Optimal Weights for Linear Estimation Using Training Images

Clayton V. Deutsch, Julián M. Ortiz and Deepak Bhandari

Centre for Computational Geostatistics (CCG)
Department of Civil and Environmental Engineering
University of Alberta

The common approach to estimation is kriging – an estimation variance is formulated and minimized in the context of a spatial random function. There are two implicit assumptions behind such an approach: stationarity and ergodicity. Stationarity is addressed by trends and locally varying parameters of estimation. Ergodicity is rarely addressed; it is fundamental to kriging. This paper considers a non-kriging based approach to determine optimal weights; specifically, optimal weights are determined using simulated annealing to minimize the mean squared error based on estimating a specified number of locations from an exhaustive training image.

Introduction

Much of geostatistics is concerned with estimation and simulation of continuous variables. Linear estimation is a common starting point:

$$z^*(\mathbf{u}) - m(\mathbf{u}) = \sum_{i=1}^{n} \lambda_i \bullet \left[z(\mathbf{u}_i) - m(\mathbf{u}_i) \right]$$

where **u** refers to a location, m refers to the mean, $z^*(\mathbf{u})$ is an estimate at location **u**, and n refers to the number of data values $z(\mathbf{u}_i)$, $i=1,\ldots,n$ and λ_i refers to their corresponding weights. An estimation variance is formulated and an estimate is calculated. The criterion used is to minimize the estimation variance.

This paper considers the use of training images to optimize the weights for linear estimates. This method is explored using a mean squared error criterion and simulated annealing as the optimization method. Weights obtained from this approach are then compared to those obtained from simple kriging and ordinary kriging for a number of different scenarios with strings of data.

Proposed Methodology

The idea is to use optimization to find the weights that are optimal for estimation under a mean squared error criterion:

$$\text{(Mean Squared Error)} \quad MSE = \frac{1}{M} \sum_{j=1}^{M} \left[z_j^* - z_j \right]^2$$

The following methodology is proposed to determine the optimal weights:

1. Assemble M sets of data and true values from a training image.
2. Start with an initial set of weights ($\lambda_i, i=1,\ldots,n$), calculate the M estimates and calculate the MSE.

3. Perturb the weights, recalculate the *M* estimates and recalculate the MSE.
4. Accept the new set of weights with a simulated annealing-type decision rule and return to step 3 until no further improvement is possible.

The next section illustrates the effectiveness of such an approach in comparison to SK and OK.

Application

Suppose we have training images at a resolution of 1000 units by 1000 units; for this example, an unconditional realization from sequential Gaussian simulation is used (Deutsch and Journel, 1998). For these training images, consider that the reference variogram is a spherical model with 10% nugget effect.

$$\gamma(h)=\begin{cases}0 \quad for \quad h=0 \\ 0.1+0.9.Sph\left(\dfrac{h}{a}\right) \quad , \quad \varepsilon<h<a \\ 1 \quad for \quad h>a\end{cases}$$

where a is the continuity range, which will be varied in subsequent analyses for sensitivity purposes. Let's consider a specific configuration of five data aligned along a string d distance units ($d=$number of blocks distance between known and estimated point) away from the location to be estimated (see Figure 1). For comparison, the proposed methodology to obtain an optimal weight along with simple kriging, ordinary kriging and an equal weighted approach will be performed for estimation of the unsampled location. Different cases are examined for these comparative analyses.

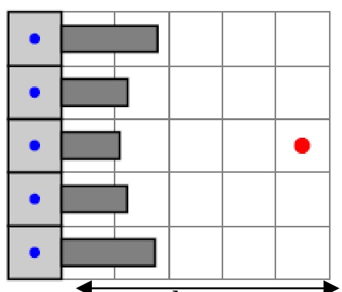

Figure 1: Configuration of data set used for different cases

Case 1: Impact of variogram range in TI

In this case we consider different TIs for different variogram ranges: 6, 10, 20, 30, 40, and 100 units (see Figure 2). For each TI, the optimal weights, SK weights, and OK weights are calculated; these are shown in Figure 3 and tabulated in Table 1. We can see that the MSE in the case of optimal weights is less than that of SK, OK and the equal weighted methods. At the same time we also see that the calculated optimal weights follow a pattern similar to the pattern of simple kriging weights; that is, end samples in the string are given higher weights than those near the centre.

Case 2: Impact of random number seed in Optimal Weights Approach

Considering the same TIs generated for Case 1 above, we now consider the optimal weights approach when different random number seeds are used. Specifically, the seeds 49049, 59059, and 69069 are considered; results are illustrated in Figure 4 and the MSE is recorded in Table 1.

Case 3: Constrain the optimal weights to sum to 1.0

For this scenario, we consider a constraint that the optimal weights must sum to one similar to OK. Figure 5 shows the results of imposing this constraint, and the MSE for this is tabulated in Table 2. The resulting weights show that imposing this constraint yields an MSE that is greater than SK, but quite close to of ordinary kriging. This appears reasonable given that the optimal weight approach has been constructed to emulate OK.

Case 4: Consider a non-Gaussian TI

Consider now that we want to move away from a Gaussian TI. For this particular case, a non-Gaussian TI can be obtained by simply squaring values in the exhaustive TI image at each location, and then perform a normal score transform. Now we get the variogram of the normal score transformed training image (see Figure 6), and calculate the optimal weights, SK and OK weights (Figure 7). Table 3 summarizes the MSE for this case; we can see that the optimal weights approach yields the minimum MSE relative to the other three estimation approaches.

Case 5: Impact of boundaries

In this case we run through two TIs and place one below the other. In the first case (1000x5,20-30) we consider a TI of 1000x4 of range 20 and another TI of size 1000x1 (fixed in all cases) with a range of 30 units. Both TIs have a common boundary in the horizontal direction. Now we consider it as one TI of size 1000x5 and calculate the optimal weights, SK and OK weights (see Figure 8). Similarly we run other cases of (1000x10 grid, with range 20 at the top and range 30 below), (1000x5 grid, with range 30 at the top and range 40 below) and (1000x10 grid, with range 30 at the top and range 40 below). Results for this case are tabulated in Table 4. In all cases, the MSE from the optimal weights approach is lower than SK, OK and the equal weighted methods.

Discussion and Conclusion

The different cases considered in this study examined the MSE from the proposed optimal weights approach in comparison with SK, OK and an equal weighted scheme for estimation of an unsampled location using a string of data. In general, the MSE for the optimal weights method is lower than the other three estimation methods considered. In presence of a horizontal boundary, similarly favourable results are obtained. In all cases, the string effect remains clearly evident and suggests that the higher weights assigned to end values are correct in kriging.

References

Deutsch, C.V., “Kriging with Strings of Data”, *Mathematical Geology*, Vol. 26, No. 5, November 1994, pp. 623-638.

Deutsch, C.V., “Kriging in a Finite Domain”, *Mathematical Geology*, Vol. 25, No. 1, January 1993, pp. 41-52.

Deutsch, C.V. and Journel, A.G., *GSLIB: Geostatistical Software Library*, Second Edition, Oxford University Press, 1998.

Table 1: Mean Squared Error (MSE) for Different Ranges (Case-1and Case-2):-

range	MSE (Optimal weight)	MSE (Optimal weight)	MSE (Optimal weight)	MSE (Simple Kriging)	MSE (Ordinary Kriging)	MSE (Equal Weight)
	seed 69069	seed 49069	seed 59069			
6	0.9866188	0.9866118	0.9866322	0.9921731	1.403826	1.426582
10	0.8772789	0.8772928	0.8773034	0.8793535	1.106586	1.118542
20	0.5925331	0.5925286	0.5925307	0.5928163	0.6599989	0.6640775
30	0.4501556	0.4501769	0.4501956	0.4502287	0.4825832	0.4845606
40	0.3745092	0.3745278	0.374524	0.3746626	0.3966955	0.3982701
100	0.2407958	0.2407897	0.2407892	0.2436695	0.2523342	0.2525712

Table 2: Mean Squared Error (MSE) for Different Ranges (Case-3):-

range	MSE (Optimal weight)	MSE (Simple Kriging)	MSE (Ordinary Kriging)	MSE (Equal Weight)
	seed 49069			
6	1.4033898	0.9921731	1.403826	1.426582
10	1.1073977	0.8793535	1.106586	1.118542
20	0.6604409	0.5928163	0.6599989	0.6640775
30	0.4825731	0.4502287	0.4825832	0.4845606
40	0.3969369	0.3746626	0.3966955	0.3982701
100	0.2521586	0.2436695	0.2523342	0.2525712

Table 3: Mean Squared Error (Case-4):-

Figure 7	MSE (Optimal Weights)	MSE (simple kriging)	MSE (ordinary kriging)	MSE (equal weights)
(a)	0.9812416	0.9829755	1.280239	1.28463
(b)	0.9258254	0.9261239	1.158582	1.163533
(c)	0.8040836	0.8041023	0.9296195	0.932699
(d)	0.7163961	0.7174662	0.7921199	0.793256
(e)	0.7240023	0.724368	0.795376	0.79614

Table 4: Mean Squared Error (Case-5):-

TI	MSE (Optimal Weights)	MSE (simple kriging)	MSE (ordinary kriging)	MSE (equal weights)
1000x5,20-30	0.6520177	0.687206	0.761826	0.7440127
1000x10,20-30	0.6160122	0.6444041	0.7406005	0.7291508
1000x5,30-40	0.4243364	0.4556494	0.4856835	0.4668692
1000x10,30-40	0.4779669	0.494923	0.5237929	0.5150857

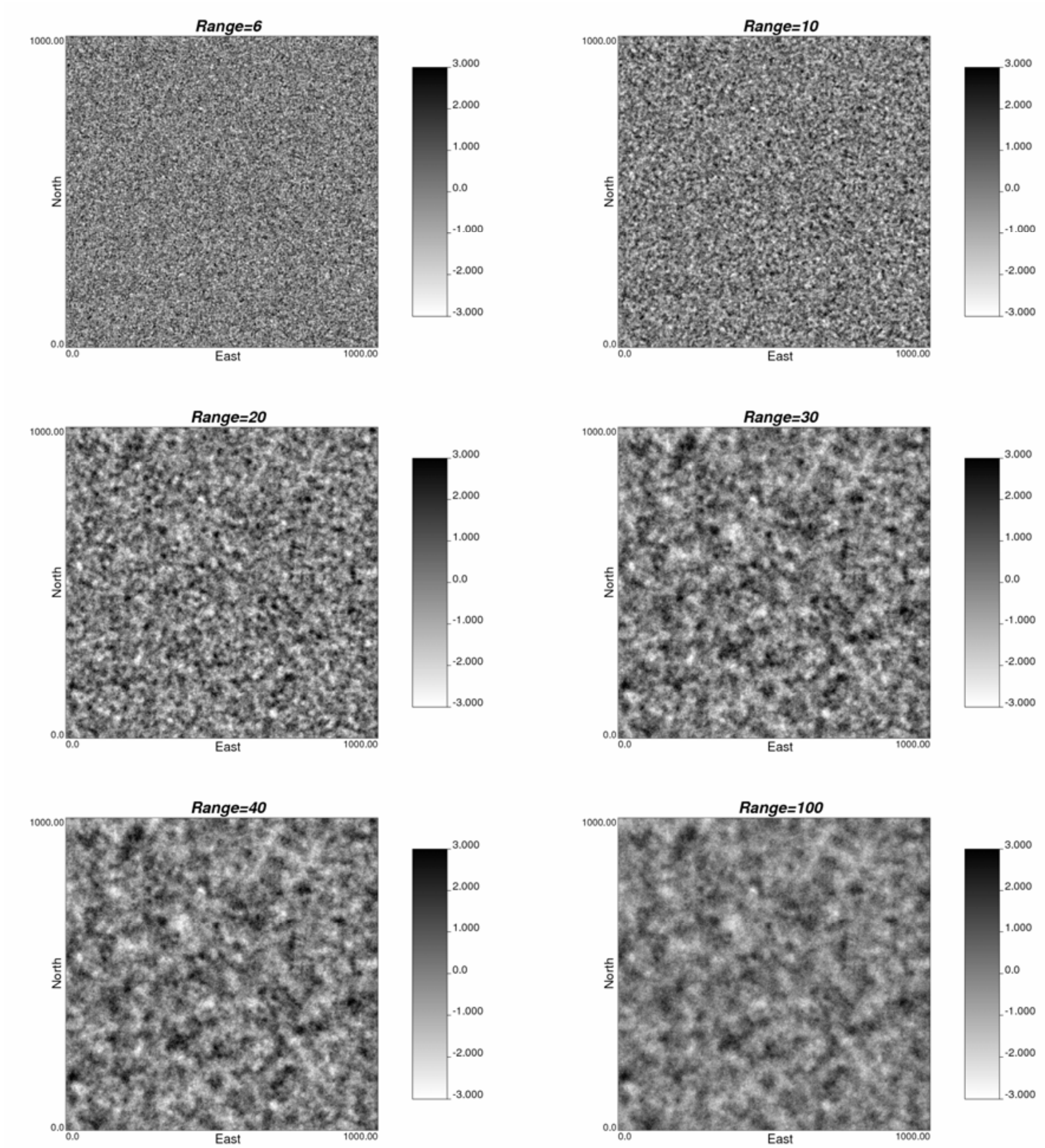

Figure 2: Training images for different ranges

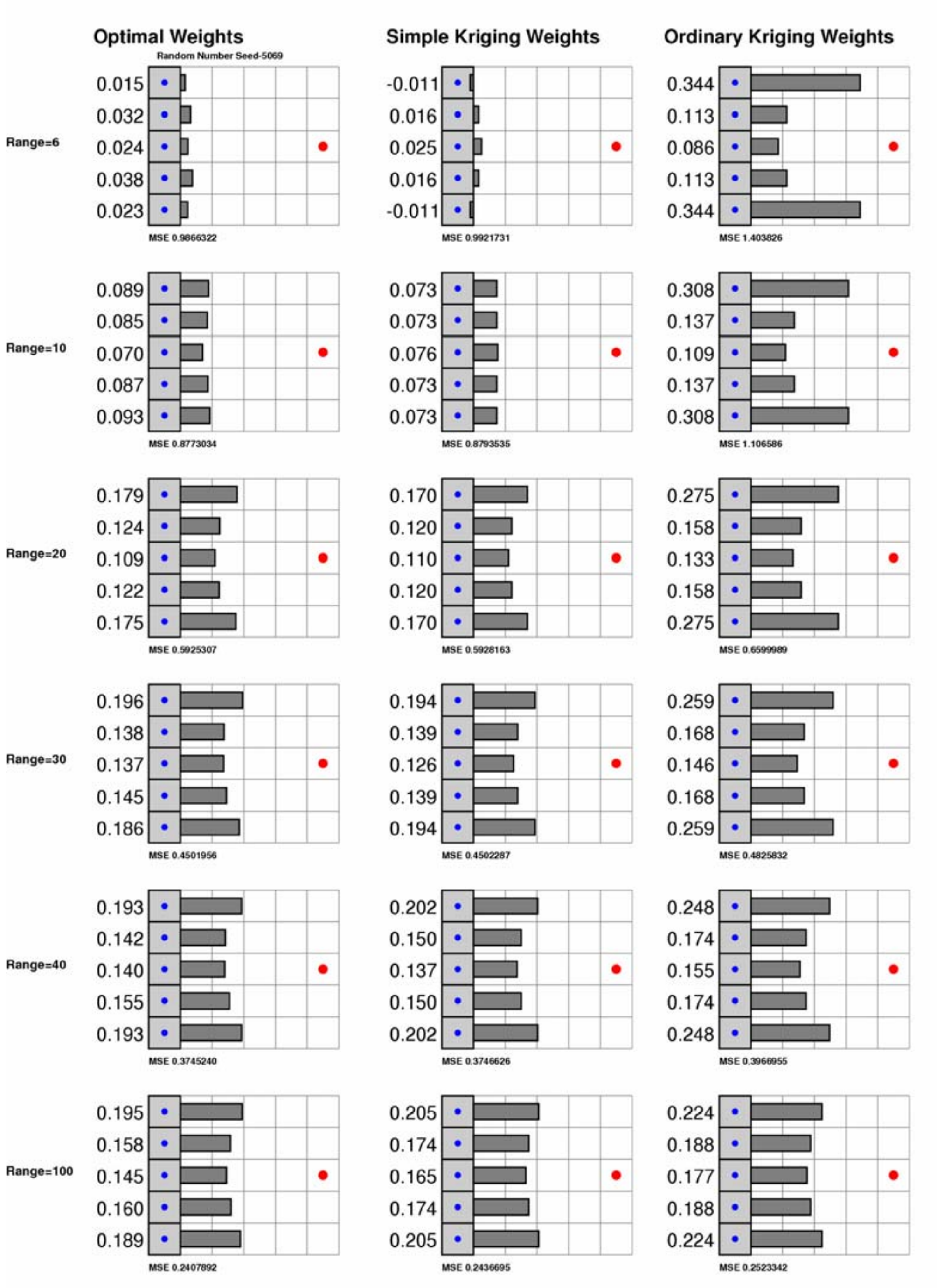

Figure 3: Comparison of estimation weights for optimal weight, simple kriging and ordinary kriging methods (Case 1).

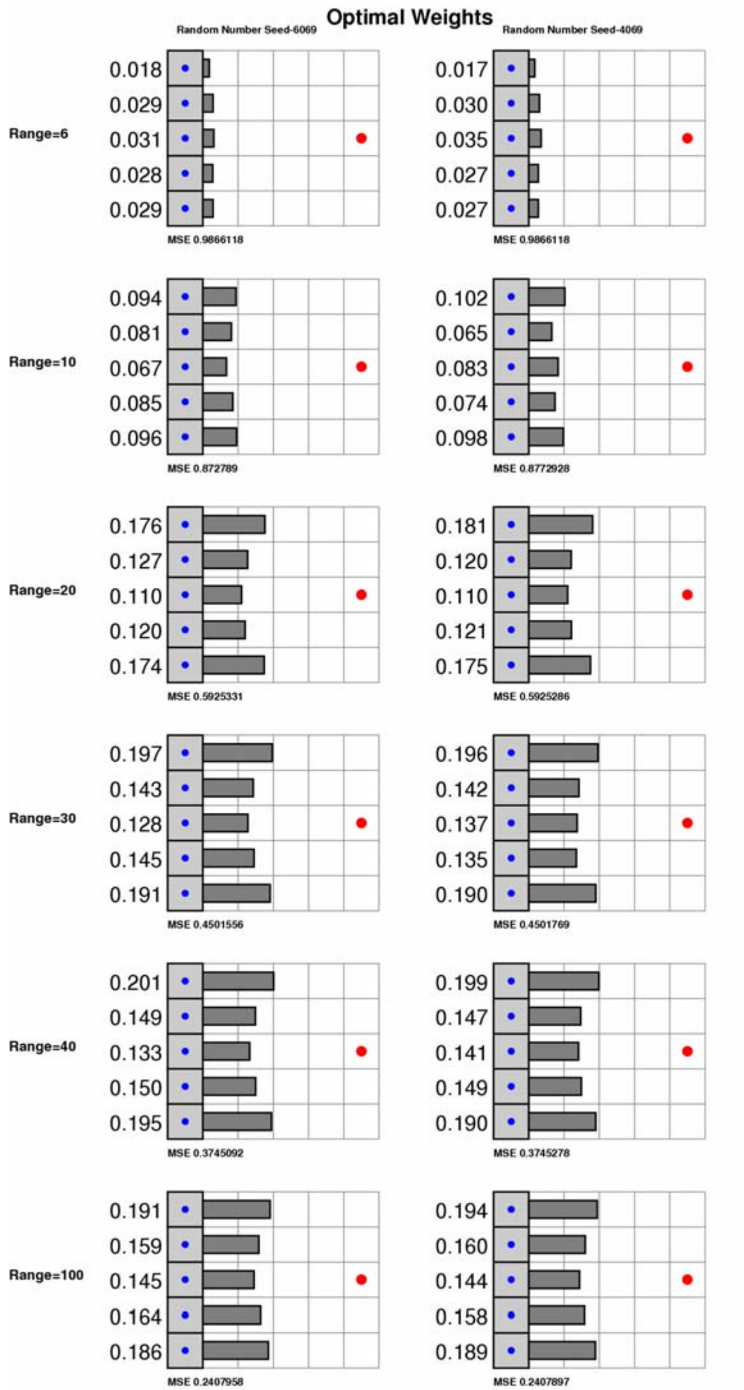

Figure 4: Comparison of estimation weights for optimal weight for different random number seeds (Case 2).

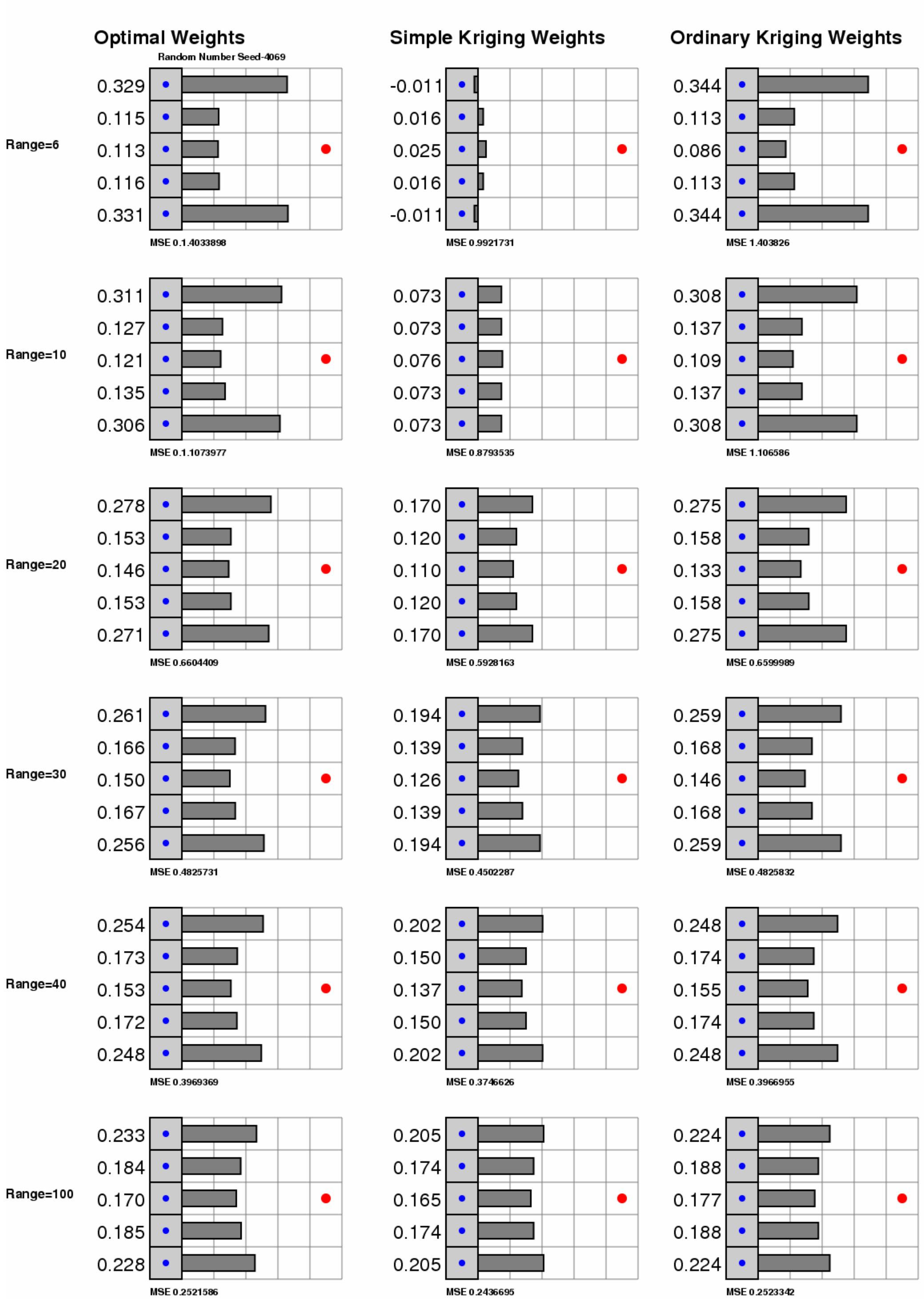

Figure 5: Comparison of estimation weights for optimal weight, simple kriging and ordinary kriging methods (Case 3).

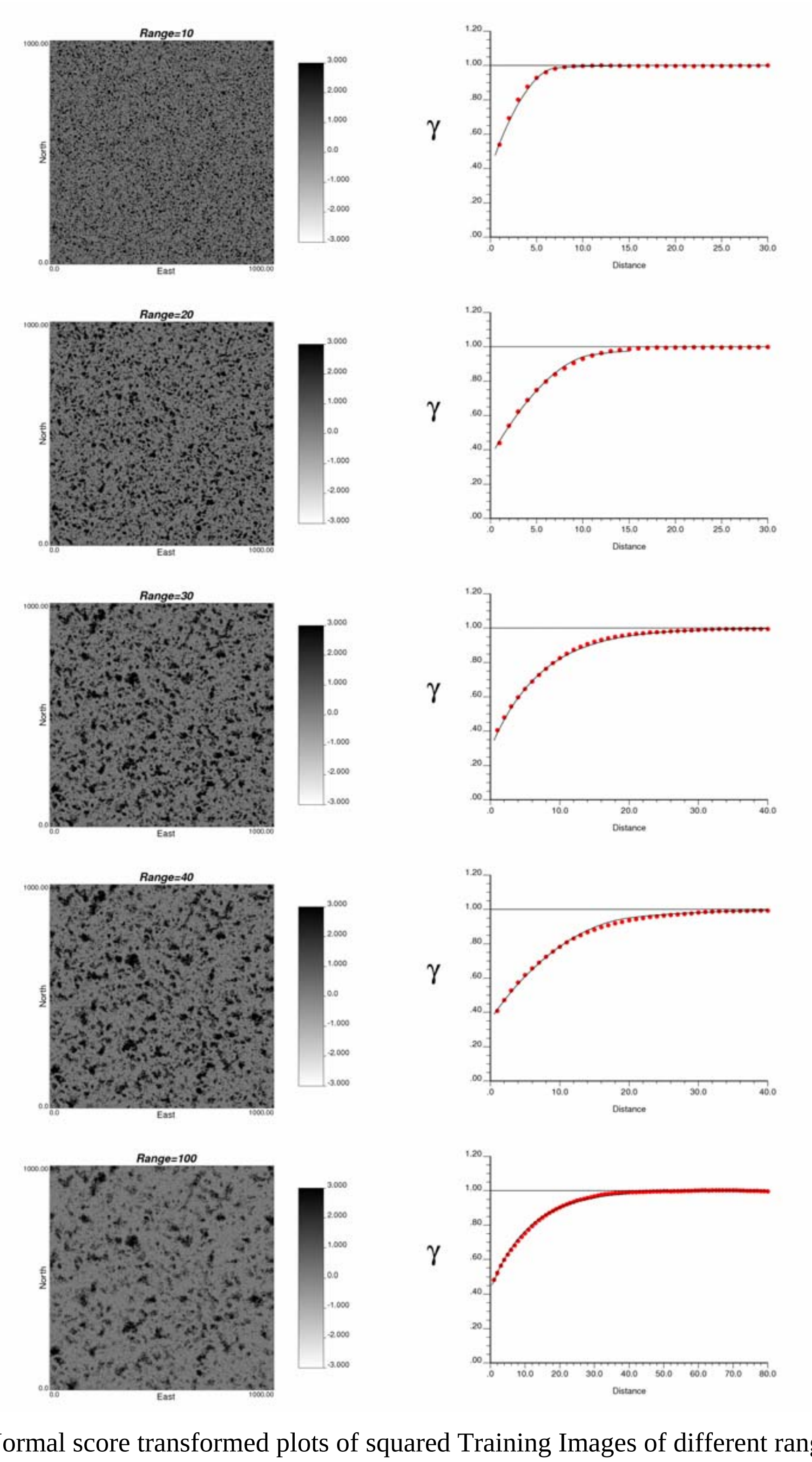

Figure 6: Normal score transformed plots of squared Training Images of different ranges and its corresponding variogram (Case 4).

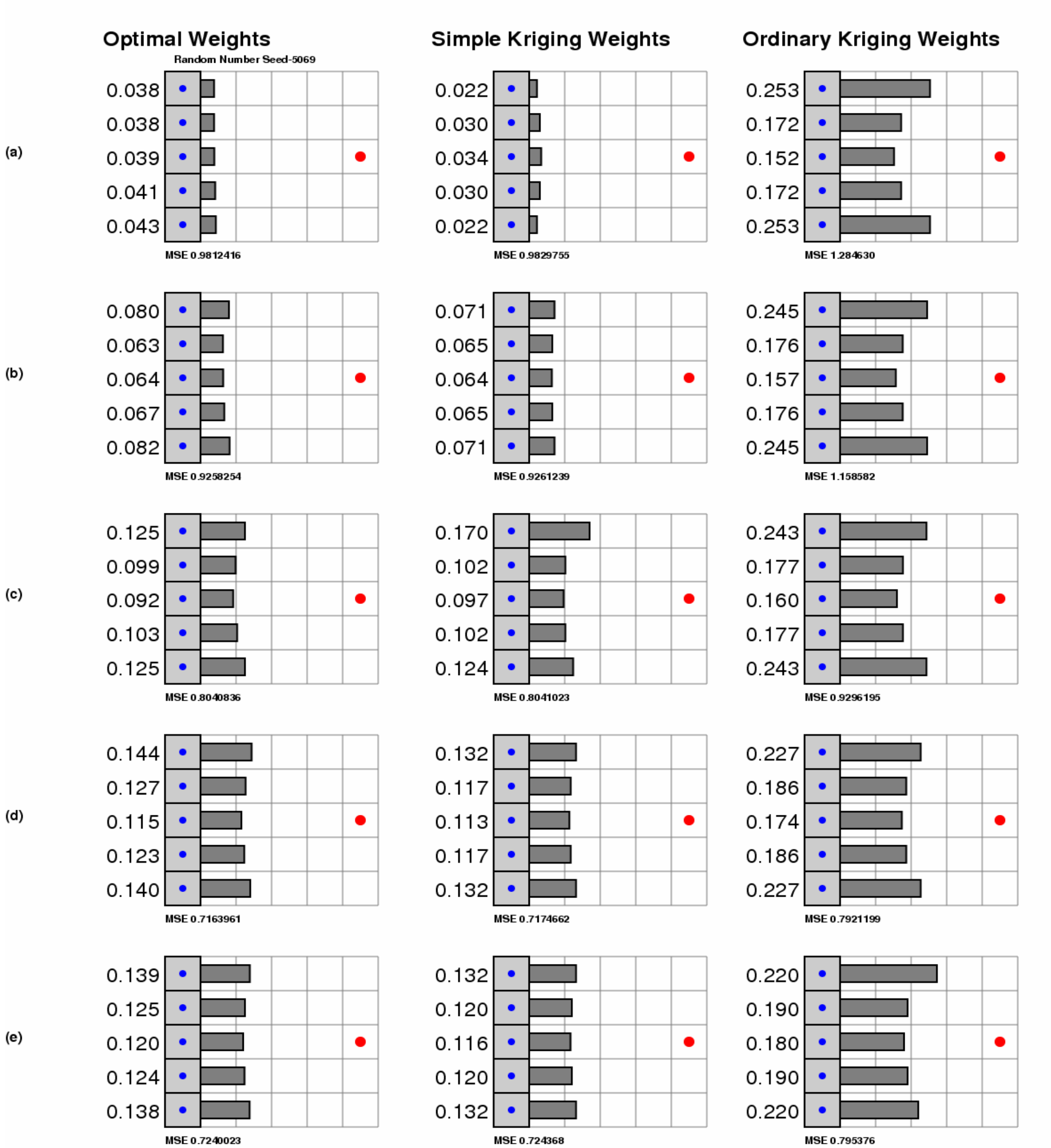

Figure 7: Comparison of estimation weights for optimal weight, simple kriging and ordinary kriging methods (Case 4).

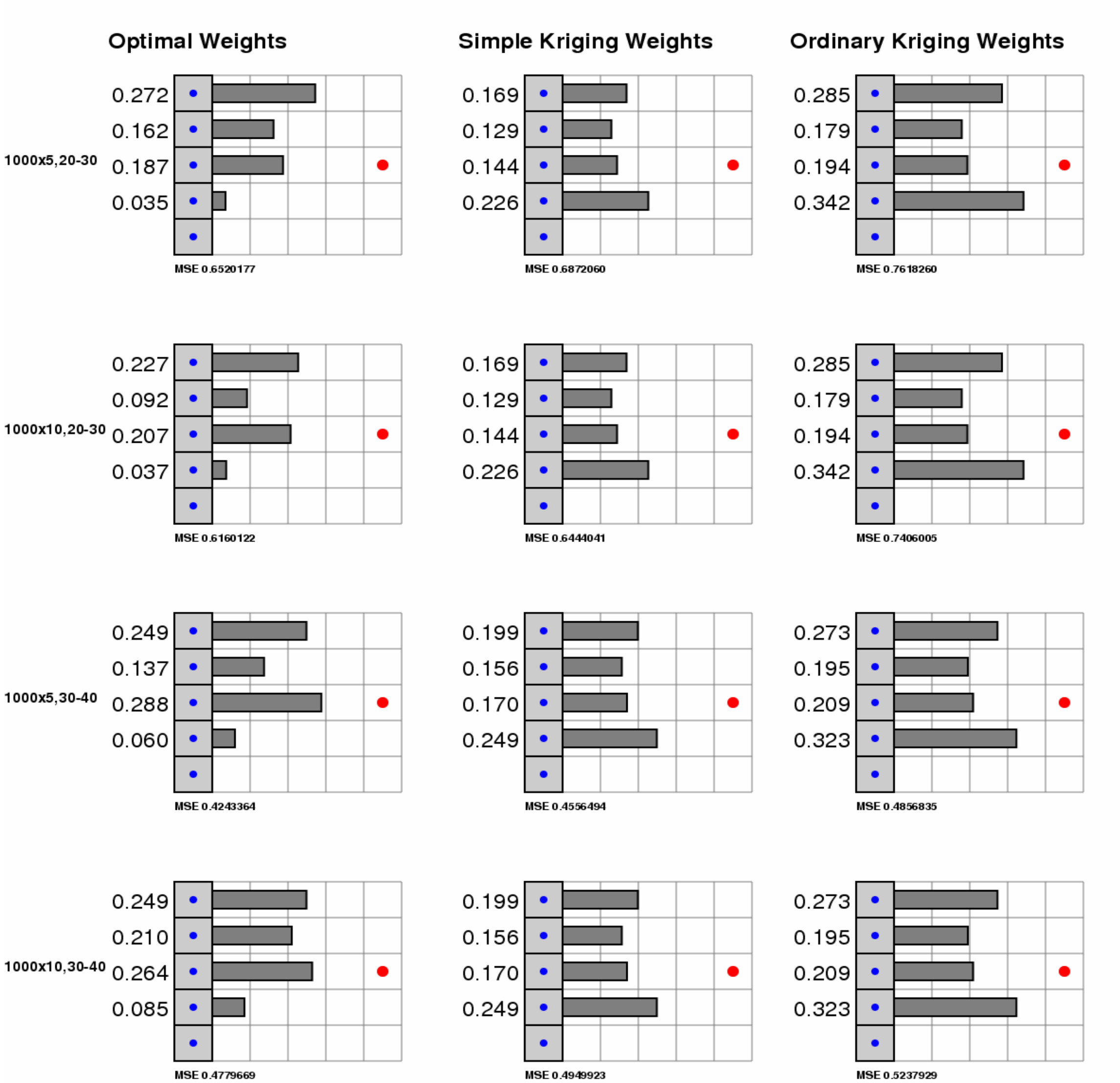

Figure 8: Comparison of estimation weights for optimal weight, simple kriging and ordinary kriging methods (Case 5).