

Supplementary materials for “Smoothing parameter selection in two frameworks for penalized splines”

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1 Estimating equations and their derivatives

In the following $\partial \mathbf{S}_\lambda / \partial \lambda = -\lambda^{-1}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)$ will be used.

1.1 Mallows' C_p

The Mallows' C_p is defined as

$$C_p(\lambda) = \frac{1}{n} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \left\{ 1 + \frac{2\text{tr}(\mathbf{S}_\lambda)}{n} \right\}.$$

Its estimation equation (obtained as $\lambda/2 \partial C_p(\lambda) / \partial \lambda$) will be denoted by $T_{C_p}(\lambda)$, which, together with its derivative, is given by

$$\begin{aligned} T_{C_p}(\lambda) &= \frac{1}{n} \left[\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{Y} \left\{ 1 + \frac{2\text{tr}(\mathbf{S}_\lambda)}{n} \right\} - \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \frac{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n} \right], \\ T'_{C_p}(\lambda) &= -\frac{1}{\lambda n} \left\{ \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (\mathbf{S}_\lambda - 3\mathbf{S}_\lambda^2) \mathbf{Y} - \frac{\text{tr}(\mathbf{S}_\lambda)}{n} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (\mathbf{I}_n - 6\mathbf{S}_\lambda + 6\mathbf{S}_\lambda^2) \mathbf{Y} \right. \\ &\quad \left. + \frac{\text{tr}(\mathbf{S}_\lambda^2)}{n} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (3\mathbf{I}_n - 4\mathbf{S}_\lambda) \mathbf{Y} - \frac{2\text{tr}(\mathbf{S}_\lambda^3)}{n} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \right\}. \end{aligned}$$

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1.1.1 Frequentist model

Let find the expectations of $T_{Cp}(\lambda)$ and $T'_{Cp}(\lambda)$, as well as the variance of $T_{Cp}(\lambda)$, under the frequentist model (1), that is for \mathbf{Y} with $E_f(\mathbf{Y}) = \mathbf{f}$ and $\text{var}_f(\mathbf{Y}) = \sigma^2 \mathbf{I}_n$.

$$\begin{aligned} E_f \{T_{Cp}(\lambda)\} &= \frac{1}{n} \left[\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} - \sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2\} \right. \\ &+ \frac{2\text{tr}(\mathbf{S}_\lambda)}{n} \{ \sigma^2 \text{tr}(2\mathbf{S}_\lambda - 3\mathbf{S}_\lambda^2 + \mathbf{S}_\lambda^3) + \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} \} \\ &\left. - \frac{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n} \{ \sigma^2 \text{tr}(\mathbf{S}_\lambda^2) + \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{f} \} \right], \end{aligned}$$

$$\begin{aligned} E_f \{T'_{Cp}(\lambda)\} &= -\frac{1}{\lambda n} \left[\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (\mathbf{S}_\lambda - 3\mathbf{S}_\lambda^2) \mathbf{f} - \sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 (2\mathbf{I}_n - 3\mathbf{S}_\lambda)\} \right. \\ &+ \frac{\text{tr}(\mathbf{S}_\lambda)}{n} \{ \sigma^2 \text{tr}(8\mathbf{S}_\lambda - 19\mathbf{S}_\lambda^2 + 18\mathbf{S}_\lambda^3 - 6\mathbf{S}_\lambda^4) - \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (\mathbf{I}_n - 6\mathbf{S}_\lambda + \mathbf{S}_\lambda^2) \mathbf{f} \} \\ &- \frac{\text{tr}(\mathbf{S}_\lambda^2)}{n} \{ \sigma^2 \text{tr}(10\mathbf{S}_\lambda - 11\mathbf{S}_\lambda^2 + 4\mathbf{S}_\lambda^3) - \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (3\mathbf{I}_n - 4\mathbf{S}_\lambda) \mathbf{f} \} \\ &\left. + \frac{2\text{tr}(\mathbf{S}_\lambda^3)}{n} \{ \sigma^2 \text{tr}(2\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) - \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{f} \} \right]. \end{aligned}$$

Under assumptions of Gaussian errors, one finds

$$\begin{aligned} \text{var}_f \{T_{Cp}(\lambda)\} &= \frac{2\sigma^2}{n^2} \left(\sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2\} + 2\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \mathbf{f} \right. \\ &+ \frac{4\text{tr}(\mathbf{S}_\lambda)}{n} \{1 + \text{tr}(\mathbf{S}_\lambda)/n\} [\sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2\} + 2\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \mathbf{f}] \\ &- \frac{2\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n} \{1 + 2\text{tr}(\mathbf{S}_\lambda)/n\} [\sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda\} + 2\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda \mathbf{f}] \\ &\left. + \frac{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)^2}{n^2} \{ \sigma^2 \text{tr}(\mathbf{I}_n - \mathbf{S}_\lambda)^4 + 2\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{f} \} \right), \end{aligned}$$

using $\text{var}_f(\mathbf{Y}^t \mathbf{A} \mathbf{Y}) = 2\sigma^4 \text{tr}(\mathbf{A}^2) + 4\sigma^2 \mathbf{f}^t \mathbf{A}^2 \mathbf{f}$ for any $n \times n$ matrix \mathbf{A} . If normality of errors is not given, but $E_f(\epsilon_i^4) =: \mu_4 < \infty$ can be assumed, then $\text{var}_f(\mathbf{Y}^t \mathbf{A} \mathbf{Y}) = 2\sigma^4 \text{tr}(\mathbf{A}^2) + 4\sigma^2 \mathbf{f}^t \mathbf{A}^2 \mathbf{f} + (\mu_4 - 3\sigma^4) \text{tr}(\mathbf{A} \circ \mathbf{A})$, for \circ denoting the Hadamard product (see e.g. Wiens, 1992). Hence, $\text{var}_f \{T_{Cp}(\lambda)\}$ has an additional term, which, using the linearity

of the Hadamard product, can be written as

$$\begin{aligned}
& (\mu_4 - 3\sigma^4) \left[\text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \circ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \} \right. \\
& + \frac{4\text{tr}(\mathbf{S}_\lambda)}{n} \{1 + 2\text{tr}(\mathbf{S}_\lambda)/n\} \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \circ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \} \\
& - \frac{2\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n} \{1 + 2\text{tr}(\mathbf{S}_\lambda)/n\} \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \circ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \} \\
& \left. + \frac{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)^2}{n^2} \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \circ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \} \right].
\end{aligned}$$

To simplify all above expressions, note that $\text{tr}(\mathbf{S}_\lambda^l) = \text{const} \lambda^{-1/(2q)}$ and $\lambda^{-1/(2q)} n^{-1} = o(1)$ due to (A3), as well as

$$\begin{aligned}
\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \mathbf{f} &= \sum_{i=1}^{k+p+1} \frac{b_i^2 (\lambda n \eta_i)^m}{(1 + \lambda n \eta_i)^{m+l}} + n I_{\{l=0\}} \frac{1}{n} \mathbf{f}^t (\mathbf{I}_n - \mathbf{\Phi}_k \mathbf{\Phi}_k^t) \mathbf{f} \\
&= \lambda n \frac{1}{n} \sum_{i=1}^{k+p+1} b_i^2 n \eta_i \frac{(\lambda n \eta_i)^{m-1}}{(1 + \lambda n \eta_i)^{m+l}} + O(k^{-2q} n) = O(\lambda n) + O(k^{-2q} n),
\end{aligned}$$

for any $m = 1, 2, \dots$ and $l = 0, 1, \dots$. Here $n^{-1} \mathbf{f}^t (\mathbf{I}_n - \mathbf{\Phi}_k \mathbf{\Phi}_k^t) \mathbf{f}$ is the average squared approximation bias, see Claeskens et al. (2009).

Next, the diagonal elements $\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda\}_{jj} = \sum_{i=q+1}^{k+p+1} \phi_{ji}^2 (\lambda n \eta_i)^2 (1 + \lambda n \eta_i)^{-3}$, so that

$$\begin{aligned}
\text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \circ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \} &= \sum_{j=1}^n \left\{ \sum_{i=q+1}^{k+p+1} \frac{\phi_{ji}^2 (\lambda n \eta_i)^2}{(1 + \lambda n \eta_i)^3} \right\}^2 \\
&\leq [\text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \}]^2 \sum_{j=1}^n \{ \max_i \phi_{ji}^2 \}^2 = O(n^{-1} \lambda^{-1/q}),
\end{aligned}$$

since $\phi_{ji}^2 = O(n^{-1})$ by definition. Similarly, one can show that the terms containing

$\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2\}_{jj} = 1 - \sum_{i=1}^{k+p+1} \phi_{ji}^2 + \sum_{i=q+1}^{k+p+1} \phi_{ji}^2 (\lambda n \eta_i)^2 (1 + \lambda n \eta_i)^{-2}$ are also negligible.

Hence, both for Gaussian and non-normal errors with $\text{E}_f(\epsilon_i^4) < \infty$, it holds

$$\begin{aligned}
\text{E}_f \{T_{Cp}(\lambda)\} &= \frac{1}{n} \left[\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} - \sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 \} + o(1) \right], \\
\text{E}_f \{T'_{Cp}(\lambda)\} &= \frac{1}{\lambda n} \left[\sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 (2\mathbf{I}_n - 3\mathbf{S}_\lambda) \} - \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 (\mathbf{S}_\lambda - 3\mathbf{S}_\lambda^2) \mathbf{f} + o(1) \right], \\
\text{var}_f \{T_{Cp}(\lambda)\} &= \frac{2\sigma^2}{n^2} \left[2\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \mathbf{f} + \sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \} + o(1) \right].
\end{aligned}$$

Note that other popular criteria like generalized cross validation (GCV) by Craven and Wahba (1978) or Akaike information criterion (AIC Akaike, 1969) are asymptotically equivalent to Mallows' C_p , so that all subsequent results for Mallows' C_p hold also for these criteria. Indeed,

$$\begin{aligned}
\text{GCV}(\lambda) &= n^{-1} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \{1 - \text{tr}(\mathbf{S}_\lambda)/n\}^{-2} \\
&= n^{-1} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \{1 + 2\text{tr}(\mathbf{S}_\lambda)/n + 3\text{tr}(\mathbf{S}_\lambda)^2/n^2 + \dots\} \\
\exp \{\text{AIC}(\lambda)\} &= n^{-1} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \exp \{2\text{tr}(\mathbf{S}_\lambda)/n\} \\
&= n^{-1} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \{1 + 2\text{tr}(\mathbf{S}_\lambda)/n + 2\text{tr}(\mathbf{S}_\lambda)^2/n^2 + \dots\},
\end{aligned}$$

where $\text{tr}(\mathbf{S}_\lambda)^2/n^2 = \text{const } \lambda^{-1/q} n^{-2} = o(\text{tr}(\mathbf{S}_\lambda)/n)$.

1.1.2 Stochastic model

To find expectations and variances under the stochastic model (4), that is for $\mathbf{Y} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n + \sigma_u^2 \tilde{\mathbf{R}})$ ($\tilde{\mathbf{R}}$ is defined in the proof of Theorem 2), note that for any $m = 1, 2, \dots$ and $l = 0, 1, \dots$

$$\begin{aligned}
\mathbb{E}_\beta \{ \mathbf{Y}^T (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \mathbf{Y} \} &= \sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \} + \sigma_u^2 \text{tr} \left\{ \mathbf{C} \tilde{\mathbf{D}}^- \mathbf{C}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \right\} \\
&\times \left[1 + \frac{\text{tr} \left\{ (\tilde{\mathbf{R}} - \mathbf{C} \tilde{\mathbf{D}}^- \mathbf{C}^t) (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \right\}}{\text{tr} \left\{ \mathbf{C} \tilde{\mathbf{D}}^- \mathbf{C}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \right\}} \right] \\
&= \sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \} \\
&+ \sigma_u^2 \lambda n \left[\text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^{m-1} \mathbf{S}_\lambda^{l+1} \} - q I_{\{m=1\}} \right] \{1 + \tilde{r}(l, m)\},
\end{aligned}$$

where

$$\text{tr} \left\{ \mathbf{C} \tilde{\mathbf{D}}^- \mathbf{C}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \right\} = \lambda n \left[\text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^{m-1} \mathbf{S}_\lambda^{l+1} \} - q I_{\{m=1\}} \right]$$

has been used and

$$\tilde{r}(l, m) = \frac{\text{tr} \left\{ (\tilde{\mathbf{R}} - \mathbf{C} \tilde{\mathbf{D}}^{-1} \mathbf{C}^t) (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \right\}}{\text{tr} \left\{ \mathbf{C} \tilde{\mathbf{D}}^{-1} \mathbf{C}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \right\}} = \begin{cases} o(1), & l, m \in \mathbb{N} \\ o(\lambda^{-1+1/(2q)}), & l = 0, m \in \mathbb{N} \end{cases},$$

is shown to hold below. With this,

$$\mathbb{E}_\beta \{T_{Cp}(\lambda)\} = \frac{1}{n} \left[\sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) o(1) + (\sigma_u^2 \lambda n - \sigma^2) \text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3) \right] \{1 + o(1)\},$$

$$\mathbb{E}_\beta \{T'_{Cp}(\lambda)\} = \frac{1}{\lambda n} \left[\sigma^2 \text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3) + (\sigma_u^2 \lambda n - \sigma^2) \text{tr}\{(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)(3\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda)\} \right] \{1 + o(1)\},$$

$$\begin{aligned} \text{var}_\beta \{T_{Cp}(\lambda)\} &= \frac{2\sigma^4}{n^2} \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2\} \{1 + o(1)\} + \frac{2(\sigma_u^2 \lambda n - \sigma^2)}{n^2} \\ &\times \left[\sigma_u^2 \lambda n \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^4\} + \sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^3 (2\mathbf{I}_n - \mathbf{S}_\lambda)\} \right] \{1 + o(1)\}. \end{aligned}$$

Since $\lambda_r = \sigma^2/(\sigma_u^2 n) = \lambda_{f|r} \{1 + o(1)\}$, all terms with the multiplier $(\sigma_u^2 \lambda_{f|r} n - \sigma^2)$ in $\mathbb{E}_\beta \{T_{Cp}(\lambda_{f|r})\}$, $\mathbb{E}_\beta \{T'_{Cp}(\lambda_{f|r})\}$ and $\text{var}_\beta \{T_{Cp}(\lambda_{f|r})\}$ are asymptotically negligible.

Let now show the order of $\tilde{r}(l, m)$. With the Demmler-Reinsch basis, one can represent $\tilde{\mathbf{R}} = \mathbf{\Phi}_n \text{diag}(\boldsymbol{\eta}_n^-) \mathbf{\Phi}_n^t$, as well as $\mathbf{C} \tilde{\mathbf{D}}^{-1} \mathbf{C}^t = \mathbf{\Phi}_k \text{diag}(\boldsymbol{\eta}_k^-) \mathbf{\Phi}_k^t$, where the eigenvalues $\boldsymbol{\eta}_k^- = (\mathbf{0}_q, \eta_{k,q+1}^{-1}, \dots, \eta_{k,k+p+1}^{-1})^t$, $\boldsymbol{\eta}_n^- = (\mathbf{0}_q, \eta_{n,q+1}^{-1}, \dots, \eta_{n,n}^{-1})^t$ and $\mathbf{\Phi}_n$ corresponds to the Demmler-Reinsch basis for $k = n$. Denote also $\mathbf{\Phi}_{kn} = \mathbf{\Phi}_k^t \mathbf{\Phi}_n$ a $(k + p + 1) \times n$ semi-orthonormal matrix, such that $\mathbf{\Phi}_{kn} \mathbf{\Phi}_{kn}^t = \mathbf{I}_{k+p+1}$. With this,

$$\begin{aligned} \tilde{r}(l, m) &= \frac{\text{tr} \left[\{ \mathbf{\Phi}_{kn} \text{diag}(\boldsymbol{\eta}_n^-) \mathbf{\Phi}_{kn}^t - \text{diag}(\boldsymbol{\eta}_k^-) \} \text{diag} \{ (\lambda n \boldsymbol{\eta}_k)^m (1 + \lambda n \boldsymbol{\eta}_k)^{-(l+m)} \} \right]}{\lambda n \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^{m-1} \mathbf{S}_\lambda^{l+1}\}} \\ &+ I_{\{l=0\}} \frac{\text{tr}\{(\text{diag}(\boldsymbol{\eta}_n^-) (\mathbf{I}_n - \mathbf{\Phi}_{kn}^t \mathbf{\Phi}_{kn}))\}}{\lambda n \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^{m-1} \mathbf{S}_\lambda^{l+1}\}}. \end{aligned}$$

First, consider the diagonal elements of $\{ \mathbf{\Phi}_{kn} \text{diag}(\boldsymbol{\eta}_n^-) \mathbf{\Phi}_{kn}^t - \text{diag}(\boldsymbol{\eta}_k^-) \}$, which are given by $\left(\sum_{i=q+1}^n \{ \mathbf{\Phi}_{kn} \}_{ij}^2 \eta_{n,i}^{-1} - \eta_{k,j}^{-1} \right)$, $j = q + 1, \dots, k + p + 1$. The elements $\{ \mathbf{\Phi}_{kn} \}_{ij}$ belong to a product of two Demmler-Reinsch bases at the same set of x -values but based on a different number of knots: $\mathbf{\Phi}_k$ and $\mathbf{\Phi}_n$. From the properties of the Demmler-Reinsch

basis it holds that $\eta_{k,i} = \eta_{n,i}\{1 + o(1)\}$, as well as $\phi_{k,i} = \phi_{n,i}\{1 + o(1)\}$, where $o(1)$ is independent of i , for $i = o\{n^{2/(2q+1)}\}$. Hence, $\{\Phi_{kn}\}_{jj}^2 = 1 + o(1)$ and $\{\Phi_{kn}\}_{ij}^2 = o(n^{-1})$, $i \neq j$. Let fix an index $j^* \propto n^{1/(2q)}$, so that $j^* = o\{n^{2/(2q+1)}\}$ is fulfilled. Then, for $j \leq j^*$

$$\sum_{i=q+1}^n \{\Phi_{kn}\}_{ij}^2 \eta_{n,i}^{-1} - \eta_{k,j}^{-1} = o(1) \sum_{i=q+1}^n \frac{(i-q)^{-2q}}{c(\rho)^{2q}} + o(1) \eta_{k,j}^{-1} = o(1) \eta_{k,j}^{-1},$$

implying

$$\begin{aligned} & \text{tr} \left[\{ \Phi_{kn} \text{diag}(\boldsymbol{\eta}_n^-) \Phi_{kn}^t - \text{diag}(\boldsymbol{\eta}_k^-) \} \text{diag} \{ (\lambda n \boldsymbol{\eta}_k)^m (1 + \lambda n \boldsymbol{\eta}_k)^{-(l+m)} \} \right] \\ &= o(1) \lambda n \text{tr} \{ \mathbf{I}_n - \mathbf{S}_\lambda \}^{m-1} \mathbf{S}_\lambda^{l+1}, \end{aligned}$$

since for $j > j^*$ the sum components of the trace are negligible. Similarly,

$$\text{tr} \{ (\text{diag}(\boldsymbol{\eta}_n^-) (\mathbf{I}_n - \Phi_{kn}^t \Phi_{kn}) \} = \sum_{i=q+1}^n \eta_{n,i}^{-1} \left(1 - \sum_{j=q+1}^{k+p+1} \{\Phi_{kn}\}_{ij}^2 \right) = o(n^{-1}),$$

so that $\tilde{r}(l, m) = o(1)$ for $l, m \in \mathbb{N}$ and $\tilde{r}(0, m) = o(\lambda^{1-1/(2q)})$, $m \in \mathbb{N}$.

1.2 Restricted maximum likelihood

The likelihood function for the model (5) is given by

$$-2l(\boldsymbol{\beta}, \sigma^2, \sigma_u^2; \mathbf{Y}) = n \log \sigma^2 + \log |\mathbf{V}_\lambda| + \sigma^{-2} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^t \mathbf{V}_\lambda^{-1} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}),$$

with $\mathbf{V}_\lambda = \mathbf{I}_n + \sigma_u^2 \mathbf{Z} \mathbf{D}^{-1} \mathbf{Z}^t / \sigma^2$. Plugging in $\tilde{\boldsymbol{\beta}} = (\mathbf{X}^t \mathbf{V}_\lambda^{-1} \mathbf{X})^{-1} \mathbf{X}^t \mathbf{V}_\lambda^{-1} \mathbf{Y}$, leads to the profile likelihood for σ^2 and σ_u^2 . However, σ^2 and $\lambda = \sigma^2 / (n\sigma_u^2)$ are better to be estimated from the restricted profile likelihood (Patterson and Thompson, 1971)

$$\begin{aligned} -2l_r(\sigma^2, \lambda; \mathbf{Y}) &= -2l(\tilde{\boldsymbol{\beta}}, \sigma^2, \sigma_u^2; \mathbf{Y}) + \log |\sigma^2 \mathbf{X}^t \mathbf{V}_\lambda^{-1} \mathbf{X}| \\ &= (n - q) \log \sigma^2 + \log |\mathbf{V}_\lambda| |\mathbf{X}^t \mathbf{V}_\lambda^{-1} \mathbf{X}| + \frac{\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y}}{\sigma^2}. \end{aligned}$$

Since $\hat{\sigma}_{ML}^2 = (n - q)^{-1} \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y}$, the profile restricted likelihood for λ results in

$$-2l_p(\lambda; \mathbf{Y}) = (n - q) \log \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y} + \log |\mathbf{V}_\lambda| |\mathbf{X}^t \mathbf{V}_\lambda^{-1} \mathbf{X}|.$$

Its first derivative equals

$$\begin{aligned} \frac{\partial l_p(\lambda; \mathbf{Y})}{\partial \lambda} &= -\frac{n - q}{2\lambda} \frac{\mathbf{Y}^t (\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{Y}}{\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y}} - \frac{1}{2} \text{tr} \left\{ (\mathbf{X} \mathbf{V}_\lambda^{-1} \mathbf{X})^{-1} \mathbf{X}^t \frac{\partial \mathbf{V}_\lambda^{-1}}{\partial \lambda} \mathbf{X} \right\} \\ &\quad - \frac{1}{2} \text{tr} \left(\mathbf{V}_\lambda^{-1} \frac{\partial \mathbf{V}_\lambda}{\partial \lambda} \right) = -\frac{n - q}{2\lambda} \frac{\mathbf{Y}^t (\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{Y}}{\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y}} + \frac{\text{tr}(\mathbf{S}_\lambda) - q}{2\lambda}. \end{aligned}$$

The estimating equation is now defined via

$$\begin{aligned} T_{ML}(\lambda) &= -\frac{2\lambda \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y}}{n(n - q)} \frac{\partial l_p(\lambda; \mathbf{Y})}{\partial \lambda} \\ &= \frac{1}{n} \left[\mathbf{Y}^t (\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{Y} - \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y} \{ \text{tr}(\mathbf{S}_\lambda) - q \} / (n - q) \right]. \end{aligned}$$

The first derivative of $T_{ML}(\lambda)$ is given by

$$\begin{aligned} T'_{ML}(\lambda) &= -\frac{1}{\lambda n} \left\{ \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda (\mathbf{I}_n - 2\mathbf{S}_\lambda) \mathbf{Y} + \mathbf{Y}^t (\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{Y} \frac{\text{tr}(\mathbf{S}_\lambda) - q}{n - q} \right. \\ &\quad \left. - \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y} \frac{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n - q} \right\}. \end{aligned}$$

1.2.1 Frequentist model

Let now find the expectations of $T_{ML}(\lambda)$ and $T'_{ML}(\lambda)$, as well as the variance of $T_{ML}(\lambda)$, under the frequentist model (1).

$$\begin{aligned} E_f \{T_{ML}(\lambda)\} &= \frac{1}{n} \left[\mathbf{f}^t (\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{f} - \sigma^2 \{ \text{tr}(\mathbf{S}_\lambda^2) - q \} \right. \\ &\quad \left. + \frac{\text{tr}(\mathbf{S}_\lambda) - q}{n - q} \{ \sigma^2 \text{tr}(\mathbf{S}_\lambda) - \sigma^2 q - \mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{f} \} \right], \end{aligned}$$

$$\begin{aligned}
\mathbb{E}_f \left\{ T'_{ML}(\lambda) \right\} &= \frac{1}{\lambda n} \left[2\sigma^2 \text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3) - \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda (\mathbf{I}_n - 2\mathbf{S}_\lambda) \mathbf{f} \right. \\
&\quad - \frac{\text{tr}(\mathbf{S}_\lambda) - q}{n - q} \left\{ \sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) + \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \mathbf{f} \right\} \\
&\quad \left. - \frac{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n - q} \left\{ \sigma^2 \text{tr}(\mathbf{S}_\lambda) - \sigma^2 q - \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{f} \right\} \right].
\end{aligned}$$

Under assumption of the Gaussian errors

$$\begin{aligned}
\text{var}_f \{ T_{ML}(\lambda) \} &= \frac{2\sigma^2}{n^2} \left(\sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2 \} + 2\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2 \mathbf{f} \right. \\
&\quad - \frac{2\{\text{tr}(\mathbf{S}_\lambda) - q\}}{n - q} \left[\sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \} + 2\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} \right] \\
&\quad \left. + \frac{\{\text{tr}(\mathbf{S}_\lambda) - q\}^2}{(n - q)^2} \left\{ \sigma^2 \text{tr}(\mathbf{I}_n - \mathbf{S}_\lambda)^2 + 2\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{f} \right\} \right).
\end{aligned}$$

If the errors are not Gaussian, but $\mathbb{E}_f(\epsilon_i^4) = \mu_4 < \infty$ holds, then $\text{var}_f \{ T_{ML}(\lambda) \}$ has an extra term given by

$$\begin{aligned}
&(\mu_4 - 3\sigma^4) \left[\text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \circ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \} \right. \\
&\quad - \frac{2\{\text{tr}(\mathbf{S}_\lambda) - q\}}{n - q} \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \circ (\mathbf{I}_n - \mathbf{S}_\lambda) \} \\
&\quad \left. + \frac{\{\text{tr}(\mathbf{S}_\lambda) - q\}^2}{(n - q)^2} \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \circ (\mathbf{I}_n - \mathbf{S}_\lambda) \} \right].
\end{aligned}$$

With the same arguments as in Section 1.1.1, one obtains

$$\begin{aligned}
\mathbb{E}_f \{ T_{ML}(\lambda) \} &= \frac{1}{n} \left[\mathbf{f}^t(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{f} - \sigma^2 \{ \text{tr}(\mathbf{S}_\lambda^2) - q \} + o(1) \right], \\
\mathbb{E}_f \left\{ T'_{ML}(\lambda) \right\} &= \frac{1}{\lambda n} \left[2\sigma^2 \text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3) - \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda (\mathbf{I}_n - 2\mathbf{S}_\lambda) \mathbf{f} + o(1) \right], \\
\text{var}_f \{ T_{ML}(\lambda) \} &= \frac{2\sigma^2}{n^2} \left[2\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2 \mathbf{f} + \sigma^2 \{ \text{tr}(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2 \} + o(1) \right].
\end{aligned}$$

Now, it is easy to verify equation (6) of the paper

$$\begin{aligned}
R(\lambda) &= \mathbb{E}_f \{ T_{ML}(\lambda) \} - \mathbb{E}_f \{ T_{Cp}(\lambda) \} = \frac{1}{n} \left[\mathbf{f}^t(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{f} - \sigma^2 \{ \text{tr}(\mathbf{S}_\lambda^2) - q \} + o(1) \right. \\
&\quad \left. - \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} - \sigma^2 \text{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 \} + o(1) \right] \\
&= \frac{1}{n} \left[\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 \mathbf{f} - \sigma^2 \{ \text{tr}(\mathbf{S}_\lambda^3) - q \} + o(1) \right].
\end{aligned}$$

Note also $E_f [\mathbf{Y}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 \mathbf{Y} - \sigma^2 \{\text{tr}(\mathbf{S}_\lambda^2) - q\}] = \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 \mathbf{f} - \sigma^2 \{\text{tr}(\mathbf{S}_\lambda^3) - q\}$.

1.2.2 Stochastic model

Applying results of Section 1.1.2 gives

$$\begin{aligned} E_\beta \{T_{ML}(\lambda)\} &= \frac{1}{n} \left\{ \text{tr}(\mathbf{S}_\lambda) o(1) + (\sigma_u^2 \lambda n - \sigma^2) \text{tr}(\mathbf{S}_\lambda^2) \right\} \{1 + o(1)\}, \\ E_\beta \{T'_{ML}(\lambda)\} &= \frac{\sigma^2}{\lambda n} \left\{ \text{tr}(\mathbf{S}_\lambda^2) + (\sigma_u^2 \lambda n - \sigma^2) \text{tr}(2\mathbf{S}_\lambda^3 - \mathbf{S}_\lambda^2) \right\} \{1 + o(1)\}, \\ \text{var}_\beta \{T_{ML}(\lambda)\} &= \frac{2}{n^2} \left[\sigma^4 \text{tr}(\mathbf{S}_\lambda^2) - (\sigma_u^2 \lambda n - \sigma^2) \sigma^2 \text{tr}\{\mathbf{S}_\lambda^3(2\mathbf{I}_n - \mathbf{S}_\lambda)\} \right. \\ &\quad \left. + \sigma_u^2 \lambda n (\sigma_u^2 \lambda n - \sigma^2) \text{tr}(\mathbf{S}_\lambda^4) \right] \{1 + o(1)\}. \end{aligned}$$

2 Detailed proof of Theorem 3

2.1 Proof for $\widehat{\lambda}_f$

From the Taylor expansion $0 = T_{Cp}(\widehat{\lambda}_f) = T_{Cp}(\lambda_f) + T'_{Cp}(\widetilde{\lambda})(\widehat{\lambda}_f - \lambda_f)$, for some $\widetilde{\lambda}$ between $\widehat{\lambda}_f$ and λ_f , it holds $\widehat{\lambda}_f - \lambda_f = -T_{Cp}(\lambda_f)/T'_{Cp}(\widetilde{\lambda})$.

Showing

$$\frac{T_{Cp}(\lambda_f) - E_f\{T_{Cp}(\lambda_f)\}}{\sqrt{\text{var}_f\{T_{Cp}(\lambda_f)\}}} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) \quad \text{and} \quad \frac{T'_{Cp}(\widetilde{\lambda})}{E_f\{T'_{Cp}(\lambda_f)\}} \xrightarrow{\mathcal{P}} 1,$$

would allow to apply Slutsky's lemma and to conclude that

$$\left(\frac{\widehat{\lambda}_f}{\lambda_f} - 1 \right) \xrightarrow{\mathcal{D}} \mathcal{N} \left(0, \frac{\text{var}_f\{T_{Cp}(\lambda_f)\}}{[\lambda_f E_f\{T'_{Cp}(\lambda_f)\}]^2} \right).$$

To find $E_f\{T'_{Cp}(\lambda_f)\}$ and $\text{var}_f\{T_{Cp}(\lambda_f)\}$, Lemma 3 is applied to get

$$\begin{aligned} \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2(\mathbf{S}_\lambda - 3\mathbf{S}_\lambda^2)\mathbf{f}|_{\lambda=\lambda_f} &= -2\sigma^2 \text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3)|_{\lambda=\lambda_f} \{1 + o(1)\}, \\ \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \mathbf{f}|_{\lambda=\lambda_f} &= o\left(\lambda_f^{-\frac{1}{2q}}\right), \end{aligned}$$

so that

$$\begin{aligned} \mathbb{E}_f \left\{ T'_{Cp}(\lambda_f) \right\} &= \frac{\sigma^2}{\lambda_f n} \operatorname{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2 (4\mathbf{I}_n - 3\mathbf{S}_\lambda) \} \Big|_{\lambda=\lambda_f} \{1 + o(1)\}, \\ \operatorname{var}_f \{ T_{Cp}(\lambda_f) \} &= \frac{2\sigma^4}{n^2} \operatorname{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \} \Big|_{\lambda=\lambda_f} \{1 + o(1)\}. \end{aligned}$$

Employing the formula

$$\operatorname{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^m \mathbf{S}_\lambda^l \} = \frac{\lambda^{-1/(2q)} \Gamma\{m + 1/(2q)\} \Gamma\{l - 1/(2q)\}}{c(\rho) 2q \Gamma(l + m)} \{1 + o(1)\},$$

as well as $\Gamma(1 + x) = x\Gamma(x)$ and $\Gamma\{1 - 1/(2q)\} \Gamma\{1/(2q)\} / (2q) = 1/\operatorname{sinc}\{\pi/(2q)\}$ allows to simplify

$$\begin{aligned} \mathbb{E}_f \left\{ T'_{Cp}(\lambda_f) \right\} &= \frac{\sigma^2 \lambda_f^{-1/(2q)-1}}{n c(\rho)} \frac{(2q-1)(4q+1)}{16q^3 \operatorname{sinc}\{\pi/(2q)\}} \{1 + o(1)\}, \\ \operatorname{var}_f \{ T_{Cp}(\lambda_f) \} &= \frac{2\sigma^4 \lambda_f^{-1/(2q)}}{n^2 c(\rho)} \frac{(2q-1)(2q+1)(4q+1)(6q+1)}{3840q^5 \operatorname{sinc}\{\pi/(2q)\}} \{1 + o(1)\}. \end{aligned}$$

Consider now

$$\begin{aligned} n T_{Cp}(\lambda_f) &= \left[\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{Y} \left\{ 1 + \frac{\operatorname{tr}(\mathbf{S}_\lambda)}{n} \right\} - \mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{Y} \frac{\operatorname{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n} \right] \Big|_{\lambda=\lambda_f} \\ &= \left[\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{Y} - \hat{\sigma}^2 \operatorname{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \right] \Big|_{\lambda=\lambda_f} + o_p(1). \end{aligned}$$

One can also represent,

$$\mathbb{E}_f \{ n T_{Cp}(\lambda_f) \} = \left[\mathbf{f}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} + \sigma^2 \operatorname{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \} - \sigma^2 \operatorname{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \right] \Big|_{\lambda=\lambda_f} + o(1).$$

Denoting $d_i = \sum_{j=1}^n \phi_{k,i}(x_j) y_j$, such that $\mathbb{E}_f(d_i^2) = b_i^2 + \sigma^2$, and noting that $\hat{\sigma}^2 = \sigma^2 \{1 + O_p(n^{-1/2})\}$, define random variables ξ_i

$$n [T_{Cp}(\lambda_f) - \mathbb{E}_f \{ T_{Cp}(\lambda_f) \}] = \sum_{i=q+1}^{k+p+1} (d_i^2 - b_i^2 - \sigma^2) \frac{(\lambda_f n \eta_i)^2}{(1 + \lambda_f n \eta_i)^3} + o_p(1) =: \sum_{i=q+1}^{k+p+1} \xi_i,$$

such that $\mathbb{E}_f(\xi_i) = o(1)$ and $s_n^2 = \sum_{i=q+1}^{k+p+1} \operatorname{var}_f(\xi_i) = 2\sigma^4 \operatorname{tr} \{ (\mathbf{I}_n - \mathbf{S}_\lambda)^4 \mathbf{S}_\lambda^2 \} \{1 + o(1)\}$. Since $s_n^2 = \operatorname{const} \lambda_f^{-1/(2q)}$ and $(\lambda_f^{1/(2q)} k)^{-1} \rightarrow 0$ according to (A2) and (A3), each $\operatorname{var}_f(\xi_i) = o(1)$

and there exist a constant B , such that $E_f|\xi_i|^2 = \text{var}_f(\xi_i) + o(1) < B$, $i = q+1, \dots, k+p+1$.

With this, the Lyapunov's condition

$$s_n^{-4} \sum_{i=q+1}^{k+p+1} E_f|\xi_i|^4 < B s_n^{-4} \sum_{i=q+1}^{k+p+1} E_f|\xi_i|^2 = B s_n^{-2} = O\left(\lambda_f^{1/(2q)}\right)$$

converges to zero as n tends to infinity. Thus, $s_n^{-1} \sum_{i=q+1}^{k+p+1} \xi_i \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$, or equivalently, $[\text{var}_f\{T_{Cp}(\lambda_f)\}]^{-1/2} [T_{Cp}(\lambda_f) - E_f\{T_{Cp}(\lambda_f)\}] \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$.

Next is shown that $\hat{\lambda}_f \xrightarrow{\mathcal{P}} \lambda_f$. From $\text{var}_f\{T_{Cp}(\lambda)\} = O(\lambda^{-1/(2q)} n^{-2}) \rightarrow 0$ for $n \rightarrow \infty$, it follows $T_{Cp}(\lambda) \xrightarrow{\mathcal{P}} E_f\{T_{Cp}(\lambda)\}$, for any λ satisfying (A3). It remains to verify that $E_f[T_{Cp}\{\lambda_f(1 - \varepsilon)\}] < 0 < E_f[T_{Cp}\{\lambda_f(1 + \varepsilon)\}]$, for any $\varepsilon \in (0, 1)$ (see Lemma 5.10 in van der Vaart, 1998). Let define $B_1(\lambda_f)$ and $B_2(\lambda_f)$ from the representation of $E_f\{T_{Cp}(\lambda_f)\}$ in terms of the Demmler-Reinsch basis.

$$\begin{aligned} E_f\{T_{Cp}(\lambda_f)\} &= \frac{1}{n} [\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f} - \sigma^2 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda^2\} + o(1)]|_{\lambda=\lambda_f} \\ &= \frac{1}{n} \sum_{i=1}^{k+p+1} \frac{b_i^2(\lambda_f n \eta_i)^2}{(1 + \lambda_f n \eta_i)^3} - \frac{\sigma^2 \lambda_f^{-\frac{1}{2q}} c(q, 2, K_q)}{4qc(\rho)n} + o(n^{-1}) \\ &=: B_1(\lambda_f) - B_2(\lambda_f) + o(n^{-1}), \end{aligned}$$

where $B_1(\lambda_f) - B_2(\lambda_f) = 0$ by definition of λ_f . Then,

$$\begin{aligned} E_f[T_{Cp}\{\lambda_f(1 - \varepsilon)\}] &= \frac{1}{n} \sum_{i=1}^{k+p+1} \frac{b_i^2\{\lambda_f(1 - \varepsilon)n\eta_i\}^2}{\{1 + \lambda_f n(1 - \varepsilon)\eta_i\}^3} \\ &\quad - (1 - \varepsilon)^{-\frac{1}{2q}} \frac{\sigma^2 \lambda_f^{-1/(2q)} c(q, 2, K_q)}{4qnc(\rho)} + o(n^{-1}) \\ &= \frac{(1 - \varepsilon)^2}{n} \left\{ \sum_{i=1}^{k+p+1} \frac{b_i^2(\lambda_f n \eta_i)^2}{(1 + \lambda_f n \eta_i)^3} + \sum_{j=1}^{\infty} \sum_{i=1}^{k+p+1} \frac{(j+2)(j+1)b_i^2(\lambda_f n \eta_i)^{2+j}}{\varepsilon^{-j} 2(1 + \lambda_f n \eta_i)^{3+j}} \right\} \\ &\quad - (1 - \varepsilon)^{-\frac{1}{2q}} B_2(\lambda_f) + o(n^{-1}) \\ &= (1 - \varepsilon)^2 B_1(\lambda_f) \left\{ 1 + \sum_{j=1}^{\infty} \frac{\varepsilon^j (j+2)(j+1)}{2} \frac{\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^{2+j} \mathbf{S}_\lambda \mathbf{f}}{\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f}} \Big|_{\lambda=\lambda_f} \right\} \\ &\quad - (1 - \varepsilon)^{-\frac{1}{2q}} B_2(\lambda_f) + o(n^{-1}). \end{aligned}$$

Since $\sum_{j=1}^{\infty} \varepsilon^j(j+1)(j+2) = 2\varepsilon(\varepsilon^2 - 3\varepsilon + 3)(1 - \varepsilon)^{-3}$ and according to Lemma 3 it holds that $\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^{2+1} \mathbf{S}_\lambda \mathbf{f}|_{\lambda=\lambda_f} = o(1) \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{f}|_{\lambda=\lambda_f}$, one gets

$$\begin{aligned} \mathbb{E}_f[T_{Cp}\{\lambda_f(1 - \varepsilon)\}] &= (1 - \varepsilon)^2 B_1(\lambda_f) \{1 + o(1)\} - (1 - \varepsilon)^{-\frac{1}{2q}} B_2(\lambda_f) \\ &= (1 - \varepsilon)^2 B_1(\lambda_f) \left\{1 - (1 - \varepsilon)^{-2 - \frac{1}{2q}} + o(1)\right\} < 0, \end{aligned}$$

for $n \rightarrow \infty$. Similarly,

$$\mathbb{E}_f[T_{Cp}\{\lambda_f(1 + \varepsilon)\}] = (1 + \varepsilon)^2 B_1(\lambda_f) \left\{1 - (1 + \varepsilon)^{-2 - \frac{1}{2q}} + o(1)\right\} > 0,$$

for $n \rightarrow \infty$, so that $\hat{\lambda}_f \xrightarrow{\mathcal{P}} \lambda_f$ follows.

Let now consider $T'_{Cp}(\tau\lambda_f)/\mathbb{E}_f\{T'_{Cp}(\lambda_f)\}$, where $\tau \in [1 - \varepsilon, 1 + \varepsilon]$ for any bounded $\varepsilon > 0$.

It is easy to see that, since $\text{var}_f\{T'_{Cp}(\tau\lambda_f)\} = (\tau\lambda_f)^{-2-1/(2q)} n^{-2} \text{const}\{1 + o(1)\}$,

$$\text{var}_f \left[\frac{T'_{Cp}(\tau\lambda_f)}{\mathbb{E}_f\{T'_{Cp}(\lambda_f)\}} \right] = O\left(\lambda_f^{1/(2q)}\right) \rightarrow 0, \quad n \rightarrow \infty.$$

Also, using Lemma 3 and the same arguments as in the proof of $\hat{\lambda}_f \xrightarrow{\mathcal{P}} \lambda_f$,

$$\begin{aligned} \mathbb{E}_f\{T'_{Cp}(\tau\lambda_f)\} &= \frac{\sigma^2}{\lambda_f \tau n} \left[\tau^{-\frac{1}{2q}} \text{tr}\{(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3)(2\mathbf{I}_n - 3\mathbf{S}_\lambda)\} + \tau^2 2\text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3) \right] \Big|_{\lambda=\lambda_f} \{1 + o(1)\} \\ &= \mathbb{E}_f\{T'_{Cp}(\lambda_f)\} \frac{4q \tau + \tau^{-1-1/(2q)}}{4q + 1} \{1 + o(1)\}, \end{aligned}$$

where

$$\frac{4q \tau + \tau^{-1-1/(2q)}}{4q + 1} = \begin{cases} 1 - \varepsilon\{1 - 1/(2q)\} + O(\varepsilon^2), & \text{for } \tau = 1 - \varepsilon \\ 1 + \varepsilon\{1 - 1/(2q)\} + O(\varepsilon^2), & \text{for } \tau = 1 + \varepsilon \end{cases},$$

so that for any fixed $\tau \in [1 - \varepsilon, 1 + \varepsilon]$ it holds $T'_{Cp}(\tau\lambda_f)/\mathbb{E}_f\{T'_{Cp}(\lambda_f)\} \xrightarrow{\mathcal{P}} 1$, as $n \rightarrow \infty$.

Since $P(|\tilde{\lambda}/\lambda_f - 1| \leq \varepsilon) \rightarrow 1$ for $n \rightarrow \infty$ and any $\varepsilon > 0$ due to $\hat{\lambda}_f \xrightarrow{\mathcal{P}} \lambda_f$, it follows

$$\frac{T'_{Cp}(\tilde{\lambda})}{\mathbb{E}_f\{T'_{Cp}(\lambda_f)\}} \xrightarrow{\mathcal{P}} 1, \quad n \rightarrow \infty.$$

Putting all together and applying Slutsky's lemma gives

$$\left(\frac{\hat{\lambda}_f}{\lambda_f} - 1\right) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, 2\lambda_f^{1/(2q)} c(\rho) \text{sinc}\{\pi/(2q)\} \frac{q(12q^2 + 8q + 1)}{15(8q^2 - 2q - 1)}\right).$$

2.2 Proof for $\hat{\lambda}_{r|f}$

Proof for $\hat{\lambda}_{r|f}$ follows the same lines, using equations derived in Section 1.2. Consider the first order Taylor expansion $0 = T_{ML}(\hat{\lambda}_r) = T_{ML}(\lambda_{r|f}) + T'_{ML}(\tilde{\lambda})(\hat{\lambda}_r - \lambda_{r|f})$, for some $\tilde{\lambda}$ between $\hat{\lambda}_r$ and $\lambda_{r|f}$ and show that

$$\frac{T_{ML}(\lambda_{r|f}) - \mathbb{E}_f\{T_{ML}(\lambda_{r|f})\}}{\sqrt{\text{var}_f\{T_{ML}(\lambda_{r|f})\}}} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) \quad \text{and} \quad \frac{T'_{ML}(\tilde{\lambda})}{\mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\}} \xrightarrow{\mathcal{P}} 1.$$

Applying Lemma 3 to see that

$$\begin{aligned} \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda (\mathbf{I}_n - 2\mathbf{S}_\lambda) \mathbf{f} \Big|_{\lambda=\lambda_{r|f}} &= -\sigma^2 \{\text{tr}(\mathbf{S}_\lambda^2) - q\} \Big|_{\lambda=\lambda_{r|f}} \{1 + o(1)\}, \\ \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2 \mathbf{f} \Big|_{\lambda=\lambda_{r|f}} &= o\left(\lambda_{r|f}^{-1/(2q)}\right), \end{aligned}$$

and simplifying Gamma functions results in

$$\begin{aligned} \mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\} &= \frac{\sigma^2 \lambda_{r|f}^{-1/(2q)-1}}{n c(\rho)} \frac{4q^2 - 1}{4q^2 \text{sinc}\{\pi/(2q)\}} \{1 + o(1)\}, \\ \text{var}_f\{T_{ML}(\lambda_{r|f})\} &= \frac{2\sigma^4 \lambda_{r|f}^{-1/(2q)}}{n^2 c(\rho)} \frac{4q^2 - 1}{48q^3 \text{sinc}\{\pi/(2q)\}} \{1 + o(1)\}. \end{aligned}$$

Consider now

$$\begin{aligned} n T_{ML}(\lambda_{r|f}) &= \left[\mathbf{Y}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \mathbf{Y} - \frac{\mathbf{Y}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{Y}}{n - q} \{\text{tr}(\mathbf{S}_\lambda) - q\} \right] \Big|_{\lambda=\lambda_{r|f}} \\ &= [\mathbf{Y}^t(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{Y} - \sigma^2 \{\text{tr}(\mathbf{S}_\lambda) - q\}] \Big|_{\lambda=\lambda_{r|f}} + o_p(1) \\ \mathbb{E}_f\{n T_{ML}(\lambda_{r|f})\} &= [\mathbf{f}^t(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \mathbf{f} + \sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) - \sigma^2 \{\text{tr}(\mathbf{S}_\lambda) - q\}] \Big|_{\lambda=\lambda_{r|f}} + o(1). \end{aligned}$$

Define random variables ξ_i by

$$n [T_{ML}(\lambda_{r|f}) - E_f\{T_{ML}(\lambda_{r|f})\}] = \sum_{i=q+1}^{k+p+1} (d_i^2 - b_i^2 - \sigma^2) \frac{\lambda_f n \eta_i}{(1 + \lambda_f n \eta_i)^2} + o_p(1) =: \sum_{i=q+1}^{k+p+1} \xi_i,$$

such that $E_f(\xi_i) = o(1)$ and $s_n^2 = \sum_{i=q+1}^{k+p+1} \text{var}_f(\xi_i) = 2\sigma^4 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2\} \{1 + o(1)\}$. Since $s_n^2 = \text{const } \lambda_f^{-1/(2q)}$ and $(\lambda_f^{1/(2q)} k)^{-1} \rightarrow 0$, according to (A2) and (A3), each $\text{var}_f(\xi_i) = o(1)$ and there exist a constant B , such that $E_f|\xi_i|^2 = \text{var}_f(\xi_i) + o(1) < B, i = q+1, \dots, k+p+1$.

With this, the Lyapunov's condition

$$s_n^{-4} \sum_{i=q+1}^{k+p+1} E_f|\xi_i|^4 < B s_n^{-4} \sum_{i=q+1}^{k+p+1} E_f|\xi_i|^2 = B s_n^{-2} = O\left(\lambda_{r|f}^{1/(2q)}\right)$$

converges to 0, $n \rightarrow \infty$ and $[\text{var}_f\{T_{ML}(\lambda_{r|f})\}]^{-1/2} [T_{ML}(\lambda_{r|f}) - E_f\{T_{ML}(\lambda_{r|f})\}] \xrightarrow{D} \mathcal{N}(0, 1)$.

Next is shown that $\hat{\lambda}_r \xrightarrow{P} \lambda_{r|f}$. From $\text{var}_f\{T_{ML}(\lambda)\} = O(\lambda^{-1/(2q)} n^{-2}) \rightarrow 0$ for $n \rightarrow \infty$, it follows $T_{ML}(\lambda) \xrightarrow{P} E_f\{T_{ML}(\lambda)\}$, for any λ satisfying (A3). It remains to verify that $E_f[T_{ML}\{\lambda_{r|f}(1 - \varepsilon)\}] < 0 < E_f[T_{ML}\{\lambda_{r|f}(1 + \varepsilon)\}]$ for $\varepsilon \in (0, 1)$. Define $B_1(\lambda_{r|f})$ and $B_2(\lambda_{r|f})$ from the representation of $E_f\{T_{ML}(\lambda_{r|f})\}$ in terms of the Demmler-Reinsch basis.

$$\begin{aligned} E_f\{T_{ML}(\lambda_{r|f})\} &= \frac{1}{n} [\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \mathbf{f} - \sigma^2 \{\text{tr}(\mathbf{S}_\lambda^2) - q\} + o(1)] \Big|_{\lambda=\lambda_{r|f}} \\ &= \frac{1}{n} \sum_{i=1}^{k+p+1} \frac{b_i^2 \lambda_{r|f} n \eta_i}{(1 + \lambda_{r|f} n \eta_i)^2} - \frac{\sigma^2 \lambda_{r|f}^{-1/(2q)} c(q, 2, K_q)}{c(\rho) n} + o(n^{-1}) \\ &=: B_1(\lambda_{r|f}) - B_2(\lambda_{r|f}) + o(n^{-1}), \end{aligned}$$

where $B_1(\lambda_{r|f}) - B_2(\lambda_{r|f}) = o(n^{-1})$ by definition of $\lambda_{r|f}$. Then,

$$\begin{aligned} E_f[T_{ML}\{\lambda_{r|f}(1 - \varepsilon)\}] &= \frac{1}{n} \sum_{i=1}^{k+p+1} \frac{b_i^2 \lambda_{r|f}(1 - \varepsilon) n \eta_i}{\{1 + \lambda_{r|f} n(1 - \varepsilon) \eta_i\}^2} \\ &\quad - (1 - \varepsilon)^{-\frac{1}{2q}} \frac{2\sigma^2 \lambda_{r|f}^{-1/(2q)} c(q, 2, K_q)}{nc(\rho)} + o(n^{-1}) \\ &= (1 - \varepsilon)^2 B_1(\lambda_{r|f}) \left\{ 1 + \sum_{j=1}^{\infty} (j+1) \varepsilon^j \frac{\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^{1+j} \mathbf{S}_\lambda \mathbf{f}}{\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \mathbf{f}} \Big|_{\lambda=\lambda_{r|f}} \right\} \\ &\quad - (1 - \varepsilon)^{-\frac{1}{2q}} B_2(\lambda_{r|f}) + o(n^{-1}). \end{aligned}$$

Since $\sum_{j=1}^{\infty} (j+1)\varepsilon^j = \varepsilon(2-\varepsilon)(1-\varepsilon)^{-2}$, and according to Lemma 3 it holds that

$\mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda)^{1+1} \mathbf{S}_\lambda \mathbf{f}|_{\lambda=\lambda_{r|f}} = o(1) \mathbf{f}^t(\mathbf{I}_n - \mathbf{S}_\lambda) \mathbf{S}_\lambda \mathbf{f}|_{\lambda=\lambda_{r|f}}$, one gets

$$\begin{aligned} \mathbb{E}_f[T_{ML}\{\lambda_{r|f}(1-\varepsilon)\}] &= (1-\varepsilon)^2 B_1(\lambda_{r|f}) \{1+o(1)\} - (1-\varepsilon)^{-\frac{2q+1}{2q}} B_2(\lambda_{r|f}) \\ &= (1-\varepsilon)^2 B_1(\lambda_{r|f}) \left\{1 - (1-\varepsilon)^{-2-\frac{1}{2q}} + o(1)\right\} < 0, \end{aligned}$$

for $n \rightarrow \infty$. Similarly,

$$\mathbb{E}_f[T_{ML}\{\lambda_{r|f}(1+\varepsilon)\}] = (1+\varepsilon)^2 B_1(\lambda_{r|f}) \left\{1 - (1+\varepsilon)^{-2-\frac{1}{2q}} + o(1)\right\} > 0,$$

for $n \rightarrow \infty$, so that $\hat{\lambda}_r \xrightarrow{\mathcal{P}} \lambda_{r|f}$ follows.

Let now consider $T'_{ML}(\tau\lambda_{r|f})/\mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\}$, where $\tau \in [1-\varepsilon, 1+\varepsilon]$, for any bounded $\varepsilon > 0$. It is easy to see that, since $\text{var}_f\{T'_{ML}(\tau\lambda_{r|f})\} = (\tau\lambda_{r|f})^{-2-1/(2q)} n^{-2} \text{const}\{1+o(1)\}$,

$$\text{var}_f \left[\frac{T'_{ML}(\tau\lambda_{r|f})}{\mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\}} \right] = O\left(\lambda_{r|f}^{1/(2q)}\right) \rightarrow 0, \quad n \rightarrow \infty.$$

Also, using Lemma 3 and the same arguments as in the proof of $\hat{\lambda}_r \xrightarrow{\mathcal{P}} \lambda_{r|f}$,

$$\begin{aligned} \mathbb{E}_f\{T'_{ML}(\tau\lambda_{r|f})\} &= \frac{\sigma^2}{\lambda_{r|f}\tau n} \left[\tau^{-\frac{1}{2q}} 2\text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3) + \tau^2 \{\text{tr}(\mathbf{S}_\lambda^2) - q\} \right] \Big|_{\lambda=\lambda_{r|f}} \{1+o(1)\} \\ &= \mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\} \frac{2q\tau + \tau^{-1-1/(2q)}}{2q+1} \{1+o(1)\}, \end{aligned}$$

where

$$\frac{2q\tau + \tau^{-1-1/(2q)}}{2q+1} = \begin{cases} 1 - \varepsilon \{1 - 1/(2q) - 1/(2q+1)\} + O(\varepsilon^2), & \text{for } \tau = 1 - \varepsilon \\ 1 + \varepsilon \{1 - 1/(2q) - 1/(2q+1)\} + O(\varepsilon^2), & \text{for } \tau = 1 + \varepsilon \end{cases},$$

so that for any fixed $\tau \in [1-\varepsilon, 1+\varepsilon]$ it holds $T'_{ML}(\tau\lambda_{r|f})/\mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\} \xrightarrow{\mathcal{P}} 1$, as $n \rightarrow \infty$.

Since $P(|\tilde{\lambda}/\lambda_{r|f} - 1| \leq \varepsilon) \rightarrow 1$ for $n \rightarrow \infty$ and any $\varepsilon > 0$ due to $\hat{\lambda}_r \xrightarrow{\mathcal{P}} \lambda_{r|f}$, it follows

$$\frac{T'_{ML}(\tilde{\lambda})}{\mathbb{E}_f\{T'_{ML}(\lambda_{r|f})\}} \xrightarrow{\mathcal{P}} 1.$$

Putting all together and applying Slutsky's lemma gives

$$\left(\frac{\widehat{\lambda}_r}{\lambda_{r|f}} - 1 \right) \xrightarrow{\mathcal{D}} \mathcal{N} \left(0, 2\lambda_{r|f}^{1/(2q)} c(\rho) \text{sinc}\{\pi/(2q)\} \frac{q}{12q^2 - 3} \right).$$

3 Detailed proof of Theorem 4

3.1 Proof for $\widehat{\lambda}_f$

All the steps of the proof are the same as in Theorem 3, that is one needs to show

$$\frac{T_{Cp}(\lambda_{f|r}) - \mathbb{E}_\beta \{T_{Cp}(\lambda_{f|r})\}}{\sqrt{\text{var}_\beta \{T_{Cp}(\lambda_{f|r})\}}} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) \quad \text{and} \quad \frac{T'_{Cp}(\widetilde{\lambda})}{\mathbb{E}_\beta \{T'_{Cp}(\lambda_{f|r})\}} \xrightarrow{\mathcal{P}} 1,$$

for some $\widetilde{\lambda}$ between $\widehat{\lambda}_f$ and $\lambda_{f|r}$. Simplifying Gamma functions in the expressions for $\mathbb{E}_\beta \{T'_{Cp}(\lambda_{f|r})\}$ and $\text{var}_\beta \{T_{Cp}(\lambda_{f|r})\}$ obtained in Section 1.1.2, results in

$$\begin{aligned} \mathbb{E}_\beta \{T'_{Cp}(\lambda_{f|r})\} &= \frac{\sigma^2 \lambda_{f|r}^{-1/(2q)-1}}{n c(\rho)} \frac{2q-1}{8q^2 \text{sinc}\{\pi/(2q)\}} \{1 + o(1)\}, \\ \text{var}_\beta \{T_{Cp}(\lambda_{f|r})\} &= \frac{2\sigma^4 \lambda_{f|r}^{-1/(2q)}}{n^2 c(\rho)} \frac{4q^2-1}{48q^3 \text{sinc}\{\pi/(2q)\}} \{1 + o(1)\}. \end{aligned}$$

Consider now

$$\begin{aligned} n T_{Cp}(\lambda_{f|r}) &= [\mathbf{Y}^t (\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda \mathbf{Y} - \sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)]|_{\lambda=\lambda_{f|r}} + o_p(1), \\ \mathbb{E}_\beta \{n T_{Cp}(\lambda_{f|r})\} &= \sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)|_{\lambda=\lambda_{f|r}} o(1). \end{aligned}$$

For $d_i = \sum_{j=1}^n \phi_{k,i}(x_j) y_j$, such that $\mathbb{E}_\beta(d_i^2) = \sigma^2 \lambda_{f|r} n \eta_i (1 + \lambda_{f|r} n \eta_i)^{-1} \{1 + o(1)\}$, let define random variables ξ_i by

$$\begin{aligned} n [T_{Cp}(\lambda_{f|r}) - \mathbb{E}_f \{T_{Cp}(\lambda_{f|r})\}] &= \sum_{i=q+1}^{k+p+1} \left[d_i^2 - \sigma^2 \frac{1 + \lambda_{f|r} n \eta_i}{\lambda_{f|r} n \eta_i} \{1 + o(1)\} \right] \frac{(\lambda_{f|r} n \eta_i)^2}{(1 + \lambda_{f|r} n \eta_i)^3} + o_p(1) \\ &=: \sum_{i=q+1}^{k+p+1} \xi_i, \end{aligned}$$

with $E_\beta(\xi_i) = o(1)$ and $s_n^2 = \sum_{i=q+1}^{k+p+1} \text{var}_\beta(\xi_i) = 2\sigma^4 \text{tr}\{(\mathbf{I}_n - \mathbf{S}_\lambda)^2 \mathbf{S}_\lambda^2\} \{1 + o(1)\}$. Since $s_n^2 = \text{const } \lambda_{f|r}^{-1/(2q)}$ and $(\lambda_{f|r}^{1/(2q)} k)^{-1} \rightarrow 0$ according to (A2), each $\text{var}_\beta(\xi_i) = o(1)$ and there exist a constant B , such that $E_\beta|\xi_i|^2 = \text{var}_\beta(\xi_i) + o(1) < B$, $i = q+1, \dots, k+p+1$. With this, the Lyapunov's condition

$$s_n^{-4} \sum_{i=q+1}^{k+p+1} E_\beta|\xi_i|^4 < B s_n^{-4} \sum_{i=q+1}^{k+p+1} E_\beta|\xi_i|^2 = B s_n^{-2} = O\left(\lambda_{f|r}^{1/(2q)}\right)$$

converges to zero as n tends to infinity. Thus, $s_n^{-1} \sum_{i=q+1}^{k+p+1} \xi_i \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$, or equivalently, $[\text{var}_\beta\{T_{Cp}(\lambda_{f|r})\}]^{-1/2} [T_{Cp}(\lambda_{f|r}) - E_\beta\{T_{Cp}(\lambda_{f|r})\}] \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$.

Next is shown that $\hat{\lambda}_f \xrightarrow{\mathcal{P}} \lambda_{f|r}$. From $\text{var}_\beta\{T_{Cp}(\lambda)\} = O(\lambda^{-1/(2q)} n^{-2}) \rightarrow 0$, for $n \rightarrow \infty$ it follows $T_{Cp}(\lambda) \xrightarrow{\mathcal{P}} E_\beta\{T_{Cp}(\lambda)\}$. It remains to verify that $E_\beta[T_{Cp}\{\lambda_{f|r}(1 - \varepsilon)\}] < 0 < E_\beta[T_{Cp}\{\lambda_{f|r}(1 + \varepsilon)\}]$, for any $\varepsilon \in (0, 1)$. Indeed,

$$\begin{aligned} E_\beta[T_{Cp}\{\lambda_{f|r}(1 - \varepsilon)\}] &= \frac{\sigma^2}{n} (1 - \varepsilon)^{-1/(2q)} \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2) \Big|_{\lambda=\lambda_{f|r}} \\ &\times \left[o(1) + \{\sigma_u^2 \lambda_{f|r}(1 - \varepsilon)n - \sigma^2\} \frac{\text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3)}{\sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)} \Big|_{\lambda=\lambda_{f|r}} \right] \{1 + o(1)\} \\ &= \left\{ -\varepsilon \frac{\text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3)}{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)} \Big|_{\lambda=\lambda_{f|r}} + o(1) \right\} \frac{\sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n(1 - \varepsilon)^{1/(2q)}} \Big|_{\lambda=\lambda_{f|r}} < 0, \end{aligned}$$

for $n \rightarrow \infty$, where $\sigma^2 = \sigma_u^2 \lambda_{f|r} n \{1 + o(1)\}$ is used. Similarly, for $n \rightarrow \infty$

$$E_\beta[T_{Cp}\{\lambda_{f|r}(1 + \varepsilon)\}] = \left\{ \varepsilon \frac{\text{tr}(\mathbf{S}_\lambda^2 - \mathbf{S}_\lambda^3)}{\text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)} \Big|_{\lambda=\lambda_{f|r}} + o(1) \right\} \frac{\sigma^2 \text{tr}(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)}{n(1 + \varepsilon)^{1/(2q)}} \Big|_{\lambda=\lambda_{f|r}} > 0.$$

Let now consider $T'_{Cp}(\tau \lambda_{f|r})/E_\beta\{T'_{Cp}(\lambda_{f|r})\}$, where $\tau \in [1 - \varepsilon, 1 + \varepsilon]$, for any bounded $\varepsilon > 0$. It is easy to see that, since $\text{var}_\beta\{T'_{Cp}(\tau \lambda_{f|r})\} = (\tau \lambda_{f|r})^{-2-1/(2q)} n^{-2} \text{const}\{1 + o(1)\}$,

$$\text{var}_\beta \left[\frac{T'_{Cp}(\tau \lambda_{f|r})}{E_\beta\{T'_{Cp}(\lambda_{f|r})\}} \right] = O\left(\lambda_{f|r}^{1/(2q)}\right) \rightarrow 0, \quad n \rightarrow \infty.$$

Also,

$$E_\beta\{T'_{Cp}(\tau \lambda_{f|r})\} = E_\beta\{T'_{Cp}(\lambda_{f|r})\} \tau^{-1-1/(2q)} [1 + (\tau - 1)\{1 - 1/(2q)\}] \{1 + o(1)\},$$

where

$$\tau^{-1-1/(2q)} [1 + (\tau - 1)\{1 - 1/(2q)\}] = \begin{cases} 1 + \varepsilon/q + O(\varepsilon^2), & \text{for } \tau = 1 - \varepsilon \\ 1 - \varepsilon/q + O(\varepsilon^2), & \text{for } \tau = 1 + \varepsilon \end{cases},$$

so that for any fixed $\tau \in [1 - \varepsilon, 1 + \varepsilon]$ it holds $T'_{Cp}(\tau \lambda_{f|r})/E_\beta\{T'_{Cp}(\lambda_{f|r})\} \xrightarrow{\mathcal{P}} 1$, as $n \rightarrow \infty$.

Since $P(|\tilde{\lambda}/\lambda_{f|r} - 1| \leq \varepsilon) \rightarrow 1$ for $n \rightarrow \infty$ and any $\varepsilon > 0$ due to $\hat{\lambda}_f \xrightarrow{\mathcal{P}} \lambda_{f|r}$, it follows

$$\frac{T'_{Cp}(\tilde{\lambda})}{E_\beta\{T'_{Cp}(\lambda_{f|r})\}} \xrightarrow{\mathcal{P}} 1.$$

Putting all together and applying Slutsky's lemma gives

$$\left(\frac{\hat{\lambda}_f}{\lambda_{f|r}} - 1\right) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0, 2\lambda_{f|r}^{1/(2q)} c(\rho) \text{sinc}\{\pi/(2q)\} \frac{4q(2q+1)}{3(2q-1)}\right).$$

3.2 Proof for $\hat{\lambda}_r$

One needs to show

$$\frac{T_{ML}(\lambda_r) - E_\beta\{T_{ML}(\lambda_r)\}}{\sqrt{\text{var}_\beta\{T_{ML}(\lambda_r)\}}} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) \quad \text{and} \quad \frac{T'_{ML}(\tilde{\lambda})}{E_\beta\{T'_{ML}(\lambda_r)\}} \xrightarrow{\mathcal{P}} 1,$$

for some $\tilde{\lambda}$ between $\hat{\lambda}_r$ and λ_r . Simplifying Gamma functions in the expressions for $E_\beta\{T'_{ML}(\lambda_r)\}$ and $\text{var}_\beta\{T_{ML}(\lambda_r)\}$ obtained in Section 1.1.2 results in

$$\begin{aligned} E_\beta\{T'_{ML}(\lambda_r)\} &= \frac{\sigma^2 \lambda_r^{-1/(2q)-1}}{n c(\rho)} \frac{2q-1}{2q \text{sinc}\{\pi/(2q)\}} \{1 + o(1)\}, \\ \text{var}_\beta\{T_{ML}(\lambda_r)\} &= \frac{2\sigma^4 \lambda_r^{-1/(2q)}}{n^2 c(\rho)} \frac{2q-1}{2q \text{sinc}\{\pi/(2q)\}} \{1 + o(1)\}. \end{aligned}$$

Consider now

$$\begin{aligned} n T_{ML}(\lambda_r) &= [\mathbf{Y}^t(\mathbf{S}_\lambda - \mathbf{S}_\lambda^2)\mathbf{Y} - \sigma^2 \text{tr}(\mathbf{S}_\lambda)]|_{\lambda=\lambda_{f|r}} + o_p(1), \\ E_\beta\{n T_{ML}(\lambda_r)\} &= \sigma^2 \text{tr}(\mathbf{S}_\lambda)|_{\lambda=\lambda_r} o(1). \end{aligned}$$

For $d_i = \sum_{j=1}^n \phi_{k,i}(x_j)y_j$, such that $E_\beta(d_i^2) = \sigma^2 \lambda_r n \eta_i (1 + \lambda_r n \eta_i)^{-1} \{1 + o(1)\}$, let define random variables ξ_i by

$$\begin{aligned} n [T_{ML}(\lambda_r) - E_f\{T_{ML}(\lambda_r)\}] &= \sum_{i=q+1}^{k+p+1} \left[d_i^2 - \sigma^2 \frac{1 + \lambda_r n \eta_i}{\lambda_r n \eta_i} \{1 + o(1)\} \right] \frac{(\lambda_r n \eta_i)}{(1 + \lambda_r n \eta_i)^2} + o_p(1) \\ &=: \sum_{i=q+1}^{k+p+1} \xi_i, \end{aligned}$$

with $E_\beta(\xi_i) = o(1)$ and $s_n^2 = \sum_{i=q+1}^{k+p+1} \text{var}_\beta(\xi_i) = 2\sigma^4 \text{tr}(\mathbf{S}_\lambda^2) \{1 + o(1)\}$. Since $s_n^2 = \text{const } \lambda_r^{-1/(2q)}$ and $(\lambda_r^{1/(2q)} k)^{-1} \rightarrow 0$ according to (A2), each $\text{var}_\beta(\xi_i) = o(1)$ and there exist a constant B , such that $E_\beta|\xi_i|^2 = \text{var}_\beta(\xi_i) + o(1) < B$, $i = q+1, \dots, k+p+1$. With this the Lyapunov's condition

$$s_n^{-4} \sum_{i=q+1}^{k+p+1} E_\beta|\xi_i|^4 < B s_n^{-4} \sum_{i=q+1}^{k+p+1} E_\beta|\xi_i|^2 = B s_n^{-2} = O(\lambda_r^{1/(2q)})$$

converges to zero as n tends to infinity. Thus, $s_n^{-1} \sum_{i=q+1}^{k+p+1} \xi_i \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$, or equivalently, $[\text{var}_\beta\{T_{ML}(\lambda_r)\}]^{-1/2} [T_{ML}(\lambda_r) - E_\beta\{T_{ML}(\lambda_r)\}] \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$.

Next is shown that $\hat{\lambda}_r \xrightarrow{\mathcal{P}} \lambda_r$. From $\text{var}_\beta\{T_{ML}(\lambda)\} = O(\lambda^{-1/(2q)} n^{-2}) \rightarrow 0$ for $n \rightarrow \infty$, it follows $T_{ML}(\lambda) \xrightarrow{\mathcal{P}} E_\beta\{T_{ML}(\lambda)\}$. It remains to verify that $E_\beta[T_{ML}\{\lambda_r(1 - \varepsilon)\}] < 0 < E_\beta[T_{ML}\{\lambda_r(1 + \varepsilon)\}]$, for any $\varepsilon \in (0, 1)$. Indeed,

$$E_\beta[T_{ML}\{\lambda_r(1 - \varepsilon)\}] = \left\{ -\varepsilon \frac{\text{tr}(\mathbf{S}_\lambda^2)}{\text{tr}(\mathbf{S}_\lambda)} \right\}_{\lambda=\lambda_r} + o(1) \left\{ \frac{\sigma^2 \text{tr}(\mathbf{S}_\lambda)}{n(1 - \varepsilon)^{1/(2q)}} \right\}_{\lambda=\lambda_r} < 0,$$

for $n \rightarrow \infty$, where $\sigma^2 = \sigma_u^2 \lambda_r n \{1 + o(1)\}$ is used. Similarly, for $n \rightarrow \infty$

$$E_\beta[T_{ML}\{\lambda_r(1 + \varepsilon)\}] = \left\{ \varepsilon \frac{\text{tr}(\mathbf{S}_\lambda^2)}{\text{tr}(\mathbf{S}_\lambda)} \right\}_{\lambda=\lambda_r} + o(1) \left\{ \frac{\sigma^2 \text{tr}(\mathbf{S}_\lambda)}{n(1 + \varepsilon)^{1/(2q)}} \right\}_{\lambda=\lambda_r} > 0.$$

Let now consider $T'_{ML}(\tau \lambda_r)/E_\beta\{T'_{ML}(\lambda_r)\}$, where $\tau \in [1 - \varepsilon, 1 + \varepsilon]$, for any bounded $\varepsilon > 0$.

It is easy to see that, since $\text{var}_\beta\{T'_{ML}(\tau \lambda_r)\} = (\tau \lambda_r)^{-2-1/(2q)} n^{-2} \text{const}\{1 + o(1)\}$,

$$\text{var}_\beta \left[\frac{T'_{ML}(\tau \lambda_r)}{E_\beta\{T'_{ML}(\lambda_r)\}} \right] = O(\lambda_r^{1/(2q)}) \rightarrow 0, \quad n \rightarrow \infty.$$

Also,

$$E_\beta \left\{ T'_{ML}(\tau \lambda_r) \right\} = E_\beta \left\{ T'_{ML}(\lambda_r) \right\} \tau^{-1-1/(2q)} [1 + (\tau - 1)\{1 - 1/(2q)\}] \{1 + o(1)\},$$

where

$$\tau^{-1-1/(2q)} [1 + (\tau - 1)\{1 - 1/(2q)\}] = \begin{cases} 1 + \varepsilon/q + O(\varepsilon^2), & \text{for } \tau = 1 - \varepsilon \\ 1 - \varepsilon/q + O(\varepsilon^2), & \text{for } \tau = 1 + \varepsilon \end{cases},$$

so that for any fixed $\tau \in [1 - \varepsilon, 1 + \varepsilon]$ it holds $T'_{ML}(\tau \lambda_r)/E_\beta\{T'_{ML}(\lambda_r)\} \xrightarrow{\mathcal{P}} 1$, as $n \rightarrow \infty$.

Since $P(|\tilde{\lambda}/\lambda_r - 1| \leq \varepsilon) \rightarrow 1$ for $n \rightarrow \infty$ and any $\varepsilon > 0$ due to $\hat{\lambda}_r \xrightarrow{\mathcal{P}} \lambda_r$, it follows

$$\frac{T'_{ML}(\tilde{\lambda})}{E_\beta \{T'_{ML}(\lambda_r)\}} \xrightarrow{\mathcal{P}} 1.$$

Putting all together and applying Slutsky's lemma gives

$$\left(\frac{\hat{\lambda}_r}{\lambda_r} - 1 \right) \xrightarrow{\mathcal{D}} \mathcal{N} \left(0, 2\lambda_r^{1/(2q)} c(\rho) \text{sinc}\{\pi/(2q)\} \frac{2q}{2q-1} \right).$$

4 Data-driven selection of q

Using the same functions f_1 and f_2 and the same setting as in Section 4 of the paper, $R^*(q)$ was calculated for $q = 2, 3, 4, 5$ and two sample sizes $n = 350$ and $n = 1000$, fixing the number of knots at $k = 40$. The results from 500 Monte Carlo replications are shown in Figure 1 and agree with the simulation results from Section 4. For f_1 using $q = 3$ or $q = 4$ for $n = 350$ and $q = 4$ for $n = 1000$ seem to do best, since the corresponding $|R^*(q)|$ is smallest. For f_2 using $q = 4$ is more advisable.

References

Akaike, H. (1969). Fitting autoregressive models for prediction. *Annals of the Institute of Statistical Mathematics*, 21:243 – 47.

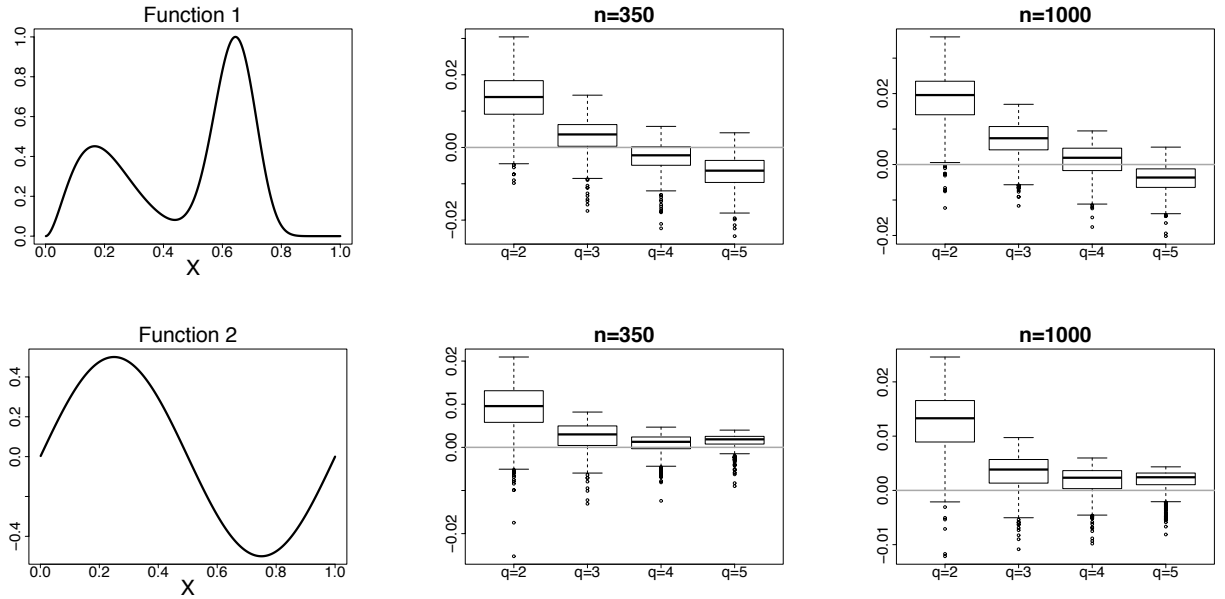


Figure 1: Choice of the optimal q : Boxplots of $R^*(q)$ for different values of q for $n = 350$ (middle plots) and $n = 1000$ (right plots) for f_1 (top left) and f_2 (bottom left).

- Claeskens, G., Krivobokova, T., and Opsomer, J. (2009). Asymptotic properties of penalized spline estimators. *Biometrika*, 96(6):529–544.
- Craven, P. and Wahba, G. (1978). Smoothing noisy data with spline functions. Estimating the correct degree of smoothing by the method of generalized cross-validation. *Numer. Math.*, 31(4):377–403.
- Patterson, H. and Thompson, R. (1971). Recovery of inter-block information when block sizes are unequal. *Biometrika*, 58(3):545–554.
- van der Vaart, A. W. (1998). *Asymptotic statistics*. Cambridge University Press, New York.
- Wiens, D. P. (1992). On moments of quadratic forms in non-spherically distributed variables. *Statistics*, 23:265–270.