

Supplementary material for Asymptotic analysis of the role of spatial sampling for covariance parameter estimation of Gaussian processes

François Bachoc^{a,b,*}

^aCEA-Saclay, DEN, DM2S, STMF, LGLS, F-91191 Gif-Sur-Yvette, France

^bLaboratoire de Probabilités et Modèles Aléatoires, Université Paris Diderot,
75205 Paris cedex 13

Abstract

In this supplementary material, we address the one-dimensional case with $p = 1$. We provide the exact expression of the asymptotic variances of ML and CV, for $\epsilon = 0$, and of the second derivative w.r.t. ϵ , at $\epsilon = 0$ for ML. We recall the notations, restate the exact expressions in proposition 2, and give the proof.

We recall the expression of Σ_{ML} , $\Sigma_{CV,1}$ and $\Sigma_{CV,2}$:

$$\frac{1}{2n} \text{Tr} \left(R^{-1} \frac{\partial R}{\partial \theta} R^{-1} \frac{\partial R}{\partial \theta} \right) \xrightarrow{n \rightarrow +\infty} \Sigma_{ML}, \quad (1)$$

with

$$M_\theta = R_\theta^{-1} \text{diag} (R_\theta^{-1})^{-2} \left\{ \text{diag} \left(R_\theta^{-1} \frac{\partial R_\theta}{\partial \theta} R_\theta^{-1} \right) \text{diag} (R_\theta^{-1})^{-1} - R_\theta^{-1} \frac{\partial R_\theta}{\partial \theta} \right\} R_\theta^{-1},$$

$$2 \frac{1}{n} \text{Tr} \left[\left\{ M_{\theta_0} + (M_{\theta_0})^t \right\} R_{\theta_0} \left\{ M_{\theta_0} + (M_{\theta_0})^t \right\} R_{\theta_0} \right] \xrightarrow{n \rightarrow +\infty} \Sigma_{CV,1}, \quad (2)$$

and

$$-8 \frac{1}{n} \text{Tr} \left\{ \text{diag} (R_{\theta_0}^{-1})^{-3} \text{diag} \left(R_{\theta_0}^{-1} \frac{\partial R_{\theta_0}}{\partial \theta} R_{\theta_0}^{-1} \right) R_{\theta_0}^{-1} \frac{\partial R_{\theta_0}}{\partial \theta} R_{\theta_0}^{-1} \right\} \quad (3)$$

$$+ 2 \frac{1}{n} \text{Tr} \left\{ \text{diag} (R_{\theta_0}^{-1})^{-2} R_{\theta_0}^{-1} \frac{\partial R_{\theta_0}}{\partial \theta} R_{\theta_0}^{-1} \frac{\partial R_{\theta_0}}{\partial \theta} R_{\theta_0}^{-1} \right\}$$

$$+ 6 \frac{1}{n} \text{Tr} \left\{ \text{diag} (R_{\theta_0}^{-1})^{-4} \text{diag} \left(R_{\theta_0}^{-1} \frac{\partial R_{\theta_0}}{\partial \theta} R_{\theta_0}^{-1} \right) \text{diag} \left(R_{\theta_0}^{-1} \frac{\partial R_{\theta_0}}{\partial \theta} R_{\theta_0}^{-1} \right) R_{\theta_0}^{-1} \right\}$$

$$\xrightarrow{n \rightarrow +\infty} \Sigma_{CV,2}.$$

The observation points $v_i + \epsilon X_i$, $1 \leq i \leq n$, $n \in \mathbb{N}^*$, are $i + \epsilon X_i$, where X_i is uniform on $[-1, 1]$, and $\Theta = [\theta_{inf}, \theta_{sup}]$.

All the covariance matrices are considered at θ_0 and so we do not write explicitly this dependence. We denote $\partial_\theta R = \frac{\partial}{\partial \theta} R$, $\partial_\epsilon R = \frac{\partial}{\partial \epsilon} R$, $\partial_{\epsilon, \theta} R = \frac{\partial}{\partial \epsilon} \frac{\partial}{\partial \theta} R$, $\partial_{\epsilon, \epsilon} R = \frac{\partial^2}{\partial \epsilon^2} R$ and $\partial_{\epsilon, \epsilon, \theta} R = \frac{\partial^2}{\partial \epsilon^2} \frac{\partial}{\partial \theta} R$.

We define the Fourier transform function $\hat{z}(\cdot)$ of a sequence s_n of \mathbb{Z} by $\hat{z}(f) = \sum_{n \in \mathbb{Z}} s_n e^{i s_n f}$ as in [1]. This function is 2π periodic on $[-\pi, \pi]$. Then

*Corresponding author: François Bachoc

CEA-Saclay, DEN, DM2S, STMF, LGLS, F-91191 Gif-Sur-Yvette, France

Phone: +33 (0) 1 69 08 97 91

Email: francois.bachoc@cea.fr

- The sequence of the $K_{\theta_0}(i)$, $i \in \mathbb{Z}$, has Fourier transform f which is even and non negative on $[-\pi, \pi]$.
- The sequence of the $\frac{\partial}{\partial \theta} K_{\theta_0}(i)$, $i \in \mathbb{Z}$, has Fourier transform f_θ which is even on $[-\pi, \pi]$.
- The sequence of the $\frac{\partial}{\partial t} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $i \in \mathbb{Z}$, has Fourier transform $i f_t$ which is odd and imaginary on $[-\pi, \pi]$.
- The sequence of the $\frac{\partial}{\partial t} \frac{\partial}{\partial \theta} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $i \in \mathbb{Z}$, has Fourier transform $i f_{t,\theta}$ which is odd and imaginary on $[-\pi, \pi]$.
- The sequence of the $\frac{\partial^2}{\partial t^2} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $i \in \mathbb{Z}$, has Fourier transform $f_{t,t}$ which is even on $[-\pi, \pi]$.
- The sequence of the $\frac{\partial^2}{\partial t^2} \frac{\partial}{\partial \theta} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $i \in \mathbb{Z}$, has Fourier transform $f_{t,t,\theta}$ which is even on $[-\pi, \pi]$.

We recall the condition on the sequences above in condition 1.

Condition 1. *There exist $C < \infty$ and $a > 0$ so that the sequences of general terms $K_{\theta_0}(i)$, $\frac{\partial}{\partial \theta} K_{\theta_0}(i)$, $\frac{\partial}{\partial t} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $\frac{\partial}{\partial t} \frac{\partial}{\partial \theta} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $\frac{\partial^2}{\partial t^2} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $\frac{\partial^2}{\partial t^2} \frac{\partial}{\partial \theta} K_{\theta_0}(i) \mathbf{1}_{i \neq 0}$, $i \in \mathbb{Z}$, are bounded by $Ce^{-a|i|}$.*

For a sequence $(z_i)_{i \in \mathbb{Z}}$ on \mathbb{Z} , or equivalently its 2π -périodic Fourier transform function f on $[-\pi, \pi]$, we denote by $T(f)$ the associated Toeplitz matrix sequence, where we do not write explicitly the dependence on n . The Toeplitz matrix sequence is defined by $T(f)_{i,j} := z_{i-j} = \int_{-\pi}^{\pi} f(t) e^{-(i-j)t} dt$. We denote by $M(f)$ the mean value of f on $[-\pi, \pi]$. Notice that $M(f) = T(f)_{0,0}$.

Then, proposition 2 gives the closed form expressions of Σ_{ML} , $\Sigma_{CV,1}$, $\Sigma_{CV,2}$ and $\frac{\partial^2}{\partial \epsilon^2} \Sigma_{ML} \Big|_{\epsilon=0}$.

Proposition 2. *Assume that f is positive on $[-\pi, \pi]$ and that condition 1 is verified.*

For $\epsilon = 0$,

$$\Sigma_{ML} = \frac{1}{2} M \left(\frac{f_\theta^2}{f^2} \right),$$

$$\begin{aligned} \Sigma_{CV,1} &= 8M \left(\frac{1}{f} \right)^{-6} M \left(\frac{f_\theta}{f^2} \right)^2 M \left(\frac{1}{f^2} \right) \\ &\quad + 8M \left(\frac{1}{f} \right)^{-4} M \left(\frac{f_\theta^2}{f^4} \right) \\ &\quad - 16M \left(\frac{1}{f} \right)^{-5} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_\theta}{f^3} \right), \end{aligned}$$

$$\Sigma_{CV,2} = 2M \left(\frac{1}{f} \right)^{-3} \left\{ M \left(\frac{f_\theta^2}{f^3} \right) M \left(\frac{1}{f} \right) - M \left(\frac{f_\theta}{f^2} \right)^2 \right\},$$

and

$$\begin{aligned}
\frac{\partial^2}{\partial \epsilon^2} \Sigma_{ML} \Big|_{\epsilon=0} &= \frac{2}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_t^2 f_\theta}{f^2} \right) \\
&- \frac{4}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta} f_t f_\theta}{f^2} \right) - \frac{4}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_{t,\theta} f_t}{f} \right) \\
&+ \frac{2}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_t^2 f_\theta^2}{f^3} \right) + \frac{2}{3} M \left(\frac{f_\theta^2}{f^3} \right) M \left(\frac{f_t^2}{f} \right) \\
&- \frac{2}{3} M \left(\frac{f_{t,t} f_\theta^2}{f^3} \right) \\
&+ \frac{2}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta}^2}{f} \right) \\
&+ \frac{2}{3} M \left(\frac{f_{t,t,\theta} f_\theta}{f^2} \right).
\end{aligned}$$

Proof. We only give the proof of the expression of $\frac{\partial^2}{\partial \epsilon^2} \Sigma_{ML} \Big|_{\epsilon=0}$, since the proofs of the expressions of Σ_{ML} , $\Sigma_{CV,1}$ and $\Sigma_{CV,2}$ are simpler and essentially follow from the results in [1].

Using proposition 3,

$$\begin{aligned}
&\frac{1}{n} \left\{ \frac{\partial^2}{\partial \epsilon^2} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\theta R) \right\} \tag{4} \\
&= 2 \frac{1}{n} \text{Tr} (R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) - 4 \frac{1}{n} \text{Tr} (R^{-1} \partial_{\epsilon,\theta} R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) \\
&\quad + 4 \frac{1}{n} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) - 2 \frac{1}{n} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_{\epsilon,\epsilon} R R^{-1} \partial_\theta R) \\
&\quad + 2 \frac{1}{n} \text{Tr} (R^{-1} \partial_{\epsilon,\theta} R R^{-1} \partial_{\epsilon,\theta} R) \\
&\quad - 4 \frac{1}{n} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_{\epsilon,\theta} R) + 2 \frac{1}{n} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_{\epsilon,\epsilon,\theta} R), \\
&= 2 \frac{1}{n} \text{Tr} (\partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1}) - 4 \frac{1}{n} \text{Tr} (\partial_{\epsilon,\theta} R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1}) \\
&\quad + 4 \frac{1}{n} \text{Tr} (\partial_\epsilon R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \partial_\theta R R^{-1}) - 2 \frac{1}{n} \text{Tr} (\partial_{\epsilon,\epsilon} R R^{-1} \partial_\theta R R^{-1} \partial_\theta R R^{-1}) \\
&\quad + 2 \frac{1}{n} \text{Tr} (\partial_{\epsilon,\theta} R R^{-1} \partial_{\epsilon,\theta} R R^{-1}) \\
&\quad - 4 \frac{1}{n} \text{Tr} (\partial_\epsilon R R^{-1} \partial_{\epsilon,\theta} R R^{-1} \partial_\theta R R^{-1}) + 2 \frac{1}{n} \text{Tr} (\partial_{\epsilon,\epsilon,\theta} R R^{-1} \partial_\theta R R^{-1}).
\end{aligned}$$

We denote as in [1], for a real $n \times n$ matrix A , $|A|^2 = \frac{1}{n} \sum_{i,j=1}^n A_{i,j}^2$ and $\|A\|$ the largest singular value of A . $|\cdot|$ and $\|\cdot\|$ are norms and $\|\cdot\|$ is a matrix norm. We denote, for two sequences of square matrices A and B , indexed by $n \in \mathbb{N}^*$, $A \sim B$ if $|A - B| \rightarrow_{n \rightarrow +\infty} 0$ and $\|A\|$ and $\|B\|$ are bounded with respect to n .

Using [1], theorems 11 and 12, we have $R^{-1} \partial_\theta R R^{-1} = T(f)^{-1} T(f_\theta) T(f)^{-1} \sim_{n \rightarrow \infty} T\left(\frac{f_\theta}{f^2}\right)$ because f and θf are C^∞ and f is positive. Hence, as the eigenvalues of $\partial_\epsilon R$ are uniformly bounded, we obtain, using [1] theorem 1

$$\partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \sim_{n \rightarrow \infty} \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right) \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right),$$

and hence

$$\frac{1}{n} \text{Tr} (\partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1}) = \frac{1}{n} \text{Tr} \left\{ \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right) \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right) \right\} + o(1).$$

The equivalence is uniform in $x = (x_1, \dots, x_n)^t \in [-1, 1]^n$. Applying this method for all the terms of (4), we obtain

$$\begin{aligned}
& \frac{1}{n} \left\{ \frac{\partial^2}{\partial \epsilon^2} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\theta R) \right\} + o(1) \\
= & 2 \frac{1}{n} \text{Tr} \left\{ \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right) \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right) \right\} - 4 \frac{1}{n} \text{Tr} \left\{ \partial_{\epsilon, \theta} R T \left(\frac{1}{f} \right) \partial_\epsilon R T \left(\frac{f_\theta}{f^2} \right) \right\} \\
& + 4 \frac{1}{n} \text{Tr} \left\{ \partial_\epsilon R T \left(\frac{1}{f} \right) \partial_\epsilon R T \left(\frac{f_\theta^2}{f^3} \right) \right\} - 2 \frac{1}{n} \text{Tr} \left\{ \partial_{\epsilon, \epsilon} R T \left(\frac{f_\theta^2}{f^3} \right) \right\} \\
& + 2 \frac{1}{n} \text{Tr} \left\{ \partial_{\epsilon, \theta} R T \left(\frac{1}{f} \right) \partial_{\epsilon, \theta} R T \left(\frac{1}{f} \right) \right\} \\
& - 4 \frac{1}{n} \text{Tr} \left\{ \partial_\epsilon R T \left(\frac{1}{f} \right) \partial_{\epsilon, \theta} R T \left(\frac{f_\theta}{f^2} \right) \right\} + 2 \frac{1}{n} \text{Tr} \left\{ \partial_{\epsilon, \epsilon, \theta} R T \left(\frac{f_\theta}{f^2} \right) \right\} + o(1).
\end{aligned}$$

For a matrix A , we define A_x by $(A_x)_{i,j} = A_{i,j} (X_i - X_j)$ and $A_{x,x}$ by $(A_{x,x})_{i,j} = A_{i,j} (X_i - X_j)^2$, where the X_i 's are the random perturbations.

We then have, since $\epsilon = 0$,

$$\begin{aligned}
R &= T(f), \\
\partial_\theta R &= T(f_\theta), \\
\partial_\epsilon R &= T_x(i f_t), \\
\partial_{\epsilon, \theta} R &= T_x(i f_{t, \theta}), \\
\partial_{\epsilon, \epsilon} R &= T_{x,x}(f_{t,t}).
\end{aligned}$$

and

$$\partial_{\epsilon, \epsilon, \theta} R = T_{x,x}(f_{t,t, \theta}).$$

With these notations,

$$\begin{aligned}
& \frac{1}{n} \left\{ \frac{\partial^2}{\partial \epsilon^2} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\theta R) \right\} \\
= & 2 \frac{1}{n} \text{Tr} \left\{ T_x(f_t) T \left(\frac{f_\theta}{f^2} \right) T_x(f_t) T \left(\frac{f_\theta}{f^2} \right) \right\} - 4 \frac{1}{n} \text{Tr} \left\{ T_x(f_{t, \theta}) T \left(\frac{1}{f} \right) T_x(f_t) T \left(\frac{f_\theta}{f^2} \right) \right\} \\
& + 4 \frac{1}{n} \text{Tr} \left\{ T_x(f_t) T \left(\frac{1}{f} \right) T_x(f_t) T \left(\frac{f_\theta^2}{f^3} \right) \right\} - 2 \frac{1}{n} \text{Tr} \left\{ T_{x,x}(f_{t,t}) T \left(\frac{f_\theta^2}{f^3} \right) \right\} \\
& + 2 \frac{1}{n} \text{Tr} \left\{ T_x(f_{t, \theta}) T \left(\frac{1}{f} \right) T_x(f_{t, \theta}) T \left(\frac{1}{f} \right) \right\} \\
& - 4 \frac{1}{n} \text{Tr} \left\{ T_x(f_t) T \left(\frac{1}{f} \right) T_x(f_{t, \theta}) T \left(\frac{f_\theta}{f^2} \right) \right\} + 2 \frac{1}{n} \text{Tr} \left\{ T_{x,x}(f_{t,t, \theta}) T \left(\frac{f_\theta}{f^2} \right) \right\} + o(1).
\end{aligned}$$

Hence, using propositions 4 and 6, we obtain

$$\begin{aligned}
& \lim_{n \rightarrow +\infty} \mathbb{E} \left[\frac{1}{n} \left\{ \frac{\partial^2}{\partial \epsilon^2} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\theta R) \right\} \right] \\
&= 2 \left\{ \frac{1}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_t f_t f_\theta}{f^2} \right) + \frac{1}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_t f_t f_\theta}{f^2} \right) \right\} \\
&\quad - 4 \left\{ \frac{1}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta} f_t f_\theta}{f^2} \right) + \frac{1}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_{t,\theta} f_t}{f} \right) \right\} \\
&\quad + 4 \left\{ \frac{1}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_t f_t f_\theta^2}{f^3} \right) + \frac{1}{3} M \left(\frac{f_\theta^2}{f^3} \right) M \left(\frac{f_t f_t}{f} \right) \right\} \\
&\quad - 2 \frac{2}{3} M \left(\frac{f_{t,t} f_\theta^2}{f^3} \right) \\
&\quad + 2 \left\{ \frac{1}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta} f_{t,\theta}}{f} \right) + \frac{1}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta} f_{t,\theta}}{f} \right) \right\} \\
&\quad - 4 \left\{ \frac{1}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_t f_{t,\theta} f_\theta}{f^2} \right) + \frac{1}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_t f_{t,\theta}}{f} \right) \right\} \\
&\quad + 2 \frac{2}{3} M \left(\frac{f_{t,t,\theta} f_\theta}{f^2} \right), \\
&= \frac{4}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_t^2 f_\theta}{f^2} \right) \\
&\quad - \frac{8}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta} f_t f_\theta}{f^2} \right) - \frac{8}{3} M \left(\frac{f_\theta}{f^2} \right) M \left(\frac{f_{t,\theta} f_t}{f} \right) \\
&\quad + \frac{4}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_t^2 f_\theta^2}{f^3} \right) + \frac{4}{3} M \left(\frac{f_\theta^2}{f^3} \right) M \left(\frac{f_t^2}{f} \right) \\
&\quad - \frac{4}{3} M \left(\frac{f_{t,t} f_\theta^2}{f^3} \right) \\
&\quad + \frac{4}{3} M \left(\frac{1}{f} \right) M \left(\frac{f_{t,\theta}^2}{f} \right) \\
&\quad + \frac{4}{3} M \left(\frac{f_{t,t,\theta} f_\theta}{f^2} \right).
\end{aligned}$$

□

Proposition 3.

$$\begin{aligned}
& \frac{\partial^2}{\partial \epsilon^2} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\theta R) \\
&= 2 \text{Tr} (R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) - 4 \text{Tr} (R^{-1} \partial_{\epsilon,\theta} R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) \\
&\quad + 4 \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) - 2 \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_{\epsilon,\epsilon} R R^{-1} \partial_\theta R) \\
&\quad + 2 \text{Tr} (R^{-1} \partial_{\epsilon,\theta} R R^{-1} \partial_{\epsilon,\theta} R) \\
&\quad - 4 \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_{\epsilon,\theta} R) + 2 \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_{\epsilon,\epsilon,\theta} R).
\end{aligned}$$

Proof. We use $\frac{\partial}{\partial \epsilon} \text{Tr} (M^2) = 2 \text{Tr} (M \frac{\partial}{\partial \epsilon} M)$. Then:

$$\begin{aligned}
\frac{\partial}{\partial \epsilon} \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\theta R) &= 2 \text{Tr} (R^{-1} \partial_\theta R (-R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R + R^{-1} \partial_{\epsilon,\theta} R)) \quad (5) \\
&= -2 \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_\epsilon R R^{-1} \partial_\theta R) + 2 \text{Tr} (R^{-1} \partial_\theta R R^{-1} \partial_{\epsilon,\theta} R).
\end{aligned}$$

We use $\frac{\partial}{\partial \epsilon} \text{Tr} (ABCDEF) = \text{Tr} (\frac{\partial}{\partial \epsilon} A B C D E F + \dots + A B C D E \frac{\partial}{\partial \epsilon} F)$. Then

$$\begin{aligned}
& \frac{\partial}{\partial \epsilon} \text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) \tag{6} \\
&= -\text{Tr} (R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) + \text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad -\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) + (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad -\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) + (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon, \theta} R), \\
&= -\text{Tr} (R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) + \text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad -2\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) + (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad + (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon, \theta} R)
\end{aligned}$$

and

$$\begin{aligned}
& \frac{\partial}{\partial \epsilon} \text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \theta} R) \tag{7} \\
&= -\text{Tr} (R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \theta} R) + \text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon, \theta} R) \\
&\quad -\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon, \theta} R) + \text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon, \theta} R).
\end{aligned}$$

Using (5), (6) and (7), and using $\text{Tr} (AB) = \text{Tr} (BA)$ we obtain

$$\begin{aligned}
& \frac{\partial^2}{\partial \epsilon^2} \text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\theta} R) \\
&= 2\text{Tr} (R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) - 2\text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad + 4\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) - 2\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad - 2\{R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon, \theta} R\} \\
&\quad - 2\text{Tr} (R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \theta} R) + 2\text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon, \theta} R) \\
&\quad - 2\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon, \theta} R) + 2\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon, \theta} R), \\
&= 2\text{Tr} (R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) - 4\text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad + 4\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\theta} R) - 2\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon} R R^{-1} \partial_{\theta} R) \\
&\quad + 2\text{Tr} (R^{-1} \partial_{\epsilon, \theta} R R^{-1} \partial_{\epsilon, \theta} R) \\
&\quad - 4\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon} R R^{-1} \partial_{\epsilon, \theta} R) + 2\text{Tr} (R^{-1} \partial_{\theta} R R^{-1} \partial_{\epsilon, \epsilon, \theta} R).
\end{aligned}$$

□

Proposition 4. *Let f_1, f_2, f_3 and f_4 some 2π -périodic and C^∞ functions on $[-\pi, \pi]$. Furthermore we suppose that f_1 and f_3 are odd and that f_2 and f_4 are even. Then*

$$\mathbb{E} \left[\frac{1}{n} \text{Tr} \{T_x (if_1) \ T (f_2) \ T_x (if_3) \ T (f_4)\} \right] \rightarrow_{n \rightarrow \infty} \frac{1}{3} M (f_2) M (f_1 f_3 f_4) + \frac{1}{3} M (f_4) M (f_1 f_2 f_3).$$

Proof. We calculate

$$\begin{aligned}
\text{Tr} (ABCD) &= \sum_{i,j=1}^n (AB)_{i,j} (CD)_{j,i}, \\
&= \sum_{i,j=1}^n \left(\sum_{k=1}^n A_{i,k} B_{k,i} \right) \left(\sum_{l=1}^n C_{j,l} D_{l,i} \right), \\
&= \sum_{i,j,k,l=1}^n A_{i,k} B_{k,j} C_{j,l} D_{l,i}.
\end{aligned}$$

Then

$$\begin{aligned}
& \frac{1}{n} \mathbb{E} [\text{Tr} \{T_x (if_1) T(f_2) T_x (if_3) T(f_4)\}] \\
&= \frac{1}{n} \mathbb{E} \left\{ \sum_{i,j,k,l=1}^n (X_i - X_k) T (if_1)_{i,k} T (f_2)_{k,j} (X_j - X_l) T (if_3)_{j,l} T (f_4)_{l,i} \right\}, \\
&= \frac{1}{n} \mathbb{E} \left\{ \sum_{i,j,k,l=1}^n T (if_1)_{i,k} T (f_2)_{k,j} T (if_3)_{j,l} T (f_4)_{l,i} (X_i X_j - X_k X_j - X_i X_l + X_k X_l) \right\}, \\
&= \frac{1}{3} \frac{1}{n} \sum_{i,k,l=1}^n T (if_1)_{i,k} T (f_2)_{k,i} T (if_3)_{i,l} T (f_4)_{l,i} - \frac{1}{3} \frac{1}{n} \sum_{i,j,l=1}^n T (if_1)_{i,j} T (f_2)_{j,j} T (if_3)_{j,l} T (f_4)_{l,i} \\
&\quad - \frac{1}{3} \frac{1}{n} \sum_{i,k,l=1}^n T (if_1)_{i,k} T (f_2)_{k,j} T (if_3)_{i,j} T (f_4)_{i,i} + \frac{1}{3} \frac{1}{n} \sum_{i,j,k=1}^n T (if_1)_{i,k} T (f_2)_{k,j} T (if_3)_{j,k} T (f_4)_{k,i}.
\end{aligned} \tag{8}$$

Then

$$\begin{aligned}
\frac{1}{n} \sum_{i,k,l=1}^n T (if_1)_{i,k} T (f_2)_{k,i} T (if_3)_{i,l} T (f_4)_{l,i} &= \frac{1}{n} \sum_{i,k=1}^n T (if_1)_{i,k} T (f_2)_{k,i} \left\{ \sum_{l=1}^n T (if_3)_{i,l} T (f_4)_{l,i} \right\}, \\
&= \frac{1}{n} \sum_{i,k=1}^n T (if_1)_{i,k} T (f_2)_{k,i} (T (if_3) T (f_4))_{i,i}, \\
&= \frac{1}{n} \sum_{i=1}^n \{T (if_3) T (f_4)\}_{i,i} \left\{ \sum_{k=1}^n T (if_1)_{i,k} T (f_2)_{k,i} \right\}, \\
&= \frac{1}{n} \sum_{i=1}^n \{T (if_3) T (f_4)\}_{i,i} \{T (if_1) T (f_2)\}_{i,i}.
\end{aligned}$$

Lemma 5. For $|A'_n - A_n| \rightarrow 0$, $|B'_n - B_n| \rightarrow 0$, $\sup_{i,j,n} |(A_n)_{i,j}| < \infty$ and $\sup_{i,j,n} |(B'_n)_{i,j}| < \infty$,
 $\left| \frac{1}{n} \sum_{i=1}^n (A'_n)_{i,i} (B'_n)_{i,i} - \frac{1}{n} \sum_{i=1}^n (A_n)_{i,i} (B_n)_{i,i} \right| \rightarrow 0$.

Proof.

$$\begin{aligned}
& \left| \frac{1}{n} \sum_{i=1}^n (A'_n)_{i,i} (B'_n)_{i,i} - \frac{1}{n} \sum_{i=1}^n (A_n)_{i,i} (B_n)_{i,i} \right|^2 \\
&\leq \frac{1}{n^2} n \sum_{i=1}^n \left\{ (A'_n)_{i,i} (B'_n)_{i,i} - (A_n)_{i,i} (B_n)_{i,i} \right\}^2, \quad \text{by Cauchy-Schwartz,} \\
&\leq \frac{1}{n} \sum_{i,j=1}^n \left\{ (A'_n)_{i,j} (B'_n)_{i,j} - (A_n)_{i,j} (B_n)_{i,j} \right\}^2, \\
&\leq 2 \frac{1}{n} \sum_{i,j=1}^n \left\{ (A'_n)_{i,j} (B'_n)_{i,j} - (A_n)_{i,j} (B'_n)_{i,j} \right\}^2 + 2 \frac{1}{n} \sum_{i,j=1}^n \left\{ (A_n)_{i,j} (B'_n)_{i,j} - (A_n)_{i,j} (B_n)_{i,j} \right\}^2, \\
&\leq 2 \sup_{i,j,n} |(B'_n)_{i,j}| \frac{1}{n} \sum_{i,j=1}^n \left\{ (A'_n)_{i,j} - (A_n)_{i,j} \right\}^2 + 2 \sup_{i,j,n} |(A_n)_{i,j}| \frac{1}{n} \sum_{i,j=1}^n \left\{ (B'_n)_{i,j} - (B_n)_{i,j} \right\}^2, \\
&\leq 2 \sup_{i,j,n} |(B'_n)_{i,j}| \cdot |A'_n - A_n| + 2 \sup_{i,j,n} |(A_n)_{i,j}| \cdot |B'_n - B_n|.
\end{aligned}$$

□

We use lemma 5 with $A'_n = T(\text{if}_1)T(f_2)$, $A_n = T(\text{if}_1f_2)$, $B'_n = T(\text{if}_3)T(f_4)$ and $B_n = T(\text{if}_3f_4)$. It is shown in [1] theorem 12 that $|A'_n - A_n| \rightarrow 0$ and $|B'_n - B_n| \rightarrow 0$. As if_1f_2 is C^∞ , the coefficients of $T(\text{if}_1f_2)$ are uniformly bounded. Finally $\{T(\text{if}_1)T(f_2)\}_{i,j} \leq \sup_{i,j,n} |T(\text{if}_1)_{i,j}| \sum_{k \in \mathbb{Z}} |T(f_2)_{k,j}|$ which is uniformly bounded because if_1 and f_2 are C^∞ .

Hence

$$\begin{aligned}
& \frac{1}{n} \sum_{i,k,l=1}^n T(\text{if}_1)_{i,k} T(f_2)_{k,i} T(\text{if}_3)_{i,l} T(f_4)_{l,i} \\
&= \frac{1}{n} \sum_{i=1}^n \{T(\text{if}_3)T(f_4)\}_{i,i} \{T(\text{if}_1)T(f_2)\}_{i,i}, \\
&= \frac{1}{n} \sum_{i=1}^n \{T(\text{if}_3f_4)\}_{i,i} \{T(\text{if}_1f_2)\}_{i,i} + o(1), \\
&\xrightarrow{n \rightarrow +\infty} M(\text{if}_3f_4)M(\text{if}_1f_2), \\
&= 0, \quad \text{because } f_3f_4 \text{ is odd.}
\end{aligned} \tag{9}$$

We show similarly

$$\frac{1}{n} \sum_{i,j,k=1}^n T(\text{if}_1)_{i,k} T(f_2)_{k,j} T(\text{if}_3)_{j,k} T(f_4)_{k,i} \rightarrow 0. \tag{10}$$

Then

$$\begin{aligned}
& \frac{1}{n} \sum_{i,j,l=1}^n T(\text{if}_1)_{i,j} T(f_2)_{j,j} T(\text{if}_3)_{j,l} T(f_4)_{l,i} \\
&= M(f_2) \frac{1}{n} \sum_{i,j,l=1}^n T(\text{if}_1)_{i,j} T(\text{if}_3)_{j,l} T(f_4)_{l,i}, \\
&= M(f_2) \frac{1}{n} \sum_{i,j=1}^n T(\text{if}_1)_{i,j} \left\{ \sum_{l=1}^n T(\text{if}_3)_{j,l} T(f_4)_{l,i} \right\}, \\
&= M(f_2) \frac{1}{n} \sum_{i,j=1}^n T(\text{if}_1)_{i,j} \{T(\text{if}_3)T(f_4)\}_{j,i}, \\
&= M(f_2) \frac{1}{n} \text{Tr} \{T(\text{if}_1)T(\text{if}_3)T(f_4)\}, \\
&\rightarrow M(f_2)M(\text{if}_1\text{if}_3f_4), \quad \text{using [1] theorem 12,} \\
&= -M(f_2)M(f_1f_3f_4).
\end{aligned} \tag{11}$$

We show similarly

$$\frac{1}{n} \sum_{i,j,k=1}^n T(\text{if}_1)_{i,k} T(f_2)_{k,j} T(\text{if}_3)_{i,j} T(f_4)_{i,i} \rightarrow -M(f_4)M(f_1f_2f_3). \tag{12}$$

We conclude with (8), (9), (10), (11) and (12). \square

Proposition 6. *Let f_1 and f_2 be 2π -périodic, C^∞ , functions on $[-\pi, \pi]$, with f_1 odd. Then*

$$\mathbb{E} \left[\frac{1}{n} \text{Tr} \{T_{x,x}(f_1)T(f_2)\} \right] \rightarrow \frac{2}{3} M(f_1f_2).$$

Proof.

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{n} \text{Tr} \{ T_{x,x} (f_1) T (f_2) \} \right] \\ &= \mathbb{E} \left\{ \frac{1}{n} \sum_{i,j=1}^n T (f_1)_{i,j} (X_i - X_j)^2 T (f_2)_{j,i} \right\}, \\ &= \frac{1}{n} \frac{2}{3} \sum_{i,j=1}^n T (f_1)_{i,j} T (f_2)_{j,i}, \quad \text{because } T (f_1)_{i,i} = M (f_1) = 0, \\ &= \frac{2}{3} \frac{1}{n} \text{Tr} \{ T (f_1) T (f_2) \}, \\ &\rightarrow \frac{2}{3} M (f_1 f_2), \text{ using [1] theorem 12.} \end{aligned}$$

□

References

- [1] R.M. Gray, Toeplitz and circulant matrices: A review, Foundations and Trends® in Communications and Information Theory 2 (2006) 155–239.