Application of 2D methods for scattered data approximation to geophysical data sets

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ABSTRACT The aim of this paper is to study the performance of three methods used in the geophysical community for the gridding of irregularly sampled data sets: the minimum curvature method, the generalized equivalent source technique and kriging. These methods are applied to synthetic and real world data sets and are compared in terms of robustness and reconstruction quality. In addition the new ACT algorithm developed by Feichtinger, Gröchenig, and Strohmer will also be applied to geophysical data sets and its practical relevance will be indicated.

1 Introduction

The aim of applied geophysics is to study the earth by measuring some of its physical properties, e.g. the magnetic field or the gravitational acceleration. Surveys in Austria are usually performed by helicopter, although special ground measurements are also quite common.

The resulting amount of data is enormous. Sampling geometries are in general irregular for a variety of reasons: ground measurements can not be made e.g. in rivers or technically disturbed areas, airborne measurements are intrinsically inhomogeneous as the sampling density along the flight path is much higher than the spacing of the profiles, and because the helicopter is influenced by wind and the topography.

For further processing and mapping it is necessary to interpolate or to approximate the data onto a grid. This problem arises not only in geophysics but in a variety of scientific fields, and a number of methods can be found in the literature (see [6] and references cited there). In the present study the focus is on three methods which are primarily used in the geophysical community, namely the minimum curvature method, the generalized equivalent source technique, and kriging. Furthermore the application of the new ACT algorithm [5] to geophysical data will be studied.

For a precise description of the problem, suppose that we have \( N \) distinct sampling points \( p_i = (x_i, y_i) \) and sampling values \( f_i \) with error \( \epsilon_i \), arising from imperfect measuring devices and preprocessing.

The task is to find a smooth function \( F(x, y) \) which satisfies \( F(x_i, y_i) = f_i + \epsilon_i \). If \( \epsilon_i \) is neglected \( F \) is an interpolating function, otherwise it represents an approximation to the data.

2 The minimum curvature method

The minimum curvature method (MNC) has first been proposed by Briggs[1] for automatic contouring of geophysical data. It solves the problem to interpolate the data onto a regular grid in the sense that a grid point value tends to an observational value if the position of the observation tends to the grid point.

For this a two-dimensional cubic spline is fit to the data by solving the corresponding difference equations, which have been set up under the conditions that the solution takes the measured values at the points of observation while keeping the total squared curvature minimal.

The curvature is constructed directly in terms of the grid point values \( F(x_i, y_k) \) and depends on the grid spacing \( h \).

The discrete total squared curvature is

\[
C(x_i, y_k) = \frac{1}{2} \left( F(x_{i+1}, y_k) + F(x_{i-1}, y_k) + F(x_i, y_{k+1}) + F(x_i, y_{k-1}) - 4F(x_i, y_k) \right) h^2.
\]

(1)

To minimize \( C \), the partial derivatives of \( C \) with respect to \( F(x_i, y_k) \) must be set to zero. The resulting equations determine a set of relations between neighboring grid point values, one for each point.

If one of the samples does not coincide with a grid point, additional difference equations are used for the grid points at the vertices of the square containing the sample, and the sampling point becomes part of the grid.

The resulting system of equations is then solved iteratively. The method is fast but has the disadvantage of being interpolating rather than approximating.

3 The generalized equivalent source technique

Dampney[3] developed the original equivalent source technique for analyzing gravity data. He showed that a collection of \( N \) point masses \( m_i \),
the equivalent sources, one located directly under each data point. The depth is constant for all sources and has to be determined empirically.

A more generalized algorithm (GEQS), which is also suitable for the 3D case, has recently been developed by Cordell[2]. She defines the set of sources \( \{m_n, (u_n, v_n, w_n)\} \) such that

\[
|f_i - \sum_{n=1}^{N} \frac{n_m}{\sqrt{(x_i - u_n)^2 + (y_i - v_n)^2 + (w_n)^2}}| < \epsilon, \tag{2}
\]

where \( u_n, v_n \) represent the \( x, y \)-coordinates of the source, \( w_n \) its depth and \( \epsilon \) some global error. The functional relationship (2) has the form of a Newtonian potential, and, in case of a gravitational potential, the \( m_n \) are proportional to point masses at \( (u_n, v_n, w_n) \).

The set of sources \( m_n \) is built up iteratively, working each time on the most anomalous data value, i.e. on the sampling point defined by \( |f_{i_n}| = \max(|f_i|) \), where \( f \) has zero mean.

Locating the source below the \( i_m \)-th sampling point and relating the depth of the source to the local data density, expressed by the distance \( d_i \) of the sampling point to its nearest neighbor, one obtains for the coordinates of the source \( (u_m, v_m, w_m) = (x_{i_m}, y_{i_m}, a d_{i_m}) \), where \( a \) is a proportionality factor, which has to be determined empirically. The source is then completely defined by \( m_n = f_{i_n} |w_n| \).

The effect of this source is removed from all the data and the next iteration starts. The algorithm stops if the maximum of the remaining set is smaller than the error \( \epsilon \).

The resulting effect of all the sources is then used to grid the data, by making use of equation (2).

The algorithm works fairly well for potential field data, but the convergence of the iterative determination of the sources is not guaranteed and depends strongly on the choice of the parameter \( a \).

4 Kriging

Kriging is a geostatistical method first mentioned by Krige[7] and developed by Matheron[8].

The idea is to regard all measurements \( f_i \) as a realization of a random process and to analyze the spatial behavior of the corresponding parameters.

The first step is the analysis of the spatial variability expressed by a function called variogram \( \gamma \), which can be calculated from the data according to

\[
\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} (f(p_{1,i}) - f(p_{2,i}))^2, \tag{3}
\]

where \( f(p_{1,i}), f(p_{2,i}) \) are \( N(h) \) pairs of sampling points approximately separated by the distance \( h \).

The experimental variogram is then replaced by a theoretical one, most often by a spherical model with

\[
\gamma(h) = \begin{cases} c[1.5a - 0.5(h/a)^3], & h \leq a \\ c, & h > a \end{cases} \tag{4}
\]

To estimate parameters at locations \( p \) where no measurements are available, one uses the known samples in order to set up a linear estimator, the kriging estimator, of the following type

\[
F(p) = \sum_{i=1}^{N} \lambda_i f(x_i, y_i). \tag{5}
\]

The weights \( \lambda_i \) are determined such that the estimator is unbiased and minimizes the error- or so called kriging-variance. This leads to a linear system of equations, which can be expressed in terms of the variogram under the assumption that the random process is stationary:

\[
\sum_{j=1}^{N} \lambda_{ij} \gamma(p_i - p_j) + \mu = \gamma(p_i - p) \tag{6}
\]

\[
\sum_{j=1}^{N} \lambda_{ij} = 1, \tag{7}
\]

where \( \mu \) is a Lagrange multiplier, arising from the minimization of the variance, and \( i = 1, \ldots, N \). The solution of this system yields the weights and thus an approximation value. In case of large data sets one uses only a small subset of the samples in the neighborhood of the point to be estimated. This splits the problem into subproblems and keeps computational expenses reasonably low.
The biggest advantages of kriging are the fact that the spatial behavior of the approximation can be controlled via the variogram, and that it is possible to incorporate secondary information by some slight modifications of the linear system of equations.

The main disadvantage is the strong influence of the variogram, which has to be fitted interactively and is thus time consuming and depending on the experience of the operator. Furthermore the algorithm is computationally expensive and can only be solved by splitting the problem into smaller subproblems.

5 The ACT method

An extremely fast method for the reconstruction of a bandlimited function from irregular samples has been developed by Feichtinger, Gröchenig and Strohmer [5]. The name ACT results from the combination of the adaptive weights method, a conjugate gradient acceleration and the use of Toeplitz matrices. A corresponding 2D-algorithm has been derived by Strohmer[9].

In detail the following algorithm is used: first of all the available data are interpreted as the scalar-products between the given, but unknown signal $F(p)$ and shifted 2D-sinc-functions.

From the data the so called frame operator $S$ may be formed, which resembles the Shannon sampling formula: for a signal $F$ we have

$$SF(p) = \sum_{i=1}^{N} f(p_i) \text{sinc}(p-p_i).$$  \hspace{1cm} (8)

The sinc-functions are constructed by the characteristic function in the Fourier domain and thus depend on the size of the spectrum.

This leads to a system of linear equations which can be solved numerically by inverting the corresponding system matrix. The approach described above has the big advantage of leading to a simple matrix with block-Toeplitz structure by choosing a suitable trigonometric basis. Furthermore each subblock is of moderate size and also of Toeplitz type. Thus they can be inverted with considerably less computational effort than matrices without special structures. It is not even necessary to build up the entire matrix in the computer memory.

This is important because it easily allows to deal with thousands of data points without splitting the problem in little subproblems.

The ACT-algorithm solves the system iteratively with the superfast conjugate gradient method, which is based on the Fast Fourier Transform and the positive definiteness of the system.

Actually, making use of the idea of adaptive weights one can show that the weighted frame operator $S_w$ of the form

$$S_w F(p) = \sum_{i=1}^{N} f(p_i) w_i \text{sinc}(p-p_i)$$  \hspace{1cm} (9)

has a much better condition number, independently of irregularities in the sampling set, such as clusters. The weight coefficients $w_i$ are chosen adaptively, depending on the geometry of the sampling set.

The main disadvantage of the algorithm is that the resulting reconstruction is periodic, coming from the Fourier approach. Another problem is the size of the spectrum, which has still to be chosen empirically.

6 Synthetic tests

In order to compare the performance of the four methods described above, a synthetic gravitational anomaly, depicted in Figure 1, was calculated. It represents the gravitational acceleration due to ten rectangular boxes of different density and depth. Small, high density objects at shallow depth give rise to the spiky small scale features, whereas big and deep ones are responsible for the overall appearance.
Table 1: Summary of the results. The errors of the reconstruction of the synthetic anomaly shown in Figure 1 relative to the approximation from the sampling sets as depicted in Figure 2 with different amount of noise are listed. The abbreviations MINC, GEQS, KRIG and ACT stand for the four methods described in this paper.

<table>
<thead>
<tr>
<th>noise</th>
<th>uniform sampling set</th>
<th>clustered sampling set</th>
<th>line type sampling set</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MINC</td>
<td>GEQS</td>
<td>KRING</td>
</tr>
<tr>
<td>no</td>
<td>7.2</td>
<td>7.4</td>
<td>7.1</td>
</tr>
<tr>
<td>2%</td>
<td>7.4</td>
<td>7.6</td>
<td>7.5</td>
</tr>
<tr>
<td>5%</td>
<td>7.8</td>
<td>8.3</td>
<td>7.6</td>
</tr>
<tr>
<td>10%</td>
<td>10.3</td>
<td>10.5</td>
<td>9.2</td>
</tr>
<tr>
<td>20%</td>
<td>16.8</td>
<td>15.9</td>
<td>11.1</td>
</tr>
</tbody>
</table>

This anomaly was then sampled according to the three main types of sampling sets that occur in the geophysical practice: the random or uniform density set, the clustered set and the line type or profile set. The sampling sets together with a contour plot of the anomaly are shown in Figure 2.

The uniform density or random set, is characterized by irregular geometries but an approximately constant number of samples per unit area. This setup is the second best after the regular case and does not occur very often in practice.

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As real world measurements have always a certain amount of error, additive white noise with a signal to noise ratio of 2%, 5%, 10%, and 20% respectively, has been added to the sampling sets.

All four methods were then used to reconstruct the anomaly in the original region. For the minimum curvature method (MINC) the computer program developed by Webring[10] was used. The approximation by the generalized equivalent source technique (GEQS) and the ACT algorithms were performed with MATLAB implementations by the author and Strohmer[9] respectively. The calculation of the variogram and kriging (KRIG) has been done with computer programs described by Deutsch and Journel[4].

To measure the quality of the approximations, the relative deviation of the reconstructed anomaly from the original one has been calculated in the $L^2$-norm.

The results are summarized in Table 1. As a graphical example the approximations from the clustered sampling sets with a signal to noise ratio of 5% are shown in Figure 4.

7 A real world example

A small scale gravity survey in the eastern part of Austria has been chosen as a real world example. The sampling geometry is depicted in Figure 3 and consists of 595 distinct sampling points. It is obvious that the set is an example of the clustered sampling set.

The sampling values are preprocessed measurements of the gravitational acceleration, representing
8 Discussion

From the results of the synthetic tests and the grid-ded real world example one can draw the following conclusions:

The quality of a reconstruction depends on two factors, one being the error arising from the sampling geometry, the other the error of the approximation method.

The uniform sampling set has the best coverage of the anomaly and allows a better reconstruction than the clustered and the line type sampling geometry, which shows the biggest errors, independent from the noise and method.

In case of uniform sampling density all methods exhibit a similar approximation quality and robustness to noise.

The minimum curvature method and the generalized equivalent source technique are more sensible to data anisotropies and noise than kriging and the ACT algorithm. The reasons are the interpolating property of MINC and the locality of the Newton potential of point sources of GEQS. This can also be seen in the noisy appearance of the surfaces in the upper panels of Figure 4.

The kriging algorithm shows the best performance and robustness to clustering and noise, as both are reflected in the variogram and are taken into consideration during the modelling stage of the method. It is the best choice for small data sets and nonautomatic implementations, because of its extremely high computational costs and interactive character.

The ACT method shows the smoothest overall appearance and a relatively high robustness to clustering, as it depends only on the average sampling density. With an increasing amount of noise, the fre-
Figure 5: Gridded real world sampling set. The upper panels show the reconstructions by the minimum curvature method and the generalized equivalent source technique, the lower panels of the kriging and the ACT algorithm respectively. Gravity is given in mGal. The sampling geometry is depicted in Figure 3.

frequencies still containing information become smaller and the algorithm gives a very good reconstruction of the low frequency part of the anomaly. This is especially useful for potential field data, as fields away from sources are smooth and can be considered as bandlimited. The periodicity of the method causes problems at the boundaries of less concentrated data sets. This is only of little practical relevance because the most interesting parts of a survey are in general in the center of the region of interest.

The ACT algorithm combines thus the robustness and smoothness which are characteristic for kriging with an high computational efficiency, and is therefore of strong practical relevance.

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References