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A Method of Choosing the Optimal Number of Singular Values in the Inverse Laplace Transform for the Two-Dimensional NMR Distribution Function *

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Two-dimensional (2D) nuclear magnetic resonance (NMR) distributions as functions of diffusion coefficient and relaxation time are powerful tools in the study of porous media. We propose a practical method to perform proper truncation of singular value decomposition (TSVD) in Laplace inversion for obtaining 2D-NMR distributions from measured NMR data. By analyzing basic algorithms for Laplace inversion, it is well known that proper TSVD does not affect the inversion result for an ill-posed problem with zero-order Tikhonov regularization, but can greatly increase the inversion speed. In this new method, the optimal number of singular values for data compression is applied to each dimension separately. The method also makes full use of the redundancy nature of the data with a finite signal-to-noise ratio and well balances the tradeoff between the speed and the bias. The method does not require the stochastic information of the estimated parameters when obtaining the optimal number of singular values.

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Nuclear magnetic resonance (NMR) relaxation time and diffusion coefficient have long been playing an important role in the study of porous media such as biological systems,[1] food,[2] building materials[3] and reservoir rocks.[4] A recently developed technique to acquire the two-dimensional diffusion-relaxation (D-T2) distribution function separates oil (especially heavy oil) from water by striking diffusivity contrast in fluids while obtaining their T2 distributions.[5] As a result, the 2D distribution functions become powerful tools in well logging and laboratory core analysis. A two-dimensional inverse Laplace transform is required to extract the 2D distribution functions from the observed data. The inversion is a typical ill-posed problem[6] with smooth kernels for the measurement of the relaxation time or the diffusion coefficient, and inverting a large data set of low signal-to-noise ratio (SNR) in a short time is a great challenge. Because of the ill-posed nature and the low SNR, proper truncation of singular value decomposition has little effect on the inversion result and it accelerates the computing speed greatly.[7] However the optimal number of singular values is unable to be predetermined before the inversion according to the above methods. An early study in image reconstruction chose the optimal number of singular values with known stochastic information of the distribution to be estimated, but the stochastic information is unavailable in most cases.

In this Letter, a diffusion editing technique with separable kernels is employed so that the compression can be carried out in each dimension. The transverse relaxation time is measured using a CPMG sequence.[8] The diffusion editing is achieved using a stimulated echo sequence with pulsed field gradients.[9] The pulse sequence for the 2D distribution function measurements has an initial editing part in place of the standard 90° pulse in CPMG sequence.

The sequence used for data simulations and experimental tests in this study is shown in Fig. 1. The observed data are composed of echo peak amplitudes in m echo trains of length n acquired with m different gradients.

In discrete form, the 2D distribution function is a density matrix F $(x \times y)$ on x different transverse relaxation times and y different diffusion coefficients. The observed data matrix M $(n \times m)$ is related to the distribution function by a two-dimensional Laplace transform with two independent kernels K_1 and K_2:

$$M = K_1 F K_2 + \varepsilon, \tag{1}$$

where ε is an additive noise with zero mean and standard deviation σ. F_{ij} is the density on the transverse relaxation time $T2_i$ and the diffusion coefficient D_j $(i \in \{1, \ldots, x\},\ j \in \{1, \ldots, y\})$. The kernels are $K_{1li} = \exp(-lt_E/T2_i)$ $(l \in \{1, \ldots, n\})$ and $K_{2jk} = \exp(-\gamma^2 g_k^2 \delta^2 D_j(\Delta - \delta/3))$ $(k \in \{1, \ldots, m\})$, where γ is the gyro-magnetic ratio.

Let singular value decomposition (SVD) of K_1 and K_2 be

$$K_1 = U_1 \Sigma_1 V_1', \quad K_2 = U_2 \Sigma_2 V_2', \tag{2}$$

where Σ_1 and Σ_2 are diagonal matrices whose elements on the diagonal are nonnegative singular values in descending order. U_1, U_2, V_1 and V_2 are unitary matrices. The prime denotes the transpose.

The first r_1 $(r_1 < x)$ columns of U_1 and V_1 form $\tilde{U}_1$ and $\tilde{V}_1$ respectively. $\tilde{\Sigma}_1$ is a matrix composed of the first r_1 rows and r_1 columns of Σ_1. $\tilde{U}_2$ and $\tilde{V}_2$ are

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the first r_2 ($r_2 < y$) columns of U_2 and V_1. $\tilde{\Sigma}_2$ is the matrix composed of the first r_2 rows and r_2 columns of Σ_2. Equation (1) is converted to

$$\tilde{M} = \tilde{K}_1 F \tilde{K}_2 + \varepsilon, \tag{3}$$

where $\tilde{M} = \tilde{U}_1' M \tilde{V}_2$, $\tilde{K}_1 = \tilde{\Sigma}_1 \tilde{V}_1'$, $\tilde{K}_2 = \tilde{U}_2 \tilde{\Sigma}_2$. Then the problem of the 2D distribution function can be converted to a 1D problem by lexicographically ordering $\tilde{M}$ and F,

$$m = Kf + \varepsilon. \tag{4}$$

Here $K = \tilde{K}_1 \otimes \tilde{K}_2'$, and $\otimes$ denotes the Kronecker product. In our method the TSVD is performed on K_1, K_2, respectively. It is more practical and faster than the method which performs the TSVD on K.[10,14] The optimization problem to find the nonnegative least square solution of Eq. (4) with a zero-order regularization functional weighted by α is posed as

$$f = \arg\min_{f\geq 0} \|m - Kf\|^2 + \alpha\|f\|^2. \tag{5}$$

It is equivalent to minimize $\psi = c'(G + \alpha I)c/2 - c'm$, where $f = K'c$ and $G = KK'$ have $r_1 \times r_2$ rows and $r_1 \times r_2$ columns.[11] Then a pure inverse Newton iterative method is performed for minimizing according to $c_{n+1} = c_n - (G + \alpha I)^{-1}((G + \alpha I)c_n - m)$. If $f_i < 0$ in the iterative course, we set the ith column of K to be zero and change G correspondingly.

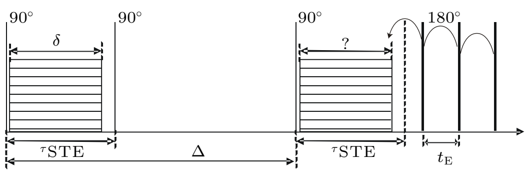

Fig. 1. The pulse sequence to measure D-T2 distribution functions with incremented gradient pulse amplitudes (rectangular area of width δ).

Without truncation of SVD ($r_1 = x, r_2 = y$), $G + \alpha I$ is too large to be inverse for standard PCs. On the contrary if r_1, r_2 are too small, the inversion result will be strongly biased. Thus the number of singular values plays a key role in the data compression.

A practical method was derived to choose the optimal number of singular values according to the number of data points and the SNR. This method is able to choose the optimal number of singular values in advance for known kernels, which makes it possible to realize real-time analysis. Since the compression is accomplished through TSVD in each dimension respectively, the method can be derived from the analysis of a 1D problem:

$$M = KF + \varepsilon. \tag{6}$$

There are n data points in data vector M and N points in distribution vector F; ε is an additive white noise with zero mean and standard deviation σ. The SVD of kernel K gives

$$K = USV', \tag{7}$$

where U ($n \times N$), V ($N \times N$) are unitary matrices. S is a diagonal matrix with singular values in descending order on the diagonal.

The least square solution to Eq. (6) is

$$F = VS^{-1}U'M. \tag{8}$$

The distribution is a sum of sub distributions corresponding to different s_i:

$$F = \sum_i v_i \frac{u_i' M}{s_i}, \tag{9}$$

with $\|v_i\| = 1$ and $\|u_i\| = 1$ in unitary matrices. Thus the noise is only amplified by small s_i. There are two approaches to avoid the noise amplification. (1) Zero-order Tikhonov regularization: the problem is regularized by a zero-order Tikhonov regularization functional weighted by a smoothing factor α. This method is equal to increasing s_i by α/s_i,

$$F = \arg\min \|M - KF\|^2 + \alpha\|F\|^2 = \sum_i v_i \frac{u_i' M}{s_i + \alpha/s_i} \tag{10}$$

(2) SVD truncation: sub-distributions corresponding to zero or very small singular values are discarded.

Some of the sub distributions in Eq. (10) can be discarded if $\alpha \gg s_i^2$ for a proper smoothing factor α.

In the first approach, the main structure of the distribution generated from the signal is $v_1 u_1' M/\hat{s}_1$ where $\hat{s}_1$ is the maximum one of $\hat{s}_i = s_i + \alpha/s$. The maximum sub distribution caused by the noise is $v_r u_r' \varepsilon/\hat{s}_r$, where $\hat{s}_r$ is the minimum one of $\hat{s}_i = s_i + \alpha/s$. To avoid the noise amplification, the sub-distributions caused by the noise should be very small compared with the main structure of the distribution generated from the signal

$$\left\| v_1 \frac{u_1' M}{\hat{s}_1} \right\| \gg \left\| v_r \frac{u_r' \varepsilon}{\hat{s}_r} \right\|. \tag{11}$$

Because of the isotropic property of white noise $\|u_r' \varepsilon\| = \sigma$, the inequality (11) can be converted to $\|u_1' M/\sigma\| \gg \|\hat{s}_1/\hat{s}_r\|$, where u_1 is the basic trend of the measured data,[7] so $u_1' M \approx M$ and $\|u_1' M/\sigma\| \approx \sqrt{n}\mathrm{SNR}(a)$. Here

$$\sqrt{n}\mathrm{SNR}(a) \gg \left\| \frac{\hat{s}_1}{\hat{s}_r} \right\|, \tag{12}$$

$\mathrm{SNR}(a)$ is related to the SNR in dB through

$$\mathrm{SNR(dB)} \approx 20 \log \mathrm{SNR}(a), \tag{13}$$

where α must be large enough to satisfy inequality (12). There are a lot of methods to choose α with a finite SNR in the literature.[11,12]

In an ill-conditioned problem, there are many singular values very close to zero;[13,15]

$$v_i \frac{u_i' M}{s_i + \alpha/s_i} \ll v_i \frac{u_i' M}{s_i},$$

when $\alpha \gg s_i^2$. The sub-distributions corresponding to the s_i can be ignored after Tikhonov regularization so that discarding such sub-distributions does not affect the result obtained through the first approach.

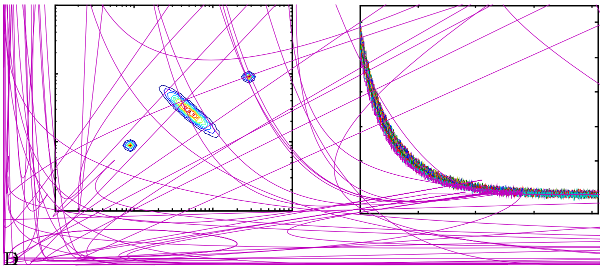

Fig. 2. The true distribution function (a) and (b) the simulated observed data (SNR = 23 dB).

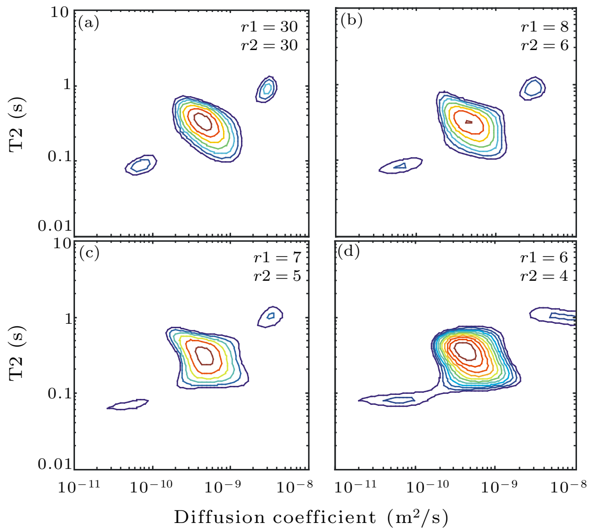

Fig. 3. D-T2 distribution inversion result for the simulated data (a) with $r_1 = 30$, $r_2 = 30$ (very large for 500 MB memory), (b) with singular values truncated according to the method in this study, (c) with $r_1 = 7$, $r_2 = 5$, and (d) with $r_1 = 6$, $r_2 = 4$.

Based on the analysis described above, the inverse problem can be solved in two steps: (1) Truncation of SVD: choose r singular values so that $\sqrt{n}\mathrm{SNR}(a) \approx \|s_1/s_r\|$. Then generate the compressed kernel and data. (2) Choose a proper smoothing factor α to satisfy inequality (12) and solve the optimization problem with nonnegative constraints according to the BRD method.

Additionally, the method we proposed chooses the smallest number of singular values when $u_1' M \approx \|M\|$. If $u_1' M < \|M\|$, the method chooses more than adequate singular values, which ensures the quality of the result.

This method is demonstrated through a set of simulations for a D-T2 model with 60 T2 parameters logarithmically spaced between 0.01 s and 10 s, and 60 diffusion coefficients logarithmically spaced between 10^{-11} m^2/s and 10^{-8} m^2/s. The echo train length is 2048 and $t_E = 1$ ms. There are 50 echo trains acquired with different gradient amplitudes logarithmically spaced between 0.005 T/m and 0.15 T/m. The duration of the gradient pulses is $\delta = 20$ ms, and the interval time between the gradient pulses is $\Delta = 50$ ms. The maximum simulated signal amplitude is 1 and the noise standard deviation is 0.00832. The SNR is 23 dB. The true distribution function and the simulated observed data are shown in Fig. 2. The distribution functions are displayed by contour plots.

In this study, $\alpha = 5$ is chosen according to the L-curve,[13] and it is large enough to satisfy inequality (11). The result with $r_1 = 8$ and $r_2 = 6$ is shown in Fig. 3(b). The result has little variation with $r_1 = 30$ and $r_2 = 30$ in Fig. 3(a), and it is severely distorted when the number of singular values is decreased by 1 in each dimension (Fig. 3(c)). Some peaks are lost completely with much smaller singular values (Fig. 3(d)).

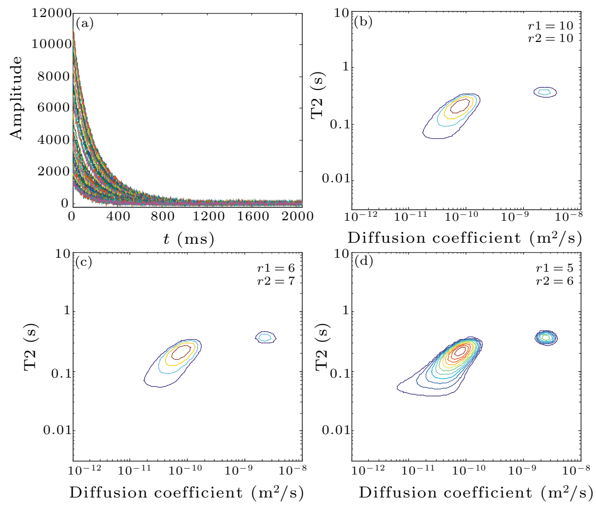

Fig. 4. D-T2 distribution inversion result of a reservoir core. (a) The experimental data for the reservoir core. (b) The distribution function obtained with $r_1 = 6$, $r_2 = 7$. (c) The distribution function obtained with $r_1 = 10$, $r_2 = 10$. (d) The distribution function obtained with $r_1 = 5$, $r_2 = 6$.

The results on simulated data show that the described method fulfills the purpose to choose the smallest number of singular values in each dimension without information loss. The inversion with the optimal number of singular values takes only a few seconds except for a period of about 2 min for SVD (on a computer with 500 MB memory and a Pentium (D) 2-core 3.00 GHz CPU). The speed is fast enough to make real time analysis for both laboratory tests and well-logging if the SVD could be carried out in advance for predetermined kernels. However, the inversion with $r_1 = 30$, $r_2 = 30$ takes more than 10 min on the same computer.

A reservoir core of 2.5 cm in diameter and 4 cm in length is initially fully saturated with 15# white oil (the viscosity of the oil is 15cp at 40℃) and then centrifuged in water with an average capillary pressure of 20 psi. The NMR experiment is conducted on a home-built NMR spectrometer (with ^{1}H Larmor frequency of 5 MHz). The D-T2 distribution function is measured with gradient duration $\delta = 40$ ms and the interval between gradient pulses $\Delta = 70$ ms. There are 40 acquisitions operated with gradient amplitudes linearly spaced between 2 mT/m and 84 mT/m. The echo train length (ETL) is 1024 with $t_{ESP} = 2$ ms. The SNR(a) = 25 is estimated from the observed data shown in Fig. 4(a) according to this method. Here $\alpha = 9$ is chosen according to the L-curve for the inversion results in Fig. 4; and $r_1 = 6$, $r_2 = 7$ are set as the optimal numbers. The corresponding result is shown in Fig. 4(b). The water and oil, whose relaxation times are very close to each other, are separated well in the D-T2 distribution function. The diffusion coefficient of the oil is much smaller than that of water. The result varies little when more singular values are involved (Fig. 4(c)), and the oil peak is strongly distorted with less singular values in each dimension (Fig. 4(d)).

In summary, a practical method is presented to make optimal TSVD in the fast inverse Laplace transform for two-dimensional NMR distribution functions. In our method the TSVD is performed in each dimension respectively. This method does not require any stochastic information of the inversion result. The method shows good performance with the smoothing factor chosen by the commonly used methods for zero-order Tikhonov regularization. For the predetermined kernels the optimal number of singular values can be determined in advance. According to this method, the inversion can be accomplished in a very short time without large computer memory requirement. The method and the inversion algorithm are expected to be suitable for most 2D inversion problems.

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