# Inverse Laplace Transforms Applied to $\beta$-NMR

Derek Fujimoto, Ryan McFadden

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Let $n$-vector $\boldsymbol{y}$ be be a set of measurements, corresponding to independent variable $\boldsymbol{x}$ of equal length. The goal is to find the vector of weights $\boldsymbol{p}$, of length $m$, which satisfies the least squares condition

$$\min ||\boldsymbol{y} - K\boldsymbol{p}||^2, \tag{1}$$

where $K$ is a $n \times m$ kernel matrix composed of function $f(x, z)$ in the following way:

$$K = \begin{pmatrix} f(x_1, z_1) & f(x_1, z_2) & f(x_1, z_3) & \dots \\ f(x_2, z_1) & \ddots & & \\ f(x_3, z_1) & & & \\ \vdots & & & \end{pmatrix}. \tag{2}$$

The final fit function to the data $\boldsymbol{y}$ is therefore $\sum_i p_i f(\boldsymbol{x}, z_i)$. Accounting for the errors in $\boldsymbol{y}$, the weighted $\chi^2_w$ is given by

$$\chi^2_w = ||\Sigma(\boldsymbol{y} - K\boldsymbol{p})||^2, \tag{3}$$

where

$$\Sigma = \begin{pmatrix} 1/\sigma_1 & & & \\ & 1/\sigma_2 & & \\ & & \ddots & \\ & & & 1/\sigma_n \end{pmatrix} \tag{4}$$

is the diagonal matrix constructed from the errors in $\boldsymbol{y}$. However, due to the noise in $\boldsymbol{y}$, the problem is ill-defined: there exist many possible weights $\boldsymbol{p}$ which produce a funtion which falls within the scatter and noise of $\boldsymbol{y}$. We introduce regularization $m \times m$ matrix $\Gamma$ in order to minimize

$$\min ||\Sigma(\boldsymbol{y} - K\boldsymbol{p})||^2 + ||\Gamma\boldsymbol{p}||^2. \tag{5}$$

This matrix is often chosen to be $\alpha I$, where the parameter $\alpha$ is a constant, and $I$ is the identity matrix. If $\alpha$ is large, this has the effect of smoothing $\boldsymbol{p}$. If $\alpha$ is too small, then $\boldsymbol{p}$ will appear to be "spiky". For the sake of generality however, we will preserve the notation of $\Gamma$ for the most of the following discussion. The solution to Equation (5) also satisfies

$$\boldsymbol{q} = L\boldsymbol{p} \tag{6}$$

where $\boldsymbol{q}$ and $L$ are the block matrices defined by

$$\boldsymbol{q} = \begin{pmatrix} \Sigma\boldsymbol{y} \\ \boldsymbol{0} \end{pmatrix} \tag{7}$$

$$L = \begin{pmatrix} \Sigma K \\ \Gamma \end{pmatrix}. \tag{8}$$

This is proven by showing that $||\boldsymbol{q} - L\boldsymbol{p}||^2 = ||\boldsymbol{y} - K\boldsymbol{p}||^2 + ||\Gamma p||^2$:

$$\begin{aligned} ||\boldsymbol{q} - L\boldsymbol{p}||^2 &= (\boldsymbol{q} - L\boldsymbol{p})^T(\boldsymbol{q} - L\boldsymbol{p}) && (9) \\ &= (\boldsymbol{q}^T - \boldsymbol{p}^T L^T)(\boldsymbol{q} - L\boldsymbol{p}) && (10) \\ &= \boldsymbol{q}^T\boldsymbol{q} - \boldsymbol{q}^T L\boldsymbol{p} - (\boldsymbol{q}^T L\boldsymbol{p})^T + \boldsymbol{p}^T L^T L\boldsymbol{p} && (11) \end{aligned}$$

where

$$\boldsymbol{q}^T\boldsymbol{q} = \begin{pmatrix} \boldsymbol{y}^T\Sigma^T & \boldsymbol{0}^T \end{pmatrix} \begin{pmatrix} \Sigma\boldsymbol{y} \\ \boldsymbol{0} \end{pmatrix} = \boldsymbol{y}^T\Sigma^T\Sigma\boldsymbol{y} \tag{12a}$$

$$\boldsymbol{q}^T L\boldsymbol{p} = \begin{pmatrix} \boldsymbol{y}^T\Sigma^T & \boldsymbol{0}^T \end{pmatrix} \begin{pmatrix} \Sigma K \\ \Gamma \end{pmatrix} \boldsymbol{p} = \boldsymbol{y}^T\Sigma^T\Sigma K\boldsymbol{p} \tag{12b}$$

$$\boldsymbol{p}^T L^T L\boldsymbol{p} = \boldsymbol{p}^T \begin{pmatrix} K^T\Sigma^T & \Gamma^T \end{pmatrix} \begin{pmatrix} \Sigma K \\ \Gamma \end{pmatrix} \boldsymbol{p} = \boldsymbol{p}^T(K^T\Sigma^T\Sigma K + \Gamma^T\Gamma)\boldsymbol{p}. \tag{12c}$$

Therefore

$$||\boldsymbol{q} - L\boldsymbol{p}||^2 = \boldsymbol{y}^T\Sigma^T\Sigma\boldsymbol{y} + \boldsymbol{y}^T\Sigma^T\Sigma K\boldsymbol{p} + \boldsymbol{p}^T K^T\Sigma^T\Sigma\boldsymbol{y} + \boldsymbol{p}^T(K^T\Sigma^T\Sigma K + \Gamma^T\Gamma)\boldsymbol{p} \tag{13}$$

$$= (\boldsymbol{y}^T\Sigma^T - \boldsymbol{p}^T K^T\Sigma^T)(\Sigma\boldsymbol{y} - \Sigma K\boldsymbol{p}) + \boldsymbol{p}^T\Gamma^T\Gamma\boldsymbol{p} \tag{14}$$

$$= ||\Sigma(\boldsymbol{y} - K\boldsymbol{p})||^2 + ||\Gamma\boldsymbol{p}||^2. \tag{15}$$

We then solve $\boldsymbol{q} = L\boldsymbol{p}$ using a non-negative least squares algorithm such that $\boldsymbol{p}$ may be identified with the vector of weights corresponding to parameters $z_i$.