

Chapter 2

Basic Mathematics

Abstract The basic mathematics useful for this book is divided into discrete least squares theory, collocation, coordinate systems, Legendre's polynomials, spherical and ellipsoidal harmonics, the fundamentals of potential theory and regularization. Most numerical applications are based on linear least squares theory, either in the spatial domain (mainly for local studies) or by spherical harmonics in regional and global applications. For example, linear regression analysis, discrete and continuous least squares collocation are described. As problems in geodesy and geophysics are frequently non-linear, the linearization of such a problem is also presented. After introducing Legendre's polynomials and spherical harmonics, the latter type of series is used for spectral smoothing and combining sets of data. The gravitational potential on and outside the ellipsoid is also presented in ellipsoidal harmonics. One section is devoted to the basics of potential theory, including some basic concepts, Newton's integral for the potential, Laplace's and Poisson's equations and Gauss' and Green's formulas, as a well as basic boundary value problems, as a background for the rest of the book. Considering that most problems related with gravity inversion are inverse problems, regularization is needed to reach a practical solution. Hence, various approaches to regularization of solutions to inverse problems are shortly described and compared.

Keywords Basic mathematics • Collocation • Coordinate systems • Least squares theory • Legendre's polynomials • Spherical harmonics • Potential theory • Regularization

2.1 Least Squares Adjustment Theory

Least squares treatment of large data sets is common in geodesy, surveying and geophysics. Least squares collocation, widely used in geodesy, is closely related with kriging, frequently applied in geophysical prospecting. This book will apply

least squares in various ways in physical geodesy and geophysics, and the basics are provided in this section.

Definition 2.1 Let x be a stochastic estimator for the parameter μ . If the stochastic expectation $E\{x\} = \mu$ holds, we say that x is an unbiased estimator of μ and its variance is given by:

$$\sigma_x^2 = E\{(x - \mu)^2\}. \quad (2.1)$$

Definition 2.2 If $E\{x\} \neq \mu$, then x is a *biased* estimator of μ , and its Mean Square Error,

$$MSE\{x\} = E\{(x - \mu)^2\} = \sigma_x^2 + bias_x^2, \quad (2.2a)$$

is the sum of its variance given by (2.1) and the bias squared, the bias given by:

$$bias_x = E\{x\} - \mu. \quad (2.2b)$$

Equation (2.2a) follows directly from the relation:

$$MSE\{x\} = E\{(x - \mu)^2\} = E\{(x - E\{x\} + E\{x\} - \mu)^2\}. \quad (2.3)$$

2.1.1 Adjustment by Elements

Let us assume that \mathbf{L} is a vector of n observations with a random error vector $\boldsymbol{\varepsilon}$. If \mathbf{L} is related with the unknown parameter vector \mathbf{X} (with $m < n$ elements) by the linear matrix equation (system of observation equations)

$$\mathbf{AX} = \mathbf{L} - \boldsymbol{\varepsilon}, \quad (2.4)$$

where \mathbf{A} is called the design matrix, assumed to be of full rank, the least squares solution to (2.4), minimizing the weighted sum of squares of errors, $\boldsymbol{\varepsilon}^T \mathbf{P} \boldsymbol{\varepsilon}$, is:

$$\hat{\mathbf{X}} = (\mathbf{A}^T \mathbf{P} \mathbf{A})^{-1} \mathbf{A}^T \mathbf{P} \mathbf{L}. \quad (2.5a)$$

The error vector and covariance matrix of the unknowns become:

$$\hat{\boldsymbol{\varepsilon}} = \mathbf{L} - \mathbf{A} \hat{\mathbf{X}} \quad (2.5b)$$

and

$$\mathbf{Q}_X = \sigma_0^2 (\mathbf{A}^T \mathbf{P} \mathbf{A})^{-1}. \quad (2.5c)$$

Here \mathbf{P} is a positive definite weight matrix among the observations, $()^{-1}$ is the inverse of the matrix in the bracket and σ_0^2 is the variance of unit weight. The latter can be unbiasedly estimated by:

$$s^2 = \hat{\boldsymbol{\varepsilon}}^T \mathbf{P} \hat{\boldsymbol{\varepsilon}} / (n - m) = \mathbf{L}^T \mathbf{P} (\mathbf{L} - \mathbf{A} \hat{\mathbf{X}}) / (n - m), \quad (2.5d)$$

where n and m are the numbers of observations and unknown parameters, respectively.

Example 1 Consider a linear regression in time (t_i) with observation equations

$$a + bt_i = l_i - \varepsilon_i; \quad i = 1, \dots, n, \quad (2.6a)$$

or, in a matrix equation

$$\begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_n \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} l_1 \\ \vdots \\ l_n \end{bmatrix} - \boldsymbol{\varepsilon} \quad (2.6b)$$

with the least squares solution for the parameters a and b

$$\begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^n t_i \\ \sum_{i=1}^n t_i & \sum_{i=1}^n t_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^n l_i \\ \sum_{i=1}^n t_i l_i \end{bmatrix} \quad (2.6c)$$

If one substitutes t_i by $\Delta t_i = t_i - t_0$, where $t_0 = (\sum_{i=1}^n t_i) / n$ is the mean of the observation times, one obtains:

$$\sum_{i=1}^n \Delta t_i = 0,$$

implying that the off-diagonal elements of the normal matrix $\mathbf{A}^T \mathbf{A}$ vanish, yielding a diagonal matrix, and the above solution is simplified to:

$$\hat{a} = \sum_{i=1}^n l_i / n \quad \text{and} \quad \hat{b} = \sum_{i=1}^n \Delta t_i l_i / \sum_{i=1}^n (\Delta t_i)^2 \quad (2.6d)$$

with standard errors

$$s_{\hat{a}} = s/\sqrt{n} \quad \text{and} \quad s_{\hat{b}} = s/\sqrt{\sum_{i=1}^n (\Delta t_i)^2}, \quad (2.6e)$$

where the variance of unit weight (s) is given by Eq. (2.5d).

This solution is useful in estimating the secular change/trend parameter b of the set of observations (l) observed at different epochs. In particular, if the time interval (Δt) between successive epochs is constant, it follows that:

$$\hat{b} = \frac{2 \sum_{i=1}^n (2i - n - 1) l_i}{\Delta t \sum_{i=1}^n (2i - n - 1)^2} \quad \text{and} \quad s_b = \frac{s}{\Delta t \sqrt{\sum_{i=1}^n (2i - n - 1)^2}}. \quad (2.6f)$$

One may also eliminate the constant a in Eq. (2.6a) by substituting each observation l_i by $l_i - \bar{l}$, where \bar{l} is the mean of the observations.

The estimated secular trend (\hat{b}) may be sensitive to periodic signals not included in the regression analysis, in particular for long-periodic terms. If the periods (T_j) are known, their causes can be included in the adjustment by the revised formula

$$a + bt_i + \sum_{j=1}^J (c_j \cos \omega_j t_i + d_j \sin \omega_j t_i) = l_i - \varepsilon_i; \quad i = 1, \dots, n, \quad (2.6g)$$

where $\omega_j = 2\pi/T_j$ and J is the number of periodic signals included in the adjustment.

If the set of observations are evenly distributed over the period and includes one or a multiple of periods, the effect of the periodic term is eliminated. More generally, the regression formula is extended to multiple regression analysis by including several types of correlated observables. Then the normal matrix $\mathbf{A}^T \mathbf{P} \mathbf{A}$ of the solution (2.5a) will be a full matrix, and, for example, the simple solution for the trend parameter in (2.6f) does not hold, implying that the unknown parameters are correlated and mutually affect the solutions of the individual parameters.

– *Special Cases:*

- Frequently the underlying function $f_i(\mathbf{X})$ for the observation l_i is *non-linear*:

$$l_i - \varepsilon_i = f_i(\mathbf{X}); \quad i = 1, \dots, n, \quad (2.7a)$$

and by Taylor expansion of all observation equations the system may be linearized to the matrix equation

$$\mathbf{A}\Delta\mathbf{X} = \Delta\mathbf{L} - \boldsymbol{\varepsilon}, \quad (2.7b)$$

where \mathbf{A} is the design matrix as above, $\Delta\mathbf{X}$ is the (unknown) improvement of \mathbf{X} versus the approximate value \mathbf{X}_0 and

$$\Delta\mathbf{L} = \mathbf{L} - [f_1(\mathbf{X}_0), \dots, f_n(\mathbf{X}_0)]^T \quad (2.7c)$$

Here \mathbf{L} is the vector of observations l_i . By solving (2.7b) as in (2.5a), the least squares solution is achieved. As the original equations are non-linear, the solution may need to be iterated for convergence.

- If there are a priori information \mathbf{X}^- of the unknown vector \mathbf{X} with covariance matrix \mathbf{Q}_X , the matrix equation (2.4) can be augmented by the equation

$$\mathbf{I}\mathbf{X} = \mathbf{X}^- - \boldsymbol{\varepsilon}_x; \quad E(\boldsymbol{\varepsilon}_x \boldsymbol{\varepsilon}_x^T) = \mathbf{Q}_X, \quad (2.8a)$$

and assuming also that the observations \mathbf{X}^- and \mathbf{L} are uncorrelated, the improved least squares solution becomes (e.g. Sjöberg 2013, Sect. 12.1):

$$\hat{\mathbf{X}} = \mathbf{N}^{-1}(\mathbf{Q}_X^{-1}\mathbf{X}^- + \mathbf{A}^T\mathbf{Q}^{-1}\mathbf{L}) \quad (2.8b)$$

or

$$\hat{\mathbf{X}} = \mathbf{X}^- + \mathbf{K}(\mathbf{L} - \mathbf{A}\mathbf{X}^-), \quad (2.8c)$$

where:

$$\mathbf{N} = \mathbf{Q}_X^{-1} + \mathbf{A}^T\mathbf{Q}^{-1}\mathbf{A} \quad \text{and} \quad \mathbf{K} = \mathbf{Q}_X\mathbf{A}^T(\mathbf{A}\mathbf{Q}_X\mathbf{A}^T + \mathbf{Q})^{-1}, \quad (2.8d)$$

and the covariance matrix of the solution vector can be written:

$$\mathbf{Q}_{\hat{\mathbf{X}}} = \mathbf{N}^{-1} = \mathbf{Q}_X - \mathbf{K}\mathbf{A}\mathbf{Q}_X. \quad (2.8e)$$

It is obvious that this solution is both more stable and precise than the original solution (2.5a).

As an example, the solution of Eqs. (2.8c) and (2.8e) is useful in gravity inversion when a preliminary model of Earth parameters (\mathbf{X}^-) are at hand from a previous analysis, and new data (\mathbf{L}) are available to improve the model. In the case that the new observation equation is non-linear, it can be linearized as described above. Several other ways of adjusting the non-linear equations in combination with the preliminary model are discussed at length in Tarantola (1987).

- Closely related adjustment schemes are condition adjustment and condition adjustment with unknowns. See, e.g. Bjerhammar (1973, Chaps. 12 and 20),

A discrete least squares problem may be *rank deficient* or *ill-conditioned*, leading to proper and numerical singularities, respectively, in the systems of equations. In the first case, there is no unique solution. In the second case, a unique solution may exist, but the system is badly conditioned such that the numerical solution may fail or be badly contaminated by errors. In solving geoscience problems by gravity inversion, the systems of equations are frequently ill-conditioned, as such problems are typically *ill-posed*, which can be handled by some type of regularization (see Sect. 2.8).

2.2 Least Squares Collocation

2.2.1 Discrete Collocation

Least Squares Collocation (LSC) is a type of interpolation and/or prediction of stochastic variables, either within one type of observable or from the observations of one type to another. In addition, the covariances among the observables as well as between these and the predicted variable are assumed to be known.

Let x and y be stochastic variables with expectations zero. The variable y is assumed to be estimated (predicted) from observations of x . The auto-covariance and error covariance matrices (**C** and **D**) among the observations in the observation matrix **X**, as well as the cross-covariance vector **c** between y and **X**, are known. Moreover, if the variance of y , σ_y^2 , is known, the prediction variance can also be estimated. In this case y can be optimally estimated/predicted in a least squares sense by the formula (Moritz 1980, Part B)

$$\hat{y} = \mathbf{c}^T (\mathbf{C} + \mathbf{D})^{-1} \mathbf{X}, \quad (2.9a)$$

and the prediction variance becomes:

$$\sigma_{\hat{y}}^2 = \sigma_y^2 - \mathbf{c}^T (\mathbf{C} + \mathbf{D})^{-1} \mathbf{c}. \quad (2.9b)$$

Proof Consider the general linear estimator

$$\tilde{y} = \mathbf{a}^T \mathbf{X}, \quad (2.10a)$$

where **a** is an arbitrary vector and the error of **X** is ϵ with expectation zero. Then the prediction error becomes:

$$\varepsilon_{\tilde{y}} = \tilde{y} - y = \mathbf{a}^T \mathbf{X} - y, \quad (2.10b)$$

and by assuming that $\boldsymbol{\varepsilon}$ and y are uncorrelated, the prediction variance becomes:

$$\begin{aligned} \sigma_y^2 &= E\{\varepsilon_y^2\} = \sigma_y^2 + \mathbf{a}^T E\{(\mathbf{X} + \boldsymbol{\varepsilon})(\mathbf{X} + \boldsymbol{\varepsilon})^T\} \mathbf{a} - 2\mathbf{a}^T E\{(\mathbf{X} + \boldsymbol{\varepsilon})y\} \\ &= \sigma_y^2 + \mathbf{a}^T (\mathbf{C} + \mathbf{D}) \mathbf{a} - 2\mathbf{a}^T \mathbf{c} = \sigma_y^2 - \mathbf{c}^T (\mathbf{C} + \mathbf{D})^{-1} \mathbf{c} \\ &\quad + \left[\mathbf{a} - (\mathbf{C} + \mathbf{D})^{-1} \mathbf{c} \right]^T (\mathbf{C} + \mathbf{D}) \left[\mathbf{a} - (\mathbf{C} + \mathbf{D})^{-1} \mathbf{c} \right] \\ &\geq \sigma_y^2 - \mathbf{c}^T (\mathbf{C} + \mathbf{D})^{-1} \mathbf{c}, \end{aligned} \quad (2.10c)$$

where $\mathbf{C} = E\{\mathbf{x}\mathbf{x}^T\}$, $\mathbf{D} = E\{\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T\}$ and $\mathbf{c} = E\{\mathbf{x}y\}$. This shows that the optimum predictor is provided for $\mathbf{a} = (\mathbf{C} + \mathbf{D})^{-1} \mathbf{c}$, and the predictor and its variance follow from (2.9a, b).

If the expectation of x does not vanish, collocation can still be applied as above after first removing the bias, trend or systematic error by a least squares adjustment by elements as above. The whole procedure, including trend removal, is the general form of least squares collocation (Moritz 1980, Parts B and C).

When collocation is applied to the gravity field of the Earth, it is unrealistic to assume that the signal (but, on the contrary, the error) is stochastic, and this can only be assumed as an approximate model. As a result, also the signal covariance functions needed are in doubt. In the application of collocation the statistical expectation operator is replaced by a space average operator, which is not trivial. Lauritzen (1973) even proved that a Gaussian stochastic process of gravity is not ergodic, implying that “even if we knew gravity all over the Earth, we would not be able to find the true covariance function”. If there is only one realization available of the stochastic process, we cannot determine the true covariance function.

Nevertheless, discrete collocation is an important method for inter- and extrapolation that also provides an approximate estimate of the prediction variance. Even if this method is not the most precise technique, it is frequently also used for determining various quantities from gravity data. However, one should also bear in mind that collocation leads to large matrix systems when many observations are at hand.

In geology and geophysics, a similar concept named kriging has been developed for applications in geostatistics (see, e.g. Matheron 1963). The essential difference to collocation is the variogram that replaces the covariance function used in collocation. See, e.g. Dermanis (1984) for further details.

2.2.2 Continuous Collocation

Let x be a continuous stochastic process on the sphere with expectation zero and auto-covariance function $c_{xx}(P, Q)$. Its observation \bar{x} is contaminated by the error ε , which is assumed to be uncorrelated with the true signal x , has expectation 0 and auto-covariance function $d(P, Q)$.

Problem It is requested to determine the least squares solution to the linear continuous estimator on the sphere:

$$\tilde{y}_P = \iint_{\sigma} h\bar{x}d\sigma, \quad (2.11)$$

where h is an unknown kernel function to be determined such that the variance of \tilde{y} is a minimum. Here σ is the unit sphere. In addition, the cross-covariance function between the signals y and x , i.e. $c_{yx}(P, Q) = c_{xy}(P, Q)$, is assumed to be known.

Solution (Sjöberg 1979): The error of \tilde{y} is:

$$\varepsilon_y = \tilde{y} - y = \iint_{\sigma} h\bar{x}d\sigma - y, \quad (2.12)$$

with the prediction variance

$$\begin{aligned} \sigma_{\tilde{y}}^2(P) = E\{(\tilde{y} - y)^2\} &= \sigma_y^2(P) - 2 \iint_{\sigma} h(P, Q)c_{yx}(P, Q)d\sigma_Q \\ &+ \iint_{\sigma} h(P, Q) \left[\iint_{\sigma} h(P, Q')\{c_{uu}(Q, Q' + d((Q, Q'))\}d\sigma_{Q'} \right] d\sigma_Q. \end{aligned} \quad (2.13)$$

It follows that the minimum prediction variance

$$\sigma_{\tilde{y}}^2(P) = \sigma_y^2(P) - 2 \iint_{\sigma} \hat{h}(P, Q)c_{yx}(P, Q)d\sigma_Q \quad (2.14)$$

is obtained by:

$$c_{yx}(P, Q) = \iint_{\sigma} \hat{h}(P, Q')\{c_{uu}(Q, Q') + d(Q, Q')\}d\sigma_{Q'}. \quad (2.15)$$

which is the so-called Wiener-Hopf integral equation for the kernel function h . The least squares solution is thus given by Eq. (2.11) with h given by Eq. (2.15).

If there are two different sets of stochastic processes, x_1 and x_2 on the sphere, observed with random errors ε_1 and ε_2 , and all covariance functions are known (with obvious notations similar to the above example), a related stochastic process y can be optimally estimated from the general combined estimator

$$\tilde{y}_P = \iint_{\sigma} (h_1(P, Q)\bar{x}_1(Q) + h_2(P, Q)\bar{x}_2(Q))d\sigma. \quad (2.16)$$

The least squares solution for functions h_1 and h_2 are the solutions to the integral equations

$$c_{yx_1}(P, Q) = \iint_{\sigma} [\hat{h}_1(P, Q') \bar{c}_{11}(Q', Q) + \hat{h}_2(P, Q') c_{12}(Q', Q)] d\sigma' \quad (2.17a)$$

and

$$c_{yx_2}(P, Q) = \iint_{\sigma} [\hat{h}_2(P, Q') \bar{c}_{22}(Q', Q) + \hat{h}_1(P, Q') c_{21}(Q', Q)] d\sigma', \quad (2.17b)$$

where:

$\bar{c}_{11} = c_{11} + d_{11}$ and $\bar{c}_{22} = c_{22} + d_{22}$; d_{ii} are the respective noise covariance functions.

The expected least squares prediction variance becomes:

$$\begin{aligned} \sigma_{\hat{y}}^2(P) = & \sigma_y^2(P) - \iint_{\sigma} \left[\hat{h}_1(P, Q) \iint_{\sigma} \{ \bar{c}_{11}(Q, Q') \hat{h}_1(P, Q) + 2c_{12}(Q, Q') \hat{h}_2(P, Q') \} d\sigma' \right] d\sigma \\ & - \iint_{\sigma} \left[\hat{h}_2(P, Q) \iint_{\sigma} \{ \bar{c}_{22}(Q, Q') \hat{h}_2(P, Q') \} d\sigma' \right] d\sigma. \end{aligned} \quad (2.18)$$

The solutions to the kernel functions h_i can be conveniently determined from Eqs. (2.17a, b) by expressing all functions in spherical harmonics (see Sect. 2.8.2). If the stochastic processes are harmonic in the exterior of the sphere (which is the case if they are related with the gravity field and there are no topographic and atmospheric masses outside the sphere), the predictions \hat{y}_p can be extended to any point on or outside the sphere (Sjöberg 1979). The Wiener filter is further discussed in Sect. 2.8.2 as a method of *regularization*.

2.3 Coordinate Systems

Consider the point P in an Earth-fixed Cartesian coordinate system (x, y, z) , with origin at the Earth's centre of gravity, the z -axis along the Earth's axis of rotation and the (x, y) -plane in the equatorial plane with the x -axis in Greenwich meridian and y -axis at right angle to the east.

Then the Cartesian coordinates can also be expressed in spherical coordinates (see Fig. 2.1)

$$\begin{aligned} x &= r \cos \psi \cos \lambda \\ y &= r \cos \psi \sin \lambda \\ z &= r \sin \psi, \end{aligned} \quad (2.19)$$

Fig. 2.1 Relation between Cartesian and spherical coordinates

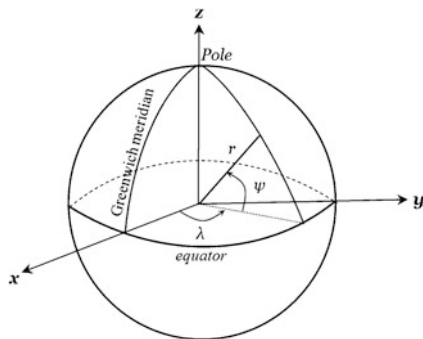
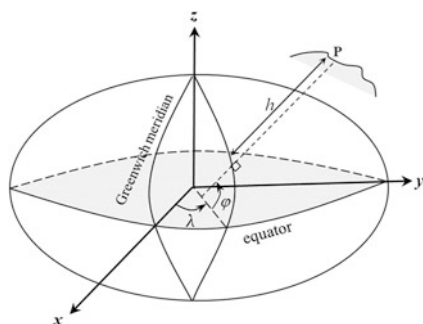


Fig. 2.2 Relation between Cartesian and geodetic coordinates



where r and ψ are the geocentric radius and latitude, respectively, and λ is the longitude.

The geodetic coordinates $(\varphi, \lambda, h) = (\text{latitude, longitude, height})$ are related to the Cartesian coordinates by the formulas (see Fig. 2.2)

$$\begin{aligned} x &= (\mathbb{N} + h) \cos \varphi \cos \lambda \\ y &= (\mathbb{N} + h) \cos \varphi \sin \lambda \\ z &= [\mathbb{N}(1 - e^2) + h] \sin \varphi, \end{aligned} \quad (2.20)$$

where:

$$\mathbb{N} = a / \sqrt{1 - e^2 \sin^2 \varphi} \quad (2.21)$$

is the radius of curvature in the prime vertical of the reference ellipsoid with semi-major and semi-minor axes a and b , and $e^2 = (a^2 - b^2)/a^2$ is the eccentricity of the ellipsoid squared.

Next we present the relationship between the Cartesian and ellipsoidal coordinates (u, β, λ) (see Fig. 2.3)

$$\begin{aligned} x &= \sqrt{u^2 + E^2} \cos \beta \cos \lambda \\ y &= \sqrt{u^2 + E^2} \cos \beta \sin \lambda \\ z &= u \sin \beta, \end{aligned} \quad (2.22)$$

where:

$$E = ae = \sqrt{a^2 - b^2}$$

is the linear eccentricity.

By considering a point on the reference ellipsoid (i.e., with $h = 0$ and $u = b$), it follows from the above equations that geocentric, geodetic and reduced latitudes (ψ, φ, β) are related by the equations

$$\frac{z}{\sqrt{x^2 + y^2}} = \tan \psi = (1 - e^2) \tan \varphi = \sqrt{1 - e^2} \tan \beta. \quad (2.23)$$

The Cartesian coordinates can be determined from the curvilinear coordinates above by straightforward transformations. The inverse transformations are much more cumbersome to derive, unless the computational point is located on the reference ellipsoid. An exception is the longitude, which for all three curvilinear coordinate systems above is the same and can be determined by:

$$\lambda = 2 \arctan \frac{y}{x + \sqrt{x^2 + y^2}}. \quad (2.24)$$

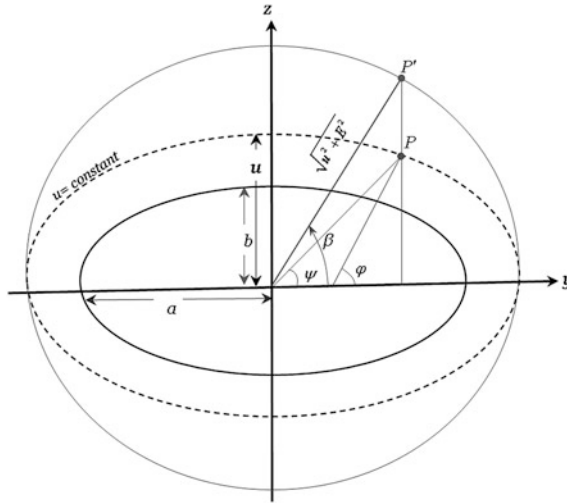


Fig. 2.3 Relations between Cartesian coordinates and geocentric, geodetic and reduced latitudes

Equation (2.19) can be inverted to provide the spherical coordinates (r, ψ) from the Cartesian ones by:

$$\tan \psi = \frac{z}{p} \quad \text{and} \quad r = \sqrt{p^2 + z^2}, \quad (2.25a)$$

where:

$$p = \sqrt{x^2 + y^2}. \quad (2.25b)$$

From Eq. (2.22) one obtains the inverse transformation from Cartesian coordinates to ellipsoidal coordinates by:

$$u = \sqrt{\left(w^2 + \sqrt{w^4 + 4E^2 z^2}\right)} / \sqrt{2} \quad (2.26a)$$

and

$$\tan \beta = \frac{z}{p} \sqrt{1 + (E/u)^2}, \quad (2.26b)$$

where:

$$w^2 = p^2 + z^2 - E^2. \quad (2.26c)$$

There are numerous solutions in the literature to the geodetic latitude φ and height h ; some solutions are iterative (e.g. Heiskanen and Moritz 1967, p. 183; Fukushima 2006; others are approximate, (e.g. Hoffmann-Wellenhof et al. 2008, p. 280):

$$\varphi = \arctan \frac{z + (e')^2 b \sin^3 o}{p - e^2 \cos^3 o}, \quad (2.27a)$$

where the auxiliary argument o is given by:

$$\tan o = z / \left(p \sqrt{1 - e^2}\right) \quad \text{and} \quad (e')^2 = (a^2 - b^2) / b^2, \quad (2.27b)$$

and there are also several exact solutions (see below).

Two efficient iterative methods were presented by Fukushima (2006) by applying Halley's third-order method to solve non-linear equations (Danby 1988). This method can be derived as follows. By squaring and adding the first two of Eq. (2.20), one obtains:

$$p = (\mathbb{N} + h) \cos \varphi, \quad (2.28)$$

and from this equation, and the last equation of (2.20) h can be eliminated, resulting in an equation in φ alone:

$$f(\varphi) = p \tan \varphi - z - e^2 a \frac{\sin \varphi}{\sqrt{1 - e^2 \sin^2 \varphi}} = 0, \quad (2.29a)$$

and by taking advantage of Eq. (2.23), one finally obtains:

$$F(T) = PT - Z - e^2 \frac{T}{\sqrt{1 + T^2}} = 0, \quad (2.29b)$$

where $P = p/a$, $Z = z/a$ and $T = \tan \beta$.

Applying Halley's third-order method, the iteration for T uses the formula

$$T_{n+1} = T_n - \frac{F(T_n)}{F'(T_n) - F''(T_n)F(T_n)/(2F'(T_n))}, \quad (2.30a)$$

where n is the iteration step and the first- and second-order derivatives are:

$$F'(T_n) = P - e^2/(1 + T_n^2)^{3/2} \quad \text{and} \quad F''(T_n) = 3e^2 T_n / (1 + T_n^2)^{5/2}. \quad (2.30b)$$

As the second-order derivative is rather cumbersome, it may be neglected, yielding Newton's second-order iteration formula

$$T_{n+1} = T_n - \frac{F(T_n)}{F'(T_n)}. \quad (2.31)$$

A suitable start value for T_n could be $T_0 = Z/[P(1 - e^2)]$.

Fukushima (2006) showed that this iterative method is faster than any of the other methods published for the transformation of Cartesian to geodetic coordinates at an accuracy within $6'' \times 10^{-6}$ for elevations ranging between -10 and $30,000$ km.

Note that the iteration using the latitude as an argument will have a problem for high latitudes. In such situations, Sjöberg (1999) proposed iteration by using the co-latitude. Another way to circumvent the problem close to the pole is to substitute the unknown latitude φ by: $\phi = \varphi \mp \pi/4$.

An exact solution of geodetic height and latitude (Sjöberg 2008; slightly revised) reads as follows.

By introducing the new unknown $k = (\mathbb{N} + h)/\mathbb{N}$ one obtains the following equations from Eqs.(2.20), (2.21) and (2.23):

$$P = (x^2 + y^2)/a^2 = k^2 \cos^2 \beta \quad (2.32a)$$

and

$$Q = z^2(1 - e^2)/a^2 = (k - e^2)^2 \sin^2 \beta, \quad (2.32b)$$

and by combining these two equations such that β is eliminated, one arrives at a fourth-order equation in k :

$$\frac{P}{k^2} + \frac{Q}{(k - e^2)^2} = 1. \quad (2.32c)$$

Using the notations

$$r = (P + Q - e^2)/6 \quad \text{and} \quad s = PQe^4/(4r^3) \quad (2.33)$$

followed by

$$t = \sqrt[3]{1 + s + \sqrt{2s + s^2}}, \quad u = r(1 + t + t^{-1}), \quad v = \sqrt{u^2 + e^4 P} \quad (2.34a)$$

and $w = e^2 \frac{v + u - P}{2v},$

the only real and positive solution for k becomes

$$k = w + \sqrt{w^2 + v + u} \quad \text{and also} \quad W = k \sqrt{\frac{1 - e^2}{k^2 - e^2 P}}. \quad (2.34b)$$

Inserting (2.21) into the definition of k above (2.32a) the geodetic height can now be determined by

$$h = \frac{a}{W}(k - 1). \quad (2.35)$$

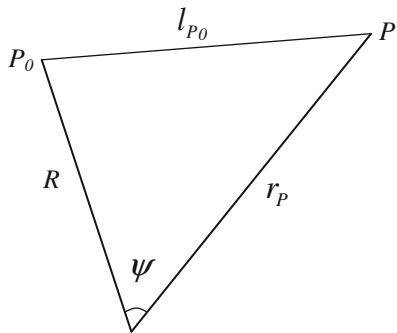
If P is small vs. Q then the latitude is given by Eq. (2.32a) as

$$\varphi = \pm \arccos(W\sqrt{P}/k) \text{ (with the same sign as } z). \quad (2.36a)$$

Otherwise Eq. (2.32b) yields

$$\varphi = \pm \arcsin\left(\frac{k}{k - e^2} \sqrt{\frac{Q}{k^2 - e^2 P}}\right) \text{ (with the same sign as } z). \quad (2.36b)$$

Fig. 2.4 Spherical distance/
geocentric angle ψ between
the radius vectors for points
 P_0 and P



2.4 Legendre's Polynomials

Legendre's polynomials and spherical harmonics are important in regional and global data representations. The generating function for Legendre polynomials is the inverse distance between two points P_0 and P , located on a sphere of radius R and outside the sphere at distance r_P from the centre of the sphere, respectively:

$$l_{P_0}^{-1} = \frac{1}{\sqrt{r_P^2 + R^2 - 2r_P R t}} = \frac{1}{r_P \sqrt{1 + s^2 - 2st}}, \quad (2.37a)$$

where $s = R/r_P$ and $t = \cos \psi$; ψ being the centric angle between the radius vectors for $P_0(R, \varphi_0, \lambda_0)$ and $P(r_P, \varphi, \lambda)$ (see Fig. 2.4). The angle is related to the latitudes and longitudes of the points by the cosine formula from spherical trigonometry:

$$\cos \psi = \sin \varphi_0 \sin \varphi + \cos \varphi_0 \cos \varphi \cos(\lambda - \lambda_0). \quad (2.37b)$$

Equation (2.37a) can be expanded as a Taylor/binomial series in s , which can be re-arranged into a series in Legendre's polynomials $P_n(t)$ as:

$$l_{P_0}^{-1} = \frac{1}{r_P} \sum_{n=0}^{\infty} s^n P_n(t); \quad s < 1. \quad (2.38a)$$

If P is located inside the sphere, the series becomes:

$$l_{P_0}^{-1} = \frac{1}{R} \sum_{n=0}^{\infty} s^{-n} P_n(t); \quad s > 1. \quad (2.38b)$$

On the sphere (with $s = 1$), the series converges for $\psi \neq 0$:

$$l_{P_0}^{-1} = \frac{1}{R} \sum_{n=0}^{\infty} P_n(t). \quad (2.38c)$$

Differentiate each side of Eq. (2.38a) w.r.t. r_P , multiply by $-2r_P$ and subtract the inverse distance. Then, after a few manipulations, one obtains *Poisson's kernel function*

$$\frac{r_P(r_P^2 - R^2)}{l_{P0}^3} = \sum_{n=0}^{\infty} \frac{(2n+1)R^n}{r_P^n} P_n(t); \quad r_P > R. \quad (2.39)$$

This function is important in solving Dirichlet's problem, the first boundary value problem of physical geodesy (see Sect. 2.7.5).

Exercise 2.1 Make a Taylor expansion of the inverse distance and compare with (2.38a) to show that $P_0(t) = 1$, $P_1(t) = t$ and $P_2(t) = (3t^2 - 1)/2$.

The solution is given in Appendix.

Legendre's polynomials have the following important properties:

$$|P_n| \leq 1, \quad P_n(1) = 1, \quad P_n(-1) = (-1)^n \quad (2.40)$$

and

$$P_n(t) = \frac{2n-1}{n} t P_{n-1}(t) - \frac{n-1}{n} P_{n-2}(t); \quad n \geq 2. \quad (2.41)$$

By the recursive formula Eq. (2.41) the Legendre's polynomial can be determined numerically to any degree.

Legendre's polynomials are orthogonal in the interval -1 to 1 , i.e.:

$$\int_{-1}^1 P_n^2(t) dt = \frac{2}{2n+1} \quad \text{and} \quad \int_{-1}^1 P_n(t) P_m(t) dt = 0, \quad \text{if } n \neq m. \quad (2.42)$$

Exercise 2.2 Verify (2.42) for $n = 0-2$.

The solution is given in Appendix.

Legendre's polynomials can also be determined by *Rodrigues's formula*:

$$P_n(t) = \frac{d^n(t^2 - 1)^n}{2^n n! dt^n}, \quad (2.43)$$

but this formula is less practical on a computer than the recursive formula.

From the ordinary Legendre's polynomials, the (*associated*) *Legendre functions* can be defined:

$$P_{nm}(t) = (1 - t^2)^{m/2} \frac{d^m P_n(t)}{dt^m}; \quad m \leq n, \quad (2.44)$$

where m is the *order*. It is a basic component in spherical harmonics.

2.5 Spherical Harmonics

A fully normalized (surface) spherical harmonic of degree n and order m can be written (Sjöberg 1975, 1978):

$$Y_{nm}(\theta, \lambda) = N_{nm} P_{n|m|}(\cos \theta) \begin{cases} \sin m\lambda & \text{if } m > 0 \\ \cos m\lambda & \text{otherwise} \end{cases}, \quad (2.45a)$$

where:

$$N_{nm} = \begin{cases} \sqrt{2(2n+1) \frac{(n-|m|)!}{(n+|m|)!}} & \text{if } m \neq 0 \\ \sqrt{2n+1} & m = 0 \end{cases} \quad (2.45b)$$

is a normalizing factor that makes the harmonics *orthonormal*, i.e., they obey:

$$\frac{1}{4\pi} \iint_{\sigma} Y_{nm}^2 d\sigma = 1, \quad (2.46)$$

where (θ, λ) are the co-latitude and longitude, and they are orthogonal to each other when averaged over the unit sphere (σ):

$$\frac{1}{4\pi} \iint_{\sigma} Y_{nm} Y_{kl} d\sigma = 0, \quad \text{if } n \neq k \text{ and/or } m \neq l. \quad (2.47)$$

Note that we use the notations $Y_{nm}(\theta, \lambda)$, Y_{nm} , $Y_{nm}(P)$ interchangeably when there could be no misunderstanding.

Let a distance between two points in space be given by $l_P = \sqrt{r_P^2 + r^2 - 2r_P r t}$, where $t = \cos \psi$ and r_P, r are the geocentric radii of the two points, separated by the geocentric angle ψ . Then Eqs. (2.38a, b) can be generalized to:

$$1/l_P = \sum_{n=0}^{\infty} \frac{r^n}{r_P^{n+1}} P_n(t); \quad r_P > r \quad (\text{external type series}) \quad (2.48a)$$

and

$$1/l_P = \sum_{n=0}^{\infty} \frac{r_P^n}{r^{n+1}} P_n(t), \quad \text{if } r_P < r \quad (\text{internal type series}) \quad (2.48b)$$

- The *Legendre's polynomial* $P_n(\cos \psi)$ is related with the spherical harmonics by the *addition theorem*

$$(2n+1)P_n(\cos \psi) = \sum_{m=-n}^n Y_{nm}(P) Y_{nm}(Q), \quad (2.49)$$

where P and Q are the endpoints of an arc on the unit sphere of geocentric angle ψ .

- Any (decent) function f on a sphere can be expanded as a harmonic series:

$$f = f(\theta, \lambda) = \sum_{n=0}^{\infty} \sum_{m=-n}^n f_{nm} Y_{nm}(\theta, \lambda), \quad (2.50a)$$

where:

$$f_{nm} = \frac{1}{4\pi} \iint_{\sigma} f Y_{nm} d\sigma. \quad (2.50b)$$

- The function f may also be written as a *Laplace series*

$$f = f(\theta, \lambda) = \sum_{n=0}^{\infty} f_n(\theta, \lambda), \quad (2.51a)$$

where:

$$f_n(\theta, \lambda) = \frac{2n+1}{4\pi} \iint_{\sigma} f P_n(\cos \psi) d\sigma, \quad (2.51b)$$

or, using the addition theorem (2.49)

$$f_n(\theta, \lambda) = \sum_{m=-n}^n f_{nm} Y_{nm}(\theta, \lambda), \quad (2.51c)$$

which relates the Laplace harmonics to the spherical harmonics.

- The truncated series

$$\hat{f}(\theta, \lambda) = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n f_{nm} Y_{nm}(\theta, \lambda) \quad (2.52a)$$

has $1 + 3 + 5 + \dots + (2n_{\max} + 1) = (1 + n_{\max})^2$ terms and an approximate resolution of:

$$v^{\circ} \approx 180^{\circ} / n_{\max}. \quad (2.52b)$$

For $n_{\max} = 2159$ (which is the case for EGM2008; see below) there are 4.665.600 terms and a resolution of about $5'$.

- The Newton integral of the Earth's potential with $\mu =$ gravitational constant times density is:

$$V(P) = \iint_{\sigma} \int_0^{r_s} \frac{\mu r^2}{l_P} dr d\sigma. \quad (2.53)$$

- It can be expanded in the external type harmonic series

$$V(P) = \sum_{n=0}^{\infty} \left(\frac{R}{r_P} \right)^{n+1} V_n(P), \quad r_P \geq (r_s)_{\max}, \quad (2.54a)$$

where:

$$V_n(P) = \sum_{m=-n}^n \frac{Y_{nm}(P)}{2n+1} \iint_{\sigma} \int_0^{r_s} \mu \frac{r^{n+2}}{R^{n+1}} dr Y_{nm} d\sigma. \quad (2.54b)$$

Here R is a selected radius (e.g. mean sea-level radius), and $r_s = r_s(\theta, \lambda)$ is the radius of the Earth's topography.

- If $r_P < (r_s)_{\max}$, the potential can be expanded in a combination of external and internal type series

$$V(P) = \sum_{n=0}^{\infty} \left(\frac{R}{r_P} \right)^{n+1} V_n^e(P) + \sum_{n=0}^{\infty} \left(\frac{r_P}{R} \right)^n V_n^i(P), \quad (2.55a)$$

where:

$$V_n^e(P) = \sum_{m=-n}^n \frac{Y_{nm}(P)}{2n+1} \iint_{\sigma} \int_{r_P}^{r_s} \mu \frac{r^{n+2}}{R^{n+1}} dr Y_{nm} d\sigma, \quad (2.55b)$$

and

$$V_n^i(P) = \sum_{m=-n}^n \frac{Y_{nm}(P)}{2n+1} \iint_{\sigma} \int_{r_P}^{r_s} \mu \frac{R^n}{r^{n-1}} dr Y_{nm} d\sigma. \quad (2.55c)$$

Note that the coefficients in (2.55b, 2.55c) change for each radius r_P .

Disregarding the atmosphere, the external type series in Eq. (2.55a) definitely converges outside the bounding sphere, the Brillouin sphere, which touches the peak of Mt. Chimborazo in Ecuador at elevation 6267 m with an Earth centre radius of 6384 km. Although, in the strict sense, the series is likely to diverge inside this sphere but be asymptotically divergent (Moritz 1980, Chaps. 6 and 7), it can be applied to very high degrees without notable commission errors also inside the sphere. However, when applied (analytically continued) inside topographic masses,

the series is biased and should be corrected for this error (see Sect. 5.2.6). This is in agreement with the approximation theorems of Runge-Krarup (Krarpup 1969) and Keldysh-Laurentiev (Bjerhammar 1975), which states that there exist harmonic series that approximate the external type harmonic series arbitrarily well above the surface and down onto the surface of the Earth, respectively, and converge all the way down to the internal (Bjerhammar) sphere.

Integral formulas and equations on the sphere can frequently be derived and solved, respectively, in the spectral domain by spherical harmonics. For examples, see Sects. 3.3, and 8.2.

2.5.1 *Spectral Filtering and Combination*

2.5.1.1 Introduction

Here we derive the local least squares spectral filter for a stochastic function on the sphere based on the spectral representation of the observable and its error covariance matrix. Second, the local least squares spectral combination of two erroneous harmonic series is derived based on their full covariance matrices. In both problems, the transition from spectral representation of an estimator to an integral representation is demonstrated. Practical examples are given for the spectral filter and for the combination of a series and an integral formula.

Taking advantage of the full covariance matrices in the spectral combination implies a huge computational burden in determining the least squares filters and combinations for high degree spherical harmonic series. A reasonable compromise could be to consider only one weight parameter/degree, yielding the optimum filtering and combination of Laplace series as outlined in Sect. 7.5.

Spectral combination of harmonic functions has proved to be a practical tool to match various observables in physical geodesy (see Sects. 2.8.4, 4.4.4–4.4.6 and Chap. 6). Early models along this line were presented by Sjöberg (1979, 1980, 1981) as well as by Wenzel (1981). In Sjöberg (1979) and partly in Sjöberg (1980), integral formulas were presented for least squares combination of stochastic, random heterogeneous data, while otherwise, more realistically, only the errors of the data were considered stochastic. All these models have in common that the correlations between different spectral degrees of errors are disregarded, and frequently the models are based on minimizing the global variance or mean square error. See also Sjöberg (1984a, b, 1986), which provide the basics of least squares modification of Stokes' formula. Also, Sjöberg (2005) presents a local modification of Stokes' formula using weighting by degrees. Considering that Earth gravitational models (EGMs) are usually provided together with their full covariance matrices, at least up to some specific degrees, and that the qualities of the models vary over the surface of the Earth, all the information contained in the covariance matrices should be utilized in the combined solutions. This article derives such solutions for filtering and combination of EGMs, as well as in the combination of an EGM with an

integral formula. See also Sjöberg (2011a). Most of the following subsection is a reprint of Sjöberg (2011b).

2.5.1.2 Local Spectral Filtering

Let the gravity field related function v be developed into a finite series of spherical harmonics $Y_{nm}(\theta, \lambda)$ on the sphere

$$v = v(\theta, \lambda) = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n v_{nm} Y_{nm}(\theta, \lambda), \quad (2.56)$$

where v_{nm} are the harmonic coefficients, n_{\max} is the maximum degree of expansion of the series and (θ, λ) is the (co-latitude, longitude) of the function. Consider the unbiased and biased estimators of v :

$$\tilde{v}' = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n \tilde{v}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{e}^T \mathbf{D} \tilde{\mathbf{v}}, \quad (2.57a)$$

and

$$\tilde{\mathbf{v}} = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n p_{nm} \tilde{v}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{p}^T \mathbf{D} \tilde{\mathbf{v}} \quad (2.57b)$$

where p_{nm} is weighting parameter to be fixed,

$$\tilde{v}_{nm} = v_{nm} + dv_{nm} \quad \text{with} \quad E\{dv_{nm}\} = 0, \quad (2.57c)$$

and \mathbf{D} is a diagonal matrix with $(n_{\max} + 1)^2$ elements $(Y_{00}, Y_{1-1}, \dots, Y_{n_{\max}n_{\max}})$. Furthermore \mathbf{p} and $\tilde{\mathbf{v}}$ are vectors with obvious elements, and $\mathbf{e}^T = (1, 1, \dots, 1)$.

The error of the unbiased and biased estimators can be written:

$$d\tilde{v}' = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n dv_{nm} Y_{nm}(\theta, \lambda) = \mathbf{e}^T \mathbf{D} d\mathbf{v} \quad (2.58a)$$

and

$$d\tilde{\mathbf{v}} = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n [p_{nm} dv_{nm} + v_{nm}(p_{nm} - 1)] Y_{nm}(\theta, \lambda) = \mathbf{p}^T \mathbf{D} d\mathbf{v} + (\mathbf{p}^T - \mathbf{e}^T) \mathbf{D} \mathbf{v}. \quad (2.58b)$$

Assuming that the covariance matrix of the error vector \mathbf{dv} is \mathbf{Q} , one obtains the following variance and Mean Square Error (MSE) of \tilde{v}' and \tilde{v} , respectively:

$$\sigma_{v'}^2 = \mathbf{e}^T \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{e} \quad (2.59a)$$

and

$$\text{MSE}(\tilde{v}) = \mathbf{p}^T \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{p} + (\mathbf{p}^T - \mathbf{e}^T) \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D} (\mathbf{p} - \mathbf{e}). \quad (2.59b)$$

The spectral filter solutions are provided by Eq. (2.2b), and the optimum filter is the one where the filter parameters p_{nm} are chosen such that the MSE is a minimum. This choice for filter parameters is thus obtained by differentiating the MSE w.r.t. \mathbf{p} and equating it to zero. The result is the matrix equation

$$(\mathbf{D} \mathbf{Q} \mathbf{D} + \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D}) \mathbf{p} - \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D} \mathbf{e} = \mathbf{0} \quad (2.60)$$

with the solution

$$\hat{\mathbf{p}} = (\mathbf{D} \mathbf{Q} \mathbf{D} + \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D})^{-1} \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D} \mathbf{e}. \quad (2.61)$$

Hence, by inserting Eq. (2.61) into Eq. (2.2b), the Local Least Squares Spectral Filter becomes:

$$\hat{v} = \mathbf{p}^T \mathbf{D} \tilde{\mathbf{v}} = \mathbf{e}^T \left[\mathbf{I} - \mathbf{D} \mathbf{Q} \mathbf{D} (\mathbf{D} \mathbf{Q} \mathbf{D} + \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D})^{-1} \right] \mathbf{D} \tilde{\mathbf{v}} \quad (2.62a)$$

with the mean square error

$$\text{MSE}\{\hat{v}\} = \mathbf{e}^T \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{e} - \mathbf{e}^T \mathbf{D} \mathbf{Q} \mathbf{D} (\mathbf{D} \mathbf{Q} \mathbf{D} + \mathbf{D} \mathbf{v} \mathbf{v}^T \mathbf{D})^{-1} \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{e}, \quad (2.62b)$$

and Eqs. (2.62a, b) can also be simplified to:

$$\hat{v} = \mathbf{e}^T \mathbf{D} \tilde{\mathbf{v}} - \mathbf{e}^T \mathbf{D} \mathbf{Q} (\mathbf{Q} + \mathbf{v} \mathbf{v}^T)^{-1} \tilde{\mathbf{v}} \quad (2.63a)$$

and

$$\text{MSE}\{\hat{v}\} = \mathbf{e}^T \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{e} - \mathbf{e}^T \mathbf{D} \mathbf{Q} (\mathbf{Q} + \mathbf{v} \mathbf{v}^T)^{-1} \mathbf{Q} \mathbf{D} \mathbf{e}. \quad (2.63b)$$

Equations (2.59a) and (2.63b) show that the MSE of \hat{v} is smaller than the variance of v' . As $\mathbf{v} \mathbf{v}^T$ is not known, there is a practical problem in applying Eqs. (2.63a, b). However, $\mathbf{Q} + \mathbf{v} \mathbf{v}^T$ is unbiasedly estimated by $\tilde{\mathbf{v}} \tilde{\mathbf{v}}^T$, and, by this substitution, the filter and its covariance matrix can be realized.

2.5.1.3 Generalized Filtering

Here we assume that a function $w(\theta, \lambda)$ is related to function $v(\theta, \lambda)$ by the harmonic series

$$w = w(\theta, \lambda) = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n k_{nm} v_{nm} Y_{nm}(\theta, \lambda), \quad (2.64)$$

where k_{nm} are known coefficients (possibly functions of radial position). In analogy with above, the general estimator

$$\tilde{w} = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n q_{nm} \tilde{v}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{q}^T \mathbf{D} \tilde{\mathbf{v}} \quad (2.65)$$

is optimized in the least squares sense by the weight vector

$$\hat{\mathbf{q}} = (\mathbf{DQD} + \mathbf{D}\mathbf{v}\mathbf{v}^T\mathbf{D})^{-1} \mathbf{D}\mathbf{v}\mathbf{v}^T\mathbf{D}\mathbf{k} = \left[\mathbf{I} - \mathbf{DQD}(\mathbf{DQD} + \mathbf{D}\mathbf{v}\mathbf{v}^T\mathbf{D})^{-1} \right] \mathbf{k}, \quad (2.66)$$

yielding the least squares estimator

$$\hat{w} = \mathbf{k}^T \mathbf{D} \tilde{\mathbf{v}} - \mathbf{k}^T \mathbf{DQ}(\mathbf{Q} + \mathbf{v}\mathbf{v}^T)^{-1} \tilde{\mathbf{v}}, \quad (2.67a)$$

with the minimum mean square error (with respect to choice of \mathbf{q})

$$\text{MSE}\{\hat{w}\} = \mathbf{k}^T \mathbf{DQDk} - \mathbf{k}^T \mathbf{DQ}(\mathbf{Q} + \mathbf{v}\mathbf{v}^T)^{-1} \mathbf{QDk}. \quad (2.67b)$$

Comparing Eqs. (2.64) and (2.67a), we notice that $\hat{q}_{nm} = \hat{p}_{nm}$, which we will take advantage of in the integral representations that follow below.

2.5.1.4 Integral Representation of the Filter

Assuming that the spherical harmonics $Y_{nm}(\theta, \lambda)$ are fully normalized, it means that they are mutually orthonormal, i.e.:

$$\iint_{\sigma} Y_{nm} Y_{kl} d\sigma = \begin{cases} 4\pi, & \text{if } (n, m) = (k, l) \\ 0 & \text{otherwise.} \end{cases} \quad (2.68)$$

Then we can express Eq. (2.67a) by the integral

$$\hat{w}_P = \frac{1}{4\pi} \iint_{\sigma} K(P, Q) \tilde{v} d\sigma, \quad (2.69a)$$

where the kernel function $K(P, Q)$ becomes:

$$K(P, Q) = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n k_{nm} \hat{p}_{nm} Y_{nm}(\theta_P, \lambda_P) Y_{nm}(\theta_Q, \lambda_Q). \quad (2.69b)$$

Here Q is the integration point on the unit sphere (denoted by σ).

Example 2.1 Use Eq. (2.69a) to estimate the disturbing potential T_P at the radius r_P from the gravity anomaly $\Delta\tilde{g}$ on the sphere of radius R .

Solution Choosing $k_{nm} = 0$ for $n < 2$ and $k_{nm} = r_P/(n-1)(R/r_P)^{n+1}$ for $n \geq 2$, the solution is obtained by:

$$\hat{T}_P = \frac{r_P}{4\pi} \iint_{\sigma} S(P, Q) \Delta\tilde{g} d\sigma, \quad (2.70a)$$

where:

$$S(P, Q) = \sum_{n=2}^{n_{\max}} \frac{1}{n-1} \left(\frac{R}{r_P}\right)^{n+1} \sum_{m=-n}^n \hat{p}_{nm} Y_{nm}(P) Y_{nm}(Q). \quad (2.70b)$$

2.5.1.5 Local Spectral Combination

Let \tilde{u} and \tilde{v} be two unbiased estimators of the finite harmonic series v , given by Eq. (2.56). Let the estimators be expressed by the series

$$\tilde{u} = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n \tilde{u}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{e}^T \mathbf{D} \tilde{\mathbf{u}} \quad (2.71a)$$

and

$$\tilde{v} = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n \tilde{v}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{e}^T \mathbf{D} \tilde{\mathbf{v}}, \quad (2.71b)$$

where both sets of coefficients \tilde{u}_{nm} and \tilde{v}_{nm} are unbiased estimates of v_{nm} with random errors du_{nm} and dv_{nm} , respectively, and the last parts of the equations are obvious matrix representations. We will assume also that the errors of the coefficients have expectations zero, and their covariance matrices will be denoted:

$$E\{\mathbf{dud}\mathbf{u}^T\} = \mathbf{\Sigma}, \quad E\{\mathbf{dv}\mathbf{d}\mathbf{v}^T\} = \mathbf{Q}, \quad \text{and} \quad E\{\mathbf{dud}\mathbf{v}^T\} = \mathbf{\Omega}. \quad (2.72)$$

The general unbiased spectral combination of the two series of Eqs. (2.71a, b) can be written:

$$\tilde{w} = \mathbf{p}^T \mathbf{D} \tilde{\mathbf{u}} + (\mathbf{e}^T - \mathbf{p}^T) \mathbf{D} \tilde{\mathbf{v}}, \quad (2.73)$$

where, again, \mathbf{p} is a weight vector. The error and variance of this estimator become:

$$dw = \mathbf{p}^T \mathbf{D} d\mathbf{u} + (\mathbf{e}^T - \mathbf{p}^T) \mathbf{D} d\mathbf{v} \quad (2.74)$$

and

$$\begin{aligned} \sigma_w^2 = E\{dw^2\} &= \mathbf{p}^T \mathbf{D} \mathbf{\Sigma} \mathbf{D} \mathbf{p} + (\mathbf{e}^T - \mathbf{p}^T) \mathbf{D} \mathbf{Q} \mathbf{D} (\mathbf{e} - \mathbf{p}) \\ &\quad + \mathbf{p}^T \mathbf{D} \mathbf{\Omega} \mathbf{D} (\mathbf{e} - \mathbf{p}) + (\mathbf{e}^T - \mathbf{p}^T) \mathbf{D} \mathbf{\Omega}^T \mathbf{D} \mathbf{p}. \end{aligned} \quad (2.75)$$

The least squares choice of \mathbf{p} minimizes the variance, and this minimum is attained by differentiating Eq. (2.75) w.r.t. \mathbf{p} and equating to zero. The result is:

$$\mathbf{D} \mathbf{M} \mathbf{D} \mathbf{p} - \mathbf{D} (\mathbf{Q} - \mathbf{\Omega}) \mathbf{D} \mathbf{e} = \mathbf{0}, \quad (2.76a)$$

where:

$$\mathbf{M} = \mathbf{\Sigma} + \mathbf{Q} - \mathbf{\Omega} - \mathbf{\Omega}^T, \quad (2.76b)$$

with the solution

$$\hat{\mathbf{p}} = (\mathbf{D} \mathbf{M} \mathbf{D})^{-1} \mathbf{D} (\mathbf{Q} - \mathbf{\Omega}) \mathbf{D} \mathbf{e} = \mathbf{D}^{-1} \mathbf{M}^{-1} (\mathbf{Q} - \mathbf{\Omega}) \mathbf{D} \mathbf{e}. \quad (2.76c)$$

Hence, the least squares spectral combination becomes:

$$\hat{w} = \mathbf{e}^T \mathbf{D} (\mathbf{Q} - \mathbf{\Omega}^T) \mathbf{M}^{-1} \tilde{\mathbf{u}} + \mathbf{e}^T \mathbf{D} (\mathbf{\Sigma} - \mathbf{\Omega}) \mathbf{M}^{-1} \tilde{\mathbf{v}} \quad (2.77a)$$

with the variance

$$\sigma_{\hat{w}}^2 = \mathbf{e}^T \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{e} - \mathbf{e}^T \mathbf{D} (\mathbf{Q} - \mathbf{\Omega}^T) \mathbf{M}^{-1} (\mathbf{Q} - \mathbf{\Omega}) \mathbf{D} \mathbf{e}. \quad (2.77b)$$

2.5.1.6 Generalization

Let us assume that the function

$$w = w(r, \theta, \lambda) = \sum_{n=0}^{n_{\max}} \left(\frac{R}{r}\right)^{n+1} \sum_{m=-n}^n w_{nm} Y_{nm}(\theta, \lambda), \quad (2.78)$$

where $r \geq R$, is a 3D function, unbiasedly estimable on and outside the sphere of radius R by the functions $\tilde{u}(\theta, \lambda)$ and $\tilde{v}(\theta, \lambda)$ on the sphere. Then the general unbiased estimators for w can be written:

$$\tilde{w}_1 = \sum_{n=0}^{n_{\max}} \left(\frac{R}{r}\right)^{n+1} \sum_{m=-n}^n f_{nm} \tilde{u}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{f}^T \mathbf{D} \tilde{\mathbf{u}} \quad (2.79a)$$

and

$$\tilde{w}_2 = \sum_{n=0}^{n_{\max}} \left(\frac{R}{r}\right)^{n+1} \sum_{m=-n}^n g_{nm} \tilde{v}_{nm} Y_{nm}(\theta, \lambda) = \mathbf{g}^T \mathbf{D} \tilde{\mathbf{v}}, \quad (2.79b)$$

where the given coefficients f_{nm} and g_{nm} bring the harmonics of u and v to those of w , i.e. $w_{nm} = f_{nm} u_{nm} = g_{nm} v_{nm}$. Also, vectors \mathbf{f} and \mathbf{g} have the elements $(R/r)^{n+1} f_{nm}$ and $(R/r)^{n+1} g_{nm}$, with $0 \leq n \leq n_{\max}$ and $-n \leq m \leq n$.

A general unbiased combined estimator for w can be written:

$$\tilde{w} = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n p_{nm} f_{nm} \tilde{u}_{nm} Y_{nm}(\theta, \lambda) + \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n (1 - p_{nm}) g_{nm} \tilde{v}_{nm} Y_{nm}(\theta, \lambda), \quad (2.80a)$$

where p_{nm} are arbitrary degree/order weights. With matrix notations the estimator becomes:

$$\tilde{w} = \mathbf{d}^T \tilde{\mathbf{u}} + (\mathbf{g}^T \mathbf{D} - \mathbf{h}^T) \tilde{\mathbf{v}}, \quad (2.80b)$$

where $\mathbf{d} = \mathbf{F}\mathbf{p}$, $\mathbf{h} = \mathbf{G}\mathbf{p}$ and \mathbf{p} is the vector with elements p_{nm} . Here \mathbf{F} and \mathbf{G} are diagonal matrices with elements from vectors \mathbf{Df} and \mathbf{Dg} , respectively.

The variance of \tilde{w} becomes:

$$\sigma_{\tilde{w}}^2 = \mathbf{d}^T \Sigma \mathbf{d} + (\mathbf{g}^T \mathbf{D} - \mathbf{h}^T) \mathbf{Q} (\mathbf{Dg} - \mathbf{h}) + \mathbf{d}^T \Omega (\mathbf{Dg} - \mathbf{h}) + (\mathbf{g}^T \mathbf{D} - \mathbf{h}^T) \Omega^T \mathbf{d}^T, \quad (2.81)$$

and its minimum is obtained by differentiating Eq. (2.81) w.r.t. \mathbf{p} and equating it to zero. The result is:

$$\mathbf{Hp} - \mathbf{GQDg} + \mathbf{F}\Omega\mathbf{Dg} = \mathbf{0}, \quad (2.82a)$$

where:

$$\mathbf{H} = \mathbf{F}\mathbf{\Sigma}\mathbf{F} + \mathbf{G}\mathbf{Q}\mathbf{G} - \mathbf{F}\mathbf{\Omega}\mathbf{G} - \mathbf{G}\mathbf{\Omega}^T\mathbf{F}. \quad (2.82b)$$

Hence, the optimum weight vector becomes:

$$\hat{\mathbf{p}} = \mathbf{H}^{-1}(\mathbf{G}\mathbf{Q} - \mathbf{F}\mathbf{\Omega})\mathbf{D}\mathbf{g}, \quad (2.83)$$

yielding the optimum estimator for w

$$\hat{w} = \hat{\mathbf{p}}^T \mathbf{F}\tilde{\mathbf{u}} + (\mathbf{g}^T \mathbf{D} - \hat{\mathbf{p}}^T \mathbf{G})\tilde{\mathbf{v}}, \quad (2.84a)$$

with the variance

$$\sigma_w^2 = \mathbf{g}^T \mathbf{D} \mathbf{Q} \mathbf{D} \mathbf{g} - \hat{\mathbf{p}}^T \mathbf{H} \hat{\mathbf{p}} = \mathbf{g}^T \mathbf{D} [\mathbf{Q} - (\mathbf{Q}\mathbf{G} - \mathbf{\Omega}^T \mathbf{F})\mathbf{H}^{-1}(\mathbf{G}\mathbf{Q} - \mathbf{F}\mathbf{\Omega})] \mathbf{D} \mathbf{g}. \quad (2.84b)$$

2.5.1.7 Integral and Series Combination

The estimator \tilde{w}_2 of Eq. (2.79b) can be expressed by the integral

$$\tilde{w}_2 = \frac{1}{4\pi} \iint_{\sigma} \tilde{M}(r, \theta, \lambda, \theta', \lambda') \tilde{v}(\theta', \lambda') d\sigma', \quad (2.85a)$$

where the kernel function is given by:

$$\tilde{M}(r, \theta, \lambda, \theta', \lambda') = \sum_{n=0}^{n_{\max}} \left(\frac{R}{r}\right)^{n+1} \sum_{m=-n}^n g_{nm} Y_{nm}(\theta, \lambda) Y_{nm}(\theta', \lambda'). \quad (2.85b)$$

It follows that Eq. (2.80a) can be rewritten as

$$\hat{w} = \frac{1}{4\pi} \iint_{\sigma} M(r, \theta, \lambda, \theta', \lambda') \tilde{v}(\theta', \lambda') d\sigma + \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n \hat{p}_{nm} f_{nm} \tilde{u}_{nm} Y_{nm}(\theta, \lambda), \quad (2.86a)$$

where:

$$M(r, \theta, \lambda, \theta', \lambda') = \sum_{n=0}^{n_{\max}} \left(\frac{R}{r}\right)^{n+1} \sum_{m=-n}^n (1 - \hat{p}_{nm}) g_{nm} Y_{nm}(\theta, \lambda) Y_{nm}(\theta', \lambda'). \quad (2.86b)$$

Example 3.1 Geoid height estimation from an EGM and an integral formula with estimated gravity anomaly $\Delta\tilde{g}$.

The least squares estimator for the geoidal height is given by Eqs. (2.86a, b) for $f_{nm} = R/\gamma$, $\tilde{u}_{nm} = \tilde{T}_{nm}$, $\tilde{v} = \Delta\tilde{g}$, $g_{nm} = R/(n-1)$, $r = R$, and the degree summation in Eq. (2.86b) starts at $n_{\min} = 2$. The result is:

$$\hat{N} = \frac{R}{4\pi\gamma} \iint_{\sigma} S(\theta, \lambda, \theta', \lambda') \Delta\tilde{g} d\sigma + \frac{R}{\gamma} \sum_{n=2}^{n_{\max}} \sum_{m=-n}^n \hat{p}_{nm} \tilde{T}_{nm} Y_{nm}(\theta, \lambda), \quad (2.87a)$$

where:

$$S(\theta, \lambda, \theta', \lambda') = \sum_{n=2}^{n_{\max}} \frac{1}{n-1} \sum_{m=-n}^n (1 - \hat{p}_{nm}) Y_{nm}(\theta, \lambda) Y_{nm}(\theta', \lambda'). \quad (2.87b)$$

The least squares weights are given by Eq. (2.83) when considering the above choices of f_{nm} and g_{nm} .

2.5.1.8 Filtering and Weighting by Laplace Harmonics

So far we considered filtering and weighting by spherical harmonics. From a numerical point of view, when considering the large dimension of the matrices to be inverted, e.g. $\mathbf{Q} + \mathbf{v}\mathbf{v}^T$ in Eq. (2.63a), it could be reasonable to modify the technique to one weight factor/degree. This is obtained by considering that Eq. (2.56) can be written as the series of Laplace harmonics

$$x_n = x_n(\theta, \lambda) = \sum_{m=-n}^n v_{nm} Y_{nm}(\theta, \lambda), \quad (2.88)$$

which yields:

$$v = \sum_{n=0}^{n_{\max}} x_n. \quad (2.89)$$

Similarly, the estimator of Eq. (2.57b) and its error can be expressed as:

$$\tilde{v} = \sum_{n=0}^{n_{\max}} p_n \tilde{x}_n = \mathbf{p}^T \tilde{\mathbf{x}} \quad (2.90a)$$

and

$$d\tilde{v} = \sum_{n=0}^{n_{\max}} [p_n d\tilde{x}_n + (p_n - 1)x_n] = \mathbf{p}^T d\mathbf{x} + (\mathbf{p}^T - \mathbf{e}^T)\mathbf{x}. \quad (2.90b)$$

Hence, the MSE of \tilde{v} becomes:

$$\text{MSE}(\tilde{v}) = \mathbf{p}^T \mathbf{Q}_{xx} \mathbf{p} + (\mathbf{p}^T - \mathbf{e}^T) \mathbf{x} \mathbf{x}^T (\mathbf{p} - \mathbf{e}) \quad (2.91)$$

with the least squares choice for the weight vector:

$$\hat{\mathbf{p}} = (\mathbf{Q}_{xx} + \mathbf{x} \mathbf{x}^T)^{-1} \mathbf{x} \mathbf{x}^T \mathbf{e}. \quad (2.92)$$

Finally, the filtered estimator becomes:

$$\hat{v} = \mathbf{e}^T \left[\mathbf{I} - \mathbf{Q}_{xx} (\mathbf{Q}_{xx} + \mathbf{x} \mathbf{x}^T)^{-1} \right] \tilde{\mathbf{x}} \quad (2.93a)$$

with the MSE

$$\text{MSE}\{\hat{v}\} = \mathbf{e}^T \mathbf{Q}_{xx} \mathbf{e} - \mathbf{e}^T \mathbf{Q}_{xx} (\mathbf{Q}_{xx} + \mathbf{v} \mathbf{v}^T)^{-1} \mathbf{Q}_{xx} \mathbf{e}. \quad (2.93b)$$

Similarly the generalized filter of Eq. (2.64) can be obtained for the restriction of the number of weights to one/degree, and the integral representation of the filter becomes:

$$\hat{w}_P = \frac{1}{4\pi} \iint_{\sigma} K(P, Q) \tilde{x} d\sigma, \quad (2.94a)$$

where:

$$K(P, Q) = \sum_{n=0}^{n_{\max}} (2n+1) k_n \hat{p}_n P_n(\cos \psi). \quad (2.94b)$$

Here $P_n(\cos \psi)$ is the n -th Legendre's polynomial, and ψ is the geocentric angle between the computation and integration points.

Finally the least square spectral combination for degree weighting corresponding to Eqs. (2.77a, b) can be written:

$$\hat{\mathbf{w}} = \mathbf{e}^T (\mathbf{Q} - \mathbf{\Omega}^T) \mathbf{M}^{-1} \tilde{\mathbf{u}} + \mathbf{e}^T (\mathbf{\Sigma} - \mathbf{\Omega}) \mathbf{M}^{-1} \tilde{\mathbf{v}} \quad (2.95a)$$

with the variance:

$$\sigma_{\tilde{w}}^2 = \mathbf{e}^T \mathbf{Q} \mathbf{e} - \mathbf{e}^T (\mathbf{Q} - \mathbf{\Omega}^T) \mathbf{M}^{-1} (\mathbf{Q} - \mathbf{\Omega}) \mathbf{e}, \quad (2.95b)$$

where $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{v}}$ now means vectors of Laplace harmonics, and $\mathbf{Q}, \mathbf{\Sigma}, \mathbf{\Omega}$ are the corresponding covariance matrices, and \mathbf{M} is again defined by Eq. (2.76b).

2.5.1.9 Conclusions

The above solutions are the locally optimum spectral filters and combinations of functions on the sphere in the sense of minimum MSE. They utilize the full covariance matrices of the stochastic errors of the parameters representing the functions. In the most advanced cases, this implies that the total covariance matrix of a given EGM is employed, implying a considerable computational burden. This workload can be relaxed by considering only spectral weighting by degree, yielding the filter and spectral combination of Laplace series (see e.g. Sects. 2.8.4 and 7.6).

The above study includes the theoretical derivations of general filters and spectral combinations of harmonic series or a harmonic series and an integral formula, and the solutions should be suitable for solving both direct and inverse problems on the sphere.

2.6 Ellipsoidal Harmonics

As the Earth is rather a two-axis ellipsoid than a sphere, ellipsoidal harmonics are better suited than spherical ones for global modelling. The relation between Cartesian and ellipsoidal coordinates was presented in Eq. (2.22). The Laplace equation in ellipsoidal coordinates and its solution for the exterior case were derived in Heiskanen and Moritz (1967, Sects. 1–19 and 1–20). The solutions are:

$$\begin{aligned} (u^2 + E^2 \cos^2 \theta) \Delta V = (u^2 + E^2) \frac{\partial^2 V}{\partial u^2} + 2u \frac{\partial V}{\partial u} + \frac{\partial^2 V}{\partial \theta^2} \\ + \cot \theta \frac{\partial V}{\partial \theta} + \frac{u^2 + E^2 \cos^2 \theta}{(u^2 + E^2) \sin^2 \theta} \frac{\partial^2 V}{\partial \lambda^2} = 0 \end{aligned} \quad (2.96a)$$

and

$$V_e(u, \theta, \lambda) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{Q_{nm}(iu/E)}{Q_{nm}(ib/E)} \tilde{A}_{nm} Y_{nm}(\theta, \lambda), \quad (2.96b)$$

where $Q_{nm}(\cdot)$ are associate Legendre's polynomials of the 2nd kind, and \tilde{A}_{nm} are normalized harmonic coefficients on the ellipsoid, while Y_{nm} are the surface harmonics. This implies that the potential on the ellipsoid can be expressed:

$$V_c(\mathbf{b}, \theta, \lambda) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \tilde{A}_{nm} Y_{nm}(\theta, \lambda), \quad (2.97)$$

where $\Omega = 4\pi ab$ is the area of the ellipsoid with a and b being the semi-axes of the ellipsoid. Starting from Eq. (2.96b), the disturbing potential, the gravity anomaly and other gravity related quantities can be represented in ellipsoidal harmonics. Equation (2.97) indicates that a series of surface spherical harmonics can represent a function (not necessarily a potential) on a rather arbitrary surface.

One important application of ellipsoidal harmonics was utilized in the development of the Earth Gravitational Model 2008 (Pavlis et al. 2012). In this technique, which was already tested in earlier OSU EGMs, a preliminary EGM is first determined from a global set of 5' equal-area mean gravity anomalies analytically downward extended to the reference ellipsoid. From this set of data, “terrestrial” ellipsoidal potential coefficients were solved from an overdetermined linear system of equations of coefficients \tilde{A}_{nm} from harmonic degree 2 complete to degree and order 2159, and these coefficients were transformed to spherical harmonics by the method of Gleason (1988, Eq. 2.10). In a second least squares adjustment, the satellite only spherical harmonic model ITG-GRACE03S, complete to degree 180, and the “terrestrial” harmonics were merged into a final solution.

2.7 Fundamentals of Potential Theory

2.7.1 Basic Concepts and Formulas

Newton’s law of gravitation is fundamental to potential theory. It states that (the magnitude of) the attracting force F between two point masses m_1 and m_2 at distance l is:

$$F = Gm_1m_2/l^2, \quad (2.98)$$

where $G (\approx 6.67 \times 10^{-11} \text{ Nm}^2/\text{kg}^2)$ is the gravitational constant. From now on, we set the attracted mass m_1 to 1 (unit mass) at point P (x, y, z) and the attracting mass $m_2 = m$ at point Q (ξ, η, ζ). Then the 3-D attraction force at P can be expressed:

$$\mathbf{F} = -G \frac{m}{l^3} \mathbf{r}, \quad (2.99)$$

or, in Cartesian components (see Fig. 2.5):

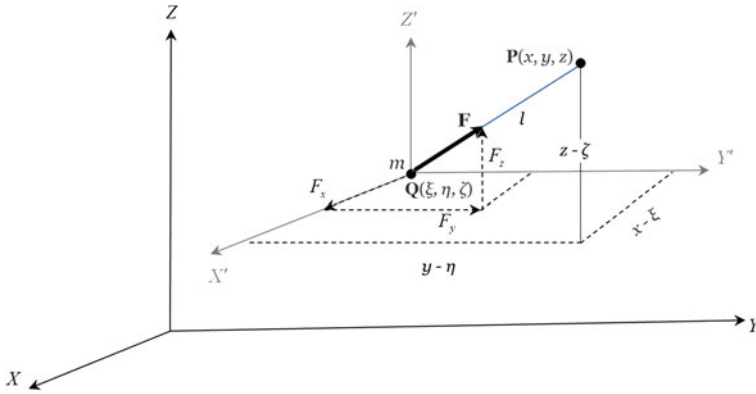


Fig. 2.5 Components of the attraction force $\mathbf{F} = \sqrt{F_x^2 + F_y^2 + F_z^2}$

$$\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} = -G \frac{m}{l^3} \begin{pmatrix} x - \xi \\ y - \eta \\ z - \zeta \end{pmatrix}. \quad (2.100)$$

The potential energy V that the unit mass experiences at point P is called *the gravitational potential at P*:

$$V = G \frac{m}{l}, \quad (2.101)$$

and the potential is thus related to the vector of attraction (gravitation) by the equation

$$\mathbf{F} = \text{grad}(V) = \left(\frac{\partial V}{\partial x} \quad \frac{\partial V}{\partial y} \quad \frac{\partial V}{\partial z} \right)^T \quad (2.102)$$

and its magnitude becomes:

$$F = \sqrt{\left(\frac{\partial V}{\partial x} \right)^2 + \left(\frac{\partial V}{\partial y} \right)^2 + \left(\frac{\partial V}{\partial z} \right)^2}. \quad (2.103)$$

The potential is a scalar quantity, and it is additive. The latter property implies that the potential at a point P_j can be determined as the sum of the potentials generated by all surrounding point masses m_i :

$$V_j = G \sum_{i=1}^n \frac{m_i}{l_{ji}}, \quad (2.104a)$$

where l_{ji} is the distance between points P_j and P_i . This equation can be generalized to a closed body with volume v and density ρ :

$$V_j = G \iiint_v \frac{dm}{l} = G \iiint_v \frac{\rho dv}{l}, \quad (2.104b)$$

where $l = l_{ji}$. According to Eq. (2.102), the force vector becomes:

$$\mathbf{F}_j = \text{grad}(V_j) = G \iiint_v \rho \left(\frac{\partial}{\partial x_j}, \frac{\partial}{\partial y_j}, \frac{\partial}{\partial z_j} \right)^T \frac{1}{l} dv. \quad (2.105)$$

- If the potential is generated by a materialized surface S with surface density $\kappa = dm/dS$, the correspondence to the 3D-Newton integral (2.104b) is given by

$$V = G \iint_S \frac{\kappa}{l} dS. \quad (2.106a)$$

This potential is continuous on and outside the surface, but its derivatives are discontinuous at the surface. Hence, the normal derivative on the surface becomes

$$\frac{\partial V}{\partial n} = G \iint_S \kappa \frac{\partial}{\partial n} \left(\frac{1}{l} \right) dS \mp 2\pi G \kappa, \quad (2.106b)$$

where the minus/plus sign applies to the exterior/internal side of the surface.

- Introducing $\mu = \text{gravitational constant times topographic density}$ into Eq. (2.104b), the Newton integral of the Earth's potential, can be written:

$$V(P) = \iint_{\sigma} \int_0^{r_s} \frac{\mu r^2}{l_p} dr d\sigma, \quad (2.107)$$

where σ is the unit sphere and r_s is the radius of the Earth's surface.

- The potential can be expanded in the external-type harmonic series

$$V(P) = \sum_{n=0}^{\infty} \left(\frac{R}{r_P} \right)^{n+1} V_n(P), \quad r_P \geq (r_s)_{\max}, \quad (2.108a)$$

where:

$$V_n(P) = \sum_{m=-n}^n \frac{Y_{nm}(P)}{2n+1} \iint_{\sigma} \int_0^{r_s} \mu \frac{r^{n+2}}{R^{n+1}} dr Y_{nm} d\sigma. \quad (2.108b)$$

Here R is a selected radius (e.g. mean sea level radius), and $r_s = r_s(\theta, \lambda)$.

- If $r_P < (r_s)_{\max}$, the potential can be expanded in a combination of external and internal type series:

$$V(P) = \sum_{n=0}^{\infty} \left(\frac{R}{r_P} \right)^{n+1} V_n^e(P) + \sum_{n=0}^{\infty} \left(\frac{r_P}{R} \right)^n V_n^i(P), \quad (2.109a)$$

where:

$$V_n^e(P) = \sum_{m=-n}^n \frac{Y_{nm}(P)}{2n+1} \iint_{\sigma} \int_{r_P}^{r_s} \mu \frac{r^{n+2}}{R^{n+1}} dr Y_{nm} d\sigma, \quad (2.109b)$$

and

$$V_n^i(P) = \sum_{m=-n}^n \frac{Y_{nm}(P)}{2n+1} \iint_{\sigma} \int_{r_P}^{r_s} \mu \frac{R^n}{r^{n-1}} dr Y_{nm} d\sigma. \quad (2.109c)$$

Note that the coefficients in (2.109b, 2.109c) change for each radius r_P .

2.7.2 Laplace's and Poisson's Equations

A function V is called harmonic if it satisfies Laplace's equation:

$$\Delta V = 0, \quad \text{where} \quad \Delta = \text{grad} \cdot \text{grad} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \quad (2.110)$$

Proposition 2.1 *Every gravitational potential is harmonic outside the attracting masses.*

Proof Applying the Laplace operator to Eq. (2.104b), one obtains:

$$\Delta V_P = \iiint_v \rho \Delta \left(\frac{1}{l_P} \right) dv = 0. \quad (2.111)$$

This is because as P is located outside the masses, $\Delta(1/l_P) = 0$ for all integration points in the body.

Corollary 2.1 (Poisson's differential equation)

If P is located inside the attracting masses, then $\Delta V_P = -4\pi G \rho_P$.

Proof The proof will be presented as an application of Gauss' theorem below.

2.7.3 Laplace's Equation and Its Solution in Spherical Coordinates

Laplace's equation in spherical coordinates reads (Heiskanen and Moritz 1967, p. 20):

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial V}{\partial r} \right) + \frac{1}{r^2} \Delta^* V = 0, \quad (2.112a)$$

where Δ^* is the *Beltrami operator* ("the Laplace operator on the sphere") defined by:

$$\Delta^* = \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \lambda^2}. \quad (2.112b)$$

By introducing V as a product of two functions that separate the variables (variable separation):

$$V(r, \theta, \lambda) = R(r)Y(\theta, \lambda), \quad (2.113)$$

Equation (2.112a) can be written:

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) = - \frac{\Delta^* Y}{Y}. \quad (2.114)$$

The two members can be separated by adding an arbitrary constant to each member. As will be shown, successful solutions are obtained by subtracting the constant $n(n+1)$ to both members of Eq. (2.114), which yields the two equations

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) - n(n+1)R = 0 \quad (2.115a)$$

and

$$\Delta^* Y + n(n+1)Y = 0. \quad (2.115b)$$

It can easily be checked that each solution to (2.115a) is an arbitrary constant times r^n or $r^{-(n+1)}$. Setting also $Y = Y_n$ in (2.115b), one can show that its solution for each n is a set of solutions of the surface spherical harmonics $Y_{nm}(\theta, \lambda)$, where m ranges from $-n$ to plus n .

Adding all partial solutions to V , its general solution becomes the sum of the external and internal types of solutions in solid spherical harmonics:

$$V = V^e + V_i, \quad (2.116a)$$

where:

$$V^e = \sum_{n=0}^{\infty} r^{-(n+1)} \sum_{m=-n}^n A_{nm} Y_{nm}(\theta, \lambda) \quad (2.116b)$$

and

$$V^i = \sum_{n=0}^{\infty} r^n \sum_{m=-n}^n B_{nm} Y_{nm}(\theta, \lambda) \quad (2.116c)$$

are the external and internal solutions to Laplace's equation, respectively. Here the constants A_{nm} and B_{nm} are arbitrary, to be fixed for each specific problem with gravitational masses at hand. On or outside the Brillouin sphere (surrounding all masses), all B_{nm} are zero, while for the topographic potential representation at or below the geoid (approximated by a sphere), all A_{nm} vanish.

Note that Eq. (2.115b) implies that:

$$\Delta^* Y_{nm} = -n(n+1)Y_{nm}, \quad \text{for all } n \text{ and } m. \quad (2.117)$$

2.7.4 Gauss' and Green's Integral Formulas

Gauss' and Green's formulas are basic formulas for potential theory. Here we present some of their varieties.

Gauss' (divergence) theorem for a closed volume v with surface S applied to the vector \mathbf{F} reads:

$$\iiint_v \text{div} \mathbf{F} dv = \iint_S \mathbf{F} \cdot \mathbf{n} dS, \quad (2.118)$$

where \mathbf{n} is the external normal unit vector to the surface S and

$$\text{div} \mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \quad (2.119)$$

is the divergence of the vector \mathbf{F} .

Assuming as above that $\mathbf{F} = \text{grad}(V)$, then $\text{div} \mathbf{F} = \Delta V$, and one obtains *Gauss' integral formula* for the potential as:

$$\iiint_v \operatorname{div} \mathbf{F} dv = \iiint_v \Delta V dv = \iint_S \frac{\partial V}{\partial n} dS. \quad (2.120)$$

Green's integral formulas are derived from Gauss' formula by specifying the components of \mathbf{F} as:

$$F_X = U \frac{\partial V}{\partial X}, \quad (2.121)$$

where $X = x, y$ or z and U and V are potentials.

Then it holds that:

$$\mathbf{F} \cdot \mathbf{n} = F_n = U \frac{\partial V}{\partial n}, \quad (2.122)$$

and from Eq. (2.119):

$$\operatorname{div} \mathbf{F} = U \Delta V + \frac{\partial U}{\partial x} \frac{\partial V}{\partial x} + \frac{\partial U}{\partial y} \frac{\partial V}{\partial y} + \frac{\partial U}{\partial z} \frac{\partial V}{\partial z}, \quad (2.123)$$

so that *Green's formula I* is obtained from Eq. (2.118) as

$$\iiint_v \left(U \Delta V + \frac{\partial U}{\partial x} \frac{\partial V}{\partial x} + \frac{\partial U}{\partial y} \frac{\partial V}{\partial y} + \frac{\partial U}{\partial z} \frac{\partial V}{\partial z} \right) dv = \iint_S U \frac{\partial V}{\partial n} dS. \quad (2.124)$$

If U and V are interchanged in Eq. (2.124), one obtains another equation, which, subtracted from Eq. (2.124), yields *Green's formula II*

$$\iiint_v (U \Delta V - V \Delta U) dv = \iint_S \left(U \frac{\partial V}{\partial n} - V \frac{\partial U}{\partial n} \right) dS. \quad (2.125)$$

In the above equations, it is assumed that U and V and their first- and second-order derivatives are finite and continuous in the region v .

Finally, specifying $U = 1/l$ in Green II yields *Green's formula III*

$$\iiint_v \frac{1}{l} \Delta V dv - pV = \iint_S \left[\frac{1}{l} \frac{\partial V}{\partial n} - V \frac{\partial}{\partial n} \left(\frac{1}{l} \right) \right] dS. \quad (2.126)$$

where:

$$p = \begin{cases} 4\pi, & \text{if } P \text{ inside } S \\ 2\pi, & \text{if } P \text{ on } S \\ 0, & \text{if } P \text{ outside } S. \end{cases} \quad (2.127)$$

Here P is the computation point.

Green III also holds if v is the exterior space to the surface S and n is the interior normal to S , where:

$$p = \begin{cases} -4\pi, & \text{if } P \text{ outside } S \\ -2\pi, & \text{if } P \text{ on } S \\ 0, & \text{if } P \text{ inside } S. \end{cases} \quad (2.128)$$

Proof of Corollary 2.1 (Poisson's differential equation)

From Eq. (2.120) one obtains for point P located inside the closed masses inside volume ϑ :

$$\begin{aligned} \iiint_{\vartheta} \Delta V_P d\vartheta &= \iiint_{\vartheta_e} \Delta V_P d\vartheta = \varepsilon^2 \iint_{\sigma_e} \frac{\partial V}{\partial r} d\sigma \\ &= G\varepsilon^2 \iint_{\sigma_e} \frac{\partial}{\partial \varepsilon} \left(\frac{\rho}{\varepsilon} \right) d\sigma \rightarrow -4\pi G\rho_P \quad \text{as } \varepsilon \rightarrow 0. \end{aligned}$$

Here ϑ_e and σ_e are the volume and surface of an infinitesimal sphere of radius ε centred at point P .

2.7.4.1 A Green's Formula on the Sphere

Meissl (1971, p. 12), with reference to Hotine (1969), presented the following integral relations derived from a Green's formula on the sphere

$$\iint_{\sigma} (\nabla^* f)^T \cdot \nabla^* g d\sigma = - \iint_{\sigma} f \Delta^* g d\sigma = - \iint_{\sigma} g \Delta^* f d\sigma, \quad (2.129a)$$

where ∇^* is the gradient operator on the unit sphere

$$\nabla^* = \left[\frac{\partial}{\partial \varphi} \quad \frac{\partial}{\cos \varphi \partial \lambda} \right]^T, \quad (2.129b)$$

which is related to the gradient operator on the sphere of radius R , ∇ , by:

$$\nabla = \frac{1}{R} \nabla^* = \left[\frac{\partial}{\partial x} \quad \frac{\partial}{\partial y} \right]^T, \quad (2.129c)$$

where x and y are local horizontal coordinates on the sphere.

If one specifies $f = Y_{nm}$ and $g = Y_{pq}$, it follows from Eqs. (2.129a) and (2.117) that:

$$\begin{aligned}
\iint_{\sigma} (\nabla^* Y_{nm})^T \cdot \nabla^* Y_{pq} d\sigma &= - \iint_{\sigma} Y_{nm} \Delta^* Y_{pq} d\sigma \\
&= \begin{cases} 4\pi n(n+1), & \text{if } (n, m) = (p, q) \\ 0 & \text{otherwise.} \end{cases}
\end{aligned} \tag{2.130}$$

i.e. also the gradients of the surface spherical harmonics are orthogonal on the sphere.

2.7.5 Boundary Value Problems

Stokes' theorem states that, for a given potential $V = V_S$ on a surface S , there is only one harmonic potential V in its exterior (if it exists).

Proof The proof follows from the following form of Green I

$$\iiint_v \left(U \Delta U + \left(\frac{\partial U}{\partial x} \right)^2 + \left(\frac{\partial U}{\partial y} \right)^2 + \left(\frac{\partial U}{\partial z} \right)^2 \right) dv = \iint_S U \frac{\partial U}{\partial n} dS. \tag{2.131}$$

Let us now assume that there are two potentials V_1 and V_2 in the exterior of S that take on the same values on S . Then the difference potential $U = V_1 - V_2$ on S and its Laplaceian ΔU in v vanish, so that the integral reduces to:

$$\iiint_v \left(\left(\frac{\partial U}{\partial x} \right)^2 + \left(\frac{\partial U}{\partial y} \right)^2 + \left(\frac{\partial U}{\partial z} \right)^2 \right) dv = 0, \tag{2.132}$$

implying that U is a constant in v . As U vanishes on S , it must vanish also outside S , and it follows that $V_1 = V_2$ in v .

Stokes' theorem confirms that the forward (direct) problem in potential theory has a unique solution. On the other hand, the inverse problem (to determine the mass distribution that generates the external gravity field) is not unique.

Here follow some specific forward problems:

Dirichlet's (exterior) problem [or the first boundary value problem (bvp) of potential theory] is to determine the potential V outside the closed surface S , given the boundary values V_S . If the surface is a sphere, the solution is Poisson's integral formula for the sphere.

Neumann's (exterior) problem [or the second bvp of potential theory] is to determine V on and in the exterior of S from the given function $\partial V / \partial n$ on S . Here n is the exterior normal to the surface. If the surface is a sphere, the solution on the sphere is Hotine's formula and in the exterior it is Hotine's extended formula.

The third bvp is to determine the potential V in the exterior of S from boundary values $aV + b\partial V / \partial n$ on S , where a and b are constants. If the boundary values are

gravity anomalies, the 3rd bvp applies for determining the disturbing potential. If S is a sphere the solution is Stokes' formula, which is the basic formula for geoid determination from gravity anomalies. As we will see in Sect. 3.3, all three bvps are useful in physical geodesy.

2.8 Regularization

Geophysicists and physical geodesists are frequently confronted with linear-inverse problems, which can be solved in various ways. An *inverse problem* generally deals with the problem of converting observations \tilde{g} to information w (of physical or other origin) that generates the observations. Frequently the problem is *ill-posed*, implying that the available (type of) observations are not sufficient to determine a unique solution for w . This can be illustrated by Poisson's integral formula in the exterior space of the sphere, Eq. (3.31a). Assuming that there are no masses outside the sphere of radius R , the forward problem to determine the disturbing potential or, in this case, the gravity anomaly Δg_P at any point P outside the sphere from gravity anomalies w on the sphere is given by the spectral solution

$$\Delta g_P = \sum_{n=0}^{\infty} \left(\frac{R}{r_P} \right)^{n+2} w_n(\theta, \lambda); \quad r_P > R \quad (2.133a)$$

where:

$$w_n(\theta, \lambda) = \sum_{m=-n}^n w_{nm} Y_{nm}(\theta, \lambda). \quad (2.133b)$$

Consider next that the gravity anomaly is known on an outer sphere of radius r_P , and the task is to solve the inverse problem of finding the anomaly on the lower sphere of radius R . Then we may develop Δg into spherical harmonics on the exterior sphere, yielding the coefficients Δg_{nm} , and, by comparing the spectral components with those in Eqs. (2.133a, b), one obtains the spectral equation and solution:

$$\Delta g_{nm} = \left(\frac{R}{r_P} \right)^{n+2} w_{nm} \Rightarrow w_{nm} = \left(\frac{r_P}{R} \right)^{n+2} \Delta g_{nm}, \quad (2.134a)$$

and formally the full solution becomes:

$$w(\theta, \lambda) = \sum_{n=0}^{\infty} \left(\frac{r_P}{R} \right)^{n+2} \Delta g_n(\theta, \lambda). \quad (2.134b)$$

In this case, as there are no masses between the spheres, the solution exists for erroneous observations, but in practice it will be severely ill-conditioned (more so in higher-degree harmonics), due to inevitable erroneous observations.

A *discrete ill-posed problem* occurs from the discretization of an ill-posed problem. A typical linear-inverse problem is that of estimating the density distribution or density structure inside the Earth from gravity or related data observed on or above the Earth's surface. Such a problem can frequently be expressed as a linear Fredholm integral equation of the 1st kind (e.g. Chambers 1976):

$$M\{K(P, Q)\tilde{w}\} = \tilde{g}(P), \quad (2.135a)$$

where $M\{\}$ is the integral over the surface of the Earth, or it is the mean value operator over the unit sphere (σ):

$$M\{\} = \frac{1}{4\pi} \iint_{\sigma} \{\} d\sigma, \quad (2.135b)$$

and $K(P, Q)$ is the kernel function that relates the observations \tilde{g} at the observation point P and \tilde{w} at the integration point Q . It goes without further discussion that solving an integral equation (inverse problem) is a much more difficult problem than that of just computing an integral formula expression (forward problem). This is particularly the case if the integral equation is ill-posed.

A more general and difficult problem is that of solving a non-linear integral equation. Such problems are treated in Ch. 8.

Below we will limit the discussion to that of solving Eq. (2.135a) in the case that the kernel function is *separable* in the form of a series of Legendre's polynomials $P_n(\cos \psi)$, i.e.

$$K(P, Q) = \sum_{n=0}^{\infty} (2n+1)k_n P_n(\cos \psi), \quad (2.136)$$

where ψ is the geocentric angle between the points P and Q . Inserting Eq. (2.136) into Eq. (2.135a) and interchanging summation and integration one obtains:

$$\sum_{n=0}^{\infty} k_n \tilde{w}_n(P) = \tilde{g}(P) = \sum_{n=0}^{\infty} \tilde{g}_n(P), \quad (2.137a)$$

where:

$$\left\{ \begin{array}{c} \tilde{w}_n(P) \\ \tilde{g}_n(P) \end{array} \right\} = \frac{2n+1}{4\pi} M \left\{ \left[\begin{array}{c} \tilde{w}(Q) \\ \tilde{g}(Q) \end{array} \right] P_n(\cos \psi) \right\} \quad (2.137b)$$

are the *Laplace harmonics* of \tilde{w} and \tilde{g} . Although these harmonics are functions of position, below we will usually not specify this unless necessary for understanding.

From Eq. (2.137a), we may identify a relation between the unknown \tilde{w}_n and the known \tilde{g}_n as:

$$k_n \tilde{w}_n = \tilde{g}_n \quad \text{or} \quad \tilde{w}_n = \frac{\tilde{g}_n}{k_n} \quad \text{if and only if } k_n \neq 0, \quad (2.138)$$

and these relations hold also for the error free harmonics w_n and g_n .

In this study, we will always assume that $k_n \neq 0$ for all degrees. Then, at least tentatively, one may come up with a solution for the unknown as:

$$\tilde{w}(P) = \sum_{n=0}^{\infty} \tilde{w}_n(P) = \sum_{n=0}^{\infty} \frac{\tilde{g}_n(P)}{k_n}. \quad (2.139)$$

However, this series does not necessarily converge, but in order to do so, \tilde{g}_n must be smoother than k_n . More precisely, a square integrable solution for \tilde{w} exists if only if the *Picard condition* is satisfied, i.e.

$$\sum_{n=0}^{\infty} \left(\frac{\tilde{g}_n}{k_n} \right)^2 < \infty. \quad (2.140)$$

This condition can be satisfied either by truncating the unknown spectrum of w to a finite degree, say, n_{\max} , by smoothing the coefficients k_n or both. In the first case, despite the truncation, the solution will be affected also by high-degree signals and the noise of the observations (spectral leakage; Trampert and Snieder 1996). In the second case, by discretizing Eq. (2.135a), one implicitly smooths the solution space to a finite set, corresponding to the selected block size on the sphere. Approximately, by choosing the block size $\nu^\circ \times \nu^\circ$, the resolution of the solution will be limited to harmonic degree $n_{\max} = 180/\nu^\circ$. The smaller the block size, the more ill-conditioned the system of equations will be. As an example, Martinec (1998, Sect. 8.6) performed a discrete downward continuation of surface gravity anomalies from elevations as high as 2.425 m to sea level in the Canadian Rocky Mountains by discretizing Poisson's integral equation Eq. (3.31a–c). The iterative solution worked well for observation grid sizes larger than or equal to 5', while it failed for block sizes of 30" \times 60" due to poor numerical conditioning.

Below we will study the solutions of Eq. (2.135a) by Tikhonov regularization, Wiener filter and spectral smoothing and combination. Other types of discrete regularization methods can be found in Hansen (1998).

2.8.1 Tikhonov Regularization

One method for regularization of an ill-posed problem originates with Phillips (1962) and AN Tikhonov in 1963 (see Tikhonov and Arsenin 1977). By this method, Eq. (2.135a) is first discretized into a matrix observation equation, where we assume that the system is over-determined, i.e. the number of observations is larger than the number of unknowns. The result is:

$$\mathbf{K}\tilde{\mathbf{w}} = \tilde{\mathbf{g}} - \boldsymbol{\varepsilon} = \mathbf{g}, \quad (2.141)$$

where \mathbf{K} , $\tilde{\mathbf{w}}$, $\tilde{\mathbf{g}}$ and $\boldsymbol{\varepsilon}$ are the design matrix, vectors of unknowns, observations and residuals, respectively. Assuming that the residuals are random with expectation zero, and that there are no correlations among the individual residuals, the related Tikhonov problem is to minimize the target function

$$E\{\boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}\} + \mathbf{w}^T \boldsymbol{\Gamma}^T \boldsymbol{\Gamma} \mathbf{w} \quad (2.142)$$

for some choice of the Tikhonov matrix $\boldsymbol{\Gamma}$. According to Ditmar et al. (2003), the problem of regularization includes two aspects: (a) the optimal choice of the regularization technique (i.e. of the regularizing functional or the regularization matrix) and (b) the optimal choice of the regularization parameter. The regularization matrix $\boldsymbol{\Gamma} = \alpha \mathbf{Q}$ can be divided into three categories: zero-order Tikhonov regularization with $\mathbf{Q} = \mathbf{I}$ and first- and second-order regularizations, where \mathbf{Q} is either first- or second-order derivative operators (see Eqs. 2.143c, 2.143d). For $\boldsymbol{\Gamma} = \alpha \mathbf{I}$, where α is a small positive constant and \mathbf{I} is the unit matrix, the solution to the minimization is given by the modified normal matrix equation

$$(\mathbf{K}^T \mathbf{K} + \alpha^2 \mathbf{I}) \hat{\mathbf{w}} = \mathbf{K}^T \tilde{\mathbf{g}} \quad (2.143a)$$

with the solution

$$\hat{\mathbf{w}} = (\mathbf{K}^T \mathbf{K} + \alpha^2 \mathbf{I})^{-1} \mathbf{K}^T \tilde{\mathbf{g}}, \quad (2.143b)$$

where the matrix $\alpha^2 \mathbf{I}$ stabilizes the original least squares solution obtained for $\alpha = 0$. As the stabilization has the less desired effect of making the solution biased, the size of α should be a compromise between the bias and the expected observation error propagation, and it must be sufficiently large to match the computer capacity to solve Eq. (2.143a). Higher-order Tikhonov regularization operators are given by (Hansen 1998, Chap. 8):

$$\mathbf{Q}_{(n-1) \times n} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \quad (2.143c)$$

and

$$\mathbf{Q}_{(n-2) \times n} = \begin{bmatrix} 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix}, \quad (2.143d)$$

which represent the first- and second-derivative operators, respectively.

Applying singular value decomposition, matrix \mathbf{K} can be decomposed into:

$$\mathbf{K} = \mathbf{U}\mathbf{D}\mathbf{V}^T, \quad (2.144)$$

where \mathbf{U} and \mathbf{V} are matrices containing all the eigen-vectors \mathbf{U}_i and \mathbf{V}_i of \mathbf{K} , and \mathbf{D} is a diagonal matrix constructed by the singular values (i.e., squares of the eigen-values λ_i of \mathbf{K}). As the eigen-vectors are orthonormal, it follows that Eq. (2.143a) has the solution

$$\hat{\mathbf{w}} = \mathbf{V}(\mathbf{D}^2 + \alpha^2 \mathbf{I})^{-1} \mathbf{D}\mathbf{U}^T \tilde{\mathbf{g}} = \sum_{i=1}^q \frac{\lambda_i^2 \mathbf{U}_i^T \tilde{\mathbf{g}}}{\lambda_i^2 + \alpha^2} \mathbf{V}_i = \sum_{i=1}^q f_i \frac{\mathbf{U}_i^T \tilde{\mathbf{g}} \mathbf{V}_i}{\lambda_i}, \quad (2.145)$$

where the filter factor $f_i = \lambda_i^2 / (\lambda_i^2 + \alpha^2)$ smooths the solution for \mathbf{w} . By taking the statistical expectation of Eq. (2.145) and inserting the expected value for $\tilde{\mathbf{g}}$ from Eqs. (2.134a, b), it follows that each component \hat{w}_i of the computed vector is biased by $-\alpha^2 w_i / (\lambda_i^2 + \alpha^2)$.

Note. Here we discuss only the simple Tikhonov regularization by Eq. (2.145). Other important methods can be found, e.g. in Hansen (1998, Sect. 5.1). In statistical literature Tikhonov's method is known as *ridge regression*, e.g. Marquardt (1970). Xu and Rummel (1994) presented such a technique, by introducing more than one regularization parameter, based on the criterion of minimizing the trace of the mean square error of the solution, to determine gravity potential harmonic coefficients from satellite gravimetric data.

Let us finally mention that one simple way of smoothing the Tikhonov type of solution is to limit the number of unknowns in Eq. (2.141), which corresponds to limiting the number of discrete surface elements in the integral of Eq. (2.135a), see for example the numerical study performed by Martinec (1998, Sect. 8.6).

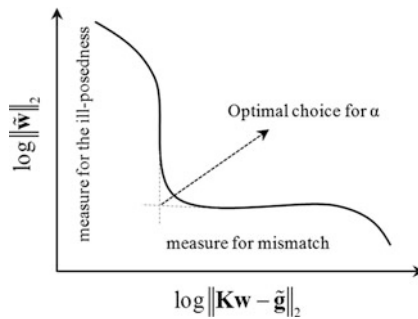
2.8.1.1 Numerical Methods for Determining the Regularization Parameter α

There are some numerical methods for computing the regularization parameter α given in Eq. (2.145). Most important are the L-curve and generalized cross-validation methods (see Hansen 1998, Sect. 2). The L-curve displays the trade-off between minimizing the residual norm ($\|\epsilon\|_2 = \|\mathbf{K}\mathbf{W} - \tilde{\mathbf{g}}\|_2$) and the solution norm ($\|\tilde{\mathbf{w}}\|_2$) in the regularization problem of Eq. (2.143a). For discrete ill-posed problems, it turns out that the L-curve, when plotted in logarithmic scale, almost always has a characteristic L-shaped appearance. Using this technique, we search for the point with maximum curvature as illustrated in Fig. 2.6. L-curve is the most suitable graphical tool to compute the regularization parameter, which is a plot for all regularization parameters of the norm of the regularized solution versus the corresponding residual norm. This method plays a major role in connection with regularization methods for discrete ill-posed problems.

Generalized cross-validation (GCV) is based on the assumption that, if the i -th arbitrary element of \mathbf{w} is left out, then the corresponding regularized solution should predict this observation well, and the choice of regularization parameter should be independent of an orthogonal transformation of \mathbf{w} . Then the regularization parameter, given in Eq. (2.145), is chosen such that the following function is a minimum:

$$GCV = \frac{\|\mathbf{K}\hat{\mathbf{w}} - \tilde{\mathbf{g}}\|_2^2}{(\text{trace}(\mathbf{I}_m - \mathbf{K}\mathbf{K}^{-1}))} \quad (2.146)$$

Fig. 2.6 The L-curve
(graphical tool for analysis of
discrete ill-posed problems)



2.8.2 Wiener Filtering

In the Wiener filter (Wiener 1949), one assumes that the signals g with w and the observation noise ε are all stationary stochastic processes with expectations zero with known spectral characteristics, i.e. their covariance and cross-covariance functions are known. The solution is practically the same as that for *least squares collocation* (Moritz 1980) and *kriging* (Matheron 1963) in geodesy and geostatistics, respectively.

Introducing a general estimator for w from a surface integral on sphere by the formula

$$\tilde{w}(P) = M_Q \{h(P, Q) \tilde{g}(Q)\}, \quad (2.147a)$$

where h is an arbitrary linear kernel function, the expected mean square error (MSE) the estimator becomes:

$$\begin{aligned} \tilde{m}^2 = E \left\{ (\tilde{w}(P) - w(P))^2 \right\} &= \sigma_w^2(P) - 2M_Q \{h(P, Q) c_{gw}(Q, P)\} \\ &+ M_Q [h(P, Q) M_X \{h(P, X) c_{gg}(Q, X)\}], \end{aligned} \quad (2.147b)$$

where c_{gw} and c_{gg} are the cross- and auto-covariance functions between the signals marked by the subscripts, and $\sigma_w^2(P)$ is the variance of w . The minimum of the MSE is obtained for h satisfying the Wiener-Hopf equation (see also Sect. 2.2.2):

$$c_{wg}(P, Q) = M_X \{ \hat{h}(P, X) c_{gg}(Q, X) \}, \quad (2.148)$$

yielding the MSE

$$\tilde{m}^2 = \sigma_w^2(P) - M_Q [\hat{h}(P, Q) M_X \{ \hat{h}(P, X) c_{gg}(Q, X) \}]. \quad (2.149)$$

Assuming that the covariance functions are homogeneous and isotropic, they can be written in the spectral forms

$$c_{gg}(X, Q) = c_{gg}(X, Q) + c_{\varepsilon\varepsilon}(X, Q) = \sum_{n=0}^{\infty} (c_n^2 + \sigma_n^2) P_n(\cos \psi), \quad (2.150a)$$

and

$$c_{wg}(P, Q) = \sum_{n=0}^{\infty} d_n P_n(\cos \psi). \quad (2.150b)$$

Here c_n^2 and σ_n^2 are the signal and error degree variances of \tilde{g} , while $d_n = d_n(P)$ are the signal degree variances of the cross-covariance function. Notice that the

latter is a function of position/elevation (only) if the estimated quantity lies outside the sphere of computation.

Inserting the above series of covariance functions, as well as the series representation for the kernel function h ,

$$h(P, Q) = \sum_{n=0}^{\infty} h_n P_n(\cos \psi) \quad (2.151)$$

into Eq. (2.148), the least squares solution for h follows as:

$$\hat{h}(P, Q) = \sum_{n=0}^{\infty} (2n+1) \frac{d_n}{c_n^2 + \sigma_n^2} P_n(\cos \psi). \quad (2.152)$$

Hence, by considering Eqs. (2.147a) and (2.149), the least squares solution for w and its mean square error become:

$$\hat{w}(P) = \sum_{n=0}^{\infty} \frac{d_n}{c_n^2 + \sigma_n^2} \tilde{g}_n \quad (2.153a)$$

and

$$\hat{m}^2 = \sigma_w^2 - \sum_{n=0}^{\infty} \frac{d_n^2}{c_n^2 + \sigma_n^2}. \quad (2.153b)$$

From Eq. (2.138), we also have the relation $w_n = g_n/k_n$, which yields:

$$\hat{w}(P) = \sum_{n=0}^{\infty} f_n k_n^{-1} \tilde{g}_n, \quad \text{where } f_n = \frac{c_n^2}{c_n^2 + \sigma_n^2} \quad (2.154a)$$

and

$$\hat{m}^2 = \sum_{n=0}^{\infty} k_n^{-2} c_n^2 - \sum_{n=0}^{\infty} k_n^{-2} \frac{c_n^4}{c_n^2 + \sigma_n^2} = \sum_{n=0}^{\infty} k_n^{-2} \frac{c_n^2 \sigma_n^2}{c_n^2 + \sigma_n^2}. \quad (2.154b)$$

As an alternative, Eq. (2.154a) can be written in the space domain as:

$$\hat{w}(P) = \frac{1}{4\pi} \iint_{\sigma} H(P, Q) \tilde{g}(Q) d\sigma_Q, \quad (2.155a)$$

where the kernel function is:

$$H(P, Q) = \sum_{n=0}^{\infty} (2n+1)k_n^{-1}f_nP_n(\cos \psi). \quad (2.155b)$$

2.8.3 Spectral Smoothing

Let us return to Eq. (2.154a)

$$\tilde{w}(P) = \sum_{n=0}^{\infty} f_n k_n^{-1} \tilde{g}_n, \quad (2.156)$$

where f_n are now arbitrary filter parameters to be estimated such that the mean square error of \tilde{w} is minimized. As the error of \tilde{w} is given by its random error and bias, i.e.

$$\varepsilon_{\tilde{w}} = \sum_{n=0}^{\infty} [f_n k_n^{-1} \varepsilon_n + (f_n - 1)k_n^{-1} g_n], \quad (2.157)$$

it follows the expected MSE becomes:

$$\tilde{m}^2 = E[M\{\varepsilon_{\tilde{w}}^2\}] = \sum_{n=0}^{\infty} k_n^{-2} [f_n^2 \sigma_n^2 + (f_n - 1)^2 c_n^2], \quad (2.158)$$

where σ_n^2 and c_n^2 are the error and signal-degree variances of \tilde{g} . The minimum MSE is achieved by differentiating the MSE w.r.t. each of the smoothing factors and equating to zero. The result is:

$$\hat{f}_n = \frac{c_n^2}{c_n^2 + \sigma_n^2}, \quad (2.159)$$

and the least squares estimator \hat{w} and its MSE are the same as in Eqs. (2.154a, b). Some of the theory and applications were presented in Sjöberg (1980, 1986, 2011a, b).

The practical formulation in the space domain again becomes Eqs. (2.154a, b).

2.8.4 Spectral Combination

We now assume that, in addition to the information given in above, there is an Earth Gravitational Model (EGM) available to degree n_{\max} that yields the unbiased estimate w_1 (unbiased through degree n_{\max})

$$w_1 = \sum_{n=0}^{n_{\max}} w_n^{GM}, \quad (2.160)$$

with the random error with expectation zero

$$dw_1 = \sum_{n=0}^{n_{\max}} w_n^{GM} \quad (2.161)$$

and the variance (composed of the error degree variances σ_n^{GM})

$$\sigma_{w_1}^2 = \sum_{n=0}^{n_{\max}} \sigma_n^{GM}. \quad (2.162)$$

A general estimator for w , unbiased through degree n_{\max} , can be formulated as:

$$\tilde{w} = \sum_{n=0}^{\infty} k_n^{-1} p_n \tilde{g}_n + \sum_{n=0}^{n_{\max}} (1 - p_n) w_n^{GM}, \quad (2.163)$$

with the MSE

$$\tilde{m}^2 = \sum_{n=0}^{\infty} \left\{ k_n^{-2} p_n^2 \sigma_n^2 + (1 - p_n)^2 d c_n^{GM} \right\}, \quad (2.164a)$$

where:

$$d c_n^{GM} = \begin{cases} \sigma_n^{GM} & \text{if } n \leq n_{\max} \\ k_n^{-2} c_n^2 & \text{otherwise.} \end{cases} \quad (2.164b)$$

Here p_n are arbitrary degree weights, which are optimized in a least squares sense by differentiating \tilde{m}^2 w.r.t. each of them and equating to zero. The result is:

$$\hat{p}_n = \begin{cases} \frac{\sigma_n^{GM}}{k_n^{-2} \sigma_n^2 + \sigma_n^{GM}} & \text{if } n \leq n_{\max} \\ \frac{c_n^2}{c_n^2 + \sigma_n^2} & \text{otherwise,} \end{cases} \quad (2.165)$$

and the MSE becomes:

$$\hat{m}^2 = \sum_{n=0}^{n_{\max}} \frac{k_n^2 \sigma_n^2 \sigma_n^{GM}}{\sigma_n^2 + k_n^2 \sigma_n^{GM}} + \sum_{n=n_{\max}+1}^{\infty} \frac{k_n^2 c_n^2}{\sigma_n^2 + k_n^2 c_n^2}. \quad (2.166)$$

Finally, the spectral combination can be formulated also as the sum of a surface integral and a spectral series:

$$\hat{w}(P) = \frac{1}{4\pi} \iint_{\sigma} K(P, Q) \tilde{g}(Q) d\sigma_Q + \sum_{n=0}^{n_{\max}} (1 - \hat{p}_n)^2 w_n^{GM}, \quad (2.167a)$$

where the kernel function is:

$$K(P, Q) = \sum_{n=0}^{\infty} (2n+1) k_n^{-1} \hat{p}_n P_n(\cos \psi). \quad (2.167b)$$

For applications of spectral smoothing and combination, see Sects. 4.4.4 and 7.5. See also Sjöberg (1981, 1986, 2011a, b).

2.8.5 Optimum Regularization

Based on the above experiences, one may ask whether Tikhonov regularization can be modified to share the properties of the Wiener filter and/or spectral smoothing, namely to be optimum in the sense of minimizing the MSE. There are numerous publications solving Tikhonov's regularization problem by minimizing the MSE of the solution. However, each such solution is optimal only w.r.t. the specified target function, Eq. (2.142), i.e. for a specified Tikhonov matrix $\mathbf{\Gamma}$. Hence, the major problem is thus to find the correct Tikhonov matrix for the optimum solution. For this purpose, we rewrite Eq. (2.135a) as:

$$M\{[K(\psi) + Q(\psi)]\tilde{w}\} = \tilde{g}(P), \quad (2.168a)$$

where:

$$Q(\psi) = \sum_{n=0}^{\infty} (2n+1) q_n P_n(\cos \psi). \quad (2.168b)$$

Here q_n are arbitrary parameters to be determined such that the target function, the expected global MSE m_w^2 of \tilde{w} , is minimized. As the spectral form of Eq. (2.168a) can be written:

$$\tilde{w}_n = \frac{\tilde{g}_n}{k_n + q_n}, \quad (2.169)$$

it follows that its error and global MSE become:

$$\varepsilon_{w_n} = \frac{\tilde{g}_n}{k_n + q_n} - \frac{g_n}{k_n} \quad \text{and} \quad m_{w_n}^2 = \frac{k_n^2 \sigma_n^2 + q_n^2 c_n^2}{k_n^4 + k_n^2 q_n^2}, \quad (2.170)$$

and, by differentiating the MSE w.r.t. q_n , one obtains the least squares choice of the parameters:

$$\hat{q}_n = k_n \sigma_n^2 / c_n^2. \quad (2.171)$$

Inserting this choice for q_n in Eq. (2.169) and summing up, one obtains the solution

$$\hat{w} = \sum_{n=0}^{\infty} \frac{c_n^2}{c_n^2 + \sigma_n^2} \frac{\tilde{g}_n}{k_n}, \quad (2.172)$$

which is the same as the solution by spectral filtering, Eqs. (2.156), with filter factors given by Eq. (2.159).

However, the kernel function Q with parameters \hat{q}_n is a divergent series, as $\sigma_n^2 / c_n^2 > 1$ for large n , which implies that the optimum regularization cannot be realized in the limiting integral equation, Eq. (2.168a). However, in the numerical approximation of the integral equation, we may approximate it by the matrix equation

$$(\mathbf{K} + \overline{\mathbf{Q}}) \mathbf{w} = \tilde{\mathbf{g}} \quad (\text{consistent}) \quad (2.173)$$

with the solution

$$\mathbf{w} = (\mathbf{K} + \overline{\mathbf{Q}})^{-1} \tilde{\mathbf{g}}, \quad (2.174)$$

where the elements of $\overline{\mathbf{Q}}$ are determined from a smoothed kernel function, Eq. (2.168b), e.g. obtained by truncating the series to a maximum degree. (Such a truncation is a reasonable approximation, as the numerical integration to a finite number of integration blocks will automatically limit the frequency contained in the solution.) In this way, the solution for \mathbf{w} will be a smoothed spectral filter/Wiener filter. The higher the degree of truncation in the kernel function for $\overline{\mathbf{Q}}$, and the more precise the numerical integration is, the closer to the Wiener filter will be the solution.

In the special case with all q_n set to a constant α^2 , the function value for $\mathbf{Q}(0)$ is still infinite, but the Tikhonov solution is consistent with the non-optimized Wiener filter

$$\hat{w} = \sum_{n=0}^{\infty} \frac{c_n^2}{c_n^2 + \alpha^2} \frac{\tilde{g}_n}{k_n}. \quad (2.175)$$

2.8.6 Spherical Harmonic Analysis

Let the unknown w be represented by the truncated series of fully normalized spherical harmonics Y_{nm} :

$$\tilde{w}(P) = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n w_{nm} Y_{nm}(P), \quad (2.176a)$$

where the harmonics are orthonormal, i.e.

$$M\{Y_{nm}Y_{rs}\} = \begin{cases} 1, & \text{if } (n, m) = (r, s) \\ 0 & \text{otherwise.} \end{cases} \quad (2.176b)$$

The task is to determine the spherical harmonic coefficients w_{nm} from Eq. (2.168a). Hence, by inserting Eq. (2.176a) and using Eq. (2.176b), we obtain:

$$\sum_{n=0}^{n_{\max}} (k_n + q_n) \sum_{m=-n}^n w_{nm} Y_{nm}(P) = \tilde{g}(P). \quad (2.177)$$

Then, by multiplying each member of this equation by $Y_{nm}(P)$ and averaging over the unit sphere, one finally arrives at the solution for the harmonic coefficients

$$w_{nm} = \frac{1}{k_n + q_n} M\{\tilde{g}(P)Y_{nm}(P)\}. \quad (2.178)$$

If q_n is chosen as $k_n \sigma_n^2 / c_n^2$, this solution for the harmonic coefficients will be optimal in the sense of minimizing the MSE. Finally, by applying these coefficients in Eq. (2.176a), the optimum, truncated estimate of w is obtained.

The solution by spherical harmonic analysis has the merits of being stable and not prone to spectral leakage as previous methods (see the different approach of Trampert and Snieder (1996) and Spetzler and Trampert (2003), which suffers from the problem of leakage). Its major drawback is the requirement of a global, homogeneous coverage of data on the sphere. Finally, we mention that if an independent set of harmonics of w is available, it can be combined with the above harmonics in an optimum sense.

This method was applied [with q_n set to 0 in Eq. (2.178)] in computing some of the OSU Earth Gravitational Models in the 1970s and 1980s; see e.g. Rapp (1981) and Rapp and Cruz (1986).

2.8.7 Comparison

Table 2.1 summarizes a comparison of the inverse solutions by Tikhonov's method, Wiener filtering and spectral smoothing and combination.

The most important results are the following:

- Tikhonov regularization is the solution by direct (approximate) solving the original integral equation. The smoothing is performed in two ways: (1) the original integral equation is approximated by a finite sum of unknowns and surface elements, and (2) by adding the smoothing term $\alpha^2 \mathbf{I}$ to the normal matrix. All other methods use a direct integral formula for the solution.
- Although the spectral solution of Tikhonov regularization (Eq. 2.145) resembles the spectral forms of the Wiener filter and spectral smoothing, they are not the same, as the Tikhonov solution includes the singular values and eigen-vectors of the normal matrix (including the smoothing term), which vary w.r.t. chosen block size and number of unknown parameters, while the latter are based on the kernel, signal and error spectra. This implies that the individual observations used in Tikhonov's method can be weighted, but the additional feature of spectral weighting in the other methods, is not possible.
- The Wiener filter and the spectral smoother are identical solutions. However, the assumptions and target functions differ. The former minimizes the (local) MSE based on the known signal and covariance functions (correlation functions), while the latter minimizes the global MSE base on known signal and error degree variances.

Table 2.1 Comparison of regularization methods (Sjöberg 2012)

Method	Equation	Extra info.	Target function	Assumptions
Tikhonov regularization	Integral equation	α	$\boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} + \alpha^2 \mathbf{I}$	$E\{\boldsymbol{\varepsilon}\} = 0$
Wiener filter	Integral formula	c_n^2, σ_n^2, d_n	MSE	Stochastic processes ^a
Spectral smoothing	Integral formula	c_n^2, σ_n^2, d_n	Global MSE	Stochastic processes ^b
Spectral combination	Integral formula	c_n^2, σ_n^2, d_n	Global MSE	Stochastic processes ^b
Optimum regularization	Integral equation	c_n^2, σ_n^2, d_n	Global MSE	Stochastic processes ^c
Harmonic analysis	Integral formula	c_n^2, σ_n^2	MSE	Global data on the sphere

^aThe stochastic processes are stationary processes with expected value zero

^bThe expected values of the observation errors are zero

^cThe optimum Q is approximated by the smoothed \mathbf{Q}

- The Wiener filter assumes stationary stochastic processes with statistical expectations zero, while spectral smoothing and combination only assumes that the observation errors are zero in expectations.
- By spectral combination the integral solution can be combined in an optimum way with a priori information of the unknown function in the spectral domain.
- The solution by optimum regularization, described in Sect. 2.8.5, is the space domain representation of spectral smoothing. The solution is a smoothed spectral/Wiener filter. In the continuous case, the problem cannot even be formulated, as the corresponding integral equation does not exist.
- Harmonic analysis needs data from all over the sphere. Among its merits are resistance to spectral leakage and ill-conditioning.

2.8.8 Concluding Remarks

As discussed above, the numerical solution to an integral equation is frequently ill-conditioned, and for ill-posed problems this is always the case. Then, a unique and stable solution can be obtained, at the prize of a bias, by introducing some kind of smoothing. The numerical Tikhonov types of solutions involve solving a matrix equation, where the biases are based on some criterions. In contrast, the solutions by Wiener filter and spectral smoothing and combination are more computationally efficient, as they employ forward integration, or, numerically, matrix multiplications. This implies that Tikhonov types of solutions are particularly sensitive to the choice of block-size in the numerical integration of the coefficients of the design matrix, and the bias term α^2 must increase when the block-size decreases. This problem is not the case for the direct integration methods of Wiener and spectral filtering and spectral combination, as well as harmonic analysis.

Finally we emphasize that spectral combination is more flexible than the other methods, as it enables an optimal (with respect to minimum MSE) merging of different data. Also, harmonic analysis (possibly including spectral combination) is a viable alternative, provided that the data can be made available globally on the sphere.

Appendix: Answers to Exercises

Exercise 2.1 From Eq. (2.37a) one obtains the Taylor series

$$\begin{aligned} l_{p0}^{-1} &= r_p^{-1} \left[1 - \frac{1}{2}(s^2 - 2st) + \frac{(-\frac{1}{2})(-1 - \frac{1}{2})}{1 \times 2}(s^2 - 2st)^2 + \dots \right] \\ &= r_p^{-1} \left[1 + st + s^2 \frac{3t^2 - 1}{2} + \dots \right], \end{aligned}$$

and by comparing with Eq. (2.38a) the solution follows.

Exercise 2.2 The left member of Eq. (2.42) yields for $n = 0, 1$ and 2:

$$\begin{aligned} \int_{-1}^1 1 dt &= 2, \quad \int_{-1}^1 t^2 dt = 2/3 \quad \text{and} \quad \int_{-1}^1 \left(\frac{3t^2 - 1}{2} \right)^2 dt \\ &= \int_{-1}^1 \left(\frac{9t^4 - 6t^2 + 1}{4} \right) dt = \frac{1}{4} \left[\frac{9t^5}{5} - \frac{6t^3}{3} + t \right]_{-1}^1 = \frac{2}{5}, \end{aligned}$$

The second equation in Eq. (2.42) is shown in the same way.

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