
Solution of a certain problem of scattering by using of the maximum entropy principle

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Abstract. This paper studies a problem of inverse scattering on the basis of maximum entropy principle. The advantage of the method implies maximization of the entropy functional, what is the main condition and the scattering data and any a priori information are considered as constraints. This rephrasing of the problem leads to significant simplifications, since the entropy functional is known to be concave. Other peculiar properties of the method include his stability to various kinds of artifacts and adaptability to various schemes of measurement.

Keywords: Inverse problems, maximum entropy, cone ray transform, computerized tomography.

AMS Subject Classification 2010: 65R10, 65R32, 65Z05, 47N50.

1 Introduction

Entropy is the concept that has played a central role in a number of fields of science, especially in statistical mechanics and information theory. The idea of the maximum entropy principle as a method of solving a wide range of physics problems with incomplete information was expressed in general form by Jaynes [12, 13]. The idea is based on the common sense and the scientific principle "... we must use that probability distribution which has maximum entropy subject to whatever is known. This is the only unbiased assignment we can make; to use any other would amount to arbitrary assumption of information which by hypothesis we do not have" [12, p.623]. Gabor T. Herman in his book [11, p.117] writes "... the maximum entropy solution has the smallest information content, and so it is least likely to mislead the user by the presence of spurious features."

The maximum entropy method is one of the methods widely used in astronomy, radio astronomy, plasma physics, [9, 10, 23], crystallography [19, 24], for the solution of integral equations [1, 7] and so on. The acquisition of experimental data is always bound up with the sort of restrictions. For instance, in practice, it is almost impossible to acquire a set of measurements over all the

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scattering angles; corruption with noise of the scattered fields measured by the detectors; distribution of scattering angles for a given energy instead of exact values given by Compton's law, etc. The maximum entropy method in these cases will yield the result maximally insensitive to the missing information [12].

The Compton effect is used to probe the electron density of matter and applied often to nondestructive material control. The data measured in Compton scattering experiments is represented by the integrals of distribution function $g(\mathbf{x})$ over the cones, which are defined by the conical transform (1), [21, p.3]. Figure 1 displays the representation of conical projections.

$$G(\mathbf{x}, \boldsymbol{\beta}, \omega) = K(\omega) \sin(\omega) \int_0^{2\pi} \int_0^{\infty} g(\mathbf{x} + r\boldsymbol{\alpha}(\varphi)) \delta(\boldsymbol{\alpha} \cdot \boldsymbol{\beta} - \cos \omega) r dr d\varphi, \quad (1)$$

where vertex $\mathbf{x} = (x_{0i}, y_{0j})$ lying on the plane $X - Y$ in 100 different positions, that is $i, j = 1 \div 10$, the vector $\boldsymbol{\beta}$ in our case coincides with the axis Z' of the rotated coordinate system, $\omega \in [0, \pi/2]$, $\varphi \in [0, 2\pi]$, $\cos(\omega) = \boldsymbol{\alpha} \cdot \boldsymbol{\beta}$, $K(\omega)$ is the Klein-Nishina distribution which describes the probability of a photon scattering with a given energy by angle ω . There is a large amount

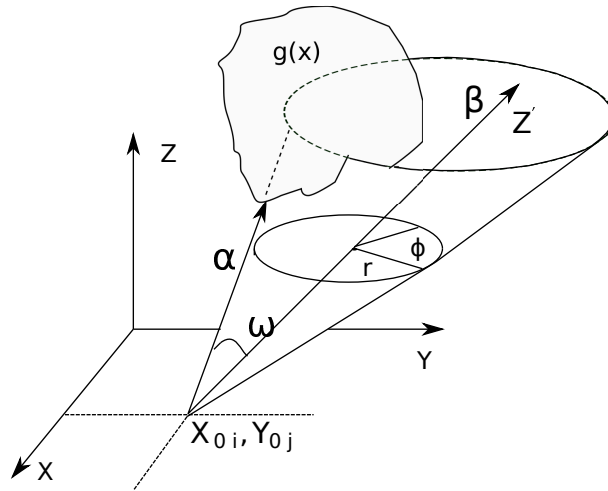


Figure 1: A sketch for measurement of scattered radiation measurement for inversion of the conical ray transform.

of publications related to the inversion of Compton scattering data. In [17, 18] an inversion of weighted cone transform is considered. In [15] provided are inversion formulas using complete Compton data for three- and two-dimensional cases. An inversion formula for the conical Radon transform arising in Compton experiments with the cylindrical camera are given in [21, 22], exact reconstruction formulas of filtered back-projection type for inverting of conical Radon transform in \mathbf{R}^d are derived in [6, 14]. The use of an orthogonal spherical expansion to convert the cone-surface integrals into plane integrals is proposed in [2]. Webber [26] has shown that the electron density may be reconstructed analytically, while using the incoherent scattered data.

An interesting inversion method has been proposed by Bruce Smith [25]. A three dimensional Compton scattering tomography problem is considered in [27]. The paper contains many good references relevant to the inversion of Compton scattering data.

In the present paper, is considered an iterative maximum entropy method of reconstruction of a scattering object from its scattered radiation data. As obvious from many numerical experiments, the maximum entropy method provides for an acceptable reconstruction even with an incomplete set of scattering data, what is important for analytical inversion methods. In practice, it is almost impossible to obtain a set of projections over all the scattering angles. With a slight correction of the program code, the algorithm solves the inversion problem for a complete data set, for data recorded by the detector located in the $X - Y$ plane with or without collimation.

The paper is organized as follows. In the Introduction, a short survey of specifics of the maximum entropy method and a number of recent publications related to Compton scattering problems are given. Section two describes the construction of the maximum entropy method. In section three, are given the results of computer simulation.

2 The inversion method

Let $g(\mathbf{x})$ be the integrable three-dimensional object function to be reconstructed in a compact support $D \subset \mathbb{B}^3 = \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \leq 1\}$. The measurable data for cone beam geometry are assumed to be defined by the formula (3) below. It is proposed to use three systems of reference: two Cartesian systems $\mathbf{x} = (x, y, z)$ and $\mathbf{x}_j = (x_j, y_j, z_j)$, i.e. the laboratory one and the reference system of scattering data registration, respectively, and cone coordinates $\mathbf{u}_j = (u_j, v_j, w_j)$ related to the coordinate system \mathbf{x}_j , as given in [20]. The transformation of the coordinate system $\mathbf{x} = (x, y, z)$ to $\mathbf{x}_j = (x_j, y_j, z_j)$ is conducted by the rotation matrix \mathbb{R}_j , $\mathbf{x}_j = \mathbb{R}_j(\alpha_i, \beta_n)\mathbf{x}$, $i = 1, \dots, I$, $n = 1, \dots, N$, j is an ordering of (i, n) , for instance, in the Fortran style, by formula $j = (n - 1) \cdot I + i$. The expression for matrix \mathbb{R}_j in terms of the Euler angles α ($0 \leq \alpha < 2\pi$), β ($0 \leq \beta \leq \pi$) is given by

$$\mathbb{R}(\alpha, \beta) = \begin{pmatrix} \cos \beta \cos \alpha & -\sin \alpha & \sin \beta \cos \alpha \\ \cos \beta \sin \alpha & \cos \alpha & \sin \beta \sin \alpha \\ -\sin \beta & 0 & \cos \beta \end{pmatrix},$$

where angle α is specified by the rotation about axis z and β is specified by the rotation about a new axis y_j . The conical coordinates (u_j, v_j, w_j) with the vertex at $z_j = -d_j$ are written in the rotated system of coordinates (x_j, y_j, z_j) by the following transformation

$$\mathbf{u}_j = \mathbb{C}(z_j) \mathbf{x}_j, \quad \mathbb{C}(z_j) = \begin{pmatrix} (1 + z_j/d_j)^{-1} & 0 & 0 \\ 0 & (1 + z_j/d_j)^{-1} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (2a)$$

$$\mathbf{x}_j = \mathbb{C}^{-1}(w_j) \mathbf{u}_j, \quad \mathbb{C}^{-1}(w_j) = \begin{pmatrix} (1 + w_j/d_j) & 0 & 0 \\ 0 & (1 + w_j/d_j) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (2b)$$

To simplify the notations, the following functional dependencies for direct and inverse transformations are used for $j = 1, 2, \dots, J$.

$$\begin{aligned} u_j &= U_j(x_j, y_j, z_j), & x_j &= X_j(u_j, v_j, w_j), \\ v_j &= V_j(x_j, y_j, z_j), & y_j &= Y_j(u_j, v_j, w_j), \\ w_j &= W_j(x_j, y_j, z_j), & z_j &= Z_j(u_j, v_j, w_j). \end{aligned}$$

Hence the relation between the unknown source function $g(\mathbf{x})$ and the scattering data functions $G_j(u, v)$ measured on the (u_j, v_j) -plane is

$$G_j(u, v) = \int_{\mathbf{R}^3} d\mathbf{x} g(\mathbf{x}) \delta(u - U_j(\mathbf{x})) \delta(v - V_j(\mathbf{x})) = \int_0^\infty dw |\mathcal{J}_j| g(\mathbf{x}(u, v, w)), \quad (3)$$

where the Jacobian matrix, \mathcal{J}_j , of the transformation is simply calculated using (2a,2b).

$$\mathcal{J}_j = \frac{\partial(x, y, z)}{\partial(u, v, w)} = (1 + w/d_j)^2.$$

The entropy functional is defined as [8, p.172]

$$E(g) = - \int_D d\mathbf{x} g(\mathbf{x}) \ln(g(\mathbf{x}) \cdot C), \quad (4)$$

where C is the normalization constant.

The reconstruction procedure conducted on the basis of the maximum entropy method is reduced to the following optimization problem with linear constraints:

$$\max_{g \in L^2(D)} E(g) \quad (5a)$$

$$G_j(u, v) = \int_0^\infty dw |\mathcal{J}_j| g(\mathbf{x}(u, v, w)). \quad (5b)$$

The problem (5a-5b) is solved by using Lagrange's method [4]. The Lagrangian writes as

$$L(g, \mathbf{\Lambda}) = E(g) - \int dudv \sum_{j=1}^J \Lambda_j(u, v) [G_j(u, v) - \int dw |\mathcal{J}_j| g(X_j, Y_j, Z_j)]. \quad (6)$$

The integration is carried out over the region of definition of the distribution function $g(\mathbf{x})$, $\mathbf{\Lambda} = (\Lambda_1, \Lambda_2, \dots, \Lambda_J)$ is the Lagrange multipliers.

The result of replacement of variables represents the second integral in (6) as follows

$$\int_D d\mathbf{u} |\mathcal{J}_j| \Lambda_j(u, v) g(\mathbf{u}) = \int_D d\mathbf{x} g(\mathbf{x}) \Lambda_j(U_j, V_j). \quad (7)$$

When taking the Fréchet derivatives of functional $L(g, \Lambda)$ and equating it to zero, one has

$$g(\mathbf{x}) = \frac{1}{e^C} \exp \left[\sum_{k=1}^J \Lambda_k(U_k(\mathbf{x}), V_k(\mathbf{x})) \right] = \frac{1}{C} \prod_{k=1}^J H_k(U_k(\mathbf{x}), V_k(\mathbf{x})), \tag{8}$$

where $e \approx 2.71828$ is the basis of the natural logarithm, $H_k(U_k, V_k) \equiv \exp(\Lambda_k(U_k, V_k) - 1/J)$. The unknown functions $H_k(U_k, V_k)$ may be evaluated by substituting equation (8) into constraints (3):

$$G_j(u, v) = \frac{1}{C} \int_{L_j(D)} dw |\mathcal{J}_j| \prod_{k=1}^J H_k(U_k, V_k). \tag{9}$$

The following equations for the functions H_j are obtained:

$$G_j(u, v) = \frac{1}{C} \cdot H_j(u, v) \int_{L_j(D)} dw |\mathcal{J}_j| \prod_{k \neq j}^J H_k(U_{kj}(u, v, w), V_{kj}(u, v, w)), \tag{10}$$

where $U_{kj} \equiv U_k(x_j, y_j, z_j), V_{kj} \equiv V_k(x_j, y_j, z_j)$.

Matrices \mathbb{C} and \mathbb{R} are used to evaluate elements $\mathbf{U}_{kj} \equiv (U_{kj}, V_{kj}, W_{kj})$ as

$$\mathbf{U}_{kj} = \mathbb{C}(z_k) \mathbb{R}_k \mathbb{R}_j^{-1} \mathbb{C}^{-1}(w_j) \mathbf{u}_j.$$

This leads to the following iterative scheme:

$$H_j^{i+1}(u, v) = \frac{G_j(u, v) \cdot C}{\int_{L_j(D)} dw |1 + w/d_j|^2 \prod_{k \neq j}^J H_k^i(U_{kj}, V_{kj})}, \quad j = i \text{ mod } (J + 1); \tag{11}$$

$$H_j^{i+1}(u, v) = H_j^i(u, v), \quad j \neq i \text{ mod } (J + 1); \tag{12}$$

$$H_j^0(u, v) = \begin{cases} 1, & \text{if } G_j(u, v) \neq 0, \\ 0, & \text{if } G_j(u, v) = 0. \end{cases} \tag{13}$$

The coefficients Λ_j in (6) may also be defined as the solution of unconstrained dual minimization problem when the equation (3) for $G_j(u, v)$ is consistent:

$$\Phi(\Lambda) = \frac{1}{e^C} \int d\mathbf{x} \exp \left[\sum_{j=1}^J \Lambda_j(U_j(\mathbf{x}), V_j(\mathbf{x})) \right] - \int dudv \sum_{j=1}^J \Lambda_j(u, v) G_j(u, v), \tag{14}$$

Since the functional (14) is strictly convex, and the minimum value of $\Phi(\Lambda_1, \dots, \Lambda_J)$ and the maximum value of $L(g, \Lambda)$ coincide [16, p.242], the iterative process above (11-13) converges. Algorithm ((11-13) is essentially one of the multiplicative algebraic methods developed taking into account the specificity of the scattering problem under consideration [5, p.135].

3 Computer simulation

This section describes the results of computer simulation for demonstrating the algorithm. The solid toroid perturbed by toroidal mode $m = 3$ with the aspect ratio $Asp = 5$ are considered as the model for the reconstruction*. We have

$$\begin{aligned} x &= (R_0 \cos(m\varphi) + r \cos \theta) \cos \varphi \\ y &= (R_0 \cos(m\varphi) + r \cos \theta) \sin \varphi \\ z &= r \cos \theta, \end{aligned} \tag{15}$$

where R_0 is the distance from the center of the tube to the center of the torus and is known as the “major radius”, the parameter r is the tube’s radius and is known as “minor radius”, θ and φ are the poloidal and toroidal angles, respectively.

The reconstructions were performed with the data spoiled by some artificial noise. The noise level was taken as 2.5% of maximum level of measured scattering data. The discrepancy between exact and reconstructed models represents the ratio of discrete analog of $L^2(D)$ norms for the exact model and the reconstructed one, respectively, and has the following form.

$$\Delta^2 = \frac{\sum_{i=0}^M (g_i - \tilde{g}_i)^2}{\sum_{i=0}^M g_i^2}.$$

Here the summation is conducted over all grid points of the 3D reconstruction domain, g_i and \tilde{g}_i are the values of the exact model and its estimation at the i -th point of the grid.

Since the scattered fields measured at the detectors are always corrupted by noise, and noise can also arise during computations, the reconstructed image is, therefore, also noisy. This is clearly seen in Fig. 2. The following procedure for smoothing a three-dimensional array have been used.

$$R_i = \begin{cases} \frac{1}{w} \sum_{j=0}^{w-1} A_{i+j-w/2}, & i = w/2, \dots, N - w \\ A_i, & \text{otherwise,} \end{cases}$$

where N is the number of elements in array A , w is the smoothing window for each dimension. For example, if $w = 3$ is used to smooth a three-dimensional array, the smoothing window will contain 27 elements, including the element being smoothed.

Fig. 4 shows the images of the exact and reconstructed models in $x - y$ (left) and $x - z$ (right) sections; **a**) the exact model; **b**) reconstruction is conducted without collimation, that is, the cone axis is fixed in the laboratory frame of reference; **c**) reconstruction is conducted with collimation, that is, the axis of the cone is oriented along the axis z_j of the rotated coordinate system. The error of reconstruction depending on the number of measurements for the three models with different toroidal modes $m = 1, 2, 3$ are given in Fig. 3. The relative error of reconstruction is not more than 10 – 15% for 100 number of measurements.

*toroidal aspect ratio is defined as $Asp = R_0/r$.

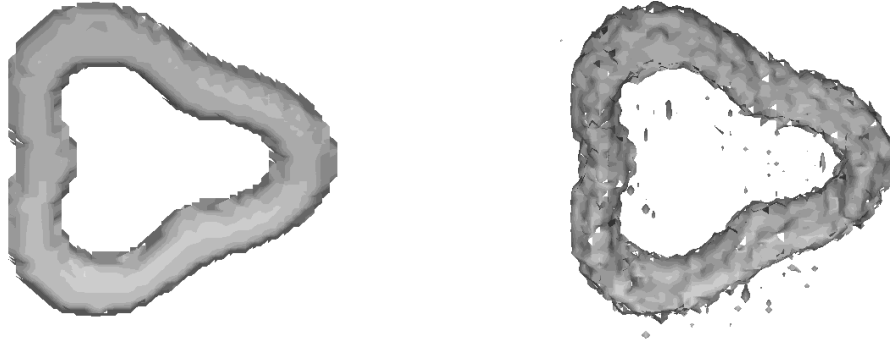


Figure 2: Perturbed by the toroidal mode $m = 3$ model toroid (left) and reconstructed one (right) with the aspect ratio $Asp = 5.0$. The relative error of reconstruction is not more than 10.5%. Reconstruction is performed with data measurements without collimation.

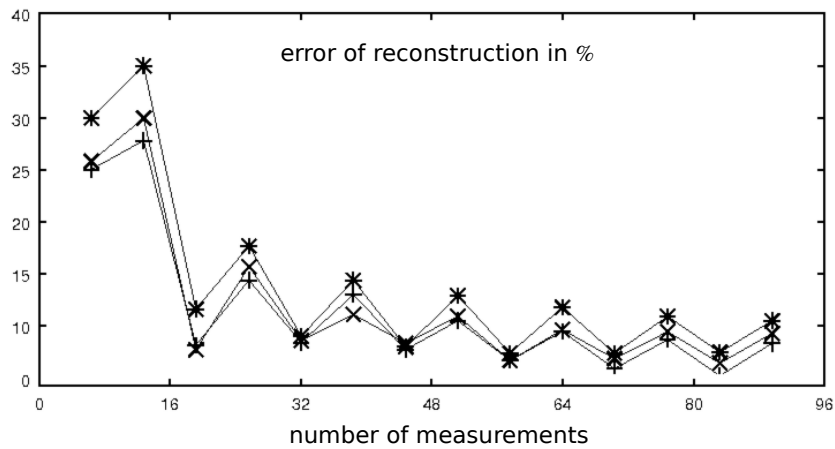


Figure 3: The reconstruction error (in per cent) against measurement numbers for different toroidal modes ($m = 1(- + -)$, $m = 2(- \times -)$, $m = 3(- * -)$).

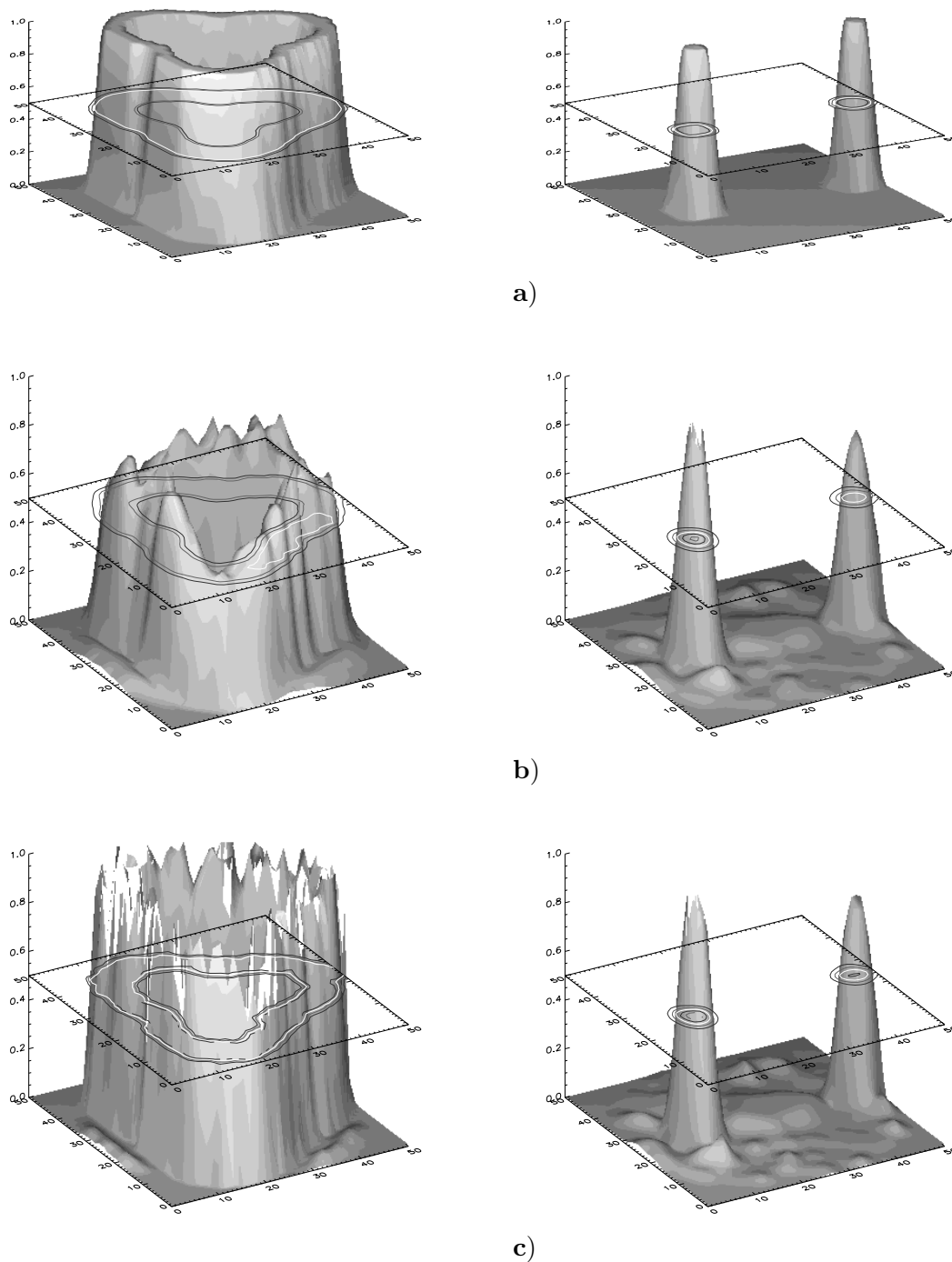


Figure 4: The images of the exact and reconstructed solid toroids in $x-y$ (left) and $x-z$ (right) sections; **a)** exact model; **b)** reconstruction is performed without collimation, that is, the cone axis is fixed in laboratory frame of reference; **c)** reconstruction is performed with collimation, that is, the axis of the cone is oriented along the axis z_j of the rotated coordinate system.

4 Conclusion

The method of reconstruction of 3D scattering object function with the use of the maximum entropy method has been developed. The method is quite resistant to noise in an experimental data. The numerical modelling conducted has shows an acceptable accuracy of reconstruction on the model with small number of measurement data. With minor modification of the program code, various schemes of measurements may be realized. The method developed can also be generalized, if necessary, for the sign-altering functions [3].

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