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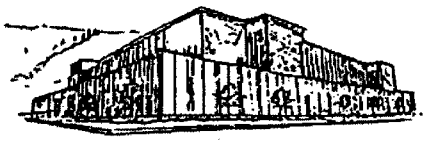
Robust variogram estimation via rank correlation and median absolute deviation correlation

Isaac C. Grenfell
The University of Montana



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ROBUST VARIOGRAM ESTIMATION VIA RANK CORRELATION AND MEDIAN ABSOLUTE DEVIATION CORRELATION

By

Isaac C Grenfell

B.A. University of Montana, 2002

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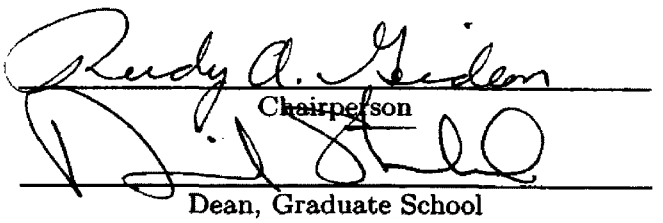

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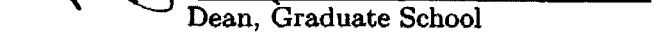

Dean, Graduate School

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Abstract

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Robust Variogram Estimation via Rank Correlation and Median Absolute Deviation Correlation

Director: Rudy Gideon

Variogram estimation via classical methods is highly sensitive to the presence of outliers in the data, as well as deviation from normality in the sampling population. To address this problem, we propose two estimation methods: one relying on the Greatest Deviation Correlation Coefficient r_{gd}, and the second based on estimates of the scale parameters and covariance through median absolute deviation (MAD). The effectiveness of these two methods is examined with computer simulation, and the methods are compared with both classical variogram estimation, and a separate robust method.

Acknowledgements

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Isaac C Grenfell

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Introduction

When conducting analysis of spatial data, a vital tool for both understanding the structure of spatial autocorrelation and the determination of kriging weights is the variogram. The most commonly used technique to estimate the variogram relies on classical statistical methods, which are very sensitive to the presence of outliers or influential observations in the data set, as well as to departure from the assumption of normality of the data. Either problem can have an ill effect on kriging weights, and therefore, kriging predictions. With real data, say from satellite imagery or field observations, it is not uncommon to have in excess of 10-15% of the observations as outliers. If an observation can be determined to be an outlier with certainty, it is best to omit the record. If it is in doubt as to whether or not an observation is an outlier, one shouldn't remove an observation without justification. This is why we seek a method that still yields meaningful results whether or not outliers are present.

Variogram Estimation

0.1 The Variogram

The objective of the variogram is to measure the association of a response variable at different distances, and possibly directions. The model of the variogram assumes intrinsic stationarity. That is, for a study region D, $E(Z_i) = E(Z_j)$, and $\text{Var}(Z_i - Z_j) = 2\gamma(\mathbf{h})$ for all points $i, j \in D$. The variogram function $2\gamma(\mathbf{h})$ is a function of the lag distance $\mathbf{h}$ that separates the points. Of interest in analyzing the variogram are three parameters: the range, sill, and nugget. The range is the lag distance at which spatial independence occurs. The sill is the value the variogram takes beyond the range. The nugget is the value the variogram takes at lag zero. We typically look at the semivariogram, which is just one half the variogram and is often referred to as the variogram.

Our goal is to estimate the function $\gamma(\mathbf{h}) = \frac{1}{2}\text{Var}(Z_i - Z_j)$ for all points i and j separated by a distance vector $\mathbf{h}$. The classical estimate of the variogram (referred to as Matheron's method in other texts) is just:

$$\widehat{\gamma}_c(\mathbf{h}) = \frac{1}{2N(\mathbf{h})} \sum_{(i,j)|h_{i,j}=\mathbf{h}} (z_i - z_j)^2 \qquad (0.1.1)$$

We do not consider the method proposed by Cressie and Hawkins [1], as its robustness has been questioned [2]. Now, if we expand the variance function, we get:

$$\begin{aligned}\gamma(\mathbf{h}) &= \frac{1}{2}\mathrm{Var}(Z_i - Z_j) \\ &= \frac{1}{2}(\sigma^2_{z_i} + \sigma^2_{z_j} - 2\,\mathrm{Cov}(z_i, z_j)) \\ &= \frac{1}{2}(\sigma^2_{z_i} + \sigma^2_{z_j} - 2\sigma_{z_i}\sigma_{z_j}\rho).\end{aligned} \tag{0.1.2}$$

where σ_{z_i} and σ_{z_j} are the standard deviations for Z_i and Z_j, and ρ is the correlation coefficient between them. In order to obtain an alternative estimate of $\gamma(\mathbf{h})$, we can simply obtain estimates of σ_{z_i}, σ_{z_j}, and ρ, and use those estimates to estimate $\gamma(\mathbf{h})$ by computing:

$$\widehat{\gamma} = \frac{1}{2}(\widehat{\sigma}^2_{z_i} + \widehat{\sigma}^2_{z_j} - 2\widehat{\sigma}_{z_i}\widehat{\sigma}_{z_j}\widehat{\rho}) \tag{0.1.3}$$

0.2 Greatest Deviation Correlation Coefficient

0.2.1 Introduction

In this section we develop a method to estimate the variogram using r_{gd}. Gideon and Hollister [3] introduced a correlation coefficient derived from the ranks of a data set, rather than the data themselves. This correlation coefficient is based on the idea of greatest deviation, where we consider only the ranks of the data and use the distribution of those ranks to obtain a correlation coefficient, which we call r_{gd}. It has several desirable characteristics. First, if we have normally distributed data, r_{gd} usually gives similar estimates to those obtained by classical techniques. If, however, we are working with a symmetric distribution such as a Student's T or a Cauchy distribution, rather than a Gaussian distribution, a good estimate of the scale parameter is attainable through r_{gd}, whereas classical methods can break down as the distribution becomes heavier in the tails. Moreover, if the data contains outliers or extreme observations, classical methods tend to give excessive weight to those observations, while methods based on r_{gd} tend be more resistant to the influence

of those observations. All of these characteristics make r_{gd} a desirable tool to estimate the variogram.

0.2.2 Method of Estimation

Let (X, Y) be bivariate normal random variables. Consider a random sample $\{(x_i, y_i)\}_{i=1}^{n}$. Sort the data by the x_i's and let p_i be the rank of the corresponding y value. Let $I(A)$ be the indicator function of the event (A) ($I(A) = 1$ if A occurs, $I(A) = 0$ if A if not), and define d_i and d_i^c in the following way:

$$d_i = \sum_{j=1}^{i} I(i < p_j) \tag{0.2.1}$$

$$d_i^c = \sum_{j=1}^{i} I(i < n + 1 - p_j) \tag{0.2.2}$$

We are now ready to define r_{gd} as:

$$r_{gd} = \frac{\max_{i=1\ldots N}(d_i^c) - \max_{i=1\ldots N}(d_i)}{\lfloor \frac{N}{2} \rfloor} \tag{0.2.3}$$

From Gideon [3], we get an estimate of ρ through the following transformation:

$$\widehat{\rho}_{gd} = \sin(\frac{\pi}{2} r_{gd}) \tag{0.2.4}$$

Now, if (X, Y)has an elliptical probability density function, we can obtain estimates of σ_x and σ_y in the following way: let $\{k_i\}_{i=1}^{n}$ be the quantiles of the standard normal distribution, and let $y_{(i)}$ be the ordered observations on Y. While there is an assumption of normality intrinsic in this method, it is not sensitive to violation of this assumption when the true distribution is symmetric [4]. From Sheng [5], our estimate of scale is the value of s that solves this equation:

$$r_{gd}(k_i, y_{(i)} - sk_i) = 0 \tag{0.2.5}$$

Using (0.2.4) together with (0.2.5), we now have a method to estimate $\gamma()$, **h** which we will call $\widehat{\gamma}_{gd}$:

$$\widehat{\gamma}_{gd}(h) = \frac{1}{2}(s_{z_i}^2 + s_{z_j}^2 - 2s_{z_i}s_{z_j}\widehat{\rho}_{gd}) \tag{0.2.6}$$

0.3 Median Absolute Deviation

0.3.1 Introduction

The MAD estimate has an intuitive appeal. It uses the median of the absolute value of the deviations from the median as an estimate of scale for a sample, and we can also obtain a direct estimate of covariance. The procedure follows from Gideon [6]. In order to achieve unbiasedness, we must rescale our estimate of scale by the 75th quantile of the hypothesized distribution. This appears to have the drawback of imposing a distributional assumption on the data, however if we look at what the actual values of these quantiles are for the T distributions, they converge quite quickly to that of the standard normal 75th quantile of 0.6745.

0.3.2 Estimation with MAD

Consider again the bivariate normal random variables (X, Y), with random sample $\{(x_i, y_i)\}_{i=1}^n$. We define MAD_x as $\text{med}(|x_i - \text{med}(x_i))$, and similarly for MAD_y. Using the MAD function, we can obtain a direct estimate of the covariance function. First, we need some results for random variables. Let $Z_x = \frac{X-\mu_x}{\sigma_x}$ and $Z_y = \frac{Y-\mu_y}{\sigma_y}$. Since X and Y are normally distributed, $P(|Z_x| \leq 0.6745) = 0.5000$. Thus, $MAD_{Z_x} = \text{med}\,|Z_x| = 0.6745$. This implies that $\frac{MAD_x}{0.6745}$ and $\frac{MAD_y}{0.6745}$ will be unbiased estimates for σ_x and σ_y [6]. Note that, $\text{Var}(Z_x + Z_y) = 2(1+\rho)$, and $\text{Var}(Z_x - Z_y) = 2(1-\rho)$. This implies that

$$\text{med}\,|Z_x + Z_y| = 0.6745\sigma_{Z_x+Z_y} = 0.6745(2(1+\rho))^{1/2} \tag{0.3.1}$$

$$\operatorname{med}|Z_x - Z_y| = 0.6745\sigma_{Z_x+Z_y} = 0.6745(2(1-\rho))^{1/2} \tag{0.3.2}$$

Now, define

$$T^+ = X - \operatorname{med} X + (Y - \operatorname{med} Y) \tag{0.3.3}$$

$$T^- = X - \operatorname{med} X - (Y - \operatorname{med} Y) \tag{0.3.4}$$

and let t^+ and t^- be the corresponding estimates. Suppose (X, Y) is bivariate normal with parameters σ_x, σ_y, and ρ. *Claim.* The covariance function $\operatorname{Cov}(X, Y)$ can be represented as:

$$\operatorname{Cov}(X, Y) = \frac{\operatorname{med}^2(|T^+|) - \operatorname{med}^2(|T^-|)}{4(0.6745)^2} \tag{0.3.5}$$

Proof. Let $\rho^* = \frac{\operatorname{med}^2(|T^+|)-\operatorname{med}^2(|T^-|)}{4(0.6745)^2}$. We now show that $\rho^* = \operatorname{Cov}(X, Y)$.

$$\rho^* = \frac{\operatorname{med}^2(|T^+|) - \operatorname{med}^2(|T^-|)}{4(0.6745)^2}$$

Using (0.3.3) and (0.3.4), this can be represented as:

$$\rho^* = \frac{\operatorname{med}^2(|X-\operatorname{med} X+Y-\operatorname{med} Y|)}{4(0.6745)^2} - \frac{\operatorname{med}^2(|X-\operatorname{med} X-Y+\operatorname{med} Y|)}{4(0.6745)^2}$$

Since $\mu_x = \operatorname{med}(X)$, $Z_x\sigma_x = X - \operatorname{med} X$:

$$\rho^* = \tfrac{1}{4(.6745)^2}(\operatorname{med}^2(|Z_x\sigma_x + Z_y\sigma_y|) - \operatorname{med}^2(|Z_x\sigma_x - Z_y\sigma_y|))$$

Using (0.3.1) and (0.3.2),

$$\rho^* = \tfrac{1}{4(.6745)^2}\left(\left(.6745\sqrt{\operatorname{Var}(Z_x\sigma_x + Z_y\sigma_y)}\right)^2 - \left(.6745\sqrt{\operatorname{Var}(Z_x\sigma_x - Z_y\sigma_y)}\right)^2\right)$$

$$= \tfrac{1}{4}\left(\left(\sqrt{\sigma_x^2 + \sigma_y^2 + 2\operatorname{Cov}(Z_x\sigma_x, Z_y\sigma_y)}\right)^2 - \left(\sqrt{\sigma_x^2 + \sigma_y^2 - 2\operatorname{Cov}(Z_x\sigma_x, Z_y\sigma_y)}\right)^2\right)$$

$$= \tfrac{1}{4}(4\sigma_x\sigma_y \operatorname{Cov}(Z_x, Z_y)) = \sigma_x\sigma_y\rho$$

$$= \operatorname{Cov}(X, Y).$$

□

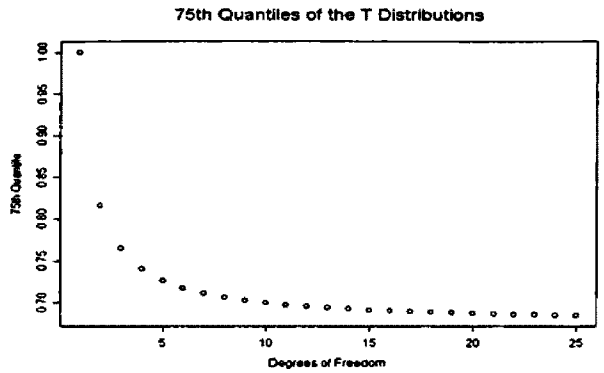

Figure 1: The 75th Quantiles of the T distributions

If (X, Y) is not normal, but still symmetric, our estimates may be biased. To see this, consider the family of T distributions. In figure 1, we see that, using 0.6745 as an estimate of the 75th quantile, we will not be far off if the degrees of freedom exceed 3 or 4. Also, the bias we observe is far smaller than if we simply took the sample standard deviation via classical methods, since the heavy-tailed distributions will produce more extreme observations. In general, MAD tends to be more robust given the presence of such observations than the sample standard deviation function.

We can now use the following sample analog as an estimate of covariance:

$$\widehat{\text{Cov}}(x, y) = \frac{\text{med}^2(|t^+|) - \text{med}^2(|t^-|)}{4(0.6745)^2} \tag{0.3.6}$$

Combining this with our estimates of scale, we get the following MAD estimate of the variogram $\gamma(\mathbf{h})$, which we will denote $\widehat{\gamma}_{mad}(\mathbf{h})$:

$$\widehat{\gamma}_{mad}(\mathbf{h}) = \frac{1}{2}\left(\left(\frac{MAD_{z_i}}{0.6745}\right)^2 + \left(\frac{MAD_{z_j}}{0.6745}\right)^2 - 2\widehat{\text{Cov}}(z_i, z_j)\right) \tag{0.3.7}$$

0.4 Simulation

To evaluate the performance of these variogram estimation methods, we perform a procedure similar to that done by Genton [2]. First, we create a spherical variogram function and use the statistical program S-plus to generate a set of 1-dimensional spatial data of 400 observations with a correlation structure imposed by this variogram. For our simulations, the variogram has a nugget of 1, a sill of 5, and a range of 7 (these values were selected arbitrarily). We then use the methods to estimate this clean data, with no imposed noise. Next, we begin taking sub-samples of this data and replace it with $100 * \epsilon\%$ of the observations with observations from an independent $N(0, \sigma^2)$ distribution. We perform this for the following values of σ and ϵ:

Simulation Conditions		
Case	ϵ	σ
I	0	1
II	0.1	5
III	0.2	5
IV	0.3	5
V	0.1	10
VI	0.1	20

Once the variograms for these different cases are obtained, we use a nonlinear-least squares method from S-plus to get estimates of the sill range and nugget. This process was repeated 40 times, yielding a table of the mean and median of the difference between the estimates and parameters via the different methods (measuring the bias of the estimates), as well as the mean squared error (MSE) and median absolute error (MAE) of the estimates (measuring the variability of the estimates).

0.5 Results and Discussion

For one set of simulations, we get the following plots, with the solid line representing the variogram function used to generate the data, and the points representing the estimate of the variogram at the given lag:

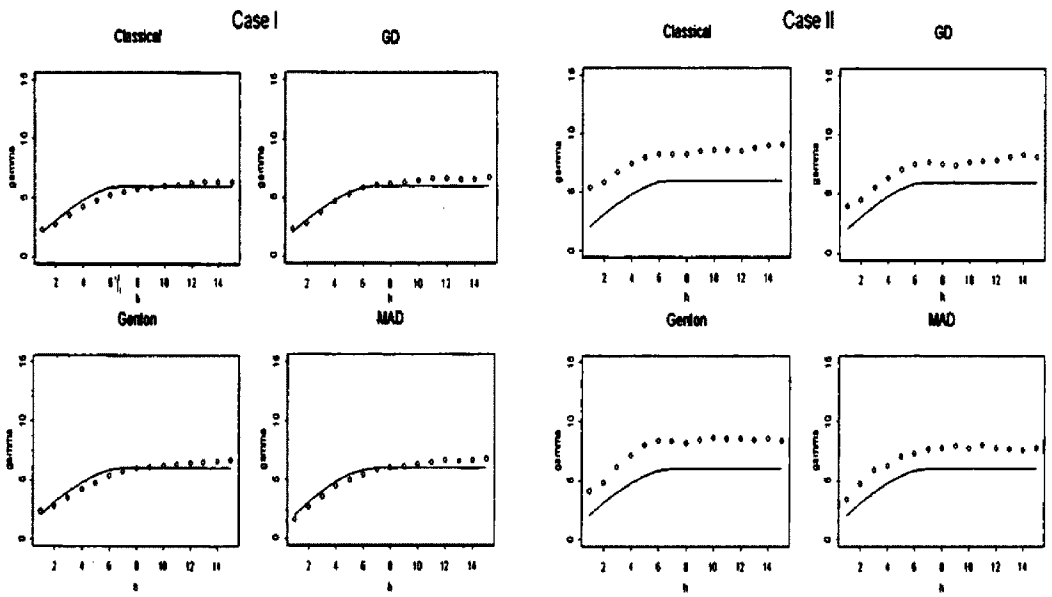

Figure 2: Cases 1 ($\epsilon = 0, \sigma = 1$) and 2 ($\epsilon = 0.10, \sigma = 5$)

For the uncontaminated data (Case I), it is apparent that all four methods perform well. As a greater proportion of the observations are replaced with outliers, however, the classical method clearly becomes worse. Genton's method appears to be overestimating the sill, indicating that the presence of the outliers is inflating the estimate of the variability. Both the r_{gd} and MAD estimates appear to miss range somewhat, but appear to be better at portraying the overall shape of the variogram.

For cases V and VI, where there is more variability in the outliers, we see again that both r_{gd} and MAD methods appear to be a little better at estimating the underlying variogram then Genton's method. Clearly, the classical method performs horribly. Note the different

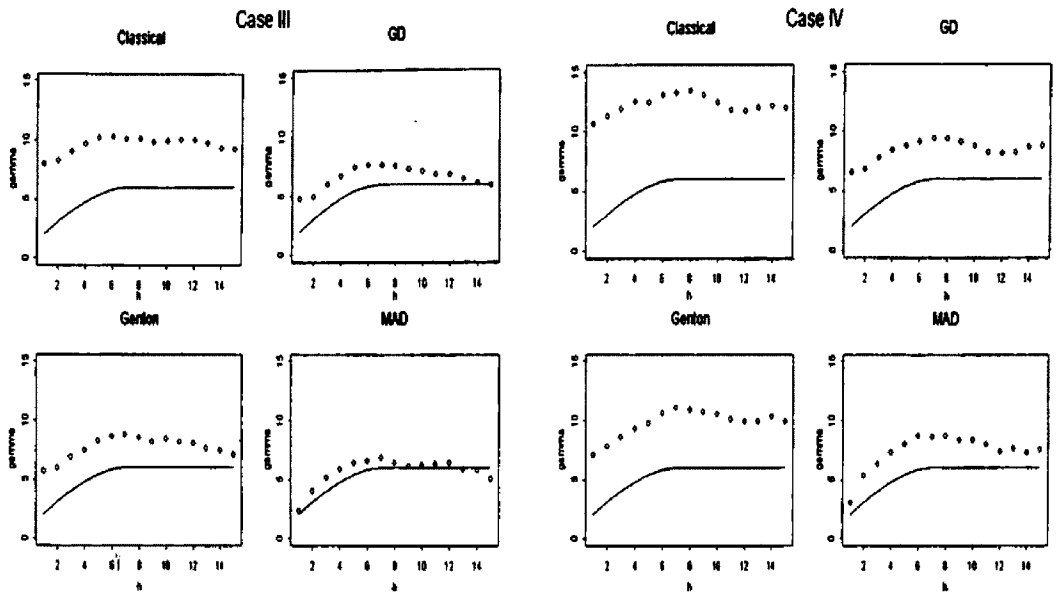

Figure 3: Cases 3 ($\epsilon = 0.20, \sigma = 5$) and 4 ($\epsilon = 0.30, \sigma = 5$)

scale for cases V and VI.

In an attempt to quantify these observations, we look at the results for 40 repetitions of this process, using a non-linear least squares function built in to S-plus to fit the variograms. For each run, we estimate the sill, range, and nugget for the variogram using a nonlinear least squares method included in S-plus. For the 40 runs, we obtain a vector of the differences between the estimates and the true parameters for each of the variogram attributes. In the table below, we give the sample mean and median of these errors, indicating the bias in the estimation method. We also include the mean-squared error and median absolute error (MSE and MAE), indicating the variability in the estimates. For the first table, we also include two columns where we scale the bias and variability statistics by the true sill and range, to get a sense of the relative errors.

For the uncontaminated data, notice that all four methods perform roughly equally well. For range estimates, the MAD method appears to be the best of the four methods, except

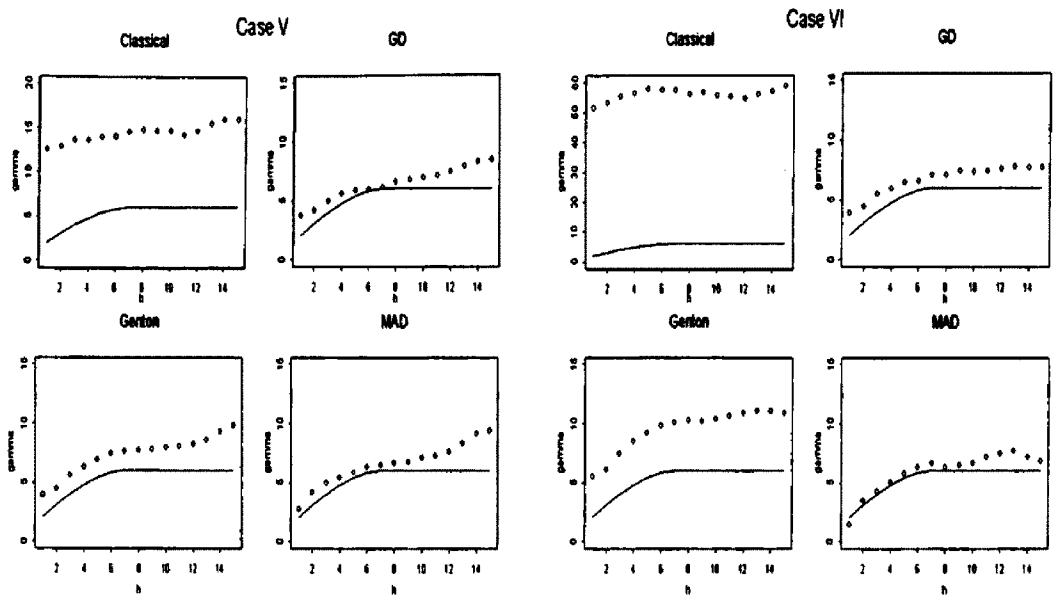

Figure 4: Cases 5 ($\epsilon = 0.10, \sigma = 10$) and 6($\epsilon = 0.10, \sigma = 20$)

when considering MAE. In terms of its overall estimation quality, MAD is better in terms of mean bias and MSE, whereas r_{gd} is better under median bias and MAE. For Case II, MAD gives better overall results than the other methods under all criteria considered. It gives the most unbiased range estimates, but Genton's method has lower MSE and MAE. For Case III, MAD is better at overall estimation again. Here it outperform's Genton's method in range estimation as well.

In Case IV, again MAD is better at overall estimation. Genton's method appears to be better at range estimation here (except for MSE). But notice a pattern here - as more and more of the data is taken up by outliers, both Genton's method and the Classical method do worse at detecting the rise (the interval from lag 0 to the range), so the variogram estimate appears to be a pure nugget effect with these methods. In this sense, it may be better to consider the overall estimation quality rather than simply considering the range.

In Case V, MAD is again better than the other methods in the overall sense, and is

Case I							
Method	*Statistic*	*Sill*	*Rel. Sill*	*Range*	*Rel. Range*	*Nugget*	*Total*
Classical	*Mean Bias*	-0.480	-0.069	0.951	0.19	0.606	2.038
	MSE	1.120	0.16	3.797	0.759	0.399	5.317
	Median Bias	-0.494	-0.071	0.628	0.126	0.587	1.709
	MAE	1.098	0.157	1.573	0.315	0.871	3.542
Genton	*Mean Bias*	-0.414	-0.059	1.161	0.232	0.581	2.155
	MSE	1.173	0.168	5.447	1.089	0.383	7.003
	Median Bias	-0.497	-0.071	0.734	0.147	0.555	1.786
	MAE	1.401	0.2	1.716	0.343	0.823	3.939
MAD	*Mean Bias*	0.696	0.099	0.031	0.006	-0.487	1.215
	MSE	1.684	0.241	2.693	0.539	0.508	4.884
	Median Bias	0.627	0.09	-0.449	-0.09	-0.524	1.600
	MAE	1.171	0.167	1.747	0.349	0.834	3.753
r_{gd}	*Mean Bias*	-0.409	-0.058	1.138	0.228	0.606	2.152
	MSE	1.427	0.204	5.920	1.184	0.471	7.818
	Median Bias	-0.309	-0.044	0.614	0.123	0.556	1.478
	MAE	1.013	0.145	1.674	0.335	0.824	5.511

better at range estimation in all senses except for MSE, where Genton's method excels. Estimation with r_{gd} gives better overall results than Genton's method. In case VI, both MAD and Genton's method have a difficult time estimating the sill, so r_{gd} provides the best overall variogram estimates for this case. The MAD method outperforms the other methods at range estimation here.

It is worth noting that this is a small study, so the conclusions may be adversely affected by this. In order to rule out this possibility, it would be necessary to conduct a more extensive study with hundreds or thousands of simulations.

0.6 Conclusion

The method of variogram estimation proposed by Cressie and Hawkins and the Classical method have been shown to fail when outliers are present in the data set [2]. I have proposed two alternatives to the method presented by Genton, and tested them via computer

Case II					
Method	*Statistic*	*Sill*	*Range*	*Nugget*	*Total*
Classical	*Mean Bias*	-1.283	1.180	3.318	5.780
	MSE	2.284	10.501	11.354	24.139
	Median Bias	-1.327	0.920	3.230	5.477
	MAE	1.967	1.662	4.788	8.418
Genton	*Mean Bias*	-0.290	1.093	1.706	3.089
	MSE	0.934	4.208	3.030	8.173
	Median Bias	-0.312	0.960	1.730	3.002
	MAE	0.946	1.783	2.564	5.293
MAD	*Mean Bias*	0.713	0.181	0.018	0.913
	MSE	1.862	4.598	0.560	7.020
	Median Bias	0.952	-0.060	-0.096	1.109
	MAE	1.591	2.529	0.803	4.922
r_{gd}	*Mean Bias*	-0.712	1.214	1.734	3.660
	MSE	1.624	5.685	3.162	10.471
	Median Bias	-0.681	1.025	1.717	3.424
	MAE	1.303	2.217	2.547	6.066

simulation. In most of the cases, the MAD method performed better than that of Genton. When the outliers have high variability compared with the clean observations, the method using r_{gd} performs well also. In light of all this, my suggestion is to use the MAD method. The Classical method only works when no outliers are present, and r_{gd} only appears to be better in the worst case.

Case III					
Method	*Statistic*	*Sill*	*Range*	*Nugget*	*Total*
Classical	*Mean Bias*	-2.108	1.052	6.120	9.280
	MSE	4.850	5.250	37.544	47.643
	Median Bias	-2.145	0.534	5.951	8.629
	MAE	3.180	1.627	8.822	13.629
Genton	*Mean Bias*	-0.074	1.084	3.328	4.486
	MSE	0.618	5.534	11.411	17.563
	Median Bias	-0.116	0.831	3.246	4.194
	MAE	0.847	1.870	4.812	7.530
MAD	*Mean Bias*	1.625	-0.371	0.320	2.316
	MSE	3.774	2.481	0.586	6.842
	Median Bias	1.559	-0.582	0.234	2.375
	MAE	2.311	1.618	0.590	4.519
r_{gd}	*Mean Bias*	-0.872	1.305	3.246	5.423
	MSE	1.607	7.310	11.042	19.958
	Median Bias	-0.807	0.914	3.234	4.955
	MAE	1.228	2.205	4.794	8.227

Case IV					
Method	*Statistic*	*Sill*	*Range*	*Nugget*	*Total*
Classical	*Mean Bias*	-2.321	1.899	8.318	12.538
	MSE	6.108	24.705	70.305	101.118
	Median Bias	-2.429	0.554	8.208	11.191
	MAE	3.601	2.686	12.169	18.457
Genton	*Mean Bias*	-0.461	0.785	5.292	6.538
	MSE	1.172	5.857	28.565	35.594
	Median Bias	-0.402	0.232	5.222	5.856
	MAE	1.054	1.665	7.742	10.461
MAD	*Mean Bias*	2.115	-1.222	0.718	4.055
	MSE	5.849	4.618	1.598	12.065
	Median Bias	2.075	-1.608	0.495	4.179
	MAE	3.076	2.857	0.942	6.875
r_{gd}	*Mean Bias*	-1.190	1.276	4.723	7.190
	MSE	2.520	8.532	23.120	34.171
	Median Bias	-1.239	0.739	4.587	6.565
	MAE	1.837	2.374	6.801	11.021

Case V					
Method	*Statistic*	*Sill*	*Range*	*Nugget*	*Total*
Classical	*Mean Bias*	-0.944	0.448	10.757	12.149
	MSE	2.432	4.152	119.872	126.456
	Median Bias	-1.222	0.239	10.668	12.129
	MAE	2.345	2.070	15.817	20.232
Genton	*Mean Bias*	1.263	1.102	2.227	4.591
	MSE	3.151	3.953	5.135	12.239
	Median Bias	1.177	1.151	2.181	4.508
	MAE	1.744	2.017	3.233	6.994
MAD	*Mean Bias*	1.749	0.373	-0.483	2.605
	MSE	4.879	4.381	0.896	10.156
	Median Bias	3.036	1.949	1.122	6.107
	MAE	3.036	1.949	1.122	6.107
r_{gd}	*Mean Bias*	-0.330	1.228	1.987	3.546
	MSE	1.389	5.676	4.140	11.204
	Median Bias	-0.343	1.120	1.980	3.443
	MAE	1.056	2.203	2.935	6.195

Case VI					
Method	*Statistic*	*Sill*	*Range*	*Nugget*	*Total*
Classical	*Mean Bias*	0.015	-0.544	40.420	40.978
	MSE	11.420	10.810	1693.190	1715.418
	Median Bias	0.152	-1.349	40.361	41.862
	MAE	3.372	4.161	59.839	67.371
Genton	*Mean Bias*	2.955	1.172	2.607	6.734
	MSE	11.183	3.971	7.033	22.187
	Median Bias	2.888	1.209	2.544	6.641
	MAE	4.282	2.015	3.771	10.068
MAD	*Mean Bias*	2.566	0.207	-1.078	3.852
	MSE	8.477	2.921	1.553	12.950
	Median Bias	2.634	-0.064	-1.050	3.748
	MAE	3.906	1.709	1.556	7.171
r_{gd}	*Mean Bias*	-0.135	1.191	2.126	3.452
	MSE	1.340	5.493	4.732	11.620
	Median Bias	-0.107	1.110	2.105	3.323
	MAE	1.231	2.254	3.121	6.605

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