

Interactive comment on “Interpolation of groundwater quality parameters with some values below the detection limit” by A. Bárdossy

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I must admit that I was very surprised by the review process of this paper. Being editor myself I know how difficult it is to get two or three reviewers for a paper. In this case five reviewers provided high quality reviews within a short time for which I can only congratulate the editor Hannah Cloke. I would like to thank all five reviewers and the two commenters for taking their time for careful reading the manuscript and for their useful suggestions. My special thanks go to Geoff Pegram who besides the scientific evaluation of the paper also took his time to correct the English of the paper.

Originally I thought that this paper is rather obscure and will mostly likely be read by a few fellow specialists. Thus it was more a kind of documentation of the methodology.

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After the reviews I tried to improve the readability of the paper. All language correction suggested by Geoff Pegram were included. I also changed the notation in some of the equations and modified several figures. The conditional interpolation equation (22) was also modified to show how inequality constraints modify the exact data based interpolation. The illustrative example (Figure 4) was replaced by a simpler but hopefully more convincing one. Meanwhile I did not add extra details and explanations on the original copula based interpolation, as that was already described elsewhere. The main focus of this paper is the statistical/geostatistical treatment of the values below the detection limit, which requires specific treatment. The most important parts of this paper, equations (2), (17) and (22) estimation of the marginals, identification of the dependence structure and the estimation of the conditional density for unobserved points are all focusing the specific problems related to non-detects.

Reply to the comments from A. Najah

The paper was revised.

1. The new version contains an updated introduction, referring also to other copula applications in hydrology.
2. Discussion of the results was extended.
3. The English of the text was corrected according to the suggestions of Prof. G. Pegram.

Reply to the comments from C.-W. Liu

The main purpose of this paper was to describe a methodology how to take values below a detection limit into account. (In fact the method can be applied for any kind of inequality constraints.) Thus my aim was not to illustrate an already published methodology but instead to provide new material the specific subject. The most important contribution of the paper is in equations (2), (17) and (22).

The parametric form of the marginal is included in the revised version.

The four corners were only used for the interpolation in the illustrative example. The method can work with any number of observations in any geometrical configuration. Thus the use in 3 dimensions is not a problem.

The interpolation of deethylatrazine was shown to illustrate how different interpolators might be depending on the assumptions and the methods. A complete discussion would require quite a few more figures.

The upper 1% of the data were removed in order to avoid the effect of outliers (such as the value of 6940 mg/l chloride compared to a mean 40 mg/l) on the traditional squared error.

Reply to the review written by Geoff Pegram

The comments in the annotated manuscript were all taken into account.

The transformation in equation (11) transforms the inequality constraints in the observation space to inequality constraints in the normal space. Due to the fact that $\Phi^{-1}(G(x))$ is monotonic the upper bounds transform to upper bounds.

Two new equations (16) and (19) are added. They demonstrate the fact that the density

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functions h_1 and h_2 are weighted sums of two/four normal densities. Thus the calculation of the integral in (20) can be done by calculating the sum of four integrals of normal densities.

I chose a new notation in equation (22) which might make it more readable.

The order of the figures was corrected.

The Figures 4 and 10 contained labeling on the submitted copy, but due to typesetting they disappeared. Unfortunately I did not recognize this during the proof reading, sorry for this.

The uncertainty measures for deethylatrazine were redrawn. For both interpolators the width of an 80% confidence interval is shown in the new version of the paper.

Reply to the review written by Jing Li

Thanks for the comments and the thorough review made by Jing Li. The paper was revised by taking the remarks into account.

1. A short remark to explain the construction of equation (2) was added.
2. n was replaced by $n_d + n_z$
3. A short explanation of the likelihood calculation and extension to multipoint cases was added after equation (12)
4. The example of interpolation using values measured at four corners of a square was changed. The present example is simpler and the corresponding figure is easier to understand.
5. All suggestions for minor changes were gratefully accepted.

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Reply to the review written by P.J. Smith

The text was partially rewritten to make it more readable. Corrections suggested by G. Pegram were included, and hopefully the paper is easier to read in its present form.

1. The two references suggested by the reviewer are valuable scientific contributions, however in my opinion only the paper by Keef et al. (2009) is relevant for this contribution. I added it to the references.
2. The problem of different detection limits makes a normal score transformation impossible. One cannot tell whether an exact value of 1.5 mg/l is greater or smaller than a value below a 5 mg/l detection limit. Even if there is a single detection limit the normal score transformation is problematic if the number of non-detects is high (often above 50 %). Further the bias caused by setting the below detects equal to an arbitrary number will remain.
3. The mixed approach in equation (2) was thought to avoid the effect of outliers. Extremes have a different importance for water quality issues - there is more interest in thresholds and their exceedences.
4. The data were separated at the beginning of the section to non detects d_i and exact measurements z_j . Thus the z -s represent exact values in equation (2).
5. The calculation of the spatial structure via maximum likelihood is restricted to a number of selected pairs. This is not only a computational advantage, but it leads to a balanced use of the available data. In geostatistics several different approaches were used to avoid the effects of observation clustering (for example in works by Journel). The suggested procedure which is a simplified version of our approach published in Bardossy and Li (2008) turned out to be a reasonable choice after a large number of simulation studies. This part of the work was not included in order to focus on the issue of non-detects.

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All minor issues were considered.

Reply to the review written by Francesco Serinaldi

Francesco Serinaldi provided several interesting comments. I am grateful for these comments, which also demonstrate that the main message of the paper could be understood even from the weak presentation. I followed Geoff Pegram's suggestions and also added a few additional explanations.

1. In equations (1) and (2) Weibull and gamma distributions were considered, but the investigation of the likelihood function I found that the exponential distribution is appropriate for all three parameters. This is now mentioned in the text.
2. The notation of the distribution function in the text was wrong. I changed F to G where necessary.
3. Ordinary kriging would provide similar results to the Gaussian copula after a normal score transformation, however note that the normal score transformation cannot be performed directly on the data due to the different detection limits. Further variogram estimation is a problem with non-detects as illustrated in the paper. The interpolation itself requires an exact value for the non detects which would lead to the same bias as the untransformed OK.
4. It is in general very difficult to find reasonable measures to evaluate the performance of the interpolators. I tried to use some of the traditional measures. Note that most measures are related to the detected values only which is often a small portion of the data. Further due to the high skew of the data and some outliers (such as the value of 6940 mg/l chloride) dominate the traditional squared error. This finally led to the decision to include the three selected measures so that

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they in combination enable a comparison. The last measure corresponding to the below detection limit probability is the only measure what I could imagine to measure the performance of the methods for the non-detects. The significance of the differences could be assessed but this would require further work. In my opinion the advantage of the suggested model lies in the low bias, the clear assessment of the spatial structure and the good uncertainty measures. For OK already the variogram assessment requires a great number of pre treatments such as the removal of the outliers, which due to the rank statistics based approach is not necessary for the copulas. Some discussion on the mean probability being below the detection limit was added.

Reply to the review written by Edzer Pebesma and Benedikt Gräler

I tried to improve the readability of the paper. In fact the paper is not easy to follow, but this is mostly due to the mathematical details. I tried to simplify the notation and added a few comments to improve readability.

1. The naming of the marginal was changed. In the whole paper $G(z)$ is the overall marginal distribution.
2. I added a few words to equation (1). In fact this is a very important modification of the original ML estimation, and enabled a outlier insensitive extension of the distribution function to the low domain.
3. The χ and the χ squared distributions have the same copula. Here the introduction of a different slope for the two sides of the transformation a new different distribution is obtained.
4. The variable y is in this case censored normal. For the below detection limit only inequality information is available.

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5. $n = 10$ to 12 points were used in the local neighborhoods. As the results were only slightly different $n = 10$ was selected in order to reduce computational efforts.
6. Results can be compared in the observational or in the probability space. I selected the LEPS score which is very frequently applied in meteorology for the evaluation of forecasts.
7. I agree that in the case of multivariate normal distributions the kriging variance is a good measure of uncertainty. However in this case the highly skewed marginals and the non-Gaussian dependence make the kriging variance inappropriate.
8. Figure 11 is exchanged, 80 % confidence intervals were calculated for ordinary kriging with setting below detects to half of the detection limit. The figure is scaled as for the copula approach and shows an unrealistic (geometrical) spatial distribution of the interpolation uncertainty.

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