Program in Applied Mathematics

A comparison of spectral estimation methods for the analysis of chaotic and stochastic dynamical systems

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Outline

1. What is the power spectrum of a stationary stochastic process?
   - Conceptual definition
   - Operation definition
2. Spectral Estimation
   - Periodogram
   - Generalized Bartlett
   - Maximal Entropy Spectral Analysis
   - Examples
3. Spectral Factorization
   - Whitening
4. Spectral Estimation (reprisal)
   - Control Variate
   - More Examples
5. Conclusions

What is power spectrum?

Conceptual

- (For ease of exposition) Start with a continuous time stochastic process $X(t)$

- We have
  - $\mu_t = \mathbb{E}X(t)$
  - $C_X(t,s) = \mathbb{E}(X(t) - \mu_t)(X(s) - \mu_s)^*$

- The process is wide-sense stationary if

$$\mu_t = \mu \qquad \text{(constant)}$$

and

$$C_X(t,s) = C_X(t-s) \qquad \text{(depends on on lag)}$$

- Center $X(t)$

$$X(t) \leftarrow X(t) - \mu$$

What is power spectrum?

Conceptual

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- From signals and systems we get the terms
  - energy

$$\text{Total energy of } X(t) \text{ over } (t_1, t_2) = \int_{t_1}^{t_2} |X(t)|^2 dt$$

  - power

$$\text{Total power of } X(t) \text{ over } (t_1, t_2) = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} |X(t)|^2 dt$$

- If $X(t)$ is **deterministic** and **periodic** with period $2T$
  - $X(t) = \sum_{n=0}^{\infty} c_n e^{i\pi nt/T}$
  - So, total power over $(-T, T) = \frac{1}{2T} \int_{-T}^{T} |X(t)|^2 dt = \sum_{n=0}^{\infty} |c_n|^2$

What is power spectrum?

Conceptual

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- Example:
  - If $X(t) = c_n e^{i\pi nt/T}$ then total power = $|c_n|^2$

interpretation

$|c_n|^2$ = contribution to the total power from the term in the Fourier series of $X(T)$ with frequency $n/2T$ Hz (or angular frequency of $\pi n/T$ radians per second).

- If $X(t)$ is **deterministic** and **nonperiodic**
  - $X(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G(\omega) e^{i\omega t} d\omega \qquad (X \in L^2(\mathbb{R}))$ Fourier integral
  - So, total energy over $\mathbb{R} = \int_{-T}^{T} |X(t)|^2 dt = \int_{-T}^{T} |G(\omega)|^2 d\omega$

interpretation

$|G(\omega)|^2 d\omega$ = contribution to the total energy from components of $X(t)$ whose frequencies lie between ω and $\omega + d\omega$ radians per second.

What is power spectrum?

Conceptual

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- If $X(t)$ is **stochastic** and **stationary**
  - take a realization of $X(t)$ $\qquad X \notin L^2$
  - $X_T(t) = X(t) I_{[-T,T]}(t) \qquad X_T \in L^2$
  - $X_T(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} G_T(\omega) e^{i\omega t} d\omega$ where $G_T(t) = \frac{1}{\sqrt{2\pi}} \int_{-T}^{T} X(\omega) e^{-i\omega t} d\omega$
  - So, we have an interpretation of $|G_T(\omega)|^2 d\omega$

interpretation

$|G_T(\omega)|^2 d\omega$ = contribution to the total energy from components of $X_T(t)$ whose frequencies lie between ω and $\omega + d\omega$ radians per second.

interpretation

$\lim_{T\to\infty} \frac{|G_T(\omega)|^2}{2T} d\omega$ = contribution to the total power from components of $X_T(t)$ whose frequencies lie between ω and $\omega + d\omega$ radians per second.

$$S_X(\omega) = \lim_{T\to\infty} \mathbb{E}\frac{|G_T(\omega)|^2}{2T}$$

interpretation

$S_X(\omega)d\omega$ = average (over all realizations) of the contribution to the total power from components in $X(t)$ with frequencies between ω and $\omega + d\omega$ radians per second.

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- Start with X_n
  - a discrete-time stochastic process,
  - wide-sense stationary, and
  - centered.
- The power spectrum $S_X(\omega)$ is define by

$$S_X(\omega) = \sum_{n=-\infty}^{\infty} C_X(n) e^{-i\omega n} = \mathcal{F}\left\{C_X\right\}(\omega) = \widehat{C_X}(\omega)$$

where $C_X(n) = \mathbb{E} X_n X_0^*$ (Fourier transform of the autocovariance function)

- The z-spectrum $\bar{S}_X(z)$ is define by

$$\bar{S}_X(\omega) = \sum_{n=-\infty}^{\infty} C_X(n) z^{-n} = \mathcal{Z}\left\{C_X\right\}(\omega)$$

(z-transform of the autocovariance function)

- Observe that, by the inverse Fourier transform formula

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

So that spectrum given the distribution of variance among the frequencies.

Mean and Covariance Estimation

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We are given data, x_n, for $n = 1, 2, 3, \dots, N$

- Assume it is be a realization of the discrete-time process X_n or observations of a continuous time process X_{t_n}.
- Assume the process X_n is stationary

How do we estimate μ?
By virtue of stationary

$$\mu = \mathbb{E}X_n \approx \frac{1}{N}\sum_{n=1}^{N} x_n =: \tilde{\mu}$$

How do we estimate $R_X(n)$?
Again, by virtue of stationary

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

Spectrum Estimation (sample spectrum)

Periodogram

How do we estimate $S_X(\omega)$? (assume X_n is mean zero)

Peridogram: (direct approach)

$$
\begin{aligned}
\tilde{S}_X(\omega) &= \sum_n \tilde{R}_X(n) e^{-in\omega} \\
&= \sum_n \frac{1}{N} \sum_j x_{n+j} x_j^* e^{-in\omega} \\
&= \frac{1}{N} \sum_k \sum_j x_k x_j^* e^{-ik\omega} e^{ij\omega} \\
&= \frac{1}{N} \left(\sum_k x_k e^{-ik\omega} \right) \left(\sum_j x_j e^{-ij\omega} \right)^* \\
&= \frac{1}{N} \hat{x}(\omega) \hat{x}(\omega)^* = \frac{1}{N} |\hat{x}(\omega)|^2 \quad (= \texttt{abs2.(fft(x))/N})
\end{aligned}
$$

Asymptotically unbiased but inconsistent (the variance does not vanish as N gets large).

How do else we estimate $S_X(\omega)$?
Bartlett's smoothing procedure: cut up the timeseries into k blocks. And approximate the peridogram $\tilde{S}_X^{(j)}(\omega)$ for each block of data $j = 1, 2, \ldots, k$.

$$\tilde{S}_X(\omega) = \frac{1}{k}\sum_{J=1}^{k}\tilde{S}_X^{(j)}(\omega)$$

This procedure allows us to control the variance, but at the expense of bias.
This procedure can be generalized.

General class of smoothed spectral estimators:
Bartlett:

$$\tilde{S}_X(\omega) = \frac{1}{k} \sum_{n=-k}^{k} \left(1 - \frac{|n|}{k}\right) \tilde{R}_X(n) e^{-in\omega}$$

General:

$$\tilde{S}_X(\omega) = \frac{1}{k} \sum_{n=-\infty}^{\infty} w(n) \tilde{R}_X(n)$$

with

$$\begin{aligned} &(1) \qquad w(0) = 1 \\ &(2) \qquad w(n) = w(-n) \\ &(3) \qquad w(n) = 0, \quad |n| \geq k, \quad k < N \end{aligned}$$

w is called a windowing function.

Most common window functions,

Bartlett:

$$w(n) = \begin{cases} 1 - \frac{|n|}{k}, & |n| \leq k \\ 0, & |n| > k \end{cases}$$

Tukey:

$$w(n) = \begin{cases} \frac{1}{2}\left(1 + \cos\frac{\pi n}{k}\right), & |n| \leq k \\ 0, & |n| > k \end{cases}$$

Parzen:

$$w(n) = \begin{cases} 1 - 6\left(\frac{n}{k}\right)^2 + 6\left(\frac{|n|}{k}\right)^3, & |n| \leq k/2 \\ 2\left(1 - \frac{|n|}{k}\right)^3, & k/2 < |n| \leq k \\ 0, & |n| > k \end{cases}$$

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What's Welch?

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- Lattice of autoregressive model of order p, $p = 1, \ldots, p_{\max}$.

$$X_n + a_{1,p}X_{n-1} + \cdots + a_{p,p}X_{n-p} = e_{n,p}$$

$$a_{p,p}X_n + a_{p-1,p}X_{n-1} + \cdots + X_{n-p} = r_{n,p}$$

- Minimize $E_p = \sum_{n=p+1}^{N} (|e_{n,p}|^2 + |r_{n,p}|^2)$
- Because of these are linear least squares coefficients

$$e_{n,p} = e_{n,p-1} + a_{p,p}r_{n-1,p-1}$$
$$r_{n,p} = a_{p,p}e_{n,p-1} + r_{n-1,p-1}$$

$$\begin{pmatrix} a_{1,p} \\ \vdots \\ a_{p-1,p} \end{pmatrix} = \begin{pmatrix} a_{1,p-1} \\ \vdots \\ a_{p-1,p-1} \end{pmatrix} + a_{p,p} \begin{pmatrix} a_{p-1,p-1} \\ \vdots \\ a_{1,p-1} \end{pmatrix}$$

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- We end up with

$$a_{p,p} = -\frac{2\sum_{n=p+1}^{N} e_{n,p-1} r_{n-1,r-1}}{\sum_{n=p+1}^{N} (e_{n,p-1}^2 + r_{n-1,r-1}^2)}$$

- For a given p the spectral estimate

$$\hat{S}_X^{\mathrm{Burg}} = \frac{\sigma_p^2}{|A(\omega)|^2} \qquad \text{where} \qquad A(\omega) = \sum_{k=0}^{p} a_{k,p} e^{-ik\omega}$$

the are a number of information criteria that can be used to select the order p.

Let us consider the stationary autoregressive process of order 2, with poles at $r_1 = .5, r_2 = -.8$

$$Y_n = (r_1 + r_2)Y_{n-1} - r_1 r_2 Y_{n-2} + e_n = -0.3Y_{n-1} + 0.4Y_{n-2} + e_n, \qquad \text{for } n > -\infty$$

for e_n are i.i.d. standard normal random variables.

One way to compute the z-spectrum is as follows. Recognize,

$$(r \star Y)_n = Y_n + 0.3Y_{n-1} - 0.4Y_{n-2} = e_n,$$

$$r = (\dots, 0, \boxed{1}, 0.3, -0.4, 0, \dots)$$

So that,

$$1 = S_e(z) = S_{(r\star Y)} = \bar{r}(z)S_Y(z)\bar{r}^*(z^{-*})$$

and

$$S_Y(z) = \frac{1}{\bar{r}(z)\bar{r}^*(z^{-*})} = \frac{1}{(1-0.5z^{-1})(1+0.8z^{-1})(1-0.5z)(1+0.8z)}$$

Example 1: AR(2) Signal

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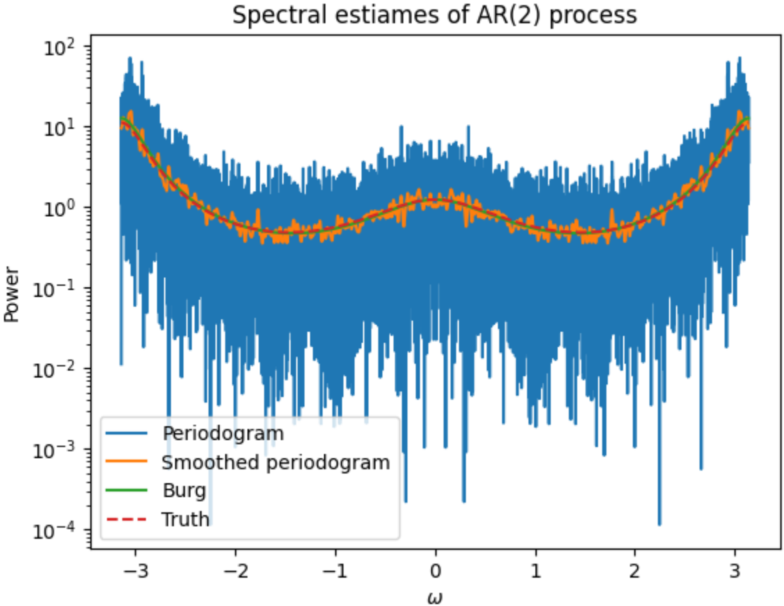
```
using DSP, PyPlot, FFTW
at  = include("../../Tools/AnalysisToolbox.jl")
se  = include("../../Tools/SpecEst.jl")
bg  = include("../../Tools/Burg.jl")

r1 = .5; r2 = -.8
r = [1, -(r1 + r2), r1*r2]
f(z) = sum(r[j]*z^(1-j) for j=1:3)

N = 10^4
fil = ZeroPoleGain(zeros(0),[r1,r2],1)
y = filt(fil,randn(N))

Sy_per = abs2.(fft(y))/N
Sy_num_gb = se.spec_GB(at.rowmatrix(y); Nex = N).S[:]
Sy_num_burg = bg.spec_mesa_sc(at.rowmatrix(y); Nex = N, p_max = 100).S[:]
Sy_ana = map(z -> 1/abs2(f(z)),exp.(2pi*im*(0:N-1)/N))

Θ = 2pi*(0:N-1)/N .- pi
title("Spectral estiames of AR(2) process")
semilogy(Θ,ifftshift(Sy_per), label = "Periodogram")
semilogy(Θ,ifftshift(Sy_num_gb), label = "Smoothed periodogram")
semilogy(Θ,ifftshift(Sy_num_burg), label = "Burg")
semilogy(Θ,ifftshift(Sy_ana), "--", label = "Truth")
ylabel("Power")
xlabel(L"\omega")
legend()
```

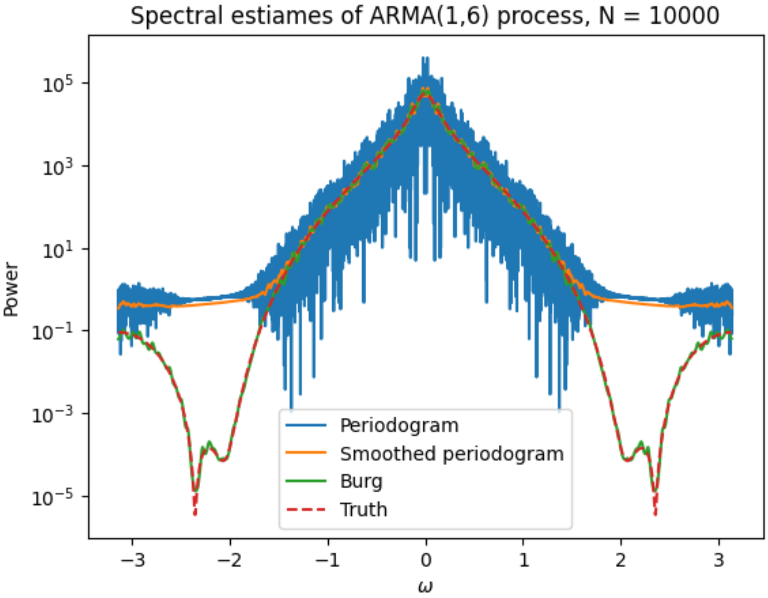


Spectral estiames of AR(2) process
Power
ω
Periodogram
Smoothed periodogram
Burg
Truth

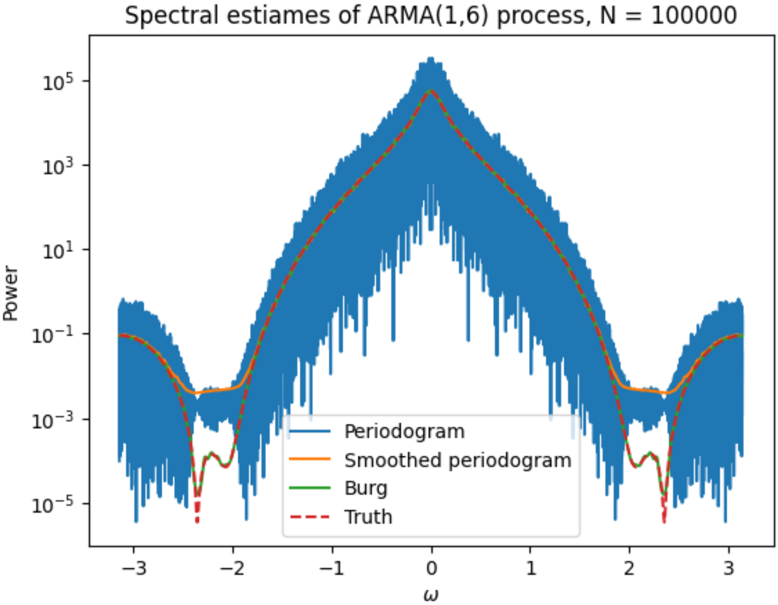
Example 2: AR(10) Signal


```
using DSP, PyPlot, FFTW, Polynomials
at  = include("../../Tools/AnalysisToolbox.jl")

Poles = [.9];

Zeros = [.99exp(1im*3pi/4); .99exp(-1im*3pi/4);
         .9exp(1im*3pi/2*.9); .9exp(-1im*3pi/2*.9);
         .9exp(1im*3pi/2*.9); .9exp(-1im*3pi/2*.9)]

spec = x -> at.poles2spec(Poles)(x) * at.zeros2spec(Zeros)(x)
spec = spec ∘ at.expi

N = 10^4
X = at.ARMA_gen(; steps = N, Poles, Zeros, rl = true)
X = at.rowmatrix(X)

Nex = 1000
L = 500

fgrid = se.θ(Nex) .- pi
SX_ana = spec.(fgrid);

SX_per = abs2.(fft(X[:]))/N
SX_num_gb = se.spec_GB(X; L, Nex).S[:]
SX_num_burg = bg.spec_mesa_sc(X; Nex, p_max = 100).S[:]

θ = 2pi*(0:N-1)/N .- pi
title("Spectral estiames of ARMA(1,6) process, N = $N")
semilogy(θ,ifftshift(SX_per), label = "Periodogram")
semilogy(fgrid,ifftshift(SX_num_gb), label = "Smoothed periodogram")
semilogy(fgrid,ifftshift(SX_num_burg), label = "Burg")
semilogy(fgrid,SX_ana, "--", label = "Truth")
ylabel("Power")
xlabel(L"\omega")
legend()
```

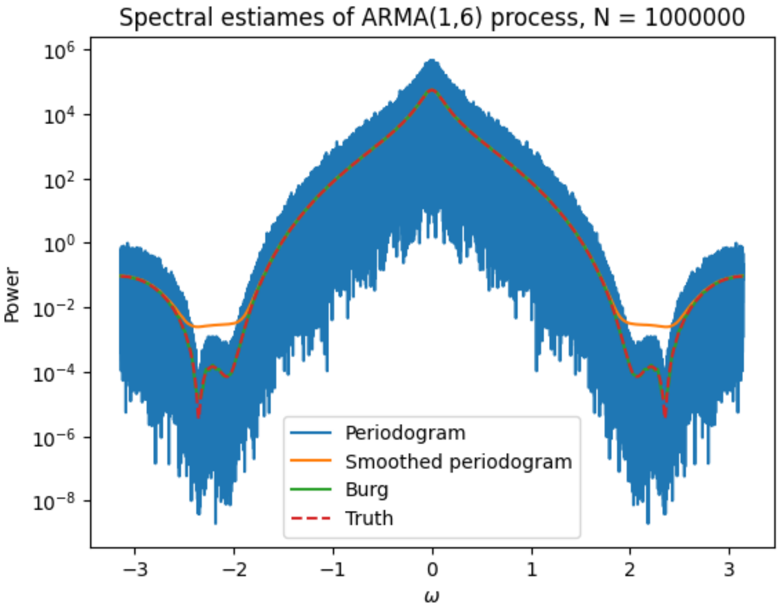
Example 2: AR(10) Signal



Example 2: AR(10) Signal



Example 2: AR(10) Signal



Now, spectral factorization!

Spectral Factorization

- For the numerical spectral factorization we do, assume $S_X(\omega)$ is rational.
- Because is a power spectrum, $S_X(\omega) \geq 0$ on $-\pi$ to π.
- So, we can factor $S_X(\omega) = L(\omega)L^*(\omega)$
  - $L(\omega) = \sqrt{S_X(\omega)}$
  - $L(\omega)$ is minimum phase
- minimum phase:
  - $\bar{S}_X(z) = \bar{L}(z)\bar{L}^*(z^{-*})$
  - $L(\omega) = \bar{L}(e^{i\omega})$
  - (minimum phase) $\bar{L}(z)$ and $\bar{L}^{-1}(z)$ are analytic on and outside the unit circle. ($\bar{L}(z)$ has all it's poles strictly inside the unit circle)

- Write $L^{-1}(\omega) = \sum_{n=-\infty}^{\infty} w_n e^{-i\omega n}$
- w_n is the Fourier coefficients of $L^{-1}(\omega)$

- It can be shown that

$$S_{w*X}(\omega) = L^{-1}(\omega) S_X(\omega) L^{-*}(\omega) = S_X(\omega)/S_X(\omega) = 1$$

- w is a whitening filter for X.

- If $L(\omega)$ is minimum phase, so is $L^{-1}(\omega)$ and

$$L^{-1}(\omega) = \sum_{n=0}^{\infty} w_n e^{-i\omega n}$$

So, $w_n = 0$ for $n < 0$, we say w is causal.

Spectral Factorization (Numerical)

Most Numerical algorithms assume $S(z)$ is rational and has the form of a Laurent Polynomial meaning it may be written as

$$S(z) = \sum_{n=-m}^{m} c_n z^{-n} \qquad \text{with } c_n = c^*_{-n}.$$

If this is assumed it may be shown that

$$S^+(z) = \sum_{n=1} L_n z^n \qquad \text{and} \qquad S^-(z) = \sum_{n=1} L^*_n z^{-n}$$

(this is what we assume here) Algorithms that use Toeplitz matrices.

- Bauer
- Schur
- Levinson-Durbin

Algorithms that use state-space formulations.

- Riccati Equation
- Kalman Filter
- Chadrasekhar-Kailath-Morf-Sidhu (CKMS)

A word about DFT

For the DFT which is used frequently in this work I use `fft` from FFTW.jl which is a Julia wrapper for the FFTW library written in C.
Here is what it does:

$$v_k = \texttt{fft}(u)_k = \sum_{j=1}^{N} u_j e^{-\frac{2\pi i}{N}(j-1)(k-1)}$$

$$u_j = \texttt{ifft}(v)_j = \frac{1}{N}\sum_{k=1}^{N} v_k e^{\frac{2\pi i}{N}(k-1)(j-1)}$$

Here is why I use it so much:
Suppose we have the function $S(z) = \sum_{j=1}^{N} c_j z^{-(j-1)}$ which we wish to evaluate at N equally-spaced, unit-circle points $z_k = e^{\frac{2\pi i}{N}(k-1)}$ for $k = 1, \ldots, N$. We need only use `fft` to get

$$S(z_k) = \sum_{j=1}^{N} c_j e^{-\frac{2\pi i}{N}(j-1)(k-1)} = \texttt{fft}(c)_k.$$

A word about DFT

So, given a causal finite impulse response (FIR) filter ℓ, it's transfer function $L(z)$ evaluated at N_{ex} evenly distributed points on the unit circle is the array

$$\left(L(z) : z = e^{2\pi ik/N_{ex}} \text{ for } k = 0, \ldots, N_{ex} - 1\right) =$$
$$\texttt{fft([}\ell\texttt{;zeros(Nex-length(}\ell\texttt{))])}$$

The first entry corresponds to $L(1)$ and the points go counterclockwise.
So, to get an approximate inverse of an causal FIR a filter.

- Parzen (1957): Error in Bartlett mainly due to variance.
- Control Variates
  - Estimate an expectation $\mu = \mathbb{E}X$, of some random variable X
  - Take n IID samples X_i of X

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} X_i.$$

  - $\hat{\mu}$ is an unbiased estimator of μ
  - $\text{var}(\hat{\mu}) = \text{var}(X)/n$.

- Suppose Y (mean zero) correlated with X.
- Take n IID samples Y_i of Y
- Consider

$$\hat{\mu}^{\mathrm{cv}} = \frac{1}{n} \sum_{i=1}^{n} X_i - \alpha Y_i$$

  - $\hat{\mu}^{\mathrm{cv}}$ is an unbiased estimator of μ
  - $\mathrm{var}(\hat{\mu}^{\mathrm{cv}}) = \frac{1}{n}\mathrm{var}(X - \alpha Y)$ and

$$\begin{aligned} \mathrm{var}(X - \alpha Y) &= \mathbb{E}(X - \alpha Y - \mu)(X - \alpha Y - \mu)^* \\ &= \mathbb{E}(X - \mu)(X - \mu)^* - \alpha \mathbb{E} Y (X - \mu)^* - \mathbb{E}(X - \mu) Y^* \alpha^* + \alpha \mathbb{E} Y Y^* \\ &= \mathrm{var}(X) - 2\mathcal{R}\{\alpha \mathrm{cov}(Y, X)\} + |\alpha|^2 \mathrm{var}(Y) \end{aligned}$$

  - minimizer $\alpha = \dfrac{\mathrm{cov}(Y, X)^*}{\mathrm{var}(Y)} = \dfrac{\mathrm{cov}(X, Y)}{\mathrm{var}(Y)}$

- So, for this $\alpha = \dfrac{\mathrm{cov}(X, Y)}{\mathrm{var}(Y)}$

$$\mathrm{var}(X - \alpha Y) = \mathrm{var}(X) - \frac{|\mathrm{cov}(X, Y)|^2}{\mathrm{var}(Y)} = \left(1 - |\rho_{XY}(0)|^2\right) \mathrm{var}(X).$$

- And,

$$\mathrm{var}(\hat{\mu}^{\mathrm{cv}}) = \frac{1 - |\rho_{XY}(0)|^2}{n} \mathrm{var}(X) = \left(1 - |\rho_{XY}(0)|^2\right) \mathrm{var}(\hat{\mu})$$

.

- So, for this $\alpha = \dfrac{\mathrm{cov}(X, Y)}{\mathrm{var}(Y)}$

$$\mathrm{var}(X - \alpha Y) = \mathrm{var}(X) - \frac{|\mathrm{cov}(X, Y)|^2}{\mathrm{var}(Y)} = \left(1 - |\rho_{XY}(0)|^2\right) \mathrm{var}(X).$$

- And,

$$\mathrm{var}(\hat{\mu}^{\mathrm{cv}}) = \frac{1 - |\rho_{XY}(0)|^2}{n} \mathrm{var}(X) = \left(1 - |\rho_{XY}(0)|^2\right) \mathrm{var}(\hat{\mu})$$

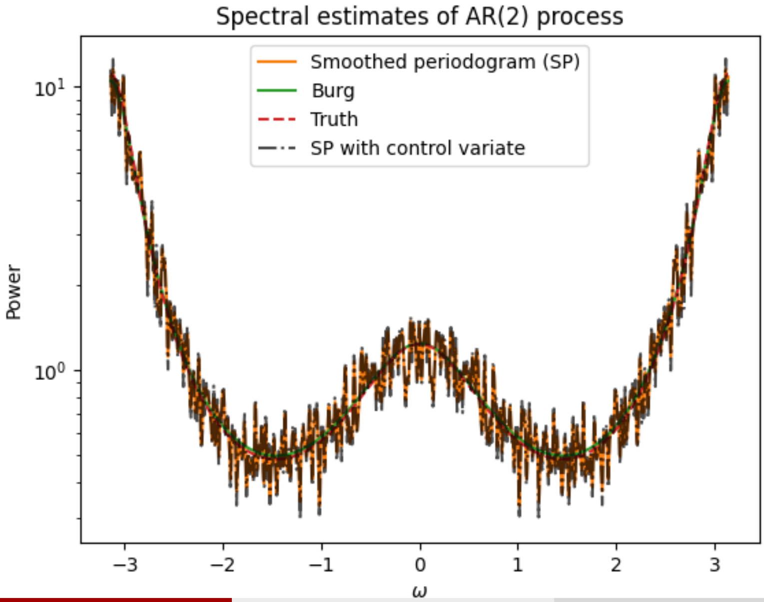
.

- How do I apply to spectral estimation?

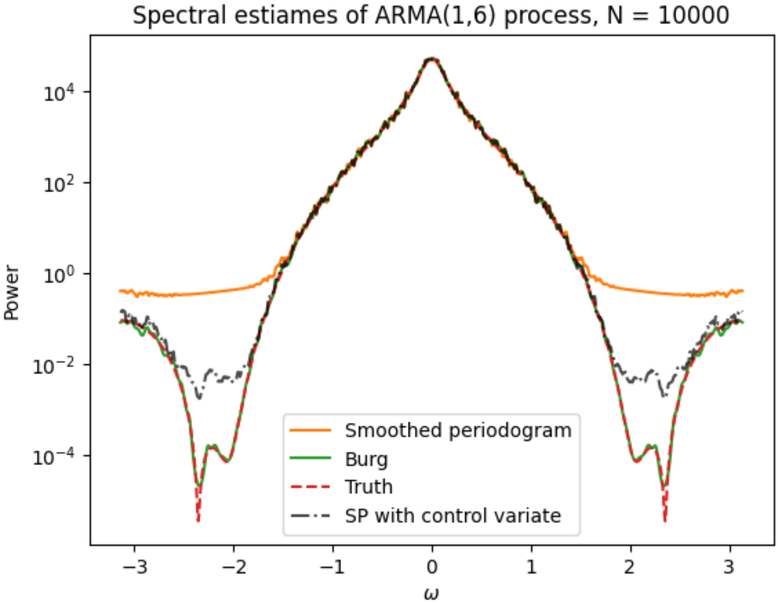
For timeseries $X = (X_j,\ j = 1, \ldots, N)$,

1. Divide the full timeseries X into K segments.
2. For each segment k, estimate the spectrum $\hat{S}^{(k)}$ and the whitened spectrum $\hat{W}^{(k)}$.
3. Take the logarithm $(\log \hat{S}^{(k)})_{k=1}^{K}$ and $(\log \hat{W}^{(k)})_{k=1}^{K}$.
4. Compute $\alpha = \frac{\mathrm{cov}_k\left(\log \hat{S}^{(k)}, \log \hat{W}^{(k)}\right)}{\mathrm{var}_k\left(\log \hat{W}^{(k)}\right)}$, at each frequency.
5. For $\hat{S}$ and $\hat{W}$, the spectrum and whitened spectrum of the full series, put

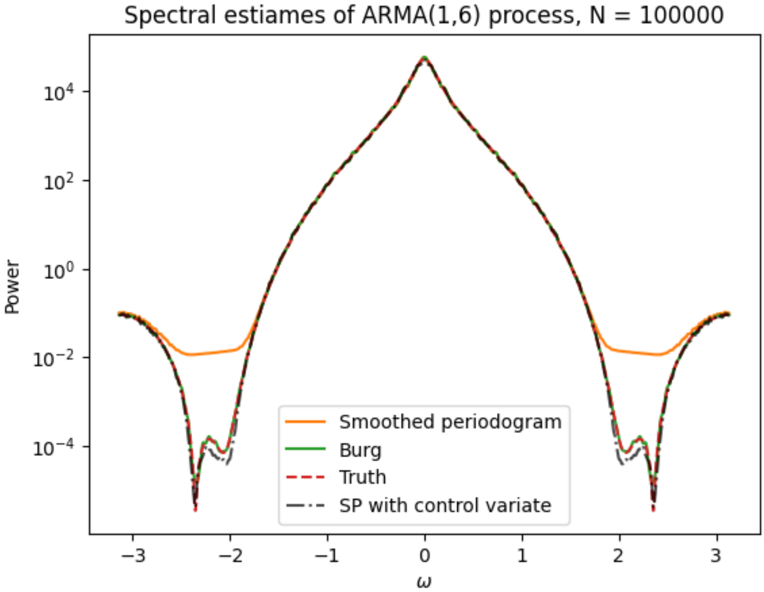
$$\hat{S}^{\mathrm{CV}} = \exp\left(\log \hat{S} - \alpha \log \hat{W}\right).$$


Spectral estimates of AR(2) process
Smoothed periodogram (SP)
Burg
Truth
SP with control variate
10^1
10^0
Power
−3
−2
−1
0
1
2
3
ω

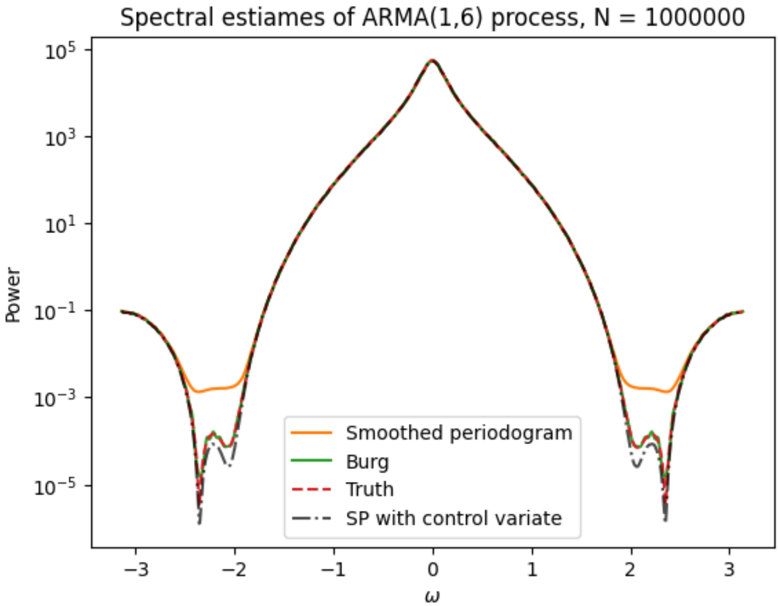
Example 2: AR(10) Signal



Example 2: AR(10) Signal



Example 2: AR(10) Signal



I first saw this while trying to whiten a KSE solution.

The Kuromoto-Sivishinsky equation (KSE) can be written as follows

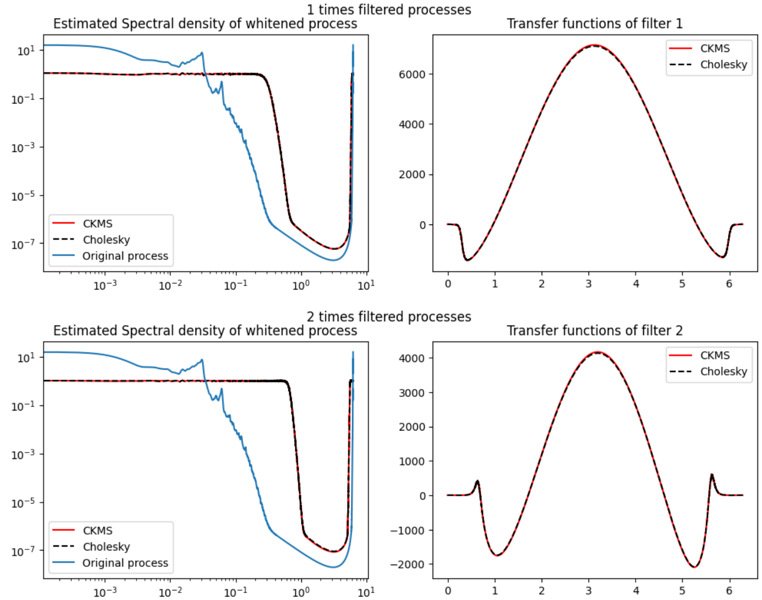
$$u_t + uu_x + u_{xx} + u_{xxxx} = 0$$

with $u(x+L,t) = u(x,t)$ for all $x \in \mathbb{R}$ and $t > 0$. And with $u(x,0) = g(x)$. Now, we use a fourier series to rewrite the KSE is Fourier space. Doing so gives

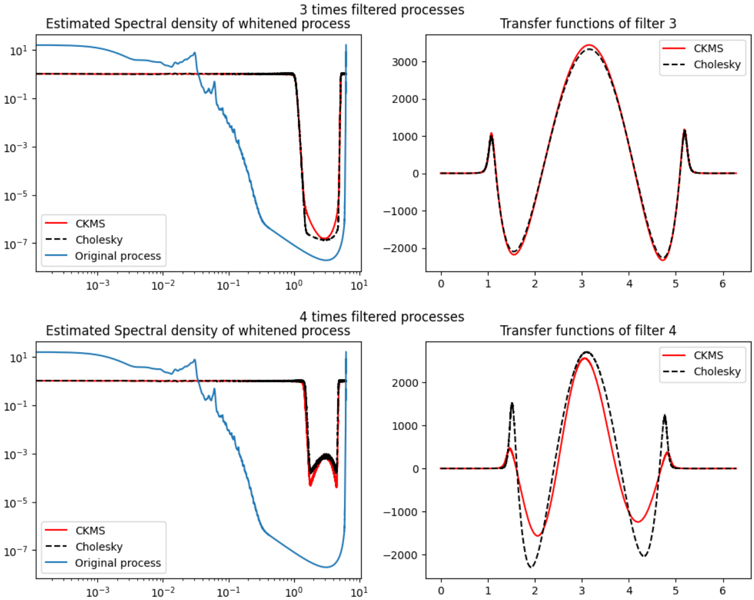
$$\dot{\hat{u}}_k = (q_k^2 - q_k^4)\hat{u}_k - \frac{iq_k}{2} \sum_{\ell=-\infty}^{\infty} \hat{u}_\ell \hat{u}_{k-\ell} \qquad (1)$$

Here, $q_k = \frac{2\pi}{L}k$. Note the trick: $uu_x = \frac{1}{2}\left(u^2\right)_x$.

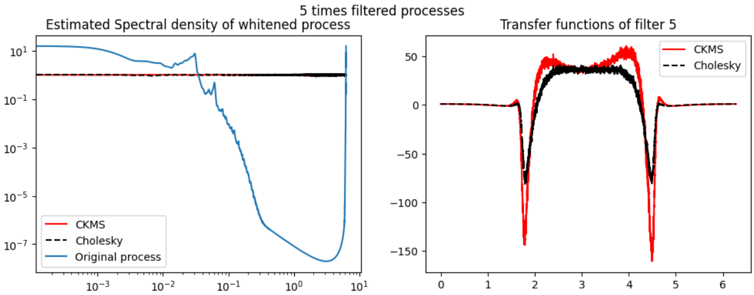
Example 3: KSE



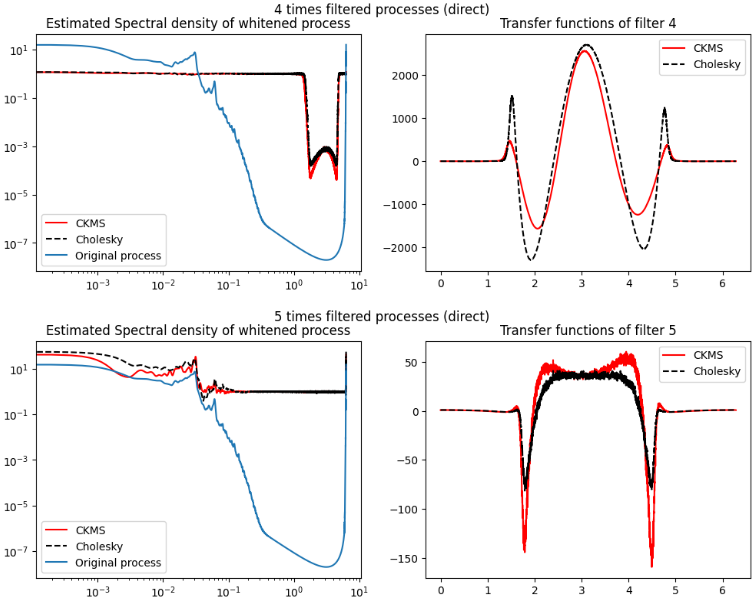
Example 3: KSE



Example 3: KSE



Example 3: KSE



Thank you!

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