Effects of low-pass filtering on inversion of airborne gravity gradient data

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EFFECTS OF LOW-PASS FILTERING ON INVERSION OF
AIRBORNE GRAVITY GRADIENT DATA

by

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Golden, Colorado

Date __May 15, 2006_______

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ABSTRACT

Airborne gravity and gravity gradiometry data used in petroleum and mining exploration are strongly affected by high-frequency noise originating from the movement of platforms. Use of low-pass filtering is necessary during data acquisition to eliminate the high-frequency noise. Such filtering, however, removes useful signal along with noise in the same frequency range. As a result, the anomalies due to geology appear wider and their amplitudes smaller. Without taking this effect into consideration, such data can lead us to wrong interpretation. For example, interpreted source bodies might appear deeper and wider than they are.

In this thesis, I first quantify the errors to be expected from directly inverting filtered data using a 2D parametric model. I then study the incorporation of the filter that is used in data acquisition phase into the forward modeling and sensitivity calculations as part of the inversion. I demonstrate that the errors can be effectively reduced and reliable results can be obtained. The same approach of incorporating filtering into the inversion is applicable to 2D and 3D problems.

The data misfit is an important component in any inversion formulated as an underdetermined problem. For instance, the optimal regularization level in a Tikhonov
inversion is determined by fitting the observations to the degree consistent with the characteristics of noise in the data. Because the noise in filtered data is correlated, I investigate the choice of data misfit function in the presence of such noise. I have found that the covariance matrix of filtered noise is singular when the filter length is greater than the data spacing. Consequently, the commonly suggested definition of data misfit based on the inverse of covariance matrix is invalid. I choose to use the traditional definition based on variances alone, and determine the expectation of such a misfit function by numerical simulation. The result is directly used to determine the proper regularization level in 3D inversion of gravity gradient data.

Combining the approach developed in the 2D parametric study and the understanding of data misfit in the presence of correlated noise resulting from low-pass filtering, I formulate a 3D inversion algorithm that accounts for the effect of filtering. The algorithm is tested on 3D synthetic and field data sets. The test results show that the new inversion algorithm clearly improves resolution of recovered source geometry in both lateral and vertical directions and produces interpretations more representative of true sources.
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Gravity and gravity gradiometry data used in petroleum and mineral exploration are commonly acquired from moving platforms (Lee, 2001; Pawlowski, 1998). Marine gravity and airborne gravity surveys are typical examples. More recently, gravity gradiometry data are acquired from marine and airborne platforms (Nabighian and Asten, 2002; Dransfield et al, 2005). Both gravity and gravity gradiometry data are highly sensitive to movement, consequently, noise associated with moving platforms severely contaminates geological signal. The magnitude of noise is often greater than wanted signal by three to four orders of magnitude in the high-frequency band, thus noise often overwhelms the signal in high frequency range (Childers et al, 1999). To obtain usable data and reduce the noise level from these surveys, acquisition systems invariably have built-in lower-pass filters to suppress the noise (Dransfield and Lee, 2004; Lane, 2004). These low-pass filters are often designed to operate on the time series of instrument output and have a given filter length in time that translates to a spatial low-pass filter of certain length. This smoothing process removes the high-frequency noise from the acquisition environment. This procedure produces a lower RMS error of data but reduces the spatial resolution. For this reason, the data accuracy is often quoted as RMS over a certain spatial wavelength (Dransfield and Lee, 2004).
This approach to noise suppression is inherently a smoothing process that wipes out a certain high-frequency band of measured data. While the filtering achieves the desired effect of noise suppression, it also removes high-frequency content from the signal at the same time. The loss of high-frequency content of signal causes the measured anomalies to become wider and their amplitudes to decrease. Figure 1.1 illustrates the effect using a synthetic data set. The jagged solid line shows a set of vertical gravity gradient data produced by a 2D dipping dyke. We have added pseudo-random Gaussian noise for the purpose of illustration. The two smoother curves are the result of applying a 7th order Butterworth filter with filtering length of 300 m and 600 m respectively. The broadening of the anomaly width and decrease of anomaly amplitude are apparent. It is clear that interpreting such filtered data without taking into consideration the filtering effect will lead to erroneous geologic interpretation.

Different systems use different filters, and some apply the low-pass filter during the acquisition in real time while others may apply additional filter during the post acquisition processing stage. For example, Bell Geospace has typically applied a cosine filter with a filter length of 1.25 km to their marine gradiometry data in their post-acquisition processing to remove high-frequency noise. Both Bell Geospace and BHPBilliton apply real-time filtering to the data from their airborne system (Dransfield et al., 2001; Murphy, 2004). Although the precise nature of these filters are not disclosed, recent work focusing on understanding the filter effect by comparing ground and airborne
data has suggested that the remaining frequency content of airborne gravity gradiometry data are consistent with the output of a Butterworth filter with varying filter lengths (Lane, 2004). Furthermore, airborne gravity data are subject to much heavier filtering because of the systems’ sensitivity to aircraft acceleration.

![Figure 1.1 Effect of low-pass filtering of vertical gravity gradient data](image)

Figure 1.1 Effect of low-pass filtering of vertical gravity gradient data. Jagged solid line is the noisy data produced by a 2D body. Smooth lines (both dotted and dashed) are the result of applying a 7th order Butterworth filter with filter length of 300 m and 600 m, respectively. Filtering reduces the original signal amplitude and makes it wider.

The measured data has high frequency noise with great power. The power spectrum shows higher power density in high frequency range, which may be larger than
that of signal in the low-frequency range. The low pass filtering can remove most banded power in high frequency range so that the low frequency area can be used for further interpretation.

Current work in published literature on inversion of gravity gradient data tends to neglect those unwanted filtering effect. Limited work is available to tackle this issue in the data processing stage. For example, Childers et al. (1999) attempt to design a special filter to minimize the loss of signal. Lyrio et al. (2004) try to separate noise from signal in the high-frequency range instead of wiping out all contents. This is achieved through the use of spatially adaptive wavelet filtering. In airborne surveys, however, the filtering is pre-chosen by the survey system, and only filtered data is available to clients and interpreter because of the proprietary nature of these acquisition systems.

Despite the possible negative effects caused by the low pass filtering on data, we can often find the inversion of various geophysical methods without consideration of the low pass filtering (Li, 2001b; Portmiaguine and Zhadanov, 2000). The problem with filtering has been recognized in other fields of geophysics. Foss (2003) showed that the filtering, which is same to smoothing, in magnetic data inversion can lead to the misinterpretation of the assumed geological target. René et al. (2004) has pointed out that filtering data can reduce the standard deviation of noise so that inversion result is improved when inverting magnetic data arising from UXO discrimination.
Thus, there is a need to answer the following two questions: (1) what is the ramification of heavily low-pass filtered gravity and gravity gradiometry data? and (2) how can we effectively interpret such filtered data without adversely affected by the filtering process? Answering these two questions is the focus of this thesis. I first consider the general problem of data filtering and its effect on quantitative data interpretation by inversion. This is accomplished by using a simple parametric model and least-square parameter estimation. The result clearly shows that direct inversion of low-pass filtered data will produce causative bodies that are deeper and wider than the true source. This result is to be expected. I recognize that inverting filtered data directly by neglecting the low-pass filter is equivalent to using a forward mapping operator inconsistent with the acquisition system. As a result, the numerically calculated field response and field data are two different quantities. To overcome this problem, I pursue an approach similar to that by René et al. (2004) and incorporate the low-pass filter into the forward operator during the inversion so that both predicted data and sensitivity calculation are consistent with the data being inverted. Incorporating the low-pass filter in this manner in the inversion dramatically reduces the errors in the recovered source parameters and demonstrates the validity of such an approach.

I then extend the work to generalized inversion for distributed density contrast and develop a practical algorithm suitable for application in large-scale problems typically
arising in resource exploration problems. The results of the density inversion by incorporating the low-pass filtering show improvement consistent with that of parametric inversion; this new algorithm improves the resolution of the source both in the lateral and vertical direction, and identifies small objects that are not shown in the inversion with the filter.

Given the application of low-pass filtering to data, the associated errors are highly correlated as expected. However, the covariance matrix of data error turns out to be singular for any filter with a length greater than the data spacing. Consequently, the accepted definition of data misfit in the presence of correlated noise (Tarantola, 1987; Scales and Smith, 1996) is no longer valid. I investigate the nature of the error covariance matrices in such situations and propose an alternative data misfit measure that is identical to the most commonly used chi-squared measure. This enables us to carry out inversion in the presence of correlated noise resulted from low-pass filtering. In addition, this research further supports the use of such a simple measure in the presence of correlated noise.

There are six chapters in my thesis. In chapter 1, this chapter, I provide an introduction to the problem of interpreting low-pass filtered gravity gradient data, summarize the current state of practice, outline the major research accomplishments resulted from my work on this problem.
Chapter 2 first presents the background of gravity gradient method, studies the errors in the inverted source parameters that result from low-pass filtering data, and examine the effectiveness of incorporating the same low-pass filter into the inversion. For generality, I use a generic density model and lower-pass filter. I use simple 2D parametric inversion algorithm to demonstrate the effect of including filter in inversion, and examine the magnitude of errors of different geometries of initial source model with various widths and depths.

Chapter 3 studies the nature of error covariance matrices for low-pass filtered data sets. I demonstrate that for any low-pass filter whose filter length is greater than the data spacing, the corresponding covariance matrix is singular. Consequently, the commonly accepted definition of data misfit based on the inverse of covariance matrix is no longer valid. I adopt the traditional chi-squared misfit as an alternative measure for use in the presence of correlated noise. Numerical simulations indicate that the expectation of such a misfit function is equal to the number of data in the low-pass filtered data set. This is a surprising result but it provides a practical misfit measure for filtered data. It also has general implications regarding the validity of using chi-squared misfit in other cases with correlated noise. This work lays the foundation for the density inversion of filtered gravity gradiometry data in Chapter 4.
Chapter 4 applies the results obtained in the two preceding chapters to more realistic gravity gradient inverse problem in 3D. In this chapter I conduct density inversion of a 3D subsurface body. I first briefly review currently used inversion algorithm for gravity gradient data, GG3D (Li, 2001a; GG3D manual), and examine the deficiencies in applying such an algorithm directly to the filtered data. I then apply the same approach used in the 2D case in Chapter 2 and incorporate the low-pass filter into the 3D forward modeling and calculation of the sensitivity matrix. To test the algorithm, I use two synthetic models. The first is a dipping dyke, and the second consists of two vertical prisms. I also investigate the use of both discrepancy principle and L-curve criterion (Hansen, 1992) in the choice of the Tikhonov regularization parameter (Tikhonov and Arsenin, 1974). The density inversion using regularization parameters selected by these two criteria produce comparable results. To evaluate the results of inversions with and without incorporating the low-pass filter, I rely on both qualitative examination of recovered density models and mass compaction indices (MCI) comparison that provides a quantitative measure of the compactness of the recovered density. The MCI of the inversion using new algorithm has much smaller value because the density distribution of recovered body in the 3D model is compact. This means that the new algorithm reduces the adverse effect of low pass filtering during the inversion process.
Chapter 5 deals with a real field data set. I use a field data set from Broken Hill, New South Wales, Australia. I apply the preceding approach in 3D density inversion of field data and control the inversion level using the number of data points as an optimal data misfit. The results show that the proposed algorithm clearly improves the resolving power in both lateral and vertical directions by reducing the low-pass filtering effect in the inversion process. The result is consistent with that of the synthetic 2D and 3D cases.

In Chapter 6, I conclude the thesis by summarizing the research accomplishments and discussing the resulting new algorithm in gravity gradient data inversion. I also discuss further recommendations and future work.
CHAPTER 2. EFFECT OF LOW-PASS FILTERING: 2D CASE

In this chapter, I examine the general problem of data filtering and its adverse effect on quantitative data interpretation by using a synthetic 2D example. For generality, I choose to use a generic model and low-pass filter instead of the parameters of a particular acquisition system. I first investigate the effect of such low-pass filtering by examining the errors which would be produced when the data are inverted directly as if no filtering had occurred. The resultant geometry without incorporating the same filter during inversion is wider and deeper than its real geometry because of the low pass filtering effect. I then develop a general approach for ameliorating the adverse filtering effect by including the filter in the inversion as an integral part of forward modeling. Comparison of results shows that one must take into account the low-pass filtering in the inversion.

2.1 Synthetic Model and Forward Modeling

For the study, I use a 2D dipping dyke model and simulate vertical gravity gradient data, $T_{zz}$. The 2D model cross-section and the simulated vertical gradient are shown in Figure 2.1. There are six model parameters that characterize the model, including the dip angle, the depth to the top, the width of dyke, its depth extent, the horizontal coordinate...
of the middle point of the top facet of the dyke, and the density contrast of the dyke. They are denoted respectively as \((\theta, h, b, t, \Delta \rho)\). For simplicity, only four parameters \((\theta, h, b, t)\) will be considered in inversion. The middle point of the top facet \(x_0\) and the density \(\Delta \rho\) are assumed to be known. Figure 2.1a shows the vertical gravity gradient data produced by the dyke model. The data have been contaminated by uncorrelated Gaussian random noise for subsequent studies.

In reality, the noise originating from the motion of platform is usually concentrated in the high-frequency band and the noise level can be three to five orders of magnitude higher than the signal at high frequencies. Such noise severely contaminates geologic signals and must be filtered out during acquisition. In the low-frequency range, the noise is relatively small. Low-pass filters used in acquisition do not in general affect either signal or noise at these low frequencies. For this reason, I have chosen to add uncorrelated Gaussian noise instead of observed noise in my study. The standard deviation of added noise is chosen to be 5% of maximum amplitude of signal. Applying low-pass filtering then primarily affects the high-frequency portion of the signal and leaves a realistic level of low-frequency noise in the data.

The true model geometry is displayed in the bottom panel Figure 2.1b. The vertical gravity gradient, \(T_z\), for given model is defined as (Telford et al., 1990),
\[ T_{zz} = 2\gamma\rho \sin \theta \{ \cos \theta \ln(r_2 r_3 / r_1 r_4) - \sin \theta (\phi_1 - \phi_2 - \phi_3 + \phi_4) \} \] (2.1)

where \( \gamma \) is the gravitational constant, \( r_i \) and \( \phi_i \) are the distance and angle between measuring point and the i’th apex of the source geometry respectively.

Figure 2.1 Profile of vertical gravity gradient for a 2D dyke model. There are six model parameters; \( h \) is the depth to top facet of dyke, \( \theta \) is dip in radian, \( b \) is the width of dyke, \( t \) is the depth extent, \( \Delta \rho \) is the density contrast, \( x_o \) is the middle point of top facet.
2.2 Parametric Inversion

Let the vertical gravity gradient data be given by,

\[
\tilde{d} = G_i(\bar{m}), \quad i = 1, \ldots, N,
\]  

(2.2)

where \( G \) is the forward operator defined in eq.(2.2) and \( \bar{m} = (\theta, h, b, t) \) is a vector of model parameters. Denoting the collection of data \( T_{zz} \) as \( d_i = (T_{zz1}, \ldots, T_{zzN})^T \), the forward modeling can be written compactly as

\[
\tilde{d} = G(\bar{m}).
\]

The purpose of inversion is to recover the unknown model parameters \( \bar{m} \) from measured vertical gravity gradient data so that the subsurface target can be characterized. In this problem, the number of data is greater than the number of unknown model parameters. Therefore, this is an over-determined problem. Thus I take the approach of least squares and minimize the L2-norm of the data misfit defined by

\[
\phi_d = \| G(\bar{m}) - \tilde{d}\text{\small{obs}} \|^2,
\]  

(2.3)
where $G(\tilde{m})$ gives the predicted data, and $\tilde{d}^{\text{obs}}$ is the observed data.

Because vertical gravity gradient data depend nonlinearly on source geometry, eq.(2.3) is a nonlinear least-squares problem. It is solved iteratively using the Gauss-Newton method. This approach starts from an initial model and successively updates the model by solving for a model perturbation at each iteration until the data misfit is minimized. Assuming we have a model $\tilde{m}^{(n)}$ at the $n^{th}$ iteration, I perform a Taylor series expansion of the forward operator and neglect higher order terms:

$$\tilde{d} \approx \tilde{d}^{(n)} + J \delta \tilde{m}, \quad \text{(2.4)}$$

where $\tilde{d}^{(n)} = G(\tilde{m}^{(n)})$ is the predicted data from the model at the $n^{th}$ iteration, $J$ is the sensitivity matrix, and $\delta \tilde{m}$ is the sought model perturbation. Substituting eq.(2.4) into eq.(2.3) and differentiating with respect to model perturbation yields,

$$\delta \tilde{m} = (J^T J)^{-1} J^T \delta \tilde{d}, \quad \text{(2.5)}$$
where $\delta \tilde{l} = \tilde{d}^{\text{obs}} - \tilde{d}^{(n)}$ is the data difference. The elements of the sensitivity matrix $J$ quantify the influence of a change in a model parameter on the predicted data and are defined as the partial derivative of a datum $d_i$ with respect to model parameter $m_j$,

$$ J_{ij} = \frac{\partial d_i}{\partial m_j} = \frac{\partial G_i(m)}{\partial m_j}. \quad (2.6) $$

Solving eq.(2.5) yields the model perturbation, and this is used to update the current model to obtain a new model,

$$ \tilde{m}^{(n+1)} = \tilde{m}^{(n)} + \alpha \delta \tilde{m}, \quad (2.7) $$

where $\alpha$ is a step length that is chosen to ensure the reduction of data misfit at each iteration. The step length is typically generated through a line search algorithm.

It is a common practice to include a diagonal term into eq.(2.5) to stabilize the solution. The corresponding equation then becomes

$$ \delta \tilde{m} = (J^T J + \mu I)^{-1} \delta \tilde{l}, \quad (2.8) $$
where $\mu$ is a damping parameter similar to the regularization parameter in distributed parameter inversion, and $I$ is an identity matrix. This is the well-known Marquardt-Levenburg method.

To further stabilize the solution, we also impose bound constraints to limit the unknown parameters to an interval that is geologically reasonable. Such constraints can be easily imposed either by nonnegative least squares (NNLS) (Lawson and Hanson, 1974) or the interior-point method (Wright, 1997).

To see the validity of preceding inversion, I invert unfiltered data shown in Figure 2.1. The inversion is set to find the four primary parameters defining the geometry of the source. The result is shown in Figure 2.2. The red jagged line in the upper panel represents the observed data with random noise, which is 5% of maximum amplitude of the anomaly. The red parallelogram in the lower panel represents a true 2D model, and blue dotted parallelogram is the recovered source geometry. The blue dotted line in the upper panel is the predicted data from the recovered model.

The recovered source geometry is a good representation of the true source body. Especially the depth and width of 2D dyke are well defined. The predicted data also matches the signal well except for a small fluctuation in the high-frequency range.
Figure 2.2 Results obtained from inverting unfiltered noisy data (red jagged line). The recovered source geometry matches the geometry of the causative body (bottom panel). The gradient response (blue dotted line) of recovered causative body follows closely the observed response used as input for the inversion process.
2.3 Error Assessment

With the inversion algorithm, I now examine the errors produced by interpreting low-pass filtered data. I first simulate a set of filtered vertical gravity gradient data from a dipping dyke, and then apply the above inversion by treating the data as if they were a geological response without any low-pass filtering. This is the current practice in industry (e.g., Christensen et al., 2001, and Zhdanov et al., 2004). The top panel in Figure 2.3 shows the original noisy data (black solid line), filtered data (red dotted line), and the predicted data (blue dashed line) from the recovered model. I simulate the low-pass filter with a 7th order Butterworth filter having a filter length of 300 m (Williams, 1981). Note that the low-pass filtering has suppressed the noise and produced a much smoother data profile, whereas the anomaly has become wider and smaller in magnitude.

As expected, the recovered model in the bottom panel is located deeper from the surface and wider than the true model, whereas the depth extent is decreased. This model reproduces the general features of the filtered data well, but there are also some long wavelength discrepancies. For example, the side lobes do not match. This reflects the commonly understood fact that filtered data do not usually correspond to geologically plausible sources. In this case, the filtered response can no longer be reproduced by that of a simple 2D dyke model.
Figure 2.3 Direct inversion of low-pass filtered data. The recovered causative body (blue dashed parallel gram) is deeper and wider than the true body (red dotted parallel gram). The vertical gravity gradient response (blue dashed line) of recovered causative body in upper panel fit the filtered data (red dotted line), but shows some discrepancy in the high frequency range.
To further examine the effect of data filtering in inversion, I invert filtered data from a variety of source bodies with different depths and widths, and evaluate the errors in the inverted parameters. The relative errors are calculated by comparing the recovered model parameters with their true values,

\[ \varepsilon(\%) = \left( \frac{m_{\text{true}} - m_{\text{rec}}}{m_{\text{true}}} \right) \times 100, \]  

where \( m_{\text{true}} \) and \( m_{\text{rec}} \) are respectively the true and recovered model parameters.

I investigate the error by varying two model parameters, namely, the depth and the width of 2D dyke. These two parameters strongly affect the frequency content in the surface response. Depth to the top facet of the dyke ranges from 50 to 250 m in 10-m increments, and the width of dyke ranges from 100 to 300 m in 10-m increments. The errors are displayed as functions of depth and width.

First, I use filtered clean data, which has no random noise. Figure 2.4 shows the error maps as functions of depth to the top and the width of the 2D dyke; four panels represent the percent error of recovered dip, depth to the top, width, and depth extent, respectively. The huge negative errors arise in narrower width and shallower depth. The
Figure 2.4 Error surfaces for model parameters recovered from filtered, noise-free data. Neglecting the filtering in the inversion leads us to large errors in the results. Error increases with decreasing depth and width of the true source. Negative errors indicate overestimation of the parameter.
negative errors indicate an overestimation; the recovered model parameters are greater than the corresponding true values. Thus, the interpreted source geometry is wider and deeper. The recovered depth extent shows positive errors, which indicate an underestimation. It is clear that data filtering leads to an overestimation of the depth and width of the causative body and underestimation of the depth extent. This result is consistent with the expectation of filtering effects shown in Figure 2.3 because low-pass filtering widens the signal and decreases its amplitude.

There is a trend that the error generally increases as the source depth and width decrease. This is also consistent with the nature of the low-pass filtering: shallower and narrower bodies have relatively more high-frequency content in their field, therefore low-pass filtering affects these data more severely.

I then simulate the realistic scenario of data being contaminated by noise prior to low-pass filtering. For each model with a given dip, depth, width, and depth extent, I generate 20 sets of data by adding 20 different realizations of random noise to the accurate response, and then perform 20 separate inversions. A mean error is then calculated from the 20 sets of results to generate a statistically reliable estimate. Figure 2.5 displays error maps generated from inverting data with random noise. These maps have similar trend to previous error maps in Figure 2.4 except small fluctuation of errors because of the random nature of the contaminating noise.
Figure 2.5 Error surfaces generated from inverting each filtered data set with 20 different realizations of noise. The surface trends mimic those in the case of noise-free data in Figure 2.4.
Data misfit of parametric inversion is important for understanding the inversion itself. In parametric inversion, the better solution to inversion is found when achieving smaller data misfit. I calculate data misfit using eq.(2.3). The mean of the data misfit of 20 parametric inversions of filtered noisy data is shown in Figure 2.6.

![Figure 2.6](image_url)

**Figure 2.6** The mean of data misfit from inverting each data set with 20 different realizations of noise. X-axis and Y-axis represent the depths to and the widths of the dipping dyke shown in Figure 2.1.

The data misfit has a maximum, around $75 \text{ Eötvös}^2$, when the true model has the smallest depth. This value is very high compared to its signal’s amplitude shown in
Figure 2.3. It decreases in direction of increasing depth and decreasing width, which is located at the right bottom in Figure 2.6.

Both errors and data misfit distribution map as functions of the depth and width of the subsurface body show strong correspondence. High values of negative error (Figure 2.5) correspond to large data misfit (Figure 2.6) in the shallow depth ranges. For the width of the source, we can see different results; the errors in the narrower ranges are larger since the low-pass filter has greater influence in high frequency range, but the data misfit shows little correlation with the width of the source.

It is clear that interpreting low-pass filtered data without considering the filter effect can lead to deeper and wider targets and erroneous source geometry. This is a limitation of the currently used method in practice, and an impetus to carrying out this research to understand the effect. The objective is, of course, to develop a method for alleviating this adverse effect. I now proceed to developing such an approach.

2.4 Incorporating Filtering Into Inversion

It is clear that ignoring the effects of the low-pass filtering can lead to large errors in the recovered model parameters. The errors increase for shallower and narrower
sources, because more high-frequency signal is lost due to filtering. Methods are needed to alleviate the errors and improve inversion results.

The errors in the direct inversion of low-pass filtered data can be considered an artifact from the loss of high-frequency information. On the other hand, these errors can also be viewed as a result of incorrect forward modeling. Since a filter has been applied to the data, the forward modeling should include not only the physical relationship between the data and sources, but also the effects of the filtering. Accordingly, practicing geophysicists have often applied filtering to the response calculated during manual forward modeling before comparing these data with field data. Jacobsen (1988) succinctly stated this as Algerlin’s Principle: “When fitting a model to processed data, one must process the model response likewise before the degree of fit can be judged.” Logically, it follows that the forward modeling and sensitivity calculation in an inversion should also incorporate the low-pass filtering. René et al. (2004) studied this approach when inverting magnetic data arising from UXO discrimination. I now proceed to examine such an algorithm in the inversion of filtered gravity gradient data.

The basic algorithm has the same structure as that presented in the preceding section. The only modification is the inclusion of low-pass filtering to mimic the effect of the filter applied to the measured data. We denote the direct forward modeling as
\( \tilde{d} = G(m) \). Let the low-pass filter be \( F[\cdot] \). The correct forward modeling incorporating the filter is then given by,

\[
\tilde{d}^F = F[G(m)], \tag{2.10}
\]

where \( \tilde{d}_i^F \) are the filtered calculated data and the corresponding data misfit is defined by

\[
\phi_d = \| F[G(m)] - \tilde{d}^{\text{obs}} \|^2. \tag{2.11}
\]

The sensitivity matrix is computed using the same forward modeling with the low-pass filter applied,

\[
J_F = \nabla_m F[G(m)]. \tag{2.12}
\]

I use eq.(2.11) and (2.12) in the inversion and the rest of the inversion algorithm proceeds in the same manner as before,

\[
\delta m = (J_T^F J_F)^{-1} \delta \tilde{d}
\]

\[
m^{(n+1)} = m^{(n)} + \alpha \delta m,
\]
As a demonstration, I apply the inversion incorporating filtering to the filtered data shown in Figure 2.3. The true model parameters are given as the starting model parameters in this iterative process. The result is displayed in Figure 2.7. Now, the source body is well recovered and the predicted data reproduce the filtered observation well. It is interesting to note that we are now able to match the side lobes of the filtered data very well. This is in sharp contrast to the result shown in Figure 2.3. Compared to Figure 2.3, the effectiveness of, and need for, incorporating the same low-pass filter during data acquisition and post-processing into the inversion is clear.

2.5 Error Assessment with Low-Pass Filtering

To investigate how including filtering in the inversion can improve the results, I repeat inversions for data sets from a wide range of source parameters in the same way as the Section 2.3. Figure 2.8 shows the result when noise-free data are used. Now, the errors in recovered parameter from filtered clean data show flat distributions around zero. The recovered models match their corresponding true models well.

Next, I evaluate the error using the noise-contaminated data and again follow the previous process by performing 20 inversions with different noise realizations for each model. The new error maps are shown in Figure 2.9. We observe that the errors now have
a significantly different distribution; they are much smaller than those produced by
inversion without incorporating filtering (Figure 2.5). The magnitudes of errors are
generally limited to less than 10%. The errors are also symmetrically distributed around
zero, as expected from results of a well-formulated inversion. Further, the errors for
different depths and widths do not show significant trends. Overall, the results
demonstrate that incorporating filtering into the inversion has largely eliminated the
errors caused by inconsistency in the data and forward modeling.

For data misfit of parametric inversion including filtering, I calculate data misfit
using eq.(2.11). The result is shown in Figure 2.10. Compared to Figure 2.6, the data
misfit shows the same trend in varying depths and widths. It decreases with increasing
depth and decreasing width. But the amplitude of data misfit is reduced as small as one
third of the data misfit without filtering in inversion. This indicates that incorporating
same filter as data acquisition ensures the consistency between numerical modeling and
field data acquisition. As a result, we can achieve better data misfit and produce better
inverse solutions.
Figure 2.7 Inversion of low-pass filtered data by including the filter in the forward modeling and the sensitivity calculation. The predicted data fit filtered data well. The recovered causative body (blue dashed parallelogram) is a good representation of the true body (red dotted parallelogram). The side lobes are well recovered. Compare to the results in Figure 2.3.
Figure 2.8. Error surfaces for accurate (noise-free) data when inversion includes the low-pass filtering used to smooth data. The errors are now negligible across the board. These results can be compared with those shown in Figure 2.4.
Figure 2.9. Error surfaces obtained from inverting 20 realizations of noisy data when the low-pass filtering is incorporated in the inversion. Compared with the surfaces in Figure 2.5, the errors in these inversions are much smaller in magnitude, distributed symmetrically around zero and do not show strong trends as a function of source depth and width.
Figure 2.10. Mean of data misfit from inverting each data set with 20 different realizations of noise.
2.6 Discussion

In this chapter, I have examined the filtering effects of noisy vertical gravity gradient data. A low-pass filtering is used to suppress unwanted high-frequency noise during acquisition, but it may lead to incorrect interpretation. Inverting such data without considering this filtering effect can produce geologic targets that are wider and deeper than those in reality. The corresponding target geometry can also be erroneous. Such errors occur because low-pass filtering decreases the amplitude of a signal and increases its width.

First, I examine the errors produced from inversion of gravity gradiometry data that have been low-pass filtered as if they were unfiltered data. This process is the currently accepted practice in industry. The inversion of filtered data without taking into account the filtering effect shows unacceptably large errors in both depth and width of the source. The errors increase with decreasing depth and width of the true source since their responses have relatively more high-frequency content that are more severely affected by the low-pass filtering.

I examine a new parametric inversion that incorporates the same filter used in data acquisition phase into the inversion process. By doing so, the predicted data and sensitivity matrix for inversion are calculated after applying low-pass filtering to the
forward modeling operator. Thus, the consistency between modeling and data acquisition is ensured. The results of new inversion clearly show improved recovery of model geometry. Thus, the adverse effect of low-pass filtering data is alleviated to a large extent.
CHAPTER 3. DATA MISFIT IN THE PRESENCE OF CORRELATED NOISE

Interpretation of gravity gradiometry data in practice often requires inversion in three dimensions. One commonly used approach is the 3D density inversion using the formalism of Tikhonov regularization. Successful application of this approach relies on the ability to misfit the observed gradiometry data to an expected level determined by the data errors. In this chapter, I examine the proper regularization of 3D inversion in order to apply the same methodology developed in the preceding chapter to 3D inversion. Presently, most inversion algorithms determine the data misfit by assuming that the noise is uncorrelated.

In this research, however, I am dealing with correlated noise so the data misfit based on correlated noise is required. This is because the low-pass filtering applied to the data in the acquisition stage causes the noise in the data to be highly correlated. To my surprise, the standard definition presented in existing literature is not valid. I therefore address this issue in this chapter.

In practice, measurements always include errors and noises. Because the observed data are contaminated, the predicted data that are generated by a forward modeling in inversion should not match observed data exactly. A proper difference between predicted
data and observed data, which might be the optimal data misfit, can be determined based on the known standard deviation of field data if the data errors are uncorrelated.

The data misfit of uncorrelated noise is well understood and used in practice. We can define the data misfit, \( \phi_d \), by the following equation,

\[
\phi_d = \sum_{i=1}^{N} \left( \frac{d_i^{\text{pre}} - d_i^{\text{obs}}}{\sigma_i} \right)^2,
\]

(3.1)

where \( d_i^{\text{pre}} \) is the predicted data, and \( d_i^{\text{obs}} \) is the observed data, and \( \sigma_i \) is the standard deviation at the i’th observation. If the observed data has Gaussian noise, the mean of the quantity inside the parenthesis in eq. (3.1) becomes unity, therefore the expected value of the data misfit, \( \phi_d \), is the same as the number of data, \( N \). Equation (3.1) can be written in matrix form as,

\[
\phi_d = (\tilde{d}^{\text{pre}} - \tilde{d}^{\text{obs}})^T W_d^T W_d (\tilde{d}^{\text{pre}} - \tilde{d}^{\text{obs}}),
\]

(3.2)

where \( W_d \) is the N by N data weighting matrix and rectangular matrix \( W_d^T W_d \) has only non-zero diagonal terms,
\[ W_d^T W_d = \begin{bmatrix}
\frac{1}{\sigma_i^2} & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & \frac{1}{\sigma_N^2}
\end{bmatrix}, \quad (3.3) \]

which is the inverse of the covariance matrix of the data noise,

\[ C_d = \begin{bmatrix}
\sigma_i^2 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & \sigma_N^2
\end{bmatrix}. \quad (3.4) \]

The covariance matrix in eq.(3.4) is clearly invertible since it is a diagonal matrix. Thus the data weighting matrix can also be equally defined by the inverse of the noise covariance matrix when the noise are uncorrelated,

\[ W_d^T W_d = C_d^{-1}. \quad (3.5) \]

Eq.(3.2) and eq.(3.5) enable us to calculate the optimal data misfit from the covariance matrix when the noise is uncorrelated. This optimal data misfit is used then to determine the level of regularization during the inversion (Menke, 1984).
In my current work, the noise is highly correlated since a low-pass filter was applied to the data in the acquisition stage and the above simple definition of data weighting matrix may not be valid anymore. It is then logical to adopt a misfit definition consistent with the nature of the correlated noise.

When the data noise is correlated, the corresponding covariance matrix is no longer diagonal and off diagonal elements that measure the correlation among errors in different data are non-zero. The covariance matrix of the correlated data is

\[
C_d = \begin{bmatrix}
\sigma_{11}^2 & \cdots & \sigma_{1y}^2 \\
\vdots & \ddots & \vdots \\
\sigma_{y1}^2 & \cdots & \sigma_{yy}^2 \\
\sigma_{y1}^2 & \cdots & \sigma_{yy}^2
\end{bmatrix}, \quad (3.6)
\]

and the data misfit is often stated as

\[
\phi_d = (\vec{d}^\text{pre} - \vec{d}^\text{obs})^T C_d^{-1} (\vec{d}^\text{pre} - \vec{d}^\text{obs}). \quad (3.7)
\]

Eq.(3.7) is accepted as a general definition for data misfit in the literature on geophysical inversion. Almost all the standard text books on geophysical inversion use this definition (Tarantola, 1987; Scales and Smith, 1999; Menke, 1984). Such a definition is predicated on the implicit assumption that the covariance matrix is invertible. A
surprising finding in my research, however, is that the covariance matrices of low-pass filtered data are generally not invertible! There has not been much discussion on this aspect in the literature. A clear understanding is crucial in order to proceed with the current work. I therefore examine the issue in this chapter. I first present a theoretic approach to estimate the covariance matrix associated with a set of low-pass filtered data, and then numerically verify it. I will then demonstrate that these covariance matrices are non-invertible. I conclude the chapter by defining a new misfit measure based on the variances of the filtered data alone and numerically estimate its expectation so that an optimal data misfit is known when a 3D inversion is carried out.

3.1 Noise Covariance Matrix of Low-Pass Filtered Data

Assume an airborne vertical gravity gradient data set $T_{zz_i}$, $i = 1, \ldots, N$, that is a sampled version of the geologic response. The sampling occurs at a given frequency along the flight line. Further we assume that the data have random Gaussian noise with zero mean and standard deviation $\sigma_i$,

$$\tilde{d} = T_{zz_i}$$
$$= \tilde{d}^i + \tilde{n}, \quad (3.8)$$
where $\tilde{d}'$ is true data and $\tilde{n}$ is noise. Such an assumption is reasonable since there are numerous noise sources during airborne acquisition and the net noise can be characterized as a normal process by central limit theorem (Saulis, 1991). I next assume that the low-pass filter is $\tilde{h}$. Then the filtered data is given by a convolution between the sampled gravity gradient and the low-pass filter,

$$
\tilde{d}' = \tilde{h} \otimes \tilde{d}
\quad = \tilde{h} \otimes \tilde{d}' + \tilde{h} \otimes \tilde{n}
\quad = \tilde{d}' + \tilde{n}_c,
$$

where $\tilde{d}'$ is the filtered version of true data, and $\tilde{n}_c$ is the filtered noise. Since any filtering will yield a correlated noise distribution, $\tilde{n}_c$ is no longer independently distributed.

This is a linear process and the errors in the filtered data are the linear combinations of the original errors. Consequently, the covariance matrix of the resulting noise can be calculated from the variance of the original noise. Now the data misfit is only related with correlated noise.
I first examine the approach based on the linear transformation. In equation 3.8, the filtered noise is

$$\tilde{n}_c = \tilde{h} \otimes \tilde{n} , \quad \tilde{h} = [h_{-K}, ..., h_0, ..., h_K]^T,$$

Or

$$n_{ci} = \sum_{j=-K}^{K} h_j n_{i+j}.$$ (3.10)

Equation (3.10) can be rewritten in the following matrix form,

$$\tilde{n}_c = L \tilde{n},$$ (3.11)

where $L$ is the filtering matrix, whose rows are given by translated filter coefficients $\tilde{h}^T$, which we denote as $\tilde{l}_i^T$.

If two vectors are related by $\tilde{y} = \tilde{l}_i^T \tilde{x}$, and the covariance matrix of the latter is given by $\text{cov}(\tilde{x}) = V$, then the elements of the filtered vector has a variance of

$$\text{Var}[y_i] = \tilde{l}_i^T V \tilde{l}_i,$$ (3.12)

and the covariance between difference elements is given by
\[
\text{Cov}[y_i, y_j] = \tilde{l}_i^T V \tilde{l}_j.
\]

For my current problem, let \( V \) be the covariance matrix of \( \tilde{n} \). Then the elements of covariance matrix of \( \tilde{n}_c \), denoted as \( V_c \), are given by

\[
\text{Var}[n_{ci}] = \tilde{l}_i^T V \tilde{l}_i, \tag{3.13}
\]

\[
\text{Cov}[n_{ci}, n_{cj}] = \tilde{l}_i^T V \tilde{l}_j, \tag{3.14}
\]

in matrix form \( V_c = L^T V L \).

Eq.(3.14) enables us to calculate the covariance matrix of the new data from that of the original data.

In the case where the filtering is done by applying a transfer function in the Fourier domain, the matrix operator can be defined by a concatenation of operators. Let \( \tilde{n} \) be the Fourier transform of \( \tilde{n} \), \( \tilde{n}_c \) be the Fourier transform of \( \tilde{n} \), \( \mathbb{F} \) be the symbolic matrix representation of the Fourier transform, \( \mathbb{F}^{-1} \) be the inverse, and \( \tilde{\eta} \) be the diagonal matrix representing the low-pass filter. Then the filtered data are given by,

\[
\tilde{n}_c = \mathbb{F}^{-1}(\tilde{\eta} \tilde{n}).
\]
\[ = \mathcal{I}^{-1} \tilde{\eta} \mathcal{I} \tilde{\eta} \mathcal{I}. \]

So linear operator, \( L \), in this case can be defined as

\[ L \equiv \mathcal{I}^{-1} \tilde{\eta} \mathcal{I}. \]  
(3.15)

The matrix \( L \) can be constructed numerically by applying (3.15) to an identity matrix.

\[ L \equiv \mathcal{I}^{-1} \tilde{\eta} \mathcal{I} \mathcal{I}. \]  
(3.16)

This is accomplished by the following steps: (1) apply Fourier transform to each column of identity matrix \( I \), (2) multiply the resulting complex by matrix \( \tilde{\eta} \) to form a new matrix, and (3) apply inverse Fourier transform to each column of the new matrix. The resultant matrix obtained by assembling the so derived columns is the matrix \( L \).

Figure 3.1 shows two different covariance matrices. Figure 3.1a is the covariance matrix of the unfiltered data and panel (b) is the simulated covariance matrix of data after being filtered with a 300-m Butterworth filter of 7th degree. The horizontal and vertical axes represent data points. The original data consist of only uncorrelated
Gaussian noise with zero mean and standard deviation of 1.0. The corresponding covariance matrix (Figure 3.1a) is diagonal. The diagonal elements are the variances of the random noise. The off-diagonal elements are zero since there is no correlation among different data points. The determinant of this covariance matrix is unity and it is invertible.

The covariance matrix of the filtered noise (Figure 3.1b) shows quite different features compared to the covariance matrix of the original data. The magnitude of main diagonal elements (variances) is drastically decreased, and the off-diagonal elements are non-zero and exhibit banding parallel to the diagonal. Furthermore, the determinant of the covariance is effectively zero. This covariance matrix is singular and has no inverse.

An alternative way to calculate the covariance matrix of filtered data is using multiple realizations of filtered data. I present this approach and the corresponding result as a verification of the result obtained using eq.(3.14) and eq.(3.16). Let us assume a set of random variables \( \bar{n} \) and their filtered version \( \bar{n}_c \) according to eq.(3.10). Knowing the distribution of the original data, we can generate multiple realizations. Each realization has a corresponding filtered version. Thus, we can obtain multiple realizations of the filtered noise and numerically calculate the mean and variance of the filtered noise.
Figure 3.1 The covariance matrices of independent noise (a) and filtered noise (b) respectively. The observation line consists of 21 data points. The amplitude of diagonal is decreased by filtering. The main diagonal terms are now different from each other, while 3.1a shows the identical main diagonal.
Assume we have $K$ realizations of the noise vector $\bar{n}_j, j = 1, \ldots, K$ and corresponding filtered noise vectors $\bar{n}_k, j = 1, \ldots, K$ resulting from the application of eq. (3.10) Now we can define $x_i$ as the column vectors consisting of the i’th element of all $K$ realizations of original noise,

$$
\begin{bmatrix}
\begin{array}{c}
\vdots \\
K \times N \\
\vdots \\
\end{array}
\end{bmatrix}
\begin{bmatrix}
\begin{array}{c}
n^1 = \begin{bmatrix} n^1_1, & \cdots, & n^1_N \end{bmatrix} \\
\vdots \\
n^K = \begin{bmatrix} n^K_1, & \cdots, & n^K_N \end{bmatrix}
\end{array}
\end{bmatrix} = 
$$

Similarly, the column vectors of the filtered noise, which is denoted as $x_{ci}$, can be defined as,

$$
\begin{bmatrix}
\begin{array}{c}
\vdots \\
K \times N \\
\vdots \\
\end{array}
\end{bmatrix}
\begin{bmatrix}
\begin{array}{c}
n^1_c = \begin{bmatrix} n^1_c, & \cdots, & n^1_{cN} \end{bmatrix} \\
\vdots \\
n^K_c = \begin{bmatrix} n^K_c, & \cdots, & n^K_{cN} \end{bmatrix}
\end{array}
\end{bmatrix} = 
$$

Thus, we can calculate the covariance matrix of the column vectors using following equation,

$$
\text{Cov}(x_i, x_j) = E[(x_i - \bar{x}_i)(x_j - \bar{x}_j)], \quad i, j = 1, \ldots, N, \quad (3.18)
$$
where $E$ is the mathematical expectation and mean $\bar{x} = E(x_i)$. 

The above process is accomplished by the following steps: (1) generate $K$ realizations of uncorrelated Gaussian noise, (2) apply low filtering to the noise sets, and (3) calculate the covariance matrix using eq.(3.18).

To carry out the simulation, I use 3000 random realizations of noise. The assumed data spacing is 50-m and the number of data points is 21. Figure 3.2 shows two different covariance matrices obtained from the simulation. Figure 3.2a is the covariance matrix of original unfiltered noise, and Figure 3.2b is the covariance matrix of noise with 300-m filtered width. Though Figure 3.2 shows slightly different features compared to Figure 3.1. The main diagonal elements of left panel are not exactly unity, and the non-diagonal elements are not exactly zero. However, since the matrix in Figure 3.2 is numerically generated, two covariance matrices are consistent with each other. If large enough number of the realizations are given, the left panel in Figure 3.2 will approach Figure 3.1. Figure 3.2a is symmetrical and its determinant is nearly unity. Thus, the matrix is invertible. Figure 3.2b is very similar to that of Figure 3.1b. It is symmetrical and the magnitude of main diagonal is decreased. Its determinant is zero so it has no inverse matrix.
Thus, I have two approaches to calculate the covariance matrix of the correlated noise resulting from low-pass filtering. The first is an analytic method based on the linear relationship between the covariance matrices of the original and filtered noise, and the second is a numerical approach based on simulation through multiple realizations. The latter provides verification. For routine applications, it is more efficient to use an analytic approach.
Figure 3.2 The covariance matrices of independent noise (a) and filtered noise (b) respectively obtained from numerical simulation using multiple noise realizations. The covariance matrices are consistent with those in Figure 3.1
3.2 Singularity of the Covariance Matrix of the Correlated Noise

The results from the preceding section show that the covariance matrix of the original noise, equivalent to being filtered with a zero-length low-pass filter, is invertible, but the covariance matrix of the 300-m low-pass filtered noise is singular. The difference suggests that there is a threshold of filter length that causes the covariance matrix to be singular. To the threshold of filter width, I apply various filter length ranging from 0 to 300 m in 25 m increments and evaluate the determinant of the resultant covariance matrices.

Figure 3.3 shows the determinant of the covariance matrix of the filtered data. When the filter width is less or equal to 50 m, the determinant has non-zero value, so the covariance matrix is invertible. When the filter width exceeds 50 m, however, all determinant values are zero. It means that these covariance matrices are singular. Several examples with changing the data spacing show that the threshold is same as the data spacing.

The previous assumption in eq.(3.6) that there is an inverse of the covariance matrix of correlated data is no longer valid. An alternative method is required. I address this in the next section.
3.3 Data Misfit of the Correlated Noise

Since the covariance matrix of filtered noise produced by a low-pass filter is singular, we can no longer use the general definition of data misfit based on the inverse
of a covariance matrix, such as eq.(3.7), for data with correlated noise. We need an alternative way to quantify the data misfit for such data.

One possibility is to work with the independent components of the data set that are identified through a principal component analysis (e.g., Yendle and MacFie, 1989; Stone and Brooks, 1990). However, such an approach introduces another layer of transformation that complicates the relationship between data and model. In addition, large data sets in exploration problems often containing thousands to tens of thousands of data points, and principal component analysis for such large data sets can be prohibitively expensive.

Alternatively, we can reconsider the simple form of data misfit in eq.(3.2) that was originally defined for uncorrelated noise. That definition can be simply understood as the $L_2$ distance between observed and predicted data when each datum is measured in the unit of its standard deviation. This quantity is always well defined. The only unknown is its expected value when the noise in data is correlated. The expected value is important since it defines the target misfit using an inversion.

To define the expected value of the data misfit in eq.(3.2) for correlated noise, I use numerical simulation. Let $\tilde{d}_j^f,(j=1,\ldots,K)$, be K realizations of the filtered noise, and
\( \sigma_{ij} \) be the standard deviation of i'th elements in the j'th realization. The true data misfit corresponding to the j'th realization is,

\[
\phi_j = \sum_{i=1}^{N} \left( \frac{d_{ij}^f}{\sigma_{ij}} \right)^2, \quad j = 1, \cdots, K
\]  

(3.19)

where \( N \) is the length of each data set such that \( \tilde{d}_j^f = (d_{i_1}, \cdots, d_{i_N})^T \). The expected value of the data misfit can then be calculated from the \( K \) realizations,

\[
E(\phi_d) = \frac{1}{K} \sum_{j=1}^{K} \phi_d^j.
\]  

(3.20)

Once the expected value is obtained as a function of number of data, it can be used to define the target data misfit in Tikhonov inversion.

I carry out this simulation using the same 3000 realizations of noise as in Section 3.1. Figure 3.4 shows the variance of the filtered data with changing the filter width. The X-axis represents the filter width and Y-axis is an arbitrary one measurement line. I apply a low-pass filtering with varying filter width on it. Because filtering process is basically smoothing process, the variance is decreased with filter width.
Figure 3.4 The variance at the each data points of the filtered noise is plotted with respect to the filter width. Y-axis, the measurement line, consists of 21 data points. The standard deviation of each point is decreased with filter length. When the filter length is less than 50 m, the data spacing, the standard deviation of all points is nearly same to each other. With filter length increasing, the standard deviation at each point is deviated from each other. This is shown Figure 3.2b.

Figure 3.5 shows the expectation of data misfit, which is the result of eq.(3.20), with respect to the changing filter width. The filter width ranges from 0 to 300 m with 25-m increments. The number of data points is 21. The expectation of the data misfit, the target data misfit, is invariant with changing filter.
Figure 3.5 The expectation of the data misfit with respect to the filter width. The expectation values converge to the number of observation points. This implies that the target data misfit of filtered data can be easily determined by its number of data points.

Figure 3.5 is important. The expectation of the data misfit, that is the target data misfit, remains the same as the number of the data points. As mentioned previously, the target data misfit of uncorrelated noise is well-known as the number of data points if we assume Gaussian statistics. Now, the optimal data misfit of filtered, correlated noise is the
same to the number of data points. We will use this target data misfit to determine the proper level of 3D inversion in the following chapter.

I also examine the variance of the data misfit with respect to changing filter width. The result is shown in Figure 3.6. The variance of data misfit shows a large range of variation as a function of filter width. When the filter width is smaller than the data spacing, the variance is equal to $2N$, where $N$ is the number of the data points. This is expected since it the noise is essentially unfiltered and the data misfit is a $\chi^2$ variable. Beyond this threshold, the variance increases monotonically with the filter width.
Figure 3.6 The variance of the data misfit with respect to changing filter width. If the filter is less than the data spacing, the variance is around $2N$, where $N$ is the number of data points. As the filter width exceed the data spacing, the values increase with the filter width monotonically.
3.4 Conclusion

I have used two methods to estimate the covariance matrices. Both methods show consistent results. If filter width increases, the covariance matrix of the filtered data becomes singular. Thus, the assumption that the covariance matrix is invertible is not valid. The singularity of the covariance matrix is related to the data spacing. If the filter width exceeds the data spacing, the covariance matrix is no longer invertible and definition of target data misfit using the inverse of the covariance matrix is not valid.

An alternative approach to define the data misfit is proposed. I use the same definition as for uncorrelated noise. The expectation is found through simulation. The results show that the expected data misfit of the filtered data is invariant with respect to the filter width, and its value is the same as the number of the data points. This result will be used in determining the 3D inversion level in the following chapter.
In this chapter, I apply the results obtained from the preceding two chapters to the 3D density inversion, which is more applicable to practical problems. Unlike parametric inversion in Chapter 2 that was solved by a least squares approach, the density inversion is formulated by simultaneous minimization of a data misfit and a model objective function. I first review the formulation of the inverse problem using Tikhonov regularization. I will then incorporate the low-pass filtering into the sensitivity to complete the algorithm. I use two synthetic examples to illustrate adverse effect of low-pass filtering and demonstrate the improvement that can be gained from the new approach.

4.1 3D Density Inversion Methodology: Algorithm-I

Parametric inversion based on assumed simple 2D source objects such as that used in Chapter 2 is helpful to understand the issues caused by low-pass filtering applied in the acquisition systems. Such a method may also be useful if isolated anomalies produced by similar causative bodies are to be interpreted. To interpret large-scale field data that may consist of multiple anomalies, however, a more general algorithm is required. A commonly used approach is the density inversion that seeks to reconstruct a density
contrast distribution as a function of subsurface position while no explicit assumptions are made regarding the number of sources present and their shapes (e.g., Li and Oldenburg, 1998; Li, 2001a). Such algorithms typically are formulated using Tikhonov regularization and a model that has certain characteristics and reproduces the observations is sought. In this section, I briefly review the algorithm described by Li (2001a) and outline its essential components. Without loss of generality, I assume the data are the vertical gravity gradient, i.e., the $T_{zz}$ component of the gradient tensor.

The $T_{zz}$ component of gravity gradient tensor produced by the density contrast $\rho(x, y, z)$ with respect of surroundings (hereafter simply referred to as density for simplicity), is given by

$$T_{zz} = \gamma \iiint \rho(x, y, z) \frac{\partial}{\partial z} \frac{1}{|\vec{r}' - \vec{r}_i|} dv,$$

where $\vec{r}_i$ is the vector denoting the i’th observation location and $\vec{r}'$ is the source location. $V$ represents the volume of the anomalous mass, and $\gamma$ is the gravitational constant. I adopt a right-hand Cartesian coordinate system with x-axis pointing toward grid north, Y-axis pointing towards the grid east, and the z-axis pointing vertically downward.
Figure 4.1 The volume of interest is expressed as a sum of serial cuboidal cells in 3D model. The model parameter vector is denoted as $\Delta \rho = (\rho_1, \rho_2, \ldots, \rho_M)^T$, and a right-handed Cartesian coordinate system is adapted. The element of sensitivity matrix $G_{ij}$ is given by the gravity gradient at the i'th observation point produced by a unit density contrast in the j’th cell.

To solve equation (4.1) numerically and to facilitate the inversion, the volume of interesting subsurface is discretized into a congregation of cuboidal prisms as shown in Figure 4.1. Each prism is assumed a constant density value. Thus, the density distribution is represented as a piece-wise constant function in 3D. The collection of the density
values in the prism for a column vector is \( \bar{\rho} = (\rho_1, \ldots, \rho_M)^T \), where \( M \) is the total number of prisms.

Given such a discretization, the i’th vertical gravity gradient, \( T^i_{zz} \), is the sum of gravity gradient contributions from all M prisms (Figure 4.1),

\[
T^i_{zz} = \sum_{j=1}^{M} \rho_j \left\{ \int_{V_j} \frac{1}{|\bar{r} - \bar{r}_i|} dV \right\} = \sum_{j=1}^{M} \rho_j G_{ij},
\]

where \( \rho_j \) and \( \Delta V_j \) are respectively the density and volume of the j’th prism, and \( G_{ij} \) is the sensitivity of i’th datum with respect to the j’th prism.

An airborne gravity gradiometry survey produces a set of data. In the same way we form a column vector of the density values, we can collect these data into a column vector \( \bar{d} = (T^1_{zz}, \ldots, T^N_{zz})^T \), where \( N \) is the number of data. The discrete equation (4.2) can be compactly written as,

\[
\bar{d} = G\bar{\rho},
\]
where $G$ is the sensitivity matrix given by

$$
G = \begin{bmatrix}
\frac{\partial d_1}{\partial \rho_1} & \ldots & \frac{\partial d_1}{\partial \rho_M} \\
\vdots & \ddots & \vdots \\
\frac{\partial d_N}{\partial \rho_1} & \ldots & \frac{\partial d_N}{\partial \rho_M}
\end{bmatrix},
$$

(4.4)

I note that each row of the sensitivity matrix corresponds to one datum.

Given the above discretization and the forward modeling expressed by Eq.(4.3), the goal of the inversion is to reconstruct the density distribution represented by the vector $\rho$. The first criterion that a candidate model in the inversion must satisfy is that it must reproduce the observed data to a reasonable degree as dictated by the errors in the data. This is measured by the data misfit function. Typically, we discretize the problem in such a way that the number of prisms is much greater than the number of data available. It is not difficult to reproduce the data to any reasonable degree. However, the crucial aspect of inversion is how to select one or more models that reproduce the data and are geologically plausible. To achieve this, we seek simplest possible model that fits the data and conforms to any known constraints such as a lower and upper bound on the density values. The simplicity of the model is measured by a model objective function. Thus the
Data misfit and model objective function are two crucial components of Tikhonov inversion.

Data misfit measures the difference between the observed data and the predicted data, and it is a critical concept of inversion. Because geophysical data always include a certain level of errors, forward modeled data from inversion result should not perfectly fit the observed data. Instead, these two data sets should be at some sufficiently small distance from each other. This distance is determined by the standard deviation of noise in the data. A commonly used measure of this distance is the $l_2$ data misfit function,

$$
\phi_d = \| W_d (\vec{d} - \vec{d}_{obs}) \|^2_2,
$$

where $W_d$ is a diagonal weighting matrix, whose i’th element is $1/\sigma_i^\prime$, where $\sigma_i^\prime$ is the standard deviation of the i’th datum of filtered data. The optimal distance between the observed and predicted data is the expected value of this function. For more details, readers are referred to Chapter 3, but it suffices here to comment that a generally applicable form of the data weighting matrix is the diagonal form that only depends on the standard deviation of the correlated error in the data.
The model objective function is the second critical component. There are many different forms of model objective functions. I use a generic model objective function (Li and Oldenburg, 1998).

\[
\phi_m(\rho) = \alpha_x \int \int \int \int \int (w(z)(\rho - \rho_o))^2 dv + \alpha_y \int \int \int \int \int \left( \frac{\partial w(z)(\rho - \rho_o)}{\partial x} \right)^2 dv + \\
\alpha_z \int \int \int \int \int \left( \frac{\partial w(z)(\rho - \rho_o)}{\partial y} \right)^2 dv + \alpha \int \int \int \int \int \left( \frac{\partial w(z)(\rho - \rho_o)}{\partial z} \right)^2 dv ,
\]

where the coefficients \(\alpha_x\), \(\alpha_y\), \(\alpha_z\), and \(\alpha\) determine the relative contribution of their corresponding terms to the objective function. \(\alpha_x\) is related to length of the model, while three other coefficients are related to the smoothness of the model. The reference model, \(\rho_o\), can be determined by local geologic information, previous investigations, or it can simply be a zero model. \(w(z)\) is a depth weighting function, which will be discussed later.

Equation (4.6) can be expressed in discrete form using finite-difference approximations as,

\[
\phi_m(\rho) = (\tilde{\rho} - \tilde{\rho}_o)^T Z^T \left( W_x^T W_x + W_y^T W_y + W_z^T W_z \right) Z (\tilde{\rho} - \tilde{\rho}_o) \\
= (\rho - \rho_o)^T W_\rho^T W_\rho (\rho - \rho_o) ,
\]

(4.7)
where \( W^T \rho W = \left( W_x^T W_x + W_y^T W_y + W_z^T W_z \right) \). Alternatively, eq.(4.7) can be expressed as an \( l_2 \) norm of the density deviation from the reference model,

\[
\phi_m = \left\| W^T (\rho - \rho_o) \right\|^2_2, \quad (4.8)
\]

As the function \( w(z) \) in eq. (4.6) is a depth weighting, and is used to compensate for the decay of the sensitivity, \( G_{ij} \), with depth. Because of non-uniqueness of gravity gradient interpretation, infinitely many density distributions can satisfy the observed data. The sensitivity, which decays predominantly with inverse depth cubed, prefers to concentrate most density near surface (Li and Oldenburg, 1998). It is necessary to use a weighting function to counteract this effect. I use the form,

\[
w(z) = \frac{1}{(z + z_o)^{3/2}}, \quad (4.9)
\]

where \( z \) is the center of the first cell of the model and \( z_o \) depends on the cell size of the model.

Inversion using the Tikhonov regularization minimizes a global objective function that consists of the data misfit and a scaled model objective function, defined as,
\[ \phi = \phi_d + \mu \phi_m, \]  

(4.10)

where \( \mu \in [0, \infty) \) is the regularization parameter, which regulates the contribution of both terms. If \( \mu \) is great, the model objective function is dominantly minimized and the data misfit will be large. If \( \mu \) is small, data misfit is dominantly minimized. Thus the choice of regularization parameter is crucial to determine optimal inversion level. With a properly chosen \( \mu \), the inversion is solved by finding a density \( \rho(\tilde{r}) \) that minimizes global objective function, \( \phi \).

I use two approaches to find a proper regularization parameter \( \mu \). The first is the commonly used discrepancy principle, which states that the optimal regularization parameter is that which produces the expected misfit. I have devoted Chapter 3 to the question of data misfit and its expected value. The result can be applied directly to the choice of regularization parameter. The data misfit is a monotonically increasing function of \( \mu \), therefore, knowing the expected misfit (also referred to as the target misfit) allows one to find the corresponding value of \( \mu \).

The second approach is the L-curve criterion (Hansen, 1992). This is a heuristic, but often robust, way to find the regularization parameter. It is known to work especially
well in the presence of correlated noise (Hansen 2001). When we plot data misfit as a function of model objective function on log-log scale to form the Tikhonov curve, it often exhibits a corner point. This corner is a turning point beyond which either model objective function or data misfit changes drastically (Lawson and Hanson, 1974). L-curve criterion states that the optimal regularization parameter is that corresponding to the corner point of L-shaped Tikhonov curve. This point is determined as the point of maximum curvature (e.g., Li and Oldenburg, 1999),

\[
2322 \cdot \frac{\phi_j \phi_j^* \phi_j \phi_j^*}{(\phi_j^*)^2 - (\phi_m^*)^2} \text{ \quad (4.11)}
\]

where \( \phi_d = \log(\phi_d) \), \( \phi_m = \log(\phi_m) \).

For density inversion, the upper and lower bounds on the density contrast are an important piece of prior information. They serve to restrict the density solutions so they are consistent with geology. Thus the inversion of gravity gradiometry data also commonly include two sets of bound constraints in the form of

\[
\rho_j^{\min} \leq \rho_j \leq \rho_j^{\max}, \quad j = 1, \cdots, M, \text{ \quad (4.12)}
\]
Where $\rho_{j}^{\text{min}}$ and $\rho_{j}^{\text{max}}$ are respectively the lower and upper bounds of the density contrast in the j’th cell. These bounds can be easily imposed using a logarithmic barrier method, which effectively represents the bound with a logarithmic term in the global objective function. Thus, the minimization associated with the inversion is

$$
\phi(\lambda) = \phi_d + \mu \phi_m - 2\lambda \sum_{j=1}^{M} \left[ \ln(\rho_j - \rho_{j}^{\text{min}}) + \ln(\rho_{j}^{\text{max}} - \rho_j) \right],
$$

where $\lambda$ is the barrier parameter. The logarithmic barrier term forms a barrier along the boundary of the feasible domain and prevents the minimization from crossing over to the infeasible region. The method solves a sequence of nonlinear minimizations with decreasing $\lambda$, and, as $\lambda$ approaches zero, the sequence of solutions approaches the solution of eq.(4.10).

4.2 Incorporating a Filter in Inversion: Algorithm-II

The 3D inversion in the preceding section assumes that the observed data has randomly distributed Gaussian noise, and does not account for any acquisition filtering in the inversion. To reduce the influence of data filtering in inversion, I incorporate into the inversion algorithm the same low-pass filter used in data acquisition phase. The justification and approach are the same as in the 2D parametric case. I incorporate the
low-pass filtering into forward modeling and sensitivity matrix calculation during the 3D inversion. I note again that this is an effective filter that describes the combined effect of several smoothing procedures in the acquisition system. These procedures are necessary to remove high frequency noise but they also remove useful geologic signal. The composite filter parameters are estimated post-acquisition.

The new algorithm (hereafter referred to as Algorithm-II) is basically the same as Algorithm-I described in the preceding section, except a low-pass filtering is included during inversion, to mimic noise filtering during the data acquisition phase. Let the low-filter be $F[\bullet]$. The forward operation including the filtering becomes

$$\tilde{d}^F = F\tilde{d} = FG\tilde{\rho}, \quad (4.14)$$

where $F$ is the matrix representation of the low-pass filter. Strictly speaking, the filtering is applied to the directly calculated data. However, the direct forward calculation is a linear process described by a matrix-vector multiplication and the sensitivity matrix is independent of the density vector. Thus, the low-pass filtering can be effectively understood as being applied to the sensitivity matrix directly:
\[ \ddot{d}^F = (FG) \ddot{\rho} \]
\[ \equiv G^F \ddot{\rho} \]  

where \( G^F \) is the filtered sensitivity matrix. Replacing eq.(4.3) with eq.(4.15) in Algorithm-I, therefore, produces the sought algorithm that incorporates the low-pass filtering. The remaining part of the inversion follows exactly as in Section 4.1.

I comment that the filter matrix F acts upon the columns of the original sensitivity matrix G. Although the matrix F can be calculated first and then applied to the sensitivity matrix, I have chosen an implementation that applies the matrix implicitly by performing the filtering directly during the sensitivity calculation. A group of rows of matrix G that corresponds to a line of filtered data is first computed. Low-pass filtering is then applied to each column of this group of rows to obtain the elements of the filtered sensitivity matrix. Completing this process for all lines in the data set builds up the entire sensitivity matrix \( G^F \). This approach has proven to be efficient in practice.

4.3 Synthetic Model

As alluded to in the introduction, the goal of this chapter is twofold. The first is to understand the effect of low-pass filtering on 3D density inversion. The second is to develop and test an algorithm that incorporates the filter and thus effectively alleviate its
effect. It is also important to gain basic understanding of the improvement that can be gained from such an algorithm. Synthetic examples allow us to examine these issues by performing numerical experiments. I now proceed with two synthetic examples. The first model is dipping slab with an anomalous density contract and the second model is made up of two vertical prisms placed side by side.

4.3.1 Dipping Slab Model: Model-A

The dipping slab (Figure 4.2) is designed as a basic test example to study the effect of low-pass filtering in 3D density inversion. It consists of a slab that is dipping 45° to the west and has a density contrast of 1000 $kg/m^3$. Within the assumed model region of 1000 by 1000 by 500 m, the dipping slab is located in 550 to 800 m in easting, 350 to 650 m in northing, and 50 to 400 m in depth.

Figure 4.3(a) shows synthetic noisy data. The data set has a station spacing of 50 m in both directions. The noise added to the data is uncorrelated Gaussian noise and its standard deviation is 2% of the datum amplitude plus a 1-eotvos minimum. Figure 4.3b shows the low-pass filtered data. I assume the low-pass filter of the acquisition system is approximated by a 7th order Butterworth filter with 300-m filter width. Note that the filtered data have not only lost the highly variable noise to some extent, the larger-scale
anomaly has also been smoothed and widened. The noisy data are presented as a reference, but it is important to remember that these data are never available in practice.

Figure 4.2 Used synthetic dipping slab (model-A). With 3D modeling, the survey area is expressed as a congregation of serial cuboidal cells. It consists of 20 by 20 by 10 cells in Easting, Northing and vertical direction respectively, and the size of each cell is 50 by 50 by 50 m. The entire dimension is 1000 by 1000 by 500 m. The dipping slab is located from 550 to 800 m in Easting, 360 to 650 m in Northing, and 50 to 400 m in depth. The dipping angle is 45 degrees to the west. The density contrast of dipping slab in purple color is 1000 kg/m$^3$ to the surroundings, which have constant density distribution.
Figure 4.3 Synthetic vertical gravity gradient data of dipping slab (model-A): (a) noisy data, (b) filtered data with 300-m filter length. Filtering is conducted in N-S direction. Note that amplitude and width of gravity anomaly are decreased and widened, respectively.
To carry out the inversion, I discretize the model region into a set of 50-m cubes. This yields 20 by 20 by 10 cells in the entire model. I first invert the unfiltered data as a reference for comparison. Although this is not available in practice, we can use it to understand the filtering effect in this and following synthetic models. Once, the optimal regularization parameter is found, I then invert the filtered data using Algorithms-I, which treats the data as if they were direct geologic responses, and Algorithm-II, which includes the low-pass filtering the forward modeling and sensitivity matrix.

The next step is to determine the proper regularization parameter for each algorithm. Figure 4.4a shows data misfit curve with respect to the regularization parameter for algorithm-I. It is clear that the data misfits over all ranges of the regularization parameter are much higher than its number of data points. Consequently, we can not find the proper regularization parameter as described in previous section. Instead, I use a trial and error in determining the regularization parameter. First, I determine the lowest data misfit which is shown in early phase of $\mu$ and multiply by 1.1 to give 10% high over the lowest data misfit. The target data misfit is given by that value.

Figure 4.4b shows data misfit curve of algorithm-II. Unlike the previous case, I can set the target data misfit of filtered data, as described in chapter 3, to be the number of data points. Next step is to find the match point between target data misfit and
discrepancy curve, then finally we can determine the regularization parameter. The number of data points is 441, and resultant regularization parameter is about 48.

Figure 4.5 shows the L-curves and maximum curvature of the two algorithms. Figure 4.5a shows two L-curves of two algorithms. With algorithm-I, the finding of corner points is very hard in the curve (blue line with circles). Meanwhile with algorithm-II, the optimal regularization parameter can be found at maximum curvature curve (red dotted line with circles). Figure 4.5b is the resultant maximum curvature of L-curve. As expected, we can easily determine maximum curvature in the graph when we use the new algorithm. Based on this graph, maximum curvature is located between $\mu = 0.46$ and $\mu = 1$. Compared to the discrepancy principle, the optimal regularization parameter determined from L-curve is lower.

Because of difficulties in determining the regularization parameter by L-curve in Algorithm-I, I use the regularization parameter determined by trial and error. Correspondingly, I use the discrepancy principle in Algorithm-II. Since the two algorithms have different process to determine the optimal regularization parameter, care is needed in comparing the two results.
Figure 4.4 Determination of the optimal regularization parameter using the discrepancy principle of model-A (one dipping slab). These are the misfit curves produced when inverting the filtered data in Figure 4.3b; (a) is using algorithm-I and (b) is using algorithm-II. As a result of Chapter 3 we can set the target data misfit be the number of data, 441. Figure 4.3a, however, shows that the data misfit cannot reach the target data misfit in Algorithm-I.
Figure 4.5 L-curves and maximum curvature of two algorithms. There is difficulty in choosing the optimal regularization parameter by finding the maximum curvature in Algorithm-I.
We now compare three inversion results with the true model by examining cross-section and plan-section slices through these models. Figure 4.6 to 4.8 show the cross-sections of the four models viewed from the west, south, and top respectively; panel (a) displays true model; (b) displays recovered model from unfiltered noisy data; panels (c) and (d) show respectively the inversion of filtered data using Algorithm-I and Algorithm-II. Three figures share several features.

It is clear that the inverted model of unfiltered noisy data is a good representation of the true model, having good definition of the lateral and vertical extent of the anomalous density block. This is an ideal scenario and serves as a basis for judging the inversion of the filtered data.

All three section maps using algorithm-I show rather poor recoveries of density distribution in both lateral and vertical directions; recovered density is spread out laterally and concentrated near the surface. The depth resolution is also poor.

The results from algorithm-II (d) clearly show the improved density model. Both lateral and vertical extents of the anomalous density block are well recovered. Those models show good comparison with models in panel (b). I note that the result from algorithm-II shows clear improvement over algorithm-I for model-A.
Figure 4.6 Four cross sections in North-South (NS) direction, viewed from West, at easting 600m of the model block. X-axis represents Northing originated from right corner, and y-axis depth. The inversion result of noisy data in (b) shows good resolution in lateral and depth. Meanwhile, the inversion result using algorithm-I (c) shows poor recovery of density distribution in both lateral and vertical direction. And recovered densities are spread and concentrated near the surface. The result from algorithm-II (d) apparently improved density recovery. I use the optimal regularization parameter, which is chosen by the discrepancy principle.
Figure 4.7 Four cross sections in West-East (WE) direction, viewed from South, at northing 500m. X-axis represents Easting originated from left corner. The density distribution in (b), which is from the inversion result of noisy data, shows good dipping recovery, and shows good recovery of depth. The inversion result using Algorithm-I (c) shows that the density distribution is concentrated near surface, and shows no. The result from algorithm-II (d) is clearly similar to (b), and shows good consistence with true model.
Figure 4.8 Plain section maps at depth 125m viewed from upside. The result from filtered data with Algorithm-I is spread, and elongated in NS direction, which coincides with filtering direction. Panel (d) shows that the algorithm-II can successively compensate for the filtering effect.
4.3.2 Quantitative Evaluation: Mass Compaction Index (MCI)

The above comparison indicates that the effect of low-pass-filtering, if not accounted for, is to produce a wider but shallower source distribution. However, such comparisons are only qualitative. To obtain a numerical measure of the differences, I compare the center of mass of the recovered density distribution and a qualitative measure of the spread of the density.

Given the density model recovered from any inversion, we can calculate the center of mass defined by,

\[
x_c = \frac{1}{m} \sum_{j=1}^{M} x_j \rho_j \Delta V_j,
\]

\[
y_c = \frac{1}{m} \sum_{j=1}^{M} y_j \rho_j \Delta V_j,
\]

\[
z_c = \frac{1}{m} \sum_{j=1}^{M} z_j \rho_j \Delta V_j,
\]

where \(x_j\) and so on denote the coordinates of the center of each cell, and \(m\) is the total mass in the recovered model,

\[
m = \sum_{j=1}^{M} \rho_j \Delta V_j.
\]
This set of coordinates gives a direct measure of the overall position, especially the depth, of the recovered density model.

Next, we can define a mass compact index (MCI) by using the concept of the moment of inertia. The moment of inertia measures indirectly the spread of mass distribution away from a central reference point. When normalized by the total mass, it provides a pure geometric measure. Thus, I define MCI as the square root of the normalized moment of inertia,

\[
I_x = \sqrt{\frac{\sum_{j=1}^{M} (x_c - x_j)^2 \rho_j \Delta V_j}{m}}, \\
I_y = \sqrt{\frac{\sum_{j=1}^{M} (y_c - y_j)^2 \rho_j \Delta V_j}{m}}, \\
I_z = \sqrt{\frac{\sum_{j=1}^{M} (z_c - z_j)^2 \rho_j \Delta V_j}{m}},
\]

which has the dimension of distance and measures how far the recovered density spreads in each axis direction. The smaller the MCI in a given direction, the more compact the recovered source is in that direction.
I note that these two sets of quantities are fundamentally the first and second order moments of a density distribution. They provide natural summary measures of the position and spread of the density function. It is also important to note that these measures do not have information about the internal structure of the density function. Therefore, they are expected to be useful for density model composed of a single density anomaly. Alternatively, they must be applied to windowed density function in 3D. For the purpose of evaluating the result from the dipping slab model, however, they are sufficient and can be used directly.

Table 4.1 shows the comparison of center of mass and the Mass Compaction Indices of three different inversion results. Column 2 display these quantities for the density model obtained from inversion of unfiltered data. These are used as the basis for comparison. The third column shows the MCI of the density model from filtered data when they are inverted directly without incorporating the filter (Algorithm-I). The Fourth column displays the relative error of these results compared to those in column-2. We note that the horizontal center of mass is nearly identical in the two models but the center of mass of the model from filtered data is significantly shallower than that from the unfiltered noisy data. Furthermore, the MCI of the density from filtered data are considerably greater in the horizontal directions.
Columns 5 and 6 in Table 4.1 display the center of mass and MCI for the density recovered using Algorithm-II and their errors compared with the model from unfiltered data. It is clear that including the filtering in the inversion has greatly improved the result. The errors are generally less than 10% whereas the errors were greater than 30% in the directions the filtering had an adverse effect. Thus Algorithm-II has successfully alleviated the effect of low-pass filtering to a certain degree. The reduction in error from over 30% less than 10% is expected to impact the interpretation in practical applications.

To summarize, I can make the following statements regarding the effect of low-pass filtering of data in 3D density inversion. First, the recovered densities without incorporating data filtering are spread out laterally to give a false impression of wider anomalies. This is consistent with the observation from the parametric study in Chapter 2. In the depth direction, the recovered densities are concentrated near the top of the true density anomalies and produce a false impression of shallower source bodies. The depth extent of the recovered density is smaller than the true extent. The former observation is contrary to the observation in the parametric case and is somewhat counterintuitive, but the latter is again consistent with the conclusion from the parametric study. The reason for such differences lies in the flexibility of cell-based density inversion. A gravity anomaly with reduced amplitude and broader width is more easily produced by a density distribution that is shallow and similarly broad.
Table 4.1 The comparison of center of mass and mass compaction index of three different inversion results for model-A. The first is from inversion of noisy data, the second is from inversion of filtered data using algorithm-I, third is from inversion using algorithm-II.

<table>
<thead>
<tr>
<th></th>
<th>Noisy model (A)</th>
<th>Filtered data, Algorithm-I (B)</th>
<th>Filtered data, Algorithm-II (C)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(B-A)/A (%)</td>
<td>(C-A)/A (%)</td>
</tr>
<tr>
<td>$x_c$</td>
<td>501.7</td>
<td>502.0</td>
<td>503.3</td>
</tr>
<tr>
<td>$y_c$</td>
<td>546.9</td>
<td>544.4</td>
<td>541.8</td>
</tr>
<tr>
<td>$z_c$</td>
<td>188.5</td>
<td>126.9</td>
<td>179.2</td>
</tr>
<tr>
<td>$I_x$</td>
<td>110.6</td>
<td>161.5</td>
<td>118.9</td>
</tr>
<tr>
<td>$I_y$</td>
<td>119.5</td>
<td>167.0</td>
<td>124.9</td>
</tr>
<tr>
<td>$I_z$</td>
<td>200.5</td>
<td>208.3</td>
<td>202.2</td>
</tr>
</tbody>
</table>

4.3.3 Two-prisms Model: Model-B

I now proceed to the second model that consists of two vertical prisms. This model is set up to illustrate the loss of lateral resolution due to low-pass filtering, and how it can be improved by the new algorithm. Figure 4.9 shows perspective view of the model. The two prisms are offset laterally in the north-south direction. The southern prism is 300 by 250 by 400 m easting, northing and vertical directions respectively. The smaller prism, located north of the first one, is 200 by 200 by 300 m in dimension. The density contrast of both prisms is 1000 kg/m³ above the surrounding.
Figure 4.9 Synthetic model with two vertical prisms (model-B). The southern prism is 300 by 250 by 400 m in the easting, northing and downward directions, respectively. The smaller prism, which is located 150 m north of first one, has 200 by 200 by 300 m dimension. The density contrast of dipping slab in purple color is 1,000 kg/m³ higher than the surroundings.

Figure 4.10 shows synthetic noisy data and filtered data from this model. The number of data points per each line is 42 and there are 42 survey lines. The total number of data points is 1,764. Similar noise has been added to the data and the same Butterworth filter is applied to simulate low-pass filtering in the acquisition system. The filtering is
applied in the north-south direction. Consequently, the gravity gradient anomalies are smoothed and widened in that direction.

**Optimal Regularization Parameter**

Figure 4.11 shows two data misfit curves of each algorithm; Figure 4.11a is for algorithm-I and 4.11b is for algorithm-II. Those curves are used to determine target data misfit. Again, it is clear that the inversion without filtering effect (Algorithm-I) cannot fit the data to the target level. Through the same process as for model-A, I determined a revised target data misfit of 7,056. In contrast, Figure 4.11b shows the data misfit curve for algorithm-II and the regularization parameter can be chosen easily. The target data misfit for model-B is 1,764, and the corresponding regularization parameter is 72.

As illustrated in the previous section on model-A, we find a similar inversion result, both with and without filter, in Figures 4.12 and 4.13. In both section maps, panel (c) in Figures 4.12 and 4.13, show poor resolution; we obtain a single causative body, which is spread out and concentrated near surface. In comparison, the inversion that accounts for the filtering (Algorithm-II) in panel (d), clearly separates the two bodies and places them in their proper locations. This is a sharp contrast between the two approaches, and suggests more accurate results from the new algorithm.
Figure 4.10 Synthetic vertical gravity gradient data of two vertical prisms (model-B): (a) random noise added data, (b) filtered data with 300-m filter length. Filtering is conducted in the N-S direction.
Figure 4.11 Determination of the optimal regularization parameter using the discrepancy principle of model-B (two vertical prisms). Those are the misfit curves produced when inverting the filtered data in Figure 4.10b; (a) is using algorithm-I and (b) is using algorithm-II. The target misfit is 1,764. Figure 4.3a again, like figure 4.4, shows that the data misfit can not reach under the target data misfit while figure (b) well matches the optimal regularization parameter, 72.
Figure 4.12 Four section maps in the NS direction of model-B at Easting 1000 m; (a) is true model, (b) is recovered model of noisy data, (c) is the recovered model using algorithm-I, and (d) is the recovered model of filtered data using algorithm-II. Panel (d) shows good recovery of the true model, while panel (c) shows that most of the density distribution is concentrated in the near surface.
Figure 4.12 Four plain-viewed maps of model-B at depth 100m; (a) is true model, (b) is recovered model of noisy data, (c) is recovered model using algorithm-I, and (d) is recovered model of filtered data using algorithm-II. The panel (b) and (d) show clear lateral discrimination of two bodies, whereas the panel (c) shows spread density distribution, so lateral density contrast is not clear. There are also unwanted density distributions in panel (c), which may be caused by artifacts during inversion.
4.4 Conclusion

In this chapter, I first briefly review the current algorithm for 3D density inversions. That algorithm does not account for the low-pass filtering used in data acquisition phase for suppression of noise. Following the approach investigated in Chapter 2, I then modify that algorithm by including the filter into forward modeling and sensitivity calculations. Both algorithms are used to understand the effect of low-pass filtering in 3D inversions and to examine the improvement that can be produced by the new algorithm.

To illustrate the effectiveness of the new algorithm over the existing one, I use two synthetic models; one is a dipping slab and another is made of two vertical prisms located close to each other. The comparison of the two algorithms on two models using visual display and quantitative evaluation based on mass compaction index (MCI) shows that there is clear improvement in inversion results when the low-pass filter is included. Without filtering in inversion (Algorithm-I), the recovered body is placed in shallow depth and spread out laterally, which is a typical adverse effect on interpretation caused by low pass filtering. Inversion result with filtering in the forward modeling and the sensitivity matrix calculation during the inversion, however shows clearly improved resolution in both lateral and vertical directions.
CHAPTER 5. FIELD EXAMPLE

In the preceding chapters, I developed algorithms that are effective in reducing the adverse effect of low-pass filtering and demonstrated the improved results using synthetic models. I will apply the new algorithm to a field data set acquired using the Falcon™ system (Lee, 2001) over Broken Hill district in Australia.

5.1 Background and Geology

The Broken Hill district is located in New South Wales, Australia (Figure 5.1) and hosts the world class multi-metal (i.e., Ag, Pb, and Zn) Broken Hill deposit. The geology of area consists of the Willyama Supergroup as a host rock, which partially contains metamorphosed clastic and volcanoclastic sediments, basic to acid volcanics and intrusions that range in age from about 1715 to 1590 Ma. The orebodies are lens or dyke shaped with northeast strike and steeply deep to the northwest. The largest orebody has about 8 km size in strike direction (Johnson and Klingner, 1974; Gibson and Nutman, 2004; Willis, 1989).

Mineralization of the area is generally understood as concurrent with, or emplaced soon after, deposition of the sediments. The main sulphides accompany mostly galena
and sphalerite with useless gangue rocks. Each lens or dyke type ore body has a specific Lead-Zinc ratio.

Figure 5.1 Location map of Broken Hill deposit. The red circled star indicates the approximate location of the airborne gravity gradiometry survey (Lane and Peljo, 2004; New South Wales in Mapquest, 2005).
The average density of the ore body is 3.4 g/cm³ (Pecanek, 1975; Kelly and Bell, 1992) and the density of host rock is estimated at 2.8 g/cm³ (Maidment et al., 1999) thus the density contrast is approximately 0.6 g/cm³. A positive gravity anomaly is expected over orebodies. Gravity methods have been used extensively as an exploration tool in this district. Broken Hill deposit was found in 1883, mining activities have continued for more than 100 years (Traicos, 2002). Exploration activities in this area continue to this day. The most recent surge in exploration occurred after the acquisition of airborne gravity gradiometry data.

5.2 Gravity Gradient Data

A FALCON™ airborne gravity gradiometer (AGG) survey was flown in the Broken Hill district early in 2003 for mineral exploration (Lane et al., 2003). The line spacing was 200 m with perpendicular 2000 m tie lines. The main flight line direction is N36E and the total survey area is 1,186 km². The average terrain clearance was 80 m.

The FALCON AGG system measures $T_{xy}$ and $T_{xx} - T_{yy}$ components of the gravity gradient tensor. These data are then transformed into the vertical gravity gradient because of its simpler anomaly pattern. The conversion from the measured horizontal gravity gradient curvature to vertical gravity gradient is done in the Fourier domain. Comparing
with upward continued ground gravity data, Lane and Peljo (2004) determined that the composite low-pass filtering caused by the acquisition system and subsequent processing is equivalent to a 6th order Butterworth filter with a 400-m filter length.

Figure 5.2 shows the gravity vertical gradient data over the entire survey data. The coordinates are MGA54 projection in GDA94 datum. The positive anomaly marked by the ellipse in the lower part of the survey area is referred to as the Goldfinger anomaly. It represents an exploration target and limited drilling has been carried out. Although little detailed geologic information is available about this anomaly, it is an ideal case for illustrating the effect of low-pass filtering and for testing my new algorithm. I have extracted a subset of the data and rotated the grid by 36° counterclockwise. Figure 5.3 shows the extracted data over a 5 by 5 km area. The flight direction now becomes N-S direction. This is the direction of low-pass filtering. The RMS error is estimated to be 5-9 Eö (Dransfield et al., 2001). The Goldefinger anomaly is located in the center of the map, with NEE elongation direction. Several smaller anomalies surround it.

5.3 Inversions of Goldfinger Data

I now apply the two inversion algorithms to the Goldfinger data shown in Figure 5.3. The data set consists of down sampled data along lines paced 100 m apart with 50 m
station spacing. The number of data points is 5151. The standard deviation of the data is assumed to be 7.5 Eötvös based on the estimates in the literature.

Figure 5.2 Converted vertical gravity gradient data over Broken Hill deposit (courtesy Richard Lane, Geoscience Australia). The line spacing was 200 m intervals and the flight was N36E with mean terrain clearance of 80m. Coordinates are for GDA94 datum and MGA54 projection.
Figure 5.3 The selected sub data set of vertical gravity gradient data $T_{zz}$. The sub data set was rotated by 36 degrees counterclockwise so that flight line is now in the grid N-S direction, which is also the filtering direction. The positive anomaly in the center is known as the Goldfinger anomaly.
I invert these data to construct the density distribution in the volume below the data area down to a depth of 500 m. This volume is discretized into uniform cells that are 50-m wide horizontally and 25-m thick vertically. Beyond this core region, I extend the volume by five padding cells with increasing sizes. The total number of cells is 140,625. Two inversions are carried out using the Algorithm-I and II respectively. Both inversions are able to fit the data reasonably well. Although the standard deviation obtained from literature is a good first estimate, I find that the data can be fit slightly closer. The final misfit value for both inversions was 0.4 times the number of data, which is equivalent to a standard deviation of 4.1 Eötvös. This is not surprising since additional smoothing of data would have occurred during the conversion to the vertical gradient $T_{zz}$. I impose a positivity constraint on the density model.

Figure 5.4 shows 3D volume-rendered density models recovered by Algorithm-I and algorithm-II, respectively. The images are generated by displaying only cells having density above a certain cut-off value and setting the lower-density cells transparent. Such a display provides a 3D representation of the major density anomalies and it is useful in this case because we are looking for high-density zones as exploration targets. The cut-off density contrast used to create these two images is $0.2 \, g/cm^3$, while the maximum density is $0.6 \, g/cm^3$. Both recovered model show the long elongated body that produced the Gold finger anomaly in Figure 5.3. Algorithm-II, which incorporates the low-pass
filtering, however has recovered more details surrounding the main anomaly. This is to be expected, based on the synthetic results we have seen so far in Chapters 2 and 4.

Although 3D images are advantageous in providing an overall view of the result, they do not show enough details. For detailed comparison, I display a plan-section at a depth of 250 m from each model. This is the depth that intersects the center of the main anomaly (Figure 5.5). The result of inversion using Algorithm-II (right panel) improves resolution and target separation of the causative bodies over the result from Algorithm-I. Note that the new algorithm also identifies more smaller bodies surrounding the main body. Furthermore, the amplitude of recovered anomaly from the Algorithm-II is higher than that from Algorithm-I. The same observations can be made in cross-sections through the model. Figure 5.6 shows two cross-sections through both models. Two sections, AA’ and BB’, are marked in the plan-sections (Figure 5.5). It is clear that the recovered source bodies from algorithm-I are wider and have smaller amplitude, whereas they appear to be more compact in the density model recovered from Algorithm-II.
Figure 5.4 3D rendered density models obtained by using Algorithm-I (top) and Algorithm-II (bottom). The cutoff density contrast is 0.2 g/cm$^3$. The elongated body with SW-NE direction in mid area represents the ore body, which contributes to the Goldfinger anomaly in Figure 5.3.
Figure 5.5 Two plan-sections at a depth of 250 m of recovered density models. The left panel shows the result when the low-pass filtering is ignored, and the panel on right shows the result when the low-pass filter is included in the inversion. Two sections, AA’ and BB’, are taken to compare the inversion results in cross-sections in Figure 5.6.

Figure 5.6 Two cross-sections from the recovered models.
5.5 Conclusion

In this chapter, I test a new algorithm incorporating the low-pass-filter on a field data set. The results of new inversion algorithm clearly suggest that better resolution of causative bodies is gained when the low-pass filter is included as a part of the forward modeling and sensitivity calculation. The result also identifies additional separate density anomalies that are not clearly visible when the data are used as direct geologic response by ignoring the filtering effect. Thus, the field data example verifies the conclusion obtained through the synthetic modeling and inversion carried out in Chapters 2 and 4.
6.1 Conclusion

Currently, all airborne gravity gradiometry acquisition systems rely on some type of low-pass filters to suppress high-frequency noise. These low-pass filters are primarily applied to time-series measurements. These measurements are associated with the platform movement, so the net result is the same as applying a spatial low-pass filter to the final gravity gradient data. Because filtering decreases the amplitude of signal and increases the anomaly width, filtering has an adverse effect on data interpretation. Since the low-pass filtering is a necessary evil in the airborne gravity gradient data acquisition phase, we must understand and quantify the effect of low-pass filtering both on the data set and the recovered source model using inversion. This is the impetus of this thesis. My results indicate that the related error generally increases with decreasing source depth and width. If not accounted for, the low-pass filtering can lead to misinterpretation.

In practice, the low pass filtering has more impact in mineral exploration since we are interested in finding orebodies within shallow depth in most cases, i.e., 500 m from surface. Orebodies at larger depth may drastically lose their economic values due to the development cost. The usual flight line spacing, which depends on the size and depth of
target body, ranges 200~1,000 m. Thus loss of information caused by low-pass filtering may be significant. Meanwhile, the exploration of oil and gas has targets at a few kilometers depth and lateral dimension of several kilometers in length. If low pass filters have a relatively small filter length, then they may have less effect on data interpretation. In general, if the filter length is comparable to the width and depth of sources, the effect is expected to be appreciable.

To deal with the problem, I develop new inversion algorithms to include the low-pass filter in both forward modeling and sensitivity matrix calculation during the inversion process. It uses same filter as used in data acquisition. Comparing the results from inversion with and without including the filter enables me to understand the nature of the errors caused by the low-pass filter.

In 2D parametric inversions, I examine the errors by comparing true 2D synthetic models with inverted models where an inversion algorithm assumes that the filtered data were solely the geological responses. The results indicate that filtering can lead to large errors, especially for models that are narrow or located at shallow depths. My simulations with a new inversion algorithm have shown that including filtering in the inversion is effective and the errors from the improved inversion are within an acceptable range. 2D parametric inversions are able to achieve much better data misfit when the low-pass
filtering is included, indicating improved consistency between the observed data and forward modeling.

For 3D inversion, I investigate the case of density inversion using Tikhonov regularization. A crucial factor in Tikhonov inversion is the expected misfit value. I first investigate the definition of data misfit in the presence of correlated random noise. This is necessary because we know the data is correlated due to the low pass filtering. In chapter 3, I focus on finding the expected data misfit of such filtered data. I demonstrate that the covariance matrix of the data noise is singular if the filter length is larger than the data spacing, which is true for most airborne data. Thus, the commonly presented data misfit function based on the inverse of the covariance matrix is invalid. I choose to return to the traditional chi-squared data misfit based on the variance alone. With such a definition, I show by simulation that the target data misfit of the filtered data is equal to the number of data points. This is quite a remarkable result, and it can be directly used in 3D inversion to select the best regularization parameter based on the discrepancy principle.

To verify the effectiveness of including filtering in 3D inversion, I compare the new inversion result with that of previous algorithm through two synthetic models. For model-A, the new algorithm clearly reduces the difference between the true and recovered models, and improves the resolution in both the lateral and depth direction. For model-B, the new algorithm can separate the two prisms, while the old algorithm only
recovers a laterally extended single body. Furthermore, the definition of depth
distribution of density is also better. Thus, I have obtained the similar improved results in
3D density inversions as in 2D parametric inversions.

I also test the new algorithm on a vertical gravity gradient field data acquired near
the Broken Hill deposit in Australia. This is a set of vertical gravity gradient data derived
from BHP’s Falcon system. The data were first inverted by assuming there is no filtering
process affecting the data. I then re-invert the data by using the filter parameters
estimated from comparison between ground and airborne data (Lane, 2004). The results
of two inversions are consistent with the synthetic inversion results. Specifically, there is
more lateral resolution when the appropriate filtering is included in the inversion.

6.2 Future Work

Because of its intrinsic function to suppress noise, low-pass filtering in data
acquisition applied either in real-time or during post-processing of airborne gravity
gradient data is inevitable. Thus, one branch of future work may be the study of the low-
pass filter. There are currently three airborne gravity gradient systems in operation and
many parts of the filtering process are not disclosed. My work has shown that this is an
important piece of information for correct interpretation of airborne gravity gradient data.
Further study on noise level of data is also anticipated. In practice, one may just neglect certain measured data as a noise. For example, any measurement under 2.5 standard deviation is regarded as useless noise in the Falcon system. However, the actual noise level in a field data set with varying geologic condition is not well understood.

Many aspects of data acquisition and post-processing can introduce errors into the data. They must be quantified in order to perform quantitative inversion. In particular, the terrain correction of airborne gravity gradiometry data is an area that requires further research. First, there is little information in published literature on the requirement of digital elevation model (DEM) and its resolution when used in terrain correction. Secondly, the consistent terrain correction must also include low-pass filtering. Otherwise, a straightforward correction is inconsistent with the data acquisition and will adversely affect the resultant data sets and subsequent interpretation.
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