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Uniform-Penalty Inversion of Multiexponential Decay Data

II. Data Spacing, T_2 Data, Systematic Data Errors, and Diagnostics

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The basic method of UPEN (uniform penalty inversion of multiexponential decay data) is given in an earlier publication (Borgia *et al., J. Magn. Reson.* 132, 65–77 (1998)), which also discusses the effects of noise, constraints, and smoothing on the resolution or apparent resolution of features of a computed distribution of relaxation times. UPEN applies negative feedback to a regularization penalty, allowing stronger smoothing for a broad feature than for a sharp line. This avoids unnecessarily broadening the sharp line and/or breaking the wide peak or tail into several peaks that the relaxation data do not *demand* to be separate. The experimental and artificial data presented earlier were T_1 data, and all had fixed data spacings, uniform in log-time. However, for T_2 data, usually spaced uniformly in linear time, or for data spaced in any manner, we have found that the data spacing does not enter *explicitly* into the computation. The present work shows the extension of UPEN to T_2 data, including the averaging of data in windows and the use of the corresponding weighting factors in the computation. Measures are implemented to control portions of computed distributions extending beyond the data range. The input smoothing parameters in UPEN are normally fixed, rather than data dependent. A major problem arises, especially at high signal-to-noise ratios, when UPEN is applied to data sets with systematic errors due to instrumental nonidealities or adjustment problems. For instance, a relaxation curve for a wide line can be narrowed by an artificial downward bending of the relaxation curve. Diagnostic parameters are generated to help identify data problems, and the diagnostics are applied in several examples, with particular attention to the meaningful resolution of two closely spaced peaks in a distribution of relaxation times. Where feasible, processing with UPEN in nearly real time should help identify data problems while further instrument adjustments can still be made. The need for the nonnegative constraint is greatly reduced in UPEN, and preliminary processing without this constraint helps identify data sets for which application of the nonnegative constraint is too expensive in terms of error of fit for the data set to represent sums of decaying positive exponentials plus random noise.

Key Words: **relaxation times; inversion; regularization; multiexponential; nuclear magnetic resonance.**

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INTRODUCTION

The basic method of UPEN (uniform penalty inversion of multiexponential decay data) is given in an earlier publication (*1*), which also discusses the effects of noise, constraints, and smoothing on the resolution or apparent resolution of features of a computed distribution of relaxation times. Numerous examples of artificial and laboratory relaxation data have been inverted by UPEN (*1, 2*) and compared with inversion employing a fixed regularizing parameter, illustrating the ability of UPEN to show, for instance, a sharp peak with a long low tail.

The examples discussed in Ref. (*1*) were of T_1 data with a uniform data density in log-time, and the present work extends the use of UPEN to T_2 data equally spaced in linear time and to multiexponential decay data spaced in any manner. Provisions are made for any necessary weighting of the input data points, including where data points are averaged in windows in order to have a manageable number of input points for computation.

The sections Inversion with Variable Smoothing and Feedback for Uniform Penalty are complete, extended, and updated versions of the corresponding sections in Ref. (*1*), with the present Eqs. [2–9] corresponding to Eqs. [2–9] of Ref. (*1*). This is to introduce and implement the windowing and weighting needed for most T_2 data and to remove the essentially unused surmise in (*1*) that, if data density is variable, it should enter *explicitly* in the UPEN computation as a factor in the smoothing penalty. Of course, denser data can force sharper detail.

Some of the symbols used in more than one section are given in the Appendix.

AVERAGING OF ECHOES IN WINDOWS

T_2 data are usually taken using some variant on CPMG, the Carr–Purcell–Meiboom–Gill method, with equal spacing in linear time. However, as many as 10^5 echoes have been taken, and it is usual to take hundreds or thousands of echoes. If any systematic data errors are smoothly varying with data time, and if the noise is additive, random, and normally distributed (or at

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least from a compact distribution), the averaging of data points into sufficiently narrow windows does not change the result with respect to that obtained by using all of the points without windowing (when this is computationally possible). The common practice of simply discarding most of the points at long times is simply a waste of good information, leading to a decreased effective signal-to-noise ratio (SNR). Numbers of points for computation can be, in some cases, reduced by orders of magnitude. A window with a full width $D = 0.05$ times its center time is narrow enough for almost all real data that we have. The first approximately $2/D$ points should be left unwindowed. These parameters are conservative, as for research use. In most applications windowing can be more severe, giving yet fewer points for computation.

If most of the original data points are subject to random noise of a given rms value, but if there are a few outliers (due to noise bursts, periodic spikes, etc.), then the editing of the data set should be done before windowing, and the windows should not span gaps in the data.

If the jth echo has amplitude s_{ej} at echo time t_{ej}, the ith window has B_i echoes in it with average signal s_i and average time t_i, $j_i = t_i/T_{EE}$ (integer or half-integer) is the index of the window center, and T_{EE} is the spacing of the echoes employed (whether even echoes or all echoes), we have $s_i = 1/B_i \sum_{j_i-(B_i-1)/2}^{j_i+(B_i-1)/2} s_{ej}$ and $t_i = 1/B_i \sum_{j_i-(B_i-1)/2}^{j_i+(B_i-1)/2} t_{ej}$. Although the sums can be evaluated exactly for an exponential signal, an integral approximation is adequate for our purposes. The noise-free part of the signal s_i is overestimated in the above average by the approximate factor

$$\frac{1}{T_{EE}B_i}\int_{-T_{EE}B_i/2}^{T_{EE}B_i/2} e^{-\tau/T}d\tau = \frac{\sinh[(T_{EE}B_i/(2T)]}{[T_{EE}B_i/(2T)]} \approx 1 + \frac{1}{6}\left(\frac{T_{EE}B_i}{2T}\right)^2, \qquad [1]$$

where T is relaxation time. If D is the relative window width (width in time divided by center time), $B_i = Dt_i/T_{EE}$. For the relaxation time T the error term in Eq. [1] gives the absolute error $(1/6)[Dt_i/(2T)]^2\exp(-t_i/T)$. The maximum value of an expression of the form x^2e^{-x} is $4/e^2 \approx 0.54$. Thus, relative to the initial signal, the error from averaging in windows is less than $0.0225\ D^2$.

INVERSION WITH VARIABLE SMOOTHING

Inversion with Fixed Smoothing and without Weighting Factors

We wish to approximate a set of relaxation data s_i, taken at times t_i equally spaced in $q_i = \ln t_i$, by a sum of M exponential components, $s_i \approx g_0 + \sum g_k\exp(-t_i/T_k)$, where T_k are the relaxation times equally spaced in $Q_k = \ln T_k$ and covering about the same range as t_i. The distribution of amplitudes at relaxation times T_k (on the logarithmic time scale) is g_k, and $g_0 = S_\infty$, the value of the signal at infinite time, may or may not be also a regression parameter. To avoid excessive detail a penalty function is added to the squared error of fit, and their sum is minimized. Common penalty functions are squares of amplitude, slope (first difference), or curvature (second difference). The function to be minimized is then of the form

$$\sum_{i=1}^{N}(g_0 + \sum_{k=1}^{M} g_k\exp(-t_i/T_k) - s_i)^2 + A\sum_{k=1}^{M} g_k^2 + D\sum_{k=1}^{M-1}(g_{k+1} - g_k)^2 + C\sum_{k=2}^{M-1}(g_{k-1} - 2g_k + g_{k+1})^2, \qquad [2]$$

where A is the coefficient for amplitude smoothing, D (difference) for slope smoothing, and C (curvature) for curvature smoothing. We do not include the g_0 term in the penalty function. Usually only one of the three kinds of smoothing is used.

Inversion with Weighting Factors and Variable Smoothing

To introduce more equitable smoothing for sharp and broad features, we make A, D, and C in Eq. [2] variable, with subscript k, and move them inside the summations. Although variable smoothing can be implemented for amplitude, slope, or curvature smoothing, we will discuss only curvature smoothing (but with feedback from both curvature and slope), which we have used for a number of years. However, outside the range of relaxation times covered by the data, we are now applying additionally an amplitude penalty, with amplitude feedback only.

The averaging of points in windows requires the introduction of the weighting factors B_i into the generalization of Eq. [2]. We apply a curvature penalty, with both curvature and slope feedback, just as in Ref. (*1*), although the compliance (or feedback) parameters α of Ref. (*1*) have been changed to β's, because the change in the assumption about the appearance of data point spacing in Eq. [9] of Ref. (*1*) inserts a factor of 0.08, the spacing used in all examples in Ref. (*1*), multiplying the former α's. The amplitude penalty now applied outside the data range adds the A-term of Eqs. [2–3]. The quantity to be minimized is now

$$\sum_{i=1}^{N} B_i(g_0 + \sum_{k=1}^{M} g_k\exp(-t_i/T_k) - s_i)^2 + \sum_{k=1}^{M} A_k g_k^2 + \sum_{k=2}^{M-1} C_k(g_{k-1} - 2g_k + g_{k+1})^2, \qquad [3]$$

where C_k will be iteratively adjusted in regions of substantial curvature to be roughly reciprocal to the local curvature squared (which itself depends on the C_k). The A_k's are zero within the range of relaxation times covered by the data. With good SNR some extrapolation of relaxation time components outside the data range is permitted. The g_0 term is used only if the asymptotic value at infinite time is a regression parameter.

We now use matrix notation for Eq. [3]. There are N data times (spaced in any manner but without big gaps), with weighting factors B_i, which are represented by the $N \times N$ diagonal matrix **B**. There are $M + M_N$ computed components, where $M_N = 1$ if the signal value at infinite time is a regression parameter, and $M_N = 0$ otherwise. The coefficients A_k are represented by the diagonal matrix **A**, with nonzero components only for relaxation times outside the range of times covered by the data.

If the components g_k, s_i, and x_i make up the vectors **g** (computed distribution, $M + M_N$ components), **s** (measured noisy signal, N components), and **x** (computed fit to the signal, N components), and if the components $\exp(-t_i/T_k)$ make up the $N \times (M + M_N)$ matrix **U**, we have $\mathbf{x} = \mathbf{Ug}$.

The first term in Eq. [3] is then $\mathbf{g}^\dagger\mathbf{U}^\dagger\mathbf{BUg} - 2\mathbf{s}^\dagger\mathbf{BUg} + \mathbf{s}^\dagger\mathbf{Bs}$, with the last of these a constant. We let $\mathbf{U}^\dagger\mathbf{BU} = \mathbf{W}$. This $(M + M_N) \times (M + M_N)$ matrix need be computed only once for the iterative computation of **g** unless changes are made in **B** or in **s** and **t**.

For the curvature penalty term in Eq. [3] we first find the contribution for unit C_k for a single k-value. This involves g_{k-1}, g_k, and g_{k+1}. The curvature (second difference) at the kth computed point is $\mathbf{V}^{(k)}\mathbf{g}$, where $\mathbf{V}^{(k)}$ is an $(M + M_N) \times (M + M_N)$ matrix containing all zero elements except for the submatrix

$$\begin{pmatrix} 0 & 0 & 0 \\ 1 & -2 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad [4]$$

centered at the kth diagonal point. The contribution to the curvature squared is $\mathbf{g}^\dagger\mathbf{V}^{(k)\dagger}\mathbf{V}^{(k)}\mathbf{g}$, where $\mathbf{V}^{(k)\dagger}\mathbf{V}^{(k)}$ is a symmetrical matrix containing all zero elements except for the submatrix

$$\begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix}, \qquad [5]$$

centered at the kth diagonal element. We now form the matrix **K** (*Krümmung:* curvature) by multiplying each matrix $\mathbf{V}^{(k)\dagger}\mathbf{V}^{(k)}$ by its curvature smoothing coefficient C_k and summing the matrices for all k-values from $2 + M_N$ to $M + M_N - 1$. The coefficients A_k for the amplitude penalty are simply added to the corresponding diagonal element of **K**. The total penalty is $\mathbf{g}^\dagger\mathbf{Kg}$. Equation [3], and the quantity to be minimized, is now given by

$$\mathbf{g}^\dagger\mathbf{Wg} - 2\mathbf{s}^\dagger\mathbf{BUg} + \mathbf{s}^\dagger\mathbf{Bs} + \mathbf{g}^\dagger\mathbf{Kg}. \qquad [6]$$

We let $\mathbf{s}^\dagger\mathbf{BU} = \mathbf{Y}$ and minimize the above expression by setting the gradient with respect to **g** to zero, giving

$$\mathbf{Wg} + \mathbf{Kg} = \mathbf{Y}; \quad \mathbf{g} = (\mathbf{W} + \mathbf{K})^{-1}\mathbf{Y}. \qquad [7]$$

FEEDBACK FOR UNIFORM PENALTY

Weighting Factors and Scaling of Signal and Noise

In Eq. [3] the weighting factor B_i for the windowed signal s_i at time t_i is normally equal to the number of data points averaged in the window for s_i. However, the inherent weight of a point, windowed or not, is inversely proportional to the square of the point's level of random noise, the noise of which is in turn proportional to the noise of the individual data points divided by the square root of the number of points averaged in the window. If different individual points have different inherent noise levels, this can be accounted for by different B_i values. If the individual data points have noise randomly selected from a Gaussian distribution of half-width R, we can either divide the B_i's by R^2 or else multiply the other terms in Eq. [3] by R^2. If we include the factor $1/R^2$ in B_i, we note that the first of the three terms in Eq. [3] becomes scale-independent. That is, the term is not changed by multiplying the input noisy signal by some scale factor. The g's are multiplied by the same factor when the data are fit, if the fit is not changed other than by scale. The noise-free signal, the noise, and the fitted function all become scaled by the same factor.

Of course, the g's in the other two terms of Eq. [3] appear quadratically, so these terms are proportional to the square of the scaling factor if the C's and the A's are left unchanged. Thus, the C's and A's are invariant with respect to scaling of the data.

In the present version of UPEN the noise R is estimated in each iteration (rather than input from separate computation, as in Ref. (*1*)) and may change significantly in the first few iterations. If the weighting factors do not change with respect to each other, it is not necessary to recompute the matrix **W**, merely to change a constant factor. Therefore, Eq. [3] is multiplied by the factor R^2, so that R^2 appears as a factor in the equations for C_k and A_k.

Feedback

To have a strictly uniform penalty, that is, the same contribution to the right side of Eq. [3] for each value of k, we would have to find a way to make C_k inversely proportional to the square of the second difference. However, when the curvature is zero or negligible, it is not possible or not meaningful to make C_k large enough to maintain a truly uniform penalty at such points. We can obtain a penalty which is the same at points of significant curvature by a series of iterations, starting

with a fixed C_k and for each new iteration letting C_k be inversely proportional to the square of the second difference from the previous iteration. This does give adequate fits to relaxation data and gives a penalty that is either zero or negligible or else a fixed value; however, this gives unsatisfactory distributions consisting of straight-line segments. This can be improved considerably by relaxing the uniform penalty requirement somewhat and using at each k the highest of the second-difference-squared values found at $k - 1$, k, or $k + 1$ from the previous iteration. That is, C_k for the next iteration is inversely proportional to the largest second-difference-squared found at k or a nearest neighbor. We can further improve appearance in many cases by using also second-nearest neighbors or points from an even wider window. However, a wide window interferes with implementing abrupt changes in smoothing coefficient. It is also possible to use only slope-squared feedback (instead of curvature feedback) for curvature smoothing. In this case it is necessary to use the highest slope-squared over a window extending about 0.3 Np in relaxation time both above and below the point k. A useful compromise was found to be the use of both curvature and slope feedback and for each k to use the highest curvature values found at the point or a nearest neighbor.

The smoothing coefficients C_k are coefficients of rigidity for the computed distributions. Therefore, the feedback to adjust the C_k to give roughly uniform penalty consists of local *compliance* contributions from both slope and curvature. To implement this we use a slope compliance parameter β_p (*pendenza:* slope) and a curvature compliance parameter β_c to define the compliance

$$c_k = \beta_p \Delta_Q^2 (g_{k+1} - g_{k-1})^2 + \beta_c \max[(g_{j-1} - 2g_j + g_{j+1})^2]_{j=k-1,k,k+1}, \quad [8]$$

where the β's are constants that are not changed from one iteration to the next nor from one data set to the next. The factor of Δ_Q^2 is to preserve the ratio of approximate first and second derivatives when the spacing Δ_Q in Nepers of computed points is changed.

Balance between Smoothing and Noise

The residuals term (left) and the penalty terms (right) of Eq. [3] should somehow be balanced in finding the quantity to be minimized to get the distribution g_k. In the vicinity of a good solution to good data the residuals term from the minimization of Eq. [3] is primarily due to the random noise. If R is the rms noise, the penalty terms in Eq. [3] should be proportional to R^2 to preserve appropriate scaling when the input noisy signal is merely multiplied by a factor. We therefore multiply the penalty terms by R^2, as mentioned above, although we could alternatively include a factor $1/R^2$ with the weighting factors **B**. For the ensemble rms noise R we use a combination of the noise estimates defined later in Eqs. [13–14]. Note that this paragraph and Eq. [9] have a substantive change from those of Ref. (*1*), in addition to extensions of the method. Removing a factor of the data spacing replaces a factor of Δ_q in Eq. [9] with 0.08, the value it had in all examples in Ref. (*1*). Another change is in defining slope between points $k + 1$ and $k - 1$ without involving point k, resulting in a 4× reduction in β_d. This is to avoid a large slope contribution from a single-point peak.

To approximate an integral of the form $\int C(Q)(d^2g/dQ^2)^2 dQ$ for the curvature penalty by a discrete sum, we include the step size Δ_Q as a factor in the coefficient C_k. We now have

$$C_k = R^2 \Delta_Q / (\beta_0 + c_k). \quad [9]$$

The C_k's from one iteration are used to give the C_k's for the next. The term β_0 is a compliance floor, which should be small enough that it would never lead to undersmoothing, but which should be large enough to be a "seed" for the development of curvature in the iteration process. For use with either low or high SNR data β_0 is now made very small (10^{-6} rather than equivalent to 80, as in Ref. (*1*), where low SNR data were not presented). It is not critical, but it cannot be zero.

The A_k term of Eq. [3] is the amplitude penalty applied for relaxation times outside the data range and is implemented by simply adding A_k to the kth diagonal element of **K** (see Eq. [6]), with $A_k = 0$ within the range of relaxation times covered by the data and

$$A_k = R^2 \Delta_Q / (\beta_0 + \beta_a g_k^2) \quad [10]$$

outside the data range, without contributions from neighboring points. The compliance parameter for amplitude feedback for the amplitude penalty is β_a (a for amplitude). The curvature penalties are applied to the entire range of relaxation times for the computed distribution, including those outside the range of data times. The relaxation times for computed points are usually extended a factor of 5 above and below the range of the data, with distribution values and slopes being zeroed at each end. That is, the first two and last two points are forced to zero, although, in the actual computation, these are virtual points and do not extend the range of the parameter space.

The current "default" values of the β's are $\beta_0 = 10^{-6}$, $\beta_a = 0.5$, $\beta_p = 0.6$, and $\beta_c = 0.3$. In addition, the program uses β_{00}, normally 1.0, which can be used to multiply all the β's to uniformly increase or decrease smoothing.

The wide possible range of the smoothing coefficient C_k is shown in Fig. 1, which is for a set of artificial data contrived to illustrate the uniform penalty feature of UPEN. The model consists of random noise of unit rms value and zero mean, a sharp line with amplitude 1000 at 2500 ms, a Gaussian line of amplitude 1000 and half-width 0.15 Np at 800 ms, a half-

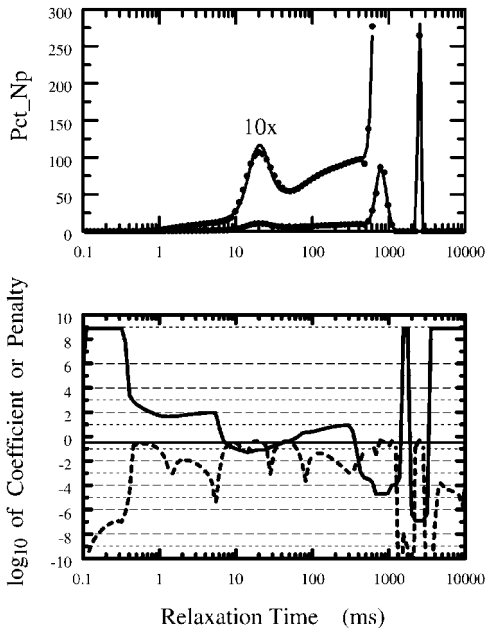

FIG. 1. The lower figure shows the smoothing coefficient C_k (heavy solid curve) and penalty $C_k(g_{k-1} - 2g_k + g_{k+1})^2$ (heavy dashed curve) for a set of artificial data with added random noise (parameters in text). The solid curve of the upper figure shows the model distribution of relaxation times, and the plotted points are g_k, the UPEN solution, with part of the curve shown also 10×. The solid horizontal line at −0.5 in the lower figure shows the uniform penalty value of the curvature penalty at most regions of significant curvature, either large or small. Under the very sharp peak in g_k at 2500 ms $C \approx 10^{-7}$, whereas $C \approx 100$ from 0.5 to 5 ms, giving a range of 10^9 for the smoothing coefficient, not counting extremes at regions of transition or baseline.

Gaussian extending downward from 800 ms with amplitude 1000 and half-width 2.5 Np, and a Gaussian line of amplitude 200 and half-width 0.3 Np at 20 ms. The UPEN solution, shown by the plotted points, is substantially identical to the above model, shown by the solid curve in the upper plot.

In the lower part of Fig. 1, the heavy solid line shows the smoothing coefficient C_k, with a value 10^{-7} under the sharp peak at 2500 ms and a value of about 100 at the foot of the very wide Gaussian near 1 ms, giving a range of a factor of 10^9. This range does not include the regions of insignificant curvature shown in the figure, such as the value 10^9 for the short section of NN-enforced baseline between the two main peaks.

The heavy dashed line shows the penalty, which is roughly uniform only in the regions of significant curvature penalty, not including inflection points and sections of baseline (including those determined by NN). The solid horizontal line at −0.5 is drawn for reference for the highest penalty regions. The penalty near 1 ms at the foot of the very wide half-Gaussian centered at 800 ms is about the same as the penalty at the very sharp peak.

Figure 1 also illustrates the ability of UPEN to show peaks at various widths without broadening the narrow ones or splitting the wide ones. Processing the data of Fig. 1 with a compromise fixed smoothing factor just small enough to resolve the two sharpest peaks almost to baseline, still greatly widening them, breaks the remaining part of the distribution into three peaks, almost to baseline. The peaks (not shown) are at 1.6, 22, 157, 680, and 2360 ms and do not represent the model well. The solution with the fixed smoothing coefficient would be strongly rejected by the diagnostic parameters to be given in a later section. Further examples are given in Refs. (*1*, *2*).

Absolute-Value Data

Most of the relaxation data processed by UPEN have been phased data, hopefully the sum of positive exponentials with added zero-mean random noise. However, data are sometimes taken as absolute-value data $S_a = \sqrt{S_p^2 + S_q^2}$, where S_p and S_q are the in-phase and quadrature signals (or signals at 90°, whatever the phases). The noise, of course, no longer averages to zero. If R is the rms single channel noise, the noise-free signal is S, and if x and y are samples of Gaussian random noise with unit rms value and zero mean, then the ensemble average of S_a is given by averaging over the possible noise values:

$$\langle S_a \rangle / R = \frac{1}{\pi} \int_{x=-\infty}^{\infty} \int_{y=0}^{\infty} \sqrt{(S/R + x)^2 + y^2} \times \exp\left[-\frac{1}{2} (x^2 + y^2) \right] dx dy. \qquad [11]$$

This can be expressed in terms of modified Bessel functions (*3*), but it is easy to compute a table of values by direct integration. The right-hand side of Eq. [11] equals S/R for large S and $\sqrt{\pi/2}$ for $S \to 0$. If Eq. [11] is used as a transform for individual data points, the estimated S-values have a bias. However, this effect is usually reduced somewhat by the fact that T_2 data at low signal values are usually at times long enough so that the processed data points represent windows in which many individual points are averaged. Reference (*4*) and references therein discuss statistical treatments of absolute-value data.

To apply transforms related to Eq. [11] one must deal separately with baseline problems if they exist. Detection circuits may have nonzero baselines, and older instruments with simple diode detection may have nonzero baselines related to a forward voltage drop in detection. Most modern relaxation data are taken with phase cycling schemes to give baselines close to zero, and, if S_∞ is a regression parameter, substantial values of S_∞/R_v for T_2 data may indicate data problems. Here, R_v is a noise estimate derived from the data and defined later in Eq. [14]. In particular, if S_∞/R_v is comparable to $\sqrt{\pi/2}$ one may suspect absolute-value recording of data. We have received numerous sets of data that are apparently absolute-value data but not identified as such.

At present we use a "quick and dirty" transform for absolute-value data rather than more elaborate statistical procedures, which do not appear justified in many applications, especially if the absolute-value recording is done because of phase problems or other data problems. We process the signal S_b given by the transform

$$S_p \approx S_b = \mathrm{sgn}(S_a - S_c)\sqrt{|S_a^2 - S_c^2|},$$
$$S_c = R_a^2[1 + (6.4S_d/(16 + S_d^4) + .5)/S_d^2],$$
$$S_d = S_a/R_a, \quad R_a = S_\infty/\sqrt{\pi/2} \quad \text{or} \quad R_v. \qquad [12]$$

In the expression for S_c the terms $1 + 0.5/S_d^2$ are from the expansion for large S_a/R_a, and the remaining part comes from a rough fit to $(\langle S_a\rangle/R)^2 - (S/R)^2 - 1 - 1/[2(\langle S_a\rangle/R)^2]$ from Eq. [11]. R_a is an estimate of R, the ensemble-average single-channel noise, and it is taken from S_∞ if available and otherwise from R_v (See later, Eq. [14]). In either case, any nonzero baseline must be known. S_a should not be much smaller than S_c and certainly not negative.

With absolute-value data it is necessary to limit the computation of the estimated noise to the data interval with substantial signal, because the noise statistics are completely different for low SNR. No attempt was made to correct the statistical treatment of the low SNR region in the regression computation.

PROBLEMS OF INVERTING "REAL" DATA

Effective Noise and Systematic Data Errors

Whatever the time sequence of the data points, equally spaced in time, log-time, or other, the denser the data the more information is available or the lower the effective noise level. We therefore define an effective noise level $R_e = R/\sqrt{(\text{data points per Neper})}$, where the noise level of the individual data points is R. By this definition, R_e is not affected by the windowing or nonwindowing of the data.

T_1 data are often taken at equal intervals in log-time, giving a constant density of data points and a constant R_e over the interval covered by the data. However, T_2 data are often taken by sequences that give data equally spaced in linear time. The point density in points per Neper is $d(t/T_{EE})/d(\ln t) = t/T_{EE}$. We then have $R_e = R/\sqrt{t/T_{EE}}$; that is, the effective signal-to-noise ratio is proportional to the square root of data time.

If the data are ideal in the sense that they consist of random noise plus the "true" decay signal, free of any systematic errors or instrumental distortions, then much more detail is available from T_2 data at long times than at short times. For instance, if we have a data point spacing $T_{EE} = 0.1$ ms and have one feature with a relaxation time of 0.5 ms and another at 5 s, the ratio of times is 10,000, and the ratio of effective noise values is $0.01 = 1/\sqrt{10{,}000}$. If the individual-point signal-to-noise ratio is SNR = 500, as is often found in laboratory measurements, for 5 s we have SNR-effective $= 500 \times \sqrt{50{,}000} = 1.1 \times 10^5$.

It is probably not possible to have sources of systematic error all smaller than 10^{-5} times the initial signal. Many factors, including constancy and accuracy of the various pulse sequences, amplifier linearity, baseline drift, and electrical interference, can lead to errors larger than the effective noise level. Even less drastic examples can give effective noise lower than plausible instrumental accuracy.

The very fact that a smoothing or "regularization" coefficient does not need to be a compromise between that needed for a sharp feature and that needed for a broad feature can lead UPEN to give spuriously sharp features on a distribution of relaxation times in response to systematic distortions of the data. A slight downward bending of the decay curve can artificially sharpen a line or even split a peak. A baseline drift can lead to artificially sharp peaks at long relaxation times.

UPEN and Diagnostics

The fact that UPEN can appropriately smooth a broad component of a distribution such as a long tail on a peak but still not oversmooth a sharp peak allows UPEN to give an adequate fit to "legitimate" data, namely, data corresponding to the sum of positive exponential components with relaxation times within the range covered by the data. Extensive testing of UPEN with artificial data yields adequate fits to all data except in a few cases, to be discussed later, of unresolved lines with SNR for the feature in the range for marginal resolution by criteria given in Ref. (*1*).

rms error of fit. If UPEN does not give an adequate fit to a set of data, it appears that some problem with the data exists. Of course, it is necessary to know the random noise level to know what fit is adequate. For many data regimes this should be known to within about a percent for diagnostic purposes. It is often difficult to know the noise this well from "blank" measurements, such as that without sample or without certain pulses. UPEN now generates several different noise parameters from the data. The parameter R, without subscript, is the assumed statistical random noise level of the individual data points, with any variability and effects of averaging in windows being indicated by the weighting factors B_i. If the residuals E_i are the errors of fit to the final (possibly windowed) data points, and the weighting factors mentioned above are B_i, and there are N (possibly windowed) points used in the computation, we define R_r as the residual error parameter,

$$R_r^2 = \sum_{i=1}^{N} B_i E_i^2/N. \qquad [13]$$

This weighting is used to give equal importance to the noise at long and short data times when relaxation times cover large ranges of times (not to give the best statistical estimate of R).

The factor of $\sqrt{B_i}$ for each factor of E_i is to offset the noise reduction by the averaging in windows or other known inherent differences in noise level. The kurtosis of the distribution of $\sqrt{B_i}E_i$ is computed to warn of wild points or major data excursions.

Random noise. R_r can, of course, be larger than the actual random noise R if the fit is not good for any reason. If there are enough data points, one can get a better estimate R_v (v for variation of E_i) of the random noise R by comparing the errors of fit of second-nearest neighbors,

$$R_v^2 = \frac{1}{2(N-2)} \sum_{i=1}^{N-2} (\sqrt{B_i}E_i - \sqrt{B_{i+2}}E_{i+2})^2. \qquad [14]$$

The intent is that R_v should not be greatly affected by slowly varying nonrandom errors of fit, thereby giving a better estimate of the random error. A useful parameter to indicate significant nonrandom errors of fit is $R_{rv} = \ln(R_r/R_v)$. This parameter should normally be negative, since the fitting procedure minimizes the errors of fit themselves (together with smoothing penalty) rather than differences of fit among neighbors.

Early signal alternation. The reason *second*-nearest neighbors were used is that a common data problem is an alternation of early data points about any plausible fit. The use of nearest neighbors would give an artificially large R_v with early point alternation. However, it is useful to have separately an indication of the early alternation problem. We define

$$R_2^2 = \frac{1}{2N_a} \sum_{i=1}^{N_a} (\sqrt{B_i}E_i - \sqrt{B_{i+2}}E_{i+2})^2, \qquad [15]$$

$$R_1^2 = \frac{1}{2N_a} \sum_{i=1}^{N_a} (\sqrt{B_i}E_i - \sqrt{B_{i+1}}E_{i+1})^2, \qquad [16]$$

where $N_a = 16$ at present. We now set $R_{12} = \ln(R_1/R_2)$. A large value indicates the early alternation problem.

Negative excursions without NN. As discussed in Ref. (*1*), the variable smoothing feature of UPEN leads to a greatly reduced dependence on NN, the nonnegative constraint. Many data sets that do not lead to sharp lines do not need NN at all. At present, UPEN executes a number of iterations without application of NN and computes the fraction of the distribution that is negative. Although without NN, sharp peaks can have substantial overshoot and undershoot, an excessive negative excursion indicates a probable data problem.

Cost of NN. Also another important diagnostic parameter is derived from the series of iterations without NN, and that is the cost of NN in terms of quality of fit. The "new" R_r (with NN) is compared to the "old" R_r (without NN) by the parameter $R_{rno} = \ln[R_r(\text{new})/R_r(\text{old})]$.

Baseline. T_2 data are usually recorded with phase cycling sequences that should produce a baseline at zero amplitude. UPEN can be run with or without S_∞, the signal at infinite time, as a regression parameter. If S_∞ is a regression parameter, a large S_∞/R_v may indicate data problems for phase-cycled T_2 data.

The UPEN output to a spreadsheet for plotting gives also the individual errors of fit. Viewing these can often help in identifying data problems, such as early signal alternation, baseline problems, oscillations at a particular frequency, or error excursions at a particular time.

Warnings and Countermeasures for Systematic Errors

UPEN posts warnings when various parameters are in ranges to suggest possible data problems or reasons to give special attention to a data set. In addition, some countermeasures are available as options to be applied either automatically or manually.

Signal alternation and data midpoints. If R_{12} is excessive, the first N_a signal values are replaced by the first N_a midpoints; that is, the first point s_1 is replaced by $\frac{1}{2}(s_1 + s_2)$, with corresponding time midpoints, etc. Under some circumstances (*5*) there is some degree of validity to the use of midpoints; in any case there is less tendency for the early alternation to distort the statistical parameters for the whole distribution. When this alternation occurs, components at very short times are subject to doubt, whatever is done in the computation. If there is reason to give more credence to certain points, such as the even points, then it is clear that the midpoints may be in error; however, if this is the case, the data points should be edited accordingly. When there are no large very short components, the use of the early midpoints does not appear to have much effect on the computed distributions. However, such diagnostic parameters as R_{rv} are much more usable, and often some obvious artifacts are eliminated at times even beyond the first N_a points. In some cases the use of the midpoints avoids wild positive or negative peaks at short times.

Clipping weighting factors on approach to baseline. Some common problems with T_2 data appear to involve the approach to baseline. The effective random noise level R_e continues to decrease at long times, and the possibility increases that systematic errors from drift may become larger than R_e. Some of these problems appear to be significantly reduced if the weighting factors B_i are clipped at the level at the longest relaxation time with significant amplitude for the distribution. Before application of NN the distribution may end with a negative peak, which may be legitimate if the distribution ends sharply, leading to undershoot; however, some distributions appear to end in negative peaks because of data problems at the longer times. With NN, a sharp final spike, possibly even separated from the rest of the distribution, may result.

The above clipping of weighting factors reduces the ability to resolve a pair of lines at the longest relaxation times about

as much as reduction of the overall compliance factor β_{00} by a factor of 2 or a decrease of the signal by a factor of $\sqrt{2}$.

Clipping weighting factors for high effective SNR. Many of the problems of systematic errors are less severe with low than with high SNR. In fact, UPEN may not function with some noiseless artificial data unless a lower limit to the computed noise is imposed. For specific data-taking conditions it may be appropriate to limit $s_1\sqrt{B_i}/R_v$, where s_1 is the initial (maximum) signal, to some maximum effective SNR.

Clipping compliances for narrow lines. It is possible to employ the negative feedback for the smoothing coefficient in UPEN for all but the narrowest lines. This is accomplished by clipping the computed compliances at a value corresponding to a peak of a given minimum width, thereby preventing excessively sharp peaks or split peaks, without oversmoothing broader features. Again, this may interfere with legitimate sharp or resolved lines from ideal data with random noise.

Excessive R_{rv} and/or R_{rno}. An excessive R_{rv} or R_{rno} indicates a bad fit to the data and probably indicates a problem with the data. One then has the opportunity to assess the problems and make decisions. For instance, plotting the errors of fit may show that the first point is bad or that a point at a very long time has been subject to drift.

Marginal resolution. Special attention is required for the case where R_{rno} has a moderate positive value and R_{rv} is comparable, here indicating a reasonable fit obtained without NN, but with a substantial cost of NN. This usually indicates data problems, but the special case of unresolved, but marginally resolvable, peaks is a possibility. If the peaks are not even close to being resolved, or if they are resolved, the cost of NN is usually not great. The marginal case may be tested somewhat by increasing β_{00} by a factor of 2 or 3 to decrease the smoothing to see if this causes resolution of some features. If it does *and* if R_r (and, usually, R_{rv} and R_{rno}) is, by the criteria in Ref. (*1*), very substantially decreased, then the resolution of the features may be meaningful. Note that an increase in β_{00} that permits an additional cycle of oscillation in a distribution allows additional accommodation of the noise (*1*).

Sharpness of detail and multimodality. A parameter F_{sd} indicating sharp detail is defined

$$F_{sd} = \left(\sum_{k=1}^{M-1} (g_{k+1} - g_k)^2 / \sum_{k=1}^{M-1} g_k^2\right)^{1/2} / \Delta_Q, \qquad [17]$$

where Δ_Q is the spacing of the computed points in Nepers, and M is the number of computed points, the first and last pairs of which are normally zero. In the limit of small Δ_Q, F_{sd}^2 is the ratio of integrals of the distribution slope squared and the amplitude squared. For many sequences of data sets a general range of F_{sd} may be found. A sequence of samples may have no very sharp peaks, often leading to F_{sd} values of the order of 1.0 or some particular range. A drastically different F_{sd}, especially a much larger one, may indicate a data problem.

A related parameter is an indicator of a multimodal character of a distribution,

$$F_{mm} = \sum_{k=1}^{M-1} |g_{k+1} - g_k| / (2g_{max}), \qquad [18]$$

where g_{max} is peak height. If the distribution is unimodal, $F_{mm} = 1$; if there are two equal and separated peaks, $F_{mm} = 2$. Thus, in some sense, F_{mm} is an index of multimodality.

Excessive $|S_\infty|$ with T_2 data. We normally use S_∞ as a regression parameter for T_1 data, because S_∞ is seldom known to an accuracy commensurate with the effective SNR. T_2 data may or may not be taken with baseline controlled to this degree. If S_∞ is made a regression parameter, it is a useful diagnostic parameter under circumstances where S_∞ should be very small compared to R_v. Of course, if baseline is *reliably* known to be very small, then the information should not be wasted by including S_∞ as a regression parameter; if S_∞ is not accurately determined by numerous baseline points, it has a smoothing effect that can in critical cases make the difference between resolution and nonresolution of a pair of peaks. On the other hand, a wrong assumption of zero baseline, when it should be slightly negative, can lead to a false apparent resolution of peaks that would not be shown as resolved when the correct baseline is used.

As has been mentioned, S_∞ values of the order of $R_v\sqrt{\pi/2}$ may indicate data recorded as absolute values.

EXAMPLES AND USE OF DIAGNOSTICS

Sets of relaxation data have been solicited from a number of sources, most of which will not be identified. All are from substantial sequences of samples for which most relaxation measurements are good according to the above criteria. The examples are shown to illustrate the use of the diagnostic features discussed above.

Distorted Relaxation Curve

Figure 2 shows several relaxation time distributions for T_2 (CPMG) data for a sample of sandstone cleaned and saturated with brine. Data were taken at two even-echo spacings T_{EE} about a factor of 3 apart. The data were windowed as described above; the weighting-factor clipping described above was used for all, and S_∞ (point at infinite time) was a regression parameter for all. The long-dashed curve is for the longer T_{EE}, and none of the diagnostic parameters suggest any problems with these data.

The remaining curves are for the shorter T_{EE}. The solid curve, which goes offscale, is with UPEN with the above parameters and $\beta_{00} = 1$. The short-dashed curve is the distri-

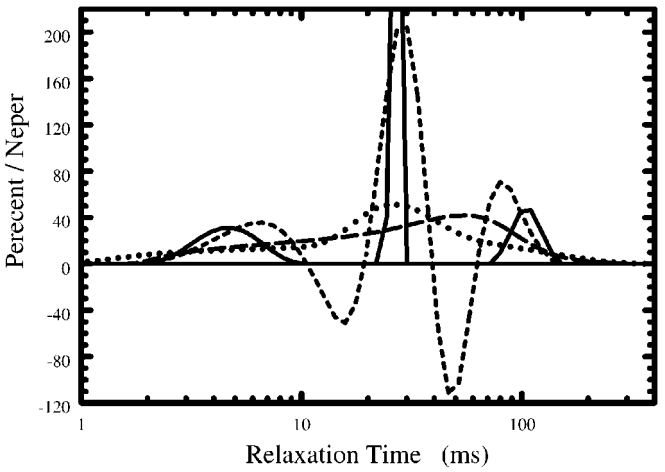

FIG. 2. Distributions of relaxation times for a porous sandstone sample saturated with brine. The long-dashed curve is for the longer of two even-echo spacings, and diagnostic parameters do not indicate data problems for this curve. The short-dashed curve is for the shorter echo spacing, with data processed with normal parameters except that NN, the nonnegative constraint, is not imposed, resulting in three peaks and in large negative excursions. The solid curve, also with three peaks, is with normal parameters, including NN. The parameter $R_{\text{rv}} = 0.185$ indicates that a good fit is not possible, and $R_{\text{rno}} = 0.08$ indicates excessive cost of NN. The dotted curve is with the overall compliance factor $\beta_{00} = 0.25$ instead of the normal 1.0, using severe oversmoothing to get a unimodal curve and a very bad fit to the data. Comparison with the curve for the good data with longer echo spacing shows that the oversmoothed curve is not even qualitatively correct.

bution without NN, the nonnegative constraint, giving a negative area 53% of the total. With NN, the parameter $R_{\text{rv}} = 0.185$, indicating a bad fit. Excessive sharp detail for this kind of sample is indicated by $F_{\text{sd}} = 12.3$. Excessive cost of NN is indicated by $R_{\text{rno}} = 0.08$, indicating a problem distribution that is essentially the opposite of the possibility discussed above of an unresolved marginally resolvable feature. The dotted curve is with the overall compliance $\beta_{00} = 0.25$, where normal is 1.0. This is equivalent to overestimating the noise R by a factor of 2. We now get a unimodal distribution with $R_{\text{rv}} = 0.8$, a huge value which indicates data problems severe enough that it is not clear what interpretation to make of this distribution. With questionable data there is diagnostic value in plotting the errors of fit. With normal processing parameters, this distribution has eight consecutive windowed data points, representing about 170 echoes, at times near 300 ms and with errors $\approx +2R_{\text{v}}$; near 180 ms there are six points, representing about 70 echoes, with errors $\approx -2R_{\text{v}}$. The relaxation curve does not represent a plausible distribution of relaxation times. By comparing this distribution with the problem-free distribution for the longer T_{EE}, we can see that the distribution for the shorter T_{EE} is probably even qualitatively wrong. The long-dashed curve for the longer T_{EE} is substantially higher in the 50–100 ms range, whereas any diffusion effect for the longer T_{EE} would only reduce the amount of signal at the longest times. Thus, we have confirmation of our diagnostic reasons not to trust the data for the shorter T_{EE}.

Marginal Resolution: One Peak or Two Peaks?

The lower part of Fig. 3 shows T_2 (CPMG, windowed) distributions for a food product. It is very clear that the distribution of relaxation times does not consist of a single sharp line. However, a common question, important for physical interpretation, is whether there are two populations of signal sources that can be reliably separated on the basis of the set of relaxation data. We will here go to considerable length to demonstrate a number of different diagnostic tests to decide whether the relaxation data alone can reliably separate the tentative two populations, and we have picked a case that leaves the answer in doubt. In most cases the relaxation data do not *rule out* two populations, but they may or may not *require* two populations.

The solid curves of the lower part of Fig. 3 are for $T_{\text{EE}} = 0.6$ ms and the dashed curves for 1.0 ms. The light curves are with the weighting-factor clipping, and the heavy curves are without. The 0.6-ms data have SNR = 580 and the 1.0-ms data 680. At 150 ms we have $\sqrt{150/0.6} = 15.8$ and $\sqrt{150/1.0} = 12.25$. Thus, effective SNRs are about 9000 and 8000, respectively.

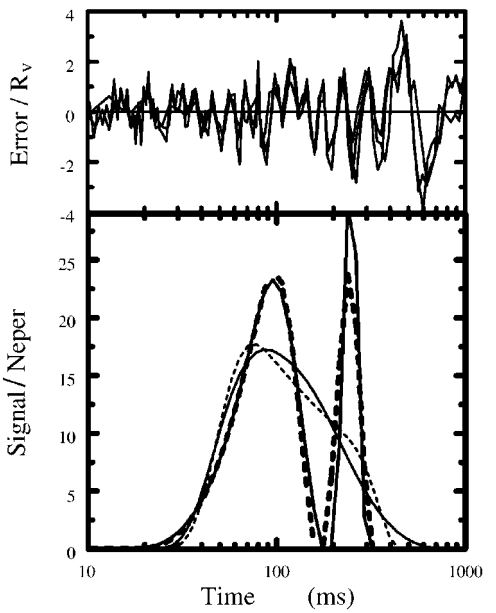

FIG. 3. Distributions of relaxation times (lower) and errors of fit (upper) for a food product. The solid curves are for an even-echo spacing $T_{\text{EE}} = 0.6$ ms, with normal parameters, giving two peaks, and with a limit on weighting factors at long times (see text), giving one peak. The dashed curves show a similar result for $T_{\text{EE}} = 1.0$ ms. The text gives criteria for resolution of two peaks, showing just adequate signal-to-noise ratio to resolve the two peaks. However, it can be noted that the errors of fit, shown in the upper part, are not random. The errors for three data sets, with $T_{\text{EE}} = 0.6$, 1.0, and 2.0 ms, are all plotted and are nearly the same, where they should be uncorrelated, and they also have large excursions at about 500 ms. We cannot safely say that there are two peaks; better data must be acquired for an answer.

However, for reliable use of such high SNR it is necessary to have correspondingly small systematic errors or data distortions. To see whether this SNR is high enough to expect, without systematic errors, to be able to reliably resolve the two peaks, we use Eqs. [11–12] from Ref. (*1*), which gives criteria for resolution of two equal sharp lines a factor Y apart: $E_2 = y^2/(6.87 + 15.9y + 7.2y^2)$, $y = (\ln Y)^2/12$, and SNR $> \sqrt{\Delta_q}/E_2$. However, the peaks in Fig. 3 have significant widths, especially the one at shorter times. The centers are separated by about 0.99 Np, and the mean halfwidth is about 0.22 Np. If we arbitrarily subtract the mean halfwidth from the separation in order to apply criteria for resolving two sharp lines, we get a reduced separation 0.77 Np, giving a separation ratio $Y = e^{0.77} = 2.16$. We get $E_2 = 0.000318 = 1/3142$. Thus, an effective SNR of the order of 3000 is required for marginal resolution, and several times that is required for firm resolution. This is just what we have for the data (8000 or 9000).

We note that the peaks in the lower part of Fig. 3 are not resolved at either T_{EE} value if the weighting-factor clipping is used and that they are resolved if it is not used. However, the diagnostics are somewhat different for the two unresolved distributions. For $T_{EE} = 0.6$ ms the maximum data time is 1200 ms, about four times the maximum relaxation time. When S_∞ is used as a regression parameter and the weighting factors are clipped at long times, there is the possibility that the regression computation can adapt S_∞ slightly to somewhat smooth the distribution at shorter times. The data are taken with many signals stacked and with phase cycling to nearly zero the baseline. For the run giving the light curve (with weighting-factor clipping), $S_\infty \approx -R_v$, or an order of magnitude larger than the effective noise even with the clipping. For the 0.6-ms data with S_∞ as a regression parameter, it was possible to raise β_{00} to very high values without resolving the two peaks. However, with $S_\infty \equiv 0$, the two peaks are resolved with $\beta_{00} = 1$. The use of S_∞ as a regression parameter also buffers the transition from no NN constraint to use of the constraint. The cost of NN, as given by R_{rno}, is small, because S_∞ can adapt to this change.

The situation is different for the $T_{EE} = 1.0$ ms data. Here the data extend to 2000 ms, which doesn't allow much adjustment of S_∞ for smoothing a feature at shorter times or adapting to the transition from no NN to NN. Even with application of the weighting-factor clipping an increase of β_{00} to 1.3 gives resolution, unlike the case for the $T_{EE} = 0.6$ data where the data extended only to 1200 ms. The parameter $R_{rno} = 0.08$, indicating excessive expense of NN, again unlike the case for $T_{EE} = 0.6$ with weight-clipping. In many cases the excessive expense is because of systematic data errors or distortions of the relaxation curves; however, here we must consider the possibility that it might be because of unresolved, marginally resolvable peaks. Removing the clipping gives resolution.

The above considerations suggest a meaningful resolution into two peaks, but without "overkill." However, the errors of fit should be examined for clues to any data distortion that might artificially sharpen or split distributions. Unfortunately, we find a repeatable, nonrandom, error pattern for the data with $T_{EE} = 0.6$ and 1.0 ms and also with a further set with $T_{EE} = 2.0$ ms, as shown in the upper part of Fig. 3. Over some regions the errors are somewhat cyclic and almost identical for three data sets, where the errors should be unrelated. Furthermore, at about 500 ms, there are groups of several points, representing many echoes, at several times the rms error. We believe that this is a case where the UPEN processing of data in nearly real time might have indicated the need for instrument adjustment while the sample was still available. Without better data, it is not safe to say that there are two separated populations.

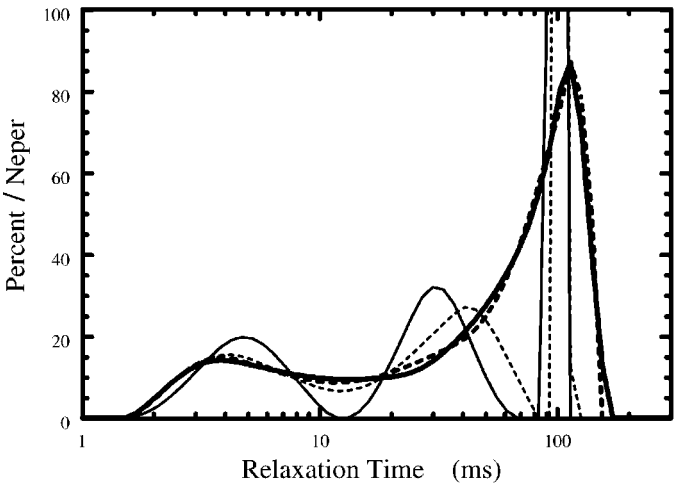

FIG. 4. Absolute-value (magnitude) data, not identified, and processed as phased data. Absolute-value data taken with effective phase cycling, with data extending to sufficiently long times, and processed with S_∞ as a regression parameter, can be recognized by a positive S_∞ of the order of $R_v\sqrt{\pi/2}$, where R_v is the noise level. The lightweight curves are from processing as if the data were phased, and the heavy curves are from processing as absolute-value data. The solid curves are with normal parameters, and the dashed curves are with the limiting of weighting factors at long times.

Absolute-Value Signal Amplitudes

Figure 4 shows a set of T_2 relaxation data apparently recorded as absolute value amplitudes rather than as phased signals, without being so designated. When processed using clipping of weighting factors, regression on S_∞, and assumption of phased data approaching a baseline (hopefully zero, but in any case with statistically stationary random noise), the thin dashed curve of Fig. 4 is obtained. The peak is unrealistically narrow, going far off scale in the figure. The thin solid line is the same without the clipping. The sharp peaks are not plausible for the particular sample, but, apart from this, the diagnostic parameters indicate data problems. For these two curves, $R_{rv} = 0.17$ and 0.09 and $R_{rno} = 0.15$ and 0.13, respectively. However, $S_\infty \approx 100$ for each, and $R_v \approx 80$ for each. For these phase-cycled data we are warned by seeing that S_∞ is about as large as the noise. When the data are processed as signal

absolute values, the square root of the sum of the squares of the in-phase and quadrature signals, we get the two heavy curves which are nearly identical. The heavy dashed curve has weighting-factor clipping, and the solid one does not. For the processing with the absolute-value assumption $R_{rv} \approx -.03$, $R_{rno} \approx 0.01$, and $S_\infty \approx -0.1 \times R_v$, all indicating a good solution to good data assumed to represent absolute values.

Peak Sharpening and Splitting by Baseline Problems

Figure 5 shows the consequences of using a wrong value of baseline signal. This can be the result of instrumental drift or other problems, but here artificial data are generated from known models and data processed with several values of the baseline signal S_∞. In Fig. 5 the dashed curves show the models, which are rectangular distributions of relaxation times; in the upper example the width is a factor of 2, and in the lower the width is a factor of 5. Random noise of unit rms value has been added, and the initial signal is 200 in both examples. After the data were generated, they were windowed as described above, using 5% relative window widths. The data extend to 1000 ms, which is only a factor of 2.5 or 2.0 beyond the longest relaxation times.

The unimodal curves approximating the dashed model curves are processed with UPEN with $S_\infty = 0$. The off-scale sharp peak in the upper figure and the bimodal curve in the lower figure are processed with $S_\infty = 1.5$, namely 1.5 times the noise. This small positive value of S_∞ has the effect of bending the logarithmic decay curves downward, tending to artificially sharpen or split peaks on relaxation time distributions. The effects of slightly negative S_∞ values (not shown) are much less pronounced. In fact, regression on S_∞ gives values of the order of -0.5, with distributions not much different from those shown for $S_\infty = 0$. Going to $S_\infty = -2.0$ (not shown) produces significant tails toward long relaxation times.

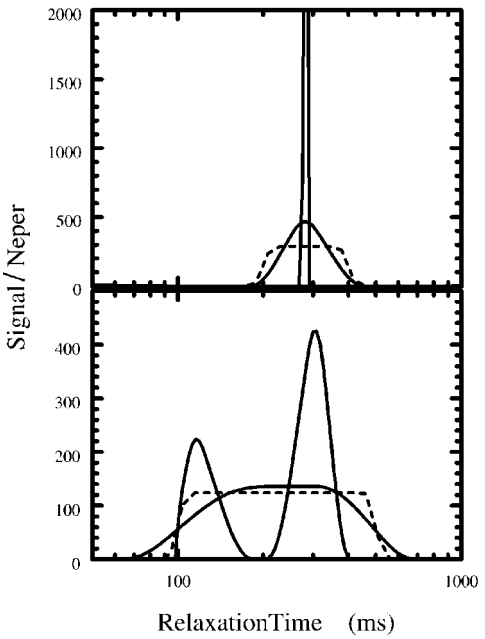

FIG. 5. Artificial T_2 data for rectangular distributions of relaxation times, with models shown as dashed curves. Width of the upper distribution is a factor of 2, and width of the lower is a factor of 5. Both have random noise with unit rms value and zero mean, and both have an initial signal of 200. Normal processing with $S_\infty = 0$ gives the solid curves approximating the models. Processing with S_∞ as a regression variable (not shown) gives nearly the same curves. The effect of baseline errors is shown by setting $S_\infty = 1.5$ (1.5 times the individual-echo rms noise), giving the sharp peak in the upper figure and the two peaks in the lower figure.

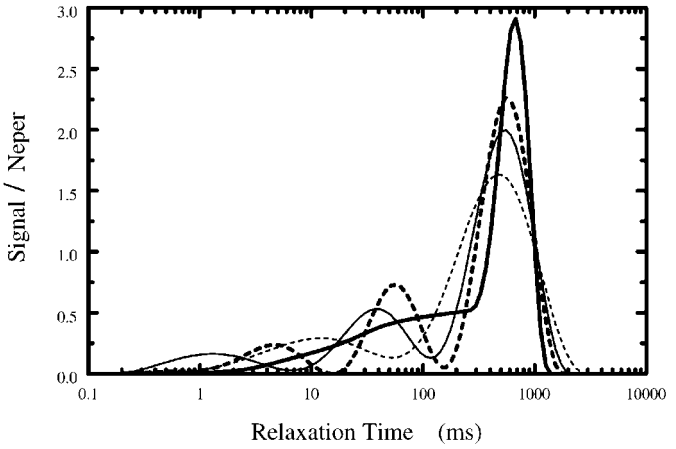

FIG. 6. Distributions for a fractured carbonate rock saturated with water. The heavy solid curve is for the UPEN solution with normal parameters. The diagnostics do not suggest any data problems. The heavy dashed curve is for curvature smoothing and a fixed smoothing coefficient giving 0.16% higher rms error of fit. Very similar curves (not shown) were obtained by use of singular value decomposition instead of a penalty function or by using slope or amplitude smoothing to give the same error of fit as by UPEN. The light solid curve is for curvature smoothing with 10 times stronger fixed coefficient and gives 27% higher error. The light dashed curve is with a further factor of 20 for a fixed smoothing coefficient and gives 2.5 times the rms error fit of the UPEN solution.

Peak with Tail

Figure 6 shows T_2 distributions for a sample of fractured carbonate rock saturated with water. In this example the diagnostics discussed above do not indicate problems with the data. The heavy solid curve shows the UPEN solution with the normal parameters. The heavy dashed curve is with a fixed smoothing coefficient, giving an rms error of fit 0.16% higher than for the UPEN solution (not significantly different). The peak is significantly wider, but the feature most easily misinterpreted is that the distribution appears to be broken into three populations. The tail of the distribution is fit too well in the sense that the oscillations allow additional fitting to the noise. The peak is not quite adequately fit, because it is oversmoothed, while the tail is undersmoothed. Very similar curves (not shown) were obtained using amplitude smoothing or slope smoothing with coefficients chosen to give the same error of fit as for the UPEN solution. Likewise, a similar solution was

obtained by using singular value decomposition (*6*) instead of a penalty function.

The thin solid curve of Fig. 6 is with the fixed smoothing coefficient increased a factor of 10, increasing the rms error of fit 27% and still leaving three peaks. Note further that the smaller peaks are not at the same times on the inversions with the different smoothing coefficients; in fact, the peak at shortest time extends to times significantly shorter than for the UPEN solution or that with the lesser fixed smoothing. Further increasing the smoothing coefficient a factor of 20 gives the light dashed curve, which has rms error of fit a factor of 2.5 worse than for the UPEN fit, and which still has a pronounced minimum.

DISCUSSION AND CONCLUSIONS

The UPEN method of inversion does not require specific input of data point spacing, whether equally spaced in time, log-time, or with other spacing schemes. However, if points have different statistical weight, the weighting factors must be used in the linear inversion done in each iteration. If T_2 data are taken with large numbers of echoes, the data can be averaged in windows as described above to give manageable numbers of data points for computation without losing significant information. Normally, there is no user adjustment of smoothing parameters, although the program computes the noise level and uses the square of this as a factor in computing a smoothing penalty.

A basic feature of UPEN is that it provides much stronger smoothing of broad slowly varying regions than it does for sharp peaks. This allows presentation of sharp peaks without unnecessarily appearing to "resolve" peaks in a broad tail. Since it is not necessary to oversmooth a sharp peak to get a reasonable overall distribution, there is the possibility of getting spurious sharp detail as a result of systematic data errors, particularly those that correspond to a slight downward bending of the logarithmic decay curve. Numerous diagnostic features are presented to try to identify data sets subject to these systematic errors. These features suggest the usefulness of running UPEN in nearly real time when taking important data, permitting attempts at improving the data while the sample is still available.

Examples of the use of diagnostic features are given, including a discussion of a case where it is important to know whether the relaxation data *require* a pair of resolved peaks or leave open the question of whether there is a single peak or two peaks.

UPEN now applies an amplitude penalty with amplitude feedback for regions of a distribution of relaxation times outside the range of the data. UPEN now goes through three cycles of computation to provide diagnostic information and to permit certain automatic changes in the computation, based on diagnostic parameters.

APPENDIX

List of Symbols

R	Noise (*rumore, Rauschen*); by itself or with one index R indicates a noise value; with two indices R indicates the log-ratio of noise values; with one index plus "*no*" ("new/old") it refers to the log-ratio of the particular category of noise after and before application of NN. Symbols defined and used only locally may not be on this list.
β_{00}	Overall multiplier for the smoothing compliances (inverse smoothing coefficient). See Feedback for the other β's.
D	Window width relative to central time. See Eqs. [1–2].
B_i	Weighting factors for windowed data (or for differences in rms noise for any reason).
E_i	Individual error of fit (usually displayed as $E_i\sqrt{B_i}$ to give uniform amplitudes for random noise).
F_{sd}	A parameter related to the form of the distribution, with large values indicating considerable sharp detail.
F_{mm}	A parameter related to the form of the distribution, with values >1 indicating multimodality.
g_k	The kth computed amplitude on relaxation time distribution.
N_{a}	Number of points used in connection with early signal alternation. See Eqs. [15–16] and Signal Alternation and Data Midpoints.
NN	The nonnegative constraint on the computed distribution.
R	Ensemble-average rms noise for a single channel (in-phase or quadrature) for individual data points (before windowing, if any).
R_{r}	rms error of fit to the data. See Eq. [13].
R_{v}	Noise computed from variation of errors of second-nearest neighbors. R_{v} is intended to reduce the effect of systematic data errors of the estimates of the noise. See Eq. [14].
R_{e}	"Effective noise" $= R/\sqrt{\text{data points per Neper in time}}$, as discussed under Effective Noise.
R_{rv}	$=\ln(R_{\mathrm{r}}/R_{\mathrm{v}})$. Substantial positive values suggest significant systematic errors.
R_{rno}	$=\ln[R_{\mathrm{r}}(\mathrm{new})/R_{\mathrm{r}}(\mathrm{old})]$, where "new" is after and "old" before application of NN. Substantial positive values suggest significant systematic errors.
R_{12}	Large R_{12} suggests alternating errors of early points. See below Eqs. [15–16].
S_∞	The asymptotic signal at infinite time, whether computed as a regression parameter or imposed.
s_i	The ith data point of a (possibly windowed) set of points used in the computation. See windowing discussion.
SNR	Signal-to-noise ratio.
t	(Lower case, perhaps with subscript) data time.
T	(Upper case, perhaps with subscript) relaxation time.

T_{EE} Time between echoes employed, whether all echoes or even echoes.

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