Geophysica (1994), 30, 1-2, 31-40

Construction of Algorithms for Optimal Fermat Ray Tracing

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(Received: December 1993; Accepted: May 1994)

Abstract

In the present paper construction of algorithms for two - point ray tracing, 2P - RT, has been carried out. The methods are based on direct optimization of the Fermat functional (OFRT). The constructed algorithms are the following: The FF - algorithm for the evaluation of the Fermat functional, the GFF - algorithm for the evaluation of the path gradient of the Fermat functional, and finally the CGFF - algorithm for the evaluation of the constrained path gradient. In this case, the construction has been carried out under two - sided inequality constraints on the path segments. By the present paper, however, the author has completed the method only for a single constraint of the above mentioned type. The idea behind the use of contraints is twofold. From one side an effort will be made to avoid the eventual flaws in computability that are caused by the method of approximation. On the other side the convergence properties of OFRT as an iterative process will be aided by an appropriate constraining.

1. Introduction

In isotropic media two - point ray tracing, or 2P - RT shortly, may be considered as an optimization (minimization) of the travel - time integral, or as favored by the present paper, the Fermat functional (FF)

$$f(\Gamma,m) = \int_{\Gamma} m \, d\sigma \tag{1}$$

In (1);

- Γ is a path (ray) connecting the two end points which are supposed to be fixed for 2P - RT,
- $\int_{\Gamma}$ is an integral along the path Γ,
- $m = \dfrac{1}{v}$ is the slowness field, and

Published by the Finnish Geophysical Society, Helsinki

- $d\sigma$ is the differential path length.

Considered as a variational problem the methods of solution of seismic 2P - RT may be classified as follows;

- as methods based on direct optimization of the FF (1).In the present paper approaches of this type will be referred to as optimal Fermat ray tracing, or OFRT shortly.
- or as methods based on solution of of the Euler equation, associated to FF, as a two - point boundary value problem.

There exist an abundance of published articles on seismic 2P - RT where the "Eulerian" point of view has been preferred over the OFRT one. For a good reference to works on this field see *Farra* (1992). As to works of OFRT type, see *Wesson* (1971), *Chander* (1975), *Kanasewich et al.* (1985), and *Chiu et al.* (1986) and *Um et al.* (1987).

By the results of the referred works one may conclude that the approaches of OFRT type to seismic 2P - RT might provide fast and versatile alternatives to the Eulerian ones.

The aims of the present paper "Construction of algorithms of optimal Fermat ray tracing" are condensed as follows: Firstly, as a working frame for constructions, a method of approximation has been developed. After that three algorithms; the FF - algorithm for path evaluation of FF, the GFF - algorithm for evaluation of the path gardient of FF and the CGFF - algorithm as an algorithm of constrained GFF will be presented.

2. *Method of approximation and construction of algorithms*

2.1 *Method of approximation*

In order to increase the consistency and systematization of the treatment it seems adviceable to introduce a formal basis for the method of approximation used in the present paper. Accordingly, two linear spaces; a path segment space (PSS) and a path coordinate space (PCS) will be introduced. Further, after a description of interrelations between the spaces to provide the path coordinate space with an inner product and a norm.

To define PSS consider a smooth and slowly varying path Γ connecting the two end points, the initial point x_0 and the final point x_{N+1}. Under these assumptions the path may be approximated to a sufficient accuracy by a piecewise smooth segment path composed of the set $\{\Gamma_1, \Gamma_2, \ldots\ldots, \Gamma_N, \Gamma_{N+1}\}$ of linear segments. Further, to construct a definite mathematical object to represent the approximate path, the segments are arranged as the (Cartesian) product,

$$\hat{\Gamma} = \{\Gamma_1, \Gamma_2, \ldots\ldots, \Gamma_N, \Gamma_{N+1}\} \tag{2}$$

As an element of PSS, the product (2), will be referred to as a segment path. The path segment space $\hat{P}$ itself is constructed as the linear span

$$\hat{P} = span\{\hat{\Gamma}\}.$$

of segment paths of the type (2).

In the context of the present paper the PSS $\hat{P}$ has only a conceptual meaning. Algorithmic constructions for computational purposes will be carried out in a path coordinate space PCS $\hat{X}$. As to a definition of PCS consider the set of nodal points

$$\left\{ x_0, x_1, \ldots\ldots, x_N, x_{N+1} \right\}$$

of a segment path. Arranged as the product,

$$\hat{x} = \left(x_0, x_1, \ldots\ldots, x_N, x_{N+1} \right), \tag{3}$$

the nodal points form a coordinate path, an element of PCS. The path coordinate space $\hat{X}$. itself will be constructed as the linear span,

$$\hat{X} = span\{\hat{x}\} ,. \tag{4}$$

of the coordinate paths of the form (3).

As a coordinate space for 2P - RT the PCS $\hat{X}$ has a special structure. Firstly, the initial and the final components, x_0 and x_{N+1}, respectively, of each $\hat{x} \in \hat{X}$ are common to all elements of $\hat{X}$. Secondly, by (3) and (4) $\hat{X}$ may be considered as a subspace of the product space

$$\prod_{j=0}^{N+1} R^n = R^n \times \ldots\ldots \times R^n.$$

Each of the component spaces R^n has been specified as R^2 in 2 - D and as R^3 in 3 - D case.

After definition of the path coordinate space $\hat{X}$ the subspace of allowable path variations $\hat{X}_0$ is defined by

$$\hat{X}_0 = \{ \hat{x} \in \hat{X} \mid x_0 = 0 \text{ and } x_{N+1} = 0 \}$$

For actual constructions of the algorithms it is helpful to introduce an inner product and a norm in $\hat{X}$. The inner product, $\hat{X}$ - IP, is defined by

$$(\hat{x}^1 \| \hat{x}^2)_{\hat{x}} = \sum_{j=0}^{N+1} x_j^1 \cdot x_j^2 . \tag{5}$$

The norm, in turn, will be defined with the aid of $\hat{X}$- IP as follows

$$\| \hat{x} \|_{\hat{x}} = (\hat{x} \| \hat{x})_x^{½}$$

As the final topic of the present section a coordinate mapping between $\hat{X}$ and $\hat{P}$ will be defined componentwise, for each $j = 1,2,......,N,N+1$, by

$$\Gamma_j = x_j - x_{j-1} .$$

2.2 *Construction of FF- algorithm*

The Fermat functional was defined as the path integral (1). Its algorithmic construction means its representation by the adopted approximation. Consequently, it is natural to refer to the following PCS - representation

$$f(\hat{x}) = \sum_{j=1}^{N+1} m_j \left\| x_j - x_{j-1} \right\|_{R^n} \tag{6}$$

as the FF - algorithm. In (6), the lengths $\left\| x_j - x_{j-1} \right\|_{R^n}$ of the path segments are defined for $j = 1,2,......,N,N+1$ by

$$\left\| x_j - x_{j-1} \right\|_{R^n} = \left\{ \left(x_j - x_{j-1} \right) \cdot \left(x_j - x_{j-1} \right) \right\}^{½} \tag{7}$$

where $\| \; \|_{R^n}$ is the R^n - *norm* and the "dot" is the R^n - dot product.

The FF - algorithm (6) is computationally fast. The reliability of the algorithm as a representation of the Fermat functional is dependent both on a dense and uniform distribution of the nodal points.

2.3 *Construction of the GFF - algorithm*

The construction is started by representing the FF - algorithm (6) with the aid of (7) in the form,

$$f(\hat{x}) = \sum_{j=1}^{n+1} m_j = \left\{ \left(x_j - x_{j-1} \right) \cdot \left(x_j - x_{j-1} \right) \right\}^{1/2}$$

Applying first variation to both sides of the above expression results in

$$\delta f(\hat{x}) = \sum_{j=1}^{n+1} m_j \, \delta = \left\{ \left(x_j - x_{j-1} \right) \cdot \left(x_j - x_{j-1} \right) \right\}^{1/2} . \tag{8}$$

It is not difficult to see that the variation of the expression with the braces in (8) is of the form

$$\delta \left\{ \left(x_j - x_{j-1} \right) \cdot \left(x_j - x_{j-1} \right) \right\}^{1/2} = \frac{\left(x_j - x_{j-1} \right) \cdot \delta \left(x_j - x_{j-1} \right)}{\left\| x_j - x_{j-1} \right\|_{R^n}} . \tag{9}$$

A substitution of (9) in (8) and carrying out the the obvious manipulations results in the following expression;

$$\delta f(\hat{x}) = \sum_{j=1}^{N} \left\{ k_j(\hat{x}) - k_{j+1}(\hat{x}) \right\} \cdot \delta x_j . \tag{10}$$

In (10), δx_j s are the components of an allowable variation $\delta x^0 \in \hat{X}_0$ of the path coordinates. Further, as notational convenience, the weighted segment direction vectors (WSDV) $k_j(\hat{x})$, for $j = 1,2,\ldots\ldots,N,N+1$, have been defined by

$$k_j(\hat{x}) = m_j \frac{x_j - x_{j-1}}{\left\| x_j - x_{j-1} \right\|_{R^n}} . \tag{11}$$

Finally, the relation between the FF and its path gradient will be expressed with the aid of the $\hat{X}$ - IP (5) by

$$\delta f(\hat{x}) = (\gamma(\hat{x}) \| \; \delta x_0)_{\hat{x}} \; . \tag{12}$$

It is easy to verify by (10), (11) and (12) that the path gradient, the GFF - algorithm, is determined by the product expression

$$\gamma(\hat{x}) = \left(0, \gamma_1(\hat{x}), \ldots\ldots, \gamma_j(\hat{x}), \ldots, \gamma_n(\hat{x}), 0 \right) \; , \tag{13}$$

where the components, for $j = 1,2,\ldots\ldots,N$, are defined by

$$\gamma_j(\hat{x}) = k_j(\hat{x}) - k_{j+1}(\hat{x}) \; . \tag{14}$$

Further, $k_j(\hat{x})$ s in (14) are the WSDV s (11).

As to the computational aspects of the GFF - algorithms (11), (13) and (14) it is seen firstly that their implementation in computer is simple. Further, their evaluation by a computer is fast. However, with respect to reliability, an iterative optimization process may favor an uneven distribution of nodal points. Consequently, either too long or too short path segments may appear at certain iteration steps. These phenomena may cause difficulties of several types; either computational problems, or lack of convergence of the optimal iterations, or appearance of "artifacts" of some kind as a result of the iterations of OFRT.

By the present paper the author has suggested a method to control these phenomena. For the representation of the method as well as its application to construction of constrained gradient algorithms, the CGFF - algorithms, see the next section.

2.4 *Construction of CGFF - algorithms*

The construction of the algorithms of constrained path gradients will be carried out by the following three stages. At the first stage, on the basis of certain inequality constraints, the segments are separated into feasible and infeasible ones. The second stage consists of introduction tangentiality constraints, again, a constraint per segment. The actual costruction of the CGFF - algorithms will be completed at the third stage.

As a notational convention the segment index set I^{seg} will be defined by

$$I^{seg} = \{ j \mid j = 1,2,\ldots\ldots,N+1 \}$$

After that a constraint function will be introduced for each segment $j \in I^{seg}$ by

$$\overset{j}{c}(\hat{x}) = \frac{1}{2} \left\{ \left\| x_j - x_{j-1} \right\|_{R^n} \right\}^2 \; . \tag{15}$$

Next, for each seqment $j \in I^{seg}$, an inequality constraint is defined by

$$\varepsilon^s \le \overset{j}{c}(\hat{x}) \le \varepsilon^l \tag{16}$$

As seen by (15), the inequalities (16) set upper and lower bounds to the lengths of the segments. Further, ε^s and ε^l are certain control parameters. By the present paper the inequality constraints (16) have been suggested to be used to control the iterations of OFRT in the following way; the segments, or equivalently the segment index set I^{seg} will be separated into feasible and infeasible segments, I^{fe} and I^{infe}, respectively. A segment is called feasible if the inequality (16) is satisfied, otherwise it is infeasible. The result of the separation may be represented by the union,

$$I^{seg} = I^{fe} \cup I^{infe}$$

The second stage in constructing algorithms of CGFF's consists of an introduction of tangentiality constraints for the path gradient. Thus, consider the CF's (15) which by (7) take, for each $j \in I^{infe}$, the form

$$\overset{j}{c}(\hat{x}) = \frac{1}{2}\left(x_j - x_{j-1}\right)\cdot\left(x_j - x_{j-1}\right) .$$

It is not difficult to verify that the first variation of each CF is defined by

$$\delta\,\overset{j}{c}(\hat{x}) = \left(x_j - x_{j-1}\right)\cdot \delta x_j - \left(x_j - x_{j-1}\right)\cdot \delta x_{j-1} . \tag{17}$$

Further, by the $\hat{X}$ - IP (5) the variation (17) may be represented as follows

$$\delta\,\overset{j}{c}(\hat{x}) = \left(\overset{j}{g}(\hat{x}) \;||\; \delta \hat{x}_0\right) \tag{18}$$

In (18), $\overset{j}{g}(\hat{x})$ is the gradient of the CF (GCF) and $\delta x_0 \in \hat{X}_0$ is an allowable path variation. A comparison of (17) and (18) results in the following expressions of the GCF:

$$\overset{j}{g}(\hat{x}) = (0,0,0,\ldots,\overset{j}{g}_{j-1}(\hat{x}),\overset{j}{g}_{j}(\hat{x}),\ldots,0,0)$$

where the components are defined by

$$\overset{j}{\underset{j}{g}}(\hat{x}) = \underset{j}{x} - \underset{j-1}{x} = -\overset{j}{\underset{j-1}{g}}(\hat{x}) \ . \tag{19}$$

After these preliminary determinations, the tangentiality constraints (TC) will be defined. For OFRT it is natural to consider path updates of gradient type; i.e. those of the form

$$\delta\hat{x}_0 = \sigma\,\gamma(\hat{x}) \ . \tag{20}$$

In (20), σ is a scaling factor and $\gamma(\hat{x})$ is the path gradient GFF. The tangentiality constraint (TC), for $j \in I^{infe}$, to $\delta x_0 \in \hat{X}_0$ and by (20) to the GFF $\gamma(\hat{x})$ is defined by

$$\left(\overset{j}{g}(\hat{x}) \parallel \gamma(\hat{x})\right)_{\hat{x}} = 0 \ . \tag{21}$$

By (20) and (21) it is seen that the role of the TC's is to prevent an "increase of infeasibility" of path segments.

It was stated previously that by the present paper the construction of the CGFF - algorithms will be carried out only for a single infeasible segment. The multi - infeasible case will be treated as a topic of the forthcoming paper. Consider now an infeasible segment $j \in I^{infe}$. With the aid of (13), (19) and (20) the TC (21) may be represented in the componentwise form

$$\overset{j}{\underset{j}{g}}(\hat{x}) \cdot \left\{ \underset{j}{\gamma}(\hat{x}) - \underset{j-1}{\gamma}(\hat{x}) \right\} = 0 \ . \tag{22}$$

However, it is easy to verify that, besides (22), even the simpler relation

$$\underset{j}{\gamma}(\hat{x}) = \underset{j-1}{\gamma}(\hat{x}) \tag{23}$$

satisfies the TC (21). As a conclusion of the previous derivations one may add that in the present case only the components $\underset{j-1}{\gamma}(\hat{x})$ and $\underset{j}{\gamma}(\hat{x})$ of the GFF are constrained by the TC (21) through (23). The other components of the GFF will remain their algorithmic expressions (14).

As to the constrained components $\underset{j-1}{\gamma}(\hat{x})$ and $\underset{j}{\gamma}(\hat{x})$ it is seen that by (14)

$$\underset{j-1}{\gamma}(\hat{x}) = \underset{j-1}{k}(\hat{x}) - \underset{j}{k}$$

and (24)

$$\gamma_j(\hat{x}) = k_j - k_{j+1}(\hat{x})$$

where k_j is an unknown WSDV for $j \in I^{infe}$. To determine k_j substitute (24) in (23) to find that

$$k_j = \frac{1}{2}\left\{ k_{j-1}(\hat{x}) + k_{j+1}(\hat{x}) \right\} . \tag{25}$$

Consequently, by (25) the constrained WSDV of an infeasible segment has to be determined as the arithmetic mean of the adjacent WSDV's. Finally, the constrained components $\gamma_{j-1}(\hat{x})$ and $\gamma_j(\hat{x})$ of the CGFF are by (24) and (25) seen to be given by

$$\gamma_{j-1}(\hat{x}) = \gamma_j(\hat{x}) = -\frac{1}{2}\left\{ k_{l+1}(\hat{x}) - k_{l-1}(\hat{x}) \right\} . \tag{26}$$

3. *Conclusions*

The following conclusions are drawn by the results of the paper:

- An approximation method for path integrals has been developed as a working frame
- On the basis of the approximation method the following algorithms have been constructed; the FF - algorithms (6) and (7) for evaluation of the Fermat functional, the GFF - algorithms (11), (13) and (14) for the evaluation of the path gradient of the Fermat functional and the CGFF - algorithms (11), (13), (14) and (26) for the evaluation of the constrained path gradient of the Fermat functional.
- A new method has been developed for a control of the lengths of the path segments. The method consists of two stages. At the first stage the path segments are divided into feasible and infeasible ones. A segment is considered feasible if it satisfies the two - sided length inequality (16). Otherwise it is infeasible. At the second stage the path gradient will be constrained tangentially with respect to the equi - surfaces of the constraint functions associated with the infeasible segments.
- In the present paper the author has applied the controlling - by - constraining method in the simplest case of a single infeasible segment. The general case will be presented as a topic of the forthcoming paper "A method for constrained optimal two - point ray tracing".

Acknowledgements

The algorithmic constructions of the paper were presented as lectures at the 1993 spring term seminar on "Constructions of algorithms of seismic tomography". The seminar was held at Institute of Seismology of University of Helsinki.

References

Chander, R., 1975: On tracing rays with specified end points, *J. Geophys.*, **41**, 173-177.

Chiu, S.K.L., Kanasewich, E.R. and Phadke, S., 1986: Three - dimensional determination of structure and velocity by seismic tomography, *Geophysics*, **51**, 1559-1571.

Farra, V., 1992: Bending method revisited: a Hamiltonian approach, *Geophys. J. Int.*, **109**, 138-150.

Kanasewich, E.R. and Chiu, S.K.L., 1985: Least squares inversion of spatial seismic refraction data, *Bull. Seism. Soc. Am.*, **75**, 865-880.

Um, J. and Thurber, C., 1987: A fast algorithm for two - point seismic ray tracing, *Bull. Seism. Soc. Am.*, **77**, 972-986.

Wesson, R.L., 1971: Travel - inversion for laterally inhomogeneous crustal velocity models, *Bull. Seism. Soc. Am.*, **61**, 729-746.