega)) \sim \frac{6}{L^2} S_X''(\omega)$$

Experiment

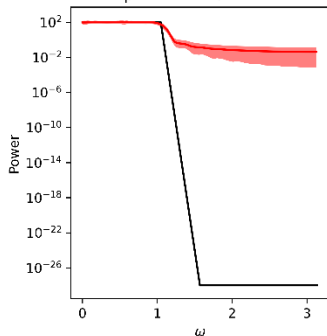
- Process know spectrum
- Large dynamic range
- $N = 1000$ (time series length)
- 100 independent time series

Three methods

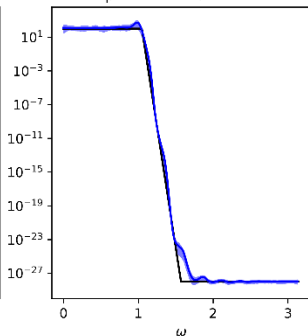
- Bartlett-Parzen
- MESA
 - $p_{\max} = 100$
- Iterated Whitening
 - 10 iterations

Mean and 90% confidence interval for each estimator

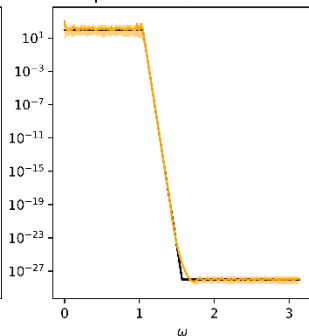
True Spectrum and BP estimate



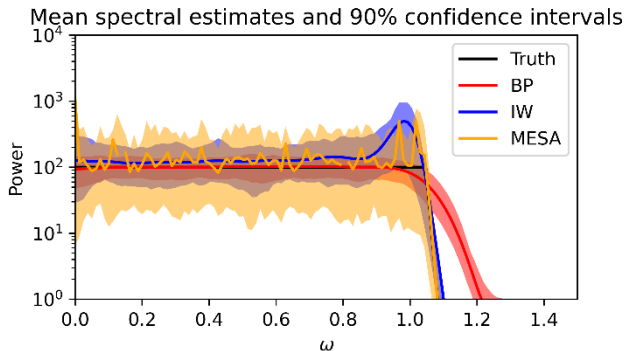
True Spectrum and IW estimate



True Spectrum and MESA estimate



- Both MESA, IW approximate full dynamic range
- MESA has numerical issues at top of large spectral ranges
- Variance of IW less than MESA top of range, smoother



Average of 100 sample times series

Method	Spec. 1 high-low	Spec. 2 low-high-low	Spec. 3 low- high
Bartlett- Parzen	$8.55 \cdot 10^{-4}$ sec	$7.82 \cdot 10^{-4}$ sec	$7.02 \cdot 10^{-4}$ sec
Iterated Whitening	0.114 sec	0.114 sec	0.114 sec
MESA	0.00207 sec	0.00171 sec	0.00189 sec

Bartlett: $O(mNd^2)$ + $O(d^2N_f \log N_f)$

MESA: $O(p_{\max}^2 Nd^2)$ + $O(p_{\max} Nd^3)$ + $O(p_{\max}^2 d^3)$

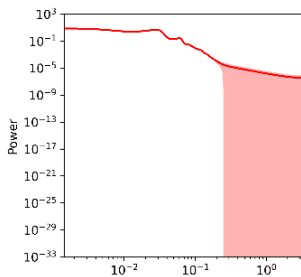
IW: $O(MmNd^2)$ + $O(MmN_{\text{SF}}d^3)$
+ $O(Md^2N_f \log N_f)$ + $O(Md^3N_f)$

- d dimension
- M # of whitening iterations
- m lag window cutoff
- p_{\max} # of Burg iterations in MESA
- N_{SF} # iterations of spectral factorization algorithm
- N_f # of points in frequency grid
- N length of time series (in steps)

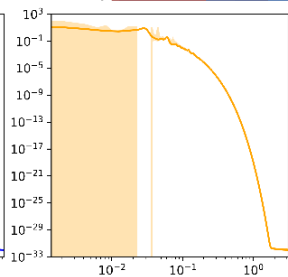
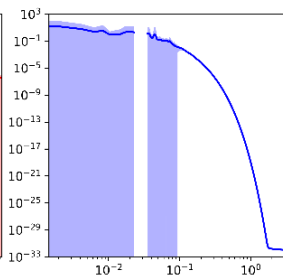
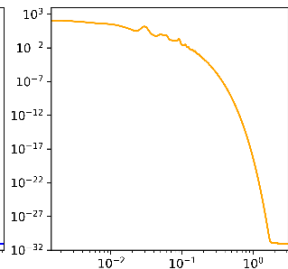
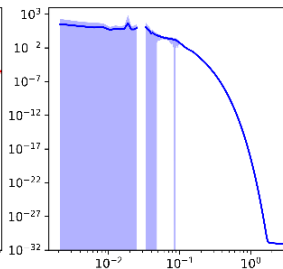
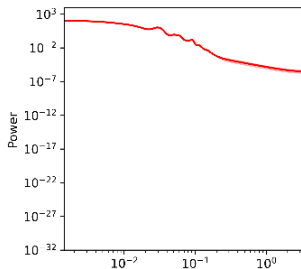
IW

First Fourier
coefficient

Bartlett



MESA

Second Fourier
coefficient

Conclusion

- IW is much more accurate than periodogram-based estimators for spectra with large dynamic range
- IW is more robust than MESA
- (noncausal) IW is simple to implement

More...Multichannel

- Control Variate model-based spectral estimation

Future Work

- Further analysis on convergence
- Apply estimator to model reduction
- Can iterated whitening address similar difficulties in phase estimation?



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- NSF
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Thank You!

Reference

- J. M., Kevin K. Lin, *A novel method for estimation of multi-scale spectra*, in preparation. 26/26