Interpolation algorithm ranking using cross-validation and the role of smoothing effect. A coal zone example

Oriol Falivene[1,3], Lluís Cabrera[1], Raimon Tolosana-Delgado[2], Alberto Sáez[1]

[1] Geomodels Institute. Group of Geodynamics and Basin Analysis. Dept. EPGM. Universitat de Barcelona, c/ Martí i Franquès s/n, Facultat de Geologia, 08028, Barcelona, Spain. email: oriolfalivene@ub.edu

[2] Laboratory of Marine Engineering, Technical University of Catalunya, 08034 Barcelona (Spain)

[3] Presently at Shell International Exploration and Production, Kessler Park 1, 2280 AB, Rijswijk (The Netherlands). Email addres: oriol.falivene@shell.com

Corresponding Author: Oriol Falivene

ABSTRACT

For a property measured at several locations, interpolation algorithms provide a unique and smooth function yielding a locally realistic estimation at any point within the sampled region. Previous studies searching for optimal interpolation strategies by measuring cross-validation error have not found consistent rankings; this fact was traditionally explained by differences in the distribution, spatial variability and sampling patterns of the datasets. This article demonstrates that ranking differences are also related to interpolation smoothing, an important factor controlling cross-validation errors that was not considered previously. Indeed, smoothing in average-based interpolation algorithms depends on the number of neighbouring data points used to obtain each interpolated value, among other algorithm parameters. A 3D dataset of calorific value measurements from a coal zone is used to demonstrate that different algorithm rankings can be obtained solely by varying the number of neighbouring points considered (i.e. whilst maintaining the distribution, spatial variability and sampling pattern of the dataset). These results suggest that cross-validation error cannot be used as a unique criterion to compare the performance of interpolation algorithms, as has

been done in the past, and indicate that smoothing should be also coupled to search for optimum and geologically realistic interpolation algorithms.

***Keywords*:** interpolation, cross-validation, smoothing effect, Kriging, inverse distance weighting

1. INTRODUCTION

Interpolation algorithms aim to predict the value of a property at a location by using values of the same property sampled at scattered neighbouring points (Journel and Huijbregts, 1978; Jones et al., 1986; Davis, 2002). These algorithms yield a unique (though different for each method) property map honouring input data. Interpolation in geosciences is widely used for both predictive and visualization purposes. A variety of algorithms have been developed to carry out interpolations (Morrisson, 1974), for example inverse distance weighting (IDW, Kane et al., 1982), Kriging, (Matheron, 1963), splines (Ahlberg et al., 1967; Mitasova and Mitas, 1993) or polynomial regression.

The selection of optimal interpolation strategies for continuous variables is an important and ongoing subject of debate (Lu and Wong, 2008; Bater and Coops, 2009). Cross-validation (CV) has often been used to compare the performance of interpolation algorithms (Table 1). CV is based on calculating the value of the variable at locations where the true value is known, but has been temporally removed from the input data, and then measuring the CV error by comparing the estimated value against the true one (Davis, 1987; Isaaks and Srivastava, 1989). Past comparisons based on CV error have yielded a variety of results, not always consistent (Table 1). For instance, in comparison of two widely used algorithms such as Kriging and IDW, some authors have found that Kriging yields better interpolations (Weber and Englund, 1994; Zimmerman et al., 1999; Goovaerts, 2000; Teegavarapu and Chandramouli, 2005; Lu and Wong, 2008), some have not found any significant differences in the results (Dirks et al., 1992; Moyeed and Papritz, 2002; Gallichand and Marcotte, 1993), and others have found that IDW yields better interpolations (Weber and Englund, 1992; Lu and Wong, 2008).

TENTATIVE POSITION FOR TABLE 1

The disparity in the results obtained from existing interpolation algorithm rankings using CV error (Table 1) motivated this research. We demonstrate that the comparisons solely based on CV error are utterly flawed. Apart from the fact that rankings may depend on some specific characteristics of the particular data set used for the comparison, we provide evidence that the size of the search neighbourhood plays a determinant role in algorithm rankings considering only CV error. The search neighbourhood is amongst the factors controlling the smoothing effect of each interpolation strategy. These findings challenge the practice of ranking and qualifying interpolation algorithms considering CV error (Table 1), and show that there is no absolute best interpolation algorithm: one has to establish a trade-off between minimum CV error and predictions with low smoothing. A representative example, derived from a real 3D dataset with calorific values from a coal mine, is used for illustration purposes (Figure 1).

TENTATIVE POSITION FOR FIGURE 1

2. METHODS

For our rankings, we considered two commonly used interpolation algorithms: IDW and Ordinary Kriging. Both methods provide an estimate Z^* of the studied variable

$Z(x_0)$ at an unsampled location x_0, by means of a linear combination of N observed values of Z, denoted as $z_1, z_2, \ldots, z_N$,

$$Z^*(x_0) = \Sigma\, w_i \cdot z_i \qquad (1)$$

For both algorithms compared, several numbers of averaged neighbours, N, ranging from 1 (nearest neighbour) to 288 were considered. Apart from well data locations (Figure 1B), interpolations were also carried out over the whole three-dimensional grid (Figure 1D) to attach a visual representation to the interpolation strategies compared by CV.

IDW is a straightforward and simple interpolation method, in which the weights w_i of Eq. (1) for each averaged neighbouring data point are assigned according to an inverse of distance criterion (Kane et al., 1982).

$$w_i = \beta^{-1} \cdot \mathrm{d}^{\alpha}(x_i, x_0), \quad \text{where} \quad \beta = \Sigma\, \mathrm{d}^{\alpha}(x_i, x_0)$$

Several distance weighting power factors were tested (α=1, 2 and 5). For the IDW interpolations the implementation in GSTAT was used (Pebesma and Wesseling, 1998).

Kriging is a geostatistical interpolation method in which the weights for each averaged neighbouring data point are defined to minimise the estimation variance (Matheron, 1963; Journel and Huijbregts, 1978; Cressie, 1990). The minimisation of this variance enables a spatial covariance criterion to be introduced, which results in weights for each data point that not only depend on the distance and direction to the grid cell being estimated (as in IDW), but also on the characteristics of the interpolated property (described by the variogram, V(h), Figure 2) and the relative positions of the averaged hard data (redundancy factor). For the Kriging interpolations the implementation in GSLIB was used (Deutsch and Journel, 1998).

As usual, CV was carried out by temporarily removing an entire well from the dataset (Deutsch, 2002), but using the model parameters derived from the exhaustive dataset to execute interpolations. CV error was taken as the average of the absolute differences between each predicted interpolation estimate and its corresponding real value. Standard deviation of the CV estimations was used to measure interpolation smoothing; their relationship is inverse (the higher the standard deviation, the lower the smoothing). Reference behaviours for the CV comparisons were defined by nearest neighbour interpolation, and random-based interpolation (i.e. assigning random values from the input distribution (Figure 1C) considering different degrees of smoothing and without considering the neighbouring data points preferentially.

3. ILLUSTRATION

3.1. Dataset, interpolation grid and interpolation parameters

The dataset used for illustration derives from the As Pontes Basin (NW Spain), a small mined non-marine basin (12 km^2) resulting from the activity of an Oligocene-Early Miocene strike-slip fault system (Bacelar et al., 1988; Santanach et al., 2005; Figure 1A). The sedimentary basin fill consists of a 350-400 m thick succession of siliciclastic facies assemblages alternating and interfingering with coal deposits (Cabrera et al., 1995, 1996; Falivene et al., 2007a, 2007b), and was extensively drilled owing to coal mining interest. Lithofacies of the continuously cored exploration wells were correlated, taking into account the settling and spreading of the major coal seams, which are bounded by isochronous or near-isochronous surfaces. Several composite sequences and intervals were identified (Ferrús, 1998; Sáez and Cabrera, 2002; Sáez et al., 2003). Dry-base calorific values sampled on coal beds in 174 wells drilled through a 30 m-thick, on average, coal-dominated interval (named 6AW, Falivene et al., 2007a) were used as the input data for the example in this study (Figure 1B and 1C). These wells were drilled along a roughly square grid at a spacing of about 105 m. Original data consisted of more than 2700 calorific value analyses spread over 4000 m of recovered core. Calorific value distribution in these coals, which form laterally continuous beds of up to several hundreds of meters, is mainly influenced by the amount of detritic material, and shows gradual lateral variations (Figure 1D and 1E).

To restore the post-depositional structural deformation (Santanach et al., 2005) and allow an easier visualization of calorific value distribution, interpolations were carried out with shifted vertical coordinates transforming the top of the 6AW zone to a horizontal datum. A grid layering combining proportional and parallel-to-the-top layering schemes was designed to mimic paleodepositional surfaces, along which calorific values and facies display the largest continuity (Figure 1D). Horizontal grid spacing was set to 20 m. Vertical cell thickness was approximately 0.15 m, in line with the resolution of core descriptions. Calorific values measured in the cores were upscaled to the size of grid cells by arithmetic averaging (Figure 1C), which averaged variability at smaller scales than the cell size. Upscaled calorific values measured in the coal beds were then transformed to normal distribution using a normal-scores transformation (Deutsch and Journel, 1998). The transformed data were the input for further analyses.

Parameters required for interpolation algorithms (i.e. variogram parameters for Ordinary Kriging and vertical-to-horizontal anisotropy ratios for IDW) were adjusted from the complete dataset (Figure 2). Anisotropy ratio (Jones et al., 1986; Falivene et al., 2007a) for IDW was approximated by the vertical-to-horizontal variogram range ratio. This factor is used to multiply the vertical coordinates prior to the interpolation in order to deal with geometric anisotropy (Kupfersberger and Deutsch, 1999). This enables assigning different weights to hard data points located at the same real distance from the point being estimated, but with different stratigraphic position, and allows reproducing flattened geometries, which are typical of sedimentary deposits.

TENTATIVE POSITION FOR FIGURE 2

3.2. Results

Results were computed directly both for the normal property and after undoing the normal scores transformation to the original data scale. As both results are qualitatively similar, for simplicity and geological relevance only the back-transformed results are shown (Figure 3, 4 and 5). Results in Figure 3 can be summarized as:

1) CV error is not independent of smoothing; for random-based interpolation, as smoothing increases, CV error decreases (Figure 3). Nearest neighbour interpolation yields the largest CV error and the lowest smoothing with respect to Kriging and IDW (Figure 3).

2) Compared to the results of random-based interpolation, by using average-based interpolation methods, the CV error and smoothing are always smaller (Figure 3).

3) When a small number of neighbouring data points are considered (Figure 4A and B), the largest CV errors are obtained (Figure 3). If the number of neighbouring data points increases (Figure 4C and D), then CV error decreases (Figure 3). In IDW, for very large numbers of neighbouring points, CV error increases slightly.

4) Smoothing always increases as the number of neighbours increases (Herzfeld et al., 1993, Figure 3).

5) For IDW, on increasing the power factor, smoothing decreases, whereas CV error tends to increase (Figure 3B and C). Increasing the power factor increases the importance of the nearest samples, thus effectively reducing the number of influential samples in the neighbourhood.

6) Depending on the degree of interpolation smoothing (i.e. on the number of neighbours considered for interpolation), completely different algorithm rankings can be obtained if only CV error is taken into account (Figure 3B and C).

TENTATIVE POSITION FOR FIGURE 3

TENTATIVE POSITION FOR FIGURE 4

4. DISCUSSION AND CONCLUSIONS

An optimal interpolation algorithm should provide minimum cross-validation (CV) error, as is common practice in the literature (Table 1). CV errors in the example presented here range between 10 to 15% of the mean measured calorific value (Figure 3). These variations are large enough to rank the different algorithms, and can be significant when predictions are made over large coal volumes. In addition, an optimal interpolation algorithm should also obtain results with relatively low interpolation smoothing (Isaaks and Srivastava, 1989; Olea and Pawlowsky, 1996; Journel et al., 2000), which seeks to preserve as much as possible the gradual lateral variation of calorific values shown in the mine (Figure 1D, compare Figure 4A to 4C, and 4B to 4D, Figure 5).

TENTATIVE POSITION FOR FIGURE 5

Variations in interpolation algorithm rankings, taking only measurements of CV error (Table 1) have been traditionally justified by the fact that the studied variables are characterized by different histogram distributions, spatial continuity or sampling patterns (Brummert et al., 1991; Zimmerman et al., 1999; Lu and Wong, 2008). For example, a general consensus exists that, in irregularly spaced data, Kriging should provide more accurate and robust results than IDW, because Kriging takes into account the relative positions of sampling points, and not only their distance from the interpolated point (Kane et al., 1982; Lebel et al., 1987; Weber and Englund, 1994; Borga and Vizzacaro, 1997; Goovaerts, 2000; Falivene et al., 2007a).

The results shown herein demonstrate that, if only CV error is considered, different algorithm rankings can be obtained by changing the number of neighbours averaged (Figures 3B and 3C). Thus, differences in algorithm rankings cannot be fully explained by intrinsic differences related to the variable studied and the sampling patterns, as suggested before. Indeed, interpolation smoothing partially controls the results of CV error (Figure 3). Interpolation smoothing is primarily controlled by the number of neighbours averaged, but also by the algorithm itself and other algorithm parameters (e.g. the semivariogram in kriging and the anisotropy ratio and the power factor in inverse distance weighting).

As a consequence, using only CV error as ranking criteria provides ambiguous results, because smoothing (relating to each particular algorithm and algorithm parameters) heavily influences the CV rankings and the appearance and continuity of the interpolation results (Figure 4 and 5). The interpolation results obtained with the largest number of neighbours are the ones that yield the lowest CV error, but Figure 4 and 5 shows that the predictions between data points in these cases tend to be too smooth, because of the increasing influence from too much data further away. Therefore, minimum CV error cannot be the unique criterion of interpolation optimality, as have been used in previous studies (Table 1). Even for the same interpolation method, the optimum number of neighbours averaged is not the one that yields minimum CV errors because the smoothing introduced in the interpolation must also be taken into account.

Multiple-criterion rankings, for instance coupling CV error and smoothing, needs to be used to search for optimum interpolation strategies. This multi-criterion would discard too smooth calorific value distributions (i.e. disconnecting large and small calorific values identified in adjacent wells), such as those in Figure 4D, even though they may yield the lowest CV error (Figure 3C). And it would favour gradual and laterally continuous, with moderate CV error and smoothing, such as those in Figure 4A or 4B (Figure 5). Therefore, in more general terms applicable to other geological situations or case studies, the analyst should search for a trade-off between geological continuity (low smoothing) and statistical optimality (low average CV error), in order to look for best interpolation practices.

5. ACKNOWLEDGEMENTS

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FIGURE AND TABLE CAPTIONS

Table 1. Summary of the results from published interpolation algorithm comparisons by means of the cross-validation (CV) check.

Figure 1. Geological setting and dataset characteristics. **(A)** Present basin boundary and areal extent of the studied 6AW interval. Coordinates are in kilometres; see location of the basin in the upper right inset. **(B)** Well distribution in the 6AW interval. The location of the reference section in Frames D and E and in Fig. 4 is shown. **(C)** Relative frequency of calorific values; plotted information corresponds to the core data upscaled to the size of grid cells. **(D)** Reference section showing upscaled calorific values in the intersected wells; calorific values in lacustrine and alluvial mudstone are null. Approximate paleodepositional surfaces are shown. **(E)** Facies distribution in the coal zone obtained by using indicator Kriging with an areal trend applied to categorical variables (for details, see Falivene et al., 2007a). Vertical exaggeration of Frames D and E is 10x.

Figure 2. Variograms for the transformed calorific values. Black dots, crosses and dashed curves correspond to the experimental variograms derived from upscaled well data. Grey continuous curves to the theoretical model fitted (Hr and Vr stand for horizontal and vertical ranges, respectively): V(h) = 0.82·Exp (Hr = 450m, Vr =2.8 m) + 0.18·Exp (Hr = 60m, Vr =100m).

Figure 3. Interpolation smoothing (measured by the standard deviation of cross validation (CV) estimates) against mean absolute CV error for all the interpolation strategies compared. The greater the standard deviation, the lower the smoothing; standard deviation in the original dataset was 650. (A) Results for several numbers of averaged neighbours (2, 4, 12, 24, 48, 96, 192 and 288). Note also the results of the nearest neighbour and random-based interpolations (i.e. assigning random values from the input distribution (with different smoothing degrees), and without considering the neighbouring points. (B) Detail with the results for 12 averaged neighbours. (C) Detail with the results for 192 averaged neighbours. Note the correspondences with frames in Figure 4.

Figure 4. (A, B, C, D) Reference section and map showing calorific value distributions in coal facies obtained by different interpolation strategies. Calorific value in alluvial and lacustrine mudstone facies shown in Figure 1E is null. **(E)** Location of the section, the map and the input data. Note that the horizontal scale of the map and the section are not the same. If the number of averaged neighbours increases, the spatial continuity of the resultant calorific value distribution in coal facies is obscured, as the result of larger interpolation smoothing. Vertical exaggeration 10x.

Figure 5. Calorific values for those cells in the intersection of the map and the section shown section in Figure 4, obtained by different interpolation strategies. Note that too smooth interpolation methods such as Kriging or IDW with 192 averaged neighbours provide interpolations that in some cases deviate largely from the closest surrounding data due to the effect of data located further away, although they yield lower CV errors than algorithms considering a smaller number of averaged neighbours.

Figure(s)

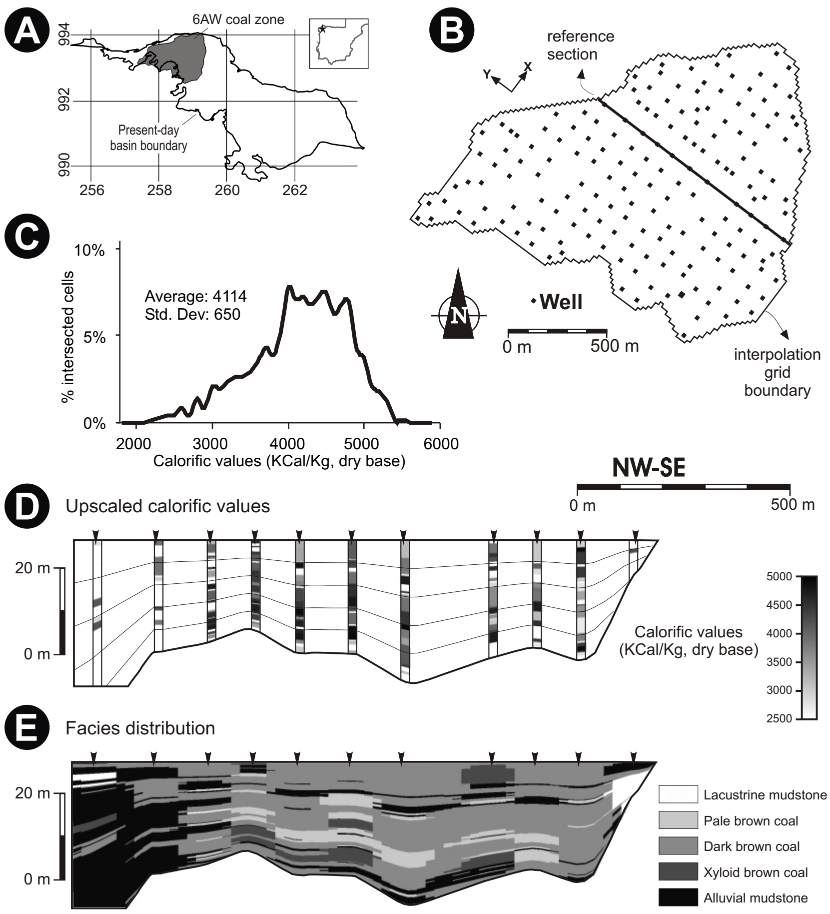
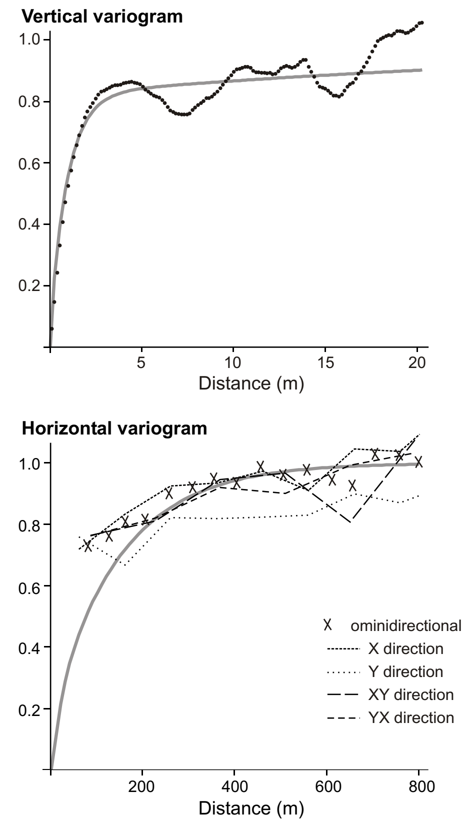


Figure 1.


Vertical variogram
1.0
0.8
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Distance (m)
Horizontal variogram
1.0
0.8
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YX direction

Figure 2.

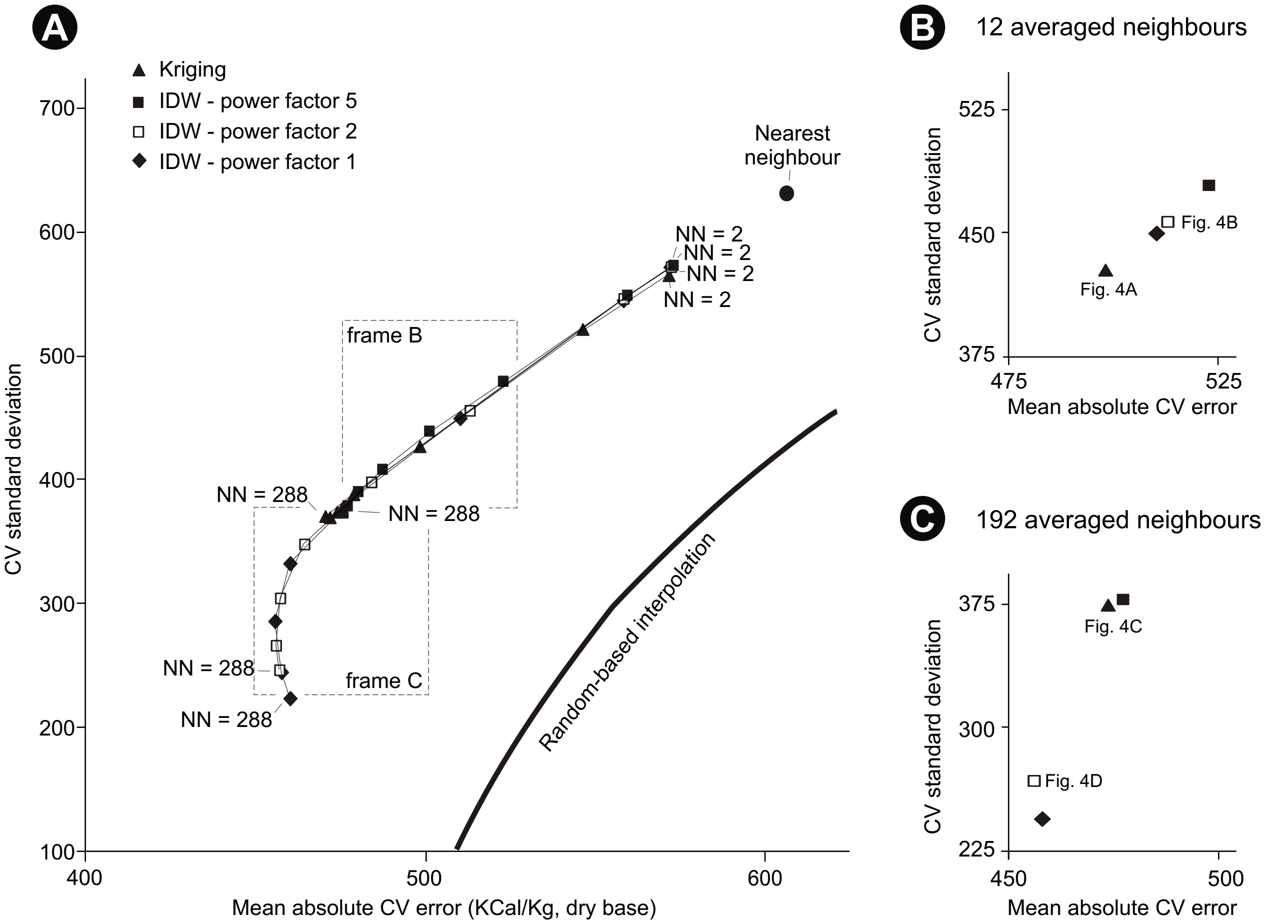

A
Kriging
IDW - power factor 5
IDW - power factor 2
IDW - power factor 1
Nearest neighbour
NN = 2
NN = 2
NN = 2
NN = 2
frame B
NN = 288
NN = 288
NN = 288
NN = 288
frame C
Random-based interpolation
CV standard deviation
700
600
500
400
300
200
100
400
500
600
Mean absolute CV error (KCal/Kg, dry base)
B
12 averaged neighbours
525
450
375
475
525
Fig. 4B
Fig. 4A
CV standard deviation
Mean absolute CV error
C
192 averaged neighbours
375
300
225
450
500
Fig. 4C
Fig. 4D
CV standard deviation
Mean absolute CV error

Figure 3.

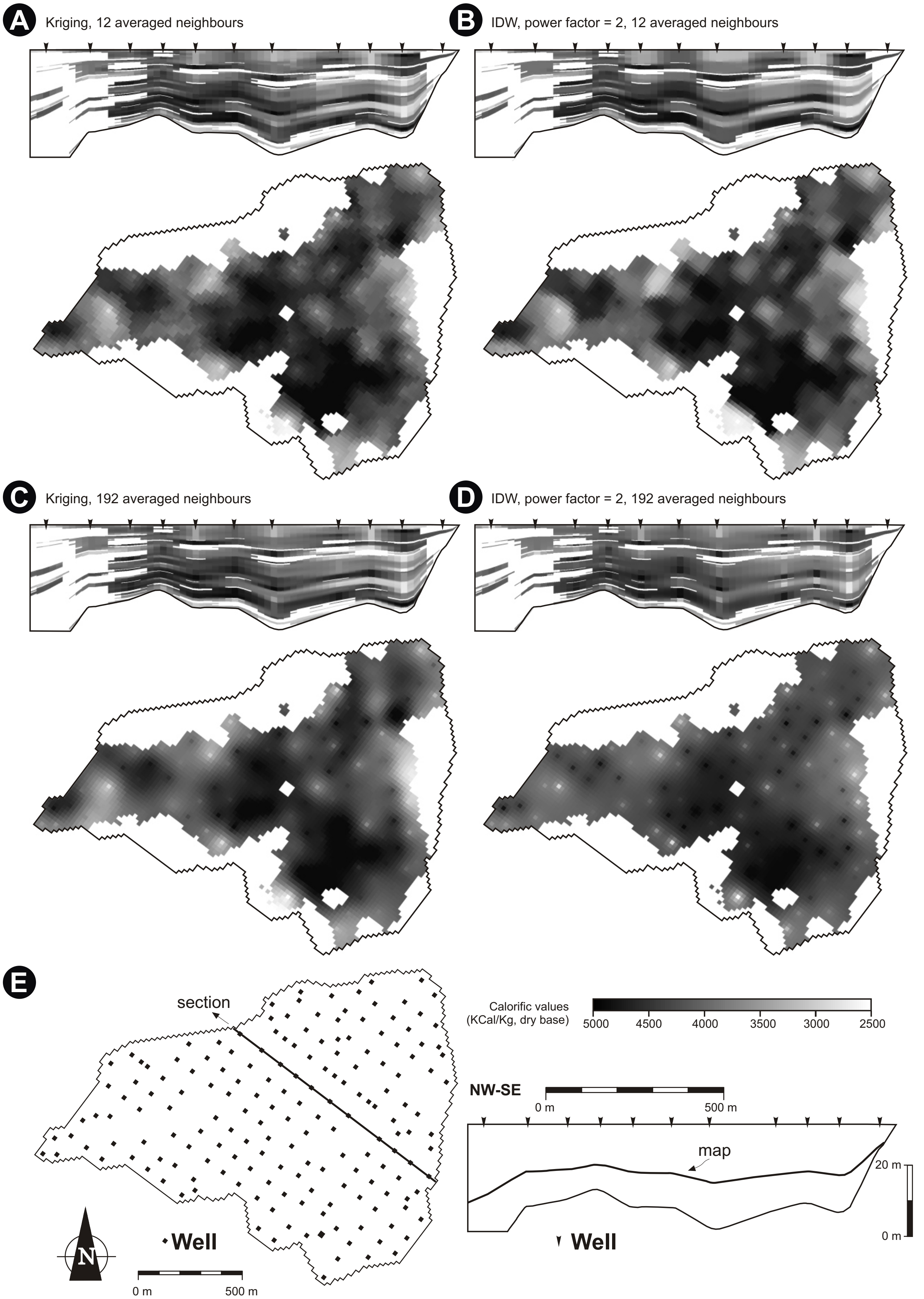
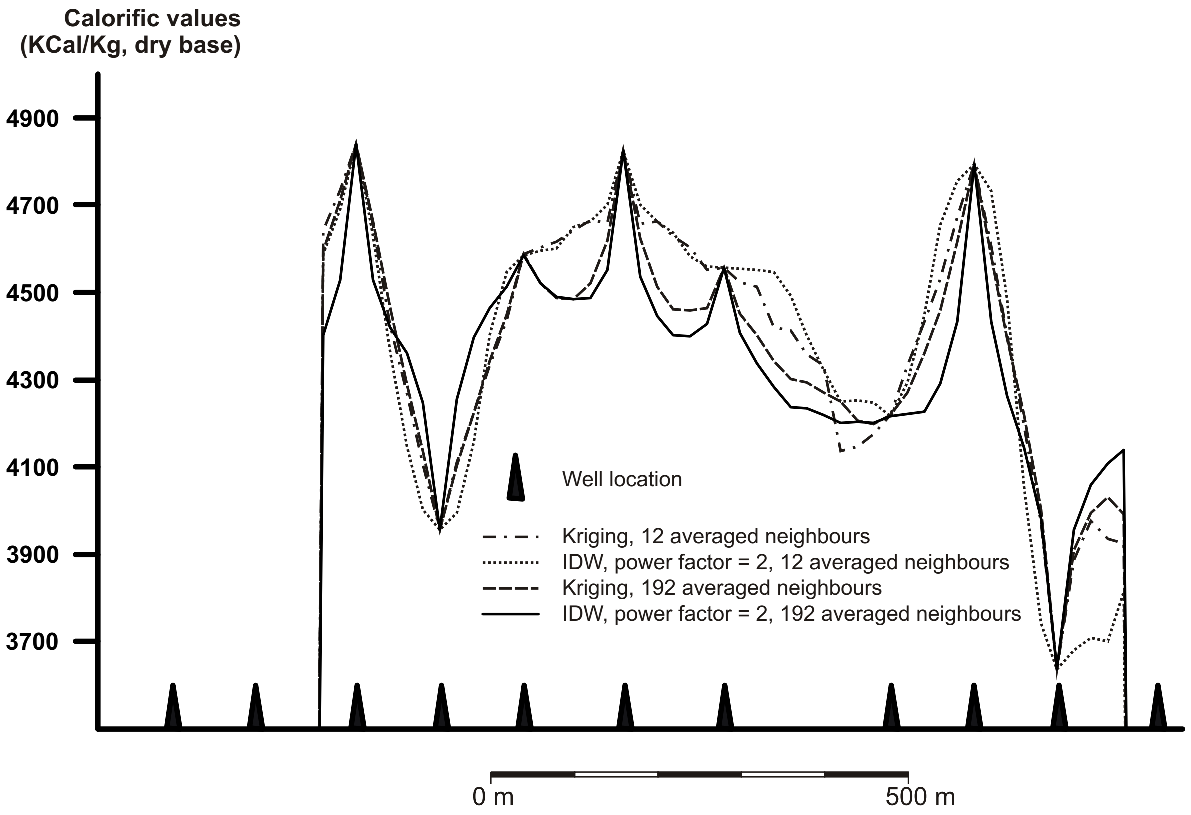

A
Kriging, 12 averaged neighbours
B
IDW, power factor = 2, 12 averaged neighbours
C
Kriging, 192 averaged neighbours
D
IDW, power factor = 2, 192 averaged neighbours
E
section
Well
0 m
500 m
Calorific values
(KCal/Kg, dry base)
5000
4500
4000
3500
3000
2500
NW-SE
0 m
500 m
map
20 m
0 m
Well

Figure 4.



Calorific values
(KCal/Kg, dry base)
4900
4700
4500
4300
4100
3900
3700
Well location
Kriging, 12 averaged neighbours
IDW, power factor = 2, 12 averaged neighbours
Kriging, 192 averaged neighbours
IDW, power factor = 2, 192 averaged neighbours
0 m
500 m

Figure 5.

Supplementary Material Captions

Supplementary Material

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Supplementary Material

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Supplementary Material

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