Chapter 1

Fundamentals of data regularization

In this chapter, I develop a general theoretical framework for addressing the data regularization problem. The problem fundamentals are traced back to statistical estimation theory. Following Claerbout (1992, 1999), I formulate data regularization as a simple linear-estimation problem.

STATISTICAL ESTIMATION

Let $\mathbf{d}$ be the vector of observed data, and $\mathbf{m}$ be the ideal underlying model. The regularized data represent the model estimate $<\mathbf{m}>$. Taking into account the lack of information about $\mathbf{m}$, we can treat both $\mathbf{m}$ and $\mathbf{d}$ as random vectors and approach the problem of finding $<\mathbf{m}>$ statistically.

For any two random vectors $\mathbf{x}$ and $\mathbf{y}$, let us denote by $\mathbf{C}_{xy}$ the mathematical expectation of the random matrix $\mathbf{x}\mathbf{y}^T$, where $\mathbf{y}^T$ denotes the adjoint of y. Analogously, $\mathbf{C}_x$ will denote the mathematical expectation of $\mathbf{x}\mathbf{x}^T$. For zero-mean vectors, the matrices $\mathbf{C}_x$ and $\mathbf{C}_{xy}$ correspond to covariances. In a more general case, they are second-moment statistics of the corresponding random processes.

Applying the Gauss-Markoff theorem, one can obtain an explicit form of the estimate $<\mathbf{m}>$ under three very general assumptions (Liebelt, 1967):

1. The estimate has a linear relationship with the input data:

$$<\mathbf{m}>=\mathbf{A}\,\mathbf{d}\,, \tag{1.1}$$

where $\mathbf{A}$ is a linear operator.

2. The estimate corresponds to the minimum of $\mathbf{C}_e = E\left(\mathbf{e}\,\mathbf{e}^T\right)$, where E is the mathematical expectation and $\mathbf{e}$ denotes the model error $\mathbf{e} = <\mathbf{m}> - \mathbf{m}$. For unbiased estimates (zero mathematical expectation of $\mathbf{e}$), the matrix $\mathbf{C}_e$ corresponds to the model error covariance. Although we do not make any explicit assumptions about the statistical distribution of the error, minimizing $\mathbf{C}_e$ is particularly meaningful in case of normal (Gaussian) distributions (Tarantola, 1987).

3. The square matrix $\mathbf{C}_d$ is invertible.

Doing a simple algebraic transformation, we find that

$$\begin{aligned}\mathbf{C}_e \;=\; & E\left[(<\mathbf{m}> - \mathbf{m})(<\mathbf{m}> - \mathbf{m})^T\right] = E\left[(\mathbf{A}\,\mathbf{d} - \mathbf{m})\left(\mathbf{d}^T\,\mathbf{A}^T - \mathbf{m}^T\right)\right] = \\ & \mathbf{A}\,\mathbf{C}_d\,\mathbf{A}^T - \mathbf{C}_{md}\,\mathbf{A}^T - \mathbf{A}\,\mathbf{C}_{md}^T + \mathbf{C}_m = \\ & \left(\mathbf{A} - \mathbf{C}_{md}\,\mathbf{C}_d^{-1}\right)\mathbf{C}_d\,\left(\mathbf{A} - \mathbf{C}_{md}\,\mathbf{C}_d^{-1}\right)^T - \mathbf{C}_{md}\,\mathbf{C}_d^{-1}\,\mathbf{C}_{md} + \mathbf{C}_m\,.\end{aligned} \tag{1.2}$$

It is evident from equation (1.2) that C_e will be minimized when $\mathbf{A} = \mathbf{C}_{md}\,\mathbf{C}_d^{-1}$. This leads immediately to the Gauss-Markoff result

$$<\mathbf{m}>=\mathbf{C}_{md}\,\mathbf{C}_d^{-1}\,\mathbf{d}\,. \tag{1.3}$$

Equation (1.3) has fundamental importance in different data regularization schemes. With some slight modifications, it appears as the basis for such methods as optimal interpolation in atmospheric data analysis (Gandin, 1965; Daley, 1991), least-squares collocation in geodesy (Moritz, 1980), and linear kriging in petroleum and mining engineering (Journel and Huijbregts, 1978; Hohn, 1999). In order to apply formula (1.3) in practice, one needs first to get an estimate of the matrices $\mathbf{C}_{md}$ and $\mathbf{C}_d$. In geostatistics, the covariance matrices are usually chosen from simple variogram models (Deutsch and Journel, 1997).

Unfortunately, a straightforward application of the Gauss-Markoff formula (1.3) is computationally unaffordable for typical seismic data applications. If the data vector contains N parameters, a straightforward application will lead to an N by N matrix inversion, which requires storage proportional to N^2 and a number of operations proportional to N^3. Although the data can be divided into local patches to reduce the computational requirements for an individual patch, the total computational complexity is still too high to be affordable for the values of N typical in 3-D seismic exploration (N as high as 10^{10}).

We can take two major theoretical steps to reduce the computational complexity of the method. The first step is to approximate the covariance matrices with sparse operators so that the matrix multiplication is reduced from N^2 operations to something linear in N. The second step is to approach model estimation as an optimization problem and to use an iterative method for solving it. The goal is to obtain a reasonable model estimate after only a small number of iterations.

REPRESENTING COVARIANCE MATRICES BY SPARSE OPERATORS

In order to understand the structure of the matrices $\mathbf{C}_{md}$ and $\mathbf{C}_d$, we need to make some assumptions about the relationship between the true model $\mathbf{m}$ and the data $\mathbf{d}$. A natural assumption is that if the model were known exactly, the observed data would be related to it by a *forward interpolation operator* $\mathbf{L}$ as follows:

$$\mathbf{d} = \mathbf{L}\,\mathbf{m} + \mathbf{n}\,, \tag{1.4}$$

where $\mathbf{n}$ is an additive observational noise. For simplicity, we can assume that the noise is uncorrelated and normally distributed around zero:

$$\mathbf{C}_{mn} = 0\,; \quad \mathbf{C}_n = \sigma_n^2\,\mathbf{I}\,, \tag{1.5}$$

where $\mathbf{I}$ is an identity matrix of the data size, and σ_n is a scalar. Assuming that there is no linear correlation between the noise and the model, we arrive at the following expressions for

the second moment matrices in formula (1.3):

$$\mathbf{C}_d = E\left[(\mathbf{L}\,\mathbf{m}+\mathbf{n})\left(\mathbf{m}^T\,\mathbf{L}^T+\mathbf{n}^T\right)\right] = \mathbf{L}\,\mathbf{C}_m\,\mathbf{L}^T+\sigma_n^2\,\mathbf{I}\,, \tag{1.6}$$

$$\mathbf{C}_{md} = E\left[\mathbf{m}\left(\mathbf{m}^T\,\mathbf{L}^T+\mathbf{n}^T\right)\right] = \mathbf{C}_m\,\mathbf{L}^T\,. \tag{1.7}$$

Substituting equations (1.6) and (1.7) into (1.3), we finally obtain the following specialized form of the Gauss-Markoff formula:

$$<\mathbf{m}>=\mathbf{C}_m\,\mathbf{L}^T\left(\mathbf{L}\,\mathbf{C}_m\,\mathbf{L}^T+\sigma_n^2\,\mathbf{I}\right)^{-1}\mathbf{d}\,. \tag{1.8}$$

Assuming that $\mathbf{C}_m$ is invertible, we can also rewrite equation (1.8) in a mathematically equivalent form

$$<\mathbf{m}>=\left(\mathbf{L}\,\mathbf{L}^T+\sigma_n^2\,\mathbf{C}_m^{-1}\right)^{-1}\mathbf{L}^T\,\mathbf{d}\,. \tag{1.9}$$

The equivalence of formulas (1.8) and (1.9) follows from the simple matrix equality

$$\mathbf{C}_m\mathbf{L}^T(\mathbf{L}\mathbf{C}_m\mathbf{L}^T+\sigma_n^2\mathbf{I})^{-1} \equiv (\mathbf{L}^T\mathbf{L}+\sigma_n^2\mathbf{C}_m^{-1})^{-1}\mathbf{L}^T\,. \tag{1.10}$$

It is important to note an important difference between equations (1.8) and (1.9): The inverted matrix has data dimensions in the first case, and model dimensions in the second case. I discuss the practical significance of this distinction in Chapter 4.

In order to simplify the model estimation problem further, we can introduce a local differential operator $\mathbf{D}$. A model $\mathbf{m}$ complies with the operator $\mathbf{D}$ if the residual after we apply this operator $\mathbf{r}=\mathbf{D}\,\mathbf{m}$ is uncorrelated and normally distributed. This means that

$$E\left[\mathbf{D}\,\mathbf{m}\,\mathbf{m}^T\,\mathbf{D}^T\right] = \mathbf{D}\,\mathbf{C}_m\,\mathbf{D}^T = \sigma_m^2\,\mathbf{I}\,, \tag{1.11}$$

where the identity matrix $\mathbf{I}$ has the model size. Furthermore, assuming that $\mathbf{D}$ is invertible, we

can represent $\mathbf{C}_m$ as follows:

$$\mathbf{C}_m = \sigma_m^2 \left(\mathbf{D}^T \mathbf{D}\right)^{-1} . \tag{1.12}$$

Substituting formula (1.12) into (1.8) and (1.9), we can finally represent the model estimate in the following equivalent forms:

$$<\mathbf{m}> = \mathbf{P}\mathbf{P}^T \mathbf{L}^T \left(\mathbf{L}\mathbf{P}\mathbf{P}^T \mathbf{L}^T + \epsilon^2 \mathbf{I}\right)^{-1} \mathbf{d} ; \tag{1.13}$$

$$<\mathbf{m}> = \left(\mathbf{L}\mathbf{L}^T + \epsilon^2 \mathbf{D}^T \mathbf{D}\right)^{-1} \mathbf{L}^T \mathbf{d} , \tag{1.14}$$

where $\mathbf{P}\mathbf{P}^T = \left(\mathbf{D}^T \mathbf{D}\right)^{-1}$ and $\epsilon = \frac{\sigma_n}{\sigma_m}$.

The first simplification step has now been accomplished. By introducing additional assumptions, we have approximated the covariance matrices $\mathbf{C}_d$ and $\mathbf{C}_{md}$ with the forward interpolation operator $\mathbf{L}$ and the differential operator $\mathbf{D}$. Both $\mathbf{L}$ and $\mathbf{D}$ act locally on the model. Therefore, they are sparse, efficiently computed operators. Different examples of operators $\mathbf{L}$, $\mathbf{D}$, and $\mathbf{P}$ are discussed later in this dissertation. In the next section, I proceed to the second simplification step.

DATA REGULARIZATION AS AN OPTIMIZATION PROBLEM

The Gauss-Markoff equation (1.3) is derived as a solution of an optimization problem – minimizing the model error covariance matrix. After simplifying this equation to the forms (1.13) and (1.14), we can again recast it as a solution to an optimization problem of a different kind. In fact, equations (1.13) and (1.14) correspond to two fundamentally different optimization formulations.

Model-space regularization

Model-space regularization implies adding equations to system

$$\mathbf{L}\mathbf{m} \approx \mathbf{d} \tag{1.15}$$

to obtain a fully constrained (well-posed) inverse problem. The additional equations take the form

$$\epsilon \mathbf{D}\mathbf{m} \approx \mathbf{0} \,. \tag{1.16}$$

The full system of equations (1.15)-(1.16) can be written in a short notation as

$$\mathbf{G_m}\mathbf{m} = \begin{bmatrix} \mathbf{L} \\ \epsilon \mathbf{D} \end{bmatrix} \mathbf{m} \approx \begin{bmatrix} \mathbf{d} \\ \mathbf{0} \end{bmatrix} = \hat{\mathbf{d}} \,, \tag{1.17}$$

where $\hat{\mathbf{d}}$ is the effective data vector:

$$\hat{\mathbf{d}} = \begin{bmatrix} \mathbf{d} \\ \mathbf{0} \end{bmatrix} , \tag{1.18}$$

and $\mathbf{G_m}$ is a *column* operator:

$$\mathbf{G_m} = \begin{bmatrix} \mathbf{L} \\ \epsilon \mathbf{D} \end{bmatrix} . \tag{1.19}$$

The estimation problem (1.17) is fully constrained. We can solve it by means of unconstrained least-squares optimization, minimizing the squared power $\hat{\mathbf{r}}^T \hat{\mathbf{r}}$ of the compound residual vector

$$\hat{\mathbf{r}} = \hat{\mathbf{d}} - \mathbf{G_m}\mathbf{m} = \begin{bmatrix} \mathbf{d} - \mathbf{L}\mathbf{m} \\ -\epsilon \mathbf{D}\mathbf{m} \end{bmatrix} . \tag{1.20}$$

The formal solution of the regularized optimization problem has a known form, which coincides with formula (1.14). One can carry out the optimization iteratively with the help of the conjugate-gradient method (Hestenes and Steifel, 1952) or its analogs (Paige and Saunders, 1982).

The next subsection introduces an alternative formulation of the optimization problem.

Data-space regularization (model preconditioning)

The data-space regularization approach is closely related to the concept of *model preconditioning* (Nichols, 1994). Regarding the operator $\mathbf{P}$ from equation (1.13) as a preconditioning operator, we can introduce a new model $\mathbf{p}$ with the equality

$$\mathbf{m} = \mathbf{P}\mathbf{p} \,. \tag{1.21}$$

The residual vector $\mathbf{r}$ for the data-fitting equation (1.4) can be defined by the relationship

$$\epsilon \mathbf{r} = \mathbf{d} - \mathbf{L}\mathbf{m} = \mathbf{d} - \mathbf{L}\mathbf{P}\mathbf{p} \,, \tag{1.22}$$

where ϵ is the scaling parameter from equation (1.13). Let us consider a compound model $\hat{\mathbf{p}}$, composed of the preconditioned model vector $\mathbf{p}$ and the residual $\mathbf{r}$. With respect to the compound model, we can rewrite equation (1.22) as

$$\left[\begin{array}{cc} \mathbf{LP} & \epsilon \mathbf{I} \end{array} \right] \left[\begin{array}{c} \mathbf{p} \\ \mathbf{r} \end{array} \right] = \mathbf{G_d}\hat{\mathbf{p}} = \mathbf{d} \,, \tag{1.23}$$

where $\mathbf{G_d}$ is a *row* operator:

$$\mathbf{G_d} = \left[\begin{array}{cc} \mathbf{LP} & \epsilon \mathbf{I} \end{array} \right] , \tag{1.24}$$

and $\mathbf{I}$ represents the data-space identity operator.

System (1.23) is clearly underdetermined with respect to the compound model $\hat{\mathbf{p}}$. If from all possible solutions of this system we seek the one with the minimal power $\hat{\mathbf{p}}^T\hat{\mathbf{p}}$, the formal (ideal) result takes the well-known form

$$<\hat{\mathbf{p}} = \left[\begin{array}{c} <\mathbf{p}> \\ <\mathbf{r}> \end{array} \right] = \mathbf{G_d}^T \left(\mathbf{G_d}\,\mathbf{G_d}^T \right)^{-1} \mathbf{d} = \left[\begin{array}{c} \mathbf{P}^T\mathbf{L}^T \left(\mathbf{L}\mathbf{P}\mathbf{P}^T\mathbf{L}^T + \epsilon^2\mathbf{I} \right)^{-1} \mathbf{d} \\ \epsilon \left(\mathbf{L}\mathbf{P}\mathbf{P}^T\mathbf{L}^T + \epsilon^2\mathbf{I} \right)^{-1} \mathbf{d} \end{array} \right] . \tag{1.25}$$

Applying equation (1.21), we obtain the corresponding estimate $<\mathbf{m}>$ for the initial model $\mathbf{m}$, which is precisely equivalent to equation (1.13). This proves the legitimacy of the alternative

Table 1.1: Comparison between model-space and data-space regularization

Regularization	*Model-space*	*Data-space*
effective model	$\mathbf{m}$	$\hat{\mathbf{p}} = \begin{bmatrix} \mathbf{p} \\ \mathbf{r} \end{bmatrix}$
effective data	$\hat{\mathbf{d}} = \begin{bmatrix} \mathbf{d} \\ \mathbf{0} \end{bmatrix}$	$\mathbf{d}$
effective operator	$\mathbf{G_m} = \begin{bmatrix} \mathbf{L} \\ \epsilon\mathbf{D} \end{bmatrix}$	$\mathbf{G_d} = \begin{bmatrix} \mathbf{LP} & \epsilon\mathbf{I} \end{bmatrix}$
optimization problem	minimize $\hat{\mathbf{r}}^T\hat{\mathbf{r}}$, where $\hat{\mathbf{r}} = \hat{\mathbf{d}} - \mathbf{G_m}\mathbf{m}$	minimize $\hat{\mathbf{p}}^T\hat{\mathbf{p}}$ under the constraint $\mathbf{G_d}\hat{\mathbf{p}} = \mathbf{d}$
formal estimate for $\mathbf{m}$	$\left(\mathbf{L}^T\mathbf{L} + \epsilon^2\mathbf{C}^{-1}\right)\mathbf{L}^T\mathbf{d}$, where $\mathbf{C}^{-1} = \mathbf{D}^T\mathbf{D}$	$\mathbf{CL}^T(\mathbf{LCL}^T + \epsilon^2\mathbf{I})^{-1}\mathbf{d}$, where $\mathbf{C} = \mathbf{PP}^T$.

data-space approach to data regularization: the model estimation is reduced to least-square minimization of the specially constructed compound model $\hat{\mathbf{p}}$ under the constraint (1.22).

I summarize the differences between model-space and data-space regularization in Table 1.1.

Although the two approaches lead to similar theoretical results, they behave quite differently in the process of iterative optimization. In Chapter 4, I illustrate this fact with many examples and show that in the case of incomplete optimization, the second (preconditioning) approach is generally preferable.

The next chapter addresses the choice of the forward interpolation operator $\mathbf{L}$ – the necessary ingredient of the iterative data regularization algorithms.

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