

Interactive comment on “Spatial mapping of ground-based observations of total ozone” by K.-L. Chang et al.

K.-L. Chang et al.

ucakkac@ucl.ac.uk

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We thank the reviewers for their detailed comments on the manuscript. Our answers are listed below.

Anonymous Referee #1

Major comment 1

If the field is Gaussian, the kriging predictor coincides with the conditional mean of the field given the data. Problems such as high computational cost or the difficulty of introducing non-stationarity are typically effects of using a covariance-based model when computing the kriging predictor, and are not caused by the fact that we are computing

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a conditional mean. Thus, saying that kriging is compared with the SPDE approach is a bit misleading, when the comparison is between using a covariance-based model, a stationary Matérn field, and a non-stationary SPDE-based model for ozone mapping.

Answer: Thanks for this clarification. Yes indeed, we compare the performance between using a covariance-based method with a stationary Matérn field, and a non-stationary SPDE-based method for ozone mapping. Thus we replaced the term “spatial kriging” by “covariance-based” kriging or model to clarify the confusion between model and method.

Major comment 2

The motivation for using the Matérn covariance function (page 3971) is incorrect: It is obviously not the “most advanced covariance function, and saying that it always outperforms all other covariance functions is just wrong. See for instance Bolin and Lindgren (2011) or Jun and Stein (2008) for examples where other covariance models outperform the Matérn model, even for Ozone data similar to the data studied in the article.

Answer: This statement was indeed wrong. We corrected the sentence as “The Matérn covariance function is an advanced covariance structure used to model dependence of spatial data on the plane. On the sphere, Guinness and Fuentes (2013) show that the kriging prediction using the Matérn function with chordal distance outperform many other types of isotropic covariance functions, both in terms of accuracy and quantification of uncertainty.”

Major comment 3

There are three possible reasons for the differences in the results:

1. Bayesian versus frequentist models and methods.
2. Non-stationarity in the mean versus non-stationarity in the covariance structure.
3. A covariance-based model using chordal distance versus a SPDE-based model

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using great circle distance on the sphere.

Clarifying to what extent each of these three factors contribute to the differences in the results is in my opinion crucial for the article.

Answer: Thanks for providing different and more detailed perspective. We have addressed these three factors below.

Firstly, we rule out the differences caused by using different spherical distances. In fact, covariance-based models using chordal (Euclidean) or great circle (geodesic) distances produce only small numerical differences in spatial estimation on our ozone data. Theoretically, the great circle Matérn function is strictly positive definite only under the smoothness parameters $\nu \in (0, 0.5]$ on the sphere (Gneiting, 2013). For our ozone data, due to the limitation of the R-INLA software, we can only fit the SPDE with $\alpha = 2$ on a spherical 2-manifold, and thus the smoothness parameter ν must be fixed at 1 (see also minor comment 4). As for covariance-based kriging, using the chordal distance, we fit a wide range of values of ν and select the best using the generalized cross validation residual variance (σ_{GCV}). We find that $\nu = 20$ minimizes the criterion on our ozone data. Therefore if the same value of ν were to be used for both techniques, the SPDE method would achieve an even larger improvement over covariance-based kriging.

Secondly, the “climatological norms” are calculated for each station and each month of the year over the whole period and then removed from the data. Therefore we perform the spatial interpolation directly through the ozone deviance. In this way we remove at least some non-stationary in the mean structure. We expect that the polynomial part in the covariance-based approach would not affect the results significantly. Therefore the second possible source should not contribute much to the differences in the results.

Thirdly, the Bayesian v. frequentist methods may be an important factor in the results. It is rather difficult to interpret these contributions for the two methods, and would require another systematic study beyond the scope of this paper. However, for the prior

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specifications of the SPDE approach, in general the prior distributions only need to be specified for the SPDE model parameters κ and τ with log normal priors by default: precision (theta.prior.prec) = 0.1, median for τ (prior.variance.nominal) = 1 and the median for κ (prior.range.nominal) depends on the mesh.

We use a regression basis of spherical harmonics for both of these parameters; therefore by default the coefficients follow the normal priors. We do not change the R-INLA default prior settings throughout the analysis. In summary, the differences in the results may mainly arise from a nonstationary-based SPDE approach v. a covariance-based method with a stationary Matérn field.

Minor comments:

1. Are the results in the article obtained for ozone data modeled in linear or transformed scale? Gaussian models typically fit well to the natural logarithm of TCO data, but not to the data in linear scale.

Answer: All the calculations in this paper are used in linear scale, but using logarithm of TCO data could have the potential to reduce the uncertainties further.

2. Page 2971, row 22: A covariance-based model is easy to use on manifolds if it is embedded in \mathbb{R}^d . One can then simply use a covariance function on \mathbb{R}^d restricted to the manifold, as pointed out in the article on page 3973. The advantage with the SPDE approach is that it will use the correct distance metric on the manifold.

Answer: The great circle distance is more physically intuitive on the sphere indeed. However, in an Euclidean space, a Gaussian process with Matérn covariance has sample paths that are $\nu - 1$ times differentiable, and the smoothness parameter ν can range between $(0, \infty)$. But the Matérn function with the great circle distance has a small range of valid smoothness parameters on the sphere, so is not generally valid on the sphere. The SPDE is directly defined on the sphere, and thus inherently uses the great circle distance (Bolin and Lindgren, 2011).

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On the other hand, as spheres are subsets of Euclidean spaces, a covariance function that is valid on a Euclidean space can be applied to a sphere of lower dimension if the Euclidean distance is used. This approach starts with a valid process on \mathbb{R}^{d+1} , and restricts it to the sphere \mathbb{S}^d , so while the process on \mathbb{S}^d is trivially valid, we must use the chordal distance in calculations of the covariance. Hence the Matérn function with chordal distance can be positive definite with the same range of smoothness parameters as in Euclidean space.

3. Page 3970, row 16: Not all statistical models assume that the unknown process is Gaussian. Even the SPDE approach can be made non-Gaussian, see Bolin (2014) or Wallin and Bolin (2015), and this could be of interest for ozone mapping.

Answer: Yes indeed, we corrected the sentence as “We consider statistical models that the unknown function assumed to be a realization of a Gaussian random spatial process.” to be more conservative.

4. Page 3973, row 24: What value of α was used for the SPDE approach? If $\nu = 20$ was used for the kriging approach, this is quite different from $\nu = 20$ which would correspond to the standard choice in INLA. If the same value of ν would be used for both models, how much do the results change?

Answer: We have discussed this point in major comment 3. If $\nu = 1$ were to be used for both techniques, the SPDE method would achieve an even larger improvement than covariance-based kriging in terms of σ_{GCV} reduction.

5. Page 3984, row 17: The parameters κ and τ need to be positive in order to have a well-defined model, but assuming that they are positive does not solve the identifiability issues if a non-stationary mean is used.

Answer: Yes we only consider a non-stationary covariance structure for the SPDE-based model. We can include the regression basis functions evaluated at the measurement locations with additional assumption for a non-stationary

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mean structure as suggested by (Bolin and Lindgren, 2011). We removed the wrong identifiability statement, and the sentence becomes “To maintain positive definiteness of a Matérn covariance function, the parameters $\kappa(\mathbf{s})$ and $\tau(\mathbf{s})$ must be positive, and their logarithm can be decomposed as:”.

Anonymous Referee #2

Major comments

As already noted by one reviewer, the comparison however doesn't make it clear what is actually being compared, as the two main approaches used differ not only in model structure, but also in the techniques used for parameter estimation. Furthermore, there is a pervasive confusion about the difference between models, estimation concepts, and computational methods. The SPDE and chordal distance covariance models used in the paper are models, whereas kriging is an estimation concept, with associated computation methods that only differ in the details between the two models; the SPDE calculations use precision matrices for basis expansion weights, and the covariance calculation use more traditional covariance matrix expressions. However, for sufficiently high resolution for the finite element construction for the SPDE model, and for covariance models equal to the covariance of solutions to the SPDE, the results should differ only in numerical details, as the calculations fundamentally target the same kriging estimate of the spatial field. This mixup between concepts unfortunately runs through the entire paper, with SPDE vs kriging instead of the perhaps more appropriate SPDE vs chordal covariance model, and the use of different statistical estimation techniques for the two models (Bayesian inference vs cross-validation) makes it very difficult to tell what the comparison results actually demonstrate.

Answer: Thanks, as explained in our answers to the other reviewer, we replace the term “spatial kriging” by “covariance-based” kriging or model to clarify the confusion

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between statistical models and computational methods. Our key sentence became “For the ozone data, we specify the Matérn covariance function defined in Eq. (2) in the covariance-based approach in order to compare the performance with the SPDE approach for exactly the same covariance function, whereas the model parameters are optimized according to different techniques.”

Specific comments

1. p3970, l16: The sentence Statistical models assumes that the unknown function is a realisation of a Gaussian random spatial process is incorrect. There are plenty of non-Gaussian spatial models, including discrete valued Markov models, point process models, and transformed Gaussian models to mention just a few. The sentence following it also confuses the model with the method; a “mean field” is naturally estimated as a part of the estimation process if it is part of the statistical model; kriging is just a word used for optimal least squares estimation of the spacial process, and in the completely Gaussian case equivalent to the conditional expectation of the field given the data.

Answer: Yes indeed, we corrected the sentence as “We consider statistical models for which the unknown functions are assumed to be realizations of a Gaussian random spatial process.” We also deleted the statement in brackets “with a mean field often estimated as well” as a mean structure is a part of the model, and with different assumptions in different computation methods (i.e. constant mean for ordinary kriging; linear or polynomial trend for universal kriging).

2. p3970, l20. Again, there is confusion between methods and models. Kriging itself has no problem with non-stationarity. That is all down to the model. It is true that it is difficult to construct general non-stationary covariance functions, but that is largely unrelated to the kriging method as such.

Answer: We corrected the sentence as “Not only large data sets can be computationally demanding for a kriging predictor, but covariance-based models strug-

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gle to take into consideration in general nonstationarity (i.e. when physical spatial correlations are different across regions), due to the fixed underlying covariance structure.”

3. p3970, l24. The year for Lindgren, Rue, and Lindström is 2011, not 2010. (This is an error in the reference list on page 3988, so correcting it there would likely fix all the references to that paper.)

Answer: Thanks, we corrected the reference in the manuscript.

4. p3972, Section 2.2. Here, there is a false opposite between the SPDE approach and spatial kriging. The Gaussian process in the spatial model, $Z(s)$, can be defined as a realisation of the process $X(s)$ from Section 2.1. The model for the observations exists independently of the kriging method, which can be applied to any model of this type; the practical details are in how the kriging estimate is computed, not in the model structure statement itself.

Answer: Yes indeed, there was a confusion. We changed the title of Section 2.2 as “Covariance-based approach” and devoted this section to the introduction of covariance-based models and precisely universal kriging. We added: “Note that the Gaussian process in the spatial model, $Z(s)$, can be defined as a realisation of the process $X(s)$ from the previous section.”

5. p3973, l13. “exactly the same covariance function appears to contradict other statements in the paper about which models were used. For example, if the SPDE models used $\alpha = 2$, then the smoothness on the sphere (a 2-manifold) is $\nu = 1$ (so the statement on page 3973, line 15, is incorrect). But on page 3974, line 8, it’s stated that the covariance based calculations were done for a model with $\nu = 20$, which is virtually indistinguishable from a squared exponential (or Gaussian) covariance, and very different from $\nu = 1$.

Answer: We corrected the sentence as ‘...for exactly the same covariance function, whereas the model parameters are optimized according to different ap-

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proaches employed'. For the model selection in the covariance based approach, yes indeed, the reviewer is right and we discussed it above.

6. p3973, line 15. $\nu = 0.5$ should most likely be $\nu = 1$ (see previous comment). The dimension d in the relation $\alpha = \nu + d/2 = 2$ is the dimension of \mathbb{R}^d for a regular Matérn model, and the relevant dimension when solving the SPDE on the 2-manifold that is the surface of the globe is $d = 2$, not 3. Further, in this paper, ν may have been fixed to 1 for the SPDE models, but the general SPDE/GMRF models have no such restriction.

Answer: Yes indeed, we corrected the manuscript.

7. p3973, l 20. model set-ups for both SPDE and kriging; again, confused comparison. An actual name for the covariance specified model is needed, as kriging is used for both that model and for the model based on an SPDE.

Answer: Yes indeed, we corrected the name to “covariance-based approach”.

8. p3973, l25 to p3974, l1. The R-INLA package does not have any default basis functions for non-stationary models (it does have helper functions for some commonly used basis functions that the user can choose to use).

Answer: We corrected the sentence to “To choose the best maximal order of the spherical harmonic basis, we fitted models with different maximal orders of spherical harmonics for the expansions of κ and τ in order to estimate them thereafter (the default formulation in the R-INLA package)”.

9. p3974, l15-20. Here, it is unclear what is really being compared. How were the parameters in the chordal distance covariance model estimated? Are the differences due to differences in statistical estimation techniques, e.g. with some models estimated with cross validation and others estimated with Bayesian inference? If a) the models are fundamentally different (different ν) and b) estimated with different methods, one should not expect the results to be comparable, as

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one combination of model and method is likely to be better than others (Even if none of them perfectly matches the data). How were the priors chosen for the weights for the basis functions for $\log \kappa$ and $\log \tau$ in the SPDE model?

Answer: We first estimate the optimized model parameters, i.e. κ and τ in a SPDE and ν in a covariance based model, by the same generalized cross validation criterion (with different computational methods, the estimated method for the chordal distance covariance model is maximum likelihood estimates), then compare the uncertainty of spatial estimation over the surface.

For the prior specifications of the SPDE approach, κ and τ follow log normal priors by default: precision (`theta.prior.prec`) = 0.1, median for τ (`prior.variance.nominal`) = 1 and median for κ (`prior.range.nominal`) depends on the mesh. We use a regression basis of spherical harmonics for both of these parameters; therefore by default the coefficients follow the log normal priors. We do not change the R-INLA default prior settings throughout the analysis.

These two sentences we added to the text for clarity.

10. p3977, l6-8. Again, kriging here should really be replaced by a name for the covariance based model! Further, is it possible that the unstable predictions are due to the ν -estimation? We are not really in the infill asymptotic domain here, so reliable estimation of ν is very difficult.

Answer: Yes indeed, we corrected the name as “covariance-based approach”. It is possible that the unstable predictions are due to unreliable ν -estimation. It is indeed difficult to have an unique reliable ν -value in all periods.

11. p3977, l8. variations. should be variation.

Answer: We corrected it in the manuscript.

12. p3980, l2. The passage underestimation and disappear of estimated annual cycle is clearly incorrect, but I am not sure what it is supposed to say. Perhaps

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disappearance of the was intended, but that would still leave a strange statement.

Answer: We corrected the sentence ‘... trigger underestimation and deflation of estimated annual cycle.’

13. p3981, l7. The statement SPDE approach is more robust than kriging against incomplete information is surprising, even when replacing the word kriging with the chordal distance covariance model. The non-stationary SPDE model has many more parameters than the explicit covariance model. Is the result that that model is more adaptive to the data? Unfortunately, since the models also appear to differ greatly in terms of smoothness (ν) and were estimated using very different estimation techniques, I don’t think one can draw any strong conclusions about which of those differences are more or less important to the results.

Answer: Thanks for this clarification. We replaced the term “robust” by “adaptive”. The covariance-based model is computing a weighted average of the neighborhood values around the location, while the SPDE model is constructed through a triangular mesh. The mesh approach can be more adaptive and flexible to irregularly distributed observations. We added this sentence.

14. p3983, l20. Why is this model completely different to the model stated in Section 2.2? Did the results using SPDE models not include any fixed/mean effects in the modelling? That could further explain some of the differences in the results.

Answer: The model in Appendix A1 is only related to Section 2.1. We do not include a mean structure in the SPDE model indeed. However, the ‘climatological norms’ are calculated for each station and each month of the year over the whole period and then removed from the data. Therefore we perform the spatial interpolation directly through the ozone deviance. In this way we remove at least some non-stationary in the mean structure. We expect that the polynomial part in the covariance-based approach would not affect the results significantly. There-

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fore the second possible source should not contribute much to the differences in the results.

15. p3984, l16-17. It is true that identifying both the mean and covariance is impossible based on a single realisation, without further modelling assumptions. However, that is completely unrelated to the statements about the κ and τ functions. Perhaps a section completing the sentence fragment To avoid this identifiability problem. is missing from the manuscript?

Answer: We corrected the sentence ‘To maintain positive definiteness of a Matérn covariance function’.

16. p3985, l15-17. In the sentence The main limitation is that R-INLA provides $0 < \alpha \leq 2$ case (though $0 < \alpha < 2$ not as extensively tested). there is a the missing after provides, and case should be cases. The statement in brackets appears to be a direct quote from Lindgren and Rue (2015), Bayesian Spatial Modelling with R-INLA, Journal of Statistical Software, 63(19) (<http://www.jstatsoft.org/v63/i19>), but that paper has not been referenced (it’s quite possible that an unpublished draft of that paper was used when preparing this paper).

Answer: The statement has indeed appeared in many R-INLA manuals or tutorials. We added a published reference in the manuscript as referee suggested.

17. p3985, l17-18. See the earlier comment about the fact that the sphere is a 2-manifold, so the relevant dimension for the smoothness relationship is 2, not 3.

Answer: Yes indeed, we corrected it in the manuscript.

References

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