On the Projection-Reconstruction NMR.*

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We discuss the recently proposed Hybrid Backprojection/Lower-Value (HBLV) algorithm and its implementation in the NMR projection-reconstruction software PR-CALC. We argue that the HBLV reconstruction is only suitable for spectra that have no negative peaks. However, in such cases HBLV becomes a straight-forward generalization of the Lower-Value reconstruction algorithm and boils down to a simple calculation, not requiring an expensive combinatorial search for the smallest sum as was originally suggested by the authors.

In the recent paper [1] Venters *et al* proposed a new version of a projection-reconstruction (PR) procedure to reconstruct multidimensional NMR spectra from a series of one-dimensional projections. (Since the acquisition dimension is treated independently, it is excluded from the consideration.) The method, named Hybrid Backprojection/Lower-Value (HBLV) algorithm is literally a hybrid of the two simpler methods proposed earlier by Kupče and Freeman, the Lower-Value (LV) Reconstruction [3] and the Backprojection (BP) Reconstruction [4]. The HBLV algorithm has been implemented by Coggins and Zhou [2] as a part of their NMR processing package PR-CALC, which may possibly have many users. In the present Communication we discuss the new reconstruction formula, namely, its applicability and algorithmic implementation. We follow the nomenclature of refs. [1, 2]; for detailed description of the PR-NMR methodology the reader is referred to the above cited papers.

The Lower-Value Reconstruction: Given n projections $P_i(r)$, for a point $(x, y, ...)$ in the spectral domain, the spectrum is reconstructed using

$$\begin{aligned} S^{\mathrm{LV}}(x,y,...) &= \mathrm{sgn}\,[P_i(r)] \min_{i=1}^{n} |P_i(r)|\,, \\ r &= x\cos\alpha_{x,i} + y\cos\alpha_{y,i} + ..., \end{aligned} \tag{1}$$

where $\alpha_{x,i},\ \alpha_{y,i}, ...$ define the projection angles and sgn is the sign function.

The Backprojection Reconstruction is given by:

$$\begin{aligned} S^{\mathrm{BP}}(x,y,...) &= \frac{1}{n}\sum_{i=1}^{n} P_i(r), \\ r &= x\cos\alpha_{x,i} + y\cos\alpha_{y,i} + ... \end{aligned} \tag{2}$$

The drawbacks of both reconstruction formulas, (1) and (2), are well documented (see, e.g., refs. [1, 4, 5]). While Eq. 1 discriminates well against false-positive peaks, it generally results in a poor signal-to-noise ratio (SNR), as picking the smallest value (out of n available values) cannot take advantage of any signal accumulation by combining the information from all the n available data sets. Moreover, due to the finite SNR, in the $n \to \infty$ limit, the spectrum reconstructed by the deterministic formula of Eq. 1 will vanish everywhere. Unlike the LV reconstruction, Eq. 2 does accumulate the signals from all the n available projections, albeit for the price of producing false cross-peaks formed by the BP ridges.

The Hybrid Backprojection-Lower-Value Reconstruction reads:

$$\begin{aligned} S^{\mathrm{HBLV}}(x,y,...) &= \frac{1}{k}\mathrm{sgn}\left[\sum_{P_j\in A_i}^{n} P_j(r)\right] \min_{i=1}^{{}_nC_k} \left|\sum_{P_j\in A_i}^{n} P_j(r)\right|, \\ r &= x\cos\alpha_{x,j} + y\cos\alpha_{y,j} + ... \end{aligned} \tag{3}$$

where A_i $(i = 1, ..., {}_nC_k)$ define all the possible choices of k projections $P_j(r)$ out of n available ones. As argued in refs. [1, 2], due to the sum over k projections, expression (3) does take advantage of signal accumulation and thus has better SNR properties than that of the LV reconstruction, while the ridge and cross-peak artifacts are still removed by the minimization step.

The striking drawback of Eq. 3 is that numerically it is by about a factor of ${}_nC_k = n!/(n-k)!k!$ more expensive than the other two expressions, (1) and (2). For example, one possibility suggested in ref. [2] corresponds to $n = 30$ and $k = 8$, in which case reconstruction by Eq. 3 at each spectral point may require to sample as many as ${}_{30}C_8 \approx 6 \times 10^6$ terms. In the case of 4D spectral reconstruction, this can make a computer cluster busy for several days. Although the authors of PR-CALC [2] did everything to carefully optimize their code for best performance, they find that because of the ${}_nC_k$ factor the use of more than about 30 projections may become prohibitive.

At this point we distinguish the following two cases. In the first case, for which the PR-NMR techniques are perhaps most suitable, the spectrum $S(x, y, ...)$ is assumed to be positive, except for negative but small noise spikes. In such a case the negative spikes in the projections $P_j(r)$ can be removed before further processing. Clearly, for

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all positive projections, the minimum arising in Eq. 3 is given by the sum of the k lowest $P_j(r)$ values:

$$\min_{i=1}^{{}_nC_k} \left| \sum_{P_j \in A_i}^{n} P_j(r) \right| = \sum_{j=1}^{k} P_j(r), \qquad (4)$$
$$0 \leq P_1(r) \leq P_2(r) \leq ... \leq P_n(r),$$

where without loss of generality we assumed that the values $P_j(r)$ have been sorted in the ascending order. So, for spectra with no negative peaks the HBLV algorithm boils down to a trivial calculation, which can be accomplished by many orders of magnitude faster than that suggested by Eq. 3. In words, for each frequency grid point of interest the value of the reconstructed spectrum is set to be equal to the arithmetic mean of the k smallest (out of n available) projection values.

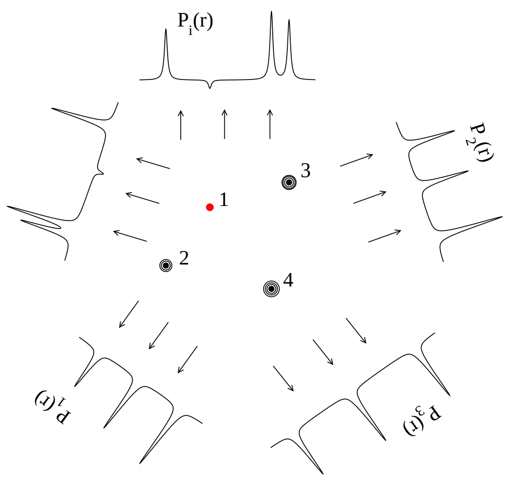

FIG. 1: Demonstration of a failure of the HBLV algorithm to reconstruct peaks with negative amplitudes (see text). The spectrum consists of one negative peak with amplitude $S_1 = -1$ and three positive peaks with amplitudes $S_2 = 7$, $S_3 = 8$ and $S_4 = 9$. The negative peak overlaps with one of the positive peaks in projections $P_j(r)$ $(j = 1, 2, 3)$.

The second case corresponds to spectra that may have genuine negative peaks. In this case the minimum in Eq. 3 is not necessarily given by the k projections with smallest magnitudes $|P_j(r)|$, because of possible cancellations of negative and positive contributions. However, these cancellations are also the reason for Eq. 3 being not a meaningful reconstruction formula, when negative peaks are encountered. Let us demonstrate this statement using a simple example shown in Fig.1. In this demonstration the true spectrum consists of only four peaks: a negative peak at point $(x_1, y_1, ...)$ with amplitude $S_1 = -1$ units, and three positive peaks with amplitudes $S_2 = 7,\ S_3 = 8,\ S_4 = 9$ units, located at three other positions. We are interested in recovering the spectrum at $(x_1, y_1, ...)$ assuming infinite SNR in all the projections. There are three projection angles at which the negative peak overlaps with one of the positive peaks. This may result in the following set of projection amplitudes:

$$P_j(r) \in \{6, 7, 8, -1, -1, -1, ...\},$$
$$r = x_1 \cos\alpha_{x_1,j} + y_1 \cos\alpha_{y_1,j} + ...,$$

where we assumed that all projections, but the first three, are due to the single negative peak. Following the suggestion of ref. [2] we set $k = 8$ and apply Eq. 3 to reconstruct the spectrum at point $(x_1, y_1, ...)$, where the negative peak is situated:

$$S^{\mathrm{HBLV}}(x_1, y_1, ...) = P_2(r) + \sum_{j=4}^{10} P_j(r) = 7 + 7 \cdot (-1) = 0,$$
$$r = x_1 \cos\alpha_{x_1,j} + y_1 \cos\alpha_{y_1,j} + ...$$

It is not hard to see that the HBLV reconstruction using $k = 7$ or $k = 9$ will also result in $S^{\mathrm{HBLV}}(x_1, y_1, ...) = 0$.

At first glance our example may seem dishonest as it was carefully designed (or "cooked-up") to make the method fail. However, we argue that in practice the situation is even worse due to the presence of a large number of positive peaks with different amplitudes overlapping with small negative peaks and thus resulting in many possibilities for similar-type cancellations. Moreover, increasing the number of projections n will only increase the chances that there will be a combination of k negative and positive terms summing to zero.

Once the fact that Eq. 3 is only applicable to spectra with no negative amplitudes is established, it becomes apparent (*cf.* Eq. 4) that the problem of combinatorial search for the smallest sum is superficial.

Eq. 3 with Eq. 4 is still a valid PR method, but its status is somewhat similar to that of Eq. 1: in the $n \to \infty$ limit with fixed value of k the HBLV spectrum will still vanish everywhere. However depending on the k/n ratio the SNR of the HBLV spectrum will be better than that of a single LV spectrum.

We also note ref. [5] discussing a variety of PR methods. For example, one of the proposed extensions of the LV algorithm (similar to that using Eq. 3 with Eq. 4) is to divide the set of n projections into k groups and apply Eq. 1 to each group independently. The resulting k LV estimates are then averaged to obtain an estimate that has better SNR properties than a single LV spectrum.

In conclusion, inspired by the above example, we propose yet another deterministic PR algorithm that is simple, numerically inexpensive, but possibly applicable to the case of negative amplitudes. Namely, for a given reconstruction point $(x, y, ...,)$, consider the set of the corresponding projection values $P_j(r)$ $(j = 1, ..., n)$ and the distribution function $g(P)$ estimated from their histogram. Assuming that $g(P)$ has a maximum at $P = P_{\max}$, the reconstructed spectrum can be estimated by setting $S(x, y, ...,) = P_{\max}$. This approach will work well for the above example or for cases with high SNR, however, it may still fail in a general situation corresponding to crowded spectra.

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