Optimization of the structural Gabor functions in a homogeneous velocity model for a zero-offset surface seismic reflection survey

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Summary

We consider the algorithm of true linearized inversion of the complete set of seismograms recorded for all shots during seismic reflection survey, based on the correspondence between the structural Gabor functions and the corresponding scattered Gaussian packets. The first step of this linearized inversion consists in specifying the finite set of structural Gabor functions to which the wanted deviations of the material parameters from the given velocity model will be decomposed. If possible, the shape of the Gabor functions should be optimized, and the Gabor functions should form a frame. We present a simple attempt to specify the finite set of structural Gabor functions for this inversion.

The shape of the Gabor functions and the space–wavenumber lattice of their central points are optimized analytically, but for a homogeneous velocity model only. The derived set of structural Gabor functions may be applied also to slightly heterogeneous models in which the shape of Gabor functions is not optimum but is still probably better than the shape of Gabor functions specified by chance. The envelopes of the structural Gabor functions are chosen isotropic, but are allowed to be complex–valued. The shape of Gabor functions is optimized for a zero–offset surface seismic reflection survey only, but is close to optimum for a narrow–offset surface seismic reflection survey.

Keywords

Gabor function, Gabor transform, frame bounds, discretization error, phase–space metric tensor, elastic waves, Gaussian packets, wavefield inversion.

1. Introduction

Klimeš (2008a) proposed the algorithm of true linearized inversion of the complete set of seismograms recorded for all shots during seismic reflection survey. The inversion is based on the correspondence the between the structural Gabor functions and the corresponding scattered Gaussian packets (Klimeš, 2007).

The first step of this linearized inversion consists in specifying the finite set of structural Gabor functions to which the wanted deviations of the material parameters from the given velocity model will be decomposed (Klimeš, 2008a, sec. 4). If possible, the shape of the Gabor functions should be optimized. If possible, the Gabor functions should form a frame. In this paper, we present a simple attempt to specify the finite set of structural Gabor functions for the above mentioned inversion.

As the first attempt should be simple enough to be completed, we optimize the shape of the Gabor functions for a homogeneous velocity model only. In this case, we can design the shape of the Gabor functions and the space–wavenumber lattice of

In: Seismic Waves in Complex 3–D Structures, Report 18 (Department of Geophysics, Charles University, Prague, 2008), pp. 115–127

their central points analytically. The optimization of the shape of the Gabor functions for a homogeneous velocity model does not mean that the velocity model must be homogeneous. We may apply the derived set of structural Gabor functions also to slightly heterogeneous models in which the shape of the Gabor functions is not optimum but is still probably better than the shape of Gabor functions specified by chance.

We choose the envelopes of the structural Gabor functions isotropic for the sake of simplicity, but allow them to be complex–valued.

The optimum shape of Gabor functions represents a compromise between the shapes optimum for various source–receiver configurations. We assume that all sources and all receivers are situated in the vicinity of a single plane, which corresponds to a surface seismic reflection survey. We consider only the receivers coinciding with the corresponding sources for our optimization. The shape of Gabor functions is thus optimized for a zero–offset seismic reflection survey, and is close to optimum for a narrow–offset seismic reflection survey.

The optimum shape of Gabor functions is proposed in Section 2. The algorithm of generating the space–wavenumber lattice of the central points of Gabor functions is then proposed in Section 3. Refer to program `sgfhom.for` of package `FORMS` (Bucha & Bulant, 2008) for the FORTRAN 77 code corresponding to this paper.

2. Optimum structural Gabor functions

We assume that the sources and receivers are situated in the vicinity of a horizontal plane in a homogeneous velocity model. We denote the horizontal coordinates by x_1, x_2, and the positive depth below the source–receiver horizontal plane by x_3.

We consider Gabor functions

$$g^\alpha(\mathbf{x}) = a^\alpha \exp[\mathrm{i}\mathbf{k}^{\alpha\mathrm{T}}(\mathbf{x}-\mathbf{x}^\alpha) - \tfrac{1}{2}(\mathbf{x}-\mathbf{x}^\alpha)^\mathrm{T}\mathbf{K}^\alpha(\mathbf{x}-\mathbf{x}^\alpha)] \quad . \tag{1}$$

These Gabor functions are centred at spatial positions $\mathbf{x}^\alpha$ and have structural wavenumber vectors $\mathbf{k}^\alpha$. The envelope and wavefront curvature of each Gabor function g^α is described by symmetric complex–valued matrix $\mathbf{K}^\alpha$ which may depend on phase–space coordinates $\mathbf{x}^\alpha$ and $\mathbf{k}^\alpha$. The real part of matrix $\mathbf{K}^\alpha$ must be positive–definite. Real–valued amplitude a^α of the envelope of the Gabor function, chosen so that the L_2 norm $|g^\alpha|$ is unit, does not influence the optimization of the shape of the structural Gabor functions.

2.1. Shape of the scattered Gaussian packet

The initial shape of a scattered Gaussian packet is determined by the initial value of the matrix of the second–order spatial derivatives of its complex–valued travel time, by the initial value of the vector of the mixed second–order space–time derivatives of its complex–valued travel time, and by the initial value of the second–order time derivative of its complex–valued travel time.

The initial value of the 2×2 matrix of the second–order spatial derivatives of the complex–valued travel time in the ray–centred coordinates reads (Klimeš, 2007, eq. 237)

$$\mathbf{M}^\alpha_{\mathrm{GP}} = \mathbf{T}^{(q)} + \mathrm{i}\omega^{-1}\mathbf{K}^{(q)} - \frac{\mathbf{k}^{(q)}}{k^{(q)}_3}\,\mathbf{m}^\mathrm{T} - \mathbf{m}\left(\frac{\mathbf{k}^{(q)}}{k^{(q)}_3}\right)^\mathrm{T} + m\,\frac{\mathbf{k}^{(q)}}{k^{(q)}_3}\left(\frac{\mathbf{k}^{(q)}}{k^{(q)}_3}\right)^\mathrm{T} \quad . \tag{2}$$

The initial value of the vector of the mixed second–order space–time derivatives of the complex–valued travel time in the ray–centred coordinates reads (Klimeš, 2007, eq. 238)

$$\mathbf{M}^{\alpha}_{\mathbf{GP}\,4} = \frac{\omega^0}{k_3^{(q)}}\left(m\frac{\mathbf{k}^{(q)}}{k_3^{(q)}} - \mathbf{m}\right) \quad . \tag{3}$$

We do not need the initial value of the second–order time derivative $M^{\alpha}_{\mathbf{GP}\,44}$ of the complex–valued travel time for optimizing the shape of the scattered Gaussian packet.

For the zero source–receiver offset, the rays of the incident wave and of the scattered Gaussian packet coincide. Matrix $\mathbf{T}^{(q)}$ then equals the matrix of the second–order derivatives of travel time in the ray–centred coordinates, and vector $\mathbf{k}^{(q)}$ vanishes.

Vector $\mathbf{m}$ in (3) reads (Klimeš, 2007, eq. 127)

$$\mathbf{m} = \mathbf{T}_3^{(q)} - \mathbf{M}_3^{\alpha} + \mathrm{i}\omega^{-1}\mathbf{K}_3^{(q)} \quad . \tag{4}$$

Vector $\mathbf{M}_3^{\alpha}$ vanishes in a homogeneous velocity model. Vector $\mathbf{T}_3^{(q)}$ vanishes for the zero source–receiver offset.

In our homogeneous velocity model, the 2×2 matrix of the second–order derivatives of travel time of the incident wave in the ray–centred coordinates reads

$$\mathbf{T}^{(q)} = V^{-1}x^{-1}\,\mathbf{1} \quad , \tag{5}$$

where V is the propagation velocity of the incident wave, x is the distance from the source, and $\mathbf{1}$ is the 2×2 identity matrix.

2.2. Isotropic envelopes of the structural Gabor functions

We are presently unable to minimize the total squared width of a Gaussian packet, but we are able to minimize the total squared width of a Gaussian beam. The total squared width of a Gaussian packet coincides with the total squared width of the Gaussian beam corresponding to matrix $\mathbf{M}^{\alpha}_{\mathbf{GP}}$ if vector $\mathbf{M}^{\alpha}_{\mathbf{GP}\,4}$ vanishes. In our case, vector $\mathbf{M}^{\alpha}_{\mathbf{GP}\,4}$ vanishes if vector $\mathbf{m}$ vanishes, and vector $\mathbf{m}$ vanishes if vector $\mathbf{K}_3^{(q)}$ vanishes. For the sake of simplicity, we thus require constraint

$$\mathbf{K}_3^{(q)} = \mathbf{0} \quad . \tag{6}$$

Then the optimum value of 2×2 matrix $\mathbf{M}^{\alpha}_{\mathbf{GP}}$ coincides with matrix $\mathbf{M}^{\alpha}$ corresponding to the optimized Gaussian beam.

For a point source in a homogeneous medium, the optimized Gaussian beams are rotationally symmetric,

$$\mathbf{M}^{\alpha\mathrm{opt}}_{\mathbf{GP}} = M^{\alpha\mathrm{opt}}\,\mathbf{1} \quad , \tag{7}$$

where $\mathbf{1}$ is the 2×2 identity matrix.

Vector $\mathbf{K}_3^{(q)}$ vanishes if the envelope of the structural Gabor function is isotropic. The simplest way, how to satisfy both equations (6) and (7), is thus to require constraint

$$\mathbf{K}^{\alpha} = K^{\alpha}\,\mathbf{1} \tag{8}$$

of the isotropic envelopes of the structural Gabor functions, where $\mathbf{1}$ is the 3×3 identity matrix. Without this constraint, matrix $\mathbf{K}^{\alpha}$, which depends on x_3^{α} and k_3^{α} as we shell see later, would depend also on k_1^{α} and k_2^{α}. The dependence of matrix $\mathbf{K}^{\alpha}$ on k_1^{α} and k_2^{α} would considerably complicate our analytical determination of the phase–space lattice of the central points of Gabor functions.

Then the 2×2 submatrix of matrix $\mathbf{K}^\alpha$ transformed to the ray–centred coordinates reads

$$\mathbf{K}^{(q)} = K^\alpha \, \mathbf{1} \quad , \tag{9}$$

where $\mathbf{1}$ is the 2×2 identity matrix. Equation (2) then reads

$$\mathbf{M}^\alpha_{\mathbf{GP}} = V^{-1} x^{-1} \, \mathbf{1} + \mathrm{i}\omega^{-1} K^\alpha \, \mathbf{1} \quad , \tag{10}$$

and the optimum isotropic envelopes of the structural Gabor functions are determined by 3×3 matrix (8) with

$$K^\alpha = \mathrm{i}\omega \, (V^{-1} x^{-1} - M^{\alpha\mathrm{opt}}) \quad , \tag{11}$$

see (7).

2.3. Narrowest Gaussian beam in a homogeneous medium

We minimize the total squared widths of the scattered Gaussian packet which equals total squared widths of the Gaussian beam corresponding to matrix $\mathbf{M}^\alpha_{\mathbf{GP}}$. For a point source in a homogeneous medium, all 2×2 matrices used by Klimeš (1989) for optimization of the shape of Gaussian beams are multiples of the identity matrix, and the optimized Gaussian beams are rotationally symmetric. We thus replace all these 2×2 matrices in the ray–centred coordinates by scalars.

To minimize the total squared widths of the scattered Gaussian packet, we take in equation (49) by Klimeš (1989)

$$U = 1 \quad , \qquad W = 0 \quad . \tag{12}$$

In a homogeneous velocity model, the geometrical–spreading components of the paraxial ray propagator matrix used for the optimization read

$$Q_1 = 1 \quad , \qquad Q_2 = \sigma \quad , \tag{13}$$

where σ is the integral of velocity with respect to the arclength along the ray to the receiver.

The integrals used for the optimization then read (Klimeš, 1989, eqs. 71 and 72)

$$B_{11} = \int_0^\sigma \mathrm{d}\sigma \, Q_1 Q_1 = \sigma \quad [1] \quad \{1\} \quad , \tag{14}$$

$$B_{12} = \int_0^\sigma \mathrm{d}\sigma \, Q_1 Q_2 = \tfrac{1}{2}\sigma^2 \quad [\tfrac{1}{2}\sigma] \quad \{\sigma\} \quad , \tag{15}$$

$$B_{22} = \int_0^\sigma \mathrm{d}\sigma \, Q_2 Q_2 = \tfrac{1}{3}\sigma^3 \quad [\tfrac{1}{2}\sigma^2] \quad \{\sigma^2\} \quad , \tag{16}$$

and (Klimeš, 1989, eq. 90)

$$C_{11} = B_{11} - B_{12}^2 B_{22}^{-1} = \tfrac{1}{4}\sigma \quad [\tfrac{1}{2}] \quad \{0\} \quad . \tag{17}$$

The values in brackets [] correspond to minimization of the squared widths of a Gaussian beam at the scatterer and receiver only, not along the whole ray. The values in braces {} correspond to minimization of the squared widths of a Gaussian beam at the receiver only, which makes sense only if the real part of M^α is for some reason fixed.

The optimum initial value $M^{\alpha\mathrm{opt}}$ of the second–order derivative of the complex–valued travel time in the ray–centred coordinates is then determined by equations (Klimeš, 1989, eq. 87)

$$\mathrm{Re}(M^{\alpha\mathrm{opt}}) = -B_{12}B_{22}^{-1} = -\tfrac{3}{2}\,\sigma^{-1} \quad \left[-\,\sigma^{-1}\right] \quad , \tag{18}$$

and (Klimeš, 1989, eq. 99)

$$\mathrm{Im}(M^{\alpha\mathrm{opt}}) = C_{11}^{\frac{1}{2}}B_{22}^{-\frac{1}{2}} = \tfrac{\sqrt{3}}{2}\,\sigma^{-1} \quad \left[\sigma^{-1}\right] \quad . \tag{19}$$

Note that the width of a Gaussian beam at the receiver is determined by

$$\mathrm{Im}(M) = \frac{\mathrm{Im}(M^{\alpha})}{(1+\sigma\,\mathrm{Re}M^{\alpha})^2 + (\sigma\,\mathrm{Im}M^{\alpha})^2} \quad . \tag{20}$$

Inserting (18) and (19) into (20), we obtain

$$\mathrm{Im}(M^{\mathrm{opt}}) = \tfrac{\sqrt{3}}{2}\,\sigma^{-1} \quad \left[\sigma^{-1}\right] \quad , \tag{21}$$

and see that the width of the optimized Gaussian beam at the receiver is equal to its initial width in a homogeneous medium, as expected.

In our homogeneous velocity model,

$$\sigma = v\,x \quad , \tag{22}$$

where v is the propagation velocity of the scattered wave and x is the distance to the receiver.

The optimum shape of the scattered Gaussian beam in a homogeneous medium is

$$M^{\alpha\mathrm{opt}} = v^{-1}x^{-1}\,M^0 \tag{23}$$

with

$$M^0 = -\tfrac{3}{2} + \mathrm{i}\tfrac{\sqrt{3}}{2} \quad \left[-\,1+\mathrm{i}\right] \quad , \tag{24}$$

which follows from equations (18) and (19) with (22).

2.4. Narrowest Gaussian beam with fixed initial wavefront curvature in a homogeneous medium

If we decide, e.g., that $\mathrm{Im}\mathbf{K}^{\alpha}$ should vanish, $\mathrm{Re}(M_{11}^{\alpha})$ is determined. In this case, we should optimize $\mathrm{Im}(M_{11}^{\alpha})$ for given $\mathrm{Re}(M_{11}^{\alpha}) = R_{11}^{\alpha}$. Then (Klimeš, 1989, eq. 102)

$$\begin{aligned}\mathrm{Im}(M^{\alpha\mathrm{opt}}) = \sqrt{C_{11}B_{22}^{-1} + (R_{11}^{\alpha} + B_{12}B_{22}^{-1})^2} &= \sqrt{\tfrac{3}{4}\sigma^{-2} + (R_{11}^{\alpha} + \tfrac{3}{2}\sigma^{-1})^2} \\ &\quad \left[\sqrt{\sigma^{-2} + (R_{11}^{\alpha} + \sigma^{-1})^2}\right] \\ &\quad \left\{\left|R_{11}^{\alpha} + \sigma^{-1}\right|\right\} \quad .\end{aligned} \tag{25}$$

For example, for

$$\mathrm{Re}(M_{11}^{\alpha}) = R_{11}^{\alpha} = \sigma^{-1} \quad , \tag{26}$$

which corresponds to $\mathrm{Im}\mathbf{K}^{\alpha} = \mathbf{0}$ and zero–offset scattering without wave conversion, we have

$$\mathrm{Im}(M^{\alpha\mathrm{opt}}) = \sqrt{7}\,\sigma^{-1} \quad \left[\sqrt{5}\,\sigma^{-1}\right] \quad \left\{2\,\sigma^{-1}\right\} \quad , \tag{27}$$

where the values in brackets [] correspond to minimization of the squared widths of a Gaussian beam at the scatterer and receiver only, and the values in braces {} correspond to minimization of the squared widths of a Gaussian beam at the receiver only.

Inserting (26) and (27) into (20), we obtain

$$\mathrm{Im}(M^{\mathrm{opt}}) = \tfrac{\sqrt{7}}{11}\,\sigma^{-1} \quad \left[\tfrac{\sqrt{5}}{9}\,\sigma^{-1}\right] \quad \left\{\tfrac{1}{4}\,\sigma^{-1}\right\} \quad . \tag{28}$$

Comparing (28) with (21), we see that constraint $\mathrm{Im}\mathbf{K}^{\alpha} = \mathbf{0}$ results in approximately twice wider Gaussian beams at the receiver than the Gaussian beams corresponding to (18) and (19).

It is thus worth to choose complex–valued $\mathbf{K}^{\alpha}$ and to optimize $\mathrm{Im}\mathbf{K}^{\alpha}$ in order to refocus the scattered Gaussian packet formed of the incident wavefield.

2.5. Optimum isotropic envelopes of the structural Gabor functions

Inserting (23) into (11), we obtain

$$K^{\alpha} = \mathrm{i}\omega\,(V^{-1}x^{-1} - v^{-1}x^{-1}M^{0}) \quad . \tag{29}$$

We express the distance x of source and receiver from the central point of the Gabor function in terms of positive x_3^{α} and negative k_3^{α},

$$x = \omega\,(V^{-1} + v^{-1})\left|\tfrac{x_3^{\alpha}}{k_3^{\alpha}}\right| \quad . \tag{30}$$

Inserting (30) into (29), we arrive at

$$K^{\alpha} = \left|\tfrac{k_3^{\alpha}}{x_3^{\alpha}}\right| K^{0} \quad , \tag{31}$$

where

$$K^{0} = \mathrm{i}\,(V^{-1} - v^{-1}M^{0})(V^{-1} + v^{-1})^{-1} = \mathrm{i}\,(v - V\,M^{0})\,(v + V)^{-1} \quad , \tag{32}$$

which simplifies to

$$K^{0} = \mathrm{i}\,\tfrac{1}{2}\,(1 - M^{0}) \tag{33}$$

for scattering without wave conversion. Equation (33) with (24) reads

$$K^{0} = \tfrac{\sqrt{3}}{4} + \mathrm{i}\,\tfrac{5}{4} \quad \left[\tfrac{1}{2} + \mathrm{i}\right] \quad . \tag{34}$$

For negative $k_3^{\alpha}/x_3^{\alpha}$, the optimum isotropic envelopes of the structural Gabor functions are determined by 3×3 matrix (8) with (31)–(34). For positive $k_3^{\alpha}/x_3^{\alpha}$, the sign of $\mathrm{Im}K^{0}$ must be changed to opposite.

3. Phase–space lattice of the central points of Gabor functions

We assume here that symmetric complex–valued matrix $\mathbf{K}^\alpha$ depends on coordinate x_3^α and wavenumber k_3^α through equation

$$\mathbf{K}^\alpha = \left|\tfrac{k_3^\alpha}{x_3^\alpha}\right| \mathbf{K}^0 \quad , \tag{35}$$

where $\mathbf{K}^0$ is a constant matrix. We denote

$$\mathbf{Y}^0 = \mathrm{Re}\mathbf{K}^0 \tag{36}$$

and

$$\mathbf{R}^0 = -\mathrm{Im}\mathbf{K}^0 \quad . \tag{37}$$

Matrix $\mathbf{Y}^0$ must be positive definite. We also assume that matrices $\mathbf{Y}^0$ and $\mathbf{R}^0$ are diagonal.

We assume here that both x_3^α and k_3^α are positive. Then, for scattering without wave conversion, the simple optimization of Section 2 resulting in equation (34) with the opposite sign of $\mathrm{Im}K^0$ yields

$$\mathbf{Y}^0 = \tfrac{\sqrt{3}}{4}\mathbf{1} \tag{38}$$

and

$$\mathbf{R}^0 = \tfrac{5}{4}\mathbf{1} \quad , \tag{39}$$

where $\mathbf{1}$ is the identity matrix. Gabor functions with negative k_3^α can be obtained by simultaneously changing the signs of k_3^α and $\mathbf{R}^0$.

3.1. Lattice in 1–D

In 1–D, we have phase space coordinates x_3 and k_3. Matrix $\mathbf{Y}^0$ reduces to a single positive number which we briefly denote here Y. Matrix $\mathbf{R}^0$ for positive x_3^α and k_3^α reduces to a single number which we denote R. In the x_3k_3 plane, we consider a lattice of discrete points $(x_3^\alpha, k_3^\alpha) = (x_{mn}, k_{mn})$ indexed by integer values of discretization coordinates $m_1 = m$ and $m_2 = n$.

We assume that the coordinates (x_3^α, k_3^α) of the lattice points are discrete values of continuous positive functions $x(m,n)$ and $k(m,n)$,

$$x_3^\alpha = x(m,n) \quad , \qquad k_3^\alpha = \pm k(m,n) \quad . \tag{40}$$

We approximate the matrix of vectorial lattice intervals by the derivatives,

$$\mathbf{D} \approx \begin{pmatrix} \frac{\partial x}{\partial m} & \frac{\partial x}{\partial n} \\ \pm\frac{\partial k}{\partial m} & \pm\frac{\partial k}{\partial n} \end{pmatrix} \quad . \tag{41}$$

The 2×2 covariant metric tensor in coordinates (x,k) reads (Klimeš, 2008b, eq. 3)

$$\mathbf{G}_{\bullet\bullet} = \begin{pmatrix} 1 & 0 \\ \mp\frac{Rk}{x} & 1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \frac{Yk}{x} & 0 \\ 0 & \frac{x}{Yk} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ \mp\frac{Rk}{x} & 1 \end{pmatrix} \quad , \tag{42}$$

and corresponding contravariant metric tensor reads (Klimeš, 2008b, eq. 4)

$$\mathbf{G}^{\bullet\bullet} = \begin{pmatrix} 1 & \pm\frac{Rk}{x} \\ 0 & 1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \frac{x}{Yk} & 0 \\ 0 & \frac{Yk}{x} \end{pmatrix} \begin{pmatrix} 1 & \pm\frac{Rk}{x} \\ 0 & 1 \end{pmatrix} \quad . \tag{43}$$

We see, that the sign of k_3^α does not influence covariant discretization metric tensor $\mathbf{D}^{\mathrm{T}}\mathbf{G}_{\bullet\bullet}\mathbf{D}$. We may thus consider just the upper sign in further derivations.

Hyperbolas

$$x\,k = c \tag{44}$$

corresponding to different constants c are equidistant with respect to metric (42), (43). The distance of two close hyperbolas is inversely proportional to the norm of the gradient of the left–hand side of (44) with respect to metric tensor (43). The square of the norm of the gradient is

$$\begin{pmatrix} k \\ x \end{pmatrix}^{\mathrm{T}} \mathbf{G}^{\bullet\bullet} \begin{pmatrix} k \\ x \end{pmatrix} = (1+R)^2 Y^{-1} x k + Y x k = [(1+R)^2 Y^{-1} + Y]\, c \quad . \tag{45}$$

We parametrize the hyperbolas by discretization coordinate n of functions (40). Then $\frac{\mathrm{d}c}{\mathrm{d}n}$ should be equal to the norm multiplied by

$$\kappa = \sqrt{\frac{2\pi}{\text{redundancy ratio}}} \quad , \tag{46}$$

$$\tfrac{\mathrm{d}c}{\mathrm{d}n} = \kappa \sqrt{[(1+R)^2 Y^{-1} + Y]\, c} \quad . \tag{47}$$

We solve this differential equation and choose

$$c = \tfrac{\kappa^2}{4} [(1+R)^2 Y^{-1} + Y]\, n^2 \quad . \tag{48}$$

We parametrize the points along individual hyperbolas by discretization coordinate m of functions (40) and express x and k in terms of function $\frac{x}{k} = \frac{x}{k}(m)$,

$$x = \sqrt{c \tfrac{x}{k}(m)} \quad , \qquad k = \sqrt{c / \tfrac{x}{k}(m)} \quad . \tag{49}$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}m} \begin{pmatrix} x \\ k \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{k}{x} \end{pmatrix} \frac{1}{2} \sqrt{\frac{c}{\frac{x}{k}}} \, \frac{\mathrm{d}\frac{x}{k}}{\mathrm{d}m} \quad . \tag{50}$$

The square of the norm of this vector with respect to metric (42) should be equal to κ^2 (Klimeš, 2008b, sec. 4.1),

$$\frac{[(1+R)^2 Y^{-1} + Y]}{4} \, \frac{c}{(\frac{x}{k})^2} \left(\frac{\mathrm{d}\frac{x}{k}}{\mathrm{d}m} \right)^2 = \kappa^2 \quad . \tag{51}$$

We insert (48), solve this differential equation, and choose

$$\tfrac{x}{k} = \exp(2\alpha \tfrac{m}{n}) \quad , \tag{52}$$

where

$$\alpha = \frac{2}{(1+R)^2 Y^{-1} + Y} \quad . \tag{53}$$

For integer values of m and positive integer values of n, we obtain lattice

$$\boxed{\begin{aligned} x(m,n) &= \tfrac{\kappa}{2} \sqrt{(1+R)^2 Y^{-1} + Y}\, n \exp(\alpha \tfrac{m}{n}) \quad , && (54) \\ k(m,n) &= \tfrac{\kappa}{2} \sqrt{(1+R)^2 Y^{-1} + Y}\, n \exp(-\alpha \tfrac{m}{n}) && (55) \end{aligned}}$$

of positive $x(m,n)$ and $k(m,n)$.

Differentiating (54) and (55) with respect to m and n, we obtain matrix (41) of vectorial lattice intervals,

$$\mathbf{D} \approx \begin{pmatrix} \alpha \frac{x}{n} & (1 - \alpha \frac{m}{n}) \frac{x}{n} \\ -\alpha \frac{k}{n} & (1 + \alpha \frac{m}{n}) \frac{k}{n} \end{pmatrix} \quad . \tag{56}$$

We calculate matrix product

$$\begin{pmatrix} 1 & 0 \\ -\frac{Rk}{x} & 1 \end{pmatrix} \mathbf{D} \approx \begin{pmatrix} \alpha\frac{x}{n} & [1-\alpha\frac{m}{n}]\frac{x}{n} \\ -\alpha(1+R)\frac{k}{n} & [1-R+\alpha(1+R)\frac{m}{n}]\frac{k}{n} \end{pmatrix} \quad . \tag{57}$$

We further multiply the matrices and, considering equations (53), (54) and (55), we arrive at

$$\begin{pmatrix} \sqrt{\frac{Yk}{x}} & 0 \\ 0 & \sqrt{\frac{x}{Yk}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{Rk}{x} & 1 \end{pmatrix} \mathbf{D} \approx \kappa \begin{pmatrix} \sqrt{\frac{\alpha Y}{2}} & \sqrt{\frac{Y}{2\alpha}}(1-\alpha\frac{m}{n}) \\ -\sqrt{\frac{\alpha}{2Y}}(1+R) & \sqrt{\frac{1}{2\alpha Y}}[1-R+\alpha(1+R)\frac{m}{n}] \end{pmatrix} . \tag{58}$$

We multiply the right–hand side of (58) from the left by unitary matrix

$$\mathbf{U} = \sqrt{\frac{1}{(1+R)^2+Y^2}} \begin{pmatrix} Y & -(1+R) \\ 1+R & Y \end{pmatrix} \tag{59}$$

and, considering (53), obtain

$$\mathbf{U} \begin{pmatrix} \sqrt{\frac{Yk}{x}} & 0 \\ 0 & \sqrt{\frac{x}{Yk}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{Rk}{x} & 1 \end{pmatrix} \mathbf{D} = \kappa \begin{pmatrix} 1 & \frac{Y^2+R^2-1}{2Y} - \frac{m}{n} \\ 0 & 1 \end{pmatrix} \quad . \tag{60}$$

We see that, in our metric, the vectorial step with respect to m is constant and that the component of the vectorial step with respect to n, perpendicular to the vectorial step with respect to m, is also constant. The lattice is thus formed by chains of points corresponding to constant n. The points within the chains are equidistant with respect to our metric. The distance between the chains is also constant in our metric.

Using matrix (60), we easily calculate covariant discretization metric tensor

$$\mathbf{D}^{\mathrm{T}}\mathbf{G}_{\bullet\bullet}\mathbf{D} \approx \kappa^2 \begin{pmatrix} 1 & \frac{Y^2+R^2-1}{2Y} - \frac{m}{n} \\ \frac{Y^2+R^2-1}{2Y} - \frac{m}{n} & 1+(\frac{Y^2+R^2-1}{2Y} - \frac{m}{n})^2 \end{pmatrix} \quad . \tag{61}$$

The rightmost matrix is symplectic, and the inverse of (61) yields contravariant discretization metric tensor

$$(\mathbf{D}^{\mathrm{T}}\mathbf{G}_{\bullet\bullet}\mathbf{D})^{-1} \approx \kappa^{-2} \begin{pmatrix} 1+(\frac{m}{n} - \frac{Y^2+R^2-1}{2Y})^2 & \frac{m}{n} - \frac{Y^2+R^2-1}{2Y} \\ \frac{m}{n} - \frac{Y^2+R^2-1}{2Y} & 1 \end{pmatrix} \quad . \tag{62}$$

Metric tensors (61) and (62) depend on m and n. This dependence is slow for large m and n. For large m and n, we may thus introduce the local upper frame bound (Klimeš, 2008b, eq. 10).

$$B = \kappa^2 \sum_{j_1,j_2} \exp\Big(-\pi^2\kappa^{-2} \{ j_1^2 + [(\tfrac{m}{n} - \tfrac{Y^2+R^2-1}{2Y})j_1 + j_2]^2 \} \Big) \quad , \tag{63}$$

and the local lower frame bound (Klimeš, 2008b, eq. 11).

$$A = 2\,\kappa^2 \sum_{j_1,j_2} \exp\Big(-(2\pi)^2\kappa^{-2} \{ j_1^2 + [(\tfrac{m}{n} - \tfrac{Y^2+R^2-1}{2Y})j_1 + j_2]^2 \} \Big) - B \quad . \tag{64}$$

However, the global upper frame bound is

$$B = \kappa^2 \sum_{j_1,j_2} \exp[-\pi^2\kappa^{-2}\,(j_1^2+j_2^2)] = \kappa^2 \Big[\sum_j \exp(-\pi^2\kappa^{-2}\,j^2) \Big]^2 \quad , \tag{65}$$

and the global lower frame bound is

$$A = 2\,\kappa^2 \sum_{j_1,j_2} \exp[-(2\pi)^2 \kappa^{-2}\,(j_1^2+j_2^2)] - B = 2\,\kappa^2 \left[\sum_j \exp[-(2\pi)^2 \kappa^{-2}\,j^2]\right]^2 - B \ . \quad (66)$$

3.2. Lattice in 2–D

In 2–D, we consider phase space coordinates x_1, x_3, k_1 and k_3. Matrices (36) and (37) read

$$\mathbf{Y}^0 = \begin{pmatrix} Y_{11}^0 & 0 \\ 0 & Y \end{pmatrix} \quad (67)$$

and

$$\mathbf{R}^0 = \begin{pmatrix} R_{11}^0 & 0 \\ 0 & R \end{pmatrix} \quad , \quad (68)$$

where we briefly denoted $Y_{33}^0 = Y$ and $R_{33}^0 = R$ as in Section 3.1.

The 4×4 covariant metric tensor reads (Klimeš, 2008b, eq. 3)

$$\mathbf{G}_{\bullet\bullet} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -\frac{R_{11}^0 k}{x} & 0 & 1 & 0 \\ 0 & -\frac{Rk}{x} & 0 & 1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \frac{Y_{11}^0 k}{x} & 0 & 0 & 0 \\ 0 & \frac{Yk}{x} & 0 & 0 \\ 0 & 0 & \frac{x}{Y_{11}^0 k} & 0 \\ 0 & 0 & 0 & \frac{x}{Yk} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -\frac{R_{11}^0 k}{x} & 0 & 1 & 0 \\ 0 & -\frac{Rk}{x} & 0 & 1 \end{pmatrix} , \quad (69)$$

and corresponding contravariant metric tensor reads (Klimeš, 2008b, eq. 4)

$$\mathbf{G}^{\bullet\bullet} = \begin{pmatrix} 1 & 0 & \frac{R_{11}^0 k}{x} & 0 \\ 0 & 1 & 0 & \frac{Rk}{x} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \frac{x}{Y_{11}^0 k} & 0 & 0 & 0 \\ 0 & \frac{x}{Yk} & 0 & 0 \\ 0 & 0 & \frac{Y_{11}^0 k}{x} & 0 \\ 0 & 0 & 0 & \frac{Yk}{x} \end{pmatrix} \begin{pmatrix} 1 & 0 & \frac{R_{11}^0 k}{x} & 0 \\ 0 & 1 & 0 & \frac{Rk}{x} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \quad (70)$$

In the x_3k_3 coordinate plane, we consider discrete points

$$x_3^\alpha = x(m_3, m_4) \quad , \qquad k_3^\alpha = k(m_3, m_4) \quad (71)$$

indexed by integer values of discretization coordinates m_3 and m_4. Functions x and k in (85) are defined by equations (54) and (55). Each of these discrete points defines plane parallel with the x_1k_1 coordinate plane. In each of these parallel planes $x_3 = x_3^\alpha$, $k_3 = k_3^\alpha$, we should choose a sublattice of discrete points parametrized by discretization coordinates m_1 and m_2.

The most primitive option is the rectangular sublattice

$$x_1^\alpha = m_2\,\Delta x_1(m_3, m_4) \quad , \qquad k_1^\alpha = m_1\,\Delta k_1(m_3, m_4) \quad . \quad (72)$$

We consider the algorithm by Klimeš (2008b, sec. 4.1). If we start with lines corresponding to constant m_2, the norm of the phase–space gradient $(1/\Delta x_1, 0, 0, 0)$ of m_2 in plane $x_3 = x_3^\alpha$, $k_3 = k_3^\alpha$ with respect to metric tensor (70) should equal $1/\kappa$,

$$\Delta x_1 = \kappa \sqrt{\frac{x}{Y_{11}^0 k}} \quad , \quad (73)$$

and the distance $(0, 0, \Delta k_1, 0$ of lattice points along lines corresponding to constant m_2 with respect to metric tensor (69) should equal κ,

$$\Delta k_1 = \kappa \sqrt{\frac{Y_{11}^0 k}{x}} \quad . \quad (74)$$

If we start with lines corresponding to constant m_1, the norm of the phase–space gradient $(0,0,1/\Delta k_1,0)$ of m_1 in plane $x_3 = x_3^\alpha$, $k_3 = k_3^\alpha$ with respect to metric tensor (70) should equal $1/\kappa$,

$$\Delta k_1 = \kappa \sqrt{\tfrac{k}{x}[Y_{11}^0 + (R_{11}^0)^2 (Y_{11}^0)^{-1}]} \quad , \tag{75}$$

and the distance $(\Delta x_1, 0, 0, 0)$ of lattice points along lines corresponding to constant m_1 with respect to metric tensor (69) should equal κ,

$$\Delta x_1 = \kappa / \sqrt{\tfrac{k}{x}[Y_{11}^0 + (R_{11}^0)^2 (Y_{11}^0)^{-1}]} \quad . \tag{76}$$

If we prefer smaller number of different values of x_1^α, option (73) and (74) is preferable to option (75) and (76).

Since the metric tensor is constant in each plane corresponding to constant x_3 and k_3, we may use more sophisticated algorithm by Klimeš (2008b, sec. 3) resulting in more regular coverage of these parallel planes $x_3 = x_3^\alpha$, $k_3 = k_3^\alpha$. In the Euclidean plane, we select regular triangular lattice of points (ξ_1, ξ_2),

$$\xi_1 = 2^{\frac{1}{2}} 3^{-\frac{1}{4}} m_1 + 2^{-\frac{1}{2}} 3^{-\frac{1}{4}} m_2 \quad , \tag{77}$$

$$\xi_2 = 2^{-\frac{1}{2}} 3^{\frac{1}{4}} m_2 \tag{78}$$

(Klimeš, 2008b, eq. 18). We then select

$$x_1^\alpha = \kappa \left(\tfrac{k}{x} Y_{11}^0\right)^{-\frac{1}{2}} \xi_2 \tag{79}$$

and

$$k_1^\alpha = \kappa \left[\left(\tfrac{k}{x} Y_{11}^0\right)^{\frac{1}{2}} \xi_1 + \tfrac{k}{x} R_{11}^0 \left(\tfrac{k}{x} Y_{11}^0\right)^{-\frac{1}{2}} \xi_2 \right] \tag{80}$$

(Klimeš, 2008b, eq. 19).

3.3. Lattice in 3–D

In 3–D, we consider phase space coordinates x_1, x_2, x_3, k_1, k_2, and k_3. Matrices (36) and (37) read

$$\mathbf{Y}^0 = \begin{pmatrix} Y_{11}^0 & 0 & 0 \\ 0 & Y_{22}^0 & 0 \\ 0 & 0 & Y \end{pmatrix} \tag{81}$$

and

$$\mathbf{R}^0 = \begin{pmatrix} R_{11}^0 & 0 & 0 \\ 0 & R_{22}^0 & 0 \\ 0 & 0 & R \end{pmatrix} \quad , \tag{82}$$

where we briefly denoted $Y_{33}^0 = Y$ and $R_{33}^0 = R$ as in Section 3.1.

The 6×6 covariant metric tensor reads (Klimeš, 2008b, eq. 3)

$$\mathbf{G}_{\bullet\bullet} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -\frac{R_{11}^0 k}{x} & 0 & 0 & 1 & 0 & 0 \\ 0 & -\frac{R_{22}^0 k}{x} & 0 & 0 & 1 & 0 \\ 0 & 0 & -\frac{Rk}{x} & 0 & 0 & 1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \frac{Y_{11}^0 k}{x} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{Y_{22}^0 k}{x} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{Yk}{x} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{x}{Y_{11}^0 k} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{x}{Y_{22}^0 k} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{x}{Yk} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -\frac{R_{11}^0 k}{x} & 0 & 0 & 1 & 0 & 0 \\ 0 & -\frac{R_{22}^0 k}{x} & 0 & 0 & 1 & 0 \\ 0 & 0 & -\frac{Rk}{x} & 0 & 0 & 1 \end{pmatrix} , \tag{83}$$

and corresponding contravariant metric tensor reads (Klimeš, 2008b, eq. 4)

$$\mathbf{G}^{\bullet\bullet} = \begin{pmatrix} 1 & 0 & 0 & \frac{R^0_{11}k}{x} & 0 & 0 \\ 0 & 1 & 0 & 0 & \frac{R^0_{22}k}{x} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{Rk}{x} \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \frac{x}{Y^0_{11}k} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{x}{Y^0_{22}k} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{x}{Yk} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{Y^0_{11}k}{x} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{Y^0_{22}k}{x} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{Yk}{x} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \frac{R^0_{11}k}{x} & 0 & 0 \\ 0 & 1 & 0 & 0 & \frac{R^0_{22}k}{x} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{Rk}{x} \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} . \tag{84}$$

In the x_3k_3 coordinate plane, we consider discrete points

$$x_3^\alpha = x(m_5, m_6) \quad , \qquad k_3^\alpha = k(m_5, m_6) \tag{85}$$

indexed by integer values of discretization coordinates m_5 and m_6. Functions x and k in (85) are defined by equations (54) and (55). Each of these discrete points defines 4–D linear subspace parallel with the $x_1x_2k_1k_2$ coordinate subspace. In each of these parallel subspaces $x_3 = x_3^\alpha$, $k_3 = k_3^\alpha$, we should choose a sublattice of discrete points parametrized by discretization coordinates m_1, m_2, m_3 and m_4.

The most primitive option is the rectangular sublattice

$$\begin{aligned} x_1^\alpha &= m_3\,\Delta x_1(m_3, m_4) \quad , \qquad & x_2^\alpha &= m_4\,\Delta x_2(m_3, m_4) \quad , \\ k_1^\alpha &= m_1\,\Delta k_1(m_3, m_4) \quad , \qquad & k_2^\alpha &= m_2\,\Delta k_2(m_3, m_4) \quad . \end{aligned} \tag{86}$$

Discretization steps Δx_1, Δx_2, Δk_1 and Δk_2 can be determined analogously as in Section 3.2.

Since the metric tensor is constant in each 4–D linear subspace corresponding to constant x_3 and k_3, we may use more sophisticated algorithm by Klimeš (2008b, sec. 3) resulting in more regular coverage of these parallel 4–D subspaces $x_3 = x_3^\alpha$, $k_3 = k_3^\alpha$. In the Euclidean 4–D space, we select regular lattice of points $(\xi_1, \xi_2, \xi_3, \xi_4)$,

$$\xi_1 = 5^{-\frac{1}{8}}\;\;2^{-\frac{1}{2}}\,(2\,m_1 + m_2 + m_3 + m_4) \quad , \tag{87}$$

$$\xi_2 = 5^{-\frac{1}{8}}\;\;6^{-\frac{1}{2}}\,(3\,m_2 + m_3 + m_4) \quad , \tag{88}$$

$$\xi_3 = 5^{-\frac{1}{8}}\,12^{-\frac{1}{2}}\,(4\,m_3 + m_4) \quad , \tag{89}$$

$$\xi_4 = 5^{-\frac{1}{8}}\,20^{-\frac{1}{2}}\;\;5\,m_4 \tag{90}$$

(Klimeš, 2008b, eq. 18). We then select

$$x_1^\alpha = \kappa\left(\tfrac{k}{x}Y^0_{11}\right)^{-\frac{1}{2}}\xi_3 \quad , \tag{91}$$

$$x_2^\alpha = \kappa\left(\tfrac{k}{x}Y^0_{22}\right)^{-\frac{1}{2}}\xi_4 \quad , \tag{92}$$

$$k_1^\alpha = \kappa\left[\left(\tfrac{k}{x}Y^0_{11}\right)^{\frac{1}{2}}\xi_1 + \tfrac{k}{x}R^0_{11}\left(\tfrac{k}{x}Y^0_{11}\right)^{-\frac{1}{2}}\xi_3\right] \quad , \tag{93}$$

$$k_2^\alpha = \kappa\left[\left(\tfrac{k}{x}Y^0_{22}\right)^{\frac{1}{2}}\xi_2 + \tfrac{k}{x}R^0_{22}\left(\tfrac{k}{x}Y^0_{22}\right)^{-\frac{1}{2}}\xi_4\right] \tag{94}$$

(Klimeš, 2008b, eq. 19).

Acknowledgements

The research has been supported by the Grant Agency of the Czech Republic under contract 205/07/0032, by the Ministry of Education of the Czech Republic within research project MSM0021620860, and by the members of the consortium “Seismic Waves in Complex 3–D Structures” (see “http://sw3d.cz”).

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