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Inverse gravimetry: background material and multiscale mollifier approaches

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Abstract This paper represents an extended version of the publications Freeden (in: Freeden, Nashed, Sonar (eds) Handbook of Geomathematics, 2nd edn, vol 1, Springer, New York, pp 3–78, 2015) and Freeden and Nashed (in: Freeden, Nashed (eds) Handbook of Mathematical Geodesy, Geosystems Mathematics, Birkhäuser, Basel, pp 641–685, 2018c). It deals with the ill-posed problem of transferring input gravitational potential information in the form of Newtonian volume integral values to geological output characteristics of the density contrast function. Some essential properties of the Newton volume integral are recapitulated. Different methodologies of the resolution of the inverse gravimetry problem and their numerical implementations are examined including their dependence on the data source. Three types of input information may be distinguished, namely internal (borehole), terrestrial (surface), and/or external (spaceborne) gravitational data sets. Singular integral theory based inversion of the Newtonian integral equation such as a Haar-type solution is handled in a multiscale framework to decorrelate specific geological signal signatures with respect to inherently given features. Reproducing kernel Hilbert space regularization techniques are studied (together with their transition to certain mollified variants) to provide geological contrast density distributions by "downward continuation" from terrestrial and/or spaceborne data. Numerically, reproducing kernel Hilbert space spline solutions are formulated in terms of Gaussian approximating sums for use of gravimeter data systems.

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1 Introduction

We begin our considerations by recapitulating some basic mathematical constituents of the theory of inverse problems:

A *direct (forward) problem* is given in the following form:

$$\text{object} \quad \longrightarrow \quad \text{data information of the object.}$$

The *inverse problem* is considered the "inverse" of the direct problem which relates the object (sub)information to the object. An *object* may be understood to be the systematic relationship of all data subinformation, object parameters, and other auxiliary information.

The object of the inverse gravimetry problem is to determine the density inside a certain subarea $\mathcal{G}$ of the Earth. If the density is supposed to be a function F of bounded signal energy in $\overline{\mathcal{G}}$, i.e.,

$$\|F\|_{L^2(\mathcal{G})} = \left(\int_{\mathcal{G}} |F(x)|^2 \, dx \right)^{1/2} < \infty, \tag{1}$$

the gravitational potential

$$V(x) = \frac{1}{4\pi} \int_{\mathcal{G}} \frac{1}{|x - y|} F(y) \, dy, \quad x \in \mathbb{R}^3 \tag{2}$$

can be calculated everywhere in $\mathbb{R}^3$ according to Newton's famous law (1687), so that the *direct gravimetry problem*

$$\underbrace{F}_{\text{= density signature}} \quad \longrightarrow \quad \underbrace{V}_{\text{= gravitational potential}} \tag{3}$$

is a matter of (approximate) integration.

Already at this stage, it should be mentioned that there is a striking dependence in the calculation of a gravitational value $V(x)$ on its position $x \in \mathbb{R}^3$. As far as the point x is situated in the "outer space" $\mathcal{G}^c = \mathbb{R}^3 \backslash \overline{\mathcal{G}}$ ($\overline{\mathcal{G}} = \mathcal{G} \cup \partial\mathcal{G}$, $\partial\mathcal{G}$ boundary surface of $\mathcal{G}$), the value $V(x)$ is obtained by a proper integral. However, for a position x in the "inner space" $\mathcal{G}$ or on the boundary $\partial\mathcal{G}$, we are confronted with an improper integral in $\mathbb{R}^3$. As a consequence, it may be expected that the *inverse gravimetry problem*

$$\underbrace{V}_{\text{= gravitational potential}} \quad \longrightarrow \quad \underbrace{F}_{\text{= density signature}} \tag{4}$$

also shows a striking difference in its solution process and dependence on the position of the gravitational data.

Inverse gravimetry is a central research area of geodesy, geophysics, and geo-exploration. It is a potential field technique which reflects variations in the Earth's gravitational field. These variations are caused by density contrasts inside the Earth. Gravimetric surveys are carried out by use of extremely sensitive instruments capable of measuring tiny variations in the gravitational field. A gravimeter is a type of an accelerometer. There are essentially two types of gravimeters, namely relative and absolute gravimeters. Absolute gravimeters measure the local gravity in absolute units. They work by directly measuring the acceleration of a mass during free fall in a vacuum. Relative gravimeters compare the value of gravity at one point with another. Most common relative gravimeters are spring-based. A spring-based relative gravimeter is basically a weight on a spring, and by measuring the amount by which the weight stretches the spring, gravitation becomes available via Hooke's law in linearized form. On a global scale gravimetric datasets are used in gravity surveys for establishing the figure of the geoid. Locally micro-gravimeters are in use, e.g., for geodetic and geophysical research, geothermal exploration, petroleum and mineral recovery.

In its simplest operator formulation, the integral equation (2) may be described as an operator equation

$$A[F] = V, \tag{5}$$

where the operator A is defined as an integral over the volume $\mathcal{G} \subset \mathbb{R}^3$

$$A[F](x) = \int_{\mathcal{G}} G(\Delta; |x - y|) \, F(y) \, dy = V(x), \quad x \in \mathbb{R}^3, \tag{6}$$

constituted by the convolution of the density contrast function F and a kernel function $G(\Delta; \cdot)$ showing the same singularity as a point mass, namely the *Newtonian kernel*

$$G(\Delta; |x - y|) = \frac{1}{4\pi} \frac{1}{|x - y|}, \quad x \in \mathbb{R}^3 \backslash \{y\}. \tag{7}$$

Apart from the sign, $G(\Delta; |x - y|)$ is known as the *fundamental solution of the Laplace equation*, so that $-\Delta_x G(\Delta; |x - y|) = 0, x \neq y$ (or in distributional jargon, $-\Delta_x G(\Delta; |x-y|) = \delta(|x-y|)$, where δ is the Dirac distribution). Roughly speaking, the operator A acts in the inner space $\mathcal{G}$ as the inverse to the negative Laplace operator,

$$- \Delta V(x) = -\Delta \, A[F](x) = - \Delta_x \int_{\mathcal{G}} G(\Delta; |x - y|) \, F(y) \, dy = F(x), \quad x \in \mathcal{G}, \tag{8}$$

which is to say (at least if the function F is Hölder continuous in a neighborhood of $x \in \mathcal{G}$) that the operation of taking the Newtonian potential of a function is a somehow "inverse operation" to the application of the negative Laplace operator.

Note that the integral (6) is named for I. Newton (1642–1720), who first discovered it and pioneered the work of P.-S. Laplace (1749–1829) and C. F. Gauss (1777–1855)

about harmonic and potential functions. Indeed, the setting (6) serves as the fundamental gravitational potential in Newton's law of gravitation (1687). In the context of this approach, the interest in our paper is laid in studying the gravitational field in macroscopic sense, where the quantum behavior of gravitation may not be taken in account.

Seen from the perspective of potential theory (see, e.g., Freeden and Gerhards 2013), Eq. (6) is in close relation to the third Green theorem of potential theory

$$
\alpha(x)\, P(x) = - \int_{\mathcal{G}} G(\Delta; |x - y|)\, \Delta P(y)\, dV(y)
$$
$$
+ \int_{\partial \mathcal{G}} \left(G(\Delta; |x - y|) \frac{\partial}{\partial \nu(y)} P(y) - P(y) \frac{\partial}{\partial \nu(y)} G(\Delta; |x - y|) \right)\, d\omega(y), \quad (9)
$$

that holds true for all twice continuously differentiable functions P on $\overline{\mathcal{G}}$, where $\alpha(x)$ is the *solid angle* subtended by the surface $\partial \mathcal{G}$ at the point $x \in \mathbb{R}^3$ characterized by

$$
\alpha(x) = - \int_{\partial \mathcal{G}} \frac{\partial}{\partial \nu(y)} G(\Delta; |x - y|)\, d\omega(y). \quad (10)
$$

From classical potential theory it is known that

$$
\alpha(x) = \begin{cases} 1, & x \in \mathcal{G}, \\ \dfrac{1}{2}, & x \in \partial \mathcal{G}, \\ 0, & x \in \mathcal{G}^c, \end{cases} \quad (11)
$$

provided that the boundary surface $\partial \mathcal{G}$ is (locally) continuously differentiable (for a more detailed analysis the reader is referred to, e.g., Freeden and Gerhards 2013).

Once more, as an immediate consequence of (9), we may expect that the discussion of $A[F](x)$, $x \in \mathbb{R}^3$, actually has to be split into three cases, in dependence on the location of $x \in \mathbb{R}^3$ as a point of the inner space $\mathcal{G}$, outer space $\mathcal{G}^c$, or the boundary $\partial \mathcal{G}$, i.e., the internal, surface (terrestrial), and external (spaceborne) input gravitational data. Compared with the integral equation (6) we are led to the conclusion that the boundary integral in (9) vanishes for the gravitational potential V provided that x is a point of the inner space $\mathcal{G}$. Moreover, a solution of (6) in $\mathcal{G}$ is not unique, since the addition of any harmonic function to V will not affect (8). In potential theory this observation can be used, for example, to prove existence and uniqueness of solutions to the Dirichlet problem for the Poisson equation inside or outside regular domains and for suitably well-behaved functions: One first applies a Newtonian potential to obtain a solution, and then adjusts it by adding a harmonic function to get the correct boundary data.

As already mentioned, the aim of this contribution is different from solving a boundary-value problem: In the language of functional analysis, we have to solve a Fredholm integral equation of the first kind (6) that canonically leads to the framework of the theory of ill-posed problems. The main difficulty, however, is that the input data

of the inverse gravimetry problem are not canonically given in the inner space $\mathcal{G}$, but usually in $\overline{\mathcal{G}^c}$. As a matter of fact, until now in physical geodesy, only measurements are taken on the surface $\partial\mathcal{G}$ (terrestrial measurements) and/or in the outer space $\mathcal{G}$ (spaceborne measurements), i.e., in the set $\overline{\mathcal{G}^c}$. Only in exceptional cases, e.g., in the neighborhood of "boreholes" of geothermal projects, the gravitational potential V and the target function F are given inside $\mathcal{G}$, so that the use of the Poisson differential equation (8) becomes applicable in the inversion process.

Typically, for inverse problems, there will also be certain *physical constraints* which will be necessary to impose on the potential pattern so that the wanted geological features of the density distribution can be approximated in some acceptable manner. Such constraints are usually referred to as conditions reflecting realizability conditions. They will be represented in our mathematical framework by requiring the density functions to lie in some appropriate subset of the output space. Under certain conditions these realizability constraints will serve to regularize the originally stated ill-posed problem, while in others, they will dictate compromises that will have to be made between requirements for accuracy of the approximating functions and the demands of meeting such *a priori* constraints. In this contribution we are essentially interested in regularization procedures based on mollifier techniques. Different types of mollifiers will be studied in more detail, namely singular integral-type mollifiers and reproducing Hilbert space kernel mollifiers.

In physical geodesy, the study of inverse gravimetry essentially started with the work of Laplace (1799, 1812a, b), Legendre (1806a, b), Poisson (1833), Green (1838), Stokes (1849a, 1867b), Gauss (1838), Helmert (1880, 1884), Lauricella (1911), Pizzetti (1909), and many others. Not only in physical geodesy, but also in inverse problem theory, there is a huge literature about the character and role of inverse gravimetry in the framework of ill-posed and inverse problems, from which we only mention a limited selection: Anger (1990), Ballani et al. (1993a, b), Ballani and Stromeyer (1983), Freeden and Gerhards (2013), Freeden and Michel (2004), Kellogg (1929), Krarup (1969), Michel (1999, 2002a, b, 2005), Michel and Fokas (2008), Parker (1975), Moritz (1990), Morozov (1984), Rummel (1992), Sansò (1980), Sansò and Rummel (1997), Sansò and Tscherning (1989), Skorvanek (1981), Tscherning (1992), Tscherning and Strykowski (1987) and Zidarov (1986, 1990) (for further details the reader is referred to the references therein). Our paper, however, follows a different approach, whose points of departure were already indicated in the introductory chapter (Freeden 2015) of the "Handbook of Geomathematics", Springer, 2015 and in the contribution (Freeden and Nashed 2018c) in "Handbook of Mathematical Geodesy", Birkhäuser, International Springer Publishing, 2018.

2 Newton volume integral

In order to handle the inverse gravimetry problem some potential-theoretic preliminaries are needed (see, e.g., Freeden and Gerhards 2013): Let $\mathcal{G}$ be a *regular region* in $\mathbb{R}^3$, i.e., a bounded region $\mathcal{G}$ dividing $\mathbb{R}^3$ uniquely into the inner space $\mathcal{G}$ and the outer space $\mathcal{G}^c = \mathbb{R}^3\backslash\overline{\mathcal{G}}$, $\overline{\mathcal{G}} = \mathcal{G} \cup \partial\mathcal{G}$, such that the boundary $\partial\mathcal{G}$ is an orientable

Lipschitzian manifold of dimension 2 (for example, ball, ellipsoid, cube and other polyhedra, spheroid, telluroid, geoid, (actual) Earth or appropriate parts of it).

2.1 Basics of potential theory

A real-valued function P is called *harmonic in* $\mathcal{G} \subset \mathbb{R}^3$ if P is of the class $C^{(2)}(\mathcal{G})$ of functions with continuous second order partial derivatives and satisfies the Laplace equation

$$\Delta P(x) = \left(\left(\frac{\partial}{\partial x_1} \right)^2 + \left(\frac{\partial}{\partial x_2} \right)^2 + \left(\frac{\partial}{\partial x_3} \right)^2 \right) P(x_1, x_2, x_3) = 0 \qquad (12)$$

for all $x = (x_1, x_2, x_3)^T$, $x \in \mathcal{G}$.

Some important examples of harmonic functions are given below in the classical nomenclature of potential theory (see, e.g., Freeden and Gerhards 2013; Freeden and Schreiner 2009).

(a) *Potential of a mass point* According to *Newton's Law of Gravitation* two points x, y with masses M_x, M_y attract each other with a force given by

$$-\frac{\gamma}{4\pi} \frac{M_x M_y}{|x - y|^3} (x - y), \quad x, y \in \mathbb{R}^3, \ x \neq y. \qquad (13)$$

The force is directed along the line connecting the two points x, y. The constant γ denotes Newton's gravitational constant (note that γ can be assumed to be equal to one in the theoretical part, but not in numerical applications).

Although the masses M_x, M_y attract each other in symmetric way, it is convenient to call one of them the *attracting mass* and the other one the *attracted mass*. Conventionally the attracted mass is set equal to unity and the attracting mass is denoted by M:

$$v(x) = -\frac{\gamma}{4\pi} \frac{M}{|x - y|^3} (x - y), \quad x \in \mathbb{R}^3 \backslash \{y\}. \qquad (14)$$

The formula (14) expresses the force exerted by the mass M on a unit mass located at the distance $|x - y|$ from M. Obviously, the intensity $|v(x)|$ of the gravitational force $v(x)$ is given by

$$|v(x)| = \frac{\gamma}{4\pi} \frac{M}{|x - y|^2}, \quad x \in \mathbb{R}^3 \backslash \{y\}. \qquad (15)$$

The scalar function V defined by

$$V(x) = \gamma M G(\Delta; |x - y|) = \gamma M \frac{1}{4\pi} \frac{1}{|x - y|}, \quad x \in \mathbb{R}^3 \backslash \{y\} \qquad (16)$$

is called the *potential of gravitation* at the point y. The force vector $v(x)$ is the gradient vector of the scalar $V(x)$:

$$v(x) = \nabla V(x), \quad x \in \mathbb{R}^3 \backslash \{y\}. \tag{17}$$

Calculating the divergence $\nabla \cdot$ of the gradient field v, it readily follows that

$$\nabla \cdot v(x) = \nabla \cdot \nabla V(x) = \Delta V(x) = 0, \quad x \in \mathbb{R}^3 \backslash \{y\}. \tag{18}$$

(note that $|y| \le \frac{|x|}{2}$ implies $|x - y| \ge ||x| - |y|| \ge \frac{1}{2}|x|$), i.e., V is regular at infinity: $V(x) = O(|x|^{-1})$, $|x| \to \infty$.

(b) *Potential of a finite mass point system* The potential for N points x_i with masses $M_i, i = 1, \ldots, N$, is the sum of the individual contributions

$$V(x) = \gamma \sum_{i=1}^{N} M_i \, G(\Delta; |x - y_i|), \quad x \in \mathbb{R}^3 \backslash \{y_1, \ldots, y_n\}. \tag{19}$$

Clearly we have

$$\Delta V(x) = 0, \quad x \in \mathbb{R}^3 \backslash \{y_1, \ldots, y_N\}. \tag{20}$$

(c) *Potential of a volume* Let $\mathcal{G} \subset \mathbb{R}^3$ be a *regular region*. The point masses are distributed continuously over $\mathcal{G} \subset \mathbb{R}^3$ with density F. Then the discrete sum (19) becomes a continuous sum, i.e., an integral over the body $\mathcal{G}$:

$$V(x) = \gamma \int_{\mathcal{G}} G(\Delta; |x - y|) F(y) \, dy. \tag{21}$$

Obviously,

$$\Delta V(x) = 0, \quad x \in \mathbb{R}^3 \backslash \overline{\mathcal{G}}. \tag{22}$$

Note that V is defined on the whole space $\mathbb{R}^3$, however, $\Delta V(x)$ may not be obtained easily by interchanging the Laplace operator and the integral over $\mathcal{G}$ for all points x inside $\mathcal{G}$. At infinity the potential behaves like $V(x) = O(|x|^{-1})$, $|x| \to \infty$, uniformly with respect to all directions, i.e., V is regular at infinity.

2.2 Properties of the Newton integral

The Newton (volume) integral (21) over a regular region $\mathcal{G}$ corresponding to a mass density distribution F satisfies the Laplace equation in the outer space $\mathcal{G}^c = \mathbb{R}^3 \backslash \overline{\mathcal{G}}$. Clearly, this property is an immediate consequence of the harmonicity of the fundamental solution for the Laplace operator (in what follows, for simplicity, we restrict ourselves to a Newton integral (21) with γ chosen to be equal to 1).

Harmonicity in $\mathcal{G}^c$. Let $F : \overline{\mathcal{G}} \to \mathbb{R}$ be an integrable bounded function. Then

$$V(x) = \int_{\mathcal{G}} G(\Delta; |x - y|) F(y) \, dy, \quad x \in \mathcal{G}^c \tag{23}$$

satisfies

$$\Delta_x \int_{\mathcal{G}} G(\Delta; |x - y|) F(y) \, dy = 0 \tag{24}$$

for all $x \in \mathcal{G}^c$, i.e., V *is harmonic in* $\mathcal{G}^c$.

Properties in $\mathcal{G}$. By one-dimensional Taylor linearization (cf. Freeden and Schreiner 2009) we obtain

$$\frac{1}{\sqrt{u}} = \frac{1}{\sqrt{u_0}} - \frac{1}{2} \frac{1}{u_0^{\frac{3}{2}}} (u - u_0) + \frac{3}{8} \frac{1}{(u_0 + \theta(u - u_0))^{\frac{5}{2}}} (u - u_0)^2 \tag{25}$$

for some $\theta \in (0, 1)$. Setting $u = r^2$ and $u_0 = \varrho^2$ we therefore find

$$\frac{1}{r} = \frac{1}{2\varrho} \left(3 - \frac{r^2}{\varrho^2} \right) + \frac{3}{8} \frac{1}{(\varrho^2 + \theta(r^2 - \varrho^2))^{\frac{5}{2}}} (r^2 - \varrho^2)^2. \tag{26}$$

In other words, by letting $r = |x - y|$ we are able to give a simple example for a "mollification" of the fundamental solution of the Laplace equation

$$G(\Delta; r) = \frac{1}{4\pi r}, \qquad r > 0, \tag{27}$$

by

$$G_\varrho^H(\Delta; r) = \begin{cases} \dfrac{1}{8\pi\varrho} \left(3 - \dfrac{1}{\varrho^2} r^2 \right), & r \le \varrho \\[3mm] \dfrac{1}{4\pi r}, & r > \varrho. \end{cases} \tag{28}$$

such that $G_\varrho^H(\Delta; \cdot)$ is continuously differentiable for all $r \ge 0$. Obviously, $G(\Delta; r) = G_\varrho^H(\Delta; r)$ for all $r > \varrho$. As a consequence,

$$G(\Delta; |x - y|) = \frac{1}{4\pi} \frac{1}{|x - y|}, \qquad |x - y| \ne 0, \tag{29}$$

admits a "mollification" (regularization) of the form

$$G_\varrho^H(\Delta; |x - y|) = \begin{cases} \dfrac{1}{8\pi\varrho} \left(3 - \dfrac{1}{\varrho^2} |x - y|^2 \right), & |x - y| \le \varrho \\[3mm] \dfrac{1}{4\pi} \dfrac{1}{|x - y|}, & \varrho < |x - y|. \end{cases} \tag{30}$$

Let $F : \overline{\mathcal{G}} \to \mathbb{R}$ be of class $C^{(0)}(\overline{\mathcal{G}})$. We set

$$V(x) = \int_{\mathcal{G}} G(\Delta; |x - y|) F(y) \, dy \tag{31}$$

and

$$V_\varrho^H(x) = \int_{\mathcal{G}} G_\varrho^H(\Delta; |x - y|) F(y) \, dy. \tag{32}$$

The integrands of V and V^ϱ differ only in the ball $\mathcal{B}_\varrho(x)$ around the point x with radius ϱ, i.e., $\mathcal{B}_\varrho(x) = \{y \in \mathbb{R}^3 : |x - y| < \varrho\}$. Because of its continuity, the function $F : \overline{\mathcal{G}} \to \mathbb{R}$ is uniformly bounded on $\overline{\mathcal{G}}$. This fact shows that

$$\left| V(x) - V_\varrho^H(x) \right| = O\left(\int_{\mathcal{B}_\varrho(x)} |G(\Delta; |x - y|) - G_\varrho^H(\Delta; |x - y|)| \, dy \right) = O(\varrho^2), \tag{33}$$

$\varrho \to 0$. Therefore, V is of class $C^{(0)}(\overline{\mathcal{G}})$ as the limit of a uniformly convergent sequence of continuous functions on $\overline{\mathcal{G}}$. Furthermore, we let

$$v(x) = \int_{\mathcal{G}} \nabla_x G(\Delta; |x - y|) F(y) \, dy \tag{34}$$

and

$$v_\varrho^H(x) = \int_{\mathcal{G}} \nabla_x G_\varrho^H(\Delta; |x - y|) F(y) \, dy. \tag{35}$$

Because of the fact

$$|\nabla_x G(\Delta; |x - y|)| = O\left(|x - y|^{-2}\right), \tag{36}$$

the integrals v and v_ϱ^H exist for all $x \in \overline{\mathcal{G}}$. It is not hard to see that

$$\sup_{x \in \overline{\mathcal{G}}} \left| v(x) - v_\varrho^H(x) \right| = \sup_{x \in \overline{\mathcal{G}}} |\nabla V(x) - \nabla V_\varrho^H(x)| = O(\varrho), \quad \varrho \to 0. \tag{37}$$

Consequently, v is a continuous vector field on $\overline{\mathcal{G}}$. Moreover, as the relation (37) holds uniformly on $\overline{\mathcal{G}}$, we obtain

$$v(x) = \nabla V(x) = \int_{\mathcal{G}} \nabla_x G(\Delta; |x - y|) F(y) \, dy. \tag{38}$$

Altogether, we are allowed to formulate the following properties:

Let $\mathcal{G}$ be a regular region. Let $F : \overline{\mathcal{G}} \to \mathbb{R}$ be of class $C^{(0)}(\overline{\mathcal{G}})$. Then V, V_ϱ^H as defined by (31), (32), respectively, are of class $C^{(1)}(\overline{\mathcal{G}})$, such that

$$\lim_{\varrho \to 0} \sup_{x \in \overline{\mathcal{G}}} |V(x) - V_\varrho^H(x)| = 0. \tag{39}$$

Furthermore, ∇V is of class $C^{(0)}(\overline{\mathcal{G}})$, such that

$$\nabla V(x) = \int_{\mathcal{G}} F(y) \, \nabla_x G(\Delta; |x - y|) \, dy, \qquad x \in \overline{\mathcal{G}}. \tag{40}$$

and

$$\lim_{\varrho \to 0} \sup_{x \in \overline{\mathcal{G}}} |\nabla V(x) - \nabla V_\varrho^H(x)| = 0. \tag{41}$$

Poisson's differential equation We next come to the *Poisson differential equation* under the assumption of μ-Hölder continuity, $\mu \in (0, 1]$, imposed on the function F on $\overline{\mathcal{G}}$. For this purpose we note that the Taylor linearization of $s^{-\frac{3}{2}}$ around s_0 is given by $s_0^{\frac{3}{2}} - \frac{3}{2} s_0^{-\frac{5}{2}}(s - s_0)$. Hence, by letting $s = r^2$ and $s_0 = \varrho^2$, we are able to replace the term r^{-3} by $\frac{1}{2\varrho^3}(5 - \frac{3}{\varrho^2} r^2)$. In consequence, as "mollification" of

$$Z(\Delta; |x - y|) = \frac{1}{4\pi |x - y|^3}, \qquad |x - y| \neq 0, \tag{42}$$

we introduce

$$Z_\varrho(\Delta; |x - y|) = \begin{cases} \dfrac{1}{8\pi \varrho^3}\left(5 - \dfrac{3}{\varrho^2}|x - y|^2\right), & |x - y| \leq \varrho \\[2ex] \dfrac{1}{4\pi |x - y|^3}, & \varrho < |x - y|. \end{cases} \tag{43}$$

The function $r \mapsto Z_\varrho(\Delta; r)$, $r \geq 0$, is continuously differentiable. Moreover, by the same arguments as above, it can be shown that the vector field

$$z_\varrho(x) = -\int_{\mathcal{G}} Z_\varrho(\Delta; |x - y|)(x - y)F(y) \, dy \tag{44}$$

converges uniformly on $\overline{\mathcal{G}}$ as $\varrho \to 0$ to the limit field

$$v(x) = \nabla V(x) = \int_{\mathcal{G}} \nabla_x G(\Delta; |x - y|)F(y) \, dy. \tag{45}$$

For all $x \in \mathcal{B}_\varrho(x)$ we obtain by a simple calculation

$$\nabla_x \cdot (Z_\varrho(\Delta; |x - y|)(x - y)) = \frac{15}{8\pi}\left(\frac{1}{\varrho^3} - \frac{|x - y|^2}{\varrho^5}\right). \tag{46}$$

Furthermore, we find

$$\int_{\mathcal{B}_\varrho(x)} \nabla_x \cdot (Z_\varrho(\Delta; |x - y|)(x - y)) \, dy = 1. \tag{47}$$

Hence, under the additional assumption of μ-Hölder continuity, $\mu \in (0, 1]$, for the function F on $\overline{\mathcal{G}}$, i.e., $|F(x) - F(y)| \leq C\,|x - y|^\mu$ for all $x, y \in \overline{\mathcal{G}}$, we obtain

$$
\begin{aligned}
\nabla \cdot z_\varrho(x) &= -\nabla_x \cdot \int_{\mathcal{G}} Z_\varrho(\Delta; |x - y|)(x - y)F(y)\,dy \\
&= -\int_{\mathcal{B}_\varrho(x)} \nabla_x \cdot \left(Z_\varrho(\Delta; |x - y|)(x - y) \right) F(y)\,dy \\
&= -\alpha(x)\,F(x) + \int_{\mathcal{B}_\varrho(x)} (F(x) - F(y))\,\nabla_x \cdot \left(Z_\varrho(\Delta|x - y|)(x - y) \right)\,dy.
\end{aligned}
\tag{48}
$$

Thus, the μ-Hölder continuity of F guarantees the estimate

$$
\sup_{x \in \overline{\mathcal{G}}} \left| \nabla \cdot z_\varrho(x) + \alpha(x)\,F(x) \right| = O(\varrho^\mu), \quad \varrho \to 0,
\tag{49}
$$

uniformly with respect to $x \in \overline{\mathcal{G}}$, where $\alpha(x)$ is the solid angle at x subtended by the surface $\partial\mathcal{G}$. In an analogous way, we are able to show that the first partial derivatives of (44) converge uniformly to continuous limit fields. Again, the uniform convergence shows that ∇V is differentiable in $\overline{\mathcal{G}}$, and we have

$$
\nabla \cdot v(x) = \Delta V(x) = \Delta_x \int_{\mathcal{G}} G(\Delta; |x - y|)F(y)\,dy = -\alpha(x)\,F(x), \quad x \in \overline{\mathcal{G}}.
\tag{50}
$$

It should be noted that the assumption of μ-Hölder continuity of F, $\mu \in (0, 1]$, is needed for the proof of (50). Indeed, Petrini (1900) showed that the μ-Hölder continuity of F, $\mu \in (0, 1]$, is necessary to imply the second continuous differentiability of the Newton volume potential.

Let $\mathcal{G}$ be a regular region. If F is of class $C^{(0,\mu)}(\overline{\mathcal{G}})$, $\mu \in (0, 1]$, in the neighborhood of $x \in \overline{\mathcal{G}}$, then the Poisson differential equation

$$
-\Delta_x \int_{\mathcal{S}} F(y)\,G(\Delta; |x - y|)\,dV(y) = \alpha(x)\,F(x)
\tag{51}
$$

holds true in the neighborhood of $x \in \overline{\mathcal{G}}$, where $\alpha(x)$ is the solid angle subtended by the surface $\partial\mathcal{G}$ at x.

3 Ill-posedness of the inverse gravimetry problem

Contrary to the case of $L^2(\partial\mathcal{G})$ (see, e.g., Freeden (1980) for more details), the class $L^2(\mathcal{G})$ of square-integrable functions on a regular region $\mathcal{G}$ is not obtainable only by the L^2-completion of a countable harmonic function system. In addition, we have to take into account a so-called "anharmonic function system" (see, e.g., Ballani et al. 1993a;

Freeden and Michel 2004; Michel 1999; Weck 1972). This observation explains the ill-posedness of the inverse gravimetry problem.

In the classical nomenclature of physical geodesy, the inversion of Newton's law of gravitation (6) from terrestrial gravitational data, i.e., the determination of the internal density contrast function from potential data on the boundary $\partial \mathcal{G}$ is known as the _terrestrial inverse gravimetry problem_ (TIGP). In other words, for a regular region $\mathcal{G} \subset \mathbb{R}^3$, (TIGP) is the problem of determining the density function $F \in L^2(\mathcal{G})$ from (information of) the gravitational potential V on $\overline{\partial \mathcal{G}}$ in accordance with the integral equation

$$V(x) = A[F](x) = \int_{\mathcal{G}} F(y) \, G(\Delta; |x - y|) \, dy, \quad x \in \partial \mathcal{G}. \tag{52}$$

In the sequel we denote the image of $X = L^2(\mathcal{G})$ under the operator A by $Y := A[L^2(\mathcal{G})]$, i.e., Y can be characterized by

$$Y = \{V : V = A[F] = \int_{\mathcal{G}} G(\Delta; |\cdot - y|) F(y) \, dy, \ F \in L^2(\mathcal{G})\}. \tag{53}$$

Furthermore, for any subset $\mathfrak{H} \subset \mathbb{R}^3$, we introduce the operator

$$A_{\mathfrak{H}} : X = L^2(\mathcal{G}) \to Y|\mathfrak{H} = A_{\mathfrak{H}}[L^2(\mathcal{G})] \tag{54}$$

(more accurately, $A_{\mathfrak{H}}^{\mathcal{G}}$), so that $Y|\mathfrak{H}$ consists of all functions $A_{\mathfrak{H}}[F]$ given by

$$\mathfrak{H} \ni x \mapsto A_{\mathfrak{H}}[F](x) = \int_{\mathcal{G}} G(\Delta; |x - y|) \, F(y) \, dy, \ F \in L^2(\mathcal{G}) \tag{55}$$

(note that A may be formally understood as $A_{\mathbb{R}^3}$ in our nomenclature). Clearly, as we already know, $Y|\mathfrak{H}$ forms a set of harmonic functions in $\mathfrak{H}$, provided that $\mathfrak{H}$ is a subset of $\mathcal{G}^c$.

In our notational framework, the _terrestrial/spaceborne inverse gravimetry problem_ (TSIGP) of classical physical geodesy can be formulated as follows:

(TSIGP): _Given $V \in C^{(0)}(\overline{\mathcal{G}^c})$, find $F \in L^2(\mathcal{G})$ with $A_{\overline{\mathcal{G}^c}}[F] = V$._

Hadamard's classification of the gravimetry problem In accordance with the famous _Hadamard's classification_ (cf. Hadamard 1902, 1923), (TSIGP) violates all criteria of well-posedness, viz. uniqueness, existence, and stability:

 (i) A solution of (TSIGP) exists only if V belongs to the space $Y|\overline{\mathcal{G}^c}$. However, it should be pointed out that this restriction does not cause any numerical difficulty since, in practice, the information of V is only finite-dimensional.
 (ii) The most serious problem is the non-uniqueness of the solution: The associated Fredholm integral operator $A_{\overline{\mathcal{G}^c}}$ has a kernel (null space) which is already known to coincide with the $L^2(\mathcal{G})$-orthogonal subspace, which is the closure of all harmonic functions on $\mathcal{G}$. More precisely, if F is a member of class $L^2(\mathcal{G})$, then $A_{\overline{\mathcal{G}^c}} : L^2(\mathcal{G}) \to Y|\mathcal{G}^c$ given by

$$V = A_{\overline{\mathcal{G}^c}}[F] = \int_{\mathcal{G}} G(\Delta; |\cdot - y|) \, F(y) \, dy \Big|_{\mathcal{G}^c}, \quad F \in L^2(\mathcal{G}), \qquad (56)$$

defines a linear operator such that $A_{\overline{\mathcal{G}^c}}[F]$ is continuous in $\overline{\mathcal{G}^c}$, harmonic in $\mathcal{G}^c$, and regular at infinity. The operator $A_{\overline{\mathcal{G}^c}}$ as defined by (56) is surjective, but it is not injective. Indeed, the null space (kernel) of $A_{\overline{\mathcal{G}^c}}$, i.e.,

$$\mathcal{N}(A_{\overline{\mathcal{G}^c}}) = AnHarm(\mathcal{G}) \qquad (57)$$

consists of all functions in $L^2(\mathcal{G})$ that are orthogonal to harmonic functions in $\mathcal{G}$. $\mathcal{N}(A_{\overline{\mathcal{G}^c}})$ is the space of anharmonic functions in $\mathcal{G}$. In fact, we have (see, e.g., Michel 1999; Weck 1972)

$$L^2(\mathcal{G}) = \overline{Harm(\mathcal{G})}^{\|\cdot\|_{L^2(\mathcal{G})}} \oplus \left(\overline{Harm(\mathcal{G})}^{\|\cdot\|_{L^2(\mathcal{G})}} \right)^{\perp}, \qquad (58)$$

hence,

$$L^2(\mathcal{G}) = Harm(\mathcal{G}) \oplus AnHarm(\mathcal{G}) = Harm(\mathcal{G}) \oplus \mathcal{N}(A_{\overline{\mathcal{G}^c}}). \qquad (59)$$

Unfortunately, the orthogonal complement, i.e., the class of *anharmonic functions*, is infinite-dimensional (see, e.g., Michel 1999; Weck 1972).

(iii) Restricting the operator $A_{\overline{\mathcal{G}^c}}$ to $Harm(\mathcal{G})$ leads to an injective mapping which, however, has a discontinuous inverse.

Concerning the historical background, the problem of non-uniqueness has been discussed extensively in literature (for a more detailed analysis see, e.g., Michel and Fokas 2008). This problem can be resolved by imposing some reasonable additional condition on the density. As we already saw, a suitable condition, suggested by the mathematical structure of the Newton potential operator A is to require that the density be harmonic. In fact, the approximate calculation of a harmonic density has already been implemented in several papers (see, e.g., Moritz 1980 and the references therein), whereas the problem of determining the anharmonic part seems to be still a great challenge.

Altogether, it should be remarked that up to now *the ill-posedness of (TSIGP) seriously limits its application in geoscience and exploration*, but sometimes in geodesy (see, e.g., Torge 1989) and particularly in geothermal research (see, e.g., Freeden and Nutz 2015), we are often able to take advantage of gravitational data systems inside the area $\mathcal{G}$ under specific consideration. However, under the knowledge of additional internal gravimeter data, the methodological situation will change, and significant improvement may be expected for practical applicability.

3.1 Spectral inversion for balls

The set $Harm(\mathcal{B}_\beta(0))$ of harmonic functions in the ball $\mathcal{B}_\beta(0)$ with radius β around the origin 0 is a closed subspace of $L^2(\mathcal{B}_\beta(0))$ (for more details see, e.g., Augustin

et al. 2018; Freeden and Gerhards 2013). Note that β can be chosen, for example, to be the radius of a *Runge (Bjerhammar) sphere* with $\beta < \inf\{|x| : x \in \partial\mathcal{G}\}$ or the (mean) Earth's radius). Moreover, the *inner harmonics* $\{H_{n,j}(\beta; \cdot)\}_{n=0,1,\dots; j=1,\dots,2n+1}$ given by

$$H_{n,j}(\beta; x) = \sqrt{\frac{2n+3}{\beta^3}} \left(\frac{|x|}{\beta}\right)^n Y_{n,j}\left(\frac{x}{|x|}\right), \quad x \in \overline{\mathcal{B}_\beta(0)}, \tag{60}$$

constitute a complete orthonormal system in the Hilbert space

$$\left(Harm(B_{\mathcal{B}_\beta(0)}), \langle\cdot, \cdot\rangle_{L^2(\mathcal{B}_\beta(0))}\right), \tag{61}$$

provided that $\{Y_{n,j}\}_{n=0,1,\dots; j=1,\dots,2n+1}$ is a complete system of spherical harmonics on the unit sphere (see, e.g., Freeden and Schreiner 2009).

The set of square–integrable harmonic functions on the outer space $\mathcal{B}_\beta^c(0) = \mathbb{R}^3 \backslash \overline{\mathcal{B}_\beta(0)}$ of a sphere $\partial\mathcal{B}_\beta(0)$ given by $Harm(\mathcal{B}_\beta^c(0))$ is a closed subspace of $L^2(\mathcal{B}_\beta^c(0))$. Moreover, the *outer harmonics* $\{H^{ext}_{-n-1,j}(\beta; \cdot)\}_{n=1,2,\dots; j=1,\dots,2n+1}$ given by

$$H_{-n-1,j}(\beta; x) = \sqrt{\frac{2n-1}{\beta^3}} \left(\frac{\beta}{|x|}\right)^{n+1} Y_{n,j}\left(\frac{x}{|x|}\right), \quad x \in \overline{\mathcal{B}_\beta^c(0)} \tag{62}$$

form a complete orthonormal system in the Hilbert space

$$\left(Harm(\mathcal{B}_\beta^c(0)), \langle\cdot, \cdot\rangle_{L^2(\mathcal{B}_\beta^c(0))}\right). \tag{63}$$

It should be remarked (cf. Michel 1999) that an outer harmonic of degree $n = 0$ is proportional to

$$\frac{1}{|x|} Y_{0,1}\left(\frac{x}{|x|}\right) = \frac{1}{\sqrt{4\pi}} \frac{1}{|x|}, \quad x \in \overline{\mathcal{B}_\beta^c(0)}. \tag{64}$$

This function, however, is not an element of $L^2(\mathcal{B}_\beta^c(0))$.
Harmonic case The operator $A_{\overline{\mathcal{B}_\beta^c(0)}}$, given by

$$A_{\overline{\mathcal{B}_\beta^c(0)}}[F](x) = \int_{\mathcal{B}_\beta(0)} G(\Delta; |x - y|)\, F(y)\, dy, \quad x \in \overline{\mathcal{B}_\beta^c(0)}, \tag{65}$$

has the null space

$$\mathcal{N}\left(A_{\overline{\mathcal{B}_\beta^c(0)}}\right) = AnHarm(\mathcal{B}_\beta(0)). \tag{66}$$

For any $F \in L^2(\mathcal{B}_\beta(0))$, there exists a unique orthogonal decomposition

$$F = P_{Harm(\mathcal{B}_\beta(0))}[F] + P_{AnGarm(\mathcal{B}_\beta(0))}[F], \tag{67}$$

where, of course, $P_{Harm(\mathcal{B}_\beta(0))}[F] \in Harm(\mathcal{B}_\beta(0))$ and $P_{AnGarm(\mathcal{B}_\beta(0))}[F] \in AnHarm(\mathcal{B}_\beta(0))$. We are allowed to represent $P_{Harm(\mathcal{B}_\beta(0))}[F]$ as a Fourier series in terms of inner harmonics

$$P_{Harm(\mathcal{B}_\beta(0))}[F] = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} \langle F, H_{n,j}(\beta; \cdot)\rangle_{L^2(\mathcal{B}_\beta(0))} \, H_{n,j}(\beta; \cdot) \qquad (68)$$

with respect to the topology of $L^2(\mathcal{B}_\beta(0))$. Suppose that $y \in \overline{\mathcal{B}_\beta^c(0)}$ is arbitrary but fixed. Then the potential at y corresponding to the mass density distribution F can be represented in the form

$$A_{\overline{\mathcal{B}_\beta^c(0)}}[F](y)$$
$$= \beta^2 \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} \frac{4\pi}{2n+1} \frac{\langle H_{n,j}\langle\beta; \cdot\rangle, F\rangle_{L^2(\mathcal{B}_\beta(0))}}{\sqrt{(2n-1)(2n+3)}} \, H_{-n-1,j}(\beta; y). \qquad (69)$$

A harmonic solution $F \in Harm(B_{\mathcal{B}_\beta(0)})$ of the problem

$$A_{\overline{\mathcal{B}_\beta^c(0)}}[F] = P, \quad P \in Harm(\mathcal{B}_\beta^c(0)) \qquad (70)$$

is unique, and it is given via its Fourier coefficients

$$\langle F, H_{n,j}(\beta; \cdot)\rangle_{L^2(\mathcal{B}_\beta(0))}$$
$$= \frac{2n+1}{4\pi\beta^2} \sqrt{(2n-1)(2n+3)} \langle P, H_{-n-1,j}(\beta; \cdot)\rangle_{L^2(\mathcal{B}_\beta^c(0))}, \qquad (71)$$

$n \in \mathbb{N}$, $j \in \{1, \ldots, 2n+1\}$, and

$$\langle F, H_{0,1}(\beta; \cdot)\rangle_{L^2(\mathcal{B}_\beta(0))} = 0. \qquad (72)$$

In other words, we have

$$F = \sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \frac{2n+1}{4\pi\beta^2} \sqrt{(2n-1)(2n+3)} \langle P, H_{-n-1,j}(\beta; \cdot)\rangle_{L^2(\mathcal{B}_\beta^c(0))} \, H_{n,j}(\beta; \cdot) \qquad (73)$$

in the sense of $L^2(\mathcal{B}_\beta(0))$.

In accordance with the Picard condition (cf. Nashed 1976), $A_{\overline{\mathcal{B}_\beta^c(0)}}[F] = P$ is solvable if and only if P is harmonic and the following series is finite, i.e.,

$$\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} n^4 \langle P, H_{-n-1,j}(\beta; \cdot)\rangle^2_{L^2(\mathcal{B}_\beta^c(0))} < \infty. \qquad (74)$$

Note that

$$\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} (2n+1)^2(2n-1)(2n+3) \langle P, H_{-n-1,j}(\beta; \cdot)\rangle^2_{L^2(\mathcal{B}_\beta^c(0))} < \infty \qquad (75)$$

is equivalent to

$$\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} n^4 \left\langle P, H_{-n-1,j}(\beta; \cdot) \right\rangle_{L^2(\mathcal{B}_\beta^c(0))}^2 < \infty. \tag{76}$$

This condition can be also motivated within the framework of harmonics by observing that

$$F \in Harm(B_{\mathcal{B}_\beta(0)}) = \overline{\left\{ H_{n,j}(\beta; \cdot) : n \in \mathbb{N}_0; j \in \{1, \ldots, 2n+1\} \right\}}^{\|\cdot\|_{L^2(\mathcal{B}_\beta(0))}}, \tag{77}$$

which implies

$$\sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} \left\langle F, H_{n,j}(\beta; \cdot) \right\rangle_{L^2(\mathcal{B}_\beta(0))}^2 < \infty. \tag{78}$$

Operators of the type $A_{\overline{\mathcal{B}_\beta^c(0)}}$ are compact, hence, we are confronted with the fact that the restricted operator

$$A_{\overline{\mathcal{B}_\beta^c(0)}} \big| Harm(B_{\mathcal{B}_\beta(0)}) : Harm(B_{\mathcal{B}_\beta(0)}) \to A_{\overline{\mathcal{B}_\beta^c(0)}} \left(Harm(B_{\mathcal{B}_\beta(0)}) \right) \tag{79}$$

is invertible, but $(A_{\overline{\mathcal{B}_\beta^c(0)}} \big|_{Harm(B_{\mathcal{B}_\beta(0)})})^{-1}$ is unbounded (equivalently, discontinuous).

Anharmonic case An orthogonal basis for $AnHarm(\mathcal{B}_\beta(0))$ (with respect to $L^2(\mathcal{B}_\beta(0))$) can be found in Ballani et al. (1993a). A different non-orthogonal anharmonic basis has been developed in Michel (1999) and Michel (2002a):

(a)   A complete $L^2(\mathcal{B}_\beta(0))$-orthogonal system in $AnHarm(\mathcal{B}_\beta(0))$ is given by

$$\left\{ x \mapsto |x|^n P_{k,n}(|x|^2) \, Y_{n,j}\left(\frac{x}{|x|}\right) \right\}_{k \in \mathbb{N}; n \in \mathbb{N}_0; j \in \{1,\ldots,2n+1\}}, \tag{80}$$

where $\{P_{k,n}\}_{k \in \mathbb{N}; n \in \mathbb{N}_0}$ is a system of polynomials defined by

$$P_{k,n}(t) = \sqrt{\frac{2}{\beta^{2n+3}}} \, G_k\left(n + \frac{3}{2}, n + \frac{3}{2}; \frac{t}{\beta^2}\right). \tag{81}$$

Here, the functions $G_k, k \in \mathbb{N}_0$, are the Jacobi polynomials, which are the only polynomials on $[0, 1]$ to satisfy the following conditions for all $n, m \in \mathbb{N}_0$:
  (i) $G_n(a, b; \cdot)$ is a polynomial of degree n on $[0, 1]$.
  (ii) $G_n(a, b; 0) = 1$.
  (iii) $\int_0^1 x^{a-1}(1 - x)^{b-a} G_n(a, b; x) \, G_m(a, b; x) \, dx = 0, \ n \neq m$,
  provided that $a > 0$ and $b > a - 1$.
(b)   A closed system in $Anharm(\overline{\Sigma_{int}})$ is given by

$$\left\{ x \mapsto \left(|x|^{n+2k} - \frac{(2n + 3)\beta^{2k}}{2n + 2k + 3} \, |x|^n \right) Y_{n,j}\left(\frac{x}{|x|}\right) \right\}_{k \in \mathbb{N}; n \in \mathbb{N}_0; j \in \{1,\ldots,2n+1\}}. \tag{82}$$

Moreover, the basis functions are polynomials of degree $\leq N \in \mathbb{N} \backslash \{1\}$ if and only if the index triple (k, n, j) is within the range $n \in \{0, \ldots, N-2\}$, $j \in \{1, \ldots, 2n+1\}$, $k \in \left\{1, \ldots, \left[\frac{N-n}{2}\right]\right\}$, where $[\,\cdot\,]$ is the Gauss bracket, defined by $[x] = \max\{\nu \in \mathbb{Z} : \nu \leq x\}$, $x \in \mathbb{R}$.

The space of anharmonic polynomials with degrees $\leq N$ has dimension $\frac{1}{6}N^3 - \frac{1}{6}N$.

The obvious advantage of the system in (a) is its orthogonality. On the other hand, the system described in (b) has a radial part (see also Freeden and Michel 2004), which is explicitly given, whereas the radial part of the orthogonal system has to be calculated iteratively by means of recurrence formulas.

The important role of the anharmonic functions in the theory of (TSIGP) is also stressed if we investigate a radially symmetric density distribution which is given for the mantle and the outer and inner core of the Earth. Such a structure of spherical layers does not give any information in the gravitational potential and, therefore, cannot be recovered by means of harmonic functions. Michel (1999), indeed, shows that a reconstruction of the (deep) Earth's interior with a harmonic function system does not make any sense. Therefore, a reliable method for the (global) approximation of the density distribution of the Earth requires a treatment of both orthogonal projections: the harmonic part and the anharmonic part.

Moreover, we recall that the contribution of $H_{-1,1}$ to an (outer) gravitational (disturbance) potential can be neglected when applying an appropriate coordinate transformation (see, e.g., Heiskanen and Moritz 1967; Hofmann-Wellenhof and Moritz 2005; Moritz 2015 for more details). Therefore, this operation can be interpreted physically as filtering out the contribution of the radially symmetric density structures in the Earth's interior (note that the total mass of an anharmonic density function is zero).

3.2 Spectral inversion for regular regions

The spherically reflected results will now be extended to the investigation of the inverse problem $A_{\overline{\mathcal{G}^c}}[F] = V$, where $A_{\overline{\mathcal{G}^c}}[F]$ is the gravitational potential of a regular region $\mathcal{G} \subset \mathbb{R}^3$ and $F \in L^2(\mathcal{G})$ is the desired mass density distribution F. As already known from (57), the null space of the operator $A_{\overline{\mathcal{G}^c}}$ is given by

$$\mathcal{N}(A_{\overline{\mathcal{G}^c}}) = AnHarm(\mathcal{G}). \tag{83}$$

A general complete orthonormal basis system for the harmonic functions inside or outside an arbitrary regular region is not available. This is the reason why the following setting is useful (cf. Michel 1999): Let the families of functions $\{H_{n,j}(\mathcal{G}; \cdot)\}_{n \in \mathbb{N}_0; j=1,\ldots,2n+1}$ and $\{H_{-n-1,j}(\mathcal{G}^c; \cdot)\}_{n \in \mathbb{N}; j=1,\ldots,2n+1}$ be complete orthonormal systems of the Hilbert spaces $\left(Harm(\mathcal{G}), \langle \cdot, \cdot \rangle_{L^2(\mathcal{G})}\right)$ and $\left(Harm(\mathcal{G}^c), \langle \cdot, \cdot \rangle_{L^2(\mathcal{G}^c)}\right)$, respectively, and $\{k_{\mathcal{G}}^{\wedge}(n)\}_{n \in \mathbb{N}_0}$ be the symbol of

$$A_{\overline{\mathcal{G}^c}} : L^2(\mathcal{G}) \to Y|\overline{\mathcal{G}^c} = \mathcal{R}(A_{\overline{\mathcal{G}^c}}) = A_{\overline{\mathcal{G}^c}}(L^2(\mathcal{G})), \tag{84}$$

given by

$$A_{\overline{\mathcal{G}^c}}[F](x) = \sum_{n=0}^{\infty} \sum_{j=1}^{2n+1} k_{\mathcal{G}}^{\wedge}(n) \left\langle F, H_{n,j}(\mathcal{G}; \cdot) \right\rangle_{L^2(\mathcal{G})} H_{-n-1,j}(\overline{\mathcal{G}^c}; x), \quad x \in \overline{\mathcal{G}^c}, \quad (85)$$

where $H_{-1,1}(\mathcal{G}; \cdot)$ is not an element of $L^2(\mathcal{G}^c)$). We assume that $k_{\mathcal{G}}^{\wedge}(n) \neq 0$ for all $n \in \mathbb{N}_0$.

If $\partial \mathcal{G}$ is a sphere with radius β around the origin, we let

$$H_{n,j}(\mathcal{G}; \cdot) := H_{n,j}(\beta; \cdot); \quad n \in \mathbb{N}_0, j \in \{1, \ldots, 2n+1\}; \quad (86)$$

$$H_{-n-1,j}(\overline{\mathcal{G}^c}; \cdot) := H_{-n-1,j}(\beta; \cdot); \quad n \in \mathbb{N}, j \in \{1, \ldots, 2n+1\}. \quad (87)$$

Moreover, we set

$$k_{\mathcal{G}}^{\wedge}(n) = k_{\beta}^{\wedge}(n) = \frac{4\pi}{2n+1} \frac{\beta^2}{\sqrt{(2n-1)(2n+3)}}. \quad (88)$$

The *inverse problem* $A_{\overline{\mathcal{G}^c}}[F] = V$ *with* $F \in Harm(\mathcal{G})$ *unknown*, is solvable if and only if $V \in Harm(\mathcal{G})$ with

$$\sum_{n=1}^{\infty} \sum_{j=1}^{2n+1} \left(\frac{\left\langle V, H_{-n-1,j}(\overline{\mathcal{G}^c}; \cdot) \right\rangle_{L^2(\mathcal{G}^c)}}{k_{\mathcal{G}}^{\wedge}(n)} \right)^2 < \infty. \quad (89)$$

In this case, the harmonic solution $F \in Harm(\mathcal{G})$ is uniquely determined and spectrally given by

$$\left\langle F, H_{0,1}(\mathcal{G}; \cdot) \right\rangle_{L^2(\mathcal{G})} = 0, \quad (90)$$

$$\left\langle F, H_{n,j}(\mathcal{G}; \cdot) \right\rangle_{L^2(\mathcal{G})} = \frac{\left\langle V, H_{-n-1,j}(\overline{\mathcal{G}^c}; \cdot) \right\rangle_{L^2(\mathcal{G}^c)}}{k_{\mathcal{G}}^{\wedge}(n)} \quad (91)$$

for $n \in \mathbb{N}, j \in \{1, \ldots, 2n+1\}$.

As already known, the inverse operator $(A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G}))^{-1}$, defined on the image $Y|\overline{\mathcal{G}^c}$, is unbounded. Due to unavoidable errors in the measurements of the gravitational field the application of this inverse operator to the observed potential for a direct reconstruction of the mass density distribution is not senseful. Therefore, we have to take into account suitable regularizations.

Indeed, the results as presented here enable us to apply projection-, multiscale-, and iterative regularization techniques in the way as indicated, e.g., in Engl (1997), Engl et al. (1996, 1997), Freeden and Nashed (2018a, b), Freeden and Schneider (1998), Groetsch (1984, 1993), Hanson (1971), Kirsch (1996), Lavrentiev (1967), Locker and Prenter (1980), Louis (1989), Louis and Maass (1989), Nashed (1971, 1980, 1981, 1987, 2010), Nashed and Wahba (1974a, b), Rieder (2003), Tikhonov (1943, 1963), Vogel (2002), and many others.

4 Mollifier methods

Next we deal with regularization methods for the Newton volume integral involving singular integral mollification. We begin with the Haar singular integral modification.

4.1 Haar-type mollifier method

We start from the differential equation

$$-\Delta_y \, G_\varrho^H(\Delta; |y - z|) = \; H_\varrho(|y - z|) \tag{92}$$

with

$$G_\varrho^H(\Delta; |y - z|) = \begin{cases} \frac{1}{8\pi\varrho}\left(3 - \frac{|y-z|^2}{\varrho^2}\right), & |y - z| \leq \varrho, \\ \frac{1}{4\pi|y-z|}, & |y - z| > \varrho, \end{cases} \tag{93}$$

where

$$H_\varrho(|y - z|) = \begin{cases} \frac{3}{4\pi\varrho^3}, & |y - z| \leq \varrho, \\ 0, & |y - z| > \varrho \end{cases} \tag{94}$$

is the so-called *Haar kernel* (note that $\|\mathcal{B}_\varrho(0)\| = \frac{4}{3}\pi\varrho^3$).

It is well-known (see, e.g., Freeden and Gerhards 2013) that the *Haar singular integral* $\{I_\varrho\}_{\varrho>0}$ defined by

$$F_\varrho^H := I_\varrho[F] = \int_{\mathcal{G}} H_\varrho(|\cdot - z|) \, F(z) \, dz, \tag{95}$$

with the *Haar kernel as mollifier* satisfies the limit relation

$$\lim_{\varrho \to 0+} I_\varrho[F] = F, \quad F \in L^2(\mathcal{G}), \tag{96}$$

in the topology of $L^2(\mathcal{G})$. Moreover, we have

$$\lim_{\varrho \to 0+} I_\varrho[F](x) = \alpha(x) \, F(x), \quad x \in \overline{\mathcal{G}}, \; F \in C^{(0)}(\overline{\mathcal{G}}), \tag{97}$$

where $\alpha(x)$ is the solid angle at x subtended by the surface $\partial\mathcal{G}$.

In constructive approximation theory, locally supported (i.e., spacelimited) functions $H_\varrho(|x - \cdot|)$, $\varrho > 0$, $x \in \mathbb{R}^3$, are nothing new, with one-dimensional counterparts having been discussed already by Haar (1910) in 1910. The primary importance of locally supported Haar kernels in the classical one-dimensional Euclidean space is that they led to the "birth" to an entire "basis family" by means of two operations, viz. dilations and translations. In other words, an entire set of approximants is available from the single locally supported "Haar mother kernel", and this basis family provides useful "building block functions" that enable the multiscale modeling and the decorrelation of data signatures.

Internal/Terrestrial Inverse Gravimetry Problem ITIGP. Correspondingly to $\{I_\varrho\}_{\varrho>0}$ we introduce the family $\{A_\varrho\}_{\varrho>0}$ given by

$$V_\varrho^H := A_\varrho^H[F] = \int_\mathcal{G} G_\varrho^H(\Delta; |\cdot - z|) \, F(z) \, dz, \tag{98}$$

such that

$$\begin{aligned}
\Delta \, A_\varrho^H[F] = \Delta \int_\mathcal{G} G_\varrho^H(\Delta; |\cdot - z|) \, F(z) \, dz \\
= -I_\varrho[F] \\
= -F_\varrho^H \\
= -\int_\mathcal{G} H_\varrho(|\cdot - z|) \, F(z) \, dz.
\end{aligned} \tag{99}$$

Multiscale mollifier approximation Next we are interested in applying the multiscale "Haar philosophy" to an approximate determination of the mass density distribution inside $\mathcal{G}$ (see Freeden and Blick 2013; Freeden and Gerhards 2013; Freeden and Nashed 2018c for the conceptual background):

Suppose that $\{\varrho_j\}_{j\in\mathbb{N}_0}$ is a positive, monotonously decreasing sequence with $\lim_{j\to\infty} \varrho_j = 0$, for example, the dyadic sequence given by $\varrho_j = 2^{-j}$. For $j \in \mathbb{N}_0$, we consider the differences

$$\Psi_{G_{\varrho_j}^H}(\Delta; |\cdot - y|) = G_{\varrho_{j+1}}^H(\Delta; |\cdot - y|) - G_{\varrho_j}^H(\Delta; |\cdot - y|) \tag{100}$$

and

$$\Psi_{H_{\varrho_j}}(|\cdot - y|) = H_{\varrho_{j+1}}(|\cdot - y|) - H_{\varrho_j}(|\cdot - y|). \tag{101}$$

$\Psi_{G_{\varrho_j}^H}(\Delta; \cdot)$ and $\Psi_{H^{\varrho_j}}$ are called "ϱ_j-*fundamental wavelet function*" and "ϱ_j-*Haar wavelet function*", respectively.

The associated "ϱ_j-*potential wavelet functions*" and the "ϱ_j-*density wavelet functions*" are given by

$$(WV)_{\varrho_j}^H = \int_\mathcal{G} \Psi_{G_{\varrho_j}^H}(\Delta; |\cdot - y|) \, F(y) \, dy \tag{102}$$

and

$$(WF)_{\varrho_j}^H = \int_\mathcal{G} \Psi_{H_{\varrho_j}}(|\cdot - y|) \, F(y) \, dy, \tag{103}$$

respectively. The ϱ_j-potential wavelet functions and the ϱ_j-density wavelet functions, respectively, characterize the successive *detail information* contained in $V_{\varrho_{j+1}}^H - V_{\varrho_j}^H$ and $F_{\varrho_{j+1}}^H - F_{\varrho_j}^H$, $j \in \mathbb{N}_0$. In other words, we are able to decorrelate the potential V and the "density signature" F, respectively, in the form of "band structures"

$$(WV)_{\varrho_j}^H = V_{\varrho_{j+1}}^H - V_{\varrho_j}^H, \tag{104}$$

and

$$(WF)^H_{\varrho j} = F^H_{\varrho j+1} - F^H_{\varrho j}. \tag{105}$$

The essential problem to be solved in multiscale extraction of geological features is to identify those detail information, i.e., band structures in (104), which contain specifically desired geological (density) characteristics in (105). Seen from a numerical point of view, it is remarkable that both wavelet functions $y \mapsto \Psi_{G^H_{\varrho j}}(\Delta; |\cdot - y|)$ and $y \mapsto \Psi_{H_{\varrho_j}}(|\cdot - y|)$ vanish outside a ball around the center x due to their construction, i.e., these functions are spacelimited showing a ball as local support. Furthermore, the ball becomes smaller with increasing scale parameter j, so that more and more high frequency phenomena can be highlighted without changing the features outside the balls.

Forming the telescoping sums

$$\sum_{j=0}^{J-1}(WV)^H_{\varrho j} = \sum_{j=0}^{J-1}\left(V^H_{\varrho j+1} - V^H_{\varrho j}\right), \tag{106}$$

and

$$\sum_{j=0}^{J-1}(WF)^H_{\varrho j} = \sum_{j=0}^{J-1}\left(F^H_{\varrho j+1} - F^H_{\varrho j}\right), \tag{107}$$

we easily arrive at the scale-discrete identities

$$V^H_{\varrho J} = V^H_{\varrho 0} + \sum_{j=0}^{J-1}(WV)^H_{\varrho j} \tag{108}$$

and

$$F^H_{\varrho J}(x) = F^H_{\varrho 0} + \sum_{j=0}^{J-1}(WF)^H_{\varrho j}. \tag{109}$$

Thus we finally end up with the following multiscale relations

$$\lim_{J \to \infty} V^H_{\varrho J} = V^H_{\varrho 0} + \sum_{j=0}^{\infty}(WV)^H_{\varrho j} \tag{110}$$

and

$$\lim_{J \to \infty} F^H_{\varrho J} = F^H_{\varrho 0} + \sum_{j=0}^{\infty}(WF)^H_{\varrho j} = -\lim_{J \to \infty}\Delta V^H_{\varrho J} = -\Delta V^H_{\varrho 0} - \sum_{j=0}^{\infty}\Delta(WV)^H_{\varrho j}. \tag{111}$$

Altogether, the potential V as well as the "density signature" F can be expressed by initial low-pass filtered signals $V^H_{\varrho 0}$ and $F^H_{\varrho 0}$ and successive addition of band-pass filtered signals $(WV)^H_{\varrho j}$ and $(WF)^H_{\varrho j}$, $j = 0, 1, \ldots$, respectively.

It should be mentioned that our multiscale approach is constructed such that, within the spectrum of all wavebands [see (104) and (105)], certain rock formations or aquifers, respectively, may be associated to a specific band characterizing typical features within the multiscale reconstruction (cf. Blick et al. 2018). Each scale parameter in the decorrelation is assigned to correspond to a low-pass approximation of the data at a particular resolution. The wavelet contributions are obtained as part within a multiscale approximation by calculating the difference between two consecutive scaling functions. In other words, the wavelet transformation (filtering) of a signal constitutes the difference of two low-pass filters, thus it may be regarded as a band-pass filter. Due to our construction, the wavelets show an increasing space localization as the scale increases. In this way, the characteristic signatures of a signal can be detected in certain frequency bands.

Finally, it should be noted that the key ideas of multiscale approximation as presented here lead back to evaluation methods proposed by Freeden and Schreiner (2006) (see also Freeden and Blick 2013, and particularly Freeden and Gerhards 2013). For the sake of simplicity, the adaptation of this approach to the requirements of gravitational potential as well as density distribution is explained only in scale discrete form, a scale continuous formulation as presented in Freeden and Schreiner (2006) is canonical. A variety of numerical tests and case studies of this approach are found in the PhD-theses Blick (2015) and Möhringer (2014).

Multiscale mollifier numerics For a sufficiently large integer J, it follows from (97) that

$$\alpha(x)\,F(x) \simeq I_{\varrho_J}[F](x) = F_{\varrho_J}^H(x) = \int_{\mathcal{G}} H_{\varrho_J}(|x-y|)F(y)\,dy, \quad x \in \overline{\mathcal{G}},\, F \in C^{(0)}(\overline{\mathcal{G}}) \tag{112}$$

(" $\simeq$ "means that the error is negligible). From (92) we obtain

$$
\begin{aligned}
\Delta\, A_{\varrho_J}^H[F](x) &= \Delta_x \int_{\mathcal{G}} G_{\varrho_J}^H(\Delta; |x-y|)F(y)\,dy \\
&= -\int_{\mathcal{G}} H_{\varrho_J}(|x-y|)F(y)\,dy \\
&\simeq -\alpha(x)\,F(x),
\end{aligned}
\tag{113}
$$

where we are aware of the fact that

$$V(x) \simeq \int_{\mathcal{G}} G_{\varrho_J}^H(\Delta; |x-y|)F(y)\,dy, \quad x \in \overline{\mathcal{G}}, \tag{114}$$

with negligible error. In order to realize a fully discrete approximation of F we have to apply approximate integration formulas leading to

$$V(x) \simeq \sum_{i=1}^{N_J} G_{\varrho_J}^H\left(\Delta; |x - y_i^{N_J}|\right)\, w_i^{N_J}\, F\left(y_i^{N_J}\right), \quad x \in \overline{\mathcal{G}}, \tag{115}$$

where $w_i^{N_J} \in \mathbb{R}$, $y_i^{N_J} \in \overline{\mathcal{G}}$, $i = 1, \ldots, N_J$, are the known weights and knots, respectively.

For numerical realization of mass density modeling by means of Haar kernels we notice that all coefficients

$$a_i^{N_J} = w_i^{N_J} F\left(y_i^{N_J}\right), \quad i = 1, \ldots, N_J, \tag{116}$$

are unknown. Then we have to solve a linear system, namely

$$V\left(x_k^{T_J}\right) = \sum_{i=1}^{N_J} G_{\varrho_J}^H\left(\Delta; |x_k^{T_J} - y_i^{N_J}|\right) a_i^{N_J}, \quad x_k^{T_J} \in \overline{\mathcal{G}}, \ k = 1, \ldots, T_J, \tag{117}$$

to determine $a_i^{N_J}$, $i = 1, \ldots, N_J$, from known gravitational values $V(x_k^{T_J})$ at knots $x_k^{T_J} \in \overline{\mathcal{G}}$, $k = 1, \ldots, T_J$.

Once all density values $F(y_i^{N_J})$, $i = 1, \ldots, N_J$, are available (note that the integration weights $w_i^{N_J}$, $i = 1, \ldots, N_J$, are known), the density distribution F can be obtained from the formula

$$F(x) \simeq F_{\varrho_J}^H(x) = \sum_{i=1}^{N_J} H_{\varrho_J}\left(|x - y_i^{N_J}|\right) \underbrace{w_i^{N_J} F\left(y_i^{N_J}\right)}_{=a_i^{N_J}}, \quad x \in \mathcal{G}. \tag{118}$$

Even better, fully discrete Haar filtered versions of F at lower scales can be derived in accordance with the approximate integration rules

$$\int_{\mathcal{G}} H_{\varrho_j}(|x - z|) F(z) \, dV(z) \simeq \sum_{i=1}^{N_j} H_{\varrho_j}\left(|x - y_i^{N_j}|\right) w_i^{N_j} F\left(y_i^{N_j}\right) \tag{119}$$

for $j = J_0, \ldots, J$, where $w_i^{N_j}$, $y_i^{N_j}$, $i = 1, \ldots, N_j$, are known weights and knots, respectively, such that $\{y_1^{N_j}, \ldots, y_{N_j}^{N_j}\} \subset \{y_1^{N_J}, \ldots, y_{N_J}^{N_J}\} \subset \overline{\mathcal{G}}$, i.e., the sequence of knots $\{y_1^{N_J}, \ldots, y_{N_J}^{N_J}\} \subset \overline{\mathcal{G}}$ shows a hierarchical positioning.

Altogether, our approach yields Haar filtered versions establishing a (space-based) multiscale decomposition $F_{\varrho_J}^H, \ldots, F_{\varrho_{J_0}}^H$ of the density distribution F, such that an entire set of approximations is available from a single locally supported "mother function", i.e., the Haar kernel function (94), and this set provides useful "building block functions", which enable decorrelation of the density signatures and suitable storage and fast decorrelation of density data. Moreover, fully discrete Haar filtered versions of F at lower scales can be derived in accordance with the approximate integration rules

$$F_{\varrho_j}^H(x) = \int_{\mathcal{G}} H_{\varrho_j}(|x-y|)\, F(y)\, dy \simeq \sum_{i=1}^{N_j} H_{\varrho_j}\left(|x-y_i^{N_j}|\right)\, w_i^{N_j} F\left(y_i^{N_j}\right), \quad x \in \mathcal{G},$$

(120)

for $j = J_0, \ldots, J$, where $w_i^{N_j}$, $y_i^{N_j}$, $i = 1, \ldots, N_j$, are known weights and knots, respectively, such that we can take adventage of the fact that $\{y_1^{N_j}, \ldots, y_{N_j}^{N_j}\} \subset \{y_1^{N_J}, \ldots, y_{N_J}^{N_J}\} \subset \overline{\mathcal{G}}$.

The serious problem of our multiscale approach, however, is that measurements of gravitation are only available in the interior $\mathcal{G}$ in exceptional cases, for example, locally in geothermal boreholes. Usually, we are able to take into account surface measurements on $\partial\mathcal{G}$, but it may be questioned in view of the ill-posedness that deep geological formations can be detected by an exclusive use of terrestrial gravitational data. Nevertheless, it should be mentioned that the multiscale method as explained above is an important postprocessing method to improve the interpretability of already available geological models as well as (wavelet) decorrelation mechanisms to extract certain local features of practical relevance in density band signatures (see Blick et al. 2018 and the references therein). In doing so, the risk of an investor involved in geothermal power plant construction may be reduced drastically.

4.2 De la Vallée Poussin-type mollifier method

The critical point in the Haar-type approach is the discontinuity of the Laplace derivative of $G_\varrho^H(\Delta; \cdot)$, i.e., the ordinary Haar function H_ϱ. In what follows we are therefore interested in a *smoothed Haar kernel variant*, called *de la Vallée Poussin kernel*.

For $x, y \in \mathbb{R}^3$ we define the de la Vallée Poussin kernel $VP_\varrho = [0, \infty) \to \mathbb{R}$, $\varrho > 0$, by

$$VP_\varrho(r) = \frac{1}{C_\varrho^{VP}} \begin{cases} \left(1 - \frac{r^2}{\varrho^2}\right), & r \le \varrho \\ 0, & r > \varrho, \end{cases}$$

(121)

where the normalization constant $C_\varrho^{VP} = \frac{8\pi}{15}\varrho^3$ is chosen in such a way that

$$\int_{\mathbb{R}^3} VP_\varrho(|x-y|)\, dy = 4\pi \int_0^\varrho VP_\varrho(r)\, r^2\, dr = 1.$$

(122)

It is easy to see that $r \mapsto -\frac{1}{6}r^2 + \frac{1}{20\varrho^2}r^4$, $r \ge 0$, satisfies

$$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\left(-\frac{1}{6}r^2 + \frac{1}{20\varrho^2}r^4\right) = 1 - \frac{r^2}{\varrho^2}, \quad r \ge 0, \ \varrho > 0.$$

(123)

As a consequence, it follows that

$$G_\varrho^{VP}(\Delta; |x-y|) = \begin{cases} \frac{1}{C_\varrho^{VP}}\left(-\frac{1}{6}|x-y|^2 + \frac{1}{20\varrho^2}|x-y|^4\right), & |x-y| \le \varrho \\ 0, & |x-y| > \varrho \end{cases}$$

(124)

satisfies

$$-\Delta_x G_\varrho^{VP}(\Delta; |x - y|) = VP_\varrho(|x - y|), \quad x, y \in \mathbb{R}^3. \tag{125}$$

An elementary calculation yields

$$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\left(1 - \frac{r^2}{\varrho^2}\right) = \frac{6}{\varrho^2}, \tag{126}$$

so that

$$-\Delta_x VP_\varrho(\Delta; |x - y|) = D_\varrho^{VP}(|x - y|), \quad x, y \in \mathbb{R}^3, \tag{127}$$

where

$$D_\varrho^{VP}(|x - y|) = \begin{cases} \frac{1}{C_\varrho^{VP}}\frac{6}{\varrho^2} = \frac{8\pi}{3}\varrho, & |x - y| \le \varrho \\ 0, & |x - y| > \varrho. \end{cases} \tag{128}$$

Clearly, all methodological concepts developed for the Haar case together with its multiscale settings remain valid. Their formulations are straightforward. The following result, however, serves as a strategic basis for our approach to density feature extraction in specific representation within the de la Vallée Poussin framework.

Theorem 1 *The "ϱ-de la Vallée Poussin potential functions"*

$$V_\varrho^{VP}(x) = \int_{\mathcal{G}} G_\varrho^{VP}(\Delta; |x - y|)F(y)\,dy \tag{129}$$

and the "ϱ-de la Vallée Poussin density function"

$$F_\varrho^{VP}(x) = \int_{\mathcal{G}} VP_\varrho(|x - y|)F(y)\,dy \tag{130}$$

satisfy the relations

$$\sup_{x \in \overline{\mathcal{G}}}|V(x) - V_\varrho^{VP}(x)| = O(\varrho^2), \quad \varrho \to 0 \tag{131}$$

and

$$\lim_{\varrho \to 0}\sup_{x \in \overline{\mathcal{G}}}|\alpha(x)F(x) - F_\varrho^{VP}(x)| = 0, \tag{132}$$

where $\alpha(x)$ is the solid angle subtended by the boundary $\partial\mathcal{G}$ at $x \in \overline{\mathcal{G}}$.

Unfortunately, de la Vallée Poussin potentials V_ϱ^{VP} do not generally show a faster convergence to V than V_ϱ^H.

Approximate mollifier solution In similarity to our previous Haar considerations we use the operators

$$A_\varrho^{VP}[F] = V_\varrho^{VP} = \int_{\mathcal{G}} G_\varrho^{VP}(\Delta; |\cdot - z|)\,F(z)\,dz, \quad F \in L^2(\mathcal{G}), \tag{133}$$

and

$$I_\varrho^{VP}[F] = F_\varrho^{VP} = \int_{\mathcal{G}} VP_\varrho(|\cdot -z|) \, F(z) \, dz, \ F \in L^2(\mathcal{G}). \tag{134}$$

We denote the image of $X = L^2(\mathcal{G})$ under the operator A_ϱ^{VP} by Y_ϱ^{VP}. So, instead of discussing the integral $A[F](x)$ we choose $A_\varrho^{VP}[F]$, $F \in L^2(\mathcal{G})$, for some sufficiently small $\varrho > 0$. We take advantage of the fact that

$$\int_{\mathcal{G}} G(\Delta; |x-z|) \, D_\varrho^{VP}(|y-z|) \, dz = VP_\varrho(|x-y|), \quad x, y \in \overline{\mathcal{G}}. \tag{135}$$

Note that

$$\Delta_x \int_{\mathcal{G}} G(\Delta; |x-z|) \, D_\varrho^{VP}(|y-z|) \, dz = \Delta_x VP_\varrho(|x-y|) = -D_\varrho^{VP}(|x-y|), \ x, y \in \overline{\mathcal{G}}. \tag{136}$$

After these preliminaries we are able to conclude that

$$\begin{aligned}
I_\varrho^{VP}[F](x) = F_\varrho^{VP}(x) &= \int_{\mathcal{G}} VP_\varrho(|x-w|) F(w) \, dw \\
&= \int_{\mathcal{G}} \left(\int_{\mathcal{G}} G(\Delta; |w-z|) \, D_\varrho^{VP}(|x-z|) \right) dz \, F(w) \, dw \\
&= \int_{\mathcal{G}} D_\varrho^{VP}(|x-z|) \left(\int_{\mathcal{G}} G(\Delta; |w-z|) F(w) \, dw \right) dz \\
&= \int_{\mathcal{G}} D_\varrho^{VP}(|x-z|) \, A[F](z) \, dz \\
&= \int_{\mathcal{G}} D_\varrho^{VP}(|x-z|) \, V(z) \, dz. \tag{137}
\end{aligned}$$

holds true for $x \in \overline{\mathcal{G}}$, so that

$$F_\varrho^{VP}(x) = \int_{\mathcal{G}} D_\varrho^{VP}(|x-z|) \, V(z) \, dz, \ x \in \mathcal{G}. \tag{138}$$

The right hand side of (138) is given analytically when the parameter ϱ is chosen appropriately. So, if we define the operator $S_\varrho : Y_\varrho^{VP} \to X$ in the form

$$F_\varrho^{VP} = S_\varrho[V], \ S_\varrho[V] = \int_{\mathcal{G}} D_\varrho^{VP}(|\cdot -z|) \, V(z) \, dz, \ x \in \mathcal{G}, \tag{139}$$

then, by (138), this operator maps the gravitational potential to mollified solutions of ITIGP. This property motivates the term *mollified inverse* of A used for S_ϱ. The discretization of the identity (139) given by

$$F_\varrho^{VP}(x) \simeq \sum_{i=1}^{N} w_i \, D_\varrho^{VP}(|x-z_i^N|) \, V(z_i^N), \ z_i^N \in \overline{\mathcal{G}}, \ x \in \mathcal{G} \tag{140}$$

may serve as an alternative to improve local density knowledge from given internal (e.g., borehole) data $V(z_i^N)$, $i = 1, \ldots, N$, where the values w_i, $i = 1, \ldots, N$, are the known integration weights.

Finally, it should be noted that, more generally, any singular integral (cf. Michlin 1965, 1975) can be chosen in analogy to the de la Vallée Poussin kernel, i.e., smoothed Haar kernel, as long as its Laplace derivative takes a reasonable role in the mollification context.

4.3 Singular integral-type mollifier method

First we recapitulate the concept of a *singular integral*: Let $\{K_\varrho\}_{\varrho>0}$ be a family of functions $r \mapsto K_\varrho(r)$, $r \geq 0$, satisfying the following conditions:

   (i) $K_\varrho(r) = 0$, $r > \varrho$,
  (ii) $K_\varrho(r) \geq 0$, $r \geq 0$,
 (iii) $K_\varrho|[0, \varrho]$ is of class $C^{(\infty)}$,
 (iii) $-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}K_\varrho(r)|_{r\in[0,\varrho]} \neq 0$,
 (iv) $4\pi \int_0^\varrho K_\varrho(r)\, r^2\, dr = 1$.

Then, the family $\{I_\varrho\}_{\varrho>0}$ of operators $I_\varrho : F \mapsto I_\varrho[F]$, $F \in X$, ($X = C^{(0)}(\mathbb{R}^3)$ or $X = L^2(\mathbb{R}^3)$), given by

$$I_\varrho[F](x) = F_\varrho(x) = \int_{\mathbb{R}^3} K_\varrho(|x - y|)\, F(y)\, dy = \int_{\mathcal{B}_\varrho(x)} K_\varrho(|x - y|)\, F(y)\, dy$$

(141)

is called a *singular integral in X*, if the following approximate identity relation holds true

$$\lim_{\varrho \to 0} \|I_\varrho[F] - F\|_X = 0$$

(142)

for all $F \in X$.

Obviously, an example of a singular integral of the aforementioned type is given by the de la Vallée Poussin kernel.

Let $\mathcal{G}$ be a regular region. Suppose that $\{K_\varrho\}_{\varrho>0}$ is a kernel constituting a singular integral in the L^2-metric, then it is not difficult to show (see, e.g., Michlin 1965, 1975) that the limit relation

$$\lim_{\varrho \to 0} \left(\int_{\mathcal{G}} \left| I_\varrho[F](x) - F(x) \right|^2\, dx \right)^{\frac{1}{2}} = 0$$

(143)

holds true for all $F \in L^2(\mathcal{G})$, while, for all $F \in C^{(0)}(\mathcal{G})$, we have

$$\lim_{\varrho \to 0} \sup_{x \in \mathcal{G}} |I_\varrho[F](x) - F(x)| = 0.$$

(144)

Correspondingly to the family $\{K_\varrho\}_{\varrho>0}$ we are led to families $\{G_\varrho\}_{\varrho>0}$ and $\{D_\varrho\}_{\varrho>0}$ such that

$$-\Delta_x G_\varrho(\Delta; |x - y|) = K_\varrho(|x - y|), \quad x, y \in \mathbb{R}^3$$

(145)

and

$$- \Delta_x K_\varrho(|x - y|) = D_\varrho(|x - y|), \quad x, y \in \mathbb{R}^3. \tag{146}$$

Our interest now is in the *terrestrial gravimetry problem* (TGP), that may be regarded as a particularly relevant problem in geoscientific practice (our considerations, however, remain valid for (ITGP)). We start from known values $V(x_i), x_i \in \partial\mathcal{G}, i = 1, \ldots, N$, given by

$$A[F](x_i) = \int_\mathcal{G} G(\Delta; |x_i - z|) \, F(z) \, dz = V(x_i), \quad x_i \in \partial\mathcal{G}, \quad i = 1, \ldots, N, \tag{147}$$

which can be thought of as resulting from moment discretization of the gravimetry integral equation (cf. (6))

$$A[F](x) = \int_\mathcal{G} G(\Delta; |x - z|) \, F(z) \, dz = V(x), \quad x \in \partial\mathcal{G}, \quad F \in L^2(\mathcal{G}). \tag{148}$$

(TGP) aims at determining an approximation of the function $F \in L^2(\mathcal{G})$ from the N equations (147). Introducing the following settings

$$^{(N)}A[F] := \left(\int_\mathcal{G} G(\Delta; |x_1 - z|) \, F(z) \, dz, \ldots, \int_\mathcal{G} G(\Delta; |x_N - z|) \, F(z) \, dz \right), \tag{149}$$

$$^{(N)}v := (V(x_1), \ldots, V(x_N))^T, \tag{150}$$

we are able to rewrite the equations (147) in operator form as follows:

$$^{(N)}A : L^2(\mathcal{G}) \to \mathbb{R}^N, \quad F \mapsto {}^{(N)}v = {}^{(N)}A\,[F]. \tag{151}$$

We look for an approximate inverse $^{(N)}S : \mathbb{R}^N \to L^2(\mathcal{G})$ for $^{(N)}A$ in the form

$$^{(N)}S\,t := \sum_{i=1}^N \underbrace{V(x_i)}_{=t_i} D(|x_i - \cdot|), \quad t = (t_1, \ldots, t_N)^T, \tag{152}$$

in terms of functions $D(|x_i - \cdot|) \in L^2(\mathcal{G}), \ i = \ldots, N$, satisfying

$$^{(N)}S\,{}^{(N)}A\,[F] = \sum_{i=1}^N \int_\mathcal{G} G(\Delta; |x_i - z|) F(z) \, dz \, D(|x_i - \cdot|)$$

$$= \int_\mathcal{G} F(z) \sum_{k=1}^N G(\Delta; |x_i - z|) \, D(|x_i - \cdot|) \, dz. \tag{153}$$

Now, the stage is set for explaining the mollifier philosophy, i.e., the sum

$$\sum_{i=1}^{N} G(\Delta; |x - x_i|) \, D(|x_i - y|) \tag{154}$$

is understood as a discrete version of the "continuous expression"

$$\int_{\mathcal{G}} G(\Delta; |x - z|) \, D(|z - y|) \, dz \simeq \delta(|x - y|) \tag{155}$$

whose "mollifier version" for some family $\{K_\varrho\}_{\varrho > 0}$ constituting a singular integral is given by

$$\int_{\mathcal{G}} G(\Delta; |x - z|) \, D_\varrho(|z - y|) \, dz = K_\varrho(|x - y|), \tag{156}$$

with sufficiently small $\varrho > 0$. This observation leads to the sum

$$^{(N)}S_\varrho \, t = \sum_{i=1}^{N} V(x_i) \, D_\varrho(|x_i - \cdot|) \tag{157}$$

and

$$^{(N)}S_\varrho \, ^{(N)}A \, [F] = \sum_{i=1}^{N} \int_{\mathcal{G}} G(\Delta; |x_i - z|) F(z) \, dz \, D_\varrho(|x_i - \cdot|)$$

$$= \int_{\mathcal{G}} F(z) \sum_{k=1}^{N} G(\Delta; |x_i - z|) \, D_\varrho(|x_i - \cdot|) \, dz. \tag{158}$$

as approximations to $^{(N)}S \, t$ and $^{(N)}S \, ^{(N)}A \, [F]$, respectively.

4.4 Moment method

Next we mention the *finite moment problem for* TIGP. For that purpose we assume that the N potential (volume integral) values

$$\int_{\mathcal{G}} G(\Delta; |x_i - y|) \, F(y) \, dy = V(x_i), \quad x_i \in \partial\mathcal{G}, \ i = 1, \dots, N. \tag{159}$$

are known.

The standard solution process (see, e.g., Engl et al. 1996; Kirsch 1996) consists of finding a linear combination in terms of the functions $x \mapsto G(\Delta; |x_i - x|), x \in \mathcal{G}, x_i \in \partial\mathcal{G}, \ i = 1, \dots, N$. In other words, the moment method looks for a function $F \in X_N$ satisfying the conditions (159), where X_N is given by

$$X_N := \operatorname{span}_{i=1,\ldots,N} G(\Delta; |x_i - \cdot|). \tag{160}$$

As a consequence, the moment solution is a harmonic function inside $\mathcal{G}$.

More formally, consider again a semi-discrete observation operator $^{(N)}A \colon L^2(\mathcal{G}) \to \mathbb{R}^N$, $F \mapsto {}^{(N)}v = {}^{(N)}A [F]$, of type (149), (150). Remembering $F \in X_N$ and choosing F as the linear combination

$$F = \sum_{k=1}^{N} \beta_i \, G(\Delta; |x_i - \cdot|) \tag{161}$$

we are led to a (uniquely solvable) linear system in the unknowns $\beta_1, \ldots, \beta_N$, viz.

$$\sum_{k=1}^{N} \beta_i \int_{\mathcal{G}} G(\Delta; |x_i - y|) \, G(\Delta; |x_j - y|) \, dy = V(x_j), \quad j = 1, \ldots, N, \tag{162}$$

that turns out to play a central role in the context of minimum norm (spline) interpolation in reproducing kernel Hilbert spaces as discussed later on.

4.5 Backus–Gilbert method

The concept originally proposed by G.E. Backus and F. Gilbert (cf. Backus and Gilbert 1967, 1968, 1970) is that one does not primarily wish to solve the finite moment problem as explained above, but rather one is interested in how well all possible candidates for solution can be recovered pointwise. More specifically, the Backus–Gilbert method is based on a *pointwise minimization criterion*: Keep $y \in \mathcal{G}$ fixed and determine the numbers $\mu_i(= \mu_i(y))$, $i = 1, \ldots, N$, , as the solution of the following minimization problem:

$$\int_{\mathcal{G}} |z - y|^2 \left| \sum_{i=1}^{N} \mu_i \, G(\Delta; |x_i - z|) \right|^2 dz \rightarrow min. \tag{163}$$

subject to $\mu \in \mathbb{R}^N$, $\mu = (\mu_1, \ldots, \mu_N)^T$ with

$$\int_{\mathcal{G}} \sum_{i=1}^{N} \mu_i \, G(\Delta; |x_i - z|) \, dz = 1. \tag{164}$$

It should be remarked that the factor $z \mapsto |z - y|^2$, $z \in \overline{\mathcal{G}}$, in the integrand of (163) is a measure for the concentration of the sum $\sum_{i=1}^{N} \mu_i \, G(\Delta; |x_i - y|)$ around the point $y \in \mathcal{G}$ under consideration. In the literature (see, e.g., Louis 1989; Rieder 2003), more generally, the term $z \mapsto |z - y|^{2\nu}$, $z \in \overline{\mathcal{G}}$, $\nu \geq 1$, is sometimes chosen. In this case, the larger ν, the more concentrated is the sum $\sum_{i=1}^{N} \mu_i \, G(\Delta; |x_i - y|)$ around $y \in \mathcal{G}$.

In matrix-vector nomenclature (thereby notationally omitting the dependence on the fixed, but arbitrary point $y \in \mathcal{G}$) we are able to rewrite the quadratic optimization problem (163), (164), in the form

$$\mu \cdot Q \mu \quad \to min. \tag{165}$$

subject to

$$\kappa \cdot \mu = 1, \tag{166}$$

where

$$(Q)_{i,j} := \int_{\mathcal{G}} |z - y|^2 \, G(\Delta; |x_i - z|) \, G(\Delta; |x_j - z|) \, dz, \; i, j = 1, \ldots, N \tag{167}$$

and

$$\kappa_j := \int_{\mathcal{G}} G(\Delta; |x_j - z|) \, dz, \quad j = 1, \ldots, N. \tag{168}$$

In fact, the formulas (165) and (166) constitute a quadratic minimization problem with only one linear equation constraint. We may assume that $\kappa = (\kappa_1, \ldots, \kappa_N)^T$ is different from 0, since otherwise the constraint (166) cannot be valid. The introduction of a Langrange multiplier well-known from optimization theory (see, e.g., Werner 1984) can be used to characterize the solvability of the resulting linear $Q\mu - \lambda\kappa = 0$ under the constraint $\kappa \cdot \mu = 1.$, i.e., existence and uniqueness. In more detail, from the integral in (163), we see that $\mu \cdot Q \mu \geq 0$ and $\mu \cdot Q \mu = 0$ implies $\sum_{i=1}^{N} \mu_i G(\Delta; |x_i - \cdot|) = 0$, so that the linear independence of the system $\{G(\Delta; |x_i - \cdot|)\}_{i=1,\ldots,N}$ shows that Q is positive definite.

Summarizing our results we therefore obtain the following statement:

The symmetric matrix $Q \in \mathbb{R}^{N \times N}$ as defined by (167) is positive definite for every $y \in \mathcal{G}$. The quadratic minimization problem (165) and (166) is uniquely solvable. The vector μ is the unique solution of (165) and (166) if and only if there exist a real number λ (the Lagrange multiplier) so that $(\mu, \lambda) \in \mathbb{R}^{N+1}$ solves the linear system $Q\mu - \lambda\kappa = 0$ under the constraint $\kappa \cdot \mu = 1$.

The Lagrange multiplier $\lambda = \mu \cdot Q \mu$ represents the minimal value of the quadratic minimization problem.

Consider the unique solution $\mu \in \mathbb{R}^N, \mu = (\mu_1, \ldots, \mu_N)^T, \mu_i = M_i(y), i = 1, \ldots, N$, of the quadratic minimization problem (165) and (166). The *Backus–Gilbert solution F_N* of the discrete version of TIGP

$$\int_{\mathcal{G}} G(\Delta; |x_i - z|) \, F_N(z) \, dz = V(x_i), \quad x_i \in \partial\mathcal{G}, \; i = 1, \ldots, N, \tag{169}$$

is defined by

$$F_N = \sum_{i=1}^{N} V(x_i) \, \mu_i \tag{170}$$

in $\mathcal{G}$. The minimal value λ (more accurately, $\lambda(y)$) is called the *spread*.

As already mentioned, the Backus–Gilbert solution (170) generally is not a solution of the finite moment problem (159). This observation is certainly a disadvantage. Therefore, the question arises if the error may be estimated in an appropriate way (see Kirsch 1996 for related work in one-dimensional context): Let $F \in L^2(\mathcal{G})$ be any solution of the finite moment problem (159). Suppose that F_N given by (170) is the Backus–Gilbert solution. Then, in connection with (164), it follows that

$$
\begin{aligned}
F_N(y) - F(y) &= \sum_{i=1}^{N} V(x_i)\, \mu_i \; - \; F(y) \int_{\mathcal{G}} \sum_{i=1}^{N} \mu_i\, G(\Delta; |x_i - z|)\, dz \\
&= \sum_{i=1}^{N} \int_{\mathcal{G}} G(\Delta; |x_i - z|)\, (F(z) - F(y))\, \mu_i\, dz
\end{aligned}
\tag{171}
$$

holds true. Consequently, we obtain

$$
|F_N(y) - F(y)| \;\le\; \int_{\mathcal{G}} \left| \sum_{i=1}^{N} G(\Delta; |x_i - z|)\, \mu_i) \right| \; |F(z) - F(y)|\, dz. \tag{172}
$$

Under the assumption of Lipschitz-continuity of F in $\overline{\mathcal{G}}$, i.e., the existence of a constant C_F so that

$$
|F(z) - F(y)| \;\le\; C_F\, |z - y|, \quad y, z \in \overline{\mathcal{G}}, \tag{173}
$$

we are able to deduce that

$$
|F_N(y) - F(y)| \;\le\; C_F \int_{\mathcal{G}} \left| \sum_{i=1}^{N} G(\Delta; |x_i - z|)\, \mu_i \right| \, |z - y|\, dz. \tag{174}
$$

By virtue of the Cauchy–Schwarz inequality we therefore obtain from (174)

$$
\begin{aligned}
|F_N(y) - F(y)| &\le C_F \int_{\mathcal{G}} 1 \cdot \left| \sum_{i=1}^{N} G(\Delta; |x_i - z|)\, \mu_i \right| \, |z - y|\, dz \\
&\le C_F \sqrt{\|\mathcal{G}\|} \left(\int_{\mathcal{G}} \left| \sum_{i=1}^{N} G(\Delta; |x_i - z|)\, \mu_i \right|^2 \, |z - y|^2\, dz \right)^{\frac{1}{2}}.
\end{aligned}
\tag{175}
$$

For $N \in \mathbb{N}$, $y \in \mathcal{G}$, we set

$$
e_N^2(y) := \min \left\{ \int_{\mathcal{G}} |Z_N(z)|^2 \, |z - y|^2\, dz : Z_N \in X_N, \int_{\mathcal{G}} Z_N(z)\, dz = 1 \right\}. \tag{176}
$$

Thus, we finally arrive at

$$|F_N(y) - F(y)| \leq C_F \sqrt{\|\mathcal{G}\|} \, e_N(y) \tag{177}$$

as pointwise *error estimate of the difference of the solution of the finite moment problem* (159) *and the Backus–Gilbert solution* (170).

We conclude our considerations with the question if the Backus-Gilbert method admits a *relation to the mollifier method*: Once again, consider the semi-discrete observation operator

$$^{(N)}A : L^2(\mathcal{G}) \to \mathbb{R}^N, \ \ F \mapsto {}^{(N)}v = {}^{(N)}A\,[F], \tag{178}$$

where

$$^{(N)}A[F] := \left(\int_{\mathcal{G}} G(\Delta; |x_1 - z|) \, F(z) \, dz, \ \dots, \ \int_{\mathcal{G}} G(\Delta; |x_N - z|) \, F(z) \, dz \right), \tag{179}$$

$$^{(N)}v := (V(x_1), \dots, V(x_N))^T. \tag{180}$$

By virtue of the operator $^{(N)}S$ given by

$$\left({}^{(N)}S\,v \right)(y) = \sum_{k=1}^{N} V(x_i)\,\mu_i(y), \quad y \in \mathcal{G}, \tag{181}$$

we have constructed a left inverse $^{(N)}S : \mathbb{R}^N \to L^2(\mathcal{G})$ such that

$$
\begin{aligned}
^{(N)}S\,^{(N)}A\,[F](y) &= \sum_{i=1}^{N} \int_{\mathcal{G}} G(\Delta; |x_i - z|) F(z)\,dz\,\mu_i(y) \\
&= \int_{\mathcal{G}} F(z) \underbrace{\left(\sum_{i=1}^{N} G(\Delta; |x_i - z|)\,\mu_i(y) \right)}_{\simeq\,\delta(|z-y|)} dz, \\
&\simeq F(y).
\end{aligned}
\tag{182}
$$

Note that we are formally allowed (in distributional context) to formulate

$$
\begin{aligned}
F(y) &= \int_{\mathcal{G}} F(z)\,\delta(|z - y|)\,dz \\
&\simeq \int_{\mathcal{G}} F(z) \int_{\mathcal{G}} G(\Delta; |x - z|)\,M(|x - y|)\,dx\,dz
\end{aligned}
\tag{183}
$$

where, in analogy to (146), we have

$$-\Delta_z\,\delta(z-y|) = M(|z-y|) \simeq -\Delta_z \sum_{i=1}^{N} G(\Delta; |x_i - z|)\,\mu_i(y). \qquad (184)$$

5 Reproducing kernel Hilbert space (RKHS) methods

Next we consider reproducing kernel Hilbert space solutions. First we discuss the classical geodetic External/Terrestrial Inverse Gravimetry Problem (ETIGP). Then we go over to the Internal/Terrestrial External Inverse Gravimetry Problem (ITEIGP), i.e., the gravimetry problem in whole Euclidean space $\mathbb{R}^3$.

5.1 Preparatory material on reproducing kernel Hilbert spaces

Since reproducing kernel Hilbert space structure plays a central role in our forthcoming mollifier approach, some preparatory aspects should be presented for the convenience of the reader (for more details see, e.g., Aronszajn 1950; Davis 1963; Hille 1972; Nashed and Walter 1991; Saitoh 1988; Xia and Nashed 1994).

A Hilbert space H of real-valued functions on a regular region $\mathcal{G}$ (e.g., a regular region) is called a *reproducing kernel Hilbert space (RKHS)* if all the evaluation functional $H \ni F \mapsto F(t) \in \mathbb{R}$ are bounded (continuous) for each fixed $t \in \mathcal{G}$, i.e., there exists a positive constant C_t for each $t \in \mathcal{G}$ such that $|F(t)| \leq C_t\,\|F\|_H$ for all $F \in H$. By the *Riesz Representation Theorem*, for each $t \in \mathcal{G}$, there exists a unique element K_t such that $F(t) = \langle F, K_t \rangle_H$ for all $F \in H$. The reproducing kernel $K(\cdot,\cdot): \mathcal{G} \times \mathcal{G} \mapsto \mathbb{R}$ of a RKHS H is defined by $K(s,t) = \langle K_s, K_t \rangle_H$, $s, t \in \mathcal{G}$.

We list some basic properties of RKHS's that are particularly relevant for our approach:

- $K(s,t) = K(t,s)$ for all $t, s \in \mathcal{G}$.
- $K(s,s) \geq 0$ for all $s \in \mathcal{G}$.
- $|K(s,t)| \leq \sqrt{K(s,s)}\sqrt{K(t,t)}$ for all $s, t \in \mathcal{G}$.
- The reproducing kernel $K(s,t)$ on $\mathcal{G} \times \mathcal{G}$ is a non-negative definite Hermitean kernel. Conversely by the *Aronszajn-Moore Theorem*, every nonnegative definite Hermitean function $K(\cdot,\cdot)$ on $\mathcal{G} \times \mathcal{G}$ determines a unique Hilbert space H_K for which $K(\cdot,\cdot)$ is a reproducing kernel (cf. Aronszajn 1950) (note that a kernel F on $\mathcal{G} \times \mathcal{G}$ is said to be positive definite if, for any n points $t_1, \ldots, t_n \in \mathcal{G}$, the matrix $A = (M(t_i, t_j))_{1 \leq i,j \leq n}$ is non-negative definite, i.e.,

$$u^H A u = \sum_{i,j=1}^{n} u_i\, M(t_i, t_j)\, u_j \geq 0 \qquad (185)$$

for all $u = (u_1, \ldots, u_n) \in \mathbb{R}^n$).

- A closed subspace $\tilde{H}$ of a RKHS H is also a RKHS. Moreover, the orthogonal projector P of H onto $\tilde{H}$ and the reproducing kernel $\tilde{K}(s, t)$ of the RKHS $\tilde{H}$ are related by $PF(s) = \langle F, \tilde{K}_s \rangle, s \in \mathcal{G}$ for all $f \in H$ where $\tilde{K}_k = PK$.
- In a RKHS, the element representing a given bounded linear functional L can be expressed by means of the reproducing kernel: $L(F) = \langle F, W \rangle_H$, where $W = L(K)$.
- If $\mathcal{G}$ is a regular region and $K(\cdot, t\cdot)$ is continuous on $\mathcal{G} \times \mathcal{G}$, then H_K is a space of continuous functions.
- If the integral relation

$$\int_{\mathcal{G} \times \mathcal{G}} |Q(s, t)|^2 \, ds \, dt < \infty, \tag{186}$$

holds true, then $Q(\cdot, \cdot)$ has a countable sequence of eigenvalues and eigenfunctions (*Theorem of Mercer*).
- $L^2(\mathcal{G})$, the space of all square-integrable functions on the regular region $\mathcal{G}$, is <u>not</u> a RKHS. Indeed, the point evaluation is not well defined. Each function $F \in L^2(\mathcal{G})$ is actually an equivalence class of functions equal to each other almost everywhere. Thus the "value" at a point has no meaning since any point has measure zero.
- Let $\{\Phi_n\}_{n \in \mathbb{N}}$ be a sequence of functions defined on $\mathcal{G}$ such that, for every $t \in \mathcal{G}$,

$$\sum_{n=1}^{\infty} |\Phi_n(t)|^2 < \infty. \tag{187}$$

For every sequence $\{c_n\}_{n \in \mathbb{N}}$ satisfying

$$\sum_{n=1}^{\infty} |c_n|^2 < \infty, \tag{188}$$

the series $\sum_{n=1}^{\infty} c_n \Phi_n(t)$ is then convergent for every $t \in \mathcal{G}$. The functions which are the sums of such series form a linear space H, on which we are able to define the structure of a separable Hilbert space by taking as scalar product, for

$$F = \sum_{n=1}^{\infty} c_n \Phi_n, \quad G = \sum_{n=1}^{\infty} d_n \Phi_n, \tag{189}$$

the number

$$\langle F, G \rangle_H = \sum_{n=1}^{\infty} c_n d_n. \tag{190}$$

This space has a reproducing kernel, namely

$$K(x, y) = \sum_{n=1}^{\infty} \Phi_n(t) \, \Phi_n(s), \quad t, s \in \mathcal{G} \times \mathcal{G}. \tag{191}$$

- Let H be a separable RKHS, then its reproducing kernel $K(\cdot, \cdot)$ has the expansion

$$K(s, t) = \sum_{n=1}^{\infty} \Phi_n(t)\, \Phi_n(s), \tag{192}$$

where $\{\Phi_n\}_{n=1}^{\infty}$ is an orthonormal basis for H (we remark that for a general separable Hilbert space H, $\sum_{n=1}^{\infty} \Phi_n(t)\, \Phi_n(s)$ is not a reproducing kernel (note that $L^2(\mathcal{G})$ is not an $RKHS$) and also that Φ_n's do not generally correspond to sampling expansions . If they do, i.e., if $\Phi_n(t) = K(t_n, t)$ for some sequence $\{t_n\}$, then we have that $F(t) = \sum_{n=1}^{\infty} F(t_n)\, \Phi_n(t)$, this constitutes a *sampling theorem*.)
- If the reproducing kernel $K(s, t)$ of a RKHS H is continuous on $\mathcal{G} \times \mathcal{G}$, then H is a space of continuous functions (uniformly continuous on a bounded $\mathcal{G}$). This follows from

$$|F(t) - F(s)| = |\langle F, K_t - K_s\rangle_H| \leq \|F\|_H \,\|K_t - K_s\|_H \tag{193}$$

and

$$\|K_t - K_s\|^2 = K(t, t) - 2K(t, s) + K(s, s) \tag{194}$$

for all $s, t \in \mathcal{G}$.
- Strong convergence in a RKHS H implies pointwise convergence and uniform convergence on compact sets, because of the fact

$$|F(t) - F_n(t)| = |\langle F - F_n, Q_t\rangle_H| \leq \sqrt{K(t, t)}\, \|F - F_n\|_H. \tag{195}$$

- Let H_K denote the RKHS with reproducing kernel K, and denote the inner product and norm in H_K by $\langle \cdot, \cdot \rangle_{H_K}$ and $\|\cdot\|_{H_K}$, respectively. Note that $K(s, s')(= K_s(s'))$ is a non-negative definite Hermitean kernel on $\mathcal{G} \times \mathcal{G}$, and that $\{K_s, s \in \mathcal{G}\}$ spans H_K since $\langle K_s, F\rangle_{H_K} = 0$, $s \in \mathcal{G}$, implies $F(s) = 0$. For more properties of reproducing kernel spaces the reader is referred to, e.g., Nashed (2010), Nashed and Sun (2013), Nashed and Wahba (1974a, b), Nashed and Walter (1991, 1995), and the references therein.
- For every positive definite kernel $K(\cdot, \cdot)$ on $\mathcal{G} \times \mathcal{G}$, there exist a zero mean Gaussian process with $K(\cdot, \cdot)$ as its covariance, giving rise to the relation between Bayes estimates, Gaussian processes, and optimization processes in RHKS (for more details the reader is referred to the geodetic literature, see e.g., Grafarend 1982; Meissl 1971, 1976; Moritz 1980, and the monographs Louis 1989; Wahba 1990).

Interest in reproducing kernel Hilbert spaces have increased in recent years, as the computer capacity has made solutions of ever larger and more complex problems practicable. Indeed, new reproducing kernel representations and new applications (in particular in physical geodesy and geophysics) are being contributed at a rapid rate. For example, a certain RHKS in terms of outer harmonics allows the adequate determination of the Earth's gravitational potential (see, e.g., Freeden 1981; Shure et al. 1982 for early spline approaches) in consistency with gravitational observables of heterogeneous type (that are interpretable as (bounded) linear functionals on the RKHS under

consideration). In our approach we are particularly interested in inverse gravimetry involved reproducing Hilbert space kernel framework, i.e., the reproducing kernel Hilbert spaces are restrictions of Y [cf. (53)] to certain subspaces of $\mathbb{R}^3$.

5.2 External/terrestrial RKHS for regular regions

Let $P_{Harm(\mathcal{G})}$ and $P_{AnHarm(\mathcal{G})}$ be the orthogonal projectors of the space $L^2(\mathcal{G})$ to $Harm(\mathcal{G})$ and $\mathcal{N}(A_{\overline{\mathcal{G}^c}}) = AnHarm(\mathcal{G})$, respectively. Then, every function F of the Hilbert space $L^2(\mathcal{G})$ can be uniquely decomposed in the form

$$F = P_{Harm(\mathcal{G})}[F] + P_{AnGarm(\mathcal{G})}[F] \tag{196}$$

such that

$$A_{\overline{\mathcal{G}^c}}[F] = A_{\overline{\mathcal{G}^c}}\left[P_{Harm(\mathcal{G})}[F]\right] + \underbrace{A_{\overline{\mathcal{G}^c}}\left[P_{AnHarm(\mathcal{G})}[F]\right]}_{=0} = A_{\overline{\mathcal{G}^c}}\left[P_{Harm(\mathcal{G})}[F]\right]. \tag{197}$$

Furthermore, it is clear that

$$\|F\|^2_{L^2(\mathcal{G})} = \left\|P_{Harm(\mathcal{G})}[F]\right\|^2_{L^2(\mathcal{G})} + \left\|P_{AnHarm(\mathcal{G})}[F]\right\|^2_{L^2(\mathcal{G})}. \tag{198}$$

In conclusion, $A_{\overline{\mathcal{G}^c}}[P_{Harm(\mathcal{G})}[F]]$ is that function of class $L^2(\mathcal{G})$, which has the smallest $L^2(\mathcal{G})$-norm among all (density) functions F in $L^2(\mathcal{G})$ generating the same potential in the space $Y|\overline{\mathcal{G}^c} = A_{\overline{\mathcal{G}^c}}(L^2(\mathcal{G}))$. Consequently, to every $P \in Y|\overline{\mathcal{G}^c}$, there corresponds a unique $F \in Harm(\mathcal{G})$ such that

$$A_{\overline{\mathcal{G}^c}}[F] = A_{\overline{\mathcal{G}^c}}[P_{Harm(\mathcal{G})}[F]] = P. \tag{199}$$

The restriction $A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G})$ is a linear bijective operator, i.e., to every $P \in Y|\overline{\mathcal{G}^c}$ there exists a unique $F \in Harm(\mathcal{G})$ such that $A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G})[F] = P$.

On the space $Y|\overline{\mathcal{G}^c}$ we are able to induce an inner product $\langle \cdot, \cdot \rangle_{Y|\overline{\mathcal{G}^c}}$ by defining

$$\left\langle A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G})[F], A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G})[G] \right\rangle_{Y|\overline{\mathcal{G}^c}} = \langle F, G \rangle_{L^2(\mathcal{G})}, \tag{200}$$

where $F, G \in L^2(\mathcal{G})$. $Y|\overline{\mathcal{G}^c}$ equipped with the inner product $\langle \cdot, \cdot \rangle_{Y|\overline{\mathcal{G}^c}}$ is a Hilbert space. $A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G})$ is an isometric operator relating $L^2(\mathcal{G})$ to $Y|\overline{\mathcal{G}^c}$. Our goal is to show that $(Y|\overline{\mathcal{G}^c}, \langle \cdot, \cdot \rangle_{Y|\overline{\mathcal{G}^c}})$ is a reproducing kernel Hilbert space, i.e., a Hilbert space equipped with the reproducing kernel $K_{Y|\overline{\mathcal{G}^c}}(\cdot, \cdot)$. It is clear that, for every $x \in \overline{\mathcal{G}^c}$, $G(\Delta; |x - \cdot|)$ is an element of $Harm(\mathcal{G})$. From well-known reproducing Hilbert space theory (see, e.g., Aronszajn 1950), it follows that any given potential $P \in Y|\overline{\mathcal{G}^c}$ can be represented in the form

$$P(x) = A_{\overline{\mathcal{G}^c}}|Harm(\mathcal{G})[F](x) = \langle\, G(\Delta; |x - \cdot|), F\rangle_{L^2(\mathcal{G})}, \quad x \in \overline{\mathcal{G}^c}, \ F \in Harm(\mathcal{G}). \tag{201}$$

For $x \in \overline{\mathcal{G}^c}$, the evaluation functional $\mathcal{E}_x[P] = P(x)$ is a bounded functional on $\overline{\mathcal{G}^c}$. Indeed, from the Cauchy-Schwarz inequality applied to (201) we obtain

$$|\mathcal{E}_x[P]| = |P(x)| \leq ||F||_{L^2(\mathcal{G})}||G(\Delta; |x - \cdot|)||_{L^2(\mathcal{G})}. \tag{202}$$

Consequently, we have

$$|\mathcal{E}_x[P]| = P(x)| \leq C_x\, \|P\|_{Y|\overline{\mathcal{G}^c}}, \quad P \in Y|\overline{\mathcal{G}^c}, \ x \in \overline{\mathcal{G}^c}. \tag{203}$$

Thus, a necessary and sufficient condition for the Hilbert space $Y|\overline{\mathcal{G}^c}$ to possess a reproducing kernel (see, e.g., Aronszajn 1950) is fulfilled. Even more, we are are able to find the explicit expression of the reproducing kernel $K_{Y|\overline{\mathcal{G}^c}}(\cdot, \cdot) : \overline{\mathcal{G}^c} \times \overline{\mathcal{G}^c} \to \mathbb{R}$ for the Hilbert space $Y|\overline{\mathcal{G}^c}$ such that, for every $P \in Y|\overline{\mathcal{G}^c}$, the reproducing property

$$P(x) = \left\langle P, K_{Y|\overline{\mathcal{G}^c}}(x, \cdot)\right\rangle_{Y|\overline{\mathcal{G}^c}}, \quad x \in \overline{\mathcal{G}^c}, \tag{204}$$

is valid. For $x \in \overline{\mathcal{G}^c}$ and $F \in Harm(\mathcal{G})$ such that $A_{\overline{\mathcal{G}^c}}[F] = P$, we obtain

$$\begin{aligned} P(x) &= \langle F, G(\Delta; |x - \cdot|)\rangle_{L^2(\mathcal{G})} \\ &= \langle A_{\overline{\mathcal{G}^c}}[F], A_{\overline{\mathcal{G}^c}}[G(\Delta; |x - \cdot|)]\rangle_{Y|\overline{\mathcal{G}^c}} \\ &= \langle P, A_{\overline{\mathcal{G}^c}}[G(\Delta; |x - \cdot|)]\rangle_{Y|\overline{\mathcal{G}^c}}. \end{aligned} \tag{205}$$

Hence, $K_{Y|\overline{\mathcal{G}^c}}(x, \cdot) = A_{\overline{\mathcal{G}^c}}[G(\Delta; |x - \cdot|)]$, i.e., we have for $x, y \in \overline{\mathcal{G}^c}$:
  The integral

$$\begin{aligned} K_{Y|\overline{\mathcal{G}^c}}(x, y) &= \langle G(\Delta; |x - \cdot|), G(\Delta; |y - \cdot|)\rangle_{L^2(\mathcal{G})} \\ &= \frac{1}{(4\pi)^2} \int_{\mathcal{G}} \frac{1}{|x - z||y - z|}\, dz \end{aligned} \tag{206}$$

represents the (unique) reproducing kernel of $Y|\overline{\mathcal{G}^c}$.

Clearly, for "geoscientifically relevant geometries" $\mathcal{G}$ such as geoid, real Earth, etc. the integral (206) has to be determined by approximate integration rules such as presented in Freeden and Gutting (2018) (see also the literature therein).

Summarizing our considerations we end up with the following result:

The class $\left(Y|\overline{\mathcal{G}^c}, \langle\cdot, \cdot\rangle_{Y|\overline{\mathcal{G}^c}}\right)$ constitutes a Hilbert space possessing the reproducing kernel (206).

5.3 External/terrestrial RKHS for balls

For the special case of a ball $\mathcal{B}_\beta(0)$ of radius β around the origin the kernel $K_{Y|\mathcal{B}_\beta^c(0)}(\cdot, \cdot)$ given by

$$K_{Y|\overline{\mathcal{B}_\beta^c(0)}}(x, y) = \frac{1}{(4\pi)^2} \int_{\mathcal{B}_\beta(0)} \frac{1}{|x - z||y - z|} \, dz, \tag{207}$$

can be expressed as series representation by use of the expansion (see, e.g., Freeden and Schreiner 2009)

$$G(\Delta; |x - y|) = \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{|y|^n}{|x|^{n+1}} P_n\left(\frac{x}{|x|} \cdot \frac{y}{|y|}\right), \quad |y| < |x|, \tag{208}$$

where P_n is the Legendre polynomial of degree n. In connection with (207) we obtain

$$K_{Y|\overline{\mathcal{B}_\beta^c(0)}}(x, y) = \frac{\beta}{4\pi} \sum_{n=0}^{\infty} \frac{1}{(2n+1)(2n+3)} \left(\frac{\beta^2}{|x||y|}\right)^{n+1} P_n\left(\frac{x}{|x|} \cdot \frac{y}{|y|}\right). \tag{209}$$

We are interested in an explicit expression of the infinite Legendre sum (209). To this end, we have a closer look at the term

$$\frac{1}{(2n+1)(2n+3)} \tag{210}$$

that can be decomposed via partial fraction decomposition in the form

$$\frac{1}{(2n+1)(2n+3)} = \frac{1}{2(2n+1)} - \frac{1}{2(2n+3)}. \tag{211}$$

As a consequence, the reproducing kernel can be rewritten in the form

$$K_{Y|\overline{\mathcal{B}_\beta^c(0)}}(x, y) = \underbrace{\frac{\beta^3}{8\pi} \frac{1}{|x||y|} \sum_{n=0}^{\infty} \frac{1}{2n+1} \left(\frac{\beta^2}{|x||y|}\right)^n P_n\left(\frac{x}{|x|} \cdot \frac{y}{|y|}\right)}_{=:\Phi_1\left(\frac{\beta}{\sqrt{|x||y|}}, \frac{x}{|x|} \cdot \frac{y}{|y|}\right)}$$
$$- \underbrace{\frac{\beta^3}{8\pi} \frac{1}{|x||y|} \sum_{n=0}^{\infty} \frac{1}{2n+3} \left(\frac{\beta^2}{|x||y|}\right)^n P_n\left(\frac{x}{|x|} \cdot \frac{y}{|y|}\right)}_{=:\Phi_2\left(\frac{\beta}{\sqrt{|x||y|}}, \frac{x}{|x|} \cdot \frac{y}{|y|}\right)}. \tag{212}$$

Case 1 We let $h := \frac{\beta}{\sqrt{|x||y|}} < 1$ and $t := \frac{x}{|x|} \cdot \frac{y}{|y|} \in (-1, 1)$. Under this assumption we consider the Legendre expansions

$$\Phi_1(h, t) = \frac{\beta}{8\pi} h \sum_{n=0}^{\infty} \frac{1}{2n+1} h^{2n+1} P_n(t), \tag{213}$$

$$\Phi_2(h, t) = \frac{\beta}{8\pi} \sum_{n=0}^{\infty} \frac{1}{2n+3} h^{2n+2} P_n(t). \tag{214}$$

Recalling the generating series by means of the Legendre polynomials (see, e.g., Abramowitz and Stegun 1964; Magnus et al. 1966)

$$\sum_{n=0}^{\infty} h^{2n} P_n(t) = \frac{1}{\sqrt{1 + h^4 - 2h^2 t}}, \quad h \in [0, 1), \ t \in [-1, 1]. \tag{215}$$

we obtain by integration of both sides of (215) with respect to h

$$\sum_{n=0}^{\infty} \frac{1}{2n+1} h^{2n+1} P_n(t) = \int \frac{1}{\sqrt{1 + h^4 - 2h^2 t}} \, dh. \tag{216}$$

The Ph.D.-thesis Kotevska (2011) provides the following representation

$$\begin{aligned}
&\Phi_1(h, t) \\
&= -i \frac{\beta}{8\pi} h \sqrt{\frac{h^2}{-t + \sqrt{t^2 - 1}} + 1} \sqrt{-\frac{h^2}{t + \sqrt{t^2 - 1}} + 1} \\
&\quad \times \frac{F\left(i \sinh^{-1}\left(h\sqrt{\frac{1}{-t+\sqrt{t^2-1}}}, \frac{t-\sqrt{t^2-1}}{t+\sqrt{t^2-1}}\right)\right)}{\sqrt{\frac{1}{-t+\sqrt{t^2-1}}} \sqrt{1 + h^4 - 2h^2 t}},
\end{aligned} \tag{217}$$

where F is the elliptic integral of the first kind (see, e.g., Magnus et al. 1966). Analogously, for the determination of $\Phi_2(h, t)$, we have

$$\sum_{n=0}^{\infty} h^{2n+2} P_n(t) = h^2 \sum_{n=0}^{\infty} h^{2n} P_n(t) = \frac{h^2}{\sqrt{1 + h^4 - 2h^2 t}}, \tag{218}$$

so that integration of the last equation with respect to h yields

$$\sum_{n=0}^{\infty} \frac{1}{2n+3} h^{2n+3} P_n(t) = \int \frac{h^2}{\sqrt{1 + h^4 - 2h^2 t}} \, dh. \tag{219}$$

By use of the elliptic integral E of the second kind (see, e.g., Magnus et al. 1966) we deduce from Kotevska (2011) that

$$\Phi_2(h, t)$$
$$= \frac{\beta}{8\pi} \frac{(\sqrt{t^2 - 1} + t)\sqrt{\frac{h^2}{-t+\sqrt{t^2-1}} + 1}\sqrt{-\frac{h^2}{t+\sqrt{t^2-1}} + 1}}{\sqrt{\frac{1}{-t+\sqrt{t^2-1}}}\sqrt{1 + h^4 - 2h^2 t}}$$

$$\times \left\{ E\left(i \sinh^{-1}\left(h\sqrt{\frac{1}{-t + \sqrt{t^2 - 1}}} \right), \frac{t - \sqrt{t^2 - 1}}{t + \sqrt{t^2 - 1}} \right) \right.$$

$$\left. - F\left(i \sinh^{-1}\left(h\sqrt{\frac{1}{-t + \sqrt{t^2 - 1}}} \right), \frac{t - \sqrt{t^2 - 1}}{t + \sqrt{t^2 - 1}} \right) \right\}. \quad (220)$$

Next we are concerned with the special cases that $t = \frac{x}{|x|} \cdot \frac{y}{|y|} = \pm 1$ and $h = \frac{\beta}{\sqrt{|x||y|}} < 1$. These cases do not need the reduction to elliptic integrals:

Case 2 We let $h = \frac{\beta}{\sqrt{|x||y|}} < 1$ and $t = \frac{x}{|x|} \cdot \frac{y}{|y|} = 1$. Now we obtain

$$\sum_{n=0}^{\infty} \frac{h^{2n+1}}{2n + 1} \underbrace{P_n(1)}_{=1} = \sum_{n=0}^{\infty} \frac{h^{2n+1}}{2n + 1} = \int \frac{1}{\sqrt{1 + h^4 - 2h^2}} \, dh = \int \frac{1}{1 - h^2} \, dh. \quad (221)$$

Note, that $h = \frac{\beta}{\sqrt{|x||y|}}$ and $1 - h^2 > 0$, since $h^2 \in [0, 1)$. Using the partial fraction $\frac{1}{1-h^2} = \frac{1}{2}\left(\frac{1}{1-h} + \frac{1}{1+h} \right)$, we are led to

$$\int \frac{1}{1 - h^2} dh = \frac{1}{2}\left(\int \frac{1}{1 - h} \, dh + \int \frac{1}{1 + h} dh \right)$$
$$= \frac{1}{2}(-\ln(1 - h) + \ln(1 + h)) = \frac{1}{2} \ln\left(\frac{1 + h}{1 - h} \right). \quad (222)$$

It follows that (note that $t = 1$)

$$\sum_{n=0}^{\infty} \frac{h^{2n+3}}{2n + 3} = \int \frac{h^2}{\sqrt{1 + h^4 - 2h^2}} \, dh = \int \frac{h^2}{1 - h^2} dh. \quad (223)$$

Using the partial fraction decomposition $\frac{h^2}{1-h^2} = \frac{1}{2}\left(-2 + \frac{1}{1-h} + \frac{1}{1+h} \right)$ we see that

$$\int \frac{h^2}{1 - h^2} \, dh = \frac{1}{2}(-2h - \ln(1 - h) + \ln(1 + h)) = \frac{1}{2}\left(\ln\left(\frac{1 + h}{1 - h} \right) - 2h \right).$$
$$(224)$$

Hence, we arrive at the following representation of the kernel $K_{Y|\mathcal{B}_\beta^c(0)}(x, y)$:

$$
K_{Y|\overline{\mathcal{B}_\beta^c(0)}}(x, y)
$$

$$
= \frac{\beta^3}{8\pi|x||y|}\left(\frac{\sqrt{|x||y|}}{2\beta}\ln\left(\frac{1+\frac{\beta}{\sqrt{|x||y|}}}{\frac{\beta}{\sqrt{|x||y|}}}\right)\right.
$$

$$
\left. -\frac{(|x||y|)^{3/2}}{2\beta^3}\left(\ln\left(\frac{1+\frac{\beta}{\sqrt{|x||y|}}}{1-\frac{\beta}{\sqrt{|x||y|}}}\right)-2\frac{\beta}{\sqrt{|x||y|}}\right)\right)
$$

$$
= \frac{1}{16\pi}\left(\left(\frac{\beta^2}{\sqrt{|x||y|}}-\sqrt{|x||y|}\right)\ln\left(\frac{\sqrt{|x||y|}+\beta}{\sqrt{|x||y|}-\beta}\right)+2\beta\right). \tag{225}
$$

Case 3 We let $h = \frac{\beta}{\sqrt{|x||y|}} < 1$ and $t = \frac{x}{|x|}\cdot\frac{y}{|y|} = -1$. Now we start from

$$
\sum_{n=0}^{\infty}\frac{h^{2n+1}}{2n+1}\underbrace{P_n(-1)}_{=(-1)^n} = \sum_{n=0}^{\infty}(-1)^n\frac{h^{2n+1}}{2n+1}
$$

$$
= \int\frac{1}{\sqrt{1+h^4+2h^2}}\,dh = \int\frac{1}{1+h^2}\,dh = \tan^{-1}(h). \tag{226}
$$

We use the partial fraction decomposition $\frac{h^2}{1+h^2} = 1 - \frac{1}{1-h^2}$ and obtain

$$
\sum_{n=0}^{\infty}(-1)\frac{h^{2n+3}}{2n+3} = \int\frac{h^2}{\sqrt{1+h^4+2h^2}}\,dh
$$

$$
= \int\frac{h^2}{\sqrt{1+h^2}}\,dh = \int 1-\frac{1}{1+h^2}\,dh = h-\tan^{-1}(h). \tag{227}
$$

As a consequence we obtain the following representation of the kernel $K_{Y|\overline{\mathcal{B}_\beta^c(0)}}(x, y)$:

$$
K_{Y|\overline{\mathcal{B}_\beta^c(0)}}(x, y)
$$

$$
= \frac{\beta^3}{8\pi|x||y|}\left(\frac{\sqrt{|x||y|}}{\beta}\tan^{-1}\left(\frac{\beta}{\sqrt{|x||y|}}\right)\right.
$$

$$
\left. -\frac{(|x||y|)^{3/2}}{\beta^3}\left(\frac{\beta}{\sqrt{|x||y|}}-\tan^{-1}\left(\frac{\beta}{\sqrt{|x||y|}}\right)\right)\right)
$$

$$
= \frac{1}{8\pi}\left(\left(\frac{\beta^2}{\sqrt{|x||y|}}+\sqrt{|x||y|}\right)\tan^{-1}\left(\frac{\beta}{\sqrt{|x||y|}}\right)-\beta\right). \tag{228}
$$

All in all, our approach shows that the reproducing kernel does not provide a closed representation even in spherical framework, since the occurring elliptic integrals

do not admit a closed form. As a consequence, suitable techniques of constructive approximation and/or numerical integration are required.

5.4 External/terrestrial/internal RKHS for regular regions

A careful look at the volume integral

$$(x, y) \mapsto \int_{\mathcal{G}} G(\Delta; |x - z|)\, G(\Delta; |z - y|)\, dz \tag{229}$$

already showed that (229) exists for all $x, y \in \mathbb{R}^3$ (with $x, y \in \mathcal{G}^c$ constituting even a regular integral expression). Furthermore, to every $F \in L^2(\mathcal{G})$, there exists a unique $V \in Y$ of the form

$$V(x) = A[F](x) = \int_{\mathcal{G}} G(\Delta; |x - y|)\, F(y)\, dy, \quad x \in \mathbb{R}^3. \tag{230}$$

On the space Y we are able to impose an inner product $\langle \cdot, \cdot \rangle_Y$ by setting

$$\langle A[F], A[G] \rangle_Y = \langle F, G \rangle_{L^2(\mathcal{G})}, \tag{231}$$

where $F, G \in L^2(\mathcal{G})$. The space Y equipped with the inner product $\langle \cdot, \cdot \rangle_Y$ is a Hilbert space.

Note that, for all $x \in \mathbb{R}^3$, the Cauchy-Schwarz inequality yields the estimate

$$|V(x)| \leq \sqrt{\int_{\mathcal{G}} |\, G(\Delta; |x - y|)|^2\, dy}\, \sqrt{\int_{\mathcal{G}} |F(y)|^2\, dy}, \tag{232}$$

where it is already known that that there exists a constant C_x such that

$$|V(x)| \leq C_x \sqrt{\int_{\mathcal{G}} |F(y)|^2\, dy} \tag{233}$$

holds true for all $x \in \overline{\mathcal{G}^c}$. Moreover, for $x \in \mathcal{G}$ and some value

$$R \geq d, \quad d = \mathrm{diam}(\mathcal{G}) = \max_{x, y \in \overline{\mathcal{G}}} |x - y|, \tag{234}$$

we are able to see that

$$\int_{\mathcal{G}} |G(\Delta; |x - y|)|^2 dy = \frac{1}{(4\pi)^2} \int_{\mathcal{G}} \frac{1}{|x - y|^2}\, dy$$
$$\leq \frac{1}{(4\pi)^2} \int_{\mathcal{B}_R(x)} \frac{1}{|x - y|^2}\, dy$$

$$= \frac{1}{(4\pi)^2} \int_0^R \int_{|x-y|=r} \frac{1}{|x-y|^2} dS(y) \, dr$$
$$= \frac{R}{4\pi}. \tag{235}$$

Altogether, we are able to conclude that for each fixed $x \in \mathbb{R}^3$, the evaluation functional $\mathcal{E}_x$ is bounded. Hence, a necessary and sufficient condition that $(Y, \langle \cdot, \cdot \rangle_Y)$ may be specified as reproducing kernel Hilbert space (see Sect. 5.1) is satisfied. In fact, for $x \in \mathcal{G}$ and $F \in L^2(\mathcal{G})$, we obtain

$$\begin{aligned} V(x) &= \langle G(\Delta; |x-\cdot|), F \rangle_{L^2(\mathcal{G})} \\ &= \langle A[G(\Delta; |x-\cdot|)], A[F] \rangle_Y \\ &= \langle A[G(\Delta; |x-\cdot|)], V \rangle_Y, \end{aligned} \tag{236}$$

so that

$$\begin{aligned} K_Y(x, y) &= \int_{\mathcal{G}} G(\Delta; |x-z|) \, G(\Delta; |z-y|) \, dz \\ &= \frac{1}{(4\pi)^2} \int_{\mathcal{G}} \frac{1}{|x-z|} \frac{1}{|z-y|} \, dz, \quad x, y \in \mathbb{R}^3, \end{aligned} \tag{237}$$

is the unique reproducing kernel of Y.

Summarizing our considerations we are finally allowed to formulate the following result:

The image space $Y = A[L^2(\mathcal{G})]$ is a reproducing kernel Hilbert space possessing the reproducing kernel

$$K_Y(x, y) = \frac{1}{(4\pi)^2} \int_{\mathcal{G}} \frac{1}{|x-z|} \frac{1}{|z-y|} \, dz, \quad x, y \in \mathbb{R}^3. \tag{238}$$

It should be remarked that reproducing kernel Hilbert space structure is of particular importance in the inversion of Newton's Law of Gravitation, since the reproducing kernel framework makes a numerical computation efficient and economical, as we shall see from the following gravimetric spline context (note that Freeden 1981, 1987, 1999; Freeden and Gerhards 2013; Freeden and Michel 2004; Freeden and Witte 1982; Shure et al. 1982 include details about harmonic splines).

5.5 External/terrestrial/internal spline theory for regular regions

Let $\mathcal{G}$ be a regular region. Suppose that $\{x_1, \ldots, x_N\}, x_i \neq x_j, i \neq j$, is a discrete set of N given points in $\mathbb{R}^3$. Assume that the values $\gamma_i = V(x_i), x_i \in \mathbb{R}^3, i = 1, \ldots, N$, constitute a given data set from the Newton potential (6). We want to find an approximation S_N^V to the potential V such that

$$S_N^V(x_i) = V(x_i) = \gamma_i, \quad i = 1, \ldots, N. \tag{239}$$

(If the data are noisy, interpolation should be replaced by smoothing (see, e.g., Freeden and Witte 1982 and the references therein)). A functional value $V(x)$ at a point $x \in \mathbb{R}^3$ can be identified with an evaluation functional

$$\mathcal{E}_x : V \mapsto \mathcal{E}_x[V] = V(x), \quad V \in Y(\overline{\mathcal{G}^c}). \tag{240}$$

For each $x \in \mathbb{R}^3$, the linear functional $\mathcal{E}_x$ defined by $\mathcal{E}_x : V \mapsto \mathcal{E}_x[V] = V(x)$, $V \in Y$, is bounded on Y, i.e, $|\mathcal{E}_x[V]| = |V(x)| \leq C_x \|V\|_Y$. Moreover, for $x \in \partial \mathcal{G}$ and for all $V \in Y$ we have $\mathcal{E}_x[V] = V(x) = (V, K_Y(x, \cdot))_Y)$.

Spline method The Newton potential V, from which the discrete data are known, is considered to be an element of the Hilbert space Y possessing the reproducing kernel $K_Y(\cdot, \cdot)$, while the observed values at the points $x_1, \ldots, x_N \in \mathbb{R}^3$ are assumed to be associated with linearly independent bounded functionals $\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}$. In doing so, we are able to find a minimum norm solution $S_N^V \in Y$ as a linear combination of the representers $\mathcal{E}_{x_i}[K_Y(\cdot, \cdot)]$ to the functionals $\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}$, i.e., S_N^V is meant as the projection of V to the N-dimensional linear subspace spanned by the linearly independent representers $\mathcal{E}_{x_i}[K_Y(\cdot, \cdot)]$, $i = 1, \ldots, N$ (see, e.g., Davis 1963).

Let $\{x_1, \ldots, x_N\} \subset \mathbb{R}^3$ be a point system, such that the evaluation functionals $\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}$ are linearly independent. Then, within the set

$$\mathcal{I}_{\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}}^V = \{U \in Y : \mathcal{E}_{x_i}[U] = \mathcal{E}_{x_i}[V] = \gamma_i, \ i = 1, \ldots, N\}, \tag{241}$$

the minimum norm interpolation problem of finding S_N^V that satisfies

$$\|S_N^V\|_Y = \inf_{U \in \mathcal{I}_{\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}}^V} \|U\|_Y \tag{242}$$

is well posed, i.e., its solution exists, is unique and depends continuously on the data $\gamma_1, \ldots, \gamma_N$. The uniquely determined solution S_N^V is given in the explicit form

$$S_N^V(x) = \sum_{i=1}^N a_i^N \mathcal{E}_{x_i}[K_Y(x, \cdot)], \quad x \in \mathbb{R}^3, \tag{243}$$

where the coefficients $a_1^N, \ldots, a_N^N$ are determined by solving the linear system of equations

$$\sum_{i=1}^N a_i^N \mathcal{E}_{x_i} \mathcal{E}_{x_j}[K_Y(\cdot, \cdot)] = \gamma_j, \quad j = 1, \ldots, N. \tag{244}$$

As a consequence of the interpolation procedure, the density inside $\mathcal{G}$ is obtained as linear combination in terms of fundamental solutions with singularities in the points $\{x_1, \ldots, x_N\}$:

$$
\begin{aligned}
S_N^F(x) &= -\Delta_x S_N^V(x) \\
&= -\sum_{i=1}^{N} a_i^N \mathcal{E}_{x_i}[G(\Delta; |x - \cdot|)] \\
&= -\sum_{i=1}^{N} a_i^N G(\Delta; |x - x_i|), \quad x \in \mathcal{G} \backslash \{x_1, \ldots, x_N\}. \quad (245)
\end{aligned}
$$

As a consequence, S_N^F is a harmonic function provided that $\{x_1, \ldots, x_N\} \subset \overline{\mathcal{G}^c}$.

Spline solutions in terms of Gaussian sums Until now, the proposed methods for numerically calculating the reproducing kernel are either to apply some cubature rule or, in the spherical context, to truncate the associated spherical harmonic expansion. However, using the truncated spherical harmonic expansion of an acceptable numerical effort usually is not accurate enough for terrestrial data points. In what follows we are interested in spline approximation as an inversion procedure based on evaluation functionals. As, in spline approximation, one needs to evaluate reproducing kernel sum expressions when calculating the full-sized spline matrix, we have to find a proper replacement of

$$
K_{A[L^2(\mathcal{G})]}(x, y) = \frac{1}{(4\pi)^2} \int_{\mathcal{G}} \frac{1}{|x - z||y - z|} \, dz, \quad x, y, \in \mathbb{R}^3, \quad (246)
$$

that can be evaluated in economic and efficient way.

Our goal is to substitute the kernel of a monopole $|x - z|^{-1}$ by a linear combination of Gaussians, i.e.,

$$
\frac{1}{|z - x|} \approx \sum_{m=1}^{M} \omega_m e^{-\alpha_m |x - z|^2}, \quad (247)
$$

so that

$$
\begin{aligned}
K_{A[L^2(\mathcal{G})]}(x, y) &= \frac{1}{(4\pi)^2} \int_{\mathcal{G}} \frac{1}{|x - z||y - z|} \, dz \\
&\simeq K_{A[L^2(\mathcal{G})]}^M(x, y) \\
&= \frac{1}{(4\pi)^2} \sum_{m=1}^{M} \sum_{n=1}^{M} \omega_m \omega_n \int_{\mathcal{G}} e^{-\alpha_m |x - z|^2} e^{-\alpha_n |y - z|^2} \, dz \quad (248)
\end{aligned}
$$

(note that the right hand side of (247) allows the separation into Cartesian coordinates; thus, multi-dimensional integrals over cuboids can be handled iteratively, just by one-dimensional integration).

The critical point concerning (247) is to specify the coefficients $\alpha_m, \omega_m, m = 1, \ldots, M$, and the integer M. Different approaches have been proposed in the literature: In Hackbusch (2010), the approximation is attacked by a Newton-type optimization procedure. In Hackbusch et al. (2005), a Remez algorithm exploits specific properties of a certain error functional (not discussed here in more detail). Fast

multipole methods (see, e.g., Cheng et al. 1999; Greengard and Rokhlin 1997) also provide tools of great numerical significance. Our approach here closely parallels the concepts presented in Beylkin and Monzón (2005, 2010). This concept starts with an initial approximation obtained by the appropriate discretization of an integral expression of $|z - x|^{-1}$. Afterwards, in order to reduce the number M of terms of the Gaussian sum on the right side of (247), an algorithm is applied based on Prony's method.

An advantage is that we are able to develop our results for the one-dimensional fuction $r \mapsto r^{-1}$, $r \in [\delta, 1]$, with some sufficiently small $\delta > 0$:

$$\frac{1}{r} \simeq \sum_{m=1}^{M} \omega_m e^{-\alpha_m r^2}, \quad r \in [\delta, 1] \tag{249}$$

(note that we can transform any closed interval to this type of interval so that we can restrict ourselves, without loss of generality to the interval $[\delta, 1]$).

Our interest is in guaranteeing that

$$\left| \frac{1}{r} - \sum_{m=1}^{M} \omega_m e^{-\alpha_m r^2} \right| \leq \frac{\varepsilon_{rel}}{r}, \quad r \in [\delta, 1], \tag{250}$$

where $\varepsilon_{rel} > 0$ is (a bound of) the *relative error of the approximation* (note that the relative error states, up to which significant digit our approximations are correct; in fact, if we compare the absolute error with the relative error via the relation $\varepsilon_{rel} = \max_{r \in [\delta, 1]}(\varepsilon_{abs} \, r)$, it becomes clear that the relative error will become larger than the absolute error under our assumptions).

Remark By choosing a scale parameter ϱ instead of δ, the Newtonian kernel $G(\Delta; |x - y|)$ admits, e.g., an "exponential Haar mollification" (regularization) of the form

$$G_\varrho^H(\Delta; |x - y|) \approx \begin{cases} \dfrac{1}{8\pi\varrho}\left(3 - \dfrac{1}{\varrho^2}|x - y|^2\right), & |x - y| \leq \varrho \\[2mm] \dfrac{1}{4\pi}\sum_{m=1}^{M} \omega_m e^{-\alpha_m |x-y|^2}, & \varrho < |x - y|. \end{cases} \tag{251}$$

Remark Suppose that an interval $[A, B]$ is given with the property $A/B \geq \delta$. Then, in the sense of (250), we are allowed to conclude that

$$\left| \frac{1}{r} - \sum_{m=1}^{M} \frac{\omega_m}{B} e^{-\frac{\alpha_m}{B^2} r^2} \right| \leq \frac{\varepsilon_{rel}}{r}, \quad r \in [A, B]. \tag{252}$$

In other words, by setting $\omega_m^{A,B} = \omega_m/B$ and $\alpha_m^{A,B} = \alpha_m/B^2$ we obtain the coefficients for an approximation of $1/r$ on the interval $[A, B]$ (note, that the (bound of the) relative error is not affected by this parametrisation).

Initial approximation We start from the integral representation

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-r^2 e^{2s} + s} \, ds, \tag{253}$$

that easily follows from

$$\frac{2}{\sqrt{\pi}} \int_a^b e^{-r^2 e^{2s} + s} \, ds = \frac{2}{\sqrt{\pi}} \int_{e^a}^{e^b} e^{-(rt)^2} \, dt$$

$$= \frac{2}{\sqrt{\pi}} \frac{1}{r} \int_{re^a}^{re^b} e^{-x^2} \, dx$$

$$= \frac{1}{r} \left(\mathrm{erf}(re^b) - \mathrm{erf}(re^a) \right) \tag{254}$$

by applying the limit relations $\lim_{b \to \infty} \mathrm{erf}(re^b) = 1$, $\lim_{a \to -\infty} \mathrm{erf}(re^a) = 0$, where erf is the *error function* given by

$$\mathrm{erf}(s) = \frac{2}{\sqrt{\pi}} \int_0^s \exp(-t^2) \, dt, \ s \geq 0. \tag{255}$$

Next we apply the composite *trapezoidal rule* (see, e.g., Freeden and Gutting 2018) to discretize the integral (253) in order to deduce an initial approximation of the form (249). In more detail, if a, b are given such that $-\infty < a < 0 < b < \infty$ and $M + 1$ is the total number of grid points in the trapezoidal rule, then using the abbreviations

$$s_m := a + mh, \ m = 0, \ldots, M \tag{256}$$

and

$$h := \frac{b - a}{M} \tag{257}$$

we are led to coefficients ω_m and α_m of the Gaussian sum (247) in the form

$$\omega_m := \frac{2h}{\sqrt{\pi}} e^{s_m}, \ m = 0, \ldots, M, \tag{258}$$

and

$$\alpha_m := e^{2s_m}, \ m = 0, \ldots, M. \tag{259}$$

So, our initial approximation is of the form

$$\frac{1}{r} \simeq \frac{2h}{\sqrt{\pi}} \sum_{m=0}^{M} e^{s_m} \exp(-e^{2s_m} r^2), \quad r \in [\delta, 1]. \tag{260}$$

Now, we are prepared to deal with the question of how to choose a, b, and M. First it is readily seen that

$$\left| 1 - r \int_a^b e^{-r^2 e^{2s} + s} \, ds \right|$$
$$= r \int_b^\infty e^{-r^2 e^{2s} + s} \, ds + r \int_{-\infty}^a e^{-r^2 e^{2s} + s} \, ds. \tag{261}$$

Our desire is to estimate the occurring integrals such that

$$r \int_{-\infty}^a e^{-r^2 e^{2s} + s} \, ds < \frac{1}{4} \varepsilon_{rel} \tag{262}$$

as well as

$$r \int_b^\infty e^{-r^2 e^{2s} + s} \, ds < \frac{1}{4} \varepsilon_{rel} \tag{263}$$

for all $r \in [\delta, 1]$. As a consequence, the error of the truncated integral in the limits from a to b is at most $\frac{1}{2} \varepsilon_{rel}$, i.e.,

$$\left| 1 - r \int_a^b e^{-r^2 e^{2s} + s} \, ds \right| < \frac{1}{2} \varepsilon_{rel}. \tag{264}$$

Observing the special structure of the definite integral (254) we are able to conclude that

$$r \int_{-\infty}^a e^{-r^2 e^{2s} + s} \, ds = |\mathrm{erf}(re^a)| \leq \mathrm{erf}(e^a) \tag{265}$$

and

$$r \int_b^\infty e^{-r^2 e^{2s} + s} \, ds = |1 - \mathrm{erf}(re^b)| \leq 1 - \mathrm{erf}(\delta e^b) \tag{266}$$

for all $r \in [\delta, 1]$. Combining these results we finally obtain for a and b the following representations:

$$a = \ln \left(\mathrm{erf}^{-1} \left(\frac{1}{4} \varepsilon_{rel} \right) \right) \tag{267}$$

and

$$b = \ln \left(\frac{1}{\delta} \mathrm{erf}^{-1} \left(1 - \frac{1}{4} \varepsilon_{rel} \right) \right). \tag{268}$$

All in all, the error of the truncated integral is assured to have a bound less than $\frac{1}{2} \varepsilon_{rel}$.

Test calculations Under the special choice $\delta = 10^{-10}$, Table 1 presents numerical quantities for the estimates (267) and (268) in dependence of various ε_{rel} (for more details the reader is referred to the thesis Burschäpers 2013).

Table 1 Upper bounds a_{up} for a (second column) and lower bounds b_{lo} for b (third column) for different ε_{rel} and the special choice $\delta = 10^{-10}$ (taken from Burschäpers 2013)

ε_{rel}	a_{up}	b_{lo}
10^{-11}	-26.836	24.626
10^{-12}	-29.139	24.670
10^{-13}	-31.441	24.711
10^{-14}	-33.744	24.748

It remains to discuss the choice of M. Since the composite trapezoidal rule converges to the integral of the order $O(M^{-2})$, it is evident that the Gaussian sum approximation becomes better the larger M is chosen. In fact, the substitution of r^{-1} by a finite sum of exponentials can be theoretically based on the following result due to Beylkin and Monzón (2005):

For any δ with $0 < \delta \leq 1$ and $0 < \varepsilon \leq \frac{1}{2}$, there exist positive numbers α_m and ω_m, such that

$$\left| \frac{1}{r} - \sum_{m=1}^{M} \omega_m \exp(-\alpha_m r^2) \right| < \frac{1}{r}\varepsilon, \quad r \in [\delta, 1], \tag{269}$$

with

$$M = \log \varepsilon^{-1}(c_0 + c_1 \log \varepsilon^{-1} + c_2 \log \delta^{-1}), \tag{270}$$

where $c_k, k = 0, 1, 2,$ are constants. For fixed δ, we have

$$M = O(\log^2(\varepsilon^{-1})). \tag{271}$$

However, this result does not provide us with the required coefficients of the Gaussian sum. Therefore, in the sequel, we are required to handle a proper determination of M in numerical way.

More concretely, for integration limits a and b fixed (as specified (267) and (268)) we are interested in M, so that the stipulated relative error ε_{rel} can be fulfilled. To this end, in view of (260), we consider the expression

$$\varepsilon(M) := \max_{r \in |\delta, 1|} \left| 1 - \frac{2h}{\sqrt{h}} \sum_{m=0}^{M} e^{s_m} \exp(-e^{2s_m} r^2) \right|, \tag{272}$$

where h and s_m are known from the trapezoidal rule setting.

Test calculations Table 2 makes the attempt to indicate numerically the break-even point M_{be} in its dependence on different relative errors ε_{rel} (note that a relative error of 10^{-14} already means, that the occurring error is at the second last significant digit in terms of double precision).

Assuming that we have $N \in \mathbb{N}$ data points for spline approximation we need exactly $\frac{N(N-1)}{2}$ evaluations of the reproducing kernel (246). In total, we have to sum up $M^2 \frac{N(N-1)}{2}$ summands, where we already have taken into account, that the spline interpolation matrix is symmetric and the matrix diagonal is explicitly calculable. Since we are not able to reduce the number of data points N—even worse, we are required

Table 2 Break-even points of $\varepsilon(M)$, such that $\varepsilon(M) < \varepsilon_{rel}$ for all $M \geq M_{be}$ (taken from Burschäpers 2013)

ε_{rel}	M_{be}	$\varepsilon(M_{be})$
10^{-11}	281	9.695×10^{-12}
10^{-12}	322	9.529×10^{-13}
10^{-13}	361	9.481×10^{-14}
10^{-14}	402	8.993×10^{-15}

to increase the number of data points N in order to get a better approximation—we are interested in reducing the number M of summands in the Gaussian sum. In order to achieve this goal, we use an algorithm proposed in Beylkin and Monzón (2010), which is based on Prony's method. As a matter of fact, this algorithm provides a significant reduction of the number of terms, if the coefficients α_m in a Gaussian sum are relatively small, without losing considerable accuracy.

Sum reduction We start our considerations from a Gaussian sum with small exponents, i.e., we let

$$E_{M_0}(r) := \sum_{m=1}^{M_0} p_m e^{-\beta_m r^2}, \tag{273}$$

where M_0 is large. Our purpose is to seek another Gaussian sum E_N possessing $N \ll M_0$ terms to approximate $E_{M_0}(r)$ in the given interval $[\delta, 1]$. Since the values β_m are supposed to be small, we are allowed to use the Taylor expansion of the exponential function up to a degree $2N - 1$, so that

$$E_{M_0}(r) \approx \sum_{m=1}^{M_0} p_m \sum_{k=0}^{2N-1} \frac{(-\beta_m r^2)^k}{k!} = \sum_{k=0}^{2N-1} \underbrace{\left(\sum_{m=1}^{M_0} p_m (-\beta_m)^k \right)}_{=:h_k} \frac{r^{2k}}{k!}. \tag{274}$$

Note that h_k is a fast decaying sequence, such that $N \ll M_0$ is resonable. Now, we express the values h_k in the form

$$h_k = \sum_{m=1}^{N} \omega_m (-\alpha_m)^k, \quad k = 0, \ldots 2N - 1, \tag{275}$$

where $\omega_m, \alpha_m \in \mathbb{R}$, $m = 1, \ldots, N$. Our goal (cf. Beylkin and Monzón 2010) is to determine the unknown coefficients ω_m, α_m using Prony's method. In more detail, the method aims at finding the coefficients of the polynomial

$$Q(x) = \prod_{m=1}^{N} (x + \alpha_m) = \sum_{k=1}^{N} q_k x^k, \tag{276}$$

where $q_N = 1$. Note that

$$\sum_{l=0}^{N} h_{k+l} q_l = \sum_{l=0}^{N} \left(\sum_{m=1}^{N} \omega_m (-\alpha_m)^{k+l} \right) q_l$$

$$= \sum_{m=1}^{N} \omega_m (-\alpha_m)^k \underbrace{\sum_{l=0}^{N} q_l (-\alpha_m)^l}_{=0}$$

$$= 0, \tag{277}$$

since $-\alpha_1, \ldots, -\alpha_N$ are the roots of the polynomial Q. As a consequence, we obtain

$$\sum_{l=0}^{N-1} h_{k+l} q_l = -h_{N+k} := b_k, \quad k = 0, \ldots, N - 1. \tag{278}$$

Thus, the vector $q = (q_0, \ldots, q_{N-1})^T$ is the solution of the vectorial system

$$Hq = b, \tag{279}$$

where $b = (b_0, \ldots, b_{N-1})^T$ and $H = \{h_{k+l}\}_{k,l=0,\ldots,N-1}$ is a $N \times N$ Hankel matrix. Solving this system in the unknowns q we obtain the coefficients of the polynomial Q, so that we are able to determine the roots α_m (if needed by a numerical method). Afterwards, we solve the Vandermonde system (275) and obtain the coefficients ω_m, $m = 1, \ldots, 2N - 1$.

By observing these preliminaries we are able to set up the desired Gaussian sum E_N to approximate E_{M_0}, i.e.,

$$E_{M_0}(r) = \sum_{m=1}^{M_0} p_m e^{-\beta_m r^2} = \sum_{k=0}^{\infty} h_k \frac{r^{2k}}{k!}$$

$$\simeq \sum_{k=0}^{\infty} \sum_{m=1}^{N} w_m (-\alpha_m)^k \frac{r^{2k}}{k!} = \sum_{m=1}^{N} \omega_m e^{-\alpha_m r^2}$$

$$= E_N(r). \tag{280}$$

Example We present the effectiveness of the reduction procedure by applying it to the initial approximation studied earlier in this section. We start from the initial approximation (260) and split it at M_0 so that

$$\sum_{m=1}^{M} \underbrace{\frac{2h}{\sqrt{\pi}} e^{s_m}}_{\omega_m} \exp\left(- \underbrace{e^{2s_m}}_{=\alpha_m} r^2 \right) = \sum_{m=1}^{M_0} \omega_m \exp\left(-\alpha_m r^2 \right)$$

$$+ \sum_{m=M_0+1}^{M} \omega_m \exp(-\alpha_m r^2). \tag{281}$$

ε_{rel}	M	$\varepsilon(M)$
10^{-11}	141	9.695×10^{-12}
10^{-12}	152	9.529×10^{-13}
10^{-13}	164	9.504×10^{-14}
10^{-14}	176	9.104×10^{-15}

Table 3 Reduced Gaussian sums for M_0 as described above and $N = 6$, i.e., $M = M_0 + N$ (taken from Burschäpers 2013)
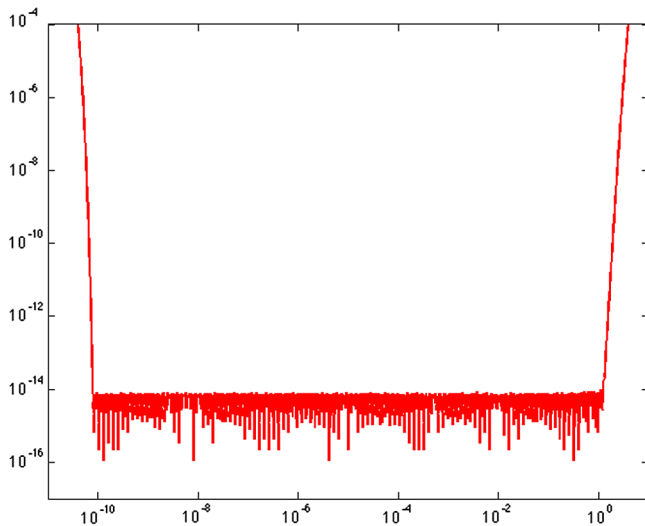
Fig. 1 Relative error (in a log–log-scale) of the reduced Gaussian sum with $M = 176$ approximating $1/r$ on the closed interval $[10^{-10}, 1]$ (taken from Burschäpers 2013)

The question is how to choose M_0 and afterwards N? We recall that the coefficients α_m have to be rather small. The decisive point here is the truncated Taylor expansion of $\exp(x)$ which provides a good approximation, e.g., on a closed interval in $[0, 1]$. This is the reason why we choose M_0 to be the maximum of all m satisfying $s_m < 0$, $m = 1, \ldots, M_0$. Then, we have $\alpha_m < 1$ for all $m = 1, \ldots, M_0$.

Numerical tests (documented in the thesis Burschäpers 2013) have shown that the choice of $N = 6$ leads to good results (for details see Table 3).

In comparison to Table 2, Table 3 demonstrates that the number of coefficients M reduces for relative errors $\varepsilon_{rel} \leq 10^{-12}$ by more than half. In fact, the reduction becomes the more efficient the smaller the prescribed relative error ε_{rel} is. It is remarkable, that there is no decrease of the order of the relative error detectable in the tests.

Another remarkable property of this approach is that we have a uniform relative error on the entire interval $[\delta, 1]$ as we can see from the illustration (Figure 1) below.

Spherical context Next we come to specific aspects in spherically refected spline approximation. To this end, we assume the reference region $\mathcal{G}$ especially to be of spherical shape, e.g., $\mathcal{G}$ is the ball $\mathcal{B}_R(0)$ of radius R around the origin. Our purpose is to calculate a representation of the reproducing kernel as explicit as desired so that

the computation time for numerical purposes can be kept short. Our option is that the results will enable us to efficiently perform spline approximation (interpolation as well as smoothing) corresponding to larger data sets.

The idea behind our concept is based on the functional equation for the exponential function. In standard spherical coordinates $z = r\xi$ with $r = |z|$ and ξ being the associated unit directional vector of z we obtain

$$
\int_{\mathcal{B}_R(0)} \frac{1}{|z-x|} \frac{1}{|z-y|} \, dz
$$
$$
= \int_0^R r^2 \int_{|\xi|=1} \frac{1}{\sqrt{|x^2|^2 + r^2 - 2r|x|(\frac{x}{|x|} \cdot \xi)}\sqrt{|y|^2 + r^2 - 2r|y|(\frac{y}{|y|} \cdot \xi)}} \, d\omega(\xi)\, dr.
$$

(282)

The inner integrand on the right side represents a spherical convolution of two zonal functions, depending only on the inner product of two unit vectors. When considering the product of two Gaussian sum approximations we are again led to a zonal function, namely

$$
\frac{1}{|z-x|} \frac{1}{|z-y|}
$$
$$
\approx \left(\sum_{m=1}^M \omega_m e^{-\alpha_m |z-y|^2} \right) \cdot \left(\sum_{k=1}^M \omega_m e^{-\alpha_k |z-y|^2} \right)
$$
$$
= \sum_{m=1}^M \sum_{k=1}^M \omega_m \omega_k e^{-\alpha_m |z-x|^2 - \alpha_k |z-y|^2}
$$
$$
= \sum_{m=1}^M \sum_{k=1}^M \omega_m \omega_k e^{-(\alpha_m + \alpha_k) r^2 - \alpha_m |x|^2 - \alpha_k |y|^2 2r |\alpha_m x + \alpha_k y| \left(\frac{\alpha_m x + \alpha_k y}{|\alpha_m x + \alpha_k y|} \cdot \xi \right)}
$$

(283)

where $z = r\xi$, with $r = |z|$ and ξ being the a unit vector, in the last step. Note, that $\zeta = \frac{a_m x + \alpha_k y}{|\alpha_m x + \alpha_k y|}$ is a unit vector depending the points x, y and the coefficients α_m and α_k.

In more detail,

$$
\int_{\mathcal{B}_R(0)} \frac{1}{|z-x|} \frac{1}{|z-y|} \, dz
$$
$$
= \int_{\mathcal{B}_R(0)} \left(\sum_{m=1}^M \omega_m e^{\alpha_m |z-x|^2} \right) \cdot \left(\sum_{k=1}^M \omega_k e^{-\alpha_k |z-y|^2} \right) dz
$$
$$
= \sum_{m=1}^M \sum_{k=1}^M \omega_m \omega_k \underbrace{\int_{\mathcal{B}_R(0)} \exp(-\alpha_m |z-x|^2 - \alpha_k |z-y|^2) \, dz}_{=:I_0(x,y)}.
$$

(284)

It remains to calculate the integral $I_0 = I_0(x, y)$ which depends on the positive values α_m, α_k. We consider two cases: The first case is $|\alpha_m x + \alpha_k y| \neq 0$. Then the integrand is a $\frac{\alpha_m x + \alpha_k y}{|\alpha_m x + \alpha_k y|}$-zonal function and the integral over the unit sphere can be calculated by a special case of the Funk–Hecke formula (see, e.g., Freeden and Gutting 2013). For the case $|\alpha_m x + \alpha_k y| = 0$, the integrand becomes a radial basis function.

Case 1 $|\alpha_m x + \alpha_k y| \neq 0$.

$$I_0 = e^{-\alpha_m |x|^2 \alpha_k |y|^2} \int_{\mathcal{B}_R(0)} \exp\left(-(\alpha_m + \alpha_k)|z|^2 + 2z \cdot (\alpha_m x + \alpha_k y)\right) dz$$

$$= 2\pi e^{-\alpha_m |x|^2 - \alpha_k |y|^2} \int_0^R r^2 \int_{-1}^1 \exp(-(\alpha_m + \alpha_k)r^2) \exp(2r|\alpha_m x + \alpha_k y|t) \, dt \, dr \quad (285)$$

so that

$$I_0 = \frac{\pi e^{-\alpha_m |x|^2 - \alpha_k |y|^2}}{|\alpha_m x + \alpha_k y|} \left(\underbrace{\int_0^R r \exp(-(\alpha_m + a_k)r^2 + 2r|\alpha_m x + \alpha_k y|) \, dr}_{= I_{1,+}} \right.$$

$$\left. - \underbrace{\int_0^R r \exp(-(\alpha_m + a_k)r^2 - 2r|\alpha_m x + \alpha_k y|) \, dr}_{= I_{1,-}} \right). \quad (286)$$

The integrals $I_{1,+}$ and $I_{1,-}$ can be calculated as follows:

$$I_{1,\pm} = e^{\frac{|\alpha_m x - \alpha_k y|^2}{\alpha_m + \alpha_k}} \int_0^R r \exp\left(-\left(\sqrt{\alpha_m + \alpha_k} r \pm \frac{|\alpha_m x + \alpha_k y|}{\sqrt{\alpha_m + \alpha_k}}\right)^2\right) dr$$

$$= \frac{e^{\frac{|\alpha_m x - \alpha_k y|^2}{\alpha_m + \alpha_k}}}{\alpha_m + \alpha_k} \left(\int_{\varphi^{-1}(0)}^{\varphi^{-1}(R)} s \exp(-s^2) \, ds \mp \frac{|\alpha_m x + \alpha_k y|}{\sqrt{\alpha_m + \alpha_k}} \int_{\varphi^{-1}(0)}^{\varphi^{-1}(R)} \exp(-s^2) \, ds\right)$$

$$= \frac{e^{\frac{|\alpha_m x - \alpha_k y|^2}{\alpha_m + \alpha_k}}}{\alpha_m + \alpha_k} \left(\left[-\frac{1}{2}\exp(s^2)\right]_{\varphi^{-1}(0)}^{\varphi^{-1}(R)} \mp \frac{\sqrt{\pi}|\alpha_m x + \alpha_k y|}{2\sqrt{\alpha_m + \alpha_k}} [\text{erf}(s)]_{\varphi^{-1}(0)}^{\varphi^{-1}(R)}\right)$$

$$= \frac{e^{\frac{|\alpha_m x - \alpha_k y|^2}{\alpha_m + \alpha_k}}}{2(\alpha_m + \alpha_k)} \left(-\exp\left(-(\alpha_m + a_k)\left(R \pm \frac{|\alpha_m x + \alpha_k y|}{\alpha_m + \alpha_k}\right)^2\right)\right.$$

$$\left. + \exp\left(\pm \frac{|\alpha_m x + \alpha_k y|^2}{\alpha_m + \alpha_k} s\right)\right)$$

$$\mp \frac{\sqrt{\pi}|\alpha_m x + \alpha_k y| e^{\frac{|\alpha_m x - \alpha_k y|^2}{\alpha_m + \alpha_k}}}{2(\alpha_m + \alpha_k)^{3/2}} \left(\text{erf}\left(\sqrt{\alpha_m + \alpha_k}\left(R \pm \frac{|\alpha_m x + \alpha_k y|}{\alpha_m + \alpha_k|}\right)\right)\right.$$

$$\left. - \text{erf}\left(\pm \frac{|\alpha_m x + \alpha_k y|}{\sqrt{\alpha_m + \alpha_k}}\right)\right), \quad (287)$$

where φ^{-1} is the transformation given by

$$s = \varphi^{-1}(r) = \sqrt{\alpha_m + \alpha_k} r \pm \frac{|\alpha_m x + \alpha_k y|}{\sqrt{\alpha_m + \alpha_k}}. \quad (288)$$

By aid of the elementary identity

$$\exp\left(\frac{|\alpha_m x + \alpha_k y|^2}{\alpha_m + \alpha_k} - \alpha_m |x|^2 - \alpha_k |y|^2\right) = \exp\left(-\alpha_m \alpha_k \frac{|x - y|^2}{\alpha_m + \alpha_k}\right), \qquad (289)$$

we obtain

$$
\begin{aligned}
I_0 &= \frac{\pi e^{-\alpha_m |x|^2 - \alpha_k |y|^2}}{|\alpha_m x + \alpha_k y|}(I_{l,+} - l_{1,-}) \\
&= \frac{\pi e^{-\alpha_m \alpha_k \frac{|x-y|^2}{\alpha_m + \alpha_k}}}{2|\alpha_m x + \alpha_k y|(\alpha_m + \alpha_k)}\left[-\exp\left(-(\alpha_m + \alpha_k)\left(R - \frac{|\alpha_m x + \alpha_k y|}{\alpha_m + \alpha_k}\right)^2\right)\right. \\
&\quad + \exp\left(-(\alpha_m + \alpha_k)\left(R + \frac{|\alpha_m x + \alpha_k y|}{\alpha_m + \alpha_k}\right)^2\right)\biggr] \\
&\quad + \frac{\pi^{3/2} e^{-\alpha_m \alpha_k \frac{|x-y|^2}{\alpha_m + \alpha_k}}}{2(\alpha_m + \alpha_k)^{3/2}}\left[\operatorname{erf}\left(\sqrt{\alpha_m + \alpha_k}\left(R - \frac{|\alpha_m x + \alpha_k y|}{\alpha_m + \alpha_k}\right)\right)\right. \\
&\quad + \operatorname{erf}\left(\sqrt{\alpha_m + \alpha_k}\left(R + \frac{|\alpha_m x + \alpha_k y|}{\alpha_m + \alpha_k}\right)\right)\biggr].
\end{aligned}
\qquad (290)
$$

Case 2 $|\alpha_m x + \alpha_k y| = 0$. In this case, the previous calculation fails, where we need to divide by $|\alpha_m x + \alpha_k y|$. Nevertheless, the calculation turns out to be shorter, since the integrand becomes a radial basis function.

$$
\begin{aligned}
I_0 &= e^{-\alpha_m |x|^2 - al_k |y|^2} \int_{\mathcal{B}_R(0)} \exp\left(-(\alpha_m + \alpha_k)|z|^2\right) dz \\
&= 4\pi e^{-\alpha_m |x|^2 - \alpha_k |y|^2} \int_0^R r^2 \exp\left(-(\alpha_m + \alpha_k)r^2\right) dr \\
&= 4\pi \frac{e^{-\alpha_m |x|^2 - \alpha_k |y|^2}}{(\alpha_m + \alpha_k)^{3/2}} \int_0^{\sqrt{\alpha_m + \alpha_k} R} s^2 \exp(-s^2) ds \\
&= 2\pi \frac{e^{-\alpha_m |x|^2 - \alpha_k |y|^2}}{(\alpha_m + \alpha_k)^{3/2}} \left[-s\exp(-s)^2 + \frac{\sqrt{\pi}}{2}\operatorname{erf}(s)\right]_0^{\sqrt{\alpha_m + \alpha_k} R} \\
&= 2\pi \frac{e^{-\alpha_m |x|^2 - \alpha_k |y|^2}}{(\alpha_m + \alpha_k)^{3/2}} \left(-\sqrt{\alpha_m + \alpha_k} R \, \exp(-(\alpha_m + \alpha_k)R^2)\right. \\
&\quad + \frac{\sqrt{\pi}}{2}\operatorname{erf}\left(\sqrt{\alpha_m + \alpha_k} R\right)\biggr).
\end{aligned}
\qquad (291)
$$

where we used the transformation $s = \varphi^{-1}(r) = \sqrt{\alpha_m + \alpha_k} r$ in the third step and integration by parts in the fourth step.

Summarizing we obtain the following Gaussian sum approximation of the reproducing kernel in spherical context

$$K_{A[L^2(\mathcal{B}_R(0))]}(x, y)$$

$$= \frac{1}{(4\pi)^2} \int_{\mathcal{B}_R(0)} \frac{1}{|z - x|} \frac{1}{|z - x|} \, dz$$

$$\simeq K^M_{A[L^2(\mathcal{B}_R(0))]}(x, y)$$

$$:= \frac{1}{(4\pi)^2} \sum_{m=1}^{M} \sum_{k=1}^{M} \omega_m \omega_k \underbrace{\int_{\mathcal{B}_R(0)} \exp(-\alpha_m |z - x|^2 - \alpha_k |z - y|^2) \, dz}_{=:I_0(x,y)} \quad (292)$$

and $I_0(x, y)$ is explicitly given by (290) and (291).

Further numerical tests and the Gaussian sum application in spline modeling relative to disturbing gravitational potential data can be found in the thesis Burschäpers (2013). All in all, we are allowed to conclude that Gaussian sums turn out to be good candidates for reducing the numerical effort in RKHS-spline approximation.

RKHS mollifier realization Instead of the "mollification" of monopoles involving Gaussian sums we now go back to the "monopole mollification" as discussed in the context of the Newton volume integral. Denoting by Y_ϱ, $\varrho > 0$, the space of all *mollified singular integral-type Newton integrals $A_\varrho[F]$* given by

$$A_\varrho[F] = \int_{\mathcal{G}} G_\varrho(\Delta; |x - y|) F(y) \, dy, \quad F \in L^2(\mathcal{G}), \quad (293)$$

with $G_\varrho(\Delta; |\cdot - \cdot|)$ given either by (251) or by (145), so that $Y_\varrho = A_\varrho[L^2(\mathcal{G})]$, we are led to an analogous result to the singular integral-type Newton integral:

The image space $Y_\varrho = A_\varrho[L^2(\mathcal{G})]$ is a reproducing kernel Hilbert space possessing the reproducing kernel

$$K_{Y_\varrho}(x, y) = \int_{\mathcal{G}} G_\varrho(\Delta; |x - z|) G_\varrho(\Delta; |z - y|) \, dz, \quad x, y \in \mathbb{R}^3. \quad (294)$$

Finally, it should be mentioned that

$$-\Delta_x K_{Y_\varrho}(x, y) = \int_{\mathcal{G}} K_\varrho(|x - z|) G_\varrho(\Delta; |z - y|) \, dz, \quad x, y \in \mathbb{R}^3. \quad (295)$$

Spline mollifier method For sufficiently small ϱ, an approximate version of the kernel

$$K_Y(x, y) = \int_{\mathcal{G}} G(\Delta; |x - z|) G(\Delta; |y - z|) \, dz \quad (296)$$

is now given by

$$K_{Y_\varrho}(x, y) = \int_{\mathcal{G}} G_\varrho(\Delta; |x - z|) G_\varrho(\Delta; |y - z|) \, dz. \quad (297)$$

Note that, from the integral in (297), we see that

$$\sum_{k=1}^{N}\sum_{i=1}^{N} a_k\, a_i \int_{\mathcal{G}} G_\varrho(\Delta; |x_k - z|)\, G_\varrho(\Delta; |x_i - z|)\, dz$$

$$= \int_{\mathcal{G}} \left| \sum_{k=1}^{N} a_k G_\varrho(\Delta; |x_k - z|) \right|^2 dz \geq 0. \tag{298}$$

Moreover, the linear independence of the system $\{G_\varrho(\Delta; |x_i - \cdot|)\}_{i=1,\ldots,N}$ implies that the Gram matrix

$$\left(\int_{\mathcal{G}} G_\varrho(\Delta; |x_i - z|)\, G_\varrho(\Delta; |x_k - z|)\, dz \right)_{k,i=1,\ldots,N} \tag{299}$$

is positive definite, so that $K_{Y_\varrho}(\cdot, \cdot)$ is a positive definite kernel.

In other words, the integral (297) defines a Hilbert space $\left(Y_\varrho, \langle \cdot, \cdot \rangle_{Y_\varrho}\right)$ possessing (297) as the reproducing kernel. In Y_ϱ, minimum norm (spline) interpolation as described above can be performed in analogous way:

Let $\{x_1, \ldots, x_N\} \subset \mathbb{R}^3$ *be a point system, such that the evaluation functionals* $\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}$ *are linearly independent. Then, within the set*

$$\mathcal{I}^V_{\mathcal{E}_{x_1},\ldots,\mathcal{E}_{x_N}} = \{U \in Y_{\varrho_J}\left(\overline{\mathcal{G}^c}\right) : \mathcal{E}_{x_i}[U] = \mathcal{E}_{x_i}[V] = \gamma_i,\ i = 1, \ldots, N\}, \tag{300}$$

the minimum norm interpolation problem of finding S_N^V *that satisfies*

$$\|S_N^V\|_{Y_\varrho} = \inf_{U \in \mathcal{I}^V_{\mathcal{E}_{x_1},\ldots,\mathcal{E}_{x_N}}} \|U\|_{Y_\varrho} \tag{301}$$

is well posed, i.e., its solution exists, is unique and depends continuously on the data $\gamma_1, \ldots, \gamma_N$. *The uniquely determined solution* S_N^V *is given in the explicit form*

$$S_N^V(x) = \sum_{i=1}^{N} a_i^N \mathcal{E}_{x_i}[K_{Y_\varrho}(x, \cdot)], \quad x \in \mathbb{R}^3, \tag{302}$$

where the coefficients $a_1^N, \ldots, a_N^N$ *are determined by solving the linear system of equations*

$$\sum_{i=1}^{N} a_i^N \mathcal{E}_{x_i} \mathcal{E}_{x_j}[K_{Y_\varrho}(\cdot, \cdot)] = \gamma_j, \quad j = 1, \ldots, N. \tag{303}$$

In this case, we obtain an approximation of the density distribution as a linear combination of singular integral-type kernels (295) which are not harmonic. Moreover, for purposes of decorrelation, we are able to take advantage of the sparse character of the resulting wavelets to reduce considerably the computational effort.

Application to geodetic observables In geodetic practice, a spline approach by means of evaluation functionals as presented until now is unrealistic. For practical purposes other geodetic observables have to come into play such as gravity anomalies, gravity disturbances, deflections of the vertical, satellite-to-satellite (SST)-data, satellite-gavity-gradiometry (SGG)-data. These observables, however, involve derivatives applied to the gravitational potential, i.e., the Newton volume integral. As long as this derivative is taken in a point of $\mathcal{G}^c$, i.e., applied to a regular Newton volume integral, the linear functionals representing these observables (cf. Freeden and Nutz 2018) are bounded on the reproducing kernel Hilbert space $Y = A[L^2(\mathcal{G})]$. However, in case of terrestrial observables, the derivative in a point on the boundary $\partial\mathcal{G}$ does not allow to guarantee the boundedness on $Y = A[L^2(\mathcal{G})]$, using a Cauchy–Schwarz estimation in standard way. The same calamity happens for derivatives in points inside $\mathcal{G}$. As a consequence, spline methods may be applied only in mollified versions, i.e., Gaussian sum approaches or (certain) mollified Hilbert spaces $Y_\varrho = A_\varrho[L^2(\mathcal{G})]$. Another spline variant for terrestrial observables involving derivatives is to introduce a Runge (Bjerhammar) ball $\mathcal{B}_R(0)$ inside $\mathcal{G}$, i.e., R is chosen such that $R < \inf_{x \in \partial\mathcal{G}} |x|$. In this case, terrestrial observables relative to $\mathcal{G}$ become inner observables relative to $(\mathcal{B}_R(0))^c$.

As prototypes for the different spline realizations we discuss *terrestrial oblique derivatives* (cf. Freeden 1987; Freeden and Gerhards 2013; Freeden and Kersten 1980, 1981; Freeden and Michel 2004), i.e., we asuume that there are known, for a point system $\{x_1, \ldots, x_N\} \subset \partial\mathcal{G}$, the linear functionals

$$\mathcal{D}_{x_i}[V] := \frac{\partial V}{\partial \lambda}(x_i) = \lambda(x_i) \cdot \nabla V(x_i) = \gamma_i, \quad i = 1, \ldots, N, \qquad (304)$$

where λ is a continuous unit vector field satisfying $\inf_{x \in \partial\mathcal{G}} \lambda(x) \cdot \nu(x) > 0$ and ν is the unit normal field on $\partial\mathcal{G}$ directed inward into $\mathcal{G}$. The occurrence of derivatives in (304) leads to the following spline variants:

RKHS mollification Let $\{x_1, \ldots, x_N\} \subset \partial\mathcal{G}$ be a point system, such that the functionals $\mathcal{D}_{x_1}, \ldots, \mathcal{D}_{x_N}$ are linearly independent. Then, within the set

$$\mathcal{I}_{\mathcal{D}_{x_1}, \ldots, \mathcal{D}_{x_N}}^V = \{U \in A_\varrho[L^2(\mathcal{G})] : \mathcal{D}_{x_i}[U] = \mathcal{D}_{x_i}[V] = \gamma_i, \ i = 1, \ldots, N\}, \quad (305)$$

the minimum norm interpolation problem of finding S_N^V *that satisfies*

$$\|S_N^V\|_{A_\varrho[L^2(\mathcal{G})]} = \inf_{U \in \mathcal{I}_{\mathcal{D}_{x_1}, \ldots, \mathcal{D}_{x_N}}^V} \|U\|_{A_\varrho[L^2(\mathcal{G})]} \qquad (306)$$

is well posed, i.e., its solution exists, is unique and depends continuously on the data $\gamma_1, \ldots, \gamma_N$. *The uniquely determined solution* S_N^V *is given in the explicit form*

$$S_N^V(x) = \sum_{i=1}^N a_i^N \mathcal{D}_{x_i}[K_{A_\varrho[L^2(\mathcal{G})]}(x, \cdot)], \quad x \in \mathbb{R}^3, \qquad (307)$$

where the coefficients $a_1^N, \ldots, a_N^N$ are determined by solving the linear system of equations

$$\sum_{i=1}^N a_i^N \mathcal{D}_{x_i} \mathcal{D}_{x_j} [K_{A_\varrho[L^2(\mathcal{G})]}(\cdot, \cdot)] = \gamma_j, \quad j = 1, \ldots, N. \tag{308}$$

RKHS Runge mollification Let $\{x_1, \ldots, x_N\} \subset \partial\mathcal{G}$ be a point system, such that the functionals $\mathcal{D}_{x_1}, \ldots, \mathcal{D}_{x_N}$ are linearly independent. Moreover, let $\mathcal{B}_R(0)$ be a Runge ball inside $\mathcal{G}$, i.e., let R be chosen such that $R < \inf_{x \in \partial\mathcal{G}} |x|$. Then, within the set

$$\mathcal{I}_{\mathcal{D}_{x_1}, \ldots, \mathcal{D}_{x_N}}^V = \{U \in A[L^2(\mathcal{B}_R(0)) : \mathcal{D}_{x_i}[U] = \mathcal{D}_{x_i}[V] = \gamma_i, \ i = 1, \ldots, N\}, \tag{309}$$

the minimum norm interpolation problem of finding S_N^V that satisfies

$$\|S_N^V\|_{A[L^2(\mathcal{B}_R(0)]} = \inf_{U \in \mathcal{I}_{\mathcal{E}_{x_1}, \ldots, \mathcal{E}_{x_N}}^V} \|U\|_{A[L^2(\mathcal{B}_R(0)]} \tag{310}$$

is well posed, i.e., its solution exists, is unique and depends continuously on the data $\gamma_1, \ldots, \gamma_N$. The uniquely determined solution S_N^V is given in the explicit form

$$S_N^V(x) = \sum_{i=1}^N a_i^N \mathcal{D}_{x_i} [K_{A[L^2(\mathcal{B}_R(0)]}(x, \cdot)], \quad x \in \mathbb{R}^3, \tag{311}$$

where the coefficients $a_1^N, \ldots, a_N^N$ are determined by solving the linear system of equations

$$\sum_{i=1}^N a_i^N \mathcal{D}_{x_i} \mathcal{D}_{x_j} [K_{A[L^2(\mathcal{B}_R(0)]}(\cdot, \cdot)] = \gamma_j, \quad j = 1, \ldots, N. \tag{312}$$

By going over to Gaussian sums we obtain the following variant:
RKHS Gaussian Runge mollification S_N^V admits a Gaussian sum approximation in the form

$$S_N^V(x) = \sum_{i=1}^N \tilde{a}_i^N \mathcal{D}_{x_i} [K_{A[L^2(\mathcal{B}_R(0)]}^M(x, \cdot)], \quad x \in \mathbb{R}^3, \tag{313}$$

where the coefficients $\tilde{a}_1^N, \ldots, \tilde{a}_N^N$ are determined by solving the linear system of equations

$$\sum_{i=1}^N \tilde{a}_i^N \mathcal{D}_{x_i} \mathcal{D}_{x_j} [K_{A[L^2(\mathcal{B}_R(0)]}(\cdot, \cdot)] = \gamma_j, \quad j = 1, \ldots, N. \tag{314}$$

These expressions are an immediate consequence of the aforementioned Runge reflected minimum norm formulation of spline interpolation to oblique derivative data.

A mollification procedure that formally simulates a minimum norm approach is as follows:

RKHS Gaussian Runge mollification S_N^V admits a Gaussian sum approximation in the form

$$S_N^V(x) = \sum_{i=1}^{N} \tilde{a}_i^N \mathcal{D}_{x_i}[K_{A[L^2(\mathcal{G})]}^M(x, \cdot)], \quad x \in \mathbb{R}^3, \tag{315}$$

where the coefficients $\tilde{a}_1^N, \ldots, \tilde{a}_N^N$ are determined by solving the linear system of equations

$$\sum_{i=1}^{N} \tilde{a}_i^N \mathcal{D}_{x_i} \mathcal{D}_{x_j}[K_{A[L^2(\mathcal{G})]}(\cdot, \cdot)] = \gamma_j, \quad j = 1, \ldots, N. \tag{316}$$

Other efficient spline solution techniques corresponding to oblique derivative data and involving fast multipole algorithms have been proposed by Gutting (2007, 2012, 2015).

6 Concluding remarks

Finally, it should be remarked that mathematical structures and results developed for the gravimetry problem enable us to apply not only new mollification techniques as presented here, but also a large variety of ideas and concepts known from the theory of ill-posed problems (see, e.g. Freeden and Nashed 2018a and the references therein for a geodetically relevant approach). These aspects, however, are straightforward, so that the details will not be considered here.

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