SPECTRAL METHODS IN GAUSSIAN MODELLING

TOPIC 4: SPECTRUM ESTIMATION

James Requiema and Wessel Bruinsma

University of Cambridge and Invenia Labs

21 January 2019

• PSD is of wide interest.

- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



• Estimators:

- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



- Estimators:
 - \bullet parametric methods

- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



- Estimators:
 - parametric methods (SSA, SMK)

- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



- Estimators:
 - parametric methods (SSA, SMK),
 - nonparametric methods

- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



- Estimators:
 - parametric methods (SSA, SMK),
 - nonparametric methods (GPCM).

- PSD is of wide interest.
- Estimation difficult: samples limited, noisy, and nonuniform.



- Estimators:
 - parametric methods (SSA, SMK),
 - nonparametric methods (GPCM).
- Novel model by Tobar (2018).

$$f \sim \mathcal{GP}(0, k(t - t')),$$
 $s(\xi) | f = |\hat{f}(\xi)|^2.$

$$f \sim \mathcal{GP}(0, k(t - t')),$$
 $s(\xi) | f = |\hat{f}(\xi)|^2.$

• Estimator: $\hat{s}(\xi) = \mathbb{E}[s(\xi) | e]$.

$$f \sim \mathcal{GP}(0, k(t - t')),$$
 $s(\xi) | f = |\hat{f}(\xi)|^2.$

- Estimator: $\hat{s}(\xi) = \mathbb{E}[s(\xi) | e]$.
- Does not work: samples from f not integrable!

$$f \sim \mathcal{GP}(0, k(t - t')),$$
 $s(\xi) | f = |\hat{f}(\xi)|^2.$

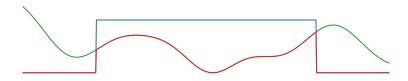
- Estimator: $\hat{s}(\xi) = \mathbb{E}[s(\xi) | e]$.
- \bullet Does not work: samples from f not integrable!
- Windowed version of f:

$$f_w(t) \mid f = f(t)w(t).$$

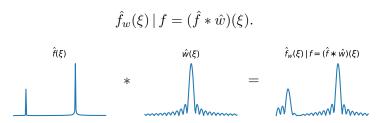
$$f \sim \mathcal{GP}(0, k(t - t')),$$
 $s(\xi) | f = |\hat{f}(\xi)|^2.$

- Estimator: $\hat{s}(\xi) = \mathbb{E}[s(\xi) | e]$.
- \bullet Does not work: samples from f not integrable!
- Windowed version of f:

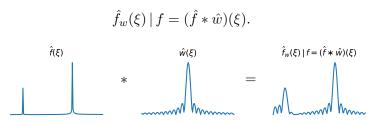
$$f_w(t) \mid f = f(t)w(t).$$



$$\hat{f}_w(\xi) \mid f = (\hat{f} * \hat{w})(\xi).$$



- Window functions:
 - algorithmic purposes (here: ensure integrability),



- Window functions:
 - algorithmic purposes (here: ensure integrability),
 - acquisition devices (e.g., sampling: $w = \coprod$).

$$f \sim \mathcal{GP}(0, k(t - t')),$$

$$f_w(t) \mid f = f(t)w(t),$$

$$s_w(\xi) \mid f_w = |\hat{f}_w(\xi)|^2.$$

$$f \sim \mathcal{GP}(0, k(t - t')),$$

$$f_w(t) \mid f = f(t)w(t),$$

$$s_w(\xi) \mid f_w = |\hat{f}_w(\xi)|^2.$$

• \hat{f}_w called local spectrum.

$$f \sim \mathcal{GP}(0, k(t - t')),$$

$$f_w(t) \mid f = f(t)w(t),$$

$$s_w(\xi) \mid f_w = |\hat{f}_w(\xi)|^2.$$

- \hat{f}_w called local spectrum.
- Estimator:

$$\hat{s}_w(\xi) = \mathbb{E}[s_w(\xi) | e] = \mathbb{E}[(\text{Re } \hat{f}_w(\xi))^2 | e] + \mathbb{E}[(\text{Im } \hat{f}_w(\xi))^2 | e].$$

$$f \sim \mathcal{GP}(0, k(t - t')),$$

$$f_w(t) \mid f = f(t)w(t),$$

$$s_w(\xi) \mid f_w = |\hat{f}_w(\xi)|^2.$$

- \hat{f}_w called local spectrum.
- Estimator:

$$\hat{s}_w(\xi) = \mathbb{E}[s_w(\xi) | e] = \mathbb{E}[(\text{Re } \hat{f}_w(\xi))^2 | e] + \mathbb{E}[(\text{Im } \hat{f}_w(\xi))^2 | e].$$

• Choices:

•
$$w(t) = \exp(-\alpha \pi^2 t^2),$$
 (tractability)

$$f \sim \mathcal{GP}(0, k(t - t')),$$

$$f_w(t) \mid f = f(t)w(t),$$

$$s_w(\xi) \mid f_w = |\hat{f}_w(\xi)|^2.$$

- \hat{f}_w called local spectrum.
- Estimator:

$$\hat{s}_w(\xi) = \mathbb{E}[s_w(\xi) | e] = \mathbb{E}[(\text{Re } \hat{f}_w(\xi))^2 | e] + \mathbb{E}[(\text{Im } \hat{f}_w(\xi))^2 | e].$$

• Choices:

•
$$w(t) = \exp(-\alpha \pi^2 t^2),$$
 (tractability)

• k = SMK or EQ in simple cases.

- Notation:
 - $k_{fg}(t, t') = \mathbb{E}[f^*(t)g(t')]$ with $k_{ff} = k_f$,

• Notation:

- $k_{fg}(t, t') = \mathbb{E}[f^*(t)g(t')]$ with $k_{ff} = k_f$,
- $\mathcal{F}_t\{f(t)\}(\xi) = \int_{-\infty}^{\infty} f(t)e^{-2\pi \iota \xi t} dt.$

- Notation:
 - $k_{fg}(t,t') = \mathbb{E}[f^*(t)g(t')]$ with $k_{ff} = k_f$,

•
$$\mathcal{F}_t\{f(t)\}(\xi) = \int_{-\infty}^{\infty} f(t)e^{-2\pi \iota \xi t} dt$$
.

• We desire

$$k_{\text{Re }\hat{f}_w}(\xi, \xi')$$

$$k_{y(\text{Re }\hat{f}_w)}(t, \xi)$$

$$k_{\text{Im }\hat{f}_w}(\xi, \xi')$$

$$k_{y(\text{Im }\hat{f}_w)}(t, \xi)$$

• Notation:

•
$$k_{fg}(t,t') = \mathbb{E}[f^*(t)g(t')]$$
 with $k_{ff} = k_f$,

•
$$\mathcal{F}_t\{f(t)\}(\xi) = \int_{-\infty}^{\infty} f(t)e^{-2\pi\iota\xi t} dt$$
.

• We desire

$$\begin{split} k_{\text{Re }\hat{f}_w}(\xi,\xi') &= \frac{1}{2} (k_{\hat{f}_w}(\xi,\xi') + k_{\hat{f}_w}(\xi,-\xi')), \\ k_{y(\text{Re }\hat{f}_w)}(t,\xi) &= \text{Re } k_{y\hat{f}_w}(t,\xi), \\ k_{\text{Im }\hat{f}_w}(\xi,\xi') &= \frac{1}{2} (k_{\hat{f}_w}(\xi,\xi') - k_{\hat{f}_w}(\xi,-\xi')), \\ k_{y(\text{Im }\hat{f}_w)}(t,\xi) &= \text{Im } k_{y\hat{f}_w}(t,\xi). \end{split}$$

$$k_{\hat{f}_w}(\xi, \xi')$$

$$k_{\hat{f}_w}(\xi, \xi') = \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')]$$

$$k_{\hat{f}_w}(\xi, \xi') = \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')]$$

= $\mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi, \xi')]$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')] \\ &= \mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi,\xi')] \\ &= (\mathcal{F}_{t,t'}\{k(t-t')\}(u,u')*\mathcal{F}_{t,t'}\{w(t)w(t')\}(u,u'))(-\xi,\xi'), \end{split}$$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')] \\ &= \mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi,\xi')] \\ &= (\mathcal{F}_{t,t'}\{k(t-t')\}(u,u')*\mathcal{F}_{t,t'}\{w(t)w(t')\}(u,u'))(-\xi,\xi'), \\ &= (\hat{k}(u)\delta(u+u')*\hat{r}_w(u,u'))(-\xi,\xi'). \end{split}$$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')] \\ &= \mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi,\xi')] \\ &= (\mathcal{F}_{t,t'}\{k(t-t')\}(u,u')*\mathcal{F}_{t,t'}\{w(t)w(t')\}(u,u'))(-\xi,\xi'), \\ &= (\hat{k}(u)\delta(u+u')*\hat{r}_w(u,u'))(-\xi,\xi'). \end{split}$$

$$\hat{r}_w(\xi+u,\xi'+u) &= \mathcal{N}(\xi-\xi';0,\alpha)\mathcal{N}(u;\frac{1}{2}(\xi+\xi'),\frac{1}{4}\alpha). \end{split}$$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')] \\ &= \mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi,\xi')] \\ &= (\mathcal{F}_{t,t'}\{k(t-t')\}(u,u') * \mathcal{F}_{t,t'}\{w(t)w(t')\}(u,u'))(-\xi,\xi'), \\ &= (\hat{k}(u)\delta(u+u') * \hat{r}_w(u,u'))(-\xi,\xi'). \\ \\ \hat{r}_w(\xi+u,\xi'+u) &= \mathcal{N}\big(\xi-\xi';0,\alpha\big)\mathcal{N}\big(u;\frac{1}{2}(\xi+\xi'),\frac{1}{4}\alpha\big). \\ \\ k_{\hat{f}_w}(\xi,\xi') &= \int \hat{k}(u)\delta(u+u')\hat{r}_w(-\xi-u,\xi'-u')\,\mathrm{d}u\,\mathrm{d}u' \end{split}$$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')] \\ &= \mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi,\xi')] \\ &= (\mathcal{F}_{t,t'}\{k(t-t')\}(u,u') * \mathcal{F}_{t,t'}\{w(t)w(t')\}(u,u'))(-\xi,\xi'), \\ &= (\hat{k}(u)\delta(u+u') * \hat{r}_w(u,u'))(-\xi,\xi'). \\ \\ \hat{r}_w(\xi+u,\xi'+u) &= \mathcal{N}\big(\xi-\xi';0,\alpha\big)\mathcal{N}\big(u;\frac{1}{2}(\xi+\xi'),\frac{1}{4}\alpha\big). \\ \\ k_{\hat{f}_w}(\xi,\xi') &= \int \hat{k}(u)\delta(u+u')\hat{r}_w(-\xi-u,\xi'-u')\,\mathrm{d}u\,\mathrm{d}u' \end{split}$$

$$k_{\hat{f}_w}(\xi, \xi') = \int \hat{k}(u)\delta(u + u')\hat{r}_w(-\xi - u, \xi' - u') du du$$
$$= \int \hat{k}(u)\hat{r}_w(\xi + u, \xi' + u) du$$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathbb{E}[\hat{f}_w^*(\xi)\hat{f}_w(\xi')] \\ &= \mathbb{E}[\mathcal{F}_{t,t'}\{f(t)f(t')w(t)w(t')\}(-\xi,\xi')] \\ &= (\mathcal{F}_{t,t'}\{k(t-t')\}(u,u') * \mathcal{F}_{t,t'}\{w(t)w(t')\}(u,u'))(-\xi,\xi'), \\ &= (\hat{k}(u)\delta(u+u') * \hat{r}_w(u,u'))(-\xi,\xi'). \end{split}$$

$$\hat{r}_w(\xi+u,\xi'+u) &= \mathcal{N}(\xi-\xi';0,\alpha)\mathcal{N}(u;\frac{1}{2}(\xi+\xi'),\frac{1}{4}\alpha). \end{split}$$

$$k_{\hat{f}_w}(\xi, \xi') = \int \hat{k}(u)\delta(u+u')\hat{r}_w(-\xi-u, \xi'-u')\,\mathrm{d}u\,\mathrm{d}u'$$

$$= \int \hat{k}(u)\hat{r}_w(\xi+u, \xi'+u)\,\mathrm{d}u$$

$$= \mathcal{N}(\xi-\xi'; 0, \alpha)\left(\hat{k}(u) * \mathcal{N}(u; 0, \frac{1}{4}\alpha)\right)\left(\frac{1}{2}(\xi+\xi')\right).$$

 $k_{y\hat{f}_w}(t,\xi)$

$$k_{y\hat{f}_w}(t,\xi) = \mathbb{E}[y^*(t)\mathcal{F}_{t'}\{f(t')w(t')\}(\xi)]$$

$$k_{y\hat{f}_w}(t,\xi) = \mathbb{E}[y^*(t)\mathcal{F}_{t'}\{f(t')w(t')\}(\xi)]$$
$$= \mathcal{F}_{t'}\{k(t-t')w(t')\}(\xi)$$

$$k_{y\hat{f}_w}(t,\xi) = \mathbb{E}[y^*(t)\mathcal{F}_{t'}\{f(t')w(t')\}(\xi)]$$
$$= \mathcal{F}_{t'}\{k(t-t')w(t')\}(\xi)$$
$$= (\hat{k}(u)e^{-2\pi\iota ut} * \mathcal{F}\{w\}(u))(\xi)$$

$$\begin{split} k_{y\hat{f}_{w}}(t,\xi) &= \mathbb{E}[y^{*}(t)\mathcal{F}_{t'}\{f(t')w(t')\}(\xi)] \\ &= \mathcal{F}_{t'}\{k(t-t')w(t')\}(\xi) \\ &= (\hat{k}(u)e^{-2\pi\iota ut} * \mathcal{F}\{w\}(u))(\xi) \\ &= \Big(\hat{k}(u)e^{-2\pi\iota ut} * \mathcal{N}\big(u;0,\frac{1}{2}\alpha\big)\Big)(\xi). \end{split}$$

$$k_{\hat{f}_w}(\xi, \xi') = \mathcal{N}\left(\xi - \xi'; 0, \alpha\right) \left(\hat{k}(u) * \mathcal{N}\left(u; 0, \frac{1}{4}\alpha\right)\right) \left(\frac{1}{2}(\xi + \xi')\right)$$

$$k_{y\hat{f}_w}(t,\xi) = \left(\hat{k}(u)e^{-2\pi\iota ut} * \mathcal{N}\left(u;0,\tfrac{1}{2}\alpha\right)\right)\!(\xi)$$

$$k_{\hat{f}_w}(\xi, \xi') = \mathcal{N}(\xi - \xi'; 0, \alpha) \left(\hat{k}(u) * \mathcal{N}(u; 0, \frac{1}{4}\alpha)\right) \left(\frac{1}{2}(\xi + \xi')\right)$$
$$\approx \mathcal{N}(\xi - \xi'; 0, \alpha) \hat{k}\left(\frac{1}{2}(\xi + \xi')\right),$$

$$k_{y\hat{f}_w}(t,\xi) = \left(\hat{k}(u)e^{-2\pi\iota ut} * \mathcal{N}\left(u;0,\frac{1}{2}\alpha\right)\right)(\xi)$$

$$\begin{split} k_{\hat{f}_w}(\xi,\xi') &= \mathcal{N}\big(\xi-\xi';0,\alpha\big) \Big(\hat{k}(u) * \mathcal{N}\big(u;0,\tfrac{1}{4}\alpha\big)\Big) \big(\tfrac{1}{2}(\xi+\xi')\big) \\ &\approx \mathcal{N}\big(\xi-\xi';0,\alpha\big) \hat{k}\big(\tfrac{1}{2}(\xi+\xi')\big), \\ k_{y\hat{f}_w}(t,\xi) &= \Big(\hat{k}(u)e^{-2\pi\iota ut} * \mathcal{N}\big(u;0,\tfrac{1}{2}\alpha\big)\Big)(\xi) \\ &\approx \hat{k}(\xi)e^{-2\pi\iota \xi t}. \end{split}$$

$$\mathbb{E}[\hat{f}_w(\xi) \mid e] = \int \hat{k}(u) \left(\sum_{i=1}^N e^{-2\pi \iota u t_i} (K_e^{-1} e)_i \right) \mathcal{N}(u; \xi, \frac{1}{2}\alpha) \, \mathrm{d}u.$$

$$\mathbb{E}[\hat{f}_w(\xi) \mid e] = \int \hat{k}(u) \left(\sum_{i=1}^N e^{-2\pi \iota u t_i} (K_e^{-1} e)_i \right) \mathcal{N}\left(u; \xi, \frac{1}{2}\alpha\right) du.$$

• Interpretation: **DFT** of whitened observations, weighted by prior, then smoothed due to window.

$$\mathbb{E}[\hat{f}_w(\xi) \mid e] = \int \hat{k}(u) \left(\sum_{i=1}^N e^{-2\pi \iota u t_i} (K_e^{-1} e)_i \right) \mathcal{N}\left(u; \xi, \frac{1}{2}\alpha\right) du.$$

- Interpretation: DFT of whitened observations, weighted by prior, then smoothed due to window.
- If prior uninformative, $K_e \approx I$, then weighted DFT in the limit:

$$\lim_{\alpha \to 0} \mathbb{E}[\hat{f}_w(\xi) \mid e] \approx \hat{k}(\xi) \sum_{i=1}^N e^{-2\pi \iota \xi t_i} e_i.$$

• Commonly used for nonuniform data.

- Commonly used for nonuniform data.
- For each ξ , LS fits a sine using least squares:

$$f(t) = A\sin(2\pi\xi t) + B\cos(2\pi\xi t).$$

- Commonly used for nonuniform data.
- For each ξ , LS fits a sine using least squares:

$$f(t) = A\sin(2\pi\xi t) + B\cos(2\pi\xi t).$$

- Commonly used for nonuniform data.
- For each ξ , LS fits a sine using least squares:

$$f(t) = A\sin(2\pi\xi t) + B\cos(2\pi\xi t).$$

BNSE:

Lomb-Scargle:

+ Probabilistic

Deterministic

- Commonly used for nonuniform data.
- For each ξ , LS fits a sine using least squares:

$$f(t) = A\sin(2\pi\xi t) + B\cos(2\pi\xi t).$$

BNSE:

+ Probabilistic

+ Nonparametric

Lomb-Scargle:

- Deterministic
- Parametric

- Commonly used for nonuniform data.
- For each ξ , LS fits a sine using least squares:

$$f(t) = A\sin(2\pi\xi t) + B\cos(2\pi\xi t).$$

BNSE:

- + Probabilistic
- + Nonparametric
- + Closed-form estimate

Lomb-Scargle:

- Deterministic
- Parametric
- Optimisation per ξ

- Commonly used for nonuniform data.
- For each ξ , LS fits a sine using least squares:

$$f(t) = A\sin(2\pi\xi t) + B\cos(2\pi\xi t).$$

BNSE:

- + Probabilistic
- + Nonparametric
- + Closed-form estimate

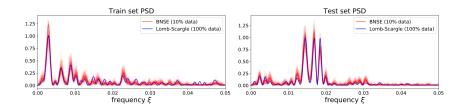
Lomb-Scargle:

- Deterministic
- Parametric
- Optimisation per ξ
- Gaussian prior on A and B: LS recovers BNSE in the limit.

• k = SMK.

- k = SMK.
- Trained on first, tested on second.

- k = SMK.
- Trained on first, tested on second.



(Figure taken from Tobar (2018).)

• BNSE (Tobar, 2018) novel nonparametric model for SE.

- BNSE (Tobar, 2018) novel nonparametric model for SE.
- Bayesian in nature: handles uncertainty automatically.



- BNSE (Tobar, 2018) novel nonparametric model for SE.
- Bayesian in nature: handles uncertainty automatically.



• Closed-form estimate of PSD.

- BNSE (Tobar, 2018) novel nonparametric model for SE.
- Bayesian in nature: handles uncertainty automatically.



- Closed-form estimate of PSD.
- \Rightarrow Can optimise to find periodicities.