ON THE DETERMINATION OF THE REGULARIZATION PARAMETER IN THE VARIATIONAL PROBLEM OF DATA PROCESSING

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Abstract. *Three different principles were considered for the determination of the regularization parameter in the variational problem of data processing. These principles are based exclusively on properties of the covariance matrixes and they are treated as analogies of traditional principles of misclosure, quasisolution and smoothing functional, respectively. It is remarkable, that the classical case of the least squares collocation (with the regularization parameter equal to 1) was obtained as one of the roots of the equation corresponding to the misclosure principle.*

Introduction

Let us consider the famous solution of well-known variational problem of data processing. The equations of observations without a systematic part (Moritz, 1980) are

$$\mathbf{l} = \mathbf{s} + \mathbf{n}, \quad (1)$$

where $\mathbf{l}$ is the observation vector, $\mathbf{s}$ is the signal vector, which is characterized by the covariance matrix $\mathbf{C}_{ss}$, and $\mathbf{n}$ is the noise vector, which is characterized by the covariance matrix $\mathbf{C}_{nn}$. By using the standard variational principle (Moritz, 1980)

$$\Phi_{\alpha,\beta} = \beta\mathbf{n}^{\mathrm{T}}\mathbf{C}_{nn}^{-1}\mathbf{n} + \alpha\mathbf{s}^{\mathrm{T}}\mathbf{C}_{ss}^{-1}\mathbf{s} = \min, \quad (2)$$

with the non-negative weighting coefficients α and β, we can obtain estimations for signal and noise in the following form:

$$\hat{\mathbf{s}} = \mathbf{C}_{ss}(\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}\mathbf{l}, \quad (3)$$

$$\hat{\mathbf{n}} = \gamma\mathbf{C}_{nn}(\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}\mathbf{l}, \quad (4)$$

where

$$\gamma = \frac{\alpha}{\beta} \geq 0. \quad (5)$$

In view of (3) and (4), we can rewrite (2) as

$$\Phi_{\gamma} = \mathbf{n}^{\mathrm{T}}\mathbf{C}_{nn}^{-1}\mathbf{n} + \gamma\mathbf{s}^{\mathrm{T}}\mathbf{C}_{ss}^{-1}\mathbf{s} = \min. \quad (6)$$

The functional (6) is nothing else but Tikhonov's smoothing functional (Tikhonov and Arsenin, 1986) in which the quadratic form $\mathbf{s}^{\mathrm{T}}\mathbf{C}_{ss}^{-1}\mathbf{s}$ is the stabilizer and γ is the regularization parameter. It is obvious, that the case $\gamma=1$ leads to the traditional least squares collocation solution. Therefore, we can treat least squares collocation as the particle case of Tikhonov's regularization (Neyman, 1979). Nevertheless, our goal consists of the determination of the regularization parameter γ in the frame of the variational problem (6).

1. Misclosure principle

Traditional approach to the determination of γ is based on misclosure principle (Tikhonov and Arsenin, 1986; Neyman, 1979; Morozov, 1987) which in the terms of (3) and (4) may be written as

$$\|\mathbf{l} - \hat{\mathbf{s}}\| = \|\hat{\mathbf{n}}\| = e_n, \quad (7)$$

where the value e_n characterizes a-priori magnitude of the misclosure (Morozov, 1987) and the norms is usual Euclidean vector norm (Horn and Johnson, 1986). However, we should keep in mind that in the model (1) the noise vector $\mathbf{n}$ is characterized by the a priori covariance matrix $\mathbf{C}_{nn}$ whereas the estimation (4) of the misclosure is characterized by the a posteriori covariance matrix

$$\hat{\mathbf{C}}_{nn} = \gamma^2\mathbf{C}_{nn}(\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}(\mathbf{C}_{ss} + \mathbf{C}_{nn}) \times (\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}\mathbf{C}_{nn}, \quad (8)$$

which may be derived in elementary way by applying the famous covariance propagation rule (Moritz, 1980) to the estimation (4). Now it would be natural to consider the next interesting case

$$\|\mathbf{C}_{nn} - \hat{\mathbf{C}}_{nn}\| = \|\Delta\mathbf{C}_{nn}\| = \min \quad (9)$$

for the further determination of γ. Here the norm is Euclidean matrix norm (Horn and Johnson, 1986):

$$\|\mathbf{A}\|^2 = \mathrm{Trace}(\mathbf{A}^{\mathrm{T}}\mathbf{A}) = \mathrm{Trace}(\mathbf{A}\mathbf{A}^{\mathrm{T}}) \quad (10)$$

and $\mathbf{A}$ is a real matrix of general kind.

After some obvious transformations, the residual matrix $\Delta\mathbf{C}_{nn}$ may be represented in the form

$$\Delta\mathbf{C}_{nn} = \mathbf{C}_{ss}(\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1} \times \left[-\gamma^2\mathbf{C}_{nn} + 2\gamma\mathbf{C}_{nn} + \mathbf{C}_{ss}\right] \times (\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}\mathbf{C}_{nn}. \quad (11)$$

Because the covariance matrixes $\mathbf{C}_{ss}$ and $\mathbf{C}_{nn}$ are positive defined (Moritz, 1980), we can see that extremal properties of the matrix $\Delta\mathbf{C}_{nn}$ are defined only by the term

$$\mathbf{D}_n(\gamma) = -\gamma^2\mathbf{C}_{nn} + 2\gamma\mathbf{C}_{nn} + \mathbf{C}_{ss}. \qquad (12)$$

As a result, the requirement

$$\|\mathbf{D}_n(\gamma)\| = \min \qquad (13)$$

may be considered as an equivalent of the requirement (9) and treated as covariance matrix analogy of misclosure principle (7).

Minimum of the norm (13) holds for those values of γ which fulfil to the equation

$$(1-\gamma)\times \left[-\gamma^2\|\mathbf{C}_{nn}\|^2 + 2\gamma\|\mathbf{C}_{nn}\|^2 + (\mathbf{C}_{ss},\mathbf{C}_{nn})\right] = 0, \qquad (14)$$

where the "scalar product" of symmetric positive defined matrixes $\mathbf{C}_{ss}$ and $\mathbf{C}_{nn}$ is introduced by analogy with the norm (10):

$$(\mathbf{C}_{ss},\mathbf{C}_{nn}) = \mathrm{Trace}(\mathbf{C}_{ss}\mathbf{C}_{nn}) = \mathrm{Trace}(\mathbf{C}_{nn}\mathbf{C}_{ss}). \quad (15)$$

From (14), we get immediately first remarkable root of this algebraic equation

$$\gamma = 1. \qquad (16)$$

It does not depend on covariance matrixes $\mathbf{C}_{ss}$ and $\mathbf{C}_{nn}$ and corresponds to traditional least squares collocation solution of the system (1). Therefore, we come to the important conclusion: in view of (9), the least squares collocation solution satisfies to the covariance matrix misclosure principle. Note here that the value (16) provides zero value of the first order derivative of the matrix (12) with respect to γ:

$$\frac{\partial}{\partial\gamma}\mathbf{D}_n(\gamma) = 2(1-\gamma)\mathbf{C}_{nn}. \qquad (17)$$

From the square equation

$$-\gamma^2\|\mathbf{C}_{nn}\|^2 + 2\gamma\|\mathbf{C}_{nn}\|^2 + (\mathbf{C}_{ss},\mathbf{C}_{nn}) = 0, \quad (18)$$

that follows from (14) for $\gamma \neq 1$, we can find second appropriate root

$$\gamma = 1 + \sqrt{1 + \frac{(\mathbf{C}_{ss},\mathbf{C}_{nn})}{\|\mathbf{C}_{nn}\|^2}}. \qquad (18)$$

This also provides minimum of the norm (13) and realizes the solution of (6) under the misclosure principle.

2. Quasisolution principle

Another principle, which can be used for the determination of the regularization parameter, is so-called quasisolution principle (Morozov, 1987). It may be written in the terms of the estimation (3) as

$$\|\hat{\mathbf{s}}\| = e_s, \qquad (19)$$

where the value e_s is connected with an a-priori information about the size of the domain which consists of the solution. In our case such information is provided by the a-priori covariance matrix of the signal vector $\mathbf{s}$ together with the a-posteriori covariance matrix of the estimation (3):

$$\hat{\mathbf{C}}_{ss} = \mathbf{C}_{ss}(\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}(\mathbf{C}_{ss} + \mathbf{C}_{nn}) \times (\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}\mathbf{C}_{ss}, \qquad (20)$$

which is obtained by applying the covariance propagation rule (Moritz, 1980) to (3). On this ground, we are considering again the next special case

$$\|\mathbf{C}_{ss} - \hat{\mathbf{C}}_{ss}\| = \|\Delta\mathbf{C}_{ss}\| = \min, \qquad (21)$$

where the residual matrix $\Delta\mathbf{C}_{ss}$ may be represented in the form

$$\Delta\mathbf{C}_{ss} = \mathbf{C}_{nn}(\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1} \times \left[\gamma^2\mathbf{C}_{nn} + 2\gamma\mathbf{C}_{ss} - \mathbf{C}_{ss}\right] \times (\mathbf{C}_{ss} + \gamma\mathbf{C}_{nn})^{-1}\mathbf{C}_{ss}. \qquad (22)$$

It is evident, that extremal properties of the matrix (22) are defined only by the term

$$\mathbf{D}_s(\gamma) = \gamma^2\mathbf{C}_{nn} + 2\gamma\mathbf{C}_{ss} - \mathbf{C}_{ss}. \qquad (23)$$

Therefore, the requirement

$$\|\mathbf{D}_s(\gamma)\| = \min \qquad (24)$$

may be considered as an equivalent of the requirement (21) and treated as covariance matrix analogy of quasisolution principle (19).

Minimum of the norm (24) holds for those values of γ which fulfil to the third-order equation

$$\gamma^3\|\mathbf{C}_{nn}\|^2 + 3\gamma^2(\mathbf{C}_{ss},\mathbf{C}_{nn}) + \gamma\left[2\|\mathbf{C}_{ss}\|^2 - (\mathbf{C}_{ss},\mathbf{C}_{nn})\right] - \|\mathbf{C}_{ss}\|^2 = 0. \qquad (25)$$

This equation may be solved by iterations on the ground of recurrence formula

$$\gamma = \frac{\|\mathbf{C}_{ss}\|^2 + \gamma(\mathbf{C}_{ss},\mathbf{C}_{nn})}{\gamma^2\|\mathbf{C}_{nn}\|^2 + 3\gamma(\mathbf{C}_{ss},\mathbf{C}_{nn}) + 2\|\mathbf{C}_{ss}\|^2} \qquad (26)$$

with the starting value $\gamma=0$. Because in (25) and (26) all matrixes are positive defined, we can see that the equation (25) has only one positive root, which belongs to the interval

$$0<\gamma<\frac{1}{2}. \qquad (27)$$

3. Smoothing functional principle

Third principle, which can be used for the determination of the regularization parameter, is so-called smoothing functional principle (Morozov, 1987), which is provided by joint application of the misclosure and quasisolution principles.

So, once again, we will study the next minimum

$$\|\mathbf{D}_n(\gamma)\|^2+\|\mathbf{D}_s(\gamma)\|^2=\min. \qquad (28)$$

In the terms of norms (13) and (24) we come to the third-order equation

$$\begin{aligned}&2\gamma^3\|\mathbf{C}_{nn}\|^2+3\gamma^2\left[(\mathbf{C}_{ss},\mathbf{C}_{nn})-\|\mathbf{C}_{nn}\|^2\right]+\\&2\gamma\left[\|\mathbf{C}_{ss}\|^2+\|\mathbf{C}_{nn}\|^2-(\mathbf{C}_{ss},\mathbf{C}_{nn})\right]+\\&(\mathbf{C}_{ss},\mathbf{C}_{nn})-\|\mathbf{C}_{ss}\|^2=0.\end{aligned} \qquad (29)$$

It may be shown, that this equation has only one positive root and may be solved by iterations with the starting value $\gamma=0$. Iterations may be realized by the Newton recurrence formula

$$\gamma=\frac{f_1(\gamma)}{2f_2(\gamma)}, \qquad (30)$$

in which

$$\begin{aligned}f_1(\gamma)=&4\gamma^3\|\mathbf{C}_{nn}\|^2+\\&3\gamma^2\left[(\mathbf{C}_{ss},\mathbf{C}_{nn})-\|\mathbf{C}_{nn}\|^2\right]+\\&\|\mathbf{C}_{ss}\|^2-(\mathbf{C}_{ss},\mathbf{C}_{nn}),\end{aligned} \qquad (31)$$

$$\begin{aligned}f_2(\gamma)=&3\gamma^2\|\mathbf{C}_{nn}\|^2+\\&3\gamma^2\left[(\mathbf{C}_{ss},\mathbf{C}_{nn})-\|\mathbf{C}_{nn}\|^2\right]+\\&\|\mathbf{C}_{ss}\|^2-(\mathbf{C}_{ss},\mathbf{C}_{nn})+\|\mathbf{C}_{nn}\|^2.\end{aligned} \qquad (32)$$

4. Numerical testing

Numerical examination of the above considered approaches to the determination of the regularization parameter was carried out on the basis of processing of 2200 modeled gravity anomalies, distributed over Austria area. In this modeling, gravity anomalies were computed by means of EGM96 (Rapp and Nerem, 1995) gravity model starting from the degree 181 up to degree 360. Such field was considered as the residual anomaly field and was processed by means of the formula (3) with adopted the variance of the noise 0.01 mGal^2 whereas the variance of the residual gravity anomalies was about 210 mGal^2. Results of the comparison of predicted signals with the modeled gravity anomalies are presented in the Table 1.

Table 1. Results (mGal) of gravity anomaly prediction

	Formula for the regularization parameter			
	(16)	(18)	(26)	(30)
Min.	-0.030	-0.485	-0.023	-0.023
Max.	0.031	0.501	0.021	0.021
Mean	0.000	0.000	0.000	0.000
Std. dev.	0.003	0.035	0.002	0.002
γ	1	144	0.499	0.499

As we can see, all approaches led to centered estimations of the signal. Moreover, value of standard deviation of residuals is dependent on the value of the regularization parameter. The last, in fact, provides a level of the signal smoothing. Although the relatively great minimal and maximal residuals take place at the border of the data area in the case of application of the misclosure principle with formula (18), we obtain the standard deviation value essentially smaller than a priori given value of errors (0.1 mGal).

Conclusions

As a result, we have realized three different principles for the determination of the regularization parameter in the variational problem of data processing. These principles are based exclusively on properties of the covariance matrixes and they are treated as analogies of traditional principles of misclosure, quasisolution and smoothing functional, respectively. It is remarkable, that the classical case of the least squares collocation (with the regularization parameter equal to 1) was obtained as one of the roots of the equation corresponding to the misclosure principle. All considered principles were tested numerically and led to appropriate results of gravity anomaly prediction.

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ПРО ВИЗНАЧЕННЯ ПАРАМЕТРУ РЕГУЛЯРИЗАЦІЇ У ВАРІАЦІЙНІЙ ЗАДАЧІ ОБРОБКИ ДАНИХ

Резюме

Розглянуті три різні принципи визначення параметру регуляризації у варіаційній задачі обробки даних. Ці принципи грунуються лише на властивостях коваріаційних мариць й трактуються як аналогії традиційних принципів нев'язки, квазірозв'язку та згладжуючого функціоналу. Класичний випадок середньої квадратичної колокації (з параметром реруляризації, рівним 1) був одержаний як один з коренів рівняння, що відповідає принципу нев'язки.

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ОБ ОПРЕДЕЛЕНИИ ПАРАМЕТРА РЕГУЛЯРИЗАЦИИ В ВАРИАЦИОННОЙ ЗАДАЧЕ ОБРАБОТКИ ДАННЫХ

Резюме

Рассмотрены три различных принципа определения параметра регуляризации в вариационной задаче обработки данных. Эти принципы основаны только на свойствах ковариационных матриц и трактуются как аналогии традиционных принципов невязки, квазирешения и сглаживающего функционала. Классический случай средней квадратической коллокации (с параметром регуляризации, равным 1) получен как один из корней уравнения, соответствующего принципу невязки.