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Original Research

Comparison of Conditioned Radial Basis Function Approach and Kriging: Estimation of Calorific Value in a Coal Field

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A B S T R A C T

Due to low production cost, coal is still the most important source of electricity production worldwide. This important position of coal also makes the evaluation of coal resources important. One of the most important attributes to be assessed in this evaluation is estimating the calorific value distribution of deposit. In geostatistical estimation currently kriging and its variants are being used widely. Alternatively new techniques are being developed and one of them is the Radial Based Functions based method. In this study, Conditioned Radial Basis Function (CRBF) is used to estimate the calorific value distribution of a coal deposit while estimations are also performed with ordinary kriging (OK). Results of both estimation methods are compared with respect to composite calorific values. Results show that CRBF produced a higher estimation range than OK with closer mean to composite. However, like OK, results are still smoother than the composite values.

Keywords: Coal, Radial basis function, Kriging, Geostatistics

Introduction

Coal is the most important natural resource used for electricity generation in the world, with a share of 38.3% in electrical energy production. In Türkiye, 37.1% of the electrical energy is covered by coal, like the world, and it takes the status of the most important electrical energy source for Türkiye which is the 19th biggest economy in the world. The total coal reserve of the world is approximately 1.07 trillion tons with annual coal consumption of 8 billion tons. The relationship between reserves and consumption in the world is similar in Türkiye while total coal reserve of the Türkiye is 19.32 billion tons, while coal consumption is around 115 million tons (Turkish Coal Enterprises, 2021). As can be seen, when the reserve and consumption rates are examined both in the world and in Türkiye, coal is the most important natural resource that supports sustainable electricity generation today. For this reason, it is of great importance to reveal the coal resources.

The most important variable in coal resources is the calorific value (Chelgani, 2021). A coal asset with insufficient calorific value cannot be considered as a coal source. The calorific value in coal beds varies depending on the location (Olea et al., 2011). It is not possible to take steps such as feasibility and production plan-

ning without modeling this variability. For this reason, the calorific value variability in coal resources and the amount of coal resources have been the subject of many studies. Fang et al. (1980) examined the usability of geostatistical methods in the estimation of coal resources. In addition, Srivastava (2013) noted the widespread use of geostatistical methods in revealing the spatial variability of coal resources and referred to many related studies. Demirel et al. (2000) performed resource estimation of the coal field in the Çanakçı, which is located in Ermenek region, using the kriging method. Tercan and Karayiğit (2001), carried out coal resource estimation studies in Kalburçayırı in Sivas - Kangal region and Tercan et al. (2013) revealed some coal resources in Western Anatolia. Whateley et al. (1997) coal resource estimations with different methods and compared the methods in the Turgut coal deposit located in Muğla-Yatağan. Inaner et al. (2008) on the other hand, made the resource estimation of the Bayır field in Yatağan. Ertunc et al. (2013) estimated the variability of calorific value in coal beds which was modeled by covariance-matched kriging. On the other hand, Afzal (2018) made a coal resource estimation using kriging and inverse distance methods in Parvadeh coal deposit in Iran and evaluated the results. Jeuken et al. (2020) compared the inverse distance weighting and kriging techniques in a coal

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deposit in Queensland, Australia. They made resource estimation using many methods. Sideri et al. (2020) estimated the mean lower calorific value of coal by using ordinary kriging methods. In this study, methods such as ordinary kriging, covariance-matching kriging and inverse distance weighting methods were used. The methods used in coal resource estimation are still in the development stage. For example, Atalay and Tercan (2017) conducted coal resource estimation with Copulas. In the framework of newly developing approaches, radial basis function estimation has never been used in the estimation of coal resources (Atalay et al. 2021).

In mineral resource estimation, in addition to classical methods such as inverse distance and kriging, relatively new advanced methods such as radial basis functions are also used. Due to the nature of the method, estimations made with radial basis functions do not meet the requirements for resource estimation to be positive definite and the estimation to be within a certain range. For this reason, direct estimation with radial basis functions will generate erroneous results. For this reason, a new approach is needed to make estimation with radial basis functions.

Since the radial basis function cannot be used in direct estimation safely, in this study, estimation is made using the conditioned radial basis function developed using radial basis functions and results were compared with kriging. For the purpose of estimation, first of all, a 3D model of the coal bed was created. After that, the kriging steps were applied. For kriging, the experimental variogram was calculated and the model variogram was fitted and the calorific value was estimated by ordinary kriging. After the kriging process, the calorific value of the coal was estimated by the conditioned radial basis function. As a result, kriging and the developed conditioned radial basis function interpolation are compared in terms of summary statistics.

1. Method

1.1. Ordinary Kriging

Kriging is basically an interpolation method based on the minimization of error variances using distance-based variability. To perform estimation using kriging, the variability depending on the distance must first be determined (Thomas, 2013). Variability due to distance is usually obtained by calculating experimental variogram values. The experimental variogram is calculated as shown in Eq. 1 (Cressie,1990, Journel and Huijbregts, 1978)

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{n} (x_i - x_{i+h})^2 \qquad (1)$$

Here; γ(h) is experimental variogram, N(h) is number of pairs and $(x_i - x_{i+h})$ is difference of pairs.

In general, experimental variogram calculation step is followed by model fitting step. Until now, many variogram models were developed like Gaussian, spherical, exponential. Among them, the spherical model is the most widely used one and is shown in Eq. 2.

$$\gamma(h) = C_o + C * \left[\frac{3}{2} \frac{h}{a} - \frac{1}{2} \left(\frac{h}{a} \right)^3 \right] \qquad (2)$$

Here; C_o is nugget effect, C is sill value, h is distance and α is range.

By fitting the variogram model, it is possible to set up kriging equations. The kriging method, like many other estimation methods, works by assigning weights to the data adjacent to the desired location (Eq. 3) (Pardo-Iquzquiza et al. 2013).

$$z(x_o) = \sum_{i=1}^{n} \lambda_i * z(x_i) \qquad (3)$$

Here; $z(x_o)$ is estimation point, λ_i is estimation weight and $z(x_i)$ shows estimation location. Estimation methods differ from each other by calculating the estimation weight in a different way (Eq. 4) (Rossi and Deutsch 2013, Rossi and Deutsch, 2014).

$$\begin{cases} \sum_{i=1}^{n} \lambda_i * z(x_i) + \mu = \gamma(x_o, x_i) \\ \sum_{i=1}^{n} \lambda_i = 1 \end{cases}, i = 1, \dots, n \qquad (4)$$

Here, is Lagrange multiplier and $\gamma(x_i, x_0)$ variogram value of that corresponds to distance between estimation point and sample point. As seen in Equation 4, the sum of the weights used in the estimation equals 1. A matrix equation that satisfies the conditions above is given in Eq. 5 (Myers,1992, Olea et al., 2011, Olea, 2012).

$$\begin{vmatrix} \gamma(x_1,x_1) & \gamma(x_1,x_2) & . & \gamma(x_1,x_n) & 1 \\ \gamma(x_2,x_1) & \gamma(x_2,x_2) & . & \gamma(x_2,x_n) & 1 \\ . & . & . & . & 1 \\ \gamma(x_n,x_1) & \gamma(x_n,x_2) & . & \gamma(x_n,x_n) & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix} \begin{vmatrix} \lambda_1 \\ \lambda_2 \\ . \\ \lambda_n \\ \mu \end{vmatrix} = \begin{vmatrix} \gamma(x_0,x_1) \\ \gamma(x_0,x_2) \\ . \\ \gamma(x_0,x_n) \\ 1 \end{vmatrix} \qquad (5)$$

By solving the kriging matrix equation, the estimation weights are calculated, and thus estimations can be performed by placing the unknown weights in Eq. 3.

1.2. Radial Basis Function

Radial basis functions are first introduced to estimate topography and other irregular surfaces while scattered data is available (Hardy, 1971). It is used for many applications in engineering problems in engineering and scientific problems while interpolation is one of them. Radial basis functions are effective tool for data interpolation problems (Schaback and Wendland,2001).

The main characteristic of the radial basis function is value of the function is changes monotonically with distance respect to central point (Orr, 1996). A radial basis function (RBF) can be defined as a function that takes values based on the distance from origin or center point (Eq. 6).

$$\emptyset(x) = \emptyset(\|x_i\|) \ or \ \emptyset(x) = \emptyset(\|x_i - c\|) \qquad (6)$$

Here $\emptyset(x)$ is radial function, is distance operator and is center.

RBF is always positively defined even though some inputs are negative. In RBF distance is generally measured in Euclidean form. Most widely used RBFs are given in Table 1.

Table 1. *Some radial basis functions (Schagen, 1979).*

RBFs	$\emptyset(\pmb{x})$
Gaussian	$e^{-(cr)^2}$
Multiquadric	$\sqrt{r^2 + c^2}$
Inverse Multiquadric	$\frac{1}{\sqrt{r^2 + c^2}}$
Inverse Quadratic	$\frac{1}{r^2 + c^2}$

In table 1 c and r parameters determine the shape of the function which affects the function output value. As seen from the table many alternative kernel functions are available. However, Gaussian kernel is the most widely used one.

Estimation with radial basis function, like in kriging, depends on the estimation of the weights associated with sampling points.

Although the method is quite similar to kriging, the only difference is that a radial basis function $\emptyset$ (II-II) processor is used instead of the variogram value of the distance between the $z(x_i)$ measurement values of the equation established on the left side of the matrix equation. Also, on the right side of the equation, the f interpolant is used in a similar way.

$$\sum_{i=1}^{n} \lambda_i * \emptyset(\|x_i - x_0\|) = f \qquad (7)$$

In this case, the matrix equation yielded for the purpose of estimation is given in the Eq. 8.

$$\begin{bmatrix} \emptyset(\|x_1 - x_1\|) & \emptyset(\|x_2 - x_1\|) & \dots & \emptyset(\|x_n - x_1\|) \\ \emptyset(\|x_1 - x_2\|) & \emptyset(\|x_2 - x_2\|) & \dots & \emptyset(\|x_n - x_2\|) \\ \vdots & \vdots & \dots & \vdots \\ \emptyset(\|x_1 - x_n\|) & \emptyset(\|x_2 - x_n\|) & \dots & \emptyset(\|x_n - x_n\|) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{bmatrix} \quad (8)$$

In Eq. 7 the distance of all values to be used in the estimation is the value of the kernel function used, and , represents the value of the function at the relevant distance. Accordingly, with the solution of the matrix equation for all λ›s, that is, the weights to be used in the estimation, the estimation process is performed as in the Eq. 3.

The estimation of radial basis functions is in the range due to the nature of the operators. However, it is not possible for mineral resources to have a negative value. In addition, mineral resources reach a limited value. For example, the average calorie of the known best quality coal occurrences is around 8000 kCal/kg. As can be seen, the radial basis function that generates estimation results in the range of can not be used directly in mineral resource estimation. For this reason, the method should be adapted to mineral resource estimation.

1.3. Conditioned Radial Basis Function

Since radial basis functions cannot be used in direct estimation, in this study, the estimation approach with conditioned radial basis functions, which is suitable for resource estimation, that guarantees positive definiteness and where the estimation results are within the desired limits, is used. This approach differs from the original approach in two points:

1) In estimation, only neighboring data is used.

2) Changing the kernel function *cr* parameter if the estimation is not within the desired range.

The goal in the first step given above is to increase the probability that the results to be in the desired range by performing regional conditioning. However, the results obtained in this step may not always be within the desired ranges. For this reason, an additional step was needed in the method. In this step, if the estimation is not within the desired range, the *cr* parameter shown in Table 1 is changed systematically. *cr* value is assigned, starting from zero, and it is checked whether the estimated value is within the desired range. The *cr* value is increased until the estimation is within the desired range.

2. Case Study

A coal field in the Türkiye-Thrace region was used for the application. A total of 128 vertical drillings with a length of 38 326 m were made in the field. The total thickness of coal cut from these drillings is 876 m. The coal seams are relatively thin, and the thickness of the coal seam is 6.5 m. The drillings made are shown in Figure 1.
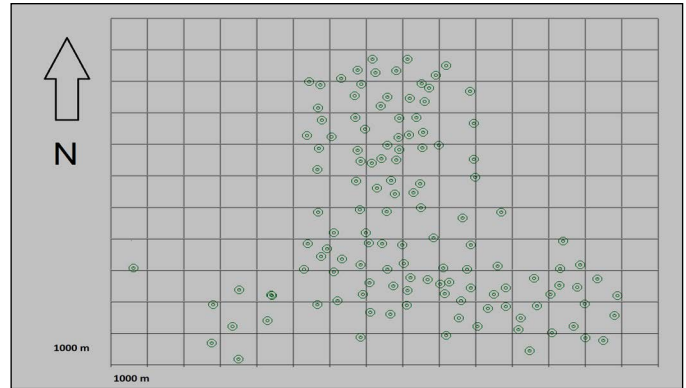

Figure 1. Plan view of the drillings

As seen in Figure 1, the average distance between the drillings is 500 m and the drilling frequency varies. Drilling frequency is approximately 800 m in the southwestern parts, while it is around 400 m in the northern parts. For the purpose of estimation, first of all, a 3D geological model of the coal seam was created. The section method, which is the most commonly used method in creating a geological model, was used and the model obtained is shown in Figure 2.
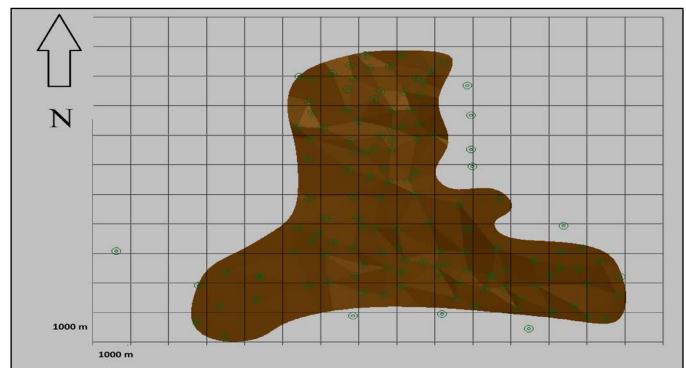

Figure 2. Solid model top view

With the creation of the 3D solid model, a block model was created to make estimations. Block dimensions were determined as 25 x 25 and 1 m in X, Y and Z directions, respectively. As a result of this process, the total blocks were created, and these are shown in Figure 3.
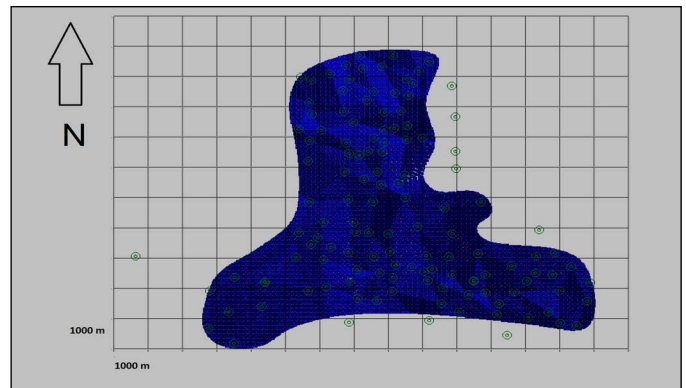

Figure 3. Block model top view

Data were composited at 1 m length for estimation with kriging and conditioned radial basis function. Summary statistics of the obtained data are shown in Table 2. Since the average distance between the data varies considerably, calculating the mean of the data directly may lead to erroneous inferences (Stein,2012, Tercan 2004). For this reason, declustered means of the data were calculated while calculating the declustered average, the existing area was divided into 1000 m x 1000 m intervals, and the data falling within these intervals was redefined according to the number of data whose weights fell on the average.

Table 2. *Summary statistics of the composites*

Number of data	Minimum	Average	Declustered Mean	Median	Maximum	Standard deviation
270	41	1428	1544	1456	3116	483

As can be seen in Table 2, the mean value and the declustered mean value are relatively different from each other. This is because the average distance between the data differs significantly. In this case, the mean for declustered data is higher than raw data. This means more frequent drilling in areas with low calorific value is made.

2.1 Estimation with Kriging

For estimation by kriging, firstly, the experimental variogram was calculated. Data frequency and spread did not allow for the computation of consistent directional variograms. For this reason, the experimental variogram was calculated and fitted as isotropic in the horizontal direction. The fitted variogram model is given in Table 3.

Table 3. *Fitted variogram model*

C_0	C	a (Horizontal, m)	a(Vertical, m)
83 000	150 000	1100	4

The cross-validation method was used to determine the usability of the adapted variogram in estimations. Cross validation results are shown in Table 4.

Table 4. *Cross validation results*

Mean	-10.23
Variance	255060
Average kriging variance	238269
Percentage of errors within two std. deviation	94.56

While the mean error was determined as low as -10 kCal/kg, the variance and mean kriging variances were close to each other. Also, Percentage of errors within two standard deviations, was a high value of 94.56%. Taking all these conditions into account, the cross-validation results show the usability of the variogram model for predictions. Estimation was performed using the fitted variogram model and summary statistics on the estimation results obtained Table 5 and the estimation map is given in Figure 4.

Table 5. *Summary statistics of kriging estimate*

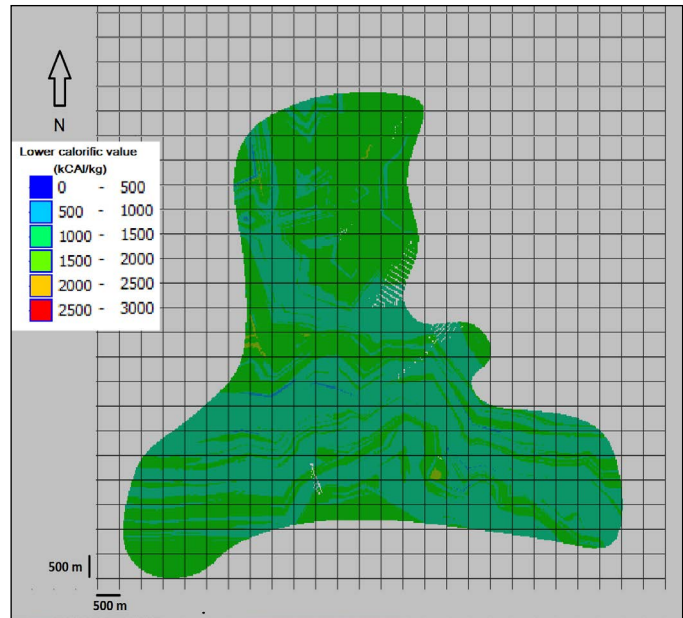| Minimum (kCal/kg)	518
Median (kCal/kg)	1506
Average (kCal/kg)	1499
Maximum (kCal/kg)	2350
Standard deviation	134.57

Figure 4. *Kriging estimate of roof of the coal model*

As can be seen in Table 5, the estimations using kriging were found between 518 and 2350 kCal/kg with an average of 1499 kCal/kg. In addition, in Figure 4, consistent with the calorific value summary statistics, the coal ceiling is with relatively low variability in the range of 1000 to 2000 kCal/kg.

2.2 Estimation with Conditioned Radial Basis Function (CRBF)

Estimation with the conditioned radial basis function is made using the steps described in the relevant section. The same block model and composites were used as in kriging. There is currently no program for estimation with conditioned radial basis functions. For this reason, the algorithm was written in MATLAB environment and a program that made predictions was written.

As seen in Table 6, there is more than one alternative that can be used as a kernel function in a radial basis function. It is necessary to determine which of these alternatives is to be used. After determining the kernel function to be used, parameter optimization of the relevant kernel function should be done. In the optimization of the kernel function and parameter, many alternatives have been tried and the option that produces the average closest to the average of the composites from these alternatives has been preferred. The estimation range was between 40 and 3000 kCal/kg, considering the lowest and highest values of the composite values. As a result, estimation was performed using the MATLAB code written to perform the estimation. Gaussian kernel function distribution parameter is preferred as 1.9 in estimation. The statistics of the obtained results are given in Table 6 and the estimation map is shown in Figure 5.

Table 6. *Summary statistics of CRBF estimate*

| Minimum (kCal/kg)	40
Median (kCal/kg)	1570
Average (kCal/kg)	1542
Maximum (kCal/kg)	3001
Standard deviation	500.47
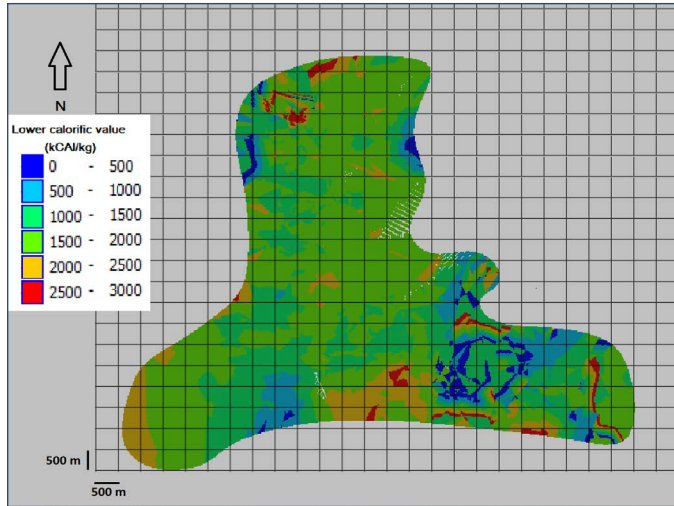
Figure 5. *CRBF estimate of roof of the coal model*

In Table 6, coal is estimated between 40 and 3001 kCal/kg with an average of 1542 kCal/kg. In addition, the standard deviation of the estimation is 500.47. Coal quality variability is relatively higher, and high-quality coal and low-quality coal are adjacent to each other in the south of the field.

In order to compare estimation results, histograms of the composites and estimation results are given in Figure 6.
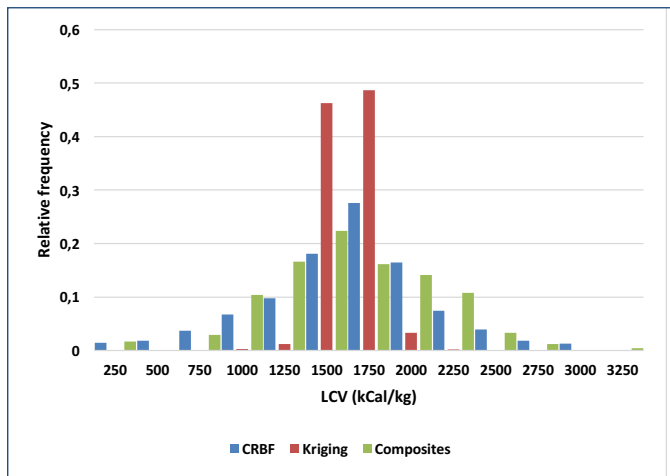
Figure 6. *Histograms of CRBF, kriging and composites*

As seen from the Figure 6 kriging estimates are centered between 1500 and 2000 kCal/kg values while it is expected due to the well-known smoothing property of the method. CRBF estimates are close to composite values while deviation exists at calorific values between 2250 and 2750 kCal/kg. To compare summary statistics of the estimate's percent of deviations from composite

statistics are are given in Table 7 while percentages of deviations are calculated as in Eq. 8.

$$Deviation\ (\%) = \frac{(Stat.of\ estimates. - Stat\ of\ composites)}{Stat.of\ composites} * 100 \qquad (8)$$

Table 7. *Deviation of summary statistics of estimates from composite summary statistics*

Deviation	CRBF	Kriging
Minimum (%)	-2.44	1163.41
Median (%)	4.28	1.37
Average (%)	7.83	3.43
Maximum (%)	-3.74	-24.60
Standard deviation(%)	3.50	-72.17

As seen from Table 7 deviation of the CRBF estimates are lower in minimum, maximum and standard deviation while kriging estimates produced closer estimates to composites in terms of median and average. The deviation of the kriging is dramatic in minimum and standard deviation which is result of smoothing.

3. Results and Discussions

In this study, Conditioned Radial Basis Function, and kriging methods for spatial estimation of quality are used and compared. For the purpose of comparison, a coal field in the Türkiye-Thrace region has been used. The spatial distribution of the coal calorific value was estimated by both methods. Experimental variograms were calculated and modeled for estimation by kriging. The experimental variogram shows that the average calorific value continuity in the field is approximately 1100 m and 4 m in horizontal and vertical directions respectively. Estimates are also made with the CRBF for comparison purposes. The Gaussian kernel function was used, and the cr was determined as 1.9.

It was observed that the average of the CRBF estimates were closer to composite estimates. In addition, the estimation interval of the CRBF is closer to the raw data. From this point of view, it has been observed that CRBF produces more desirable results in terms of estimation. However, the minimum value obtained with CRBF is 1 kCal/kg lower than the composite minimum values. Although this value may seem insignificant, it may indicate one of the flaws of estimation with CRBF. Because, in general, estimators are expected to interpolate, but as it can be seen, CRBF estimated a value outside the range of composites, albeit at an insignificant level. The highest estimate values obtained by both methods were lower than the composite estimates.

Estimation steps with both methods are similar while only attachment of the weights associated with the sampling points are only the difference. In estimation with kriging variogram values were used while in CRBF kernel function used instead. No variogram modelling is required in estimation with CRBF instead estimation of cr value is required. Results show that CRBF can be used as an alternative to kriging while technique can be used to check the estimations with kriging.

The parameters used in the method were determined by trial-and-error method. This approach is troublesome and the kernel function to be used may differ depending on the person using the method. Similarly, the parameters of the kernel function were determined by trial-and-error method. For this reason, it is necessary to develop standard methods for the determination of the kernel function and its related parameter. The method has been tried for the first time in the coal field. Testing the method with

other coal quality variables is important in terms of testing the usability of the method.

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