COMPUTATION OF PSEUDO-DIFFERENTIAL OPERATORS

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IMA Preprint Series # 1045

November 1992

Computation of Pseudo-Differential Operators [1]

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Abstract

A simple algorithm is described for computing general pseudo-differential operator actions. Our approach is based on the asymptotic expansion of the symbol together with the Fast Fourier Transform (FFT). The idea is motivated by the characterization of pseudo-differential operator algebra. We show that the algorithm is efficient through analyzing its complexity. Some of numerical experiments are also presented.

Key words. pseudo-differential operators, fast Fourier transform, spatially varying filters, microlocal cut-off, data processing

Abbreviated title: COMPUTATION OF PSEUDODIFFERENTIAL OPERATORS

AMS(MOS) subject classification: 35S05, 65T20, 86A22

1 Introduction

The theory of pseudo-differential operators ($\Psi.D.O.$s) has made many important contributions to the development of partial differential equations. It provides a natural way to

[1]This work was partially supported by the National Science Foundation under grant DMS 89-05878, by the Office of Naval Research under contracts N00014-J-89-1115, by AFOSR 89-0363, and by the Geophysical Parallel Computation Project (State of Texas).

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decompose a differential operator which may be difficult to study directly into several pieces with simple structure. A precise way to describe propagation of singularities for differential equations is in terms of $\Psi.D.O.$s. Pseudo-differential operators may be viewed as spatially varying filters with simple asymptotics at high frequencies. Pseudo-differential operators differentiate waves and wave-like signals according to directions of propagation. Pseudo-differential operators also arise naturally in diverse fields (often under different names!) such as Wave Propagation, Electrical Engineering, and Geophysics.

Although the theory of pseudo-differential operators, or more generally microlocal analysis, has been well established since 60's, little attention appears to have been paid to the computation of pseudo-differential operators. In this paper, we present a simple algorithm for computation of general $\Psi.D.O.$ actions. Our idea is based on the following characterization of $\Psi.D.O.$s:

Fact: The pseudo-differential operator algebra is generated by all differential operators and all powers of the Laplacian.

More precisely, partial differential operators and many functions of these (inverse, powers, $\cdots$) are included in $\Psi.D.O.$s in the high frequency asymptotic sense.

See Kohn & Nirenberg [3] for a detailed discussion.

2 Pseudo-differential Operators

Here, we shall give a brief introduction to a class of $\Psi.D.O.$s. For a complete account of $\Psi.D.O.$s as well as the calculus, the reader is referred to Taylor [5], Nirenberg [4], or Hörmander [2].

We begin with the introduction of Fourier transform and inverse Fourier transform. The Fourier transform acting on a "nice" function u defined in $\mathbb{R}^n$ is:

$$\mathcal{F}(u) = \hat{u} = (2\pi)^{-n} \int u(x) e^{-ix\cdot\xi} dx$$

and the inverse Fourier transform is defined by

$$\mathcal{F}^{-1}(u) = \int \hat{u}(\xi) e^{ix\cdot\xi} d\xi \ .$$

Remark. A number of algorithms for numerical computation of (discrete) Fourier transforms have been made available. We shall use a version of the Fast Fourier Transform in our numerical work. A detailed description may be found in Conte and De Boor [1]. See also Van Loan [6] for the most recent development in the field.

Pseudo-differential operators are usually defined in terms of symbols, which are smooth functions of both space and frequency variables satisfying certain estimates. More precisely, $q(x,\xi)$ is a member of the symbol class $S^m_{1,0}(\mathbb{R}^n)$ iff $q(x,\xi)$ is a smooth function and for any compact subset K of $\mathbb{R}^n$, and real α,β, there exists a constant $C_{K,\alpha,\beta}$, such that

$$|D^\alpha_x D^\beta_\xi q(x,\xi)| \le C_{K,\alpha,\beta}(1+|\xi|)^{m-|\beta|}$$

for all $x \in K$ and $\xi \in \mathbb{R}^n$.

In this paper, we shall confine ourselves to a subclass of $S^m_{1,0}$, the class S^m, which is the most natural class and sufficient for many applications. A function $q(x,\xi)$ is in S^m if $q(x,\xi) \in S^m_{1,0}$ and there are smooth $q_{m-j}(x,\xi)$, homogeneous of degree $m-j$ in ξ for $|\xi| \ge 1$, *i.e.*,

$$q_{m-j}(x, r\xi) = r^{m-j} q_{m-j}(x,\xi), \quad |\xi| \ge 1\ , \ \ r \ge 1$$

such that

$$q(x,\xi) \sim \sum_{j\ge 0} q_{m-j}(x,\xi) \tag{2.1}$$

in the sense that

$$q(x,\xi) - \sum_{j=0}^{N} q_{m-j}(x,\xi) \in S^{m-N-1}_{1,0}\ ,$$

where $q_m(x,\xi)$ is called the principal symbol, or principal part of $q(x,\xi)$ which carries the most important information about q.

Then the operator Q defined by

$$Q(x, D_x)u = \int q(x,\xi)\hat{u}(\xi)e^{ix\cdot\xi}d\xi$$

is called a $\Psi.D.O.$ of order m or $Q \in OPS^m(\mathbb{R}^n)$.

In particular, differential operators with smooth coefficients are $\Psi.D.O.$s. Indeed, for such a differential operator of order m, the corresponding symbol is a polynomial in ξ of degree m, and consequently is a symbol in S^m. The asymptotic expansion of a symbol, (2.1), is unique up to smoothing operators.

3 Algorithm

In this section we describe the algorithm explicitly. Its complexity will be examined in the section that follows. For the sake of simplicity, we shall only describe the idea of computing two-dimensional $\Psi.D.O.$s. Some obvious modifications may be made to compute $\Psi.D.O.$s of arbitrary dimension. Throughout, we shall always assume that the action of Q on u is meaningful. The precise conditions may be found in any one of the above references.

Given the symbol $q(x,z,\xi,\eta)$ of a $\Psi.D.O.$ $Q(x,z,D_x,D_z) \in OPS^m$ and a function $u(x,z)$. Let us assume that the asymptotic expansion of the symbol is given by

$$q(x,z,\xi,\eta) \sim \sum_{j\geq 0} q_{m-j}(x,z,\xi,\eta) \tag{3.2}$$

where $q_{m-j}(x,z,r\xi,r\eta) = r^{m-j}q_{m-j}(x,z,\xi,\eta)$ for $(|\xi|,\ |\eta| \geq 1)$. Again, q_m denotes the principal symbol of q.

Knowing the asymptotic expansion of q we compute the $\Psi.D.O.$ action Qu through computing $Q_{m-j}u$ for $j \geq 0$. We describe the calculation for $j = 0$, as it is representative. That is we will describe an algorithm for computing the action of the principal part of a $\Psi.D.O.$. Evidently this algorithm could be applied recursively to compute general $\Psi.D.O.$ actions. However the principal part gives the dominant effect on high frequency inputs, which is most important for our intended applications. Thus for us, computation of the principal part above is sufficient.

Let $\xi = \omega cos\theta$, $\eta = \omega sin\theta$, $\omega = \sqrt{\xi^2+\eta^2}$, then the homogeneity of q_m in ξ and η yields that

$$q_m(x,z,\xi,\eta) = q_m(x,z,\omega cos\theta,\omega sin\theta) = \omega^m \tilde{q}_m(x,z,\theta)$$

where $\tilde{q}_m(x,z,\theta)$ is defined to be $q_m(x,z,cos\theta,sin\theta)$.

Since $\tilde{q}_m$ is periodic in θ, the Fourier series expansion can be employed to give

$$\tilde{q}_m(x,z,\theta) = \sum_{l=-\infty}^{\infty} c_l(x,z)e^{il\theta} \ \simeq \ \sum_{l=-K/2}^{K/2} c_l(x,z)e^{il\theta}$$

$$= \sum_{l=-K/2}^{K/2} c_l(x,z)(cos\theta + isin\theta)^l \,. \qquad (3.3)$$

It follows that from the definition

$$\begin{aligned} Q_m u &\simeq \int\int d\xi d\eta e^{i(x\xi+z\eta)} \sum_{l=-K/2}^{K/2} \omega^m c_l(x,z)(cos\theta + isin\theta)^l \hat{u}(\xi,\eta) \\ &= \sum_{l=-K/2}^{K/2} c_l(x,z) \int\int d\xi d\eta \omega^m e^{i(x\xi+z\eta)}(cos\theta + isin\theta)^l \hat{u}(\xi,\eta) \\ &= \sum_{l=-K/2}^{K/2} c_l(x,z)\mathcal{F}^{-1}[\omega^{m-l}(\xi + i\eta)^l \hat{u}(\xi,\eta)] \end{aligned}$$

where to obtain the last equality, we have used the relations $cos\theta = \xi/\omega$ and $sin\theta = \eta/\omega$. Observe that ω^{m-l} is the symbol of the $(m-l)/2$-power of the (negative) Laplacian, while ξ and η are symbols of differential operators $D_x = -i\partial_x$ and $D_z = -i\partial_z$, respectively.

The procedure implicit in the above formulae leads to an algorithm to evaluate $Q_m u$ approximately, as follows. Assume that u is sampled on a discrete grid,

$$\begin{aligned} U_{i,j} &= u(x_0 + (i-1)\Delta x, z_0 + (j-1)\Delta z) \\ & \quad i = 1,\cdots,M, \;\; j = 1,\cdots,N \end{aligned}$$

with spacings Δx, $\Delta z > 0$. Assume similarly that a sampling of $\tilde{q}_m$ is given,

$$\begin{aligned} &Q_{i,j,k} = \tilde{q}_m(x_0 + (i-1)\Delta x, z_0 + (j-1)\Delta z, k\Delta\theta) \\ &i = 1,\cdots,M, \; j = 1,\cdots,N, \; k = -K/2,\cdots,K/2 \end{aligned}$$

with $X = (M-1)\Delta x$, $Z = (N-1)\Delta z$, the sample rates in the frequency domain are $\Delta\xi = 1/X$, $\Delta\eta = 1/Z$, so the (unaliased) samples of the symbols of the Laplacian, D_x, and D_z are

$$\begin{aligned} &\Omega_{p,r} = 2\pi\sqrt{(p\Delta\xi)^2 + (r\Delta\eta)^2} \\ &\Xi_{p,r} = 2\pi p\Delta\xi \\ &Z_{p,r} = 2\pi r\Delta\eta \\ &p = -M/2,\cdots,M/2, \; r = -N/2,\cdots,N/2 \end{aligned}$$

respectively.

Procedure for Computing $Q_m u$

1. Compute the discrete Fourier transform $\hat{U}$ of U.

2. For each $i \in \{1, \cdots, M\}$ and $j \in \{1, \cdots, N\}$, compute the discrete Fourier transform $\hat{Q}_{i,j} = \{Q_{i,j,l}\}_{l=-K/2}^{K/2}$ of $Q_{i,j} = \{Q_{i,j,k}\}_{k=-K/2}^{K/2}$.

3. Initialize $(QU)_{i,j} = 0.0$, $i = 1, \cdots, M$, $j = 1, \cdots, N$.

DO $l = -K/2,\ K/2$

a compute the inverse transform $\{R_{i,j}^l\}_{i=1,j=1}^{M,N}$ of

$$\Omega_{p,r}^{m-l}(\Xi_{p,r} + iZ_{p,r})^l \hat{U}_{p,r}$$

for $p = -M/2, \cdots, M/2$ and $r = -N/2, \cdots, N/2$.

b accumulate

$$(QU)_{i,j} = (QU)_{i,j} + \hat{Q}_{i,j,l} R_{i,j}^l$$

END DO

4 Complexity Analysis

We return to the general case. The complexity will be analyzed by the number of multiplications. We also make a few remarks about accuracy of the algorithm.

The direct method of computing the $\Psi.D.O.$ action is by straightforward discretization of the definition.

$$\begin{aligned} Q_m u &= \int\int q_m(x,\xi)\hat{u}(\xi)e^{ix\cdot\xi}d\xi \\ &= \mathcal{F}^{-1}[q_m(x,\xi)\hat{u}(\xi)] . \end{aligned}$$

Let us assume that the input function is discretized on a regular d-dimensional grid, as is the symbol q_m. We denote by N the number of grid points in each direction, assuming these are roughly similar. Assuming also that the discrete Fourier transforms are computed using a Fast Fourier transform algorithm, we then have the following result.

Lemma 4.1 *The direct algorithm has $O(N^{2d} log N)$ complexity.*

This is an immediate consequence of the well known fact that the FFT exhibits $O(N log N)$ complexity, where N is the length of the input sequence.

We next discuss the complexity of the new algorithm. For simplicity, we once again consider the 2-D case. The approximate complexity orders of the steps in the algorithm proposed above are:

1. $N^2 log N$

2. $N^2 K log K$

3. a. $KN^2 log N$; b. KN^2.

Hence the total complexity is $O(KN^2(log N + log K))$ in two dimension.

In general, when the number of dimension is d, a similar calculation will yield

Lemma 4.2 *The new algorithm exhibits $O(K^{d-1}N^d(log N + log K))$ complexity.*

Remarks. The new algorithm is significantly superior to the direct method. The number of terms K in the finite θ-Fourier series approximation of q_m ought to be chosen so that the sup norm error is small. Then the error in the computation of Q_m, modulo compact operators, will also be small (Taylor [5], p. 52). In particular the error will be small for oscillatory inputs u. Note that K is completely independent of N in this regard. Thus in effect the complexity of our algorithm is $O(N^d log N)$!

5 Numerical Experiments

In this section, we present the results of some numerical experiments carried out with the $\Psi.D.O.$ calculation algorithm. We calculated actions involving several microlocal cutoff operators, *i.e.* operators whose symbols are asymptotically 1 in some conic set and asymptotically zero in the complement of another conic set (essential support or aperture). These are the simplest indecomposable order zero $\Psi.D.O.$s. The examples exhibit some of the interesting features of $\Psi.D.O.$s.

We began with convolutional $\Psi.D.O.$s, which are $\Psi.D.O.$s that are independent of spatial variables. Obviously convolutional operators are natural extension of differential operators with constant coefficients. For this class of operators, it is easy to show that

$$\mathcal{F}(Qu) = Q(\xi)\hat{u}(\xi) \ ,$$

which is useful in verifying the code. In fact, according to this simple identity, one can recover the symbol from Qu and $\hat{u}$. A symbol that characterizes a microlocal cutoff is specified by Figure 1, where the symbol was designed to be a C^2 function. The next figure displays the symbol function in terms of the angle θ. From this one dimensional array, the $\Psi.D.O.$ algorithm was employed to compute the action, and hence the 2-D symbol function Q. The result, Figure 3, shows the symbol when the number of terms in Fourier series expansion of the symbol $k = 4$. It is easy to see that the symbol in Figure 3 illustrates the right direction but wrong amplitude within the aperture. As we increased k, the recovery of the symbol became better and better. Figure 4 shows that the symbol was perfectly recovered after several steps. Again, we want to emphasize that the number k only depends on the smoothness of the symbol.

The next experiment concerned the rotation of apertures for convolutional operators. The function plotted in Figure 5 is a slightly smoothed characteristic function of a circle. We applied a $\Psi.D.O.$ cutoff whose symbol was given in Figure 6 to this function. Just as the theory predicts, the high frequency information of the resulting function (Figure 7) was preserved within the aperture. We then rotated the symbol (Figure 8 and Figure 10), and again the high frequency information were preserved in Figure 9 and Figure 11, respectively. These examples are only illustrative, as the discrete Fourier transform allows a very simple and fast computation of convolution operators. Our next example is meant to illustrate the success of our algorithm with nonconvolutional $\Psi.D.O.$s. Figure 12 shows the symbol of a 2-D $\Psi.D.O.$ which is spatially varying (in z direction). It was generated from $q(z,\theta) = q_0(\theta + \delta\theta sin(\pi z/z_{max}))$ where q_0 was given in Figure 6, $\delta\theta$ was selected to be $\pi/2$, and $z \in [0, z_{max}]$. Thus, as z increases, the symbol rotates smoothly, in particular the symbol will be equal to q_0 as z reaches its maximum. Once again, we used the function u in Figure 5. The result, as shown in Figure 13, agreed with the theory. Observe that the aperture is vertical for z near 0. Then the symbol rotates as z increases, so we start to see some high frequency horizontal components. When z is getting close to its maximum, the symbol rotates back, and the aperture becomes vertical again.

Our final example demonstrates an important application of the $\Psi.D.O.$ algorithm to the seismic data processing in reflection seismology. The basic objective of all seismic processing is to convert the information recorded in a field into a form that most greatly facilitates geological interpretation of such field. Evidently, real reflection data, which carry most of the information of the mechanical properties of the earth, are what geophysicists most interested in obtaining through this process. Thus, an essential object of the processing is to eliminate or suppress all signals not associated with reflections. Figure 14 displays a seismogram, *i.e.* the recorded seismic data at receivers on the surface of the earth after an energy source is fired. As one can see clearly that the dark area that contains very strong signals represents the early arrivals (direct and head waves). In the area below, there are other signals (reflections) which are not nearly as strong as the early arrivals. Unfortunately, the direct and head waves do not penetrate the earth, so contain no information about the subsurface that we are interested in. The useful reflection energy is only contained in the lower part. This can be observed more clearly if one increase the amplitude of the seismogram as in Figure 15. The question arose: Can one remove the early arrivals and yet keep the useful information of reflections? Applying the $\Psi.D.O.$ computation algorithm, we were able to design a microlocal cutoff ($\Psi.D.O.$) whose action on the seismogram is shown in Figure 16. The result appears to be very encouraging. The amplitude of the early arrivals is reduced dramatically, and meanwhile information of reflections is well preserved. We tried the same $\Psi.D.O.$ filter on the resulted data set one more time to obtain Figure 17. The early arrivals are essentially gone, while again most of the reflections are preserved. We believe the noise left in the region where the early arrivals resided was caused by numerical scales, hence can be eliminated. This processing technique is actually used in reflection seismology, where it is called "f-k dip filtering", *e.g.* Yilmaz [7], pp 69-78. Our $\Psi.D.O.$ algorithm yields an accurate and efficient means of "spatially variable dip filtering", for which we envision numerous uses.

6 Concluding Remarks

A simple algorithm for the computation of a class of $\Psi.D.O.$s is introduced in this work. We exhibit some of the features of the algorithm. The complexity analysis indicates that the algorithm is much more efficient than the direct computation. Because of the simple structure, various massive parallel computers may be used to implement this algorithm so long as a fast FFT routine and fast array operations are available. In fact, some of our numerical experiments reported in this paper were obtained by using the Connection Machine.

We anticipate many applications of this algorithm. For example, $\Psi.D.O.$s are expected to play an important role in regularizing a class of ill-posed problems in multi-dimensional wave propagation arisen naturally in seismic inversion, oil and gas exploration, and many other related geophysical problems. Our experiment indicates the usefulness of microlocal (or $\Psi.D.O.$) cutoff in seismic data processing, *i.e.*, sorting of waves according to direction in seismic data.

Mathematically, this algorithm should provide a way to compute the so called microlocal norms of microlocal Sobolev spaces, which in turn would help us testing the sharpness of various results on propagation of singularities for partial differential equations. This algorithm should also have some impact on signal processing, where $\Psi.D.O.$s form a class of spatially varying filters.

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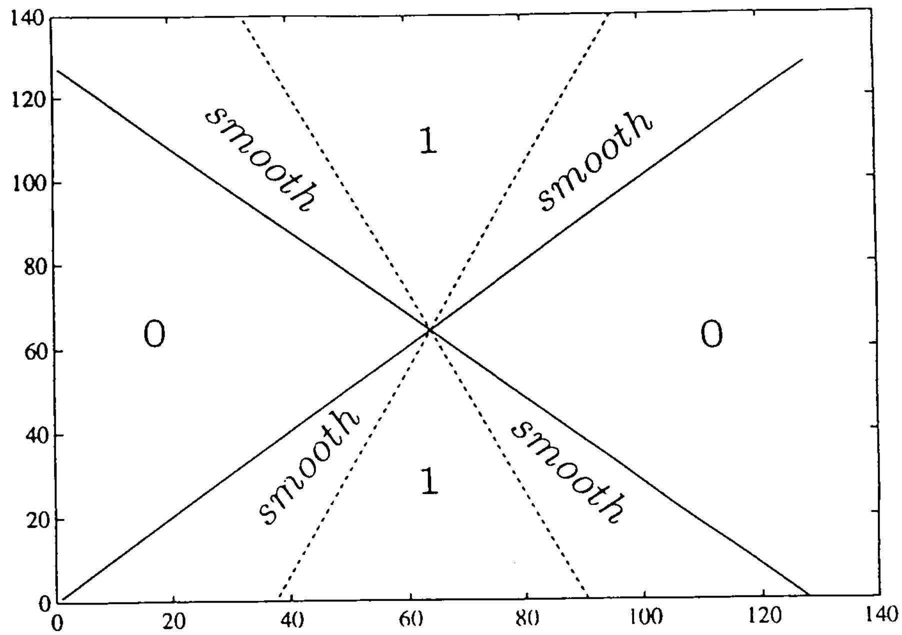

Figure 1: the symbol of a convolutional operator.

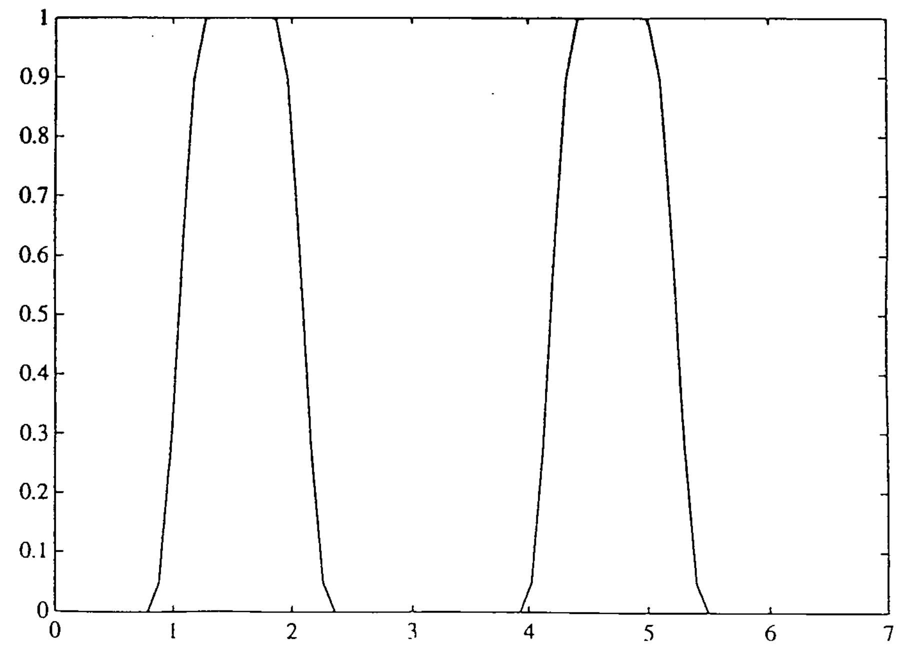

Figure 2: the same symbol as a function of θ: the angle with the horizontal axis.

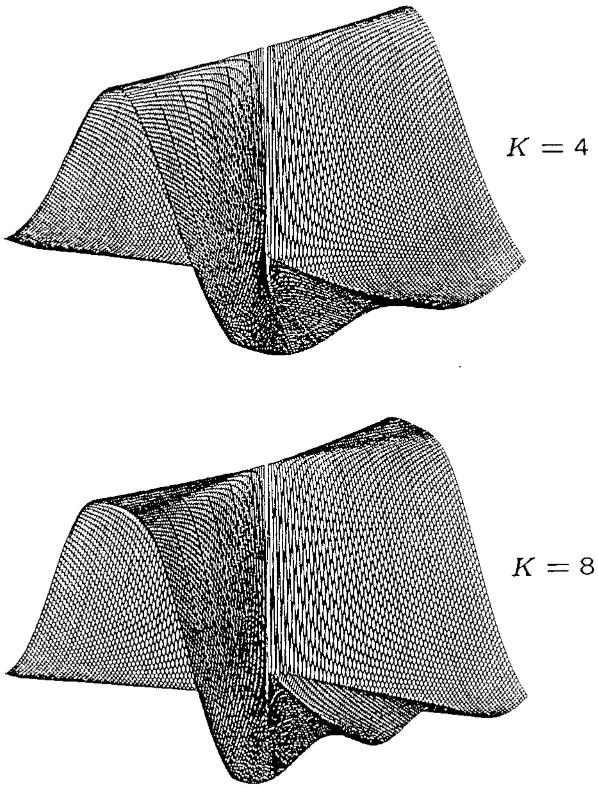

Figure 3: symbol recovery: $k = 4$.

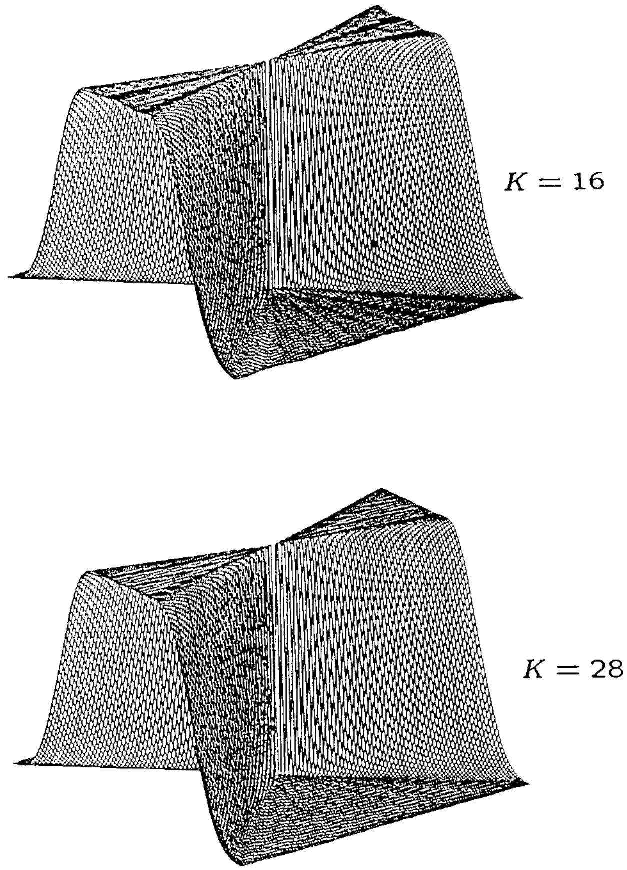

Figure 4: symbol recovery: $k = 28$.

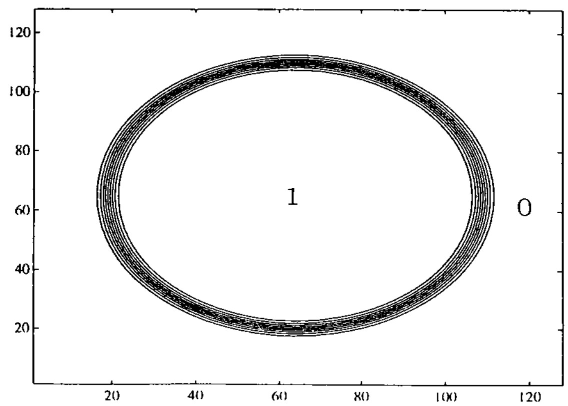

Figure 5: function u.

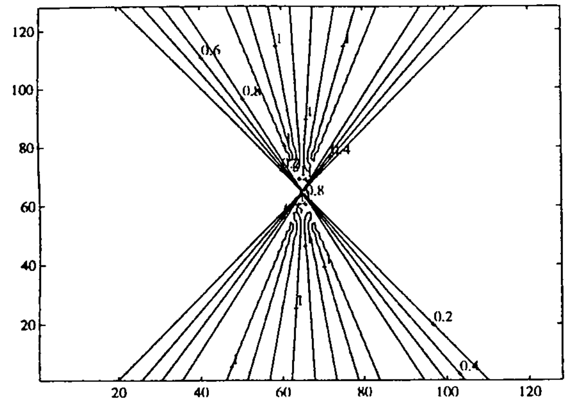

Figure 6: symbol q_0.

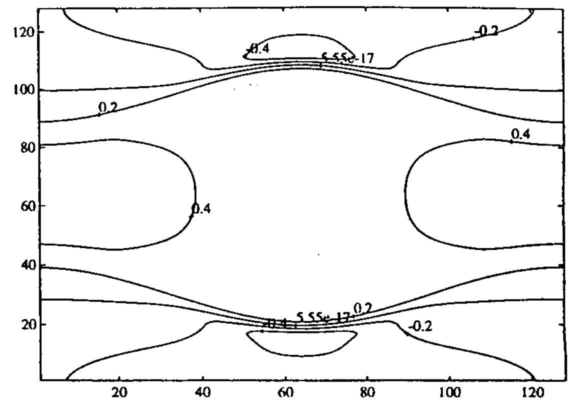

Figure 7: the action $q_0 u$.

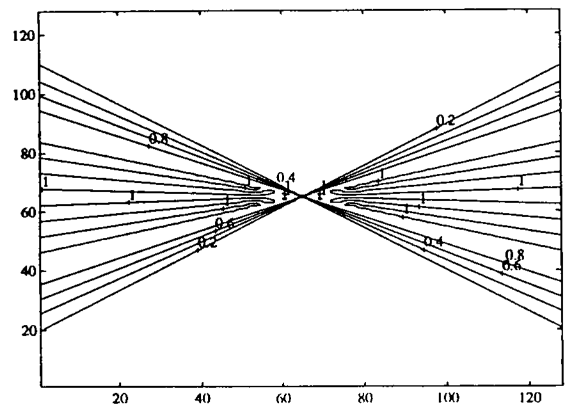

Figure 8: symbol rotation 1.

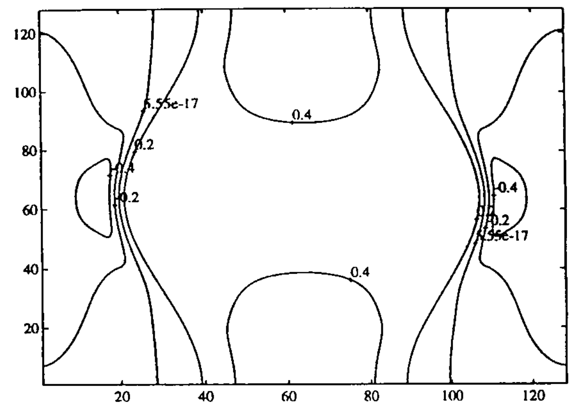

Figure 9: the action for rotation 1.

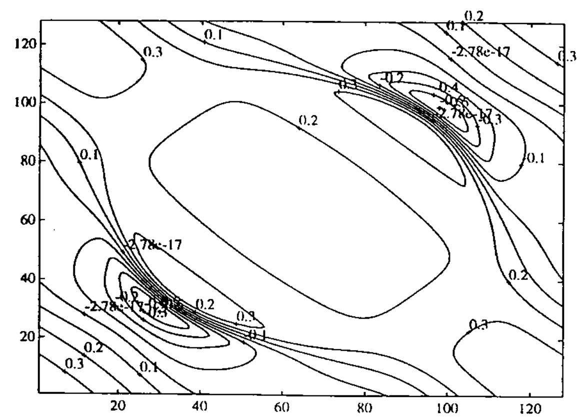

Figure 10: symbol rotation 2.

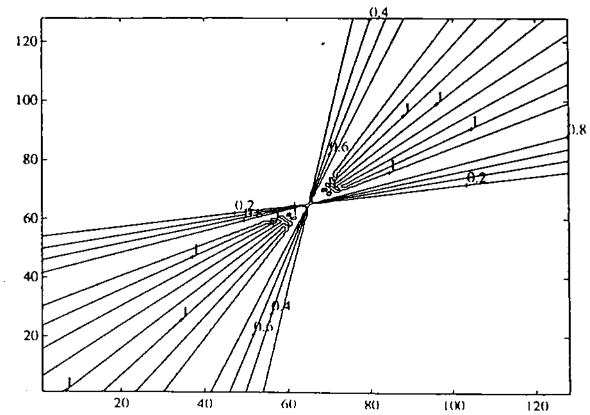

Figure 11: the action for rotation 2.

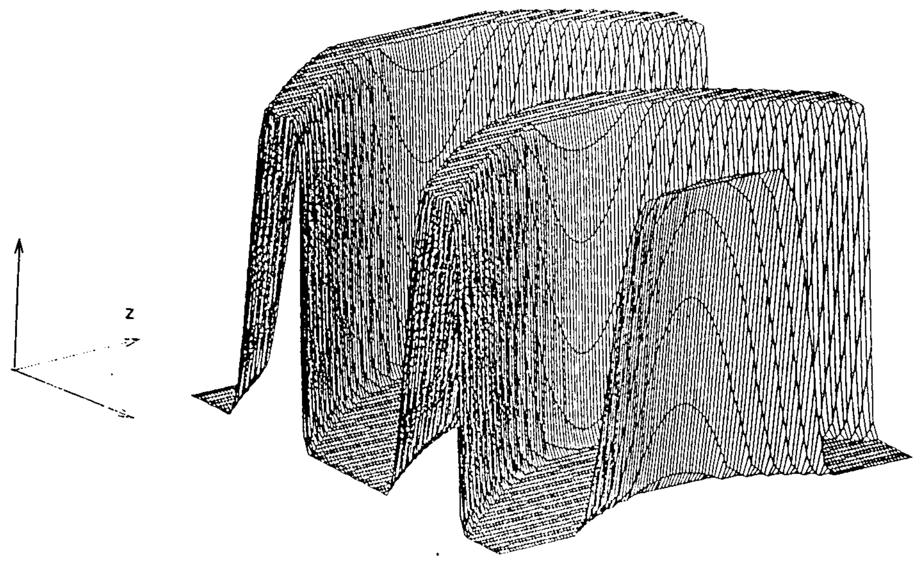

Figure 12: a spatially varying symbol.

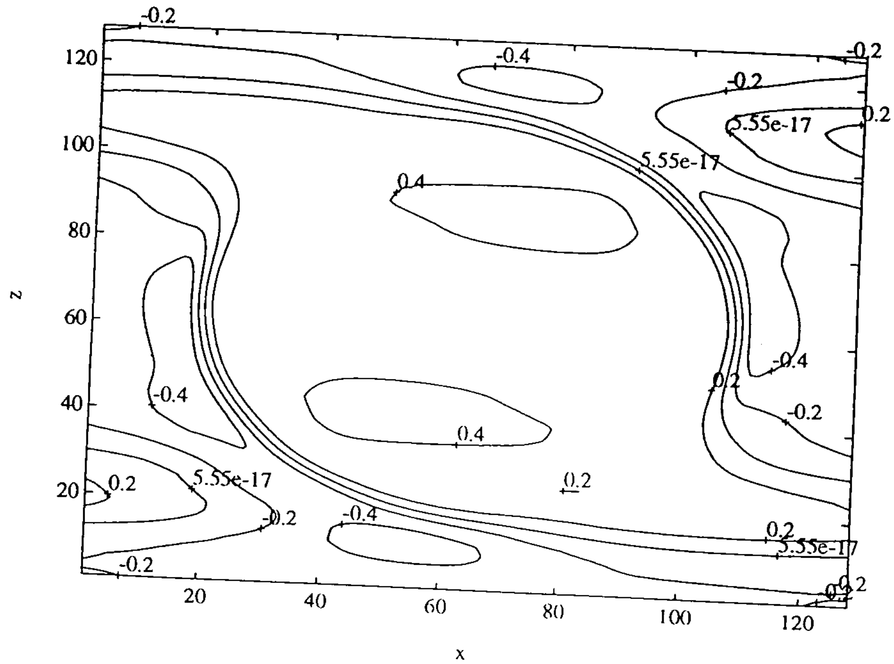

Figure 13: the action for the spatially varying symbol.

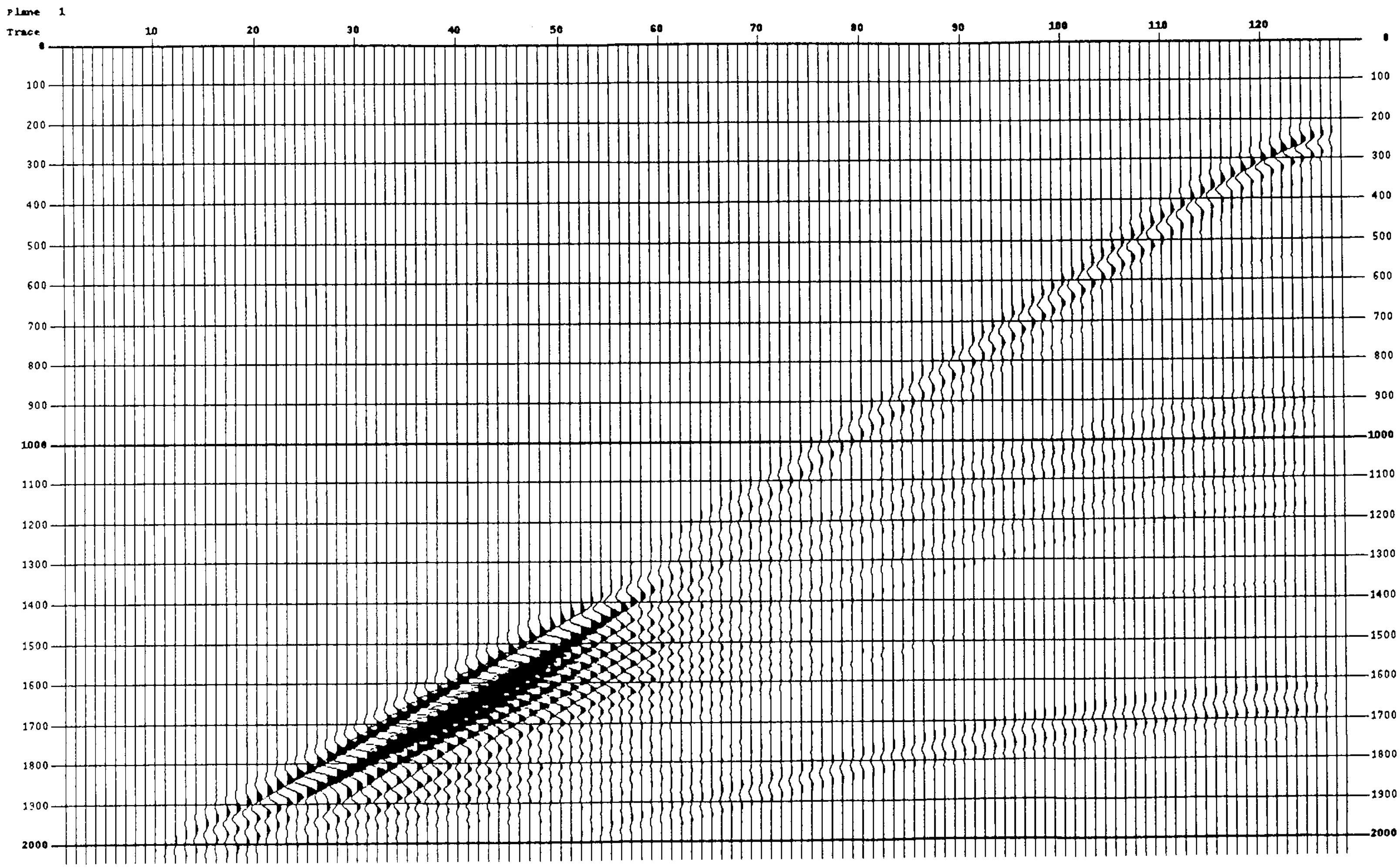

Figure 14: seismogram.

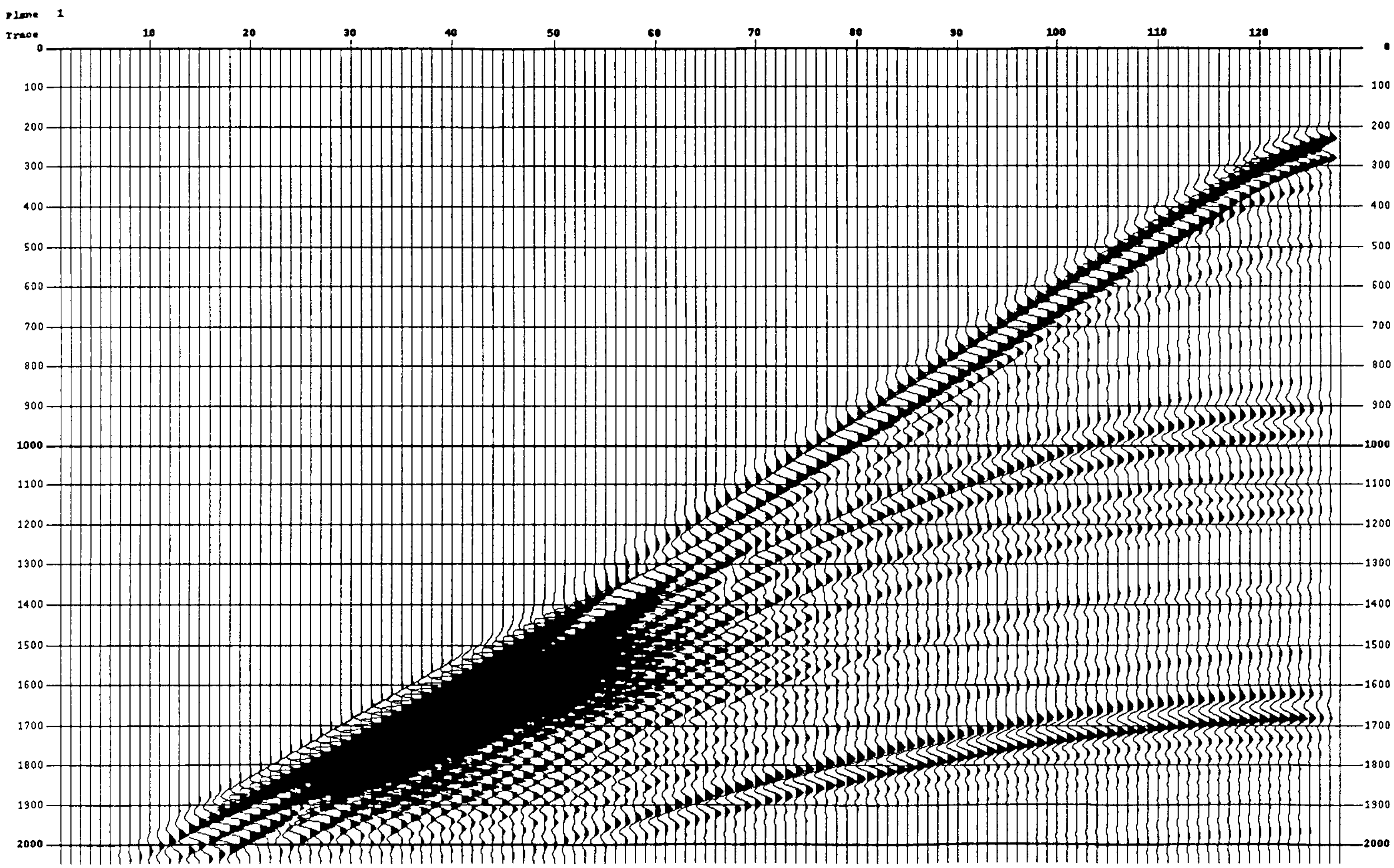

Figure 15: seismogram with increased amplitude.

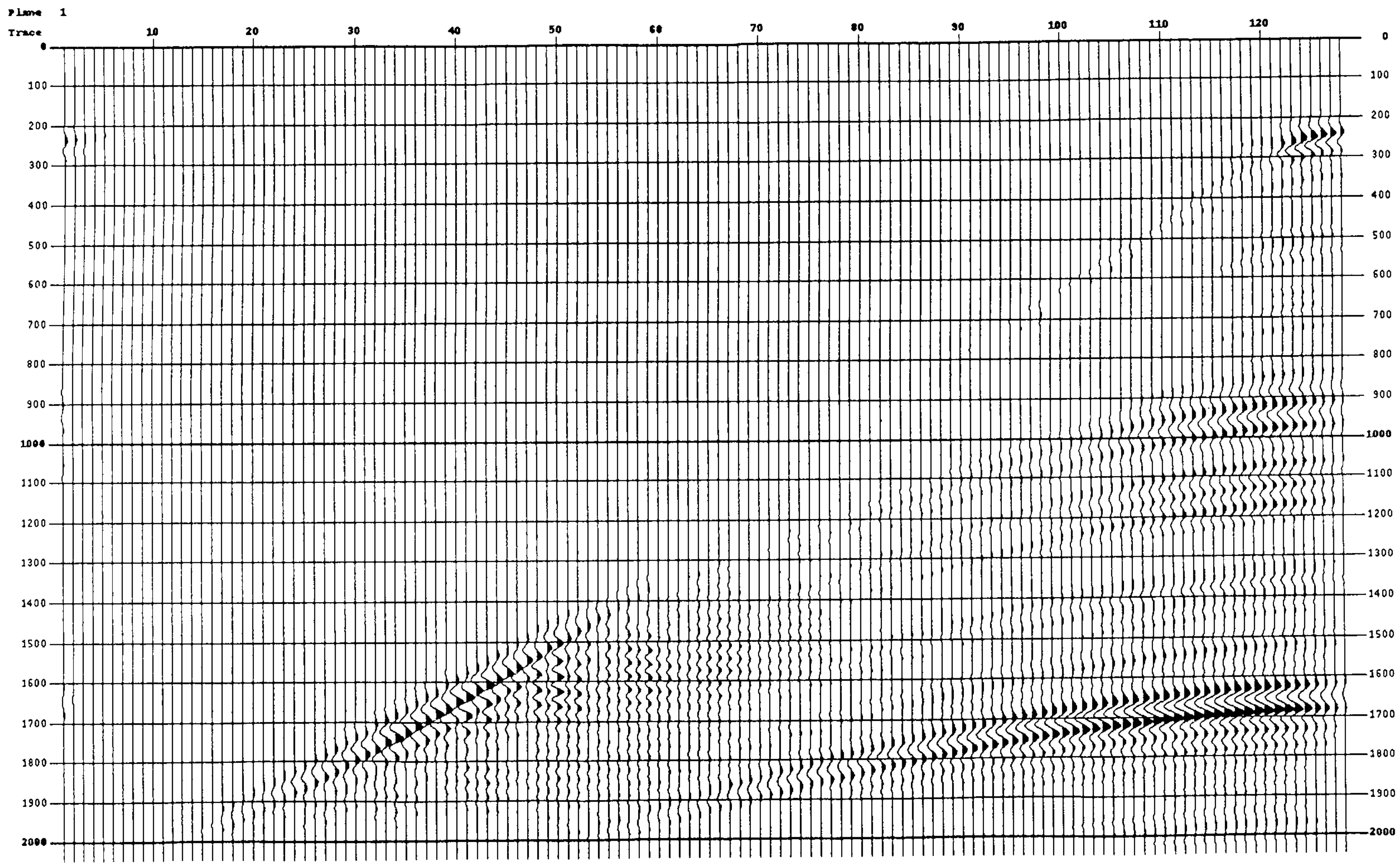

Figure 16: the result after applying the filter.

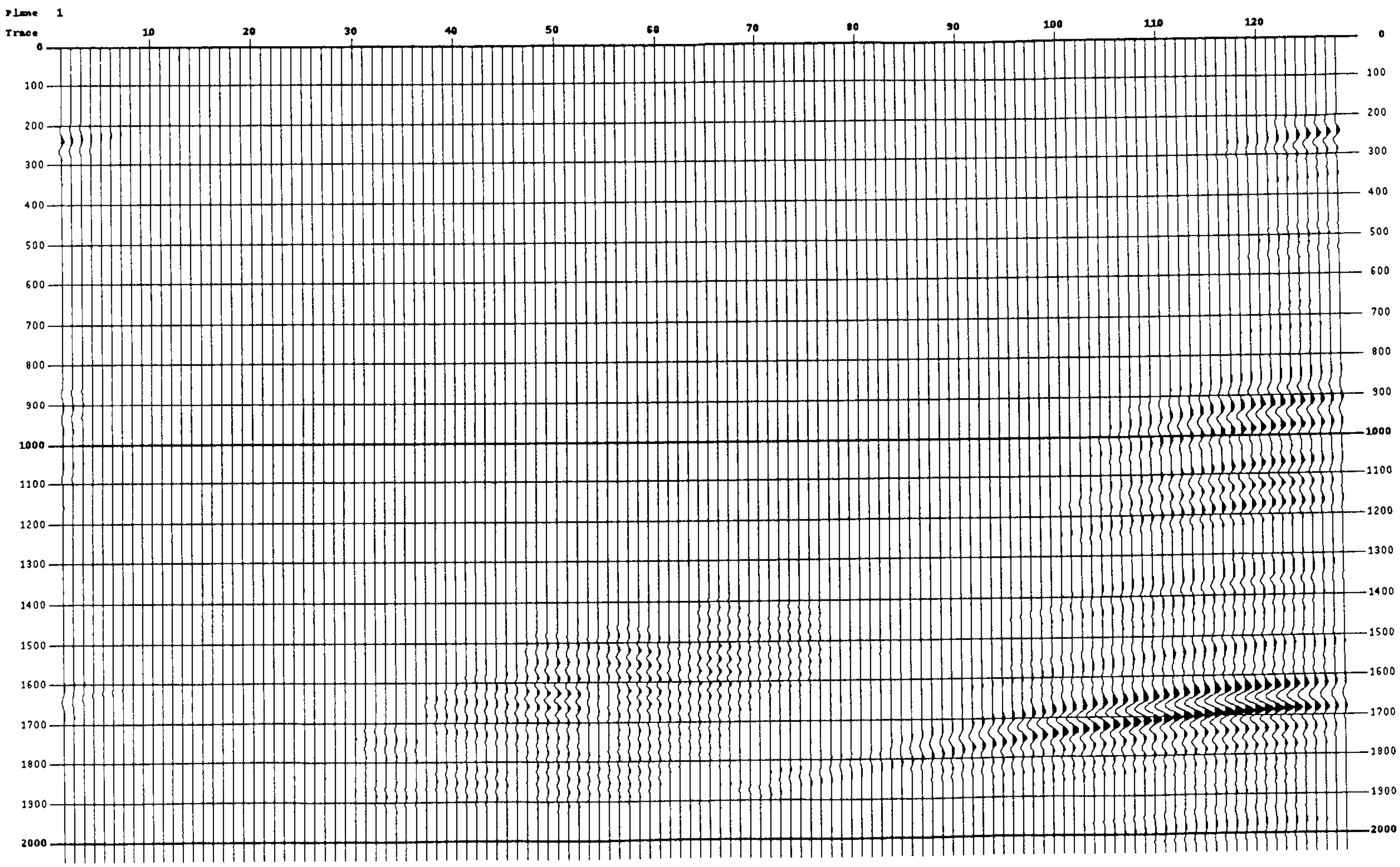

Figure 17: the result after applying the filter twice.

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1003	**Kenneth R. Driessel and Wasin So**, Linear operators on matrices: Preserving spectrum and displacement structure	
1004	**Carolyn Eschenbach**, Idempotence for sign pattern matrices	
1005	**Carolyn Eschenbach, Frank J. Hall and Charles R. Johnson**, Self-inverse sign patterns	
1006	**Marc Moonen, Paul Van Dooren and Filiep Vanpoucke**, On the QR algorithm and updating the SVD and URV decomposition in parallel	
1007	**Paul Van Dooren**, Upcoming numerical linear algebra issues in systems and control theory	
1008	**Avner Friedman and Juan J.L. Velázquez**, The analysis of coating flows near the contact line	
1009	**Stephen J. Kirkland and Michael Neumann**, Convexity and concavity of the Perron root and vector of Leslie matrices with applications to a population model	
1010	**Stephen J. Kirkland and Bryan L. Shader**, Tournament matrices with extremal spectral properties	
1011	**E.G. Kalnins, Willard Miller, Jr. and Sanchita Mukherjee**, Models of q-algebra representations: Matrix Elements of $U_q(su_2)$	
1012	**Zhangxin Chen and Bernardo Cockburn**, Error estimates for a finite element method for the drift-diffusion semiconductor device equations	
1013	**Chaocheng Huang**, Drying of gelatin asymptotically in photographic film	
1014	**Richard E. Ewing and Hong Wang**, Eulerian-Lagrangian localized adjoint methods for reactive transport in groundwater	
1015	**Bing-Yu Zhang**, Taylor series expansion for solutions of the Korteweg-de Vries equation with respect to their initial values	
1016	**Kenneth R. Driessel**, Some remarks on the geometry of some surfaces of matrices associated with Toeplitz eigenproblems	
1017	**C.J. Van Duijn and Peter Knabner**, Flow and reactive transport in porous media induced by well injection: Similarity solution	
1018	**Wasin So**, Rank one perturbation and its application to the Laplacian spectrum of a graph	
1019	**G. Baccarani, F. Odeh, A. Gnudi and D. Ventura**, A critical review of the fundamental semiconductor equations	
1020	**T.R. Hoffend Jr.**, Magnetostatic interactions for certain types of stacked, cylindrically symmetric magnetic particles	
1021	**IMA Summer Program for Graduate Students**, Mathematical Modeling	
1022	**Wayne Barrett, Charles R. Johnson, and Pablo Tarazaga**, The real positive definite completion problem for a simple cycle	
1023	**Charles A. McCarthy**, Fourth order accuracy for a cubic spline collocation method	

1024 **Martin Hanke, James Nagy, and Robert Plemmons**, Preconditioned iterative regularization for I11-posed problems
1025 **John R. Gilbert, Esmond G. Ng, and Barry W. Peyton**, An efficient algorithm to compute row and column counts for sparse Cholesky factorization
1026 **Xinfu Chen**, Existence and regularity of solutions of a nonlinear nonuniformly elliptic system arising from a thermistor problem
1027 **Xinfu Chen and Weiqing Xie**, Discontinuous solutions of steady state, viscous compressible Navier-Stokes equations
1028 **E.G. Kalnins, Willard Miller, Jr., and Sanchita Mukherjee**, Models of q-algebra representations: Matrix elements of the q-oscillator algebra
1029 **W. Miller, Jr. and Lee A. Rubel**, Functional separation of variables for Laplace equations in two dimensions
1030 **I. Gohberg and I. Koltracht**, Structured condition numbers for linear matrix structures
1031 **Xinfu Chen**, Hele-Shaw problema nd area preserved curve shortening motion
1032 **Zhangxin Chen and Jim Douglas, Jr.** Modelling of compositional flow in naturally fractured reservoirs
1033 **Harald K. Wimmer**, On the existence of a least and negative-semidefinite solution of the discrete-time algebraic Riccati equation
1034 **Harald K. Wimmer**, Monotonicity and parametrization results for continuous-time algebraic Riccati equations and Riccati inequalities
1035 **Bart De Moor, Peter Van Overschee, and Geert Schelfhout**, H_2 model reduction for SISO systems
1036 **Bart De Moor**, Structured total least squares and L_2 approximation problems
1037 **Chjan Lim**, Nonexistence of Lyapunov functions and the instability of the Von Karman vortex streets
1038 **David C. Dobson and Fadil Santosa**, Resolution and stability analysis of an inverse problem in electrical impedance tomography – dependence on the input current patterns
1039 **C.N. Dawson, C.J. van Duijn, and M.F. Wheeler**, Characteristic-Galerkin methods for contaminant transport with non-equilibrium adsorption kinetics
1040 **Bing-Yu Zhang**, Analyticity of solutions of the generalized Korteweg-de Vries equation with respect to their initial values
1041 **Neerchal K. Nagaraj and Wayne A. Fuller**, Least squares estimation of the linear model with autoregressive errors
1042 **H.J. Sussman & W. Liu**, A characterization of continuous dependence of trajectories with respect to the input for control-affine systems
1043 **Karen Rudie & W. Murray Wonham**, Protocol verification using discrete-event systems
1044 **Rohan Abeyaratne & James K. Knowles**, Nucleation, kinetics and admissibility criteria for propagating phase boundaries
1045 **Gang Bao & William W. Symes**, Computation of pseudo-differential operators
1046 **Srdjan Stojanovic**, Nonsmooth analysis and shape optimization in flow problem
1047 **Miroslav Tuma**, Row ordering in sparse QR decomposition
1048 **Onur Toker & Hitay Özbay**, On the computation of suboptimal H^∞ controllers for unstable infinite dimensional systems
1049 **Hitay Özbay**, H^∞ optimal controller design for a class of distributed parameter systems
1050 **J.E. Dunn & Roger Fosdick**, The Weierstrass condition for a special class of elastic materials
1051 **Bei Hu & Jianhua Zhang**, A free boundary problem arising in the modeling of interanl oxidation of binary alloys
1052 **Eduard Feireisl & Enrique Zuazua**, Global attractors for semilinear wave equations with locally distributed nonlinear damping and critical exponent
1053 **I-Heng McComb & Chjan C. Lim**, Stability of equilibria for a class of time-reversible, $D_n xO(2)$-symmetric homogeneous vector fields
1054 **Ruben D. Spies**, A state-space approach to a one-dimensional mathematical model for the dynamics of phase transitions in pseudoelastic materials
1055 **H.S. Dumas, F. Golse, and P. Lochak**, Multiphase averaging for generalized flows on manifolds
1056 **Bei Hu & Hong-Ming Yin**, Global solutions and quenching to a class of quasilinear parabolic equations
1057 **Zhangnxin Chen**, Projection finite element methods for semiconductor device equations
1058 **Peter Guttorp**, Statistical analysis of biological monitoring data
1059 **Wensheng Liu & Héctor J. Sussmann**, Abnormal sub-Riemannian minimizers
1060 **Chjan C. Lim**, A combinatorial perturbation method and Arnold's whiskered Tori in vortex dynamics
1061 **Yong Liu**, Axially symmetric jet flows arising from high speed fiber coating
1062 **Li Qui & Tongwen Chen**, $\mathcal{H}_2$ and $\mathcal{H}_\infty$ designs of multirate sampled-data systems
1063 **Eduardo Casas & Jiongmin Yong**, Maximum principle for state-constrained optimal control problems covered by quasilinear elliptic equations
1064 **Suzanne M. Lenhart & Jiongmin Yong**, Optimal control for degenerate parabolic equations with logistic growth
1065 **Suzanne Lenhart**, Optimal control of a convective-diffusive fluid problem