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

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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 $\Sigma_{CV,2}$:

$$\frac{1}{2n}\mathrm{Tr}\left(\mathrm{R}^{-1}\frac{\partial \mathrm{R}}{\partial \theta}\mathrm{R}^{-1}\frac{\partial \mathrm{R}}{\partial \theta}\right) \underset{\mathrm{n}\to+\infty}{\to} \Sigma_{\mathrm{ML}}, \tag{1}$$

with

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

$$2\frac{1}{n}\mathrm{Tr}\left[\left\{M_{\theta_0} + \left(M_{\theta_0}\right)^t\right\}R_{\theta_0}\left\{M_{\theta_0} + \left(M_{\theta_0}\right)^t\right\}R_{\theta_0}\right] \underset{n\to+\infty}{\to} \Sigma_{CV,1}, \tag{2}$$

and

$$\begin{aligned}
&-8\frac{1}{n}\mathrm{Tr}\left\{diag\left(R_{\theta_0}^{-1}\right)^{-3}diag\left(R_{\theta_0}^{-1}\frac{\partial R_{\theta_0}}{\partial\theta}R_{\theta_0}^{-1}\right)R_{\theta_0}^{-1}\frac{\partial R_{\theta_0}}{\partial\theta}R_{\theta_0}^{-1}\right\} \\
&+2\frac{1}{n}\mathrm{Tr}\left\{diag\left(R_{\theta_0}^{-1}\right)^{-2}R_{\theta_0}^{-1}\frac{\partial R_{\theta_0}}{\partial\theta}R_{\theta_0}^{-1}\frac{\partial R_{\theta_0}}{\partial\theta}R_{\theta_0}^{-1}\right\} \\
&+6\frac{1}{n}\mathrm{Tr}\left\{diag\left(R_{\theta_0}^{-1}\right)^{-4}diag\left(R_{\theta_0}^{-1}\frac{\partial R_{\theta_0}}{\partial\theta}R_{\theta_0}^{-1}\right)diag\left(R_{\theta_0}^{-1}\frac{\partial R_{\theta_0}}{\partial\theta}R_{\theta_0}^{-1}\right)R_{\theta_0}^{-1}\right\} \\
\underset{n\to+\infty}{\to}\ &\Sigma_{CV,2}.
\end{aligned} \tag{3}$$

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

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- 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}\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\theta R\right)\right\} \qquad (4)\\
=\ & 2\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) - 4\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right)\\
& +4\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) - 2\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon} R\ R^{-1}\ \partial_\theta R\right)\\
& +2\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_{\epsilon,\theta} R\right)\\
& -4\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) + 2\frac{1}{n}\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon,\theta} R\right),\\
=\ & 2\frac{1}{n}\mathrm{Tr}\left(\partial_\epsilon \mathrm{R}\ \mathrm{R}^{-1}\ \partial_\theta \mathrm{R}\ \mathrm{R}^{-1}\ \partial_\epsilon \mathrm{R}\ \mathrm{R}^{-1}\ \partial_\theta \mathrm{R}\ \mathrm{R}^{-1}\right) - 4\frac{1}{\mathrm{n}}\mathrm{Tr}\left(\partial_{\epsilon,\theta} \mathrm{R}\ \mathrm{R}^{-1}\ \partial_\epsilon \mathrm{R}\ \mathrm{R}^{-1}\ \partial_\theta \mathrm{R}\ \mathrm{R}^{-1}\right)\\
& +4\frac{1}{n}\mathrm{Tr}\left(\partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\theta R\ R^{-1}\right) - 2\frac{1}{n}\mathrm{Tr}\left(\partial_{\epsilon,\epsilon} R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\theta R\ R^{-1}\right)\\
& +2\frac{1}{n}\mathrm{Tr}\left(\partial_{\epsilon,\theta} R\ R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\right)\\
& -4\frac{1}{n}\mathrm{Tr}\left(\partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_\theta R\ R^{-1}\right) + 2\frac{1}{n}\mathrm{Tr}\left(\partial_{\epsilon,\epsilon,\theta} R\ R^{-1}\ \partial_\theta R\ R^{-1}\right).
\end{aligned}$$

We denote as in [1], for a real $n \times n$ matrix A, $|A|^2 = \frac{1}{n}\sum_{ij,=1}^n A_{i,j}^2$ and $||A||$ the largest singular value of A. $|.|$ and $||.||$ are norms and $||.||$ 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 $|A - B| \to_{n\to+\infty} 0$ and $||A||$ and $||B||$ are bounded with respect to n.

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

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

and hence

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

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

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

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 $\epsilon = 0$,

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

and

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

With these notations,

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

Hence, using propositions 4 and 6, we obtain

$$
\begin{aligned}
& \underset{n\to+\infty}{lim} \mathbb{E}\left[\frac{1}{n}\left\{\frac{\partial^2}{\partial\epsilon^2}\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\theta R\right)\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\} \\
& -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\} \\
& +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\} \\
& -2\frac{2}{3}M\left(\frac{f_{t,t}\ f_\theta^2}{f^3}\right) \\
& +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\} \\
& -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\} \\
& +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) \\
& -\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) \\
& +\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) \\
& -\frac{4}{3}M\left(\frac{f_{t,t}\ f_\theta^2}{f^3}\right) \\
& +\frac{4}{3}M\left(\frac{1}{f}\right)M\left(\frac{f_{t,\theta}^2}{f}\right) \\
& +\frac{4}{3}M\left(\frac{f_{t,t,\theta}\ f_\theta}{f^2}\right).
\end{aligned}
$$

□

Proposition 3.

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

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

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

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

$$\begin{aligned}
& \frac{\partial}{\partial \epsilon} \mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) \qquad (6)\\
= \;& -\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) + \mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right)\\
& -\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) + \left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon} R\ R^{-1}\ \partial_\theta R\right)\\
& -\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) + \left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right),\\
= \;& -\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) + \mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right)\\
& -2\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) + \left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon} R\ R^{-1}\ \partial_\theta R\right)\\
& + \left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right)
\end{aligned}$$

and

$$\begin{aligned}
& \frac{\partial}{\partial \epsilon} \mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) \qquad (7)\\
= \;& -\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) + \mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_{\epsilon,\theta} R\right)\\
& -\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) + \mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon,\theta} R\right).
\end{aligned}$$

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

$$\begin{aligned}
& \frac{\partial^2}{\partial \epsilon^2} \mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\theta R\right)\\
= \;& 2\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) - 2\mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right)\\
& +4\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) - 2\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon} R\ R^{-1}\ \partial_\theta R\right)\\
& -2\left\{R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right\}\\
& -2\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) + 2\mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_{\epsilon,\theta} R\right)\\
& -2\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) + 2\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon,\theta} R\right),\\
= \;& 2\mathrm{Tr}\left(R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) - 4\mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right)\\
& +4\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_\theta R\right) - 2\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon} R\ R^{-1}\ \partial_\theta R\right)\\
& +2\mathrm{Tr}\left(R^{-1}\ \partial_{\epsilon,\theta} R\ R^{-1}\ \partial_{\epsilon,\theta} R\right)\\
& -4\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_\epsilon R\ R^{-1}\ \partial_{\epsilon,\theta} R\right) + 2\mathrm{Tr}\left(R^{-1}\ \partial_\theta R\ R^{-1}\ \partial_{\epsilon,\epsilon,\theta} R\right).
\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*

$$\mathbb{E}\left[\frac{1}{n}\mathrm{Tr}\left\{T_x(\mathrm{i}f_1)\ T(f_2)\ T_x(\mathrm{i}f_3)\ T(f_4)\right\}\right] \to_{n\to\infty} \frac{1}{3}M(f_2)\,M(f_1f_3f_4) + \frac{1}{3}M(f_4)\,M(f_1f_2f_3).$$

Proof. We calculate

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

Then

$$\frac{1}{n}\mathbb{E}\left[\mathrm{Tr}\left\{T_x\left(\mathrm{i}f_1\right)\ T\left(f_2\right)\ T_x\left(\mathrm{i}f_3\right)\ T\left(f_4\right)\right\}\right] \tag{8}$$

$$= \frac{1}{n}\mathbb{E}\left\{\sum_{i,j,k,l=1}^{n}\left(X_i - X_k\right)T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,j}\left(X_j - X_l\right)T\left(\mathrm{i}f_3\right)_{j,l}T\left(f_4\right)_{l,i}\right\},$$

$$= \frac{1}{n}\mathbb{E}\left\{\sum_{i,j,k,l=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,j}T\left(\mathrm{i}f_3\right)_{j,l}T\left(f_4\right)_{l,i}\left(X_iX_j - X_kX_j - X_iX_l + X_kX_l\right)\right\},$$

$$= \frac{1}{3}\frac{1}{n}\sum_{i,k,l=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,i}T\left(\mathrm{i}f_3\right)_{i,l}T\left(f_4\right)_{l,i} - \frac{1}{3}\frac{1}{n}\sum_{i,j,l=1}^{n}T\left(\mathrm{i}f_1\right)_{i,j}T\left(f_2\right)_{j,j}T\left(\mathrm{i}f_3\right)_{j,l}T\left(f_4\right)_{l,i}$$

$$-\frac{1}{3}\frac{1}{n}\sum_{i,j,k=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,j}T\left(\mathrm{i}f_3\right)_{i,j}T\left(f_4\right)_{i,i} + \frac{1}{3}\frac{1}{n}\sum_{i,j,k=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,j}T\left(\mathrm{i}f_3\right)_{j,k}T\left(f_4\right)_{k,i}.$$

Then

$$\begin{aligned}
\frac{1}{n}\sum_{i,k,l=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,i}T\left(\mathrm{i}f_3\right)_{i,l}T\left(f_4\right)_{l,i} &= \frac{1}{n}\sum_{i,k=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,i}\left\{\sum_{l=1}^{n}T\left(\mathrm{i}f_3\right)_{i,l}T\left(f_4\right)_{l,i}\right\},\\
&= \frac{1}{n}\sum_{i,k=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,i}\left(T\left(\mathrm{i}f_3\right)T\left(f_4\right)\right)_{i,i},\\
&= \frac{1}{n}\sum_{i=1}^{n}\left\{T\left(\mathrm{i}f_3\right)T\left(f_4\right)\right\}_{i,i}\left\{\sum_{k=1}^{n}T\left(\mathrm{i}f_1\right)_{i,k}T\left(f_2\right)_{k,i}\right\},\\
&= \frac{1}{n}\sum_{i=1}^{n}\left\{T\left(\mathrm{i}f_3\right)T\left(f_4\right)\right\}_{i,i}\left\{T\left(\mathrm{i}f_1\right)T\left(f_2\right)\right\}_{i,i}.
\end{aligned}$$

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

Proof.

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

□

We use lemma 5 with $A'_n = T(\mathrm{i}f_1)\,T(f_2)$, $A_n = T(\mathrm{i}f_1 f_2)$, $B'_n = T(\mathrm{i}f_3)\,T(f_4)$ and $B_n = T(\mathrm{i}f_3 f_4)$. It is shown in [1] theorem 12 that $|A'_n - A_n| \to 0$ and $|B'_n - B_n| \to 0$. As $\mathrm{i}f_1 f_2$ is C^∞, the coefficients of $T(\mathrm{i}f_1 f_2)$ are uniformly bounded. Finally $\{T(\mathrm{i}f_1)\,T(f_2)\}_{i,j} \leq \sup_{i,j,n} \left|T(\mathrm{i}f_1)_{i,j}\right| \sum_{k\in\mathbb{Z}} \left|T(f_2)_{k,j}\right|$ which is uniformly bounded because $\mathrm{i}f_1$ and f_2 are C^∞.

Hence

$$\begin{aligned} & \frac{1}{n}\sum_{i,k,l=1}^{n} T(\mathrm{i}f_1)_{i,k}\,T(f_2)_{k,i}\,T(\mathrm{i}f_3)_{i,l}\,T(f_4)_{l,i} \qquad (9)\\ = & \frac{1}{n}\sum_{i=1}^{n} \{T(\mathrm{i}f_3)\,T(f_4)\}_{i,i}\,\{T(\mathrm{i}f_1)\,T(f_2)\}_{i,i}\,,\\ = & \frac{1}{n}\sum_{i=1}^{n} \{T(\mathrm{i}f_3 f_4)\}_{i,i}\,\{T(\mathrm{i}f_1 f_2)\}_{i,i} + o(1)\,,\\ \underset{n\to+\infty}{\to} & M(\mathrm{i}f_3 f_4)\,M(\mathrm{i}f_1 f_2)\,,\\ = & 0, \quad \text{because } f_3 f_4 \text{ is odd.} \end{aligned}$$

We show similarly

$$\frac{1}{n}\sum_{i,j,k=1}^{n} T(\mathrm{i}f_1)_{i,k}\,T(f_2)_{k,j}\,T(\mathrm{i}f_3)_{j,k}\,T(f_4)_{k,i} \to 0. \qquad (10)$$

Then

$$\begin{aligned} & \frac{1}{n}\sum_{i,j,l=1}^{n} T(\mathrm{i}f_1)_{i,j}\,T(f_2)_{j,j}\,T(\mathrm{i}f_3)_{j,l}\,T(f_4)_{l,i} \qquad (11)\\ = & M(f_2)\,\frac{1}{n}\sum_{i,j,l=1}^{n} T(\mathrm{i}f_1)_{i,j}\,T(\mathrm{i}f_3)_{j,l}\,T(f_4)_{l,i}\,,\\ = & M(f_2)\,\frac{1}{n}\sum_{i,j=1}^{n} T(\mathrm{i}f_1)_{i,j}\left\{\sum_{l=1}^{n} T(\mathrm{i}f_3)_{j,l}\,T(f_4)_{l,i}\right\},\\ = & M(f_2)\,\frac{1}{n}\sum_{i,j=1}^{n} T(\mathrm{i}f_1)_{i,j}\,\{T(\mathrm{i}f_3)\,T(f_4)\}_{j,i}\,,\\ = & M(f_2)\,\frac{1}{n}\mathrm{Tr}\,\{T(\mathrm{i}f_1)\,T(\mathrm{i}f_3)\,T(f_4)\}\,,\\ \to & M(f_2)\,M(\mathrm{i}f_1\mathrm{i}f_3 f_4)\,, \quad \text{using [1] theorem 12,}\\ = & -M(f_2)\,M(f_1 f_3 f_4)\,. \end{aligned}$$

We show similarly

$$\frac{1}{n}\sum_{i,j,k=1}^{n} T(\mathrm{i}f_1)_{i,k}\,T(f_2)_{k,j}\,T(\mathrm{i}f_3)_{i,j}\,T(f_4)_{i,i} \to -M(f_4)\,M(f_1 f_2 f_3)\,. \qquad (12)$$

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

□

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

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

Proof.

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

□

References

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