Covariance estimation based on *Slow Fourier Transforms*

Seminaris d'Estadística

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outline

- what is a (cross)-covariance function?
- characterization of covariance functions: Bochner's Theorem
- why not **fft**?
- alternative: **sft**
- **sft** to model covariances

Cross-covariance functions

- random field, random function, stochastic process:

$$Z(\vec{x}), \vec{x} \in \mathcal{D} \subset \mathbb{R}^4$$

- stationarity of the mean:

$$\mathsf{E}\left[Z(\vec{x}_n)\right] = \mu$$

- auto-covariance function:

$$\mathsf{Cov}\left[Z(\vec{x}_n), Z(\vec{x}_m)\right] = C(\vec{x}_n - \vec{x}_m) = C(\vec{h})$$

- cross-covariance function:

$$\mathsf{Cov}\left[Z_i(\vec{x}_n), Z_j(\vec{x}_m)\right] = C_{ij}(\vec{x}_n - \vec{x}_m) = C_{ij}(\vec{h})$$

Bochner's Theorem (1D)

- covariances $C(\vec{h})$ must be positive definite (PD)
- **Theorem:** In $1D$, a continuous real function $C(\vec{h})$, with $\vec{h} \in \mathbb{R}^p$, is PD if and only if it is the FT of a positive symmetric bounded measure $F(\underline{\omega})$,

$$C(\vec{h}) = \int_{\mathbb{R}^p} e^{2\pi i \langle \vec{h}, \vec{\omega} \rangle} dF(\vec{\omega}) = \int_{\mathbb{R}^p} \cos\left(2\pi \langle \vec{h}, \vec{\omega} \rangle\right) dF(\vec{\omega}),$$

  with $dF(\vec{\omega}) \geq 0$ and $\int dF(\vec{\omega}) < \infty$ (Bochner, 1959).
- in practical cases $dF(\omega) = f(\omega) d\omega$ (regularity)
- if $C(\vec{0}) = 1$ (correlogram), then $F(\mathbb{R}^p) = 1$ (PdF)

fft *for covariance estimation (1D)*

Rehman (1995), covariance modelling fitting spectral decomposition series

Yao and Journel (1998), automatic modelling of covariance tables by **fft**

- estimate $\rho_n = \rho(\vec{h}_n)$ for all $\vec{h}_n$
- fill the empty cells by applying "kernels"
- check $f_k = f(\omega_k) \geq 0$ for all ω_k
- if not, smooth ρ_n by moving windows
- if the window is too big, trim $f_k = 0$
- restandardize to ensure $\rho(0) = 1$ (ad-hoc weights)

Why not Fast Fourier Transform (fft)?

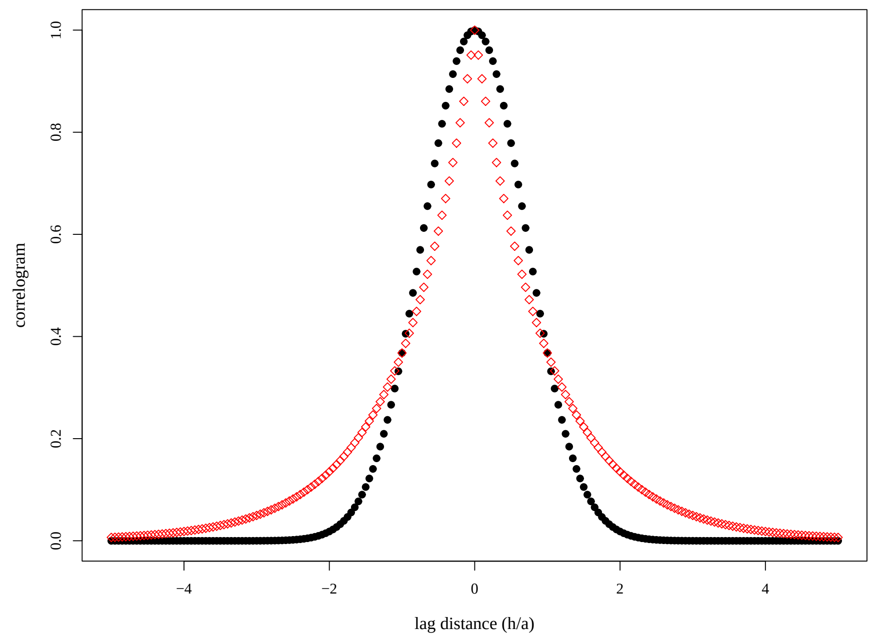
$$f_k^* = f^*(\omega_k) = \sum_{n=0}^{N-1} f(x_n) e^{-2\pi i \omega_k x_n} = \sum_{n=0}^{N-1} f_n e^{-2\pi i (k\Delta\omega)(n\Delta x)},$$

imposed limitations on the frequencies:

- periodic beyond $\rightarrow$ smallest $\omega_1 = 1/T$ (*Nyquist*)
- between the nodes? $\rightarrow$ discrete ω domain: $\omega_n = n \cdot \omega_1$
- only whole cycles $\rightarrow$ highest $\omega_{max} = \frac{\Delta x}{2} = \frac{N}{2T} = \omega_{N/2}$
- symmetry on the frequencies: $f^*_{N/2+k} = f^*_{N/2-k}$

why not Fast Fourier Transform (fft)?

- undesirable characteristics of **fft**
  - resolution concentrated in high ω (discontinuity, nugget, linear behaviour near the origin)
  - poor resolution in low ω (hole effects, range)



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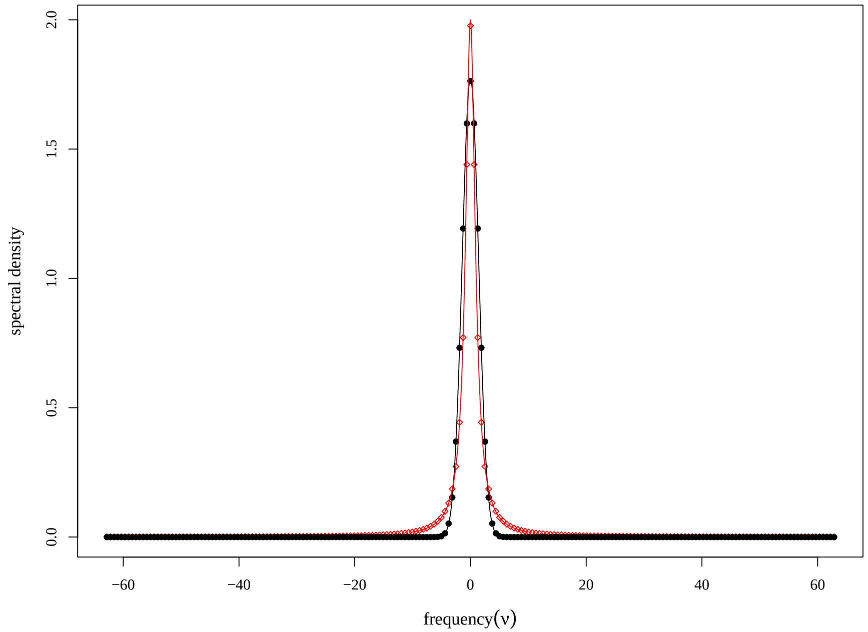

why not Fast Fourier Transform (fft)?

- undesirable characteristics of **fft**
  - resolution concentrated in high ω (discontinuity, nugget, linear behaviour near the origin)
  - poor resolution in low ω (hole effects, range)
  - the denser the lags, the higher ω
  - the higher the maximum lag distance, the better ω precision
- reasonable helpful assumptions for $C(\vec{h})$
  - continuous and smooth
  - bounded outside the estimated lag range

Slow Fourier Transform (sft)

$$f^*(\omega) = \int_{\mathbb{R}} f(x) e^{-2\pi i \omega x} dx,$$

- complementary information:
  - bounded beyond the limits $\longrightarrow f^*(0) < \infty$
  - smooth between the nodes $\longrightarrow \omega \longrightarrow \infty \quad f^*(\omega) \longrightarrow 0$
  - partial cycles $\longrightarrow$ interpolation on ω
- we can acceptably compute $f^*(\omega)$ at any *desired* frequency

Slow Fourier Transform (*sft*)

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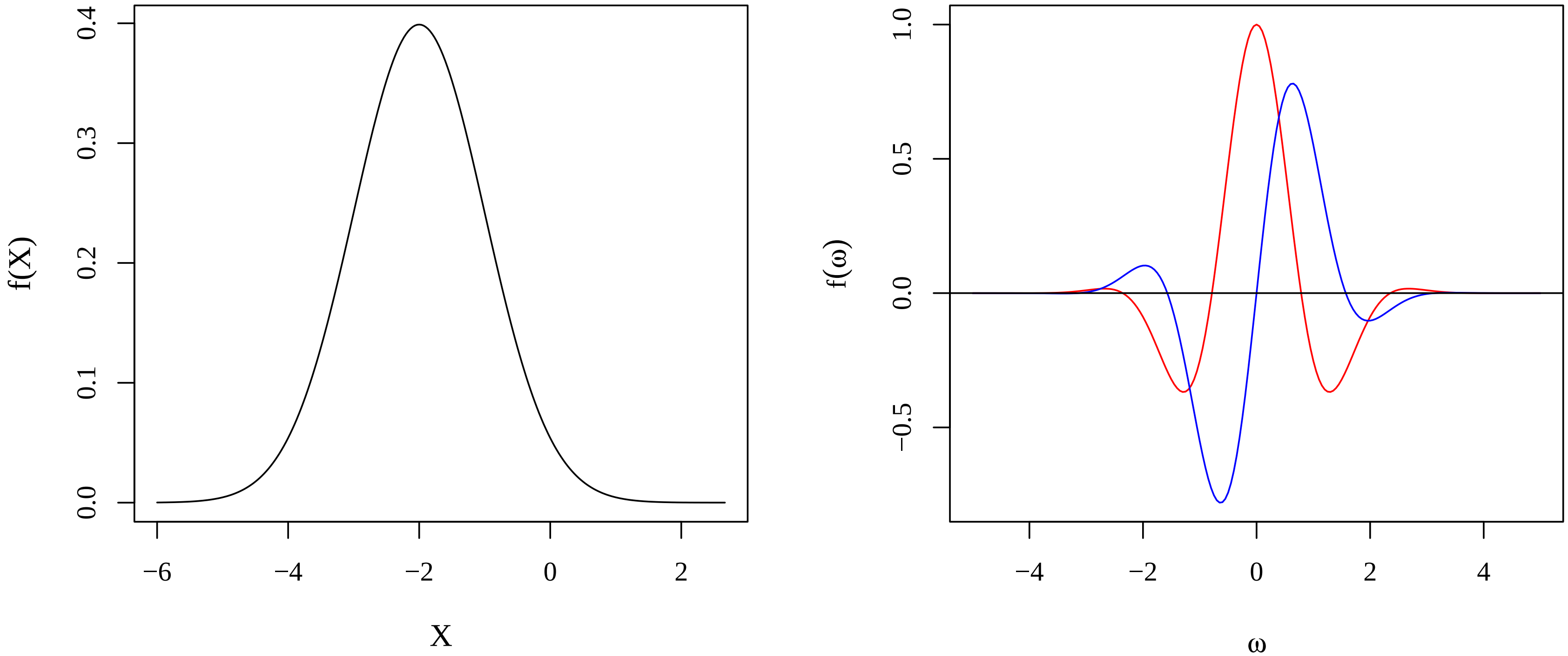
sft to approximate FT



sft to approximate FT

$$f^*(\vec{\omega}) = \int_{\mathbb{R}^{N+1}} f(\vec{x}) e^{-2\pi i \langle \vec{\omega}, \vec{x} \rangle} d\vec{x} = \mathsf{E}\left[e^{-2\pi i \langle \vec{\omega}, \vec{x} \rangle}\right]$$

$$f^*(\vec{\omega}) \approx \sum_{\vec{x}} e^{-2\pi i \langle \vec{\omega}, \vec{x} \rangle}$$

where

$$\vec{x} \sim f(\vec{x})$$

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where

$$\vec{x} \sim U(\mathcal{D}om(\vec{X}))$$

inverse sft to approximate FT^{-1}

$$f(\vec{x}) = \int_{\mathbb{R}^{N+1}} f^*(\vec{\omega}) e^{+2\pi i \langle \vec{\omega}, \vec{x} \rangle} d\vec{\omega}$$

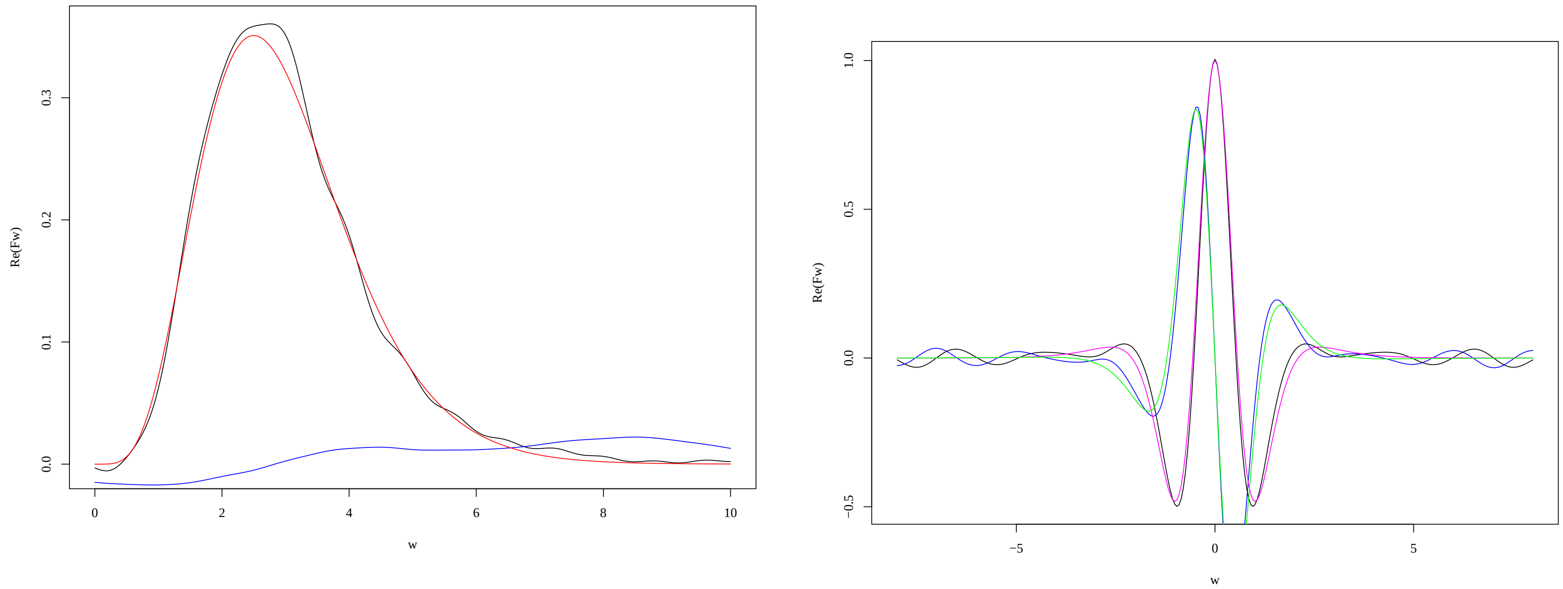
$$f(\vec{x}) \approx \sum_{\vec{\omega}} f^*(\vec{\omega}) e^{+2\pi i \langle \vec{\omega}, \vec{x} \rangle}$$

where

$$\vec{\omega} \sim U(\mathcal{D}om(\vec{\omega}))$$

for the observed values $x_1, x_2, \ldots x_N$, and all possible values of X_0 we get $f(x_0)$

a round-trip using sft



$$X \sim \Gamma(\lambda = 1/3, r = 6) \qquad f^*(\omega) = \left(\frac{\lambda}{\lambda + 2i\pi\omega}\right)^r$$

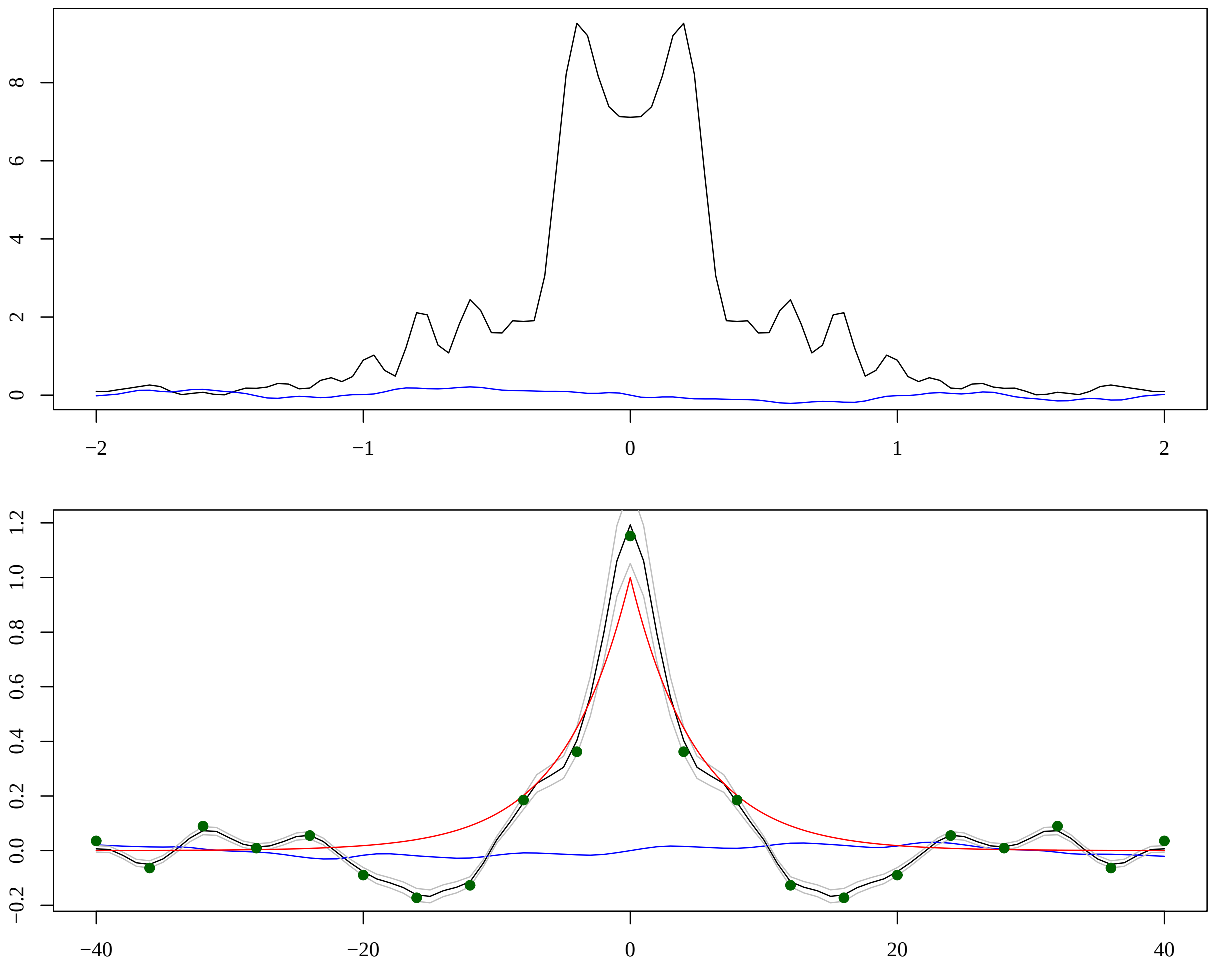
why better sft?

- maximum h: either fixed by data or user, $C(h) = 0$
- maximum ω: fixed by "model", $\nu = 2\pi\omega a, \tau = \frac{2\pi a}{t}$,

model	density	5% interval	1% interval
spherical	(naf)	7.90	22.12
exponential	Cauchy	12.71	31.82
gaussian	normal	2.77	3.29
hole effect	$\frac{\pi+\arctan(\nu+\tau)+\arctan(\nu-\tau)}{2\pi}$		

- precision on h: what needed (kriging, simulation)
- precision on ω: computation/storage/time limits

example: sft for covariance estimation (1D)



sft for covariance estimation (+D)

Proposition: The continuous $C_{jk}(\vec{h})$ are the elements of a valid covariance function matrix of a D-dim 2^{nd}-order SRF $Z(\vec{x}) \iff$ they are the FT of spectra $F_{jk}(\vec{\omega})$ which form a PD matrix for any (Borel) set $B \in \mathbb{R}^p$,

- namely

$$\sum_{j=1}^{D}\sum_{k=1}^{D} \lambda_j F_{jk}(B)\overline{\lambda_k} \geq 0$$

for any set of complex coefficients $\lambda_1, \lambda_2 \ldots \lambda_D$ (Cramér, 1940).

sft for covariance estimation (+D)

Proposition: The continuous $C_{jk}(\vec{h})$ are the elements of a valid covariance function matrix of a D-dim 2^{nd}-order SRF $Z(\vec{x}) \iff$ they are the FT of spectra $F_{jk}(\vec{\omega})$ which form a PD matrix for any (Borel) set $B \in \mathbb{R}^p$,

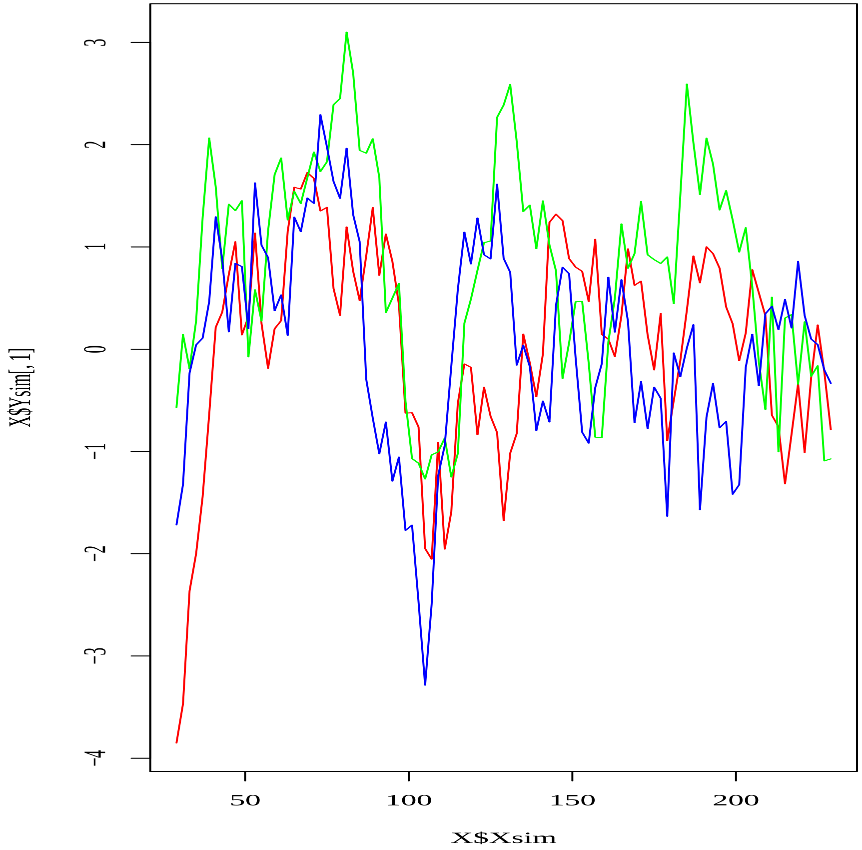
- if $\int |C_{jk}(\vec{h})| < \infty$ is absolutely integrable, then $f_{jk}(\vec{\omega})$ is continuous and bounded, and can be computed by Inverse FT
- ensure that the matrix $F(\vec{\omega}) = (f_{jk}(\vec{\omega}))$ is PD for any $\vec{\omega}$
- functional PD of $C(\vec{h}) \Longrightarrow$ matricial PD of $F(\vec{\omega})$ for all $\vec{\omega}$

sft *for covariance estimation (+D):*
Algorithm

- estimate $C_{ij}(\vec{h})$ from data
- choose an interval for ω
- estimate $f_{ij}(\vec{\omega})$ with **sft**
- compute svd of $F(\vec{\omega})$ for all $\vec{\omega}$
- ensure positivity of all eigenvalues (*e.g.* trim)
- recover a PD $F(\vec{\omega})$
- fix the set of $\vec{h}$ where a $C_{ij}(\vec{h})$ is needed
- backtransform $f_{ij}(\vec{\omega})$ with inverse **sft** for chosen $\vec{h}$

sft for covariance estimation (+D):

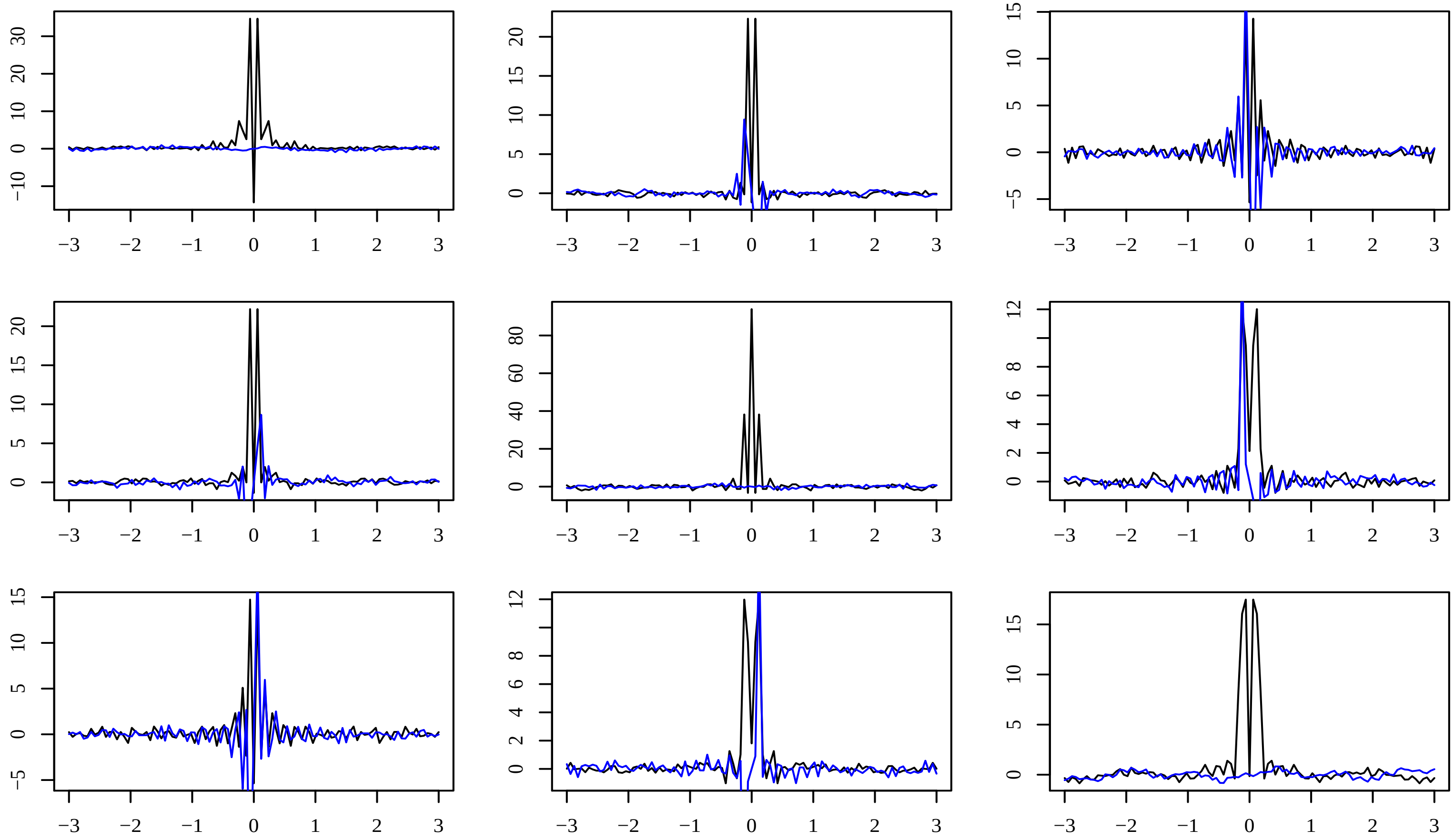
Example: simulated data set



- exponential covariances
- sills = 1
- eff. ranges = $30u$
- delay 2,3 = $10u$
- corr = 0.3
- LU sim: $\sim 750nod$

sft for covariance estimation (+D):

Example: covariances and spectra



sft for covariance estimation (+D):
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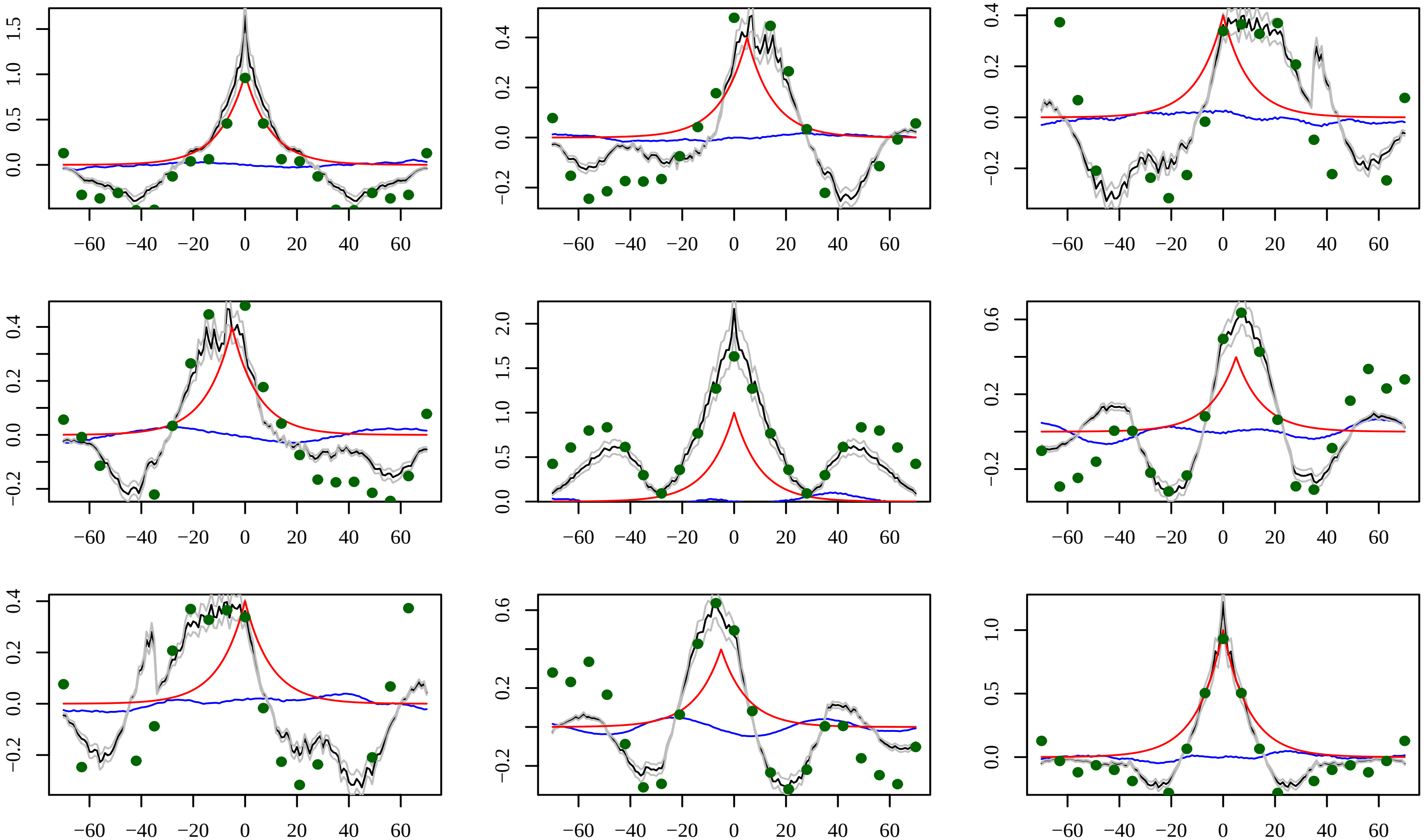
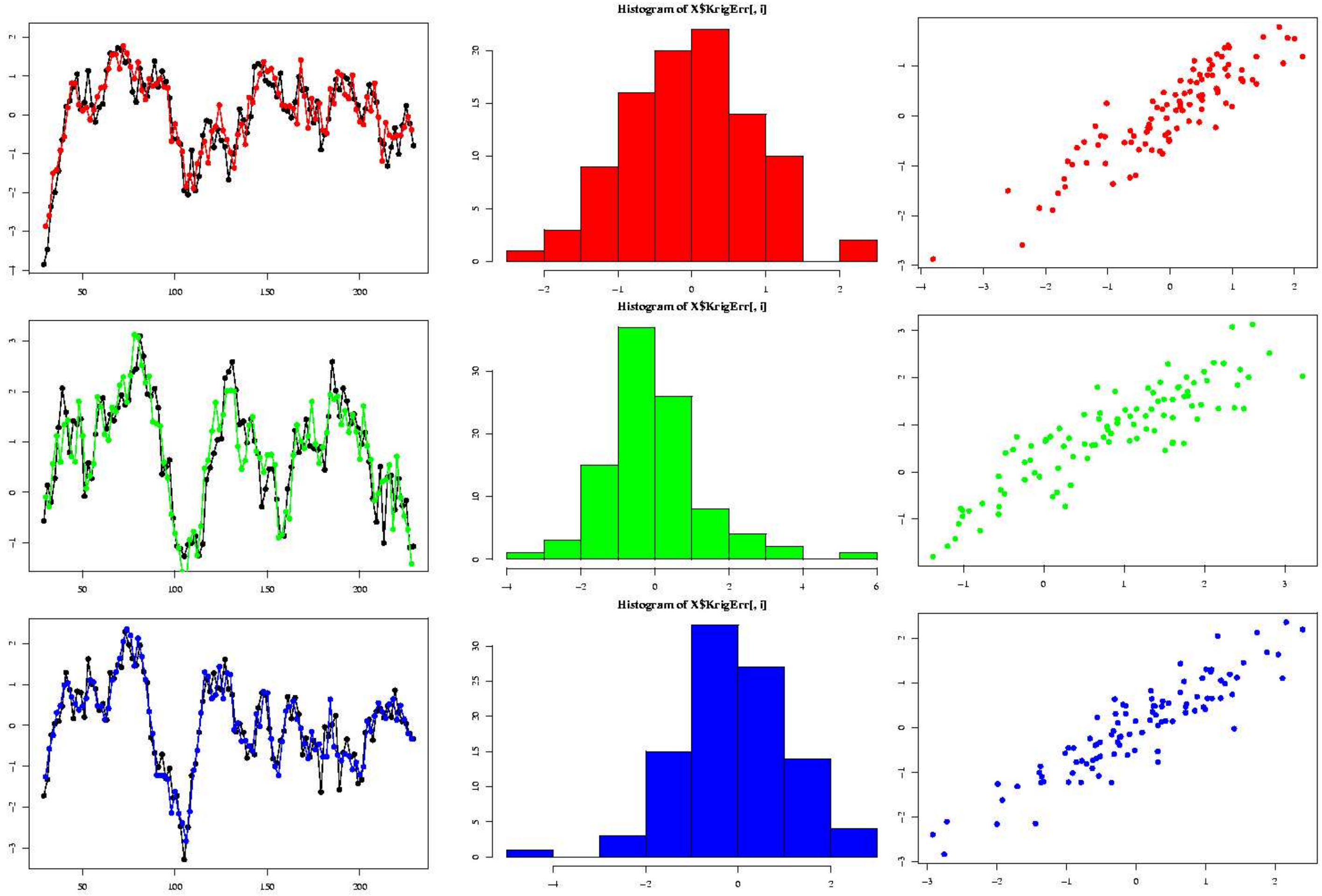


sft for covariance estimation (+D):

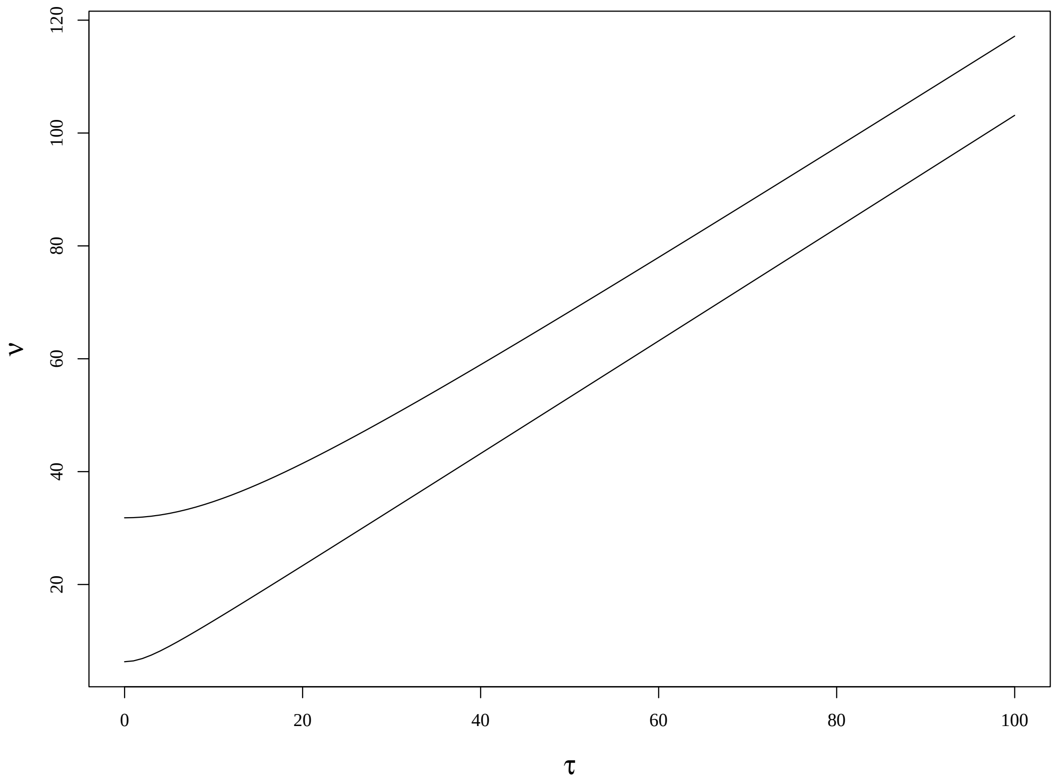
Example: estimation



final comments

- in general
  - difficult to go against "tradition"
  - **fft**: inadequate frequency domain
  - **sft**: slow, imprecise, limited
  - it provides (quite) good results
- for covariances
  - not clear how to smooth-validate
  - SK is very sensitive

hole effect intervals



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