Using Genetic Algorithms with *a Priori* Knowledge for Quantitative NMR Signal Analysis

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Genetic algorithms (GA) have been successfully applied to solve many optimization problems in science and engineering. In this work, we demonstrate by using *a priori* knowledge, that GA, are useful in NMR parameter estimation, especially when the signal-to-noise ratio is low. Moreover, different combinations of reproduction, recombination, and mutation schemes can greatly affect the optimization accuracy and efficiency.

INTRODUCTION

Genetic algorithms (GAs) are robust, global optimization methods introduced by John Holland.[1] GAs can be viewed as an evolutionary process wherein a population of candidate solutions to a problem evolves over a sequence of generations. During each generation, the "fitness" of the solutions is evaluated. Based on the principle of "survival of the fittest", the better solutions will have a higher probability to be selected for reproduction than poorer solutions, which then become extinct. Although the basic concept is simple, GAs are an effective and efficient method for tackling complex, large scale optimization problems.[2,3] Compared to gradient descent techniques, GAs are superior because the search is not biased towards locally optimal solutions. Also, calculation of parameter derivatives, usually required for optimization methods, is not required in GA. GAs are also superior to random sampling algorithms because their ability to direct the search towards the globally optimal solution.

The parameters to be fitted by the GA method are encoded into *chromosomes*, and each unknown parameter is represented by a *gene*.[2] Initially, a population of chromosomes is created by assigning a random value to each gene. After the chromosomes are generated, the fitness of each chromosome is evaluated by calling the objective function. The objective function is problem specific, and this fitness evaluation process is usually the rate-determined step in the whole optimization algorithm. A new population is then created from the current population based on this evaluated fitness. Chromosomes with higher fitness have greater probabilities of being selected for further reproduction. After reproduction, the chromosomes in the pool are mated at random by a crossover operator. The crossover is controlled by a user-defined parameter called *crossover probability* (p_c). Each time two chromosomes are drawn from the pool, a random number in the range [0 1] is generated. The two chromosomes then undergo a crossing over only if the random number is smaller than p_c. By so varying the parameter p_c, the crossover process is controlled. In a simple one-point crossover, another random number r in the range [1 L-1] is generated where L is the number of genes on the chromosomes. The crossover process can be represented as follows:

Before crossover,

$$\mathit{chromo}1 = [g_1, g_2, ..., g_L]$$

$$\mathit{chromo}2 = [g'_1, g'_2, ..., g'_L]$$

After crossover,

$$\mathit{chromo}1' = [g_1, ..., g_r, g'_{r+1}, ..., g'_L]$$

$$\mathit{chromo}2' = [g'_1, ..., g'_r, g'_{r+1}, ..., g_L]$$

Although reproduction and crossover are quite simple, the power of GAs arises from them. The reproduction process selects the "good" chromosomes and eliminates those "bad" ones, whereas crossover causes randomized exchange of genetic material between chromosomes. This exchange can lead to the production of "better" chromosomes. In addition to reproduction and crossover, another operator that is commonly applied to the population of chromosomes is called mutation. To prevent the premature convergence of the GAs to suboptimal solutions, one needs to constantly explore other areas in the parameter space (in biological terms, to explore other potentially useful genetic material). A mutation operator achieves this purpose by modifying the value of each gene of a chromosome with a small probability p_m. The processes of reproduction, crossover, and mutation are repeated until a certain termination criterion is fulfilled.

In this present work, the use of GAs in NMR spectral estimation is explored.[4] Spectral quantification and estimation is one of the crucial steps in NMR spectroscopic studies. Conventionally, this process is accomplished with the use of fast Fourier transformation (FFT).[5] However, because of the intrinsic limitation of FFT, such as low resolution for the truncated signal or side lobes due to windowing, numerous alternative methods have been proposed to overcome these limitations. Among these are the matrix pencil method (MPM),[6,7] linear prediction method (LP),[8−11] total least square method (TLS),[12] and the maximum likelihood

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method (ML).[13,14] These methods outperform FFT when the data size is small. However, most of these break down when the signal-to-noise ratio (SNR) is lower than 10 dB.[5] By combining GA with *a priori* knowledge, we demonstrate that GAs are superior to other methods in spectral estimations when the SNR is low.

THEORY AND METHOD

Model of NMR Signals. One-dimensional NMR FID data can be modeled as a sum of K exponentially damped sinusoids embedded in random noise. The experimental data points x_n of a 1D FID signal of N equally spaced complex data points can be expressed as

$$x_n = \sum_{k=1}^{K} \{a_k \exp[\mathrm{i}\phi_k]\} \exp[(\alpha_k + \mathrm{i}2\pi f_k)n\Delta t] + \epsilon_\mathrm{n} \quad (1)$$

where $\mathrm{i} = \sqrt{-1}$ and $n = 0, 1, 2, ..., N - 1$; a_k, ϕ_k, α_k, and f_k are the signal amplitude, phase, damping factor, and frequency, respectively, and ϵ_n is an additive Gaussian noise factor. The goal of spectral quantification and estimation is to solve for the amplitudes and other parameters in the presence of noise. Equation 1 can also be expressed as,

$$x_n = \sum_{k=1}^{K} c_k z_k^n + \epsilon_n = x'_n + \epsilon_n \quad (2)$$

where $c_k = a_k \exp[\mathrm{i}\phi_k]$ and $z_k = \exp[(\alpha_k + \mathrm{i}2\pi f_k)\Delta t]$. From eq 2 it is evident that c_k can be derived separately based on a linear fitting after the z_k terms are estimated. The term x'_n in eq 2 can be written in matrix form,

$$x' = \Omega c' \quad (3)$$

where $x' = [x'_0, x'_1, ..., x'_{N-1}]^\mathrm{T}$ denotes the vector of noiseless data. The parameter $c' = [c'_1, c'_2, ..., c'_K]^\mathrm{T}$ is a vector of complex amplitudes, and the matrix Ω is an NxK matrix with elements $\Omega_{ij} = z_j^{i-1}$; the superscript $^\mathrm{T}$ indicates the transposition. Under a white Gaussian noise assumption, the goal of the parameter fitting is to minimize the error $E = ||x - x'||$, where $||\cdot||$ represents the Euclidean norm. For any Ω, the optimal estimate of c' is,

$$c' = (\Omega^+\Omega)^{-1}\Omega^+ x \quad (4)$$

Hence, the least square error is

$$E = ||x - x'|| = x^+(I - P_\Omega)x \quad (5)$$

where $^+$ denotes the Hermitian conjugate operator and $P_\Omega = \Omega(\Omega^+\Omega)^{-1}\Omega^+$ is the projection matrix of Ω.

Objective Function and Fitness. Because c_k can be derived separately based on linear fitting after the z_k terms are estimated, only z_k terms are treated as unknown parameters in the GA optimization and encoded (in real value) as genes in the chromosomes. The fitness of the chromosomes should be inversely proportional to the least square error E. To restrict the range of the objective function value to [0 1], it is defined as

$$f(x) = \exp(-E') \quad (6)$$

where *f(x)* is the objective function value, $E' = E/(N\cdot K\cdot \mathrm{ave})$, ave is the average of the absolute magnitude of the data points in the FID, and N and K are the number of data points and signal poles, respectively.

Reproduction, Crossover, and Mutation. After the objective function values of the chromosomes are evaluated, they are subjected to the reproduction process. Four selection schemes for reproduction are used and their performances are compared.[15] The first one is the classic roulette wheel method.[2] Each chromosome in the population has a roulette wheel slot sized in proportion to its objective function value

$$\mathrm{slot}_i = \frac{\mathrm{ov}_i}{\sum_{i=1}^{\mathrm{pop}} \mathrm{ov}_i} \quad (7)$$

where ov_i is the objective function value of the ith chromosome and pop is the size of the population. To reproduce, we simply spin the roulette wheel. In this way, the chromosomes with higher fitness will have more offspring in the succeeding generation.

The second selection scheme is the so-called linear rank-based selection.[16] In linear rank-based selection, the population is sorted in ascending order according to their objective function values. The fitness value of each chromosome is then calculated as

$$\mathrm{fitness}(i) = (2 - \mathrm{SP}) + 2\frac{(\mathrm{SP} - 1)(R(i) - 1)}{(\mathrm{pop} - 1)} \quad (8)$$

where fitness(i) and $R(i)$ are the fitness value and the rank of the ith chromosome, respectively, and SP is the selective pressure that can be varied in the range [1.0, 2.0]. In this work, we set it to be equal to 2 (maximum selectivity). The probability of each chromosome being selected for reproduction is its fitness, normalized by the total fitness of the population. Because the probability of reproduction for each chromosome is limited, it prevents any individual from generating excessive offspring in the next generation.

Another selection scheme is the so called tournament selection.[17] A number t of chromosomes is chosen randomly from the pools and the one with the highest objective function value is selected for reproduction. The process is repeated until the population of the new generation is all created. In this work, we arbitrarily set t equal to 2. In practice, t can be any value from 2 to pop. The last selection scheme that was incorporated is truncation selection.[18] In truncation selection, the chromosomes are sorted according to their objective function values. Only a certain percentage of chromosomes with the highest objective function values are selected for reproduction at uniform probability. One can control this selection process by varying the percentage of chromosomes to be selected. Usually, the range is 10−50%.

After the reproduction process is complete, the crossover or recombination operators are applied to the newly generated population. There are many proposed methods for applying crossover and recombination in the literature. In this work, we tested four of these methods; they are: single-point crossover; two-point crossover; discrete recombination, and intermediate recombination. The following is the pseudocodes that represent these methods.

```
single-point crossover
{
 pop = the population;
 gene_no = number of genes on each chromosome;
 pc = probability of crossover (defined by user) ;
 for i=1 to pop/2 {
  randomly choose two chromosomes from the pools;
  randnum = randomly generated number in the range [0 1];
  if (pc > randnum) {
   k = random number in [1 (gene_no -1 )];
   for(j=1;j<=k;j++) {
     child 1[j] = chromosome 1[j];
     child 2[j] = chromosome 2[j];
   }
   for(j=k+1;j<=gene_no;j++) {
    child 1[j] = chromosome 2[j];
    child 2[j] = chromosome 1[j];
   }
  }
  else {
   copy chromosome 1 as child 1;
   copy chromosome 2 as child 2;
  }
 }
}
```

The chromosomes that were previously chosen from the pool are discarded and the new children that are generated are put into another pool. The probability of crossover (p_c) can be any value between 0 and 1. Usually, a value closes to 1 is chosen.

The two-point crossover is very similar to the single-point crossover, except that two points on the chromosomes are selected as crossover point. For example, if the two random numbers generated are k and m, then

```
if (pc > randnum)
{
 for(i=1;i<=k;i++) {
     child 1[i] = chromosome 1[i];
     child 2[i] = chromosome 2[i];
 }
 for(j=k+1;j<=m;j++) {
     child 1[j] = chromosome 2[j];
     child 2[j] = chromosome 1[j];
 }
 for(i=m+1;i<=gene_no;i++) {
     child 1[i] = chromosome 1[i];
     child 2[i] = chromosome 2[i];
}
else {
     copy chromosome 1 as child 1;
     copy chromosome 2 as child 2;
}
```

For discrete recombination,[18] the following operation takes place if the random number generated is greater than the probability of crossover, p_c. Otherwise, the two children chromosomes are just duplicates of their parents. Discrete recombination causes the exchange of gene values between the chromosomes.

```
two chromosomes selected : chromo1 chromo2
For example, there are six genes on each chromosome.
chromo1 : a-b-c-d-e-f
chromo2 : A-B-C-D-E-F

For each child, six random numbers that are equal to
either 1 or 2 are generated.
rand1 : 1-2-2-1-1-2
rand2 : 2-2-1-1-1-2

The children generated are:
child1 : a-B-C-d-e-F
child2 : A-B-c-d-e-F
```

Intermediate recombination[18] is different from discrete recombination as the gene values of the children are generated somewhere around the gene values of their parent.

```
two chromosomes selected : chromo1 chromo2
For example, there are six genes on each chromosome.
chromo1 : 11.0-12.0-13.0-14.0-15.0-16.0
chromo2 : 31.0-32.0-33.0-34.0-35.0-36.0

For each child, six numbers chose uniformly at random over the
range [-d (1+d)] are generated, where d  is an extension
factor pre-defined.  In this work, we set d to be equal to 0.25.
rand1 : -0.2-0.7-1.0-1.1-0.2
rand2 : 0.5-0.3-1.1-0.6-0.9-0.05

child1[i] = chromo1[i] + rand1[i] * (chromo2[i] - chromo1[i] )
child2[i] = chromo1[i] + rand2[i] * (chromo2[i] - chromo1[i] )
```

In addition to the exchange of gene values between the parents, intermediate recombination also provides a way for the children to have gene values slightly extend from their parents.

After crossover or recombination, the offspring may undergo mutation. Each gene value on the chromosomes is possibly mutated by adding a random number to it. A probability variable controls the mutation process and is therefore called the probability of mutation p_m. Usually, p_m has a small value inversely proportional to the number of genes. A mutation probability of $1/n$ (n = number of genes) is reported to produce good results for many test functions. There are different methods for mutation and in this work, we used the breeder mutation proposed by Mühlenbein et. al.[18]

Breeder mutation:
*(gene value after mutation) = (gene value before mutation) ± (range * Δ) ;*
where + and - are with equal probability.
*range = 0.5 * domain of the variable.*

$$\Delta = \sum_{i=1}^{m} a(i) * 2^{-(i-1)} \qquad \text{where } a(i) = 1 \text{ with probability } 1/m, \text{ else } a(i) = 0.$$

The processes of reproduction, recombination, or crossover and mutation are repeated until the predefined maximum number of the generation is reached.

RESULTS AND DISCUSSION

Simulated one-dimensional NMR FID data are used to evaluate the performance of different combinations of reproduction and recombination schemes. The parameters

Table 1. Parameters Used To Simulate the FID Data Sets[a]

amplitude (a_k)	phase (ϕ_k), °	damping factor (α_k)	searching range of α_k	frequency ($2\pi f_k$), rad/s	searching range of $2\pi f_k$
40.0	70	−18.0	[−20.0, 0]	3100.0	[2800, 3140]
30.0	80	−7.0	[−20.0, 0]	2400.0	[2000, 2700]
30.0	30	−9.0	[−20.0, 0]	1900.0	[1300, 2300]
25.0	150	−15.0	[−20.0, 0]	1400.0	[1000, 1800]
20.0	90	−13.0	[−20.0, 0]	1200.0	[800, 1600]
15.0	180	−12.0	[−20.0, 0]	−140.0	[−300, 700]

[a] Δt was set equal to 0.001 s in the simulation.

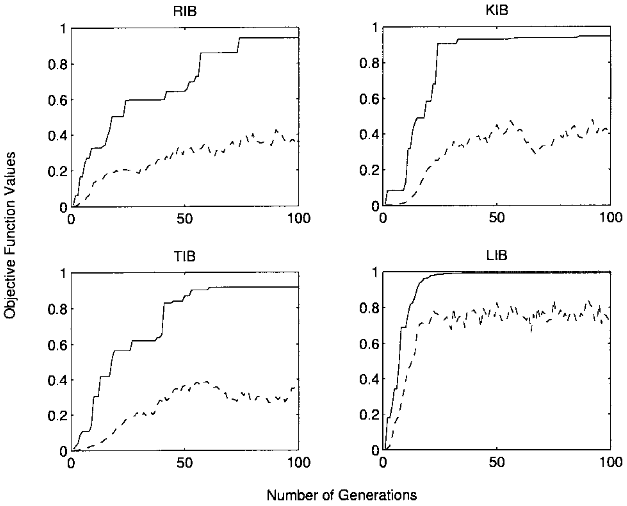

Figure 1. Solid lines show the objective function values of the best chromosomes in different generations. Broken lines show the average objective function values of the population in different generations. The codes of the methods used are the same as in Table 2.

used to simulate the FIDs are shown in Table 1. Two simulated FID data sets, each with 128 data points are generated. The first data set is noiseless and the second data set has SNR = 5dB of white noise. The SNR is defined as

$$\mathrm{SNR} = 10 \log \frac{a_{\max}{}^2}{\sigma^2} \qquad (9)$$

where $a_{\max}$ and σ are the maximum amplitude value and the variance of added noise, respectively. The signals that have comparably small amplitudes will have even lower SNR.

With *a priori* knowledge, constraints on the searching intervals for the α_k and f_k variables in eq 1 are imposed. The results of GA optimization are shown in Table 2. For each method reported in Table 2, five trials were done, each with a different initial population of chromosomes. The probability of crossover p_c is set equal to 0.9 and the probability of mutation is set equal to 0.1. For the truncation selection method, only the top 20% best of the chromosomes are selected for reproduction. For each experiment, the size of population and the number of generation are set to be equal to 100. The objective function shown in eq 6 is used to evaluate the fitness of the chromosomes.

The results in Table 2 clearly show that the intermediate recombination method (KIB, TIB, RIB, and LIB) outperforms the other three crossover or recombination methods in the optimization (the definition of the method codes can be found in the caption of Table 2). For the noiseless FID data set, the objective function value is equal to 1 for a perfect parameter set. Figure 1 shows the performance of different reproduction schemes working with intermediate recombination and breeder mutation. Truncation selection is the best among the four in terms of efficiency. By using the truncation selection method together with intermediate recombination for the noiseless tested FID data, a parameter set with a 0.99 objective function value can be obtained after <50 generations. The method has also been tested on some other noisy FID data sets (SNR = 5dB) composed of 4−12 exponentially damped sinusoid signals. Fifty generations are shown to be enough for the convergence in all these cases. Because the number of parameters used in the GA fitting is exactly equal to two times (one for α_k and one for f_k) the number of signals in the FID, the over-fitting problem is not observed.

In the truncation selection method, we also studied the effect of the percentage of the best chromosomes selected on the efficiency of optimization. The percentage of truncation was varied from 10 to 40%, and the results are shown in Table 3 and Figure 2 . Variation of the percentage of selection has no significant effect on the performance of the optimization. However, we can see that the performance of the *LIB* method is the best when the percentage of truncation is set equal to 20%.

All the optimizations just described use *a priori* knowledge of the parameters as constraints for searching the parameter space. In NMR spectroscopy, both the frequencies and damping factors of some peaks are usually known *a priori*. Incorporation of this knowledge into the GA optimization is expected to improve the accuracy of the parameter estimation. Table 4 shows the objective function values of the best chromosomes in the populations after 100 generations in the presence and the absence of frequency constraints. The results clearly shown that with the frequency constraints, a higher objective function value can be achieved

Table 2. Performances of Different GA Methods

	objective function value															
experiment	RSB	KSB	TSB	LSB	RMB	KMB	TMB	LMB	RDB	KDB	TDB	LDB	RIB	KIB	TIB	LIB
1[b]	0.755	0.875	0.765	0.747	0.740	0.775	0.813	0.742	0.785	0.625	0.762	0.799	0.926	0.936	0.929	0.990
2[c]	0.415	0.543	0.461	0.581	0.418	0.493	0.519	0.567	0.424	0.374	0.480	0.614	0.385	0.427	0.377	0.756
3[d]	0.0205	0.0206	0.0215	0.0188	0.0227	0.0220	0.0218	0.0202	0.0208	0.0193	0.0200	0.0194	0.0231	0.0243	0.0240	0.0248
4[e]	0.0116	0.0136	0.0143	0.0154	0.0122	0.0148	0.0154	0.0162	0.0121	0.0132	0.0131	0.0157	0.0089	0.0126	0.0113	0.0196

[a] The first characters stand for the selection schemes for the reproduction used: R, roulette wheel method; K, rank-based method; T, tournament method; and L, truncation selection method. [b] The averaged objective function values of the best chromosomes (after 100 generation) of the five trials (the simulated FID contains no noise). [c] The average of the average objective function values of the population (after 100 generation) of the five trials. [d] The averaged objective function values of the best chromosomes (after 100 generation) of the five trials (SNR = 5dB). [e] The average of the average objective function values of the population (after 100 generation) of the five trials (SNR = 5dB).

Table 3. Performances of the LIB Method with Varying Percentages of Truncation

	performance of LIB method			
experiment	10% trunc[a]	20% trunc	30% trunc	40% trunc
1[b]	0.978	0.990	0.982	0.988
2[c]	0.746	0.756	0.749	0.755

[a] Truncation. [b] Average objective function values. [c] Average objective function values of the whole population after 100 generations.

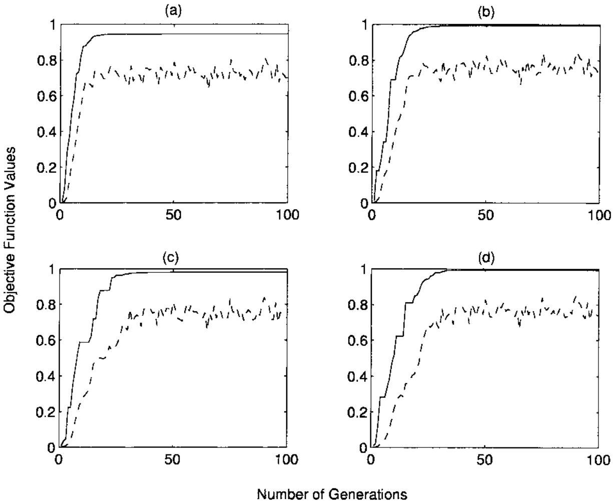

Figure 2. Performance of the LIB method with varying percentage of truncation (trunc). trunc = 10%, (b) trunc = 20%, (c) trunc = 30%, and (d) trunc = 40%.

Table 4. Averaged Objective Function Values of the Best Chromosomes in Five Trials

	average objective function			
trial	∞ dB	15 dB	10 dB	5 dB
with constraints	0.990	0.603	0.244	0.0248
without constraints	0.961	0.557	0.216	0.0230

within the same number of generations. From Figure 3, we can also find that the GA method achieves the "best" parameter set after fewer generations, if frequency constraints are provided.

We compared the GA parameter estimation with the IQML method.[19] A new set of parameters was used to generate a simulated FID data set (with 256 complex data points, SNR = 5dB). Table 5 shows the parameters used for this simulation. There are eight damped sinusoids signals, and their frequencies, damping factors, and amplitudes are randomly selected in ranges [$-3000/2\pi$, $3000/2\pi$], [-30, -10], and [20, 40] respectively. Ten trials were performed for each method and, in each trial, different random noise was added to the FID. The estimated parameters were then used to reconstruct the FIDs. Figure 4 shows the results of such calculations. From the spectra it is clear that with *a priori* knowledge, GAs perform better than IQML method in extracting NMR signal parameters from low SNR FID data. Moreover, the ranges of frequency constraints do not need to be narrow, so knowledge of the exact location of signals is not necessary. This factor is significant when some peaks are partially overlapped and the exact frequency location of the signals cannot be determined *a priori*. On the other hand, without the incorporation of *a priori* knowledge, in only two out of 10 trials can IQML extracts all eight signal poles (in four trials, IQML extracted only seven signals and in the other four trials, only six signals were extracted.)

In conclusion, we demonstrate that the GAs, with appropriate combination of reproduction and recombination

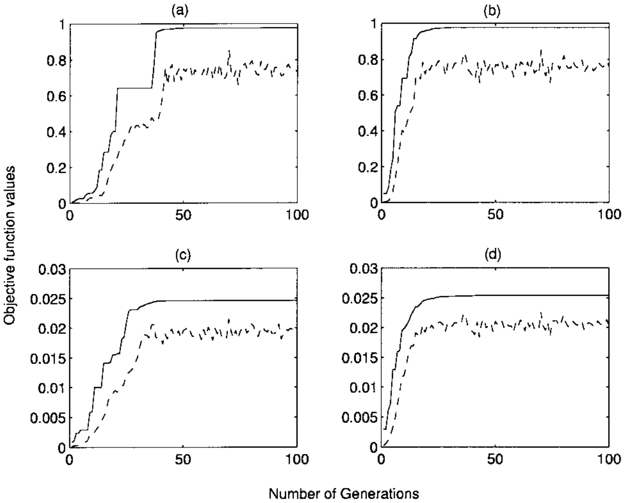

Figure 3. (a) Noiseless FID with no frequency constraints. (b) Noiseless FID with frquency constraints. (c) FID with SNR = 5dB, and no frequency constraints. (d) FID with SNR = 5dB, and with frequency constraints. Solid lines show the objective function values of the best chromosomes in different generations and broken lines show the average objective function values of the population in different generations.

Table 5. Parameters Used To Simulate the New FID Data Set

peak number	amplitude (a_k)	damping factor (a_k)	frequency ($2\pi f_k$), rad/s
1	23.0	−15.0	2274.0
2	34.0	−22.0	382.0
3	40.0	−24.0	312.0
4	37.0	−26.0	−468.0
5	34.0	−18.0	−1086.0
6	28.0	−23.0	−2014.0
7	36.0	−23.0	2166.0
8	33.0	−19.0	−2754.0

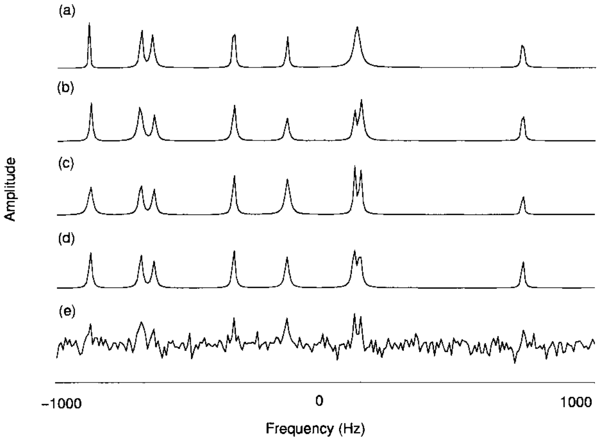

Figure 4. (a) FFT of the FID (average of 10 trials) reconstructed by IQML methods (window size used is equal to 48). (b) FFT of the FID (average of 10 trials) reconstructed by GA method. For frequencies, f_k, the constraints used are $f_k \pm (300/2\pi)$ rad/s, and for the damping factors, which are searched in the range [-10, -30] rad/s. (c) same as (b), only the frequency constraints of peaks #1, #2, #3, and #7 are changed to [-2242, -2090], [347, 417], [282, 347], and [-2090, -1938], respectively. (d) FFT of the noiseless FID. (e) FFT of one of the noise FID in the 10 trials.

schemes, can be used in NMR signal parameter estimations. Moreover, *a priori* knowledge can be incorporate into the GA in a straightforward manner, giving improved accuracy of the GA optimization approach and thereby making the algorithms more efficient. However, the computational time for GA optimization is longer than other conventional methods. The program is written in C, and for a FID with 128 data points and six signals (typical for some *in vivo* NMR FID), 50 s of cpu time on a Pentium 200MHz PC is needed for parameter estimation. Instead of using GA to replace more conventional parameter estimation methods, GA can be used as a complementary method when the SNR of the FID is low. In addition GAs can be applied to different models of data fitting by simply modifying the objective function. Work on improving the GA method and applying it to different models of NMR data are in progress.

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