INVERSE PROBLEM OF SPACE DEPENDENT ALBEDO ESTIMATION WITH ARTIFICIAL NEURAL NETWORKS AND HYBRID METHODS

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Abstract. *In the present work the Levenberg-Marquardt method (LM), Artificial Neural Networks (ANNs) and a hybridization ANN-LM are used for the solution of the inverse radiative transfer problem of estimating the space dependent albedo in one-dimensional heterogeneous participating media. The unknown function is expanded as a series of known functions, and a finite dimensional optimization problem is then solved for the estimation of the expansion coefficients. Test case results are presented.*

Keywords: *Radiative transfer, Inverse problems, Space dependent albedo, Artificial Neural Networks, Levenberg-Marquardt method.*

1. Introduction

Garcia and Siewert (1982) and Cengel et al. (1984) investigated the solution of the direct radiative transfer problem in one-dimensional heterogeneous plane-parallel media with space dependent scattering albedo.

The solution of inverse problems in participating heterogeneous media have recently been the subject of several works with applications in different areas such as engineering and medicine (Zhou et al., 2000, 2002, Boulanger and Charette, 2005, Zhang et al., 2004).

When formulated implicitly (Silva Neto, 2002) the inverse problem of radiative properties estimation usually involves the solution of an optimization problem. Silva Neto and Özisik (1995) used the Levenberg-Marquardt method (LM), Silva Neto and Silva Neto (2003) used an interior points method, Silva Neto and Soeiro (2002, 2003) used combinations of deterministic and stochastic method, Souto et al. (2005) used the Ant Colony System (ACS) algorithm as well as a hybridization ACS-LM, and Sousa et al. (2005) used the Generalized Extremal Optimization algorithm (GEO) for the estimation of radiative transfer properties in one-dimensional homogeneous media. Soeiro et al. (2004, 2004a) used Artificial Neural Networks (ANN) and the hybridization (ANN-LM) for the same purpose.

Faure et al. (2001) and Atzberger (2004) used ANNs for the estimation of space dependent radiative properties. More recently Silva Neto and Soeiro (2005) used the Simulated Annealing method (SA) and the hybridization SA-LM for the estimation of the space dependent scattering albedo, and Souto et al. (2005a) have used the ACS and a hybridization ACS-LM for the solution of the same problem.

In the present work we implement a hybridization ANN-LM for the solution of the inverse radiative transfer problem of estimating the space dependent albedo in one-dimensional heterogeneous media.

The unknown function is expanded as a series of known functions (in fact a polynomial representation is used), and a finite dimensional optimization problem is then solved for the estimation of the expansion coefficients.

The present work extends our previous results, being considered a more general and difficult physical situation involving heterogeneous participating media. Test case results are presented.

2. Mathematical formulation and solution of the direct problem

Considerer a one-dimensional heterogeneous, gray and isotropically scattering medium, of optical thickness τ_0, with transparent boundaries. The boundary at $\tau = 0$ is subjected to an external isotropic radiation source with intensity A_1 and no radiation comes into the medium through the boundary $\tau = \tau_0$.

The mathematical formulation of the interaction of the radiation with the participating medium in the case of azymuthal symmetry and a space-dependent albedo is written in the dimensionless form as (Özisik, 1973)

$$\mu \frac{\partial I(\tau,\mu)}{\partial \tau} + I(\tau,\mu) = \frac{\omega(\tau)}{2} \int_{-1}^{1} I(\tau,\mu')d\mu' \text{, in } 0 < \tau < \tau_0 \text{, } -1 \le \mu \le 1 \quad \text{(1a)}$$

$$I(0,\mu) = A_1 \text{, } \mu > 0 \quad \text{(1b)}$$

$$I(\tau_0,\mu)=0\ ,\ \mu<0 \tag{1c}$$

where I is the radiation intensity, τ is the optical variable , μ is the cosine of the polar angle, and $\omega(\tau)$ is the space dependent albedo which is here represented in the following polynomial form

$$\omega(\tau)=\sum_{k=0}^{K} D_k \tau^k \tag{2}$$

When the radiative properties and the boundary conditions are known, problem (1) can be solved in order to determine the value of the radiation intensity in the spatial and angular domains, i.e. $0<\tau<\tau_0$ and $-1\le\mu\le1$. This is the so called direct radiative transfer problem. Here we have used Chandrasekhar's discrete ordinates method (Chandrasekhar, 1960) and the finite difference method for the solution of the direct problem.

When the radiative properties or boundary conditions are unknown, but experimental data on the radiation intensity are available, one may try to estimate the unknowns. This is the so called inverse problem which will be described in the next section.

3. Mathematical formulation and solution of the direct problem

3.1. Inverse problem formulation

Consider that the space dependent albedo $\omega(\tau)$ represented in the polynomial form given in Eq. (2) is unknown, i.e. the coefficients D_k, $k=0,1,\ldots,K$, are the elements of the vector of unknowns

$$\vec{Z}=\{D_0,\ D_1,\ldots,\ D_k\} \tag{3}$$

but on the other hand consider that experimental data acquired at both boundaries of the medium, at different polar angles, are available, i.e. Y_i, $i=0,1,\ldots,N_d$, where N_d is the total number of experimental data.

The inverse radiative transfer problem is then solved as a finite dimensional optimization problem in which we seek to minimize the cost function given by the summation of the squared residues

$$Q(\vec{Z})=\sum_{i=1}^{N_d}\left[I_i(\vec{Z})-Y_i\right]^2=\vec{R}^T\vec{R} \tag{4}$$

where I_i and Y_i are the calculated and measured values of the radiation intensity, respectively.

As real experimental data were not available, we simulated the measured intensities, Y_i, by calculating the exact values I_{exact_i} using the exact values of the coefficients, i.e. $\vec{Z}_{exact}$, and then adding a computer generated noise,

$$Y_i=I_{exact_i}(\vec{Z}_{exact})+\sigma\, l_i,\qquad i=1,2,\ldots,N_d \tag{5}$$

where l_i is a pseudo-random number in the range [-1,1] and σ emulates the standard deviation of the measurement errors.

The inverse problem described here is somewhat artificial for two reasons. In first place the optical thickness of the medium, τ_0, is considered known, but in fact it is dependent on the scattering and absorption coefficients, which are unknown. Besides that, the total number of coefficients, K, should also be considered unknown. These two aspects will be investigated in the future.

3.2. Solution of the inverse problem

3.2.1. Levenberg-Marquardt method (LM)

Starting with an initial guess for the unknowns $\vec{Z}^0$, new estimates are obtained with

$$\vec{Z}^{n+1}=\vec{Z}^n+\Delta\vec{Z}^n,\quad n=0,1,2,\ldots \tag{6}$$

where the vector of corrections $\Delta\vec{Z}^n$ are obtained from the solution of the following system of linear algebraic equations

$$\left[\left(J^T\right)^n J^n + \lambda^n I\right]\Delta\vec{Z}^n = -\left(J^T\right)^n \vec{R}\left(\vec{Z}^n\right) \tag{7}$$

where I is the identity matrix, n is the iteration index, λ^n is a damping parameter which is reduced along the iterative procedure, and the elements of the Jacobian matrix J^n and the elements of the vector of residues $\vec{R}^n$ are given by

$$J_{ij}^n = \left.\frac{\partial I_i\left(\vec{Z}\right)}{\partial \vec{Z}_j}\right|_{\vec{Z}=\vec{Z}^n}, \quad i=1,2,\ldots,N_d, \quad j=0,1,\ldots,K \tag{8}$$

$$R_i^n = I_i\left(\vec{Z}^n\right) - Y_i, \; i=1,2,\ldots,N_d \tag{9}$$

The iterative procedure of calculating the vector of corrections $\Delta\vec{Z}^n$ and new estimates $\vec{Z}^{n+1}$ with Eqs. (7) and (6), respectively, is interrupted when a stopping criterion such as

$$\left|\frac{\Delta\vec{Z}_j^n}{\vec{Z}_j^n}\right| < \delta, \; j=0,1,\ldots,K \tag{10}$$

is satisfied, where δ is a small tolerance, say 10^{-5}.

Details on the derivation of the Levenberg-Marquardt method can be found in (Silva Neto and Özisik, 1995, Silva Neto and Soeiro, 2005).

3.2.1. Artificial Neural Network (ANN)

Here a multi-layer perception (MLP) neural network (Haykin, 1994, Bishop, 1995) was used. In Fig. 1 a representation of a MLP with the input and output layers, and one hidden layer (Soeiro et al., 2004a) is given.

The MLP is a collection of connected processing elements called nodes or neurons, arranged in layers. Signals (the measured values of the radiation intensity, Y_i, $i=1,2,\ldots,K$) pass into the input layer nodes, progress through the

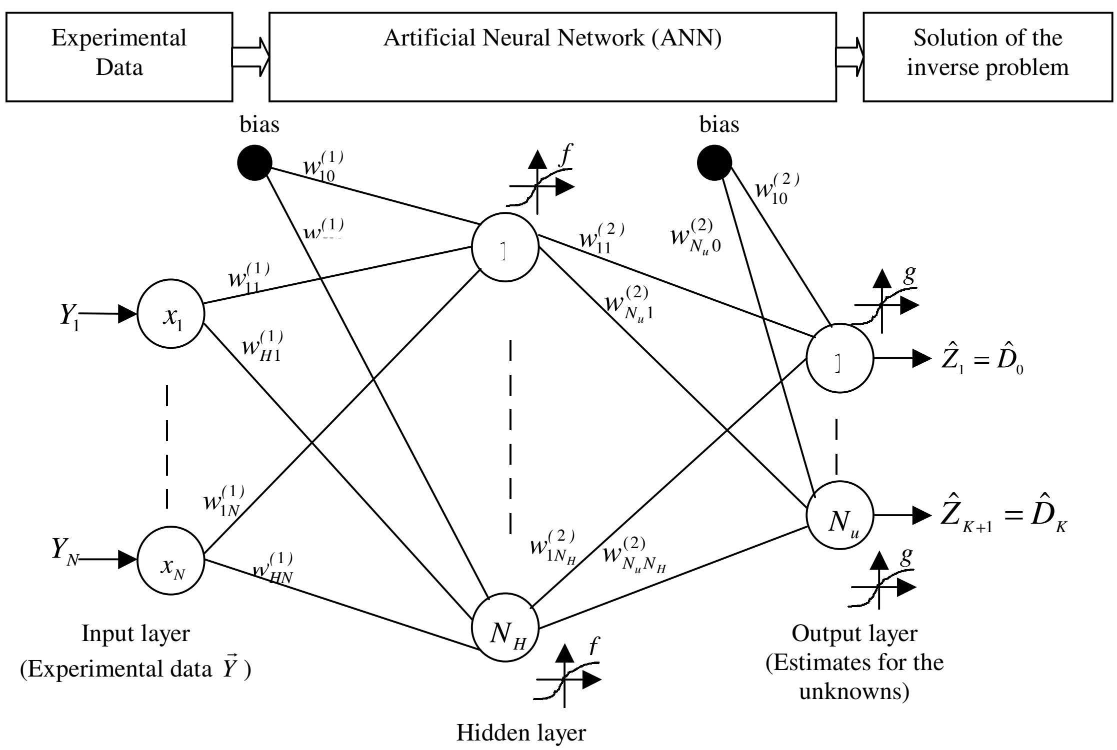

Figure 1. Multi-layer perceptron neural network with one hidden layer for the inverse radiative transfer problem.

network hidden layer and finally emerge from the output layer (yielding the estimated values for the unknowns). $\hat{\vec{Z}} = \{\hat{D}_0, \hat{D}_1, ..., \hat{D}_k\}$. In Fig. 1 the total number of unknowns Nu corresponds to the $K+1$ coefficients to be estimated. Each node i is connected to each node j in its preceding layer through a connection of weight w_{ij}, and similarly to nodes in the following layer. A weighted sum is performed at neuron i of all the signals x_j from the preceding layer, yielding the excitation of the node which is then passed through a nonlinear activation function, f, to emerge as the output of the node i,

$$Y_i = f\left(\sum_j \omega_{ij} x_j\right) \tag{11}$$

Various choices for the activation function f are possible. In this work we have used the hyperbolic tangent function.

The first stage of using an ANN to model an input-output system is to establish the appropriate values for the connection weights w_{ij}. This is the “training” or learning phase. Training is accomplished using a set of network inputs for which the desired outputs are known. These are the so called patterns, which are used in the training stage of the ANN. The patterns were generated with the solution of the direct problem given by Eqs. (1a-c).

In order to solve the inverse radiative transfer problem with ANNs we have used the Neural Networks toolbox of MATLAB package.

Several algorithms could then be used in order to determine the connection weights w_{ij} in the back-propagation process . We have chosen the Levenberg-Marquardt method for that purpose.

The presentation of a full set of patterns is denominated epoch. After one epoch is completed the set of patterns is presented again in a different (random order). After a number of epochs, once the comparison error between the target values (the expected values for the output layer used to generate the patterns) and the calculated values at the neurons in the output layer (as given by Eq. (11)) is reduced to an acceptable prescribed level over the whole training set, the training phase ends and the ANN is established. Therefore, in our inverse radiative transfer problem estimates for the unknowns $\hat{\vec{Z}}$ (output layer) can be obtained using the experimental data $\vec{Y}$ as the input to the ANN (input layer) and the simple forward sweep described by (see Fig. 1)

$$Z_k = g(\sum_{j=1}^{N_H} \omega_{kj}^{(2)} f(\sum_{i=1}^{N} \omega_{ji}^{(1)} Y_i + \omega_{j0}^{(1)}) + \omega_{k0}^{(2)}), \qquad k = 1,2,...,N_u \tag{12}$$

where f and g are the activation functions in the hidden and output layers, respectively, N is the number of neurons in the input layer, i.e. $N = N_d$, N_H is the number of neurons in the hidden layer, which is usually chosen in the range $N \le N_H \le 2N$, and N_u is the number of unknowns, i.e. $N_u = K+1$.

Here we have considered $N_H = N = N_d$.

With Eq. (12) the parameters of a model $(\vec{Z})$ can be determined using the experimental data $(\vec{Y})$. This is the generalization stage in the use of the ANN.

3.2.3 Hybrid method ANN-LM

Due to the complexity of the design space, if convergence is achieved with a gradient based method, such as LM, it may in fact lead to a local minimum.

The ANN is stochastic in its nature, but in the end provides an interpolation from the patterns used in the determination of the weights of the connections. Even though reasonable estimates are obtained with the ANN described in the previous section, a refined solution usually requires a careful fine tuning of several parameters such as number of patterns, number of epochs and number of neurons in the hidden layer, among others. Instead of following this parth, we decided to use a not refined ANN trained with a small number of patterns in order to generate an initial guess to be used in the gradient based method LM, i. e. $\vec{Z}^0 = \hat{\vec{Z}}_{ANN}$. This approach has been used by Soeiro et al. (2004, 2004a) for the solution of inverse heat conduction and radiative transfer problems.

Silva Neto and Soeiro (2002, 2003, 2005) and Souto et al. (2005), have used this strategy in order to reduce the CPU time when the Simulating Annealing, Genetic Algorithms and Ant Colony System were used for the solution of inverse radiative transfer problems. This is not the case in the present work.

The training stage of the ANN, which is the most computationally intensive part of the algorithm, was reasonably fast. Our objective with the hybridization ANN-LM is to obtain a refined solution, as will be demonstrated in the next section of the paper.

4. Results and discussion

In order to evaluate the efficacy of the use of the Levenberg-Marquardt method (LM), the Artificial Neural Network (ANN) and the hybridization ANN-LM in the solution of the inverse radiative transfer problem of space dependent albedo estimation we have considered the test cases shown in Table 1.

Also in Table 1, in the last column, it is shown if convergence is achieved when only the LM is used. The difference between the test cases with labels A and B is only related to the initial guess used for the LM. For all test cases with label B convergence was not achieved because the initial guess was not in the convergence region.

In test cases 1-3 noiseless data were used, i. e. $\sigma = 0$ in Eq. (5). In test cases 4-6 noisy data were considered.

In Table 2 the estimated values for the unknowns $\hat{\vec{Z}}$ using the LM and ANN separately are shown.

Two ANNs were used. The first one was trained using 500 patterns and the second one with 100 patterns. In Table 3 are summarized the information related to the ANNs.

In Tables 4 and 5 the results obtained with a combination of ANN (with 100 patterns in the training set) with LM using noiseless and noisy data, respectively, are shown. The objective of such runs is to obtain a refined estimate for the coefficients $\hat{D}_k$, $k = 0,1,...,K$. Here the estimates obtained with the ANN are used as the initial guess for the LM, i. e. $\vec{Z}^0_{LM} = \hat{\vec{Z}}_{ANN}$.

For all test cases presented here we have considered a medium with optical thickness $\tau_0 = 1$. The information on the CPU time is related to a Pentium IV 2.8GHz processor.

5. Conclusions

In the present work three approaches were used for the solution of an inverse radiative transfer problem in which we were interested in estimating the space dependent single scattering albedo. First we used the Levenberg- Marquardt method, after that we used Artificial Neural Networks, and finally we used a combination of these methods.

When used separately, the LM did not converge for some cases, and the solution of the ANN could be improved by a fine tuning of the “control parameters” of the method. Instead of refining the ANN we decides to combine it with the LM. The estimated values obtained with the ANN were then used as the initial guesses for the LM. The results demonstrated that good estimates were obtained using this strategy.

In future works we will investigate the simultaneous estimation of the single scattering albedo and optical thickness.

6. Acknownledgements

The authors acknownledge the financial support provided by CNPq, Conselho Nacional e Tecnológico, and FAPERJ, Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro.

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Table 1. Test Cases. $\vec{Z}_{exact} = \{D_0^{exact}, D_1^{exact}, D_2^{exact}\}$. $\vec{Z}^0 = \{D_0^0, D_1^0, D_2^0\}$ for the Levenberg-Marquardt method (LM).

Test Case	$\vec{Z}_{exact}$			$\vec{Z}^0$ (for LM)			σ (Eq. (5))	Level of Noise in Experimental Data	Convergence with LM
	D_0^{exact}	D_1^{exact}	D_2^{exact}	D_0^0	D_1^0	D_2^0			
1 A	0.5	0.0	0.0	1.0	1.0	1.0	0	0%	Yes
1 B	0.5	0.0	0.0	-2.0	-2.0	-2.0	0	0%	No
2 A	0.9	-0.8	0.0	0.5	0.5	0.5	0	0%	Yes
2 B	0.9	-0.8	0.0	-2.0	-2.0	-2.0	0	0%	No
3 A	0.2	0.2	0.6	0.5	0.5	0.5	0	0%	Yes
3 B	0.2	0.2	0.6	-2.0	-2.0	-2.0	0	0%	No
4 A	0.5	0.0	0.0	1.0	1.0	1.0	0.003	< 6%	Yes
4 B	0.5	0.0	0.0	-2.0	-2.0	-2.0	0.003	< 6%	No
5 A	0.9	-0.8	0.0	0.5	0.5	0.5	0.001	< 4%	Yes
5 B	0.9	-0.8	0.0	-2.0	-2.0	-2.0	0.001	< 4%	No
6 A	0.2	0.2	0.6	0.5	0.5	0.5	0.003	< 7%	Yes
6 B	0.2	0.2	0.6	-2.0	-2.0	-2.0	0.003	< 7%	No

Table 2. Estimated values for the vector of unknowns $\hat{\vec{Z}} = \{\hat{D}_0, \hat{D}_1, \hat{D}_2\}$ obtained with the Levenberg-Marquardt method (LM) and Artificial Neural Network (ANN) separately.

Test Case	$\vec{Z}_{exact}$			Noise in Experimental Data	LM					ANN[1] (500 patterns)			ANN[2] (100 patterns)		
	D_0^{exact}	D_1^{exact}	D_2^{exact}		$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	$Q(\vec{Z}), Eq.(4)$	(Iterations)/ CPU time(s)	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$
1	0.5	0.0	0.0	0%	0.500	0.000	0.000	4.73E-28	(20)/40.17s	0.505	-2.40E-03	-1.50E-03	0.498	0.018	-1.56E-02
2	0.9	-0.8	0.0	0%	0.900	-0.800	-1.24E-12	4.08E-27	(8)/16.14s	0.900	-0.808	8.00E-4	0.893	-0.798	-9.20E-03
3	0.2	0.2	0.6	0%	0.200	0.199	0.600	7.41E-24	(19)/39.87s	0.197	0.209	0.602	0.205	0.210	0.585
4	0.5	0.0	0.0	< 6%	0.490	0.087	-0.101	1.38E-04	(19)/39.85s	0.485	0.137	-0.146	0.475	0.130	-0.102
5	0.9	-0.8	0.0	< 4%	0.899	-0.788	-2.03E-02	9.44E-06	(7)/14.14s	0.903	-0.822	0.012	0.892	-0.796	-0.014
6	0.2	0.2	0.6	< 7%	0.210	0.170	0.640	1.81E-04	(6)/12.15s	0.210	0.217	0.570	0.197	0.268	0.539

[1] 500 patterns were used in the training of the ANN

[2] 100 patterns were used in the training of the ANN

Table 3. Summary of the Artificial Neural Networks information.

Neural Network	Number of patterns in the training of the ANN	$N = N_d$	N_H	N_u	CPU time generating patterns	CPU required in the training of the ANN
ANN[1]	500	20	20	3	71.89 s	118.8 s
ANN[2]	100	20	20	3	14.39 s	21.07 s

Table 4. Estimated values for the vector of unknowns, $\hat{\vec{Z}}$, with the Levenberg- Marquardt method (LM) initial guesses the estimates obtained with the Artificial Neural Network (ANN) trained with 100 patterns, $\vec{Z}_{LM}^{0} = \hat{\vec{Z}}_{ANN}$.

Experimental data without noise.

4(a) Test Case 1. Noiseless data. CPU time for LM=7.95s.

Iteration	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	Objective Function
0	0.4976	0.0180	-0.015	2.55E-06
1	0.4999	1.67E-05	-1.21E-05	1.00E-11
3	0.4999	1.40E-12	-1.61E-12	7.26E-24

4(b) Test Case 2. Noiseless data. CPU time for LM=8.21s.

Iteration	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	Objective Function
0	0.8930	-0.7977	-0.0092	1.93E-04
1	0.9000	-0.7999	5.45E-05	9.43E-09
4	0.8999	-0.7999	-9.39E-13	6.73E-27

4(c) Test Case 3. Noiseless data. CPU time for LM=8.15s.

Iteration	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	Objective Function
0	0.2046	0.2095	0.5845	4.03E-05
1	0.2000	0.2000	0.5998	5.35E-10
4	0.1999	0.2000	0.5999	1.22E-19

Table 5. Estimated values for the vector of unknowns, $\hat{\vec{Z}}$, with the Levenberg- Marquardt method (LM) using as initial guesses the estimates obtained with the Artificial Neural Network (ANN) trained with 100 patterns, $\vec{Z}_{LM}^{0} = \hat{\vec{Z}}_{ANN}$.

Experimental data with noise.

5(a) Test Case 4. $\sigma = 0.003$ (< 6 % error). CPU time for LM= 10.15s.

Iteration	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	Objective Function
0	0.4747	0.1298	-0.1021	1.84E-04
1	0.4931	2.20E-02	-1.94E-02	9.75E-05
4	0.4931	2.20E-02	-1.94E-02	9.74E-05

5(b) Test Case 5. $\sigma = 0.001$ (< 4 % error). CPU time for LM= 10.20s.

Iteration	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	Objective Function
0	0.8920	-0.7961	-0.0140	3.14E-04
1	0.9008	-0.7955	-8.9E-03	1.09E-05
4	0.9008	-0.7957	-8.89E-03	1.08E-05

5(c) Test Case 6. $\sigma = 0.003$ (< 7 % error). CPU time for LM= 10.25s.

Iteration	$\hat{D}_0$	$\hat{D}_1$	$\hat{D}_2$	Objective Function
0	0.1968	0.2684	0.5389	2.83E-04
1	0.2027	0.1717	0.6316	1.20E-04
4	0.2027	0.1707	0.6326	1.19E-04

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8. Responsibility notice

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