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Uncertainty quantification of interpolated maps derived from observations with different accuracy levels

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Abtract
Most practical applications of spatial interpolation ignore that some measurements may be more accurate than others. As a result all measurements are treated equally important, while it is intuitively clear that more accurate measurements should carry more weight than less accurate measurements. Geostatistics provides the tools to perform spatial interpolation using measurements with different accuracy levels. In this short paper we use these tools to explore the sensitivity of interpolated maps to differences in measurement accuracy for a case study on mapping topsoil clay content in Namibia using kriging with external drift (KED). We also compare the kriging variance maps and show how incorporation of different measurement accuracy levels influences estimation of the KED model parameters.

Keywords
Africa, geostatistics, interpolation, kriging, measurement error, regression, soil

Spatial interpolation errors are an important source of uncertainty in many spatial modelling applications and analyses. Geostatistics provides the tools to quantify interpolation error through the so-called kriging variance or by using spatial stochastic simulation, but in standard kriging the measurement error of individual observations is rarely addressed explicitly. It is usually represented as a component of the nugget variance of the semivariogram, but this implicitly assumes that all measurements are unbiased and have the same random measurement error variance. In reality, different measurement precisions and accuracies may occur because the data used may be a merge of field estimates and laboratory measurements, may be measured using different instruments and laboratory methods, or may be derived using the same methods but in different laboratories. Often data are also measured indirectly through proxies, such as when soil properties are estimated from soil spectroscopy signals that are converted to soil property values using statistical methods such as Partial Least Squares Regression (Brown et al. 2006, Leone et al. 2012). In recent years observations are also increasingly generated through crowd-sourcing and volunteered geographic information initiatives, which may suffer from large measurement errors (Goodchild and Li 2012). These initiatives can yield large volumes of data at cheap or zero cost, but their accuracy will usually be less than that of institutional data. In this work we extend kriging with external drift to the case in which each individual observation can have a different measurement error variance. As a result observations with small measurement error variance carry more weight than observations with large measurement error variance, both in regression modelling and kriging.

The methodology builds on well-known approaches in geostatistics that go back as far as Delhomme (1978) and is also presented in text books such as Chilès and Delfiner (1999, Section 3.7.1). It boils down to modification of the kriging matrix by adding the measurement error variances to the diagonal elements of the covariance matrix. In case of correlated errors, the off-diagonal elements will also be affected. Solving the kriging system using the modified kriging matrix automatically decreases the kriging weights of observations with larger measurement error variances. Also, the influence of measurements on estimation of the trend coefficients is reduced when the measurement error variance is larger. While this is all well known, it is rarely applied in practice. This is unfortunate, because differences in measurement errors may have a large impact on resulting maps and hence the prediction accuracy can be markedly improved if these differences were taken into account. Differences in measurement error variances are typically also not included in estimation of the semivariogram and trend coefficients. In this presentation we show that measurement error variance can fairly easily be included in parameter estimation (both for estimation of the variogram parameters and regression coefficients) by taking a maximum likelihood estimation approach. Further to that, we account for systematic measurement errors by representing the (unknown) systematic error as a zero-mean random variable that is equal for all observations from the same source. Uncertainty about the variogram parameters can be incorporated by taking a Markov Chain Monte Carlo approach.

The statistical methodology is largely known and fairly straightforward but requires adaptations of existing software implementations. We implemented the methodology as R scripts, which in future will be extended to scalable R functions. We use a digital soil mapping application using topsoil texture data from the Africa Soil Profiles database (Leenaars 2013) and the LandPKS project (Herrick et al. 2013) to map topsoil clay content for Namibia. We compare prediction maps and prediction error variance maps with those obtained when measurement error is ignored. Results show marked differences and indicate that measurement errors should not be ignored, particularly when there are large differences in accuracy levels between observations within the conditioning dataset. We also explore the sensitivity of mapping results for different degrees of spatial autocorrelation of measurement errors.

One important reason that the methodology has not often been applied in practice is that it requires that the measurement error variances of all observations are known. In reality, this is seldomly the case because data come from many sources and their accuracies are rarely recorded. In our case study we used the texture triangle and expert judgement and expert elicitation (O' Hagan et al., 2006) to quantify the measurement error variances, but these are no substitute for real values and hence it is important that point data used for spatial interpolation are routinely accompanied by measures of their accuracy.

Extension from linear multiple regression and regression kriging to non-linear machine-learning regression methods, such as artificial neural networks, support vector machines and random forests, is less obvious. One approach might be to duplicate more accurate observations or assign weights to observations depending on their measurement error variance, but this can only partly solve the problem and has a large ad hoc character. More satisfactory solutions should be found, but these should be sufficiently generic and work for the entire family of machine-learning methods, because in many practical machine-learning applications blends of multiple algorithms are used to optimise performance. This is important too, because in recent decades spatial interpolation makes use more and more of explanatory information contained in covariates and machine-learning algorithms are increasingly popular because they are more flexible than linear methods and usually produce more accurate predictions (e.g. Hengl et al, 2015).

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