Constrained Reconstruction Applied to 2-D Chemical Shift Imaging

Keith A. Wear,* Member, IEEE, Kyle J. Myers, Sunder S. Rajan, and Laurence W. Grossman

Abstract—The method of constrained reconstruction, previously applied to magnetic resonance imaging (MRI), is extended to magnetic resonance spectroscopy. This method assumes a model for the MR signal. The model parameters are estimated directly from the phase encoded data. This process obviates the need for the fast Fourier transform (FFT) (which often exhibits limited resolution and ringing artifact). The technique is tested on simulated data, phantom data, and data acquired from human liver in vivo. In each case, constrained reconstruction offers spatial resolution superior to that obtained with the FFT.

Index Terms—Constrained reconstruction, localization, magnetic resonance spectroscopy.

I. INTRODUCTION

In two-dimensional (2-D) chemical shift imaging (CSI) [2D CSI], a set of phase-encoded free induction decay signals is acquired. Phase encoding is performed in two dimensions. The three-dimensional (3-D) Fourier transform of this data set yields a 2-D grid of spectra which corresponds to a plane in the human body [1]. Additional localization may be achieved through use of a surface coil.

The most common method for Fourier transform estimation is the discrete Fourier transform (DFT) [2]. The DFT may be computed efficiently using the fast Fourier transform (FFT) [3]. If short record lengths (either in time domain or k-space) are used, the DFT exhibits limited resolution in the transform domain. In addition, the DFT may produce Gibbs ringing artifacts.

Numerous authors have proposed alternatives to the FFT in magnetic resonance imaging (MRI) and spectroscopy. Haacke et al. have developed a method called constrained reconstruction which they have demonstrated to exhibit superior resolution (compared with the FFT) in MRI [4]. In Haacke’s approach, the spin density can be modeled as an adaptive superposition of piece-wise local polynomials. Perhaps the most simple model is a series of contiguous boxcar shaped functions. The boxcar function model is a particular case of the more general implementation of the method and is commonly preferred because of its stability. In this case, the derivative of the phase encoded data can be shown to be a summation of exponentials. A modified version of Prony’s method using singular value decomposition (SVD) may be used to solve for the parameters of the reconstruction (amplitudes, widths, and positions of boxcar functions) [5], [6].

Other approaches have been developed in order to cope with the problems associated with cross-voxel contamination in magnetic resonance spectroscopy. A comprehensive review has been written by Liang et al. [7]. Hu and co-workers [8] have developed a method called spectral localization by imaging (SLIM) with which they incorporate prior knowledge obtained from the conventional MR image in the localization algorithm. This approach can reduce the number of input signals required and, therefore, reduce clinical examination time. A modification of this method, called generalized SLIM (GSLIM) is reported to reduce spectral leakage in CSI and inhomogeneity errors in SLIM [9]. Von Kienlin and Mejia [10] have developed another localization method based on a priori image information, called spectral localization with optimized pointspread function (SLOOP), which provides voxels of arbitrary shape and improves signal-to-noise ratio (SNR).

Plevritis and Macovski [11], [12] have developed a method in which anatomical information from the proton image is incorporated in an algorithm to enhance resolution in spectroscopic images. They have also proposed an alternative k-space sampling distribution which can enhance resolution in spectroscopic images [13]. Maudsley and co-workers [14] have developed a reduced k-space sampling method which exhibits substantial improvements of SNR at the cost of a small loss of resolution. Parker et al. and Hu et al. have proposed strategies in which phase encodes (spatial frequencies) are measured with varying amounts of repetition or varying repetition times in order to reduce ringing artifact [15]–[17]. Hu and Stillman have developed a method for obtainingCSI with reduced ringing using anatomical information [18]. Autoregressive approaches have been proposed for MRI by Smith et al. [19], Martin and Tirendi [20], Barone and Sebastiani [21], and for spectroscopy by Wear et al. [22]. Hendrich and co-workers [23] have utilized a 2-D Fourier series window (FSW) approach and circular voxels.

The present study is an application of constrained reconstruction to 2D CSI. Constrained reconstruction is applied to simulated data, phantom data, and $^{31}$P data obtained from normal human liver in vivo. In the latter case, one main issue of interest is resolution of $^{31}$P signals from muscle and liver.

Manuscript received December 8, 1995; revised July 15, 1996. The Associate Editor responsible for coordinating the review of this paper and recommending its publication was Z.-P. Liang. Asterisk indicates corresponding author.

*K. A. Wear is with the Center for Devices and Radiological Health, Food and Drug Administration, 12720 Twinbrook Parkway, Rockville, MD 20852 USA (e-mail: kaw@fdafr.cdrh.fda.gov).
K. J. Myers and L. W. Grossman are with the Center for Devices and Radiological Health, Food and Drug Administration, Rockville, MD 20852 USA.
S. S. Rajan is with Bracco Diagnostics Inc., Princeton, NJ 08543-5225 USA.

Publisher Item Identifier S 0278-0062(97)07588-5.
“Bleeding” of signals from one tissue into the other is often observed in DFT-based spectroscopic reconstructions. The application of constrained reconstruction to spectroscopy is somewhat more challenging than that for MRI for the following reasons. First, in CSI, far fewer data samples are typically acquired in one phase encode dimension (here eight, as opposed to, say, 256 in MRI). Therefore, much less data is available to be fit to the reconstruction. Second, spectroscopic data tends to be noisier than MRI data (SNR typically on the order of 8:1 as opposed to typically 100:1).

II. METHODS

A. Data Acquisition

A Siemens 1.5-T Magnetom clinical scanner and a custom designed surface coil were used to acquire data. The surface coil was used for both transmission and reception of radio frequency (rf) signals. A “BIR4 adiabatic” pulse was used (for shimming as well as for acquisition of rf data) [28]. The pulse duration was 2.56 ms. Data was phase encoded in two dimensions. A 24-cm × 24-cm × 4-cm field of view (FOV) was divided into an 8 × 8 grid of 3-cm × 3-cm × 4-cm voxels. (A 4-cm slice select was performed in the direction orthogonal to the phase encode dimensions). The data acquisition delay was 2 ms. The sampling rate was 2 kHz (dwell time = 500 μs).

Data were acquired (at 31P resonance frequency) from a syringe (diameter = 2.75 cm) containing an inorganic phosphate (P2) solution. The syringe was positioned vertically within a tube which was placed in a water tank. The chemical shift image corresponded a longitudinal section of the syringe. One signal was acquired for each phase encode. Repetition time (TR) was 2 s.

Data were also acquired from the liver of a normal human subject, positioned supine in the scanner. The surface coil (with its axis oriented horizontally) was placed on the subject’s right side, near the third rib. With this geometry, the FOV consisted of (in order of increasing distance from the coil) skin, fat, muscle, and then liver. The spectra exhibited peaks due to adenosine triphosphate (ATP) (α, β, and γ), phosphocreatine (PCr), phosphodiesters (PDE), inorganic phosphate (P1), and phosphomonoesters (PME). Since PCr is prevalent in muscle and not present in liver, the PCr peak could be used to identify signal from muscle [24]–[27]. Fifteen acquired signals were averaged for each phase encode. TR was 1 s.

B. Simulation

Simulated data were also generated. The number of phase encodes, gradient strengths, FOV, voxel size, and dwell time were the same as above. The object consisted of two boxes (length × width × thickness = 3 cm × 6 cm × 4 cm and 10.5 cm × 6 cm × 4 cm). Each box contained the same substance whose spectrum was characterized by a single peak. The concentration of the substance in the smaller box was twice that in the larger box. The spatial frequency data were generated by taking a DFT of a finely sampled discrete version of the object. Gaussian white noise was added to the Lorentzian line shape function prior to inverse Fourier transformation to produce simulated free induction decay signals. Since noise level was independent of frequency (chemical shift) and the signal exhibited a Lorentzian frequency dependence, SNR was a function of frequency, being maximum at the peak frequency. The SNR of the data set was characterized by the peak frequency SNR. The SNR values investigated were 0, 3, 6, 10, 20, and 30 dB, and infinite.

C. Data Analysis

A thorough explanation of the constrained reconstruction algorithm is provided by Haacke and co-workers [4]. A related algorithm was developed independently by Martin and Tirendi [20]. The object to be imaged is modeled, in one dimension, as a weighted sum of contiguous boxcar functions of varying amplitudes and widths. Each boxcar corresponds to a different tissue or structure in the body. The phase-encoded data (the sampled Fourier transform of the object) may be expressed as the weighted sum of functions of the form sinc(παk) exp(−i2πβk) where sinc(z) = sin(z)/z. k is sampled spatial frequency (determined by the phase encode gradients), and α and β correspond to the widths and centers of the boxcar functions. If this sum is multiplied by k, it then becomes a weighted sum of terms of the form sinc(παk) exp(−i2πβk) = exp(iπαk) − exp(−iπαk) exp(−i2πβk)/2. Thus, the product of the phase-encoded data with k is a simple sum of complex exponentials. The widths and centers of the constituent boxcars may be obtained from the frequencies of the exponentials.

In general, the frequencies of the exponentials may be estimated using a SVD method outlined by Haacke and co-workers [4]. If the number of boxcars is small, however, easier approaches may be implemented. For example, for a single boxcar object (see below), the magnitude of the phase-encoded data may be least squares fit to the functional form |sinc(παk)| and the phase may be least squares fit to a line, −2πβk. Once the widths and centers are known, the amplitudes of the boxcars may be obtained from a linear least squares procedure [4].

The two main tissues contributing 31P peaks in typical human liver spectroscopy are muscle and liver. The main species of interest (ATP, PDE, P1, and PME) are found in both tissues. PCr exists in muscle but not in liver. Therefore, at frequencies (chemical shifts) corresponding to PCr, the data could be modeled as a single boxcar (muscle). The locations of the boundaries of the muscle (skin-fat/muscle and muscle/liver interfaces) were estimated by applying a single component boxcar model to the data (at PCr frequencies) as described above. The remaining boundary of interest (determined by the sensitivity volume of the surface coil) was determined from the 1H image. The single boxcar model was used for the syringe containing P1. As stated above, once the boundaries (or equivalently, the widths and centers) of the boxcars had been determined, the amplitudes could be obtained from a linear least squares procedure. Since the concentrations of the various metabolites were not equal, the least squares procedure had to be repeated for each frequency (chemical shift).
The simulated data corresponded to a two-boxcar model. In this case, the modified least squares Prony method [29], [30] was used to estimate the location of the interface between the two boxcars. The locations of the outer surfaces of the boxes were determined from the proton image. Average error magnitude was computed by comparing reconstructions to the known object.

An FFT was used for transformation from time domain to temporal frequency (chemical shift) domain. An exponential line broadening filter (20 Hz) was applied to each free induction decay (FID) prior to Fourier transformation. For the simulation and for human data, constrained reconstruction was used for one transform from spatial frequency to position (for the direction in which high resolution was critical) while an FFT was used for the remaining spatial frequency-to-position transform. For the syringe containing 31P, constrained reconstruction was used in both spatial directions. A 3-D FFT was also computed in all cases for the purpose of comparison. Generally, rectangular windows in both spatial dimensions were used. The one exception is that, in the case of liver data, a Hamming window was applied in the direction orthogonal to the direction in which high resolution was required. The Hamming window produced smoothing in the chemical shift image. (The SNR in 31P liver CSI is sufficiently low that noise reduction techniques, such as windowing, are often desirable provided that their concomitant resolution loss is tolerable. Although application of the Hamming window degraded 3 dB resolution from 0.89 to 1.30 voxels, it reduced the highest sidelobe level from -13 to -43 dB [31]. The Hamming window was used for both the constrained reconstruction/FFT/FFT method and the 3-D FFT method). The real part of the spectrum corresponding to a voxel in the normal human liver reconstruction with high PCR content (i.e., including muscle) was selected for analysis.

The effect of reconstruction algorithm on SNR was investigated as follows. The real part of the spectrum corresponding to PCR in a voxel in the normal human liver reconstruction with high PCR content (i.e., including muscle) was selected for analysis. The SNR of the PCR peak was estimated as the ratio of the square of the PCR peak height to the variance of the spectrum taken over a large range of frequencies (chemical shifts) which included no major peaks. This approach assumes that: 1) noise is independent of frequency and 2) signal dominates noise in the PCR peak. SNR was computed for four voxels in each reconstruction.

III. RESULTS

A simulated proton image of the two-boxcar (infinite SNR) object is shown in Fig. 1. A 2 x 8 subset of the 8 x 8 phase-encode grid is superimposed. The 3-D FFT of the data set is shown in Fig. 2. The dashed line indicates the theoretical value that the peak should attain in each voxel. This reconstruction illustrates the common artifacts associated with the DFT. First, the signal is not confined to the voxels corresponding to the true location of the object (between boundaries one and six). In addition, ringing is evident. The voxels corresponding to the large low-intensity box (between boundaries one and
Fig. 2. Three-dimensional fast Fourier transform (3-D FFT) reconstruction of the simulated object shown in Fig. 1. The dashed line corresponds to the correct theoretical values for peak heights. This reconstruction exhibits artifacts commonly associated with the DFT. The signal is not confined to the voxels corresponding to the true location of the object (between boundaries one and six, see Fig. 1). An oscillation (ringing) is present, due to the "bleeding" of the signal from the small high-intensity box into the long low-intensity box and into the region outside the boxes. The average error in peak area (relative to the theoretical average peak area per voxel) is 18.4%.

Fig. 3. Constrained reconstruction of the simulated object shown in Fig. 1. The dashed line corresponds to the correct theoretical values for peak heights. The reconstruction is confined to the true location of the object (between boundaries one and six, see Fig. 1). Ringing is suppressed. The average error in peak area (relative to the theoretical average peak area per voxel) is 2.7%.

Fig. 4. Dependences of average error magnitude on SNR for FFT (solid line) and constrained reconstruction (dash dot line) for the simulation. The asymptotes, which correspond to the infinite SNR trials, are shown for FFT (short dash line) and constrained reconstruction (long dash line). Error bars denote standard deviations of results of repeated trials of the simulation with different random number generator seeds. Constrained reconstruction exhibited a substantial improvement over a wide range of SNR.

Fig. 5. Proton image of syringe containing inorganic phosphate (P$_4$). The syringe is immersed in a water tank. The vertically oriented bright object, just right of center, is the syringe. A 5 x 5 subset of the original 8 x 8 grid of voxels is superimposed. The voxel dimensions are: length $\times$ width $\times$ thickness = 3 cm $\times$ 3 cm $\times$ 4 cm.

A proton image of the syringe containing the P$_4$ solution is shown in Fig. 5. A 5 x 5 subset of the 8 x 8 phase-encode grid is shown. The vertically oriented bright object, just right of center, is the syringe. The fluid in the syringe occupies portions of six voxels in the image. The 3-D FFT of the spectroscopic data set is shown in Fig. 6. The signal occupies not only the six proper voxels, but many others as well. Ringing is apparent. In the constrained reconstruction, shown in Fig. 7, the signal is confined to the region corresponding to the true location.
WEAR et al.: CONSTRAINED RECONSTRUCTION APPLIED TO 2-D CHEMICAL SHIFT IMAGING

Fig. 6. Three-dimensional fast Fourier transform (3-D FFT) of syringe containing inorganic phosphate (P<sub>i</sub>)(see proton image in Fig. 5). The signal occupies not only the six proper voxels, but many others as well. In addition, ringing is apparent.

Fig. 7. Constrained reconstruction of syringe containing inorganic phosphate (P<sub>i</sub>). Constrained reconstruction was applied in both directions. Using the proton image (see Fig. 5) as a reference, it can be seen that the constrained reconstruction performs better than the 3-D FFT (see Fig. 6) in that 1) the reconstruction is confined to the true location of the object and 2) ringing is suppressed.

Fig. 8. Proton image of liver of normal human subject. A 3 × 5 subset of the original 8 × 8 grid of voxels is superimposed.

Fig. 9. Three-dimensional FFT of normal human liver in vivo (see proton image in Fig. 8). The vertical dotted lines correspond to the chemical shift for PCr. The arrows in the lower-right corner indicate the presence of PCr in voxels which do not contain muscle and, therefore, should not contain PCr. In particular, notice that in the right-most column, PCr, which should be confined to the top row (where muscle is located), has been vertically smeared into the two deeper voxels due to the sinc convolution effect inherent in the FFT process.

Figs. 9 and 10. The average SNR was 30.8 dB for the FFT and 32.4 dB for constrained reconstruction. (Use these numbers for comparison only. They are extremely high by spectroscopic standards because they are based on PCr, the peak in the phosphorus spectrum which has the highest SNR by far. In addition, they were obtained from voxels close to the surface coil which exhibit higher SNR than deeper voxels).

IV. DISCUSSION

The FFT suffers from a fundamental resolution limitation and from the Gibbs artifact. These effects degrade chemical shift images and hamper localization. Compared with the FFT, constrained reconstruction offers superior resolution and more-accurate quantitation. These benefits are achieved without degradation of SNR and can be realized over a wide range of the P<sub>i</sub> solution. (Constrained reconstruction was applied in both spatial dimensions in this example).

A proton image corresponding to the normal human liver is shown in Fig. 8. A 3 × 5 subset of the 8 × 8 phase-encode grid is shown. The muscle layer lies beneath the skin. With the geometry exhibited in Fig. 8, the direction in which the potential for “bleeding” of muscle signal into liver is greatest is the vertical direction. Therefore, constrained reconstruction was applied in the vertical direction while an FFT was used in the horizontal direction.

It is instructive to examine phosphocreatine (PCr) peaks in the reconstructions since PCr exists in muscle but not in liver. In the 3-D FFT (Fig. 9), PCr peaks are found not only in voxels corresponding to muscle, but also in some voxels corresponding to the interior of the liver (see arrows in the lower-right portion of the image). The vertical dotted line marks the frequency for PCr. With constrained reconstruction applied in the vertical direction (Fig. 10), PCr peaks do not appear in interior voxels. This can also be seen in the PCr spectral maps shown in Figs. 11 and 12.

SNR (for PCr) was estimated, as described above, using four voxels (all except the left one) from the top rows of
Fig. 10. Constrained reconstruction of normal human liver in vivo (see proton image in Fig. 8). Constrained reconstruction was applied in the vertical direction, while an FFT was applied in the horizontal direction. The vertical dotted lines correspond to the chemical shift for PCr. The erroneous PCr signals in the 3-D FFT reconstruction are not present in the constrained reconstruction (see arrows in the lower-right corners of Figs. 9 and 10). The PCr peak corresponding to the top-right voxel has not been smeared (due to the sinc convolution effect) into the two deeper voxels as was the case with the 3-D FFT. Hence, it has a greater magnitude than in the 3-D FFT (compare with Figs. 8 and 9).

Fig. 11. PCr map corresponding to the 3-D FFT in Fig. 9 (see proton image in Fig. 8). Note the muscle contamination in the lower-right portion.

Thus, to a certain extent, a tradeoff has been made. Resolution was sacrificed in one direction (horizontal in Figs. 8–10) so that it could be enhanced in the other direction (vertical). This choice was made because the predominant direction of potential muscle contamination into liver was the vertical. For higher SNR data sets (e.g., brain), spatial averaging via methods such as the Hamming window may not be necessary. Even in the liver, substitution of the linear prediction singular value decomposition (LPSVD) method [4], [6] for the modified least squares prony method may reduce noise sensitivity and obviate the need for spatial averaging.

Constrained reconstruction requires prior determination of the number of compartments or boxcars in the object. In the examples considered here, this number was known a priori. In cases in which it is not known, it may be determined using the SVD approach outlined by Haacke et al. [4]

There is a fundamental limitation on the number of compartments in the reconstruction relative to the number of phase encodes. Using \( n \) phase encodes will yield \( 2n \) parameters (\( n \) complex numbers) in each \( k \)-space vector requiring transformation. Each boxcar in the model is specified by four parameters (amplitude, phase, center, and width). In order that the problem remain over-determined (so that parameters may be estimated by some least squares procedure), the number of boxcars must be less than \( 2n/4 \). If the locations of outer boundaries are determined from the proton image, this information may be used to prefilter the \( k \)-space vector data so that only the internal boundaries need to be solved for [29], [30]. Therefore, the maximum number of compartments (boxcars) in the reconstruction becomes \( (2n + 2)/4 = (n + 1)/2 \). Depending on SNR, this limit may or may not be achievable in practice. It is reasonable to expect the performance of constrained reconstruction to decrease with increasing numbers of compartments. Prior knowledge of object geometry may be used to influence phase-encoding strategy in order to maximize the ratio of the number of phase encodes to the number of compartments in the dimension in which constrained reconstruction is to be applied.
It is interesting to note that, in the case of the 3-D FFT reconstruction of the syringe, substantial bleeding is apparent in the horizontal direction but not in the vertical direction. This is because, for the specific geometry of this object and the phase-encode grid, the transitions from negative to positive (and vice versa) in the vertical oscillatory ringing pattern happen to occur near horizontal grid lines in the reconstruction. For single-boxcar objects, it is possible to optimize the location of the grid relative to the object in such a way as to minimize apparent ringing. However, for more realistic (multiple boxcar) objects this would not be a practical approach for suppression of ringing.

For in vivo measurements, in which the true spatial distribution of chemical shifts is unknown, an objective criterion upon which to base an optimization scheme is not generally available. Thus, in order to demonstrate typical artifacts that can be encountered in clinical situations, the location of the grid relative to the syringe was not “optimized” in this experiment.

The analysis presented here assumes spectra in all voxels to be perfectly aligned. Spectral shifts due to inhomogeneities in the static magnetic field may complicate matters. Although inhomogeneities typically plague in vivo acquisition of $^{31}$P data from liver, the constrained reconstruction of the in vivo human liver data (Fig. 10) was quite good. (As an index of inhomogeneity, the standard deviation of chemical shift of the ATP $\alpha$ peak was measured to be 0.2 parts per million (ppm) for the human data.)

Constrained reconstruction requires more computing time than the FFT. If constrained reconstruction is used for all (1024) frequencies (chemical shifts), then the reconstruction in Fig. 10 requires about three and a half minutes on a DEC Alpha (150 MHz). However, in order to increase processing speed, the algorithm described in Section II may be applied only for frequencies at which the energy exceeds a certain threshold. For frequencies at which energy is below this threshold (i.e., noisy regions far removed from principal spectral peaks), conventional 3-D FFT processing may be employed. This can typically reduce processing time by a factor of ten.

REFERENCES


