SUPPLEMENT TO "ESTIMATION OF THE STRUCTURAL SIMILARITY INDEX FOR REMOTE SENSING DATA"

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Supplementary Material

In this supplement we derived an explicit expression for the expected information matrix and provide some details about the computational implementation of the gradient statistic for the nonlinear regression model with multiplicative noise described at Section II from the manuscript.

Supplement I: Fisher information matrix for the nonlinear regression model with multiplicative noise

In this appendix we derive the differentials $\mathsf{d}^2_\psi\,\ell(\boldsymbol{\psi})$, $\boldsymbol{\psi} = (\boldsymbol{\theta}^\top, \phi)^\top$ for the heteroscedastic nonlinear regression model defined in Section II from manuscript. The Fisher information matrix $\boldsymbol{\mathcal{F}}(\boldsymbol{\psi})$ is obtained efficiently using the differentiation method and by applying some identification theorems discussed in Magnus and Neudecker (2007).

The log-likelihood function for the nonlinear regression model defined by Equation (4) from Section II is

$$\begin{aligned}\ell(\boldsymbol{\psi}) = &-\frac{n}{2}\log 2\pi - \frac{n}{2}\log g^2(\phi) - \frac{1}{2}\log|\boldsymbol{W}(\boldsymbol{\theta})| \\ &- \frac{1}{2g^2(\phi)}(\boldsymbol{Z} - \phi\boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})(\boldsymbol{Z} - \phi\boldsymbol{f}(\boldsymbol{\theta})),\end{aligned}$$

Differentiating $\ell(\boldsymbol{\psi})$ with respect to $\boldsymbol{\theta}$, we obtain

$$\begin{aligned}\mathsf{d}_\theta\,\ell(\boldsymbol{\psi}) &= -\frac{1}{2}\operatorname{tr}\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{W}(\boldsymbol{\theta}) + \frac{\phi}{g^2(\phi)}(\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}) \\ &\quad + \frac{1}{2g^2(\phi)}\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}) \\ &= \frac{\phi}{g^2(\phi)}(\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})(\boldsymbol{Z} - \phi\boldsymbol{f}(\boldsymbol{\theta})) \\ &\quad - \frac{1}{2}\operatorname{tr}\boldsymbol{W}^{-1}(\boldsymbol{\theta})\Big(\boldsymbol{W}(\boldsymbol{\theta}) - \frac{\boldsymbol{r}(\boldsymbol{\theta})\boldsymbol{r}^\top(\boldsymbol{\theta})}{g^2(\phi)}\Big)\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{W}(\boldsymbol{\theta}).\end{aligned}$$

Thus, using the properties of the trace operator, it is possible to write the first differential $\mathsf{d}_\theta\,\ell(\boldsymbol{\psi})$, as

$$\begin{aligned}\mathsf{d}_\theta\,\ell(\boldsymbol{\psi}) = &\frac{\phi}{g^2(\phi)}(\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})(\boldsymbol{Z} - \phi\boldsymbol{f}(\boldsymbol{\theta})) \\ &- \frac{1}{2}(\mathsf{d}_\theta\operatorname{vec}\boldsymbol{W}(\boldsymbol{\theta}))^\top(\boldsymbol{W}^{-1}(\boldsymbol{\theta})\otimes\boldsymbol{W}^{-1}(\boldsymbol{\theta}))\operatorname{vec}\Big(\boldsymbol{W}(\boldsymbol{\theta}) - \frac{\boldsymbol{r}(\boldsymbol{\theta})\boldsymbol{r}^\top(\boldsymbol{\theta})}{g^2(\phi)}\Big).\end{aligned}$$

Applying the first identification theorem given in Magnus and Neudecker (2007) we arrive to Equation (A.1) from Appendix A of the manuscript.

Taking the differential of $\mathsf{d}_\theta\, \ell(\boldsymbol{\psi})$ with respect to $\boldsymbol{\theta}$, we get

$$\begin{aligned}
\mathsf{d}^2_\theta\, \ell(\boldsymbol{\psi}) &= \frac{1}{2}\operatorname{tr} \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{W}(\boldsymbol{\theta}) - \frac{1}{2}\operatorname{tr} \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}^2_\theta\, \boldsymbol{W}(\boldsymbol{\theta}) \\
&\quad - \frac{\phi^2}{g^2(\phi)}(\mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}) - \frac{2\phi}{g^2(\phi)}(\mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}) \\
&\quad + \frac{\phi}{g^2(\phi)}(\mathsf{d}^2_\theta\, \boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}) + \frac{1}{2g^2(\phi)}\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}^2_\theta\, \boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}) \\
&\quad - \frac{1}{g^2(\phi)}\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}).
\end{aligned}$$

Using that

$$\mathrm{E}\{\boldsymbol{r}(\boldsymbol{\theta})\} = \boldsymbol{0}, \quad \text{and} \quad \mathrm{E}\{\boldsymbol{r}(\boldsymbol{\theta})\boldsymbol{r}^\top(\boldsymbol{\theta})\} = g^2(\phi)\boldsymbol{W}(\boldsymbol{\theta}). \tag{S.1}$$

Yields that the negative of the expectation of the second differential of $\ell(\boldsymbol{\psi})$ with respect to $\boldsymbol{\theta}$ assumes the form

$$\begin{aligned}
\mathrm{E}\{-\,\mathsf{d}^2_\theta\, \ell(\boldsymbol{\psi})\} &= \frac{1}{2}\operatorname{tr} \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}\, \boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{W}(\boldsymbol{\theta}) + \frac{\phi^2}{g^2(\phi)}(\mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}) \\
&= \frac{\phi^2}{g^2(\phi)}(\mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}))^\top \boldsymbol{W}^{-1}(\boldsymbol{\theta})\, \mathsf{d}_\theta\, \boldsymbol{f}(\boldsymbol{\theta}) \\
&\quad + \frac{1}{2}(\mathsf{d}_\theta \operatorname{vec} \boldsymbol{W}(\boldsymbol{\theta}))^\top (\boldsymbol{W}^{-1}(\boldsymbol{\theta}) \otimes \boldsymbol{W}^{-1}(\boldsymbol{\theta}))\, \mathsf{d}_\theta \operatorname{vec} \boldsymbol{W}(\boldsymbol{\theta}).
\end{aligned}$$

Thus, applying the second identification theorem by Magnus and Neudecker (2007), leads to

$$\mathrm{E}\Big\{-\frac{\partial^2 \ell(\boldsymbol{\psi})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^\top}\Big\} = \frac{\phi^2}{g^2(\phi)}\boldsymbol{F}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{F}(\boldsymbol{\theta}) + \frac{1}{2}\boldsymbol{H}^\top(\boldsymbol{\theta})(\boldsymbol{W}^{-1}(\boldsymbol{\theta}) \otimes \boldsymbol{W}^{-1}(\boldsymbol{\theta}))\boldsymbol{H}(\boldsymbol{\theta}),$$

where $\boldsymbol{H}(\boldsymbol{\theta}) = (\operatorname{vec}(\partial \boldsymbol{W}(\boldsymbol{\theta})/\partial\theta_1), \dots, \operatorname{vec}(\partial \boldsymbol{W}(\boldsymbol{\theta})/\partial\theta_p)) \in \mathbb{R}^{n^2\times p}$.

Taking the first and second differential of $\ell(\boldsymbol{\psi})$ with respect to ϕ we have

$$\begin{aligned}
\mathsf{d}_\phi\, \ell(\boldsymbol{\psi}) &= -\frac{n}{2}\frac{\mathsf{d}\, g^2(\phi)}{2g^2(\phi)} + \frac{\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\, \mathsf{d}\,\phi}{g^2(\phi)} + \frac{\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\, \mathsf{d}\, g^2(\phi)}{2g^4(\phi)} \\
\mathsf{d}^2_\phi\, \ell(\boldsymbol{\psi}) &= -\frac{n}{2}\Big[\frac{g^2(\phi)\, \mathsf{d}^2\, g^2(\phi) - \mathsf{d}\, g^2(\phi)\, \mathsf{d}\, g^2(\phi)}{g^4(\phi)}\Big] - \frac{\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{f}(\boldsymbol{\theta})\, \mathsf{d}\,\phi\, \mathsf{d}\,\phi}{g^2(\phi)} \\
&\quad - \frac{2\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\, \mathsf{d}\,\phi\, \mathsf{d}\, g^2(\phi)}{g^4(\phi)} + \frac{\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\, \mathsf{d}^2\, g^2(\phi)}{2g^4(\phi)} \\
&\quad - \frac{\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\, \mathsf{d}\, g^2(\phi)\, \mathsf{d}\, g^4(\phi)}{g^8(\phi)}.
\end{aligned}$$

Noticing

$$\mathsf{d}\, g^2(\phi) = 2\phi(2\phi^2 - 1)\, \mathsf{d}\,\phi, \qquad \mathsf{d}\, g^4(\phi) = 4\phi^3(2\phi^4 - 3\phi^2 - 1)\, \mathsf{d}\,\phi, \tag{S.2}$$

yields that the first differential of $\ell(\boldsymbol{\psi})$ with respect to ϕ can be written as:

$$\mathsf{d}_\phi\, \ell(\boldsymbol{\psi}) = \frac{\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})}{g^2(\phi)}\, \mathsf{d}\,\phi - \frac{2\phi^2 - 1}{\phi^3(\phi^2 - 1)}\big[n\phi^2 - \boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\big]\, \mathsf{d}\,\phi.$$

From (S.1) and (S.2) and using simple algebra, we obtain

$$\begin{aligned}\mathrm{E}\{-\mathsf{d}^2_{\phi}\,\ell(\boldsymbol{\psi})\} &= \frac{1}{g^2(\phi)}\Big[\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{f}(\boldsymbol{\theta})\,\mathsf{d}\,\phi\,\mathsf{d}\,\phi - \frac{n}{2}\frac{\mathsf{d}\,g^2(\phi)}{g^2(\phi)}\Big\{\mathsf{d}\,g^2(\phi) - \frac{\mathsf{d}\,g^4(\phi)}{g^2(\phi)}\Big\}\Big]\\ &= \frac{1}{g^2(\phi)}\Big[\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{1}(\boldsymbol{\theta})\boldsymbol{f}(\boldsymbol{\theta}) + \frac{2nq(\phi)}{(\phi^2-1)^2}\Big]\,\mathsf{d}\,\phi\,\mathsf{d}\,\phi,\end{aligned}$$

with $q(\phi) = (2\phi^2-1)(2\phi^4-3\phi^2+1)$. Applying the second identification theorem by Magnus and Neudecker (2007) we arrive to $\mathcal{F}_{\phi\phi}(\boldsymbol{\psi})$ given in Appendix B from the manuscript.

Differentiating $\mathsf{d}_{\phi}\,\ell(\boldsymbol{\psi})$ with respect to $\boldsymbol{\theta}$ we have

$$\begin{aligned}\mathsf{d}^2_{\theta\phi}\,\ell(\boldsymbol{\psi}) &= \frac{\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta})\,\mathsf{d}\,\phi}{g^2(\phi)} - \frac{\phi\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta})\,\mathsf{d}\,\phi}{g^2(\phi)}\\ &- \frac{\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\,\mathsf{d}\,\phi}{g^2(\phi)} - \frac{\phi\,\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta})\,\mathsf{d}\,g^2(\phi)}{g^4(\phi)}\\ &- \frac{\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{W}(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\,\mathsf{d}\,g^2(\phi)}{2g^4(\phi)}\end{aligned}$$

Taking expectations and using Equation (S.2), we obtain

$$\mathrm{E}\{-\mathsf{d}^2_{\theta\phi}\,\ell(\boldsymbol{\psi})\} = \frac{\phi}{g^2(\phi)}\big[\boldsymbol{f}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{f}(\boldsymbol{\theta}) + (2\phi^2-1)\,\mathrm{tr}\,\boldsymbol{W}^{-1}(\boldsymbol{\theta})\,\mathsf{d}_\theta\,\boldsymbol{W}(\boldsymbol{\theta})\big]\,\mathsf{d}\,\phi.$$

Thus, the second identification theorem by Magnus and Neudecker (2007) allow us to write

$$\mathrm{E}\Big\{-\frac{\partial^2\ell(\boldsymbol{\psi})}{\partial\boldsymbol{\theta}\partial\phi}\Big\} = \frac{\phi}{g^2(\phi)}\big[\boldsymbol{F}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{f}(\boldsymbol{\theta}) + (2\phi^2-1)\boldsymbol{H}^\top\,\mathrm{vec}\,\boldsymbol{W}^{-1}(\boldsymbol{\theta})\big].$$

Supplement II: A note about the computation of score function for the nonlinear regression model with multiplicative noise

Below we describe the computational strategy adopted in our C routines to evaluate the score function for the heteroscedastic regression model defined in Equation (4) from manuscript. We have that the score function $\boldsymbol{U}(\boldsymbol{\theta}) = \partial\ell(\boldsymbol{\psi})/\partial\boldsymbol{\theta}$, can be written as:

$$\boldsymbol{U}(\boldsymbol{\theta}) = \boldsymbol{U}_1(\boldsymbol{\theta}) + \boldsymbol{U}_2(\boldsymbol{\theta}),$$

with

$$\boldsymbol{U}_1(\boldsymbol{\theta}) = \frac{\phi}{g^2(\phi)}\boldsymbol{F}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})(\boldsymbol{Z} - \phi\boldsymbol{f}(\boldsymbol{\theta})),$$

whereas $\boldsymbol{U}_2(\boldsymbol{\theta})$ corresponds to the second term of Equation (A.1) from Appendix A of the manuscript. Such equation has conceptual advantages, however its storage requirements can be quite high. Thus, we exploit the diagonal structure of $\boldsymbol{W}(\boldsymbol{\theta})$ to compute the elements of $\boldsymbol{U}_2(\boldsymbol{\theta})$ in a computationally efficient fashion. Noticing that

$$\frac{\partial\boldsymbol{W}(\boldsymbol{\theta})}{\partial\theta_j} = 2\,\mathrm{diag}(f_1(\boldsymbol{\theta})\dot{f}_{1j}(\boldsymbol{\theta}),\dots,f_n(\boldsymbol{\theta})\dot{f}_{nj}(\boldsymbol{\theta})),$$

where $\dot{f}_{ij}(\boldsymbol{\theta}) = \partial f_i(\boldsymbol{\theta})/\partial\theta_j$, for $i = 1,\dots,n$; $j = 1,\dots,p$, yields that the the jth element of $\boldsymbol{U}_2(\boldsymbol{\theta})$ takes the form

$$-\,\mathrm{tr}\,\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{W}_j(\boldsymbol{\theta}) + \frac{1}{g^2(\phi)}\boldsymbol{r}^\top(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{W}_j(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}), \qquad \text{(S.3)}$$

for $j = 1, \dots, p$, with $\boldsymbol{W}_j(\boldsymbol{\theta}) = \frac{1}{2}\partial \boldsymbol{W}(\boldsymbol{\theta})/\partial\theta_j$ and $\boldsymbol{r}(\boldsymbol{\theta}) = \boldsymbol{Z} - \phi \boldsymbol{f}(\boldsymbol{\theta})$. Simple calculations allow us to note that the first term of Equation (S.3) is given by

$$\operatorname{tr} \boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{W}_j(\boldsymbol{\theta}) = \sum_{i=1}^n \frac{\partial f_i(\boldsymbol{\theta})/\partial\theta_j}{f_i(\boldsymbol{\theta})}, \tag{S.4}$$

which is equivalent to adding all the elements of the jth column of the matrix $\boldsymbol{W}^{-1/2}(\boldsymbol{\theta})\boldsymbol{F}(\boldsymbol{\theta})$. Moreover, the second term of (S.3) assumes the form

$$\frac{1}{g^2(\phi)}\{\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta})\}^\top \boldsymbol{W}_j(\boldsymbol{\theta})\boldsymbol{W}^{-1}(\boldsymbol{\theta})\boldsymbol{r}(\boldsymbol{\theta}) = \frac{1}{g^2(\phi)}\sum_{i=1}^n \Big(\frac{r_i(\boldsymbol{\theta})}{f_i^2(\boldsymbol{\theta})}\Big)^2 \frac{\partial f_i(\boldsymbol{\theta})}{\partial\theta_j}. \tag{S.5}$$

Our implementation computes efficiently the score $\boldsymbol{U}(\boldsymbol{\theta})$ evaluating (S.4) and (S.5), as well as the cross product defined by $\boldsymbol{U}_1(\boldsymbol{\theta})$ by using the Fortran routine `dgemm` from the BLAS library (Lawson et al., 1979) included in the R software (R Core Team, 2014).

References

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