Sobolev scalar products in the construction of velocity models

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Summary

The Sobolev scalar products are defined, and discussed from the point of view of the application to model fitting and smoothing.

Keywords

Model specification, smoothing, inversion, wave propagation, ray methods.

1 Introduction

The Sobolev scalar product of two functions is a linear combination of the L_2 Lebesgue scalar products of the zero, first, second or higher derivatives of the functions. The linear combination should preserve the properties demanded on scalar products (symmetry and positiveness).

Note that if the linear combination defining the Sobolev scalar product does not contain the Lebesgue scalar product of the zero derivatives of the functions, the Sobolev scalar product of a constant function with any function is zero. In this case, the Sobolev scalar product is not positive–definite, but only positive–semidefinite. However, we may factorize the considered linear space of functions with respect to the space of functions keeping the Sobolev scalar product identical to zero. In the factor space, the Sobolev scalar product becomes positive–definite and the corresponding Sobolev seminorm becomes a norm. We will thus always speak of the "Sobolev norm", even in the situations where words "Sobolev seminorm" would be more appropriate.

Minimization of a Sobolev norm during the linearized inversion enables to control the model parameters unresolved by the data being fit. For example, if the interface is formed by a part of zero isosurface of a smooth function, the data tend just to minimize the deviations of the function from zero along the interface. In order not to obtain an entirely zero function, we have to fix the functional value at least at one point distant from the interface. The behaviour of the function at other parts of the model volume may then be controlled by minimizing the given Sobolev norm.

Even if a reasonably looking model can be obtained without minimizing a Sobolev norm, it may be too rough for some computational methods. The errors of many computational methods may be approximated by a function dependent on the Sobolev norms of functions describing the model. We may thus construct models optimally smooth for given computational methods.

Probably the smoothest models are required by the ray methods. In complex models, the behaviour of rays becomes chaotic and the geometrical spreading, number of arrivals and density of caustic surfaces are exponentially increasing with travel time. The exponential increment may be quantitatively described in terms of the "average

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Lyapunov exponent" for the model. The "average Lyapunov exponent" may be approximated by the square root of the corresponding Sobolev norm of the model. This enables to determine quantitative criteria on models, so as to be suitable for ray tracing, in terms of Sobolev scalar products. The criteria then allow to construct the optimum models of geological structures for ray tracing either by smoothing given rough models or by inversion of seismic data.

The aim of this introductory paper is to define the Sobolev scalar products, the corresponding matrices used in the last version of the SW3D software to specify the Sobolev scalar products, and to discuss the properties of various Sobolev norms from the point of view of the application of Sobolev norms to model fitting and smoothing.

Note that this preliminary version of the paper will require future revisions and extensions, because some analyses are not finished or included at all. For example, the study of the properties of interpolation between discrete values by minimizing the third derivatives is missing in Section 5.1.4, where the present version has been restricted to the first and second derivatives. Numerical examples and illustrations should be supplemented, too.

2 Sobolev scalar products

We define the Sobolev scalar product of functions f and g as

$$((f,g)) = \left[\int \mathrm{d}\mathbf{x}\right]^{-1} \sum_{ij\ldots} \sum_{ab\ldots} \int \mathrm{d}\mathbf{x}\; b_{ij\ldots|ab\ldots}\; f^*_{,ij\ldots}(x_p)\; g_{,ab\ldots}(x_q) \quad . \tag{1}$$

Note that the domain of integration is determined by the B-spline grid in the current SW3D Fortran code. It is limited by the outermost B-spline gridlines. The asterisk denoting complex–conjugacy is included just for completeness here. We shall consider real–valued functions and real–valued coefficients $b_{ij\ldots|ab\ldots}$ in this paper. Considering the symmetry of the scalar product, we assume that real–valued coefficients $b_{ij\ldots|ab\ldots}$ are symmetric with respect to the multiindices,

$$b_{ij\ldots|ab\ldots} = b_{ab\ldots|ij\ldots} \quad , \tag{2}$$

which is a special case of Hermitean complex–valued coefficients,

$$b_{ij\ldots|ab\ldots} = b^*_{ab\ldots|ij\ldots} \quad . \tag{3}$$

Considering the symmetry of the derivatives, we assume that coefficients $b_{ij\ldots|ab\ldots}$ are symmetric with respect to the permutation of indices $_{ij\ldots}$ and also $_{ab\ldots}$. To remove the corresponding multiplicity of indices $b_{ij\ldots|ab\ldots}$, we define coefficients $B_{IJK\,ABC}$ by equation

$$((f,g)) = \left[\int \mathrm{d}\mathbf{x}\right]^{-1} \sum_{IJK} \sum_{ABC} \int \mathrm{d}\mathbf{x}\; B_{IJK\,ABC}\; \frac{\partial^{I+J+K} f^*}{\partial x_1^I \partial x_2^J \partial x_3^K}\; \frac{\partial^{A+B+C} g}{\partial x_1^A \partial x_2^B \partial x_3^C} \quad . \tag{4}$$

We assume that real–valued coefficients $B_{IJK\,ABC}$ are symmetric with respect to the triplets of indices,

$$B_{IJK\,ABC} = B_{ABC\,IJK} \quad , \tag{5}$$

which is a special case of Hermitean complex–valued coefficients,

$$B_{IJK\,ABC} = B^*_{ABC\,IJK} \quad . \tag{6}$$

Coefficients $b_{ij\ldots|ab\ldots}$ and $B_{IJK\,ABC}$ are thus two equivalent representations of a particular Sobolev norm. For example,

$$B_{100\,100} = b_{1|1}\,,\ \ B_{002\,200} = b_{33|11}\,,\ \ B_{110\,110} = 4\,b_{12|12}\,,\ \ B_{121\,211} = 144\,b_{1223|1123}\ . \tag{7}$$

In this paper, we shall consider the coefficients constant with respect to spatial coordinates. Note that higher than the third derivatives should be avoided in the current SW3D Fortran code, because the corresponding Sobolev scalar products of cubic, bicubic or tricubic splines could be infinite, because the third homogeneous partial derivatives of the B-splines are discontinuous. We shall thus concentrate on the first, second and third derivatives.

2.1 Isotropic Sobolev scalar products

The isotropic Sobolev scalar products are invariant to rotations of coordinates. In this paper, we shall primarily concentrate on the isotropic Sobolev scalar products in order to decrease the number of independent coefficients specifying the scalar products. Anisotropic Sobolev scalar products can be obtained from the isotropic Sobolev scalar products by linear coordinate transformations. In this way, some of the properties of anisotropic Sobolev scalar products may be derived from the properties of the isotropic Sobolev scalar products.

Coefficients $b_{ij\ldots|ab\ldots}$ of the isotropic Sobolev scalar products form isotropic tensors. $b_{ij\ldots|ab\ldots}$ is an isotropic tensor if

$$U_{i'i}U_{j'j}\ \ldots\ U_{a'a}U_{b'b}\ \ldots\ b_{ij\ldots|ab\ldots} = b_{i'j'\ldots|a'b'\ldots} \tag{8}$$

for all unitary matrices U_{ij}. We shall list here linearly independent tensors $b_{ij\ldots|ab\ldots}$ of the respective symmetries, which generate the isotropic Sobolev scalar products composed of the first, second and third partial derivatives.

Scalar products

$$((f,g)) = \left[\int\!\mathrm{d}\mathbf{x}\right]^{-1} \int\!\mathrm{d}\mathbf{x} \sum_i f^*_{,i}\, g_{,i}\ , \quad ((f,g)) = \left[\int\!\mathrm{d}\mathbf{x}\right]^{-1} \int\!\mathrm{d}\mathbf{x} \sum_i \sum_j f^*_{,ij}\, g_{,ij}\ ,$$

$$((f,g)) = \left[\int\!\mathrm{d}\mathbf{x}\right]^{-1} \int\!\mathrm{d}\mathbf{x} \sum_i \sum_j \sum_k f^*_{,ijk}\, g_{,ijk}\ , \quad \ldots\ , \tag{9}$$

corresponding to the norms of the derivatives are described by coefficients

$$b^{11\mathrm{N}}_{ia} = \delta_{ia} \quad , \qquad b^{22\mathrm{N}}_{ijab} = \frac{1}{2}\delta_{\substack{ia\\ib}}\,\delta_{\substack{jb\\ja}} \quad , \qquad b^{33\mathrm{N}}_{ijkabc} = \frac{1}{6}\delta_{\substack{ia\\ia\\ib\\ib\\ic\\ic}}\,\delta_{\substack{jb\\jb\\ja\\ja\\ja\\ja}}\,\delta_{\substack{kc\\kc\\kc\\kc\\kb\\kb}} \quad , \qquad \ldots\ . \tag{10}$$

We introduced here the multiple rows of indices in order to make the equations more concise and easy to survey. For example,

$$\delta_{\substack{ia\\ib}}\,\delta_{\substack{jb\\ja}} \tag{11}$$

stands for

$$\delta_{ia}\delta_{jb} + \delta_{ib}\delta_{ja}\quad . \tag{12}$$

The coefficients are equivalently represented by matrix

$$
\mathbf{B}^{11\mathrm{N}} = \begin{array}{c} \\ \scriptstyle 100 \\ \scriptstyle 010 \\ \scriptstyle 001 \end{array}
\begin{array}{c} \begin{array}{ccc} \scriptstyle 100 & \scriptstyle 010 & \scriptstyle 001 \end{array} \\
\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{array}
\tag{13}
$$

stored in file "`sob11.dat`", matrix

$$
\mathbf{B}^{22\mathrm{N}} = \begin{array}{c|cccccc}
 & \scriptstyle 200 & \scriptstyle 020 & \scriptstyle 002 & \scriptstyle 011 & \scriptstyle 101 & \scriptstyle 110 \\
\hline
\scriptstyle 200 & 1 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 020 & 0 & 1 & 0 & 0 & 0 & 0 \\
\scriptstyle 002 & 0 & 0 & 1 & 0 & 0 & 0 \\
\scriptstyle 011 & 0 & 0 & 0 & 2 & 0 & 0 \\
\scriptstyle 101 & 0 & 0 & 0 & 0 & 2 & 0 \\
\scriptstyle 110 & 0 & 0 & 0 & 0 & 0 & 2
\end{array}
\tag{14}
$$

stored in file "`sob22n.dat`", and matrix

$$
\mathbf{B}^{33\mathrm{N}} = \begin{array}{c|cccccccccc}
 & \scriptstyle 300 & \scriptstyle 120 & \scriptstyle 102 & \scriptstyle 030 & \scriptstyle 210 & \scriptstyle 012 & \scriptstyle 003 & \scriptstyle 201 & \scriptstyle 021 & \scriptstyle 111 \\
\hline
\scriptstyle 300 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 120 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 102 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 030 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 210 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 012 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\
\scriptstyle 003 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
\scriptstyle 201 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\
\scriptstyle 021 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\
\scriptstyle 111 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6
\end{array}
\tag{15}
$$

stored in file "`sob33n.dat`", respectively.

Scalar products corresponding to the norms of the derivatives of the Laplace operator are described by coefficients

$$
b^{22\mathrm{L}}_{ijab} = \delta_{ij}\,\delta_{ab} \quad , \qquad b^{33\mathrm{L}}_{ijkabc} = \frac{1}{9}\delta_{\substack{ia\\ib\\ic\\ja\\jb\\jc\\ka\\kb\\kc}}\;\delta_{\substack{jk\\jk\\jk\\ik\\ik\\ik\\ij\\ij\\ij}}\;\delta_{\substack{bc\\ac\\ab\\bc\\ac\\ab\\bc\\ac\\ab}} \quad , \qquad \ldots \quad . \tag{16}
$$

The coefficients are equivalently represented by matrix

$$
\mathbf{B}^{22\mathrm{L}} = \begin{array}{c|cccccc}
 & \scriptstyle 200 & \scriptstyle 020 & \scriptstyle 002 & \scriptstyle 011 & \scriptstyle 101 & \scriptstyle 110 \\
\hline
\scriptstyle 200 & 1 & 1 & 1 & 0 & 0 & 0 \\
\scriptstyle 020 & 1 & 1 & 1 & 0 & 0 & 0 \\
\scriptstyle 002 & 1 & 1 & 1 & 0 & 0 & 0 \\
\scriptstyle 011 & 0 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 101 & 0 & 0 & 0 & 0 & 0 & 0 \\
\scriptstyle 110 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
\tag{17}
$$

stored in file "`sob221.dat`", and matrix

$$
\mathbf{B}^{33\mathrm{L}} = \begin{array}{rl}
 & \begin{array}{cccccccccc} 300 & 120 & 102 & 030 & 210 & 012 & 003 & 201 & 021 & 111 \end{array} \\
\begin{array}{c} 300 \\ 120 \\ 102 \\ 030 \\ 210 \\ 012 \\ 003 \\ 201 \\ 021 \\ 111 \end{array} &
\left(\begin{array}{cccccccccc}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right)
\end{array} \tag{18}
$$

stored in file "`sob331.dat`", respectively.

Lebesgue scalar product of a function times minus the Laplace operator is described by coefficients

$$
b^{02}_{|jk} = b^{20}_{jk|} = -\delta_{jk} \quad . \tag{19}
$$

The coefficients are equivalently represented by matrix

$$
\mathbf{B}^{02} = (\mathbf{B}^{20})^{\mathrm{T}} = \begin{array}{rl}
 & \begin{array}{ccc} 200 & 020 & 002 \end{array} \\
000 & \left(\begin{array}{ccc} -1 & -1 & -1 \end{array}\right)
\end{array} \quad . \tag{20}
$$

Lebesgue scalar product of the gradient times the gradient of minus the Laplace operator is described by coefficients

$$
b^{13}_{i|abc} = b^{31}_{abc|i} = -\frac{1}{3}\delta_{\substack{ia\\ib\\ic}}\,\delta_{\substack{bc\\ac\\ab}} \quad . \tag{21}
$$

The coefficients are equivalently represented by matrix

$$
\mathbf{B}^{13} = (\mathbf{B}^{31})^{\mathrm{T}} = \begin{array}{rl}
 & \begin{array}{cccccccccc} 300 & 120 & 102 & 030 & 210 & 012 & 003 & 201 & 021 & 111 \end{array} \\
\begin{array}{c} 100 \\ 010 \\ 001 \end{array} &
\left(\begin{array}{cccccccccc}
-1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & 0
\end{array}\right)
\end{array} \quad . \tag{22}
$$

A general isotropic Sobolev scalar product composed of the first partial derivatives is described by matrix $S^2\mathbf{B}^{11}$, where S is the scaling factor.

A general isotropic Sobolev scalar product composed of the second partial derivatives is described by matrix $S^2\mathbf{B}^{22}(L)$, where

$$
\mathbf{B}^{22}(L) = (1-L)\mathbf{B}^{22\mathrm{N}} + L\mathbf{B}^{22\mathrm{L}} \quad , \tag{23}
$$

with

$$
-\tfrac{1}{2} \le L^{(3\mathrm{D})} \le 1 \tag{24}
$$

in 3-D and

$$
-1 \le L^{(2\mathrm{D})} \le 1 \tag{25}
$$

in 2-D to keep matrix $\mathbf{B}^{22}(L)$ positive–semidefinite. There is no difference between matrices $\mathbf{B}^{22\mathrm{N}}$, $\mathbf{B}^{22\mathrm{L}}$ and $\mathbf{B}^{22}(L)$ in 1-D.

A general isotropic Sobolev scalar product composed of the third partial derivatives is described by matrix $S^2\mathbf{B}^{33}(L)$, where

$$\mathbf{B}^{33}(L) = (1-L)\mathbf{B}^{33\mathrm{N}} + L\mathbf{B}^{33\mathrm{L}} \quad , \tag{26}$$

with

$$-\tfrac{3}{2} \le L^{(3\mathrm{D})} \le 1 \tag{27}$$

in 3-D and

$$-3 \le L^{(2\mathrm{D})} \le 1 \tag{28}$$

in 2-D to keep matrix $\mathbf{B}^{33}(L)$ positive–semidefinite. There is no difference between matrices $\mathbf{B}^{33\mathrm{N}}$, $\mathbf{B}^{33\mathrm{L}}$ and $\mathbf{B}^{33}(L)$ in 1-D.

2.2 Completely symmetric tensors of coefficients

When smoothing the model for particular computational methods, we often encounter tensors obtained by averaging a unit vector over all directions,

$$b^{11}_{i|a} = \langle e_i e_a \rangle \quad , \tag{29}$$

$$b^{22}_{ij|ab} = \langle e_i e_j e_a e_b \rangle \quad , \tag{30}$$

$$b^{33}_{ijk|abc} = \langle e_i e_j e_k e_a e_b e_c \rangle \quad . \tag{31}$$

Here e_i is a unit vector and $\langle ... \rangle$ means averaging over all possible directions of the unit vector.

The averages over directions can be calculated analytically. In 2-D, we obtain

$$\langle (e_1)^{2K} (e_2)^{2M} \rangle = \frac{1\cdot 3\cdot \ldots \cdot (2K-1) \cdot 1\cdot 3 \cdot \ldots \cdot (2M-1)}{2\cdot 4 \cdot \ldots \cdot (2K+2M)} \quad . \tag{32}$$

In 3-D, we have

$$\langle (e_1)^{2K} (e_2)^{2M} (e_3)^{2N} \rangle = \frac{1\cdot 3\cdot \ldots \cdot (2K-1) \cdot 1\cdot 3 \cdot \ldots \cdot (2M-1) \cdot 1\cdot 3 \cdot \ldots \cdot (2N-1)}{3\cdot 5 \cdot \ldots \cdot (2K+2M+2N+1)} \quad . \tag{33}$$

Generally in d-D for $d=1$, $d=2$ or $d=3$, we may write

$$\langle (e_1)^{2K} (e_2)^{2M} (e_3)^{2N} \rangle = \frac{1\cdot 3\cdot \ldots \cdot (2K-1) \cdot 1\cdot 3 \cdot \ldots \cdot (2M-1) \cdot 1\cdot 3 \cdot \ldots \cdot (2N-1)}{d\cdot (d+2) \cdot \ldots \cdot (d+2K+2M+2N-2)} \quad . \tag{34}$$

Completely symmetric tensor (29) may then be expressed as

$$b^{11}_{i|a} = \frac{b^{11\mathrm{N}}_{i|a}}{d} \quad . \tag{35}$$

These coefficients are represented by matrices

$$\mathbf{B}^{11(1\mathrm{D})} = \mathbf{B}^{11\mathrm{N}} \quad , \qquad \mathbf{B}^{11(2\mathrm{D})} = \frac{1}{2}\mathbf{B}^{11(1\mathrm{D})} \quad , \qquad \mathbf{B}^{11(3\mathrm{D})} = \frac{1}{3}\mathbf{B}^{11(1\mathrm{D})} \quad . \tag{36}$$

Completely symmetric tensor (30) may be expressed as

$$b^{22}_{ij|ab} = \frac{2\, b^{22\mathrm{N}}_{ij|ab} + b^{22\mathrm{L}}_{ij|ab}}{d\,(d+2)} \quad . \tag{37}$$

The coefficients are represented by matrices

$$\mathbf{B}^{22(1\mathrm{D})} = \frac{2}{3}\mathbf{B}^{22\mathrm{N}} + \frac{1}{3}\mathbf{B}^{22\mathrm{L}} \quad , \qquad \mathbf{B}^{22(2\mathrm{D})} = \frac{3}{8}\mathbf{B}^{22(1\mathrm{D})} \quad , \qquad \mathbf{B}^{22(3\mathrm{D})} = \frac{1}{5}\mathbf{B}^{22(1\mathrm{D})} \quad . \tag{38}$$

Matrix

$$\mathbf{B}^{22(1\mathrm{D})} = \begin{array}{c} \\ \scriptstyle 200 \\ \scriptstyle 020 \\ \scriptstyle 002 \\ \scriptstyle 011 \\ \scriptstyle 101 \\ \scriptstyle 110 \end{array} \begin{array}{c} \begin{array}{cccccc} \scriptstyle 200 & \scriptstyle 020 & \scriptstyle 002 & \scriptstyle 011 & \scriptstyle 101 & \scriptstyle 110 \end{array} \\ \begin{pmatrix} 1 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & 1 & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{4}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{4}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{4}{3} \end{pmatrix} \end{array} \quad , \tag{39}$$

stored in file "`sob22.dat`", is a special case of matrix $\mathbf{B}^{22}(L)$ for

$$L = \frac{1}{3} \quad . \tag{40}$$

Completely symmetric tensor (31) may be expressed as

$$b^{33}_{ijk|abc} = \frac{6\ b^{33\mathrm{N}}_{ijk|abc} + 9\ b^{33\mathrm{L}}_{ijk|abc}}{d\,(d+2)\,(d+4)} \quad . \tag{41}$$

The coefficients are represented by matrices

$$\mathbf{B}^{33(1\mathrm{D})} = \frac{2}{5}\mathbf{B}^{33\mathrm{N}} + \frac{3}{5}\mathbf{B}^{33\mathrm{L}} \quad , \qquad \mathbf{B}^{33(2\mathrm{D})} = \frac{5}{16}\mathbf{B}^{33(1\mathrm{D})} \quad , \qquad \mathbf{B}^{33(3\mathrm{D})} = \frac{1}{7}\mathbf{B}^{33(1\mathrm{D})} \quad . \tag{42}$$

Matrix

$$\mathbf{B}^{33(1\mathrm{D})} = \begin{array}{c} \\ \scriptstyle 300 \\ \scriptstyle 120 \\ \scriptstyle 102 \\ \scriptstyle 030 \\ \scriptstyle 210 \\ \scriptstyle 012 \\ \scriptstyle 003 \\ \scriptstyle 201 \\ \scriptstyle 021 \\ \scriptstyle 111 \end{array} \begin{array}{c} \begin{array}{cccccccccc} \scriptstyle 300 & \scriptstyle 120 & \scriptstyle 102 & \scriptstyle 030 & \scriptstyle 210 & \scriptstyle 012 & \scriptstyle 003 & \scriptstyle 201 & \scriptstyle 021 & \scriptstyle 111 \end{array} \\ \begin{pmatrix} 1 & \frac{3}{5} & \frac{3}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{5} & \frac{9}{5} & \frac{3}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{5} & \frac{3}{5} & \frac{9}{5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \frac{3}{5} & \frac{3}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{5} & \frac{9}{5} & \frac{3}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{5} & \frac{3}{5} & \frac{9}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & \frac{3}{5} & \frac{3}{5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{5} & \frac{9}{5} & \frac{3}{5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{5} & \frac{3}{5} & \frac{9}{5} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{12}{5} \end{pmatrix} \end{array} \quad , \tag{43}$$

stored in file "`sob33.dat`", is a special case of matrix $\mathbf{B}^{33}(L)$ for

$$L = \frac{3}{5} \quad . \tag{44}$$

3 Objective function with the Sobolev norm for inversion of seismic data

The Sobolev norm is usually included into the inversion of seismic data (e.g., of travel times) if the numerical method to be applied to the model requires a smooth model. We assume the objective function for the inversion of slowness or velocity $u(\mathbf{x})$ in the form of

$$y = \left[\int \mathrm{d}\mathbf{x}\right]^{-1} \int \mathrm{d}\mathbf{x}\, C(\mathbf{x},\mathbf{x}) + S^2((\tilde{u},\tilde{u})) \quad , \tag{45}$$

where

$$\tilde{C}(\mathbf{x},\mathbf{x}') = <[\tilde{u}(\mathbf{x}) - u(\mathbf{x})][\tilde{u}(\mathbf{x}') - u(\mathbf{x}')]> \tag{46}$$

is the covariance function describing the deviation of the model $\tilde{u}(\mathbf{x})$ from the geological structure $u(\mathbf{x})$ (Klimeš 1997a), and S is the scaling factor of the Sobolev norm.

If u represents the propagation velocity or slowness, the first term in (45) is related to the local relative travel–time standard deviation $\rho\tau_{\mathrm{model}}(\mathbf{x})$ describing the difference between the model and geological structure,

$$\tilde{C}(\mathbf{x},\mathbf{x}) = [\tilde{u}(\mathbf{x})\ \rho\tau_{\mathrm{model}}(\mathbf{x})]^2 \quad . \tag{47}$$

It is then advantageous if the inaccuracy of the numerical method under consideration can be approximately characterized by the local relative travel–time standard deviation $\rho\tau(\mathbf{x})$ describing the difference between the exact and numerical results in the model, and if the square $[\rho\tau(\mathbf{x})]^2$ of the deviation bilinearly depends on the derivatives of the interpolated parameter (slowness or velocity),

$$[\rho\tau(\mathbf{x})\ \tilde{u}(\mathbf{x})]^2 \approx S^2\, b_{ij...|ab...}\ \tilde{u}_{,ij...}(\mathbf{x})\ \tilde{u}_{,ab...}(\mathbf{x}) \quad . \tag{48}$$

The Sobolev scalar product is then defined by coefficients $b_{ij...|ab...}$ from approximation (48) and the objective function (45) has a clear physical meaning.

If the square

$$[\overline{\rho\tau}]^2 = \left[\int \mathrm{d}\mathbf{x}\right]^{-1} \int \mathrm{d}\mathbf{x}\, [\rho\tau(\mathbf{x})]^2 \tag{49}$$

of the relative deviation, averaged over the model volume, is not proportional to the square $((\tilde{u},\tilde{u}))$ of any Sobolev norm, but can still be expressed as a function of the square of a Sobolev norm,

$$[\rho\tau(\mathbf{x})\ \tilde{u}(\mathbf{x})]^2 \approx F\,[((\tilde{u},\tilde{u}))] \quad , \tag{50}$$

objective function

$$y = \left[\int \mathrm{d}\mathbf{x}\right]^{-1} \int \mathrm{d}\mathbf{x}\, C(\mathbf{x},\mathbf{x}) + F\,[((\tilde{u},\tilde{u}))] \tag{51}$$

is no longer bilinear with respect to the model parameters, but can be iteratively approximated by the bilinear one. We denote $\tilde{u}$ from the previous iteration by $\tilde{u}_0$ and approximate $F\,[((\tilde{u},\tilde{u}))]$ by the linear Taylor expansion from $((\tilde{u}_0,\tilde{u}_0))$,

$$F\,[((\tilde{u},\tilde{u}))] \approx F\,[((\tilde{u}_0,\tilde{u}_0))] + F'\,[((\tilde{u}_0,\tilde{u}_0))]\ \ [((\tilde{u},\tilde{u})) - ((\tilde{u}_0,\tilde{u}_0))] \quad . \tag{52}$$

Objective function (51) can then be approximated in each iteration by bilinear objective function (45) with

$$S^2 = F'\,[((\tilde{u}_0,\tilde{u}_0))] \quad . \tag{53}$$

We shall now illustrate selection of the Sobolev scalar products by examples related to particular numerical methods.

3.1 Centred finite differences of the second order

Let us consider the full–wave elastic centred finite differences of the second order in $d \le 3$ dimensions. Assume that $\tilde{u}$ represents slowness. The most important component

$$\Delta^{(1)}_{\max} \approx \frac{\omega^2 h^2 \tilde{u}^2}{24} \tag{54}$$

(Klimeš 1996a, eqs. 108, 110) of the relative travel–time error corresponding to the grid dispersion along gridlines is independent of the model smoothness. Here ω is the circular frequency and h is the finite–difference grid step. The error component dependent on the first slowness derivatives is

$$\Delta^{(2)} \approx -\frac{\omega h^2}{6} \sum_{i=1}^{d} \tilde{u}_{,i} [e_i]^3 \tag{55}$$

(Klimeš 1996a, eq. 143), where e_i is a unit vector in the direction of propagation. The relevant Sobolev norm is then characterized by coefficients

$$S^2 b_{i|a} = \frac{\omega^2 h^4 \tilde{u}^2}{36} \langle (e_i)^3 (e_a)^3 \rangle = \frac{15 \omega^2 h^4 \tilde{u}^2}{36\ d\ (d+2)\ (d+4)} b^{11\mathrm{N}}_{i|a} \quad . \tag{56}$$

i.e.,

$$S^2 b_{i|a} \approx \frac{10 h^2 \Delta^{(1)}_{\max}}{d\ (d+2)\ (d+4)} b^{11(1\mathrm{D})}_{i|a} \quad . \tag{57}$$

The error component dependent on the third slowness derivatives is

$$\Delta^{(3)} \approx -\frac{h^2}{6 \omega \tilde{u}^2} \sum_{i=1}^{d} \tilde{u}_{,iii} e_i \tag{58}$$

(Klimeš 1996a, eq. 150), where we neglected the product of the first and second partial derivatives. The relevant Sobolev norm is not isotropic, but can be limited from above by the isotropic Sobolev norm characterized by coefficients

$$S^2 b_{ijk|abc} = \left[\frac{h^2}{6 \omega \tilde{u}} \right]^2 b^{33\mathrm{N}}_{ijk|abc} \quad . \tag{59}$$

The Sobolev norms approximating errors of other finite–difference schemes may be derived analogously.

3.2 Network shortest–path ray tracing

Let us consider the network shortest–path ray tracing in $d \le 3$ dimensions according to Klimeš & Kvasnička (1994). The relative travel–time error is roughly proportional to the square root of the isotropic Sobolev norm of the second slowness derivatives. The iterative minimization of an objective function of kind (51) thus takes place. We may use equations by Klimeš & Kvasnička (1994) to approximately estimate the explicit dependence of the relative travel–time error $\rho\tau$ on the Sobolev norm and use (53) with $F[((\tilde{u}, \tilde{u}))] = c\sqrt{((\tilde{u}, \tilde{u}))}$, where c is the relevant constant. Here we present an analogous approach, in which the numerical calculations performed by the network ray tracing program "`net.for`" substitute rough analytical approximations. This leads to much simpler derivation and to more accurate determination of scaling constant (53).

The relative trave–time error dependent on the second slowness derivatives is

$$\rho\tau_2 \approx \frac{h^2 N_{\rm FS}^2}{12\tilde{u}} \tilde{u}_{,ij} e_i e_j \tag{60}$$

(Klimeš & Kvasnička 1994, eq. 26), where e_i is a unit vector in the direction of propagation, h is the grid step and $N_{\rm FS}$ is the size of the forward star. The relevant Sobolev norm is then characterized by coefficients

$$S^2 b_{ij|ab} = \frac{h^4 \langle N_{\rm FS}^4 \rangle}{144} \langle e_i e_j e_a e_b \rangle \quad , \tag{61}$$

i.e.,

$$S^2 b_{ij|ab} = \frac{h^4 \langle N_{\rm FS}^4 \rangle}{48\, d\, (d+2)} b_{ij|ab}^{22(\rm 1D)} \quad . \tag{62}$$

We calculate $\langle N_{\rm FS}^4 \rangle$ in the model resulting from the previous iteration. Gridded forward–star size $N_{\rm FS}$ can be calculated by program "`net.for`", and average $\langle N_{\rm FS}^4 \rangle$ over the whole grid can be calculated by program "`grdnorm.for`".

3.3 First–arrival travel times by 2-D Podvin's method

The local relative travel–time error of the 2-D first–order travel–time tracing method of Podvin & Lecomte (1991) due to the first slowness derivatives is

$$\rho\tau \approx -\frac{h}{2\tilde{u}} \big| |e_2| - |e_1| \big| T_{12} \tag{63}$$

(Klimeš 1996b, eq. 82), where

$$T_{12} = |e_1|^3 \tilde{u}_{,2} \mathrm{sgn}(e_2) + |e_2|^3 \tilde{u}_{,1} \mathrm{sgn}(e_1) \tag{64}$$

(Klimeš 1996b, eq. 83). Here e_i is a unit vector in the direction of propagation. Then

$$(\rho\tau)^2 \approx \left[\frac{h}{2\tilde{u}}\right]^2 \left[(e_1)^2 - 2|e_1 e_2| + (e_2)^2\right] \left[(e_1)^6 (\tilde{u}_{,2})^2 + 2(e_1)^3 (e_2)^3 \tilde{u}_{,1} \tilde{u}_{,2} + (e_2)^6 (\tilde{u}_{,1})^2\right] \ . \tag{65}$$

The relevant Sobolev norm is then characterized by coefficients

$$S^2 b_{i|a} = \frac{h^2}{4} \langle [(e_1)^2 - 2|e_1 e_2| + (e_2)^2] (e_i)^3 (e_a)^3 \rangle \quad . \tag{66}$$

Inserting (32) and

$$\langle |e_1| |e_2|^7 \rangle = \frac{1}{4\pi} \quad , \tag{67}$$

we arrive at

$$S^2 b_{i|a} = \frac{h^2}{4} \left[\frac{35}{128} - \frac{2}{4\pi} + \frac{5}{128}\right] b_{i|a}^{11(\rm 1D)} \quad , \tag{68}$$

which reads

$$S^2 b_{i|a} = \frac{h^2}{8} \left[\frac{5}{8} - \frac{1}{\pi}\right] b_{i|a}^{11(\rm 1D)} \quad . \tag{69}$$

3.4 2-D second–order grid travel time tracing

The local relative travel–time error of the 2-D second–order grid travel–time tracing method of Klimeš (1996b) due to the second slowness derivatives is

$$\rho\tau \approx \frac{h^2}{12\tilde{u}}\left[3\tilde{u}_{,11}\left|\frac{e_1}{e_2}\right| - 2\tilde{u}_{,11}\left|\frac{e_1}{e_2}\right|^2 + \tilde{u}_{,22} + 2\tilde{u}_{,12}\frac{e_1}{e_2}\right] \tag{70}$$

(Klimeš 1996b, eq. 73) for $|e_1| \leq |e_2|$. For $|e_1| \geq |e_2|$, subscripts $_1$ and $_2$ in (70) have to be exchanged. Here e_i is a unit vector in the direction of propagation. The relevant Sobolev norm is then characterized by coefficients

$$S^2 b_{11|11} = S^2 b_{22|22} = \left[\frac{h^2}{12}\right]^2 \left\{\frac{1}{2} + \frac{2}{\pi}\int_0^{\frac{\pi}{4}} \left[9\tan^2\alpha - 12\tan^3\alpha + 4\tan^4\alpha\right] \mathrm{d}\alpha\right\} \quad , \tag{71}$$

$$S^2 b_{11|22} = \left[\frac{h^2}{12}\right]^2 \frac{4}{\pi}\int_0^{\frac{\pi}{4}} \left[3\tan\alpha - 2\tan^2\alpha\right] \mathrm{d}\alpha \quad , \tag{72}$$

$$S^2 b_{12|12} = \left[\frac{h^2}{12}\right]^2 \frac{4}{\pi}\int_0^{\frac{\pi}{4}} \tan^2\alpha \; \mathrm{d}\alpha \tag{73}$$

and

$$S^2 b_{11|12} = S^2 b_{22|12} = 0 \quad . \tag{74}$$

Calculating the above integrals, we arrive at

$$S^2 b_{11|11} = S^2 b_{22|22} = \left[\frac{h^2}{12}\right]^2 \left\{\frac{1}{2} + \frac{2}{\pi}\left[9\left(1 - \frac{\pi}{4}\right) - 12\left(\frac{1}{2} - \frac{1}{2}\ln 2\right) + 4\left(-\frac{2}{3} + \frac{\pi}{4}\right)\right]\right\} \quad , \tag{75}$$

$$S^2 b_{11|22} = \left[\frac{h^2}{12}\right]^2 \frac{4}{\pi}\left[3\frac{1}{2}\ln 2 - 2\left(1 - \frac{\pi}{4}\right)\right] \tag{76}$$

and

$$S^2 b_{12|12} = \left[\frac{h^2}{12}\right]^2 \frac{4}{\pi}\left[1 - \frac{\pi}{4}\right] \quad . \tag{77}$$

After rearranging the terms, these equations read

$$S^2 b_{11|11} = S^2 b_{22|22} = \left[\frac{h^2}{12}\right]^2 \left[\frac{2}{3\pi} + \frac{12\ln 2}{\pi} - 2\right] = \left[\frac{h^2}{12}\right]^2 0.860 \quad , \tag{78}$$

$$S^2 b_{11|22} = \left[\frac{h^2}{12}\right]^2 \left[\frac{6\ln 2}{\pi} - \frac{8}{\pi} + 2\right] = \left[\frac{h^2}{12}\right]^2 0.777 \tag{79}$$

and

$$S^2 b_{12|12} = \left[\frac{h^2}{12}\right]^2 \left[\frac{4}{\pi} - 1\right] = \left[\frac{h^2}{12}\right]^2 0.273 \quad . \tag{80}$$

This Sobolev norm is not isotropic, but is close, e.g., to isotropic Sobolev norm (14) with $L = \frac{2}{3}$, which has $b^{22}_{11|11}(\frac{2}{3}) = b^{22}_{22|22}(\frac{2}{3}) = 1$, $b^{22}_{11|22}(\frac{2}{3}) = \frac{2}{3}$ and $b^{22}_{12|12}(\frac{2}{3}) = \frac{1}{6}$,

$$S^2 b_{ij|ab} \approx \left[\frac{h^2}{12}\right]^2 b^{22}(\tfrac{2}{3})_{ij|ab} \quad . \tag{81}$$

3.5 Lyapunov exponents for ray tracing

Unfortunately, we still have no quantitative criteria of applicability and accuracy of ray methods or their extensions. On the other hand, the feasibility and efficiency of ray tracing puts relatively strong requirements on the smoothness of the velocity models.

In complex models, the behaviour of rays becomes chaotic and the geometrical spreading, number of arrivals and density of caustic surfaces are exponentially increasing with travel time. The exponential increment may be quantitatively described in terms of the "average Lyapunov exponent" $\overline{\lambda}$ for the model. The "average Lyapunov exponent" may roughly be approximated by the square root of the corresponding Sobolev norm of the model. This enables to determine quantitative criteria on models, so as to be suitable for ray tracing, in terms of Sobolev scalar products.

A 2-D numerical example by Klimeš (1999b, 2000) suggests that the average number $\overline{N}$ of travel times for a point source is increasing with travel time τ approximately as

$$\overline{N} = \tfrac{1}{2}\exp(\overline{\lambda}\tau) \quad . \tag{82}$$

The maximum number of travel times seems to be roughly twice greater. If we wish average number $\overline{N}$ of travel times at travel time $\tau_{\rm max}$ not to exceed $\overline{N}_{\rm max}$, we need

$$\overline{\lambda} \le \frac{\ln \overline{N}_{\rm max} + \ln 2}{\tau_{\rm max}} \quad . \tag{83}$$

According to equation (51) of Klimeš (1999b), the average Lyapunov exponent may be approximated by

$$\overline{\lambda} \approx \overline{\Lambda} + \overline{\Delta\Phi} \quad , \tag{84}$$

where

$$\overline{\Lambda} = (d-1)\left[\int\!{\rm d}\mathbf{x}\; v^{-1}\right]^{-1} \int\!{\rm d}\mathbf{x}\; \sqrt{{\rm neg}(v_{,ij})e_i e_j v^{-1}} \quad , \tag{85}$$

and $\overline{\Delta\Phi}$ is the compensation for the defocusing low–velocity zones. Here e_i is a unit vector perpendicular to the direction of propagation. We assume that the model is so smooth that there is a small number $K_{\rm osc}$ of velocity oscillations along rays of length corresponding to $\tau_{\rm max}$,

$$K_{\rm osc} = \frac{\tau_{\rm max}}{\overline{\tau}_{\rm osc}} \quad , \tag{86}$$

where $\overline{\tau}_{\rm osc}$ is the average wavelength of the velocity oscillations in the smoothed model, expressed in the travel–time units. Under this assumption, equation (51) of Klimeš (1999b) allows for approximation

$$\overline{\Delta\Phi} \approx -\frac{\ln 2}{\overline{\tau}_{\rm osc}} = -\frac{K_{\rm osc}\ln 2}{\tau_{\rm max}} \quad . \tag{87}$$

Considering inequality (83) with approximations (84) and (87), we require

$$\overline{\Lambda} \le \frac{\ln \overline{N}_{\rm max} + K\ln 2}{\tau_{\rm max}} \quad , \tag{88}$$

where

$$K = K_{\rm osc} + 1 \tag{89}$$

for a point source. On the other hand,

$$K = K_{\rm osc} + 2 \tag{90}$$

for a prestack depth migration, where we shoot rays both from sources and receivers, $\overline{N}_{\max}$ corresponds to the product of the numbers of travel times calculated from both points and $\tau_{\max}$ is the reference (maximum) sum of travel times to the target zone. Note that we still speak about a 2-D case, $d=2$. Equations in the remaining part of this section are derived only for $d=2$, but their applicability to $d=3$ have not been excluded yet. We now perform several successive approximations to express $\overline{\Lambda}$ in terms of the Sobolev norm of slowness u in the model without interfaces,

$$\overline{\Lambda} \approx (d-1) \left[\int \mathrm{d}\mathbf{x}\ u \right]^{-1} \int \mathrm{d}\mathbf{x}\ \sqrt{\mathrm{pos}(u_{,ij}) e_i e_j u^{-1}} \quad , \tag{91}$$

$$\overline{\Lambda} \approx \frac{d-1}{2} \left[\int \mathrm{d}\mathbf{x}\ u^{\frac{3}{2}} \right]^{-1} \int \mathrm{d}\mathbf{x}\ \sqrt{|u_{,ij} e_i e_j|} \quad , \tag{92}$$

and

$$\overline{\Lambda} \approx \frac{d-1}{2} [u_0]^{-\frac{3}{2}} \left\{ \left[\int \mathrm{d}\mathbf{x} \right]^{-1} \int \mathrm{d}\mathbf{x}\ (u_{,ij} e_i e_j)^2 \right\}^{\frac{1}{4}} \quad , \tag{93}$$

where

$$u_0 = \left\{ \left[\int \mathrm{d}\mathbf{x} \right]^{-1} \int \mathrm{d}\mathbf{x}\ u^{\frac{3}{2}} \right\}^{\frac{3}{2}} \quad . \tag{94}$$

Calculating average (30) over the directions of e_i, we arrive at

$$\overline{\Lambda} \approx \frac{d-1}{2} \left[\frac{3}{d\,(d+2)} \right]^{\frac{1}{4}} u_0^{-\frac{3}{2}} \sqrt{\|u\|} \quad , \tag{95}$$

where Sobolev norm $\|u\|$ is given by matrix $\mathbf{B} = \mathbf{B}^{22(1\mathrm{D})}$, see (37). This approximation may also be expressed as

$$\|u\|^2 \approx u_0^2\, \frac{d\,(d+2)}{3} \left[\frac{2}{d-1}\ \overline{\Lambda} u_0 \right]^4 \quad . \tag{96}$$

In terms of propagation velocity v, we arrive at analogous approximations

$$\overline{\Lambda} \approx \frac{d-1}{2} \left[\frac{3}{d\,(d+2)} \right]^{\frac{1}{4}} v_0^{\frac{1}{2}} \sqrt{\|v\|} \tag{97}$$

and

$$\|v\|^2 \approx v_0^2\, \frac{d\,(d+2)}{3} \left[\frac{2}{d-1}\, \frac{\overline{\Lambda}}{v_0} \right]^4 \quad , \tag{98}$$

where the same Sobolev norm as for slowness is used and

$$v_0 = \left\{ \left[\int \mathrm{d}\mathbf{x} \right]^{-1} \int \mathrm{d}\mathbf{x}\ v^{-\frac{1}{2}} \right\}^{-2} \quad . \tag{99}$$

The presented approximations allow to construct the models of geological structures, optimum for ray tracing, by smoothing given rough models or by inversion of seismic data.

3.6 Paraxial ray methods

There are errors of ray and similar high–frequency asymptotic methods, which are related to neglected derivatives in the Taylor expansion of travel time.

For example, if the geometrical spreading is large, the distance between a receiver and the best two–point ray corresponds to the geometrical spreading times the smallest step in ray parameters. The error of travel–time, linearly extrapolated from the ray endpoint, may then be related to the neglected second travel–time derivatives in the Taylor expansion.

Paraxial Gaussian beams may be used as another example. The error of their complex–valued travel time may be related to the neglected third travel–time derivatives at the distances corresponding to the half–width of the beams. The half–width of the Gaussian beams is proportional to the "norm" of their complex–valued geometrical spreading.

In general, we may consider the travel–time error proportional to the N^{th} travel–time derivatives times the N^{th} power of the geometrical spreading. The product of N^{th} travel–time derivatives with the N^{th} power of the geometrical spreading is roughly proportional to the ray length times the Sobolev norm of the N^{th} slowness derivatives times the N^{th} power of the geometrical spreading averaged along rays (Klimeš 1997b, 1999a).

4 Fitting known structure by a smooth model — wavenumber filtering

Let us assume here that we know the structure $u(\mathbf{x})$ and wish to approximate it by a smooth model $\tilde{u}(\mathbf{x})$. Then the objective function is analogous to (45),

$$y = \left[\int \mathrm{d}\mathbf{x}\right]^{-1} \int \mathrm{d}\mathbf{x}\, |\tilde{u}(\mathbf{x}) - u(\mathbf{x})|^2 + S^2(\!(\tilde{u},\tilde{u})\!) \quad . \tag{100}$$

If we neglect the boundary effects due to the limited model volume, we may express the equivalent objective function in the wavenumber domain as

$$\widehat{y} = \int \mathrm{d}\mathbf{k} |\widehat{\tilde{u}}(\mathbf{k}) - \widehat{u}(\mathbf{k})|^2 + \sum_{ij\ldots} \sum_{ab\ldots} \int \mathrm{d}\mathbf{k}\; S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots\; |\widehat{\tilde{u}}(\mathbf{k})|^2 \; . \tag{101}$$

The objective function is minimized by smoothed model

$$\widehat{\tilde{u}}(\mathbf{k}) = \frac{1}{1 + S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots} \widehat{u}(\mathbf{k}) \quad . \tag{102}$$

We see that the Sobolev norm included in the objective function acts as a low–pass wavenumber filter. The difference between the model and the given structure is

$$\widehat{\tilde{u}}(\mathbf{k}) - \widehat{u}(\mathbf{k}) = \frac{-S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots}{1 + S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots} \widehat{u}(\mathbf{k}) \quad . \tag{103}$$

Squared Lebesgue L_2 norm of the difference is proportional to

$$\int \mathrm{d}\mathbf{k} |\widehat{\tilde{u}}(\mathbf{k}) - \widehat{u}(\mathbf{k})|^2 = \int \mathrm{d}\mathbf{k} \frac{[S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots]^2}{[1 + S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots]^2} |\widehat{u}(\mathbf{k})|^2 \quad , \tag{104}$$

and the squared Sobolev norm of the smoothed model is proportional to

$$\int \mathrm{d}\mathbf{k}\; b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots\; |\widehat{\tilde{u}}(\mathbf{k})|^2 = \int \mathrm{d}\mathbf{k} \frac{b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots}{[1 + S^2 b_{ij\ldots|ab\ldots}\; k_i k_j\; \ldots\; k_a k_b\; \ldots]^2} |\widehat{u}(\mathbf{k})|^2 \; . \tag{105}$$

5 Regularization of ill–conditioned inversion

Typical example of strongly ill–conditioned inversion is fitting structural interface by implicit function. Assume that the discrete points at the interface are given and that the interface cannot be fitted by explicit function, e.g., as $x_3 = w(x_1, x_2)$, but has to be described as the zero isosurface of function $f(x_1, x_2, x_3)$. We then minimize the deviations of function $f(x_1, x_2, x_3)$ from zero at the given points. Without additional a priori requirements, we would thus obtain an entirely zero function. One of agreeable requirements is to fix the functional value at a specified point and to minimize the square of a suitable Sobolev norm. The specified point should be sufficiently distant from the interface. For the closed surface, it may be located inside the block limited by the surface.

To understand the properties of various Sobolev scalar products, we shall demonstrate them on a rotationally symmetric analytical example.

5.1 Rotationally symmetric analytical example

Assume the spherical (circular in 2-D) surface of radius 1 inside the spherical (circular in 2-D) model volume of radius R. We fix the functional value at the central point to 1. For an isotropic Sobolev scalar product, the function implicitly describing the surface is rotationally symmetric, depending just on the radius r,

$$f = f(r) \quad , \qquad r = \sqrt{(x_1)^2 + (x_2)^2 + (x_3)^2} \quad . \tag{106}$$

In 2-D, $x_3 = 0$, and in 1-D also $x_2 = 0$. We assume that the Sobolev norm is selected in such a way, that it does not distort the given functional values,

$$f(0) = 1 \quad , \qquad f(1) = 0 \quad . \tag{107}$$

The partial derivatives of function f are

$$f_{,i} = f' r_{,i} \quad , \tag{108}$$

$$f_{,ij} = f'' r_{,i} r_{,j} + f' r_{,ij} \tag{109}$$

and

$$f_{,ijk} = f''' r_{,i} r_{,j} r_{,k} + f'' r_{\substack{,i\\,j\\,k}} \, r_{\substack{,jk\\,ik\\,ij}} + f' r_{,ijk} \quad , \tag{110}$$

where

$$r_{,i} = x_i r^{-1} \quad , \tag{111}$$

$$r_{,ij} = \delta_{ij} r^{-1} - x_i x_j r^{-3} \quad , \tag{112}$$

$$r_{,ijk} = 3 x_i x_j x_k r^{-5} - x_{\substack{i\\j\\k}} \, \delta_{\substack{jk\\ik\\ij}} \, r^{-3} \quad . \tag{113}$$

We now insert the above equations into the expressions for various Sobolev norms.

5.1.1 Sobolev norms for the rotationally symmetric example

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{11\mathrm{N}}$, see (13), is

$$\|f\|^2 = \left[\int_0^R r^{d-1}\mathrm{d}r\right]^{-1}\int_0^R r^{d-1}[f']^2\mathrm{d}r = dR^{-d}\int_0^R r^{d-1}[f']^2\mathrm{d}r \quad . \tag{114}$$

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{22\mathrm{N}}$, see (14), is

$$\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\left[(f'')^2 + (d-1)r^{-2}(f')^2\right]\mathrm{d}r \quad . \tag{115}$$

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{22\mathrm{L}}$, see (17), is

$$\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\left[f'' + (d-1)r^{-1}f'\right]^2\mathrm{d}r \quad . \tag{116}$$

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{22}(L)$, see (23), is then

$$\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\left[(f'')^2 + 2L(d-1)r^{-1}f''f' + [L(d-2)+1](d-1)r^{-2}(f')^2\right]\mathrm{d}r \; . \tag{117}$$

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{33\mathrm{N}}$, see (15), is

$$\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\left[(f''')^2 + 3(d-1)r^{-2}(f'')^2 - 6(d-1)r^{-3}f''f' + 3(d-1)r^{-4}(f')^2\right]\mathrm{d}r \; . \tag{118}$$

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{33\mathrm{L}}$, see (18), is

$$\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\left[f''' + (d-1)r^{-1}f'' - (d-1)r^{-2}f'\right]^2\mathrm{d}r \quad . \tag{119}$$

The square of the Sobolev norm corresponding to matrix $\mathbf{B}^{33}(L)$, see (26), is then

$$\begin{aligned}\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\Big[&(f''')^2 + 2L(d-1)r^{-1}f'''f'' + [L(d-4)+3](d-1)r^{-2}(f'')^2 \\ -2L(d-1)r^{-2}f'''f' &- 2[L(d-4)+3](d-1)r^{-3}f''f' + [L(d-4)+3](d-1)r^{-4}(f')^2\Big]\mathrm{d}r \; ,\end{aligned} \tag{120}$$

which may be also written as

$$\begin{aligned}\|f\|^2 = dR^{-d}\int_0^R r^{d-1}\Big[&(f''')^2 + 2L(d-1)r^{-1}f'''(f'' - r^{-1}f') \\ &+[L(d-4)+3](d-1)r^{-2}(f'' - r^{-1}f')^2\Big]\mathrm{d}r \; .\end{aligned} \tag{121}$$

5.1.2 Differential equations for the rotationally symmetric example

Minimization of a Sobolev norm leads to the differential equations obtained by the Gâteaux variation of the objective function, with the given boundary conditions at the given points, lines or surfaces. Additional boundary conditions at the boundary of the model volume may also be derived from the Gâteaux variation of the objective function. In an alternative approach, used here, additional boundary conditions at the boundary of the model volume are not specified and the objective function is minimized in the linear space of the solutions of the partial differential equation.

Variation of equation (114) leads to differential equation

$$(r^{d-1}f')' = 0 \quad , \tag{122}$$

corresponding to Sobolev scalar product given by matrix $\mathbf{B}^{11\mathrm{N}}$, see (13). Variation of equation (117) leads to differential equation

$$(r^{d-1}f'')'' + L(d-1)[(r^{d-2}f')' - (r^{d-2}f'']' - [L(d-2)+1](d-1)(r^{d-3}f')' = 0 \quad . \tag{123}$$

The terms with L mutually cancel to yield

$$(r^{d-1}f'')'' - (d-1)(r^{d-3}f')' = 0 \quad . \tag{124}$$

This differential equation, corresponding to Sobolev scalar product given by matrix $\mathbf{B}^{22}(L)$, see (23), can be expressed in the form of

$$\{r^{d-1}[r^{1-d}(r^{d-1}f')']'\}' = 0 \quad . \tag{125}$$

Variation of equation (120) leads to differential equation

$$\begin{aligned}(r^{d-1}f''')''' + L(d-1)[(r^{d-2}f'')' - (r^{d-2}f''')]'' - [L(d-4)+3](d-1)(r^{d-3}f'')''\\ -L(d-1)[(r^{d-3}f')'' + (r^{d-3}f''')]'\\ +[L(d-4)+3](d-1)[(r^{d-4}f')' - (r^{d-4}f'')]' + [L(d-4)+3](d-1)(r^{d-5}f')' = 0 \ ,\end{aligned} \tag{126}$$

which reads

$$\begin{aligned}(r^{d-1}f''')''' + L(d-1)(d-2)(r^{d-3}f'')'' - [L(d-4)+3](d-1)(r^{d-3}f'')''\\ -L(d-1)[(r^{d-3}f'')' + (r^{d-3}f'')']' - L(d-1)(d-3)[(r^{d-4}f')' - (r^{d-4}f'')]'\\ +[L(d-4)+3](d-1)(d-4)(r^{d-5}f')' + [L(d-4)+3](d-1)(r^{d-5}f')' = 0 \ .\end{aligned} \tag{127}$$

The terms with L mutually cancel to yield

$$(r^{d-1}f''')''' - 3(d-1)(r^{d-3}f'')'' + 3(d-1)(d-3)(r^{d-5}f')' = 0 \ . \tag{128}$$

This differential equation, corresponding to Sobolev scalar product given by matrix $\mathbf{B}^{33}(L)$, see (26), can be expressed in the form of

$$\{\!\{r^{d-1}[\![r^{1-d}\{r^{d-1}[r^{1-d}(r^{d-1}f')']'\}']\!]'\}\!\}' = 0 \quad . \tag{129}$$

5.1.3 Solutions of the differential equations

A general solution of equations (122) for $d \neq 2$, (125) for $d \neq 2$ and $d \neq 4$, or (129) for $d \neq 2$ and $d \neq 4$ and $d \neq 6$, is

$$f = c_0 + c_1 r^{2-d} + c_2 r^2 + c_3 r^{4-d} + c_4 r^4 + c_5 r^{6-d} \quad , \tag{130}$$

where $c_2 = c_3 = c_4 = c_5 = 0$ for equation (122), and $c_4 = c_5 = 0$ for equation (125). The derivatives are

$$f' = (2-d)c_1 r^{1-d} + 2c_2 r + (4-d)c_3 r^{3-d} + 4c_4 r^3 + (6-d)c_5 r^{5-d} \quad , \tag{131}$$

$$f'' = (1-d)(2-d)c_1 r^{-d} + 2c_2 + (3-d)(4-d)c_3 r^{2-d} + 12c_4 r^2 + (5-d)(6-d)c_5 r^{4-d} \quad , \tag{132}$$

$$f''' = -d(1-d)(2-d)c_1 r^{-1-d} + (2-d)(3-d)(4-d)c_3 r^{1-d} + 24c_4 r + (4-d)(5-d)(6-d)c_5 r^{3-d} \, . \tag{133}$$

A general solution of equation (122), (125) or (129) for $d = 2$ is

$$f = c_0 + c_1 \ln r + c_2 r^2 + c_3 r^2 \ln r + c_4 r^4 + c_5 r^4 \ln r \quad , \tag{134}$$

where $c_2 = c_3 = c_4 = c_5 = 0$ for equation (122), and $c_4 = c_5 = 0$ for equation (125). Term $c_1 \ln r$ is singular at $r = 0$. The derivatives are

$$f' = c_1 r^{-1} + (2c_2 + c_3) r + 2c_3 r \ln r + (4c_4 + c_5) r^3 + 4c_5 r^3 \ln r \quad , \tag{135}$$

$$f'' = -c_1 r^{-2} + (2c_2 + 3c_3) + 2c_3 \ln r + (12c_4 + 7c_5) r^2 + 12c_5 r^2 \ln r \quad , \tag{136}$$

$$f''' = 2c_1 r^{-3} + 2c_3 r^{-1} + (24c_4 + 26c_5) r + 24c_5 r \ln r \quad . \tag{137}$$

Inside the unit sphere

For $d > 2$, term $c_1 r^{2-d}$ is singular at $r = 0$ and we thus regularize it inside the unit sphere as follows

$$\text{for } d > 2: \quad c_1 r^{2-d} \longrightarrow c_1 \varepsilon^{d-2} (r^2 + \varepsilon^2)^{1-\frac{d}{2}} \quad . \tag{138}$$

For $d = 3$, its squared Sobolev norm (114) corresponding to matrix $\mathbf{B}^{11\mathrm{N}}$ is zero,

$$\| \varepsilon^{d-2} (r^2 + \varepsilon^2)^{1-\frac{d}{2}} \|^2 = \frac{3\pi}{16} \varepsilon = 0 \quad , \tag{139}$$

but its squared Sobolev norm (117) corresponding to matrix $\mathbf{B}^{22}(L)$, and its squared Sobolev norm (120) corresponding to matrix $\mathbf{B}^{33}(L)$ are infinite.

For $d = 2$, term $c_1 \ln r$ is singular at $r = 0$ and we thus regularize it inside the unit sphere as follows

$$c_1 \ln r \longrightarrow c_1 \frac{\ln(r^2 + \varepsilon^2)}{2 \ln \varepsilon} \quad . \tag{140}$$

Its squared Sobolev norm (114) corresponding to matrix $\mathbf{B}^{11\mathrm{N}}$ is zero,

$$\left\| \frac{\ln(r^2 + \varepsilon^2)}{2 \ln \varepsilon} \right\|^2 = \frac{1}{-\ln \varepsilon} = 0 \quad , \tag{141}$$

but its squared Sobolev norm (117) corresponding to matrix $\mathbf{B}^{22}(L)$, and its squared Sobolev norm (120) corresponding to matrix $\mathbf{B}^{33}(L)$ are infinite.

Both functions (138) and (140) converge point by point to function $D(r)$, which is unit at $r = 0$ and zero otherwise,

$$D(0) = 1 \quad , \qquad D(r) = 0 \ \text{ for } \ r > 0 \quad . \tag{142}$$

Squared Sobolev norm (117) of $c_3 r^{4-d}$ is finite for $d < 4$, and squared Sobolev norm (120) of $c_3 r^{4-d}$ is finite for $d < 2$ but infinite for $d \geq 2$. Squared Sobolev norm (117) of $c_3 r^2 \ln r$ is finite for $d = 2$, but squared Sobolev norm (120) of $c_3 r^2 \ln r$ is infinite for $d = 2$.

Now we summarize the results the above considerations inside the unit sphere:
For Sobolev norm (114) given by matrix $\mathbf{B}^{11\mathrm{N}}$, $d = 1$, there is no free coefficient,

$$c_0 = 1 \ , \qquad c_1 = -1 \ . \tag{143}$$

For Sobolev norm (114) given by matrix $\mathbf{B}^{11\mathrm{N}}$, $d = 2$, there is no free coefficient,

$$c_0 = 0 \ , \qquad c_1 = 1 \ . \tag{144}$$

For Sobolev norm (114) given by matrix $\mathbf{B}^{11\mathrm{N}}$, $d = 3$, there is no free coefficient,

$$c_0 = 0 \ , \qquad c_1 = 1 \ . \tag{145}$$

For Sobolev norm (117) given by matrix $\mathbf{B}^{22}(L)$, $d = 1$, there is 1 free coefficient c_3,

$$c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 - c_3 \ , \quad f'(1) = -2 + c_3 \ . \tag{146}$$

For Sobolev norm (117) given by matrix $\mathbf{B}^{22}(L)$, there is 1 free coefficient c_3,

$$c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 \ , \quad f'(1) = -2 + c_3 \ . \tag{147}$$

For Sobolev norm (117) given by matrix $\mathbf{B}^{22}(L)$, there is 1 free coefficient c_3,

$$c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 - c_3 \ , \quad f'(1) = -2 - c_3 \ . \tag{148}$$

For Sobolev norm (120) given by matrix $\mathbf{B}^{33}(L)$, $d = 1$, there are 3 free coefficients c_3, c_4 and c_5,

$$\begin{gathered} c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 - c_3 - c_4 - c_5 \ , \\ f'(1) = -2 + c_3 + 2c_4 + 3c_5 \ , \quad f''(1) = -2 + 4c_3 + 10c_4 + 18c_5 \ . \end{gathered} \tag{149}$$

For Sobolev norm (120) given by matrix $\mathbf{B}^{33}(L)$, $d = 2$, there are 2 free coefficients c_4 and c_5,

$$\begin{gathered} c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 - c_4 \ , \quad c_3 = 0 \ , \\ f'(1) = -2 + 2c_4 + c_5 \ , \quad f''(1) = -2 + 10c_4 + 7c_5 \ . \end{gathered} \tag{150}$$

For Sobolev norm (120) given by matrix $\mathbf{B}^{33}(L)$, $d = 3$, there are 2 free coefficients c_4 and c_5,

$$\begin{gathered} c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 - c_4 - c_5 \ , \quad c_3 = 0 \ , \\ f'(1) = -2 + 2c_4 + c_5 \ , \quad f''(1) = -2 + 10c_4 + 4c_5 \ . \end{gathered} \tag{151}$$

Outside the unit sphere

Outside the unit sphere, squared Sobolev norm (114) corresponding to matrix $\mathbf{B}^{11\mathrm{N}}$ is minimized by zero function for all d. Functions minimizing Sobolev norm $\mathbf{B}^{11\mathrm{N}}$ in 1-D, 2-D and 3-D are shown in Figures 1, 2 and 3, respectively.

We denote coefficients c_α outside the unit sphere by $\tilde{c}_\alpha$. The function has to be continuous at $r = 1$. Squared Sobolev norm (117) corresponding to matrix $\mathbf{B}^{22}(L)$ also needs to fit the first derivative $f'(1)$. There are then 2 additional free coefficients $\tilde{c}_2$ and $\tilde{c}_3$ for Sobolev norm given by matrix $\mathbf{B}^{22}(L)$:
For $d = 1$, we have

$$\tilde{c}_0 = -\tilde{c}_1 - \tilde{c}_2 - \tilde{c}_3 \ , \quad \tilde{c}_1 = -2 + c_3 - 2\tilde{c}_2 - 3\tilde{c}_3 \ . \tag{152}$$

For $d=2$, we have

$$\tilde{c}_0 = -\tilde{c}_2 \ , \quad \tilde{c}_1 = -2 + c_3 - 2\tilde{c}_2 - \tilde{c}_3 \ . \tag{153}$$

For $d=3$, we have

$$\tilde{c}_0 = -\tilde{c}_1 - \tilde{c}_2 - \tilde{c}_3 \ , \quad \tilde{c}_1 = 2 + c_3 + 2\tilde{c}_2 + \tilde{c}_3 \ . \tag{154}$$

Squared Sobolev norm (120), corresponding to matrix $\mathbf{B}^{33}(L)$, needs to fit the first and second derivatives $f'(1)$ and $f''(1)$. There are then 3 additional free coefficients $\tilde{c}_3$, $\tilde{c}_4$ and $\tilde{c}_5$ for Sobolev norm $\mathbf{B}^{33}(L)$:
For $d=1$, we have

$$\tilde{c}_0 = -\tilde{c}_1 - \tilde{c}_2 - \tilde{c}_3 - \tilde{c}_4 - \tilde{c}_5 \ , \quad \tilde{c}_1 = f'(1) - 2\tilde{c}_2 - 3\tilde{c}_3 - 4\tilde{c}_4 - 5\tilde{c}_5 \ ,$$
$$\tilde{c}_2 = \tfrac{1}{2}f''(1) - 3\tilde{c}_3 - 6\tilde{c}_4 - 10\tilde{c}_5 \ . \tag{155}$$

For $d=2$, we have

$$\tilde{c}_0 = -\tilde{c}_2 - \tilde{c}_4 \ , \quad \tilde{c}_1 = \tfrac{1}{2}[f'(1) - f''(1)] + \tilde{c}_3 + 4\tilde{c}_4 + 3\tilde{c}_5 \ ,$$
$$\tilde{c}_2 = \tfrac{1}{4}[f'(1) + f''(1)] - \tilde{c}_3 - 4\tilde{c}_4 - 2\tilde{c}_5 \ . \tag{156}$$

For $d=3$, we have

$$\tilde{c}_0 = -\tilde{c}_1 - \tilde{c}_2 - \tilde{c}_3 - \tilde{c}_4 - \tilde{c}_5 \ , \quad \tilde{c}_1 = \tfrac{1}{3}[f''(1) - f'(1)] + \tfrac{1}{3}\tilde{c}_3 - \tfrac{8}{3}\tilde{c}_4 - \tilde{c}_5 \ ,$$
$$\tilde{c}_2 = \tfrac{1}{6}[2f'(1) + f''(1)] - \tfrac{1}{3}\tilde{c}_3 - \tfrac{10}{3}\tilde{c}_4 - 2\tilde{c}_5 \ . \tag{157}$$

5.1.4 Functions minimizing Sobolev norm $\mathbf{B}^{22}(L)$

For $d \neq 2$, we insert derivatives (131) and (132) into squared Sobolev norm (117) corresponding to matrix $\mathbf{B}^{22}(L)$,

$$\begin{aligned}\|f\|^2 = dR^{-d} \int_0^R \Big\{ & (d-2)^2(d-1)d(1-L)\ (c_1)^2\ r^{-d-1} \\ & +4\ d\ [L(d-1)+1]\ (c_2)^2\ r^{d-1} \\ & +2\ (d-4)(d-2)^2(d-1)(1-L)\ c_1 c_3\ r^{-d+1} \\ & -8\ (d-4)[L(d-1)+1]\ c_2 c_3\ r \\ & +(d-4)^2 [\![(d-3)^2 + [L(4-d)+1](d-1)]\!]\ (c_3)^2\ r^{-d+3} \Big\} \mathrm{d}r \quad . \end{aligned} \tag{158}$$

For $d=1$, equation (158) reads

$$\|f\|^2 = dR^{-1} \int_0^R \big\{ 4\ (c_2)^2 + 24\ c_2 c_3\ r + 36\ (c_3)^2\ r^2 \big\} \mathrm{d}r \ . \tag{159}$$

For $d=3$, equation (158) reads

$$\begin{aligned}\|f\|^2 = dR^{-3} \int_0^R \Big\{ & 6\ (1-L)\ (c_1)^2\ r^{-4} \\ & +12\ (1+2L)\ (c_2)^2\ r^2 \\ & -4\ (1-L)\ c_1 c_3\ r^{-2} \\ & +8\ (1+2L)\ c_2 c_3\ r \\ & +2\ (1+L)\ (c_3)^2\ \Big\} \mathrm{d}r \quad . \end{aligned} \tag{160}$$

For $d = 2$, we insert derivatives (135) and (136) into squared Sobolev norm (117) corresponding to matrix $\mathbf{B}^{22}(L)$,

$$\begin{aligned} \|f\|^2 = dR^{-d} \int_0^R & \{2\,(1-L)\,(c_1)^2\, r^{-3} \\ & -4\,(1-L)\; c_1 c_3\; r^{-1} \\ & +[8(1+L)(c_2)^2 + 16(1+L)c_2c_3 + (10+6L)(c_3)^2]\, r \\ & +16\,(1+L)\,(c_2+c_3)\; c_3\; r \ln r \\ & +8\,(1+L)\,(c_3)^2\; r\,(\ln r)^2\; \}\mathrm{d}r \quad . \end{aligned} \tag{161}$$

One–dimensional case

Integration of (159) yields

$$\begin{aligned} \|f\|^2 = dR^{-1}\{ & 4\,(c_2)^2 + 12c_2c_3 + 12\,(c_3)^2 \\ & +4\,(\tilde c_2)^2(R-1) + 12\tilde c_2 c_3(R^2-1) + 12\,(\tilde c_3)^2(R^3-1)\}\ . \end{aligned} \tag{162}$$

Inserting (146), we obtain expression

$$\begin{aligned} \|f\|^2 = dR^{-1}\{ & 4 - 12c_3 + 12\,(c_3)^2 \\ & +4\,(\tilde c_2)^2(R-1) + 12\tilde c_2 c_3(R^2-1) + 12\,(\tilde c_3)^2(R^3-1)\}\ , \end{aligned} \tag{163}$$

for the 1-D solution corresponding to matrix $\mathbf{B}^{22}(L)$, which is minimized by coefficients

$$c_0 = 1\ ,\quad c_1 = 0\ ,\quad c_2 = -\tfrac{3}{2}\ ,\quad c_3 = \tfrac{1}{2}\ ,\quad \tilde c_0 = \tfrac{3}{2}\ ,\quad \tilde c_1 = -\tfrac{3}{2}\ ,\quad \tilde c_2 = 0\ ,\quad \tilde c_3 = 0 \tag{164}$$

describing natural cubic 1-D spline, see Figure 4.

Two–dimensional case

Integration of (161), for $c_1 = 0$ inside the unit sphere, yields

$$\begin{aligned} \|f\|^2 = dR^{-d}\{ & 4(1+L)(c_2)^2 + 8(1+L)c_2c_3 + (5+3L)(c_3)^2 \\ & -4\,(1+L)\,(c_2+c_3)\,c_3 \\ & +2\,(1+L)\,(c_3)^2 \\ & -(1-L)\,(\tilde c_1)^2\,(R^{-2}-1) \\ & -4\,(1-L)\;\tilde c_1\tilde c_3 \ln R \\ & +[4(1+L)(\tilde c_2)^2 + 8(1+L)\tilde c_2\tilde c_3 + (5+3L)(\tilde c_3)^2]\,(R^2-1) \\ & +4\,(1+L)\,(\tilde c_2+\tilde c_3)\,\tilde c_3\,(2R^2\ln R - R^2 + 1) \\ & +2\,(1+L)\,(\tilde c_3)^2\;[2R^2(\ln R)^2 - 2R^2\ln R + R^2 - 1]\ \}\quad , \end{aligned} \tag{165}$$

which can be slightly rearranged to read

$$\begin{aligned} \|f\|^2 = dR^{-d}\{ & 4(1+L)(c_2)^2 + 4(1+L)c_2c_3 + (3+L)(c_3)^2 \\ & -(1-L)\,(\tilde c_1)^2\,(R^{-2}-1) \\ & -4\,(1-L)\;\tilde c_1\tilde c_3 \ln R \\ & +[4(1+L)(\tilde c_2)^2 + 4(1+L)\tilde c_2\tilde c_3 + (3+L)(\tilde c_3)^2]\,(R^2-1) \\ & +8\,(1+L)\;\tilde c_2\tilde c_3\, R^2\ln R \\ & +4\,(1+L)\,(\tilde c_3)^2\; R^2[(\ln R)^2 + \ln R]\ \}\quad . \end{aligned} \tag{166}$$

Inserting (147) and (153), we obtain expression

$$\begin{aligned}\|f\|^2 = dR^{-d}\{&4(1+L) - 4(1+L)c_3 + (3+L)(c_3)^2 \\ &-(1-L)\,(-2+c_3-2\tilde{c}_2-\tilde{c}_3)^2\,(R^{-2}-1) \\ &-4\,(1-L)\,(-2+c_3-2\tilde{c}_2-\tilde{c}_3)\,\tilde{c}_3\ln R \\ &+[4(1+L)(\tilde{c}_2)^2+4(1+L)\tilde{c}_2\tilde{c}_3+(3+L)(\tilde{c}_3)^2]\,(R^2-1) \\ &+8\,(1+L)\,\tilde{c}_2\tilde{c}_3\,R^2\ln R \\ &+4\,(1+L)\,(\tilde{c}_3)^2\,R^2\,[(\ln R)^2+\ln R]\,\}\quad . \end{aligned} \tag{167}$$

Differentiating the expression with respect to coefficients c_3, $\tilde{c}_2$ and $\tilde{c}_3$, we obtain equations

$$\begin{aligned}&-2\,(1+L)+(3+L)\,c_3 \\ &-(1-L)(-2+c_3-2\tilde{c}_2-\tilde{c}_3)\,(R^{-2}-1) \\ &-2\,(1-L)\,\tilde{c}_3\ln R = 0\quad , \end{aligned} \tag{168}$$

$$\begin{aligned}&\;2\,(1-L)(-2+c_3-2\tilde{c}_2-\tilde{c}_3)\,(R^{-2}-1) \\ &+4\,(1-L)\,\tilde{c}_3\ln R \\ &+2(1+L)(2\tilde{c}_2+\tilde{c}_3)\,(R^2-1) \\ &+4\,(1+L)\,\tilde{c}_3\,R^2\ln R = 0\quad , \end{aligned} \tag{169}$$

$$\begin{aligned}&\;(1-L)(-2+c_3-2\tilde{c}_2-\tilde{c}_3)\,(R^{-2}-1) \\ &-2\,(1-L)(-2+c_3-2\tilde{c}_2-2\tilde{c}_3)\ln R \\ &+[2(1+L)\,\tilde{c}_2+(3+L)\tilde{c}_3]\,(R^2-1) \\ &+4\,(1+L)\,\tilde{c}_2\,R^2\ln R \\ &+4\,(1+L)\,\tilde{c}_3\,R^2\,[(\ln R)^2+\ln R] = 0\quad . \end{aligned} \tag{170}$$

Multiplying equation (169) by $[(R^{-2}-1)^{-1}\ln R - \frac{1}{2}]$ and adding to equation (170), all terms with c_3 and $\tilde{c}_2$ cancel, and we obtain $\tilde{c}_3 = 0$. Coefficients c_3 and $\tilde{c}_2$ may then be determined from equations (168) and (169). The 2-D solution for the Sobolev norm corresponding to matrix $\mathbf{B}^{22}(L)$ reads

$$\begin{aligned}&c_0 = 1\ ,\quad c_1 = 0\ ,\quad c_2 = -1\ ,\quad c_3 = \frac{2(1+L)R^2}{2(1+L)R^2+(1-L)}\ , \\ &\tilde{c}_0 = 1-c_3\ ,\quad \tilde{c}_1 = -c_3\ ,\quad \tilde{c}_2 = -1+c_3\ ,\quad \tilde{c}_3 = 0\ . \end{aligned} \tag{171}$$

We thus have one–parametric system of solutions controlled by coefficient c_3, depending on L and R, see Figure 5. Due to inequalities (25), the range of coefficient c_3 extends from $c_3 = 0$ for $L = -1$ to $c_3 = 1$ for $L = 1$,

$$0 \leq c_3 \leq 1\ . \tag{172}$$

For practical values of L and R, coefficient c_3 is close to $c_3 = 1$ (red line in Figure 5).

Three–dimensional case

Integration of (160), for $c_1 = 0$ inside the unit sphere, yields

$$\begin{aligned}\|f\|^2 = dR^{-3}\{&4\,(1{+}2L)\,(c_2)^2\\ &+4\,(1{+}2L)\,c_2c_3\\ &+2\,(1{+}L)\,(c_3)^2\\ &-2\,(1{-}L)\,(\tilde{c}_1)^2\,(R^{-3}-1)\\ &+4\,(1{+}2L)\,(\tilde{c}_2)^2\,(R^3-1)\\ &+4\,(1{-}L)\,\tilde{c}_1\tilde{c}_3\,(R^{-1}-1)\\ &+4\,(1{+}2L)\,\tilde{c}_2\tilde{c}_3\,(R^2-1)\\ &+2\,(1{+}L)\,(\tilde{c}_3)^2\,(R{-}1)\,\}\quad .\end{aligned}\tag{173}$$

Inserting (148) and (154), we obtain expression

$$\begin{aligned}\|f\|^2 = dR^{-3}\{&4\,(1{+}2L)\,(c_3+1)\\ &+2\,(1{+}L)\,(c_3)^2\\ &-2\,(1{-}L)\,(2{+}c_3{+}2\tilde{c}_2{+}\tilde{c}_3)^2\,(R^{-3}-1)\\ &+4\,(1{+}2L)\,(\tilde{c}_2)^2\,(R^3-1)\\ &+4\,(1{-}L)\,(2{+}c_3{+}2\tilde{c}_2{+}\tilde{c}_3)\,\tilde{c}_3\,(R^{-1}-1)\\ &+4\,(1{+}2L)\,\tilde{c}_2\tilde{c}_3\,(R^2-1)\\ &+2\,(1{+}L)\,(\tilde{c}_3)^2\,(R{-}1)\,\}\quad .\end{aligned}\tag{174}$$

Differentiating the expression with respect to coefficients c_3, $\tilde{c}_2$ and $\tilde{c}_3$, we obtain equations

$$\begin{aligned}&(1{+}2L)\\ &+(1{+}L)\,c_3\\ &-(1{-}L)(2{+}c_3{+}2\tilde{c}_2{+}\tilde{c}_3)(R^{-3}-1)\\ &+(1{-}L)\,\tilde{c}_3(R^{-1}-1) = 0\quad ,\end{aligned}\tag{175}$$

$$\begin{aligned}&-2\,(1{-}L)(2+c_3{+}2\tilde{c}_2{+}\tilde{c}_3)(R^{-3}-1)\\ &+2\,(1{+}2L)\,\tilde{c}_2(R^3-1)\\ &+2\,(1{-}L)\,\tilde{c}_3(R^{-1}-1)\\ &+(1{+}2L)\,\tilde{c}_3(R^2-1) = 0\quad ,\end{aligned}\tag{176}$$

$$\begin{aligned}&-(1{-}L)(2+c_3{+}2\tilde{c}_2{+}\tilde{c}_3)(R^{-3}-1)\\ &+(1{-}L)(2+c_3{+}2\tilde{c}_2{+}2\tilde{c}_3)(R^{-1}-1)\\ &+(1{+}2L)\,\tilde{c}_2(R^2-1)\\ &+(1{+}L)\,\tilde{c}_3(R{-}1) = 0\quad .\end{aligned}\tag{177}$$

Multiplying equation (176) by $\frac{1}{2}(R^3{-}1)^{-1}(R^2{-}1)$ and subtracting from equation (177), all terms with c_3 and $\tilde{c}_2$ cancel, and we obtain $\tilde{c}_3 = 0$. Coefficients c_3 and $\tilde{c}_2$ may then be determined from equations (175) and (176). The 3-D solution for the Sobolev norm corresponding to matrix $\mathbf{B}^{22}(L)$ reads

$$c_0 = 1 \ , \quad c_1 = 0 \ , \quad c_2 = -1 - c_3 \ , \quad c_3 = -\frac{3(1+2L)R^3}{2(1+2L)R^3 + (1-L)} \ ,$$

$$\tilde{c}_0 = 1 + c_3 \ , \quad \tilde{c}_1 = -\tfrac{1}{3}c_3 \ , \quad \tilde{c}_2 = -1 - \tfrac{2}{3}c_3 \ , \quad \tilde{c}_3 = 0 \ . \tag{178}$$

We thus have one–parametric system of solutions controlled by coefficient c_3, depending on L and R, see Figure 6. Due to inequalities (24), the range of coefficient c_3 extends from $c_3 = 0$ for $L = -\frac{1}{2}$ to $c_3 = -\frac{3}{2}$ for $L = 1$,

$$-\tfrac{3}{2} \le c_3 \le 0 \ . \tag{179}$$

Coefficient c_3 controls the sharpness of the conical peak at $r = 0$. For practical values of L and R, coefficient c_3 is close to $c_3 = -\frac{3}{2}$ (red line in Figure 6), which means that there is a sharp cone at $r = 0$.

5.2 Fitting discrete values

Assume that we are fitting discrete values u_α at points $\mathbf{x}^\alpha$ inside the model volume by minimizing objective function

$$y = \sum_\alpha [\tilde{u}(\mathbf{x}^\alpha) - u^\alpha]^2 [\Delta u^\alpha]^{-2} + S^2((\tilde{u}, \tilde{u})) \quad . \tag{180}$$

For very small weighting factor S^2, the solution corresponds to the minimization of objective function

$$y = ((\tilde{u}, \tilde{u})) \tag{181}$$

with boundary conditions

$$\tilde{u}(\mathbf{x}^\alpha) = u^\alpha \quad . \tag{182}$$

The minimizing functions have to satisfy partial differential equation

$$\sum_{ij\ldots} \sum_{ab\ldots} [b_{ij\ldots|ab\ldots} u_{,ij\ldots}]_{,ab\ldots} = 0 \tag{183}$$

with boundary conditions (182). Additional boundary conditions at the boundary of the model volume may also be derived from the variation of the objective function. In an alternative approach, used in Section 5.1, additional boundary conditions at the boundary of the model volume are not specified and the objective function is minimized in the linear space of the solutions of the partial differential equation. For constant $b_{ij\ldots|ab\ldots}$ inside the model, equation (183) simplifies to

$$\sum_{ij\ldots} \sum_{ab\ldots} b_{ij\ldots|ab\ldots} u_{,ij\ldots ab\ldots} = 0 \quad . \tag{184}$$

Using the results of Section 5.1, we briefly discuss the properties of interpolation between discrete values by means of minimizing the squares of Sobolev norms.

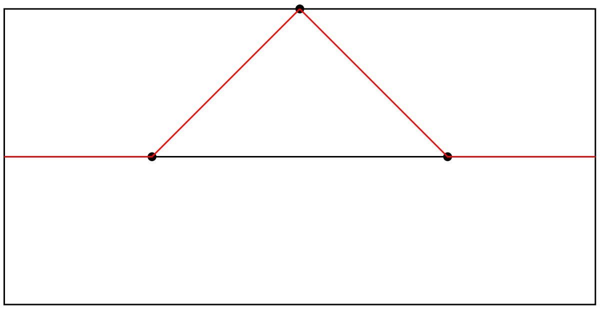

Figure 1. 1-D interpolation using the Sobolev scalar product given by matrix $\mathbf{B}^{11(1\mathrm{D})}$, see (13), is displayed in red. The black dots denote the interpolated data.

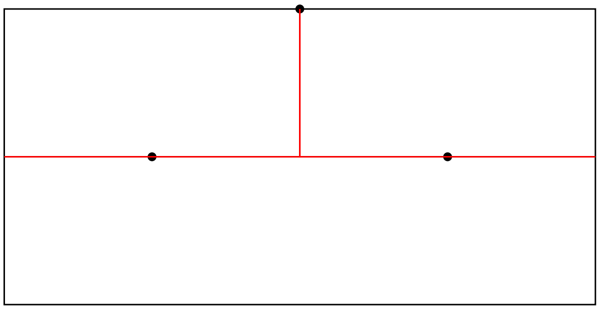

Figure 2. 2-D interpolation using the Sobolev scalar product given by matrix $\mathbf{B}^{11(1\mathrm{D})}$, see (13), is displayed in red. The black dots denote the interpolated data.

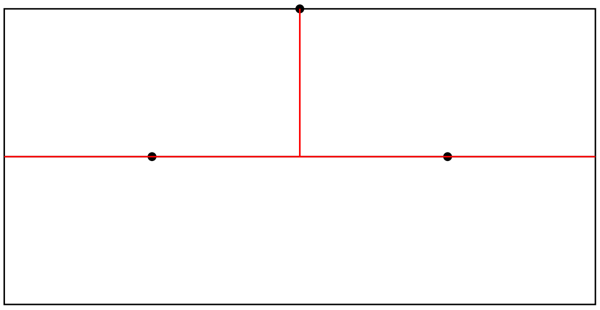

Figure 3. 3-D interpolation using the Sobolev scalar product given by matrix $\mathbf{B}^{11(1\mathrm{D})}$, see (13), is displayed in red. The black dots denote the interpolated data.

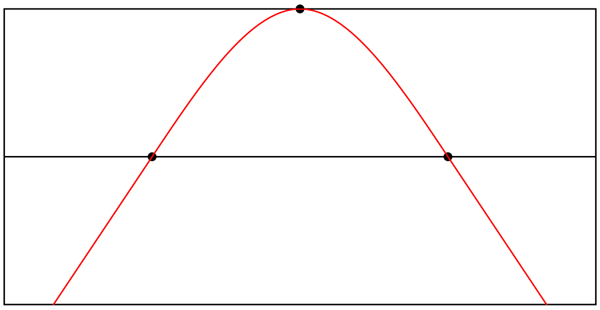

Figure 4. 1-D interpolation using the Sobolev scalar product given by matrix $\mathbf{B}^{22}(L)$, see (23), is displayed in red. The black dots denote the interpolated data.

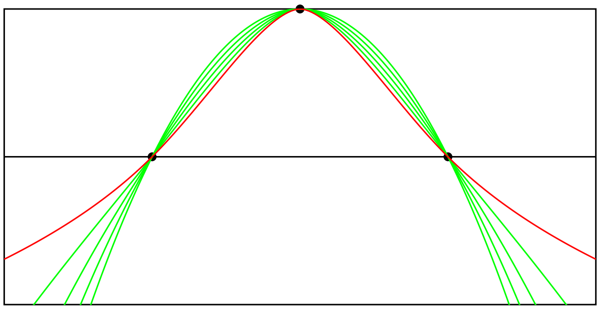

Figure 5. 2-D interpolation using the Sobolev scalar product given by matrix $\mathbf{B}^{22}(L)$, see (23). The red line corresponds to the typical interpolation, obtained for $c_3 = 1$. The green lines correspond to other values of c_3, with step 0.25. The black dots denote the interpolated data.

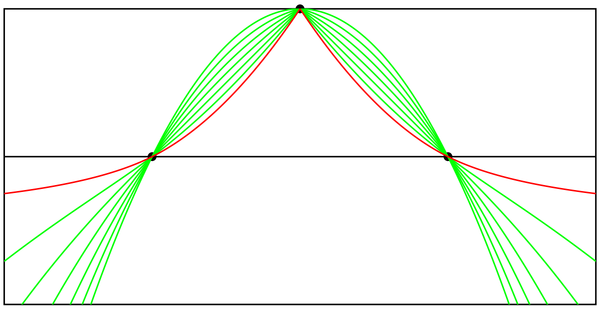

Figure 6. 3-D interpolation using the Sobolev scalar product given by matrix $\mathbf{B}^{22}(L)$, see (23). The red line corresponds to the typical interpolation, obtained for $c_3 = -3/2$. The green lines correspond to other values of c_3, with step 0.25. The black dots denote the interpolated data.

Minimization of the first derivatives

- For discrete points in 1-D, piecewise linear interpolation is obtained, see Figure 1.
- For discrete lines in 2-D, the minimizing function resembles piecewise linear interpolation.
- For discrete points in 2-D and 3-D, and discrete lines in 3-D, the interpolation tends to produce a constant function with singular spikes at the given points or lines. The value of the constant function is probably the least–square mean of the given values.

Minimization of the second derivatives

- For discrete points in 1-D, cubic splines are obtained, see Figure 4.
- For discrete lines in 2-D, smooth interpolation with continuous second derivatives, resembling cubic splines, is probably obtained.
- For discrete points in 2-D and discrete lines in 3-D, smooth interpolation with continuous first derivatives is obtained, see Figure 5.
- For discrete points in 3-D, smooth interpolation with continuous first derivatives between the given points, but with conical peaks at the given points, is obtained. The discontinuity of the first derivatives at the given points might be removed by selecting $L = -\frac{1}{2}$ in (23), but this may lead to strong oscillations and is not recommended by the author without further study.

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