# Minimum Message Length Estimate of Parameters of Laplace Distribution

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**Editor:** Cheng Soon Ong and Tu Bao Ho

## Abstract

The Laplace distribution offers a number of uses in statistical inference and modelling on symmetric data with long tails. We report here for the first time the derivation of the minimum message length (MML) estimates of location ($\mu$) and scale ($b$) parameters of the Laplace distribution for any observed data. We demonstrate an application of this work to compare and contrast the quality of orthogonal superposition of two (spatial) vector sets under $L^1$ and $L^2$ norm.

**Keywords:** Laplace distribution, Normal distribution, MML, Monte Carlo simulation

## 1. Introduction

Laplace distribution is a continuous probability density function which is dependent on the absolute value of the difference between the mean and the data point. Because of this characteristic, inference of parameters of this distribution (based on some empirical data) is not severely affected in the presence of outliers. Laplace distribution is a model of choice in areas as diverse as signal processing (Eltoft et al., 2006), image denoising (Rabbani et al., 2006), gene expression studies (Bhowmick et al., 2006), market risk prediction (Haas et al., 2005), and machine learning (Cord et al., 2006). In most of these applications, a mixture model of Laplace distributions is used.

Normal distribution, on the other hand, is sensitive to outliers because of the quadratic nature of the contributions of individual terms. In the presence of outliers, the inference of parameters is skewed to dampen the effect of their residuals with respect to the model. In many problems, formulating an objective function (that needs to be optimized) as sum of squared deviations (the $L^2$ norm) results in a closed form solution. Its $L^1$ equivalent, however, does not have an analytical solution (for data with more than one dimension).

We show this in the context of superposition of vector sets and use Monte Carlo simulation to optimize the objective function when it is formulated using $L^1$ norm. We compare the superpositions resulting from using the two versions of objective functions using the minimum message length (MML) criterion. MML is used to adjudicate which is better on individual test cases.

The MML expression for the Normal distribution has been worked out previously (Wallace and Boulton, 1968; Wallace, 2005), while the MML estimates for the Laplace distribution have not been characterized. The main contribution of this work is the derivation of the message length expression and estimation of the MML parameters for the Laplace distribution. The general procedure to formulate the message length expression for transmitting data using some statistical model is outlined in Wallace and Freeman (1987) and is referred to as Strict Message Length (SMML) Inference. This is computationally infeasible and is shown to be NP-hard (Farr and Wallace, 2002). Wallace and Freeman (1987) provide an approximate form which is commonly referred to as the *Wallace-Freeman* approximation. The MML method of estimating parameters for a number of distributions using this approximation has been well established (Wallace, 2005). In this paper, we use the Wallace-Freeman's quadratic approximation to derive the the message length expression for the Laplace distribution.

MML is an information theoretic way of Bayesian inference (Wallace and Boulton, 1968). MML is best understood through a communication process between an imaginary pair of transmitter and receiver connected over a Shannon channel. The method involves encoding the model and its fit to the data. A model that results in the smallest total message length is inferred as the most suitable under this criterion. Indeed the message length paradigm provides an objective means to differentiate between competing models and select the best one. In this paper, we use this intuition to evaluate the overall fit when the data is modelled using a Normal and a Laplace distribution.

The results demonstrate the use of Laplace estimates in two cases. The first scenario involves data being randomly generated from a Laplace distribution. This data is then fitted using both Normal and Laplace models. We use the derived formulation of Laplace MML to compute the Laplace fit. This is then compared against the fit using a Normal distribution.

As a demonstration of a practical real world application, we consider the problem of superposition of vector sets. The objective function for the superposition problem can be formulated where the deviations of the corresponding vectors are calculated using the $L^1$ norm or the $L^2$ norm. In MML parlance, the optimal superposition would correspond to stating the deviations concisely. We encode the deviations using both Normal and Laplace distributions. The distribution which results in the best compression is chosen to be the best model for those two vector sets.

## 2. The Minimum Message Length (MML) Framework

### 2.1. Inductive Inference

Wallace and Boulton (1968) developed the first practical criterion for model selection using information theory. MML provides an elegant framework to compare any two competing hypotheses that model some observed data. The hypothesis that results in the shortest overall message length is chosen as the best one, in line with traditional statistical inference using the Bayesian method.[1] Using Bayes's theorem to explain some observed data $D$ by

[1] http://allisons.org/ll/MML/

hypothesis $H$, we get:

$$\Pr(H\&D) = \Pr(H) \times \Pr(D|H) = \Pr(D) \times \Pr(H|D)$$

where $\Pr(H\&D)$ is the joint probability of data $D$ and hypothesis $H$, $\Pr(H)$ is the prior probability of hypothesis $H$, $\Pr(D)$ is the prior probability of probability of data $D$, $\Pr(H|D)$ is the posterior probability of $H$ given $D$, and $\Pr(D|H)$ is the likelihood. MML uses the following result from information theory: given an event $E$ with a probability $\Pr(E)$, the message length $I(E)$ for an optimal code is given by $I(E) = -\log_2(\Pr(E))$ bits (Shannon, 1948). Applying this insight to the Bayes's theorem, we get the following relationship between conditional probabilities in terms of optimal message lengths:

$$I(H\&D) = I(H) + I(D|H) = I(D) + I(H|D)$$

In the traditional Bayesian framework, the hypothesis $H$ with the largest posterior probability $\Pr(H|D)$ is often preferred. Among the terms in the above equation, $\Pr(H)$ (and hence $I(H)$) can usually be estimated well for some *reasonable* prior(s) on hypotheses. Given the data $D$ and a chosen prior $H$, the likelihood $\Pr(D|H)$ can also be estimated. Whilst comparing two competing hypotheses, the prior of observed data $\Pr(D)$ can be ignored as it is a common factor. Hence, for two competing hypotheses, $H$ and $H'$, we have:

$$I(H|D) - I(H'|D) = I(H) + I(D|H) - I(H') - I(D|H')$$

The discriminative ability of MML lies in its consideration of the model complexity and the error of the fit. In the MML setting, the net message, therefore, involves statement cost of the hypothesis (given by $I(H)$) and statement cost of the data given the hypothesis (given by $I(D|H)$).

### 2.2. Parameter Estimation using MML

The hypothesis is a statistical model which is characterized by its parameters. MML accounts for both the model complexity and its explanatory power of the data observed. MML works by maximizing the expectation of the posterior probability and this is where it differs from the traditional Bayesian methods. This involves determining the *accuracy of parameter values (AOPV)* for continuous parameters. AOPV is a measure of the uncertainty in stating a parameter and it is this region over which the expectation is maximized. As per MML, a parameter need not be stated very accurately. The optimal precision to which it needs to be stated is computed as part of the MML inference. A good description of the procedure is outlined in Oliver and Baxter (1994).

## 3. Message Length of Laplace distribution

Wallace and Freeman (1987) derived the approximation to the code length of the two part message as

$$\begin{aligned} I(\bar{\theta}, D) &= I(\bar{\theta}) + I(D|\bar{\theta}) \\ &\approx \underbrace{\frac{d}{2}\log \kappa_d - \log h(\bar{\theta}) + \frac{1}{2}\log(det\, F(\bar{\theta}))}_{\text{part1}} + \underbrace{L(\bar{\theta}) + \frac{d}{2}}_{\text{part2}} \end{aligned} \tag{1}$$

where $\bar{\theta}$ is the set of model parameters, $d$ is the number of parameters, $\kappa_d$ is the $d$-dimensional lattice quantization constant (Conway and Sloane, 1984), $h(\bar{\theta})$ is the prior probability of the parameters, $det(\mathrm{F}(\bar{\theta}))$ is the determinant of the expected Fisher matrix, and $L(\bar{\theta})$ is the negative log likelihood of observed data. The MML estimates $\hat{\bar{\theta}}_{\mathrm{MML}}$ of the parameters are determined by minimizing (1).

### 3.1. Laplace distribution

The contribution of this paper is in the derivation of the MML estimates of the parameters of the Laplace distribution which have not been characterized previously. The parameters describing a Laplace distribution are the location($\mu$) and the scale ($b$). The probability density function (pdf) is given in (2).

$$\mathrm{pdf}(x) = \frac{1}{2b}\exp\left(-\frac{|x-\mu|}{b}\right) \tag{2}$$

To derive the MML estimates, we use the Wallace-Freeman approximation (Wallace and Freeman, 1987). This estimation as per (1) requires the likelihood function, the Fisher information matrix, and the prior distributions on the parameters. Let $D = \{x_1, x_2, \ldots, x_N\}$ be the observed data containing $N$ samples and $\epsilon$ be the precision to which each datum is stated. Let $\mathrm{R}_\mu$, $\mathrm{R}_b$ be the range of $\mu$ and $\log b$ respectively ($\epsilon$, $\mathrm{R}_\mu$, $\mathrm{R}_b$ are hyperparameters which are introduced in Wallace (2005)). Using (2), the *likelihood function* is given by

$$f(D|\bar{\theta}) = \prod_{n=1}^{N} \frac{\epsilon}{2b} e^{-\frac{|x_n-\mu|}{b}}$$

and, hence, the *negative log-likelihood* is computed as

$$\begin{aligned} L(\bar{\theta}) &= -\log f(D|\bar{\theta}) \\ &= N\log\left(\frac{2}{\epsilon}\right) + N\log b + \frac{1}{b}\sum_{n=1}^{N}|x_n-\mu| \end{aligned} \tag{3}$$

The maximum likelihood (ML) estimates for $\mu$ and $b$ are given by

$$\begin{aligned} \hat{\mu}_{\mathrm{ML}} &= \mathrm{median}\{x_n\} \\ \hat{b}_{\mathrm{ML}} &= \frac{1}{N}\sum_{n=1}^{N}|x_n - \hat{\mu}_{\mathrm{ML}}| \end{aligned}$$

#### Computation of Fisher information $\mathbf{F}(\bar{\boldsymbol{\theta}})$

The Fisher information matrix is given by

$$\mathrm{F}(\mu, b) = \begin{pmatrix} \mathrm{E}\left[\frac{\partial^2 L}{\partial \mu^2}\right] & \mathrm{E}\left[\frac{\partial^2 L}{\partial \mu \partial b}\right] \\ \mathrm{E}\left[\frac{\partial^2 L}{\partial b \partial \mu}\right] & \mathrm{E}\left[\frac{\partial^2 L}{\partial b^2}\right] \end{pmatrix}$$

where E[.] is the expected value of that quantity. Using (3),

$$\frac{\partial^2 L}{\partial b^2} = -\frac{N}{b^2} + \frac{2}{b^3}\sum_{n=1}^{N}|x_n - \mu|$$

$$\mathrm{E}\left[\frac{\partial^2 L}{\partial b^2}\right] = -\frac{N}{b^2} + \frac{2}{b^3}\mathrm{E}\left[\sum_{n=1}^{N}|x_n - \mu|\right]$$

$$\begin{aligned}
\mathrm{E}\left[|x-\mu|\right] &= \int\limits_{-\infty}^{\infty} |x-\mu| . \frac{1}{2b} . e^{-\frac{|x-\mu|}{b}}\,dx \\
&= \frac{1}{2b}\int\limits_{-\infty}^{\mu} -(x-\mu)e^{\frac{(x-\mu)}{b}}\,dx + \int\limits_{\mu}^{\infty}(x-\mu)e^{-\frac{(x-\mu)}{b}}\,dx \\
&= b
\end{aligned}$$

$$\text{Therefore,}\quad \mathrm{E}\left[\frac{\partial^2 L}{\partial b^2}\right] = -\frac{N}{b^2} + \frac{2}{b^3}(Nb) = \frac{N}{b^2} \tag{4}$$

$$\frac{\partial L}{\partial \mu} = -\frac{1}{b}\sum_{n=1}^{N}\frac{(x_n-\mu)}{|x_n-\mu|} \qquad \left(\text{using}\frac{d}{dx}|x| = \frac{d}{dx}\sqrt{x^2} = \frac{x}{|x|}\right)$$

This is discontinuous as it is piecewise constant. Hence to calculate $\frac{\partial^2 L}{\partial \mu^2}$, the following approach is adopted: Assume that the actual distribution has parameters $m$ and $b$. The receiver, however, decodes the mean as $\mu$ to an accuracy of parameter value $\delta$. As such $\mu$ is a random variable and it is fair to reason out that $\mu \in \left[m - \frac{\delta}{2}, m + \frac{\delta}{2}\right]$. It is assumed that $\mu$ follows a uniform distribution in this range. Using this assumption, now we compute the $\mathrm{E}\left[\frac{\partial L}{\partial \mu}\right]$ and subsequent calculations. From our assumptions, pdf$(\mu) = \frac{1}{\delta}$.

$$\therefore \frac{\partial L}{\partial \mu} \approx \mathrm{E}\left[\frac{\partial L}{\partial \mu}\right] = -\frac{1}{b}\mathrm{E}\left[\sum_{n=1}^{N}\frac{x_n-\mu}{|x_n-\mu|}\right]$$

$$\begin{aligned}
\mathrm{E}\left[\frac{x-\mu}{|x-\mu|}\right] &= \int\limits_{-\infty}^{\infty}\frac{x-\mu}{|x-\mu|} . \frac{1}{2b} . e^{\frac{|x-m|}{b}}\,dx \\
&= \int\limits_{-\infty}^{\mu} -\frac{1}{2b}e^{-\frac{|x-m|}{b}}\,dx + \int\limits_{\mu}^{\infty}\frac{1}{2b}e^{-\frac{|x-m|}{b}}\,dx
\end{aligned}$$

(i) Let $\mu < m$

$$\begin{aligned}
\therefore \mathrm{E}\left[\frac{x-\mu}{|x-\mu|}\right] &= \int\limits_{-\infty}^{\mu} -\frac{1}{2b}e^{\frac{x-m}{b}}\,dx + \int\limits_{\mu}^{m}\frac{1}{2b}e^{\frac{x-m}{b}}\,dx + \int\limits_{m}^{\infty}\frac{1}{2b}e^{-\frac{x-m}{b}}\,dx \\
&= 1 - e^{\frac{\mu-m}{b}}
\end{aligned}$$

(ii) Let $\mu > m$

$$\begin{aligned}\therefore \mathrm{E}\left[\frac{x-\mu}{|x-\mu|}\right] &= \int\limits_{-\infty}^{m} -\frac{1}{2b}e^{\frac{x-m}{b}}dx + \int\limits_{m}^{\mu} -\frac{1}{2b}e^{-\frac{x-m}{b}}dx + \int\limits_{\mu}^{\infty} \frac{1}{2b}e^{-\frac{x-m}{b}}dx \\ &= -(1-e^{-\frac{\mu-m}{b}})\end{aligned}$$

(i) and (ii) can be merged and hence, $\mathrm{E}\left[\frac{x-\mu}{|x-\mu|}\right] = -sgn(\mu-m)(1-e^{-\frac{|\mu-m|}{b}})$. From the argument above,

$$\begin{aligned}\frac{\partial L}{\partial \mu} \approx \mathrm{E}\left[\frac{\partial L}{\partial \mu}\right] &= -\frac{1}{b}\mathrm{E}\left[\sum_{n=1}^{N}\frac{x_n-\mu}{|x_n-\mu|}\right] \\ &= \frac{N}{b}sgn(\mu-m)(1-e^{-\frac{|\mu-m|}{b}}) \qquad (5) \\ \therefore \frac{\partial^2 L}{\partial \mu^2} &= \frac{N}{b^2}e^{\frac{-|\mu-m|}{b}} \\ \mathrm{E}\left[\frac{\partial^2 L}{\partial \mu^2}\right] &= \frac{N}{b^2}\mathrm{E}\left[e^{\frac{-|\mu-m|}{b}}\right]\end{aligned}$$

$$\begin{aligned}\mathrm{E}\left[e^{\frac{-|\mu-m|}{b}}\right] &= \int\limits_{m-\frac{\delta}{2}}^{m+\frac{\delta}{2}} e^{\frac{-|\mu-m|}{b}}.\frac{1}{\delta}.d\mu \\ &= \frac{1}{\delta}\int\limits_{m-\frac{\delta}{2}}^{m} e^{\frac{\mu-m}{b}}d\mu + \int\limits_{m}^{m+\frac{\delta}{2}} e^{-\frac{\mu-m}{b}}d\mu \\ &= 2b\left(\frac{1-e^{-\frac{\delta}{2b}}}{\delta}\right) \\ &= 2b\left(\frac{1}{2b}-\frac{1}{2b}\mathcal{O}\left(\frac{\delta}{2b}\right)\right) \qquad \text{(assuming} \quad \delta \ll 2b) \\ &\approx 1\end{aligned}$$

$$\text{Therefore,} \quad \mathrm{E}\left[\frac{\partial^2 L}{\partial \mu^2}\right] = \frac{N}{b^2}(1) = \frac{N}{b^2} \tag{6}$$

Using (5),

$$\begin{aligned}\frac{\partial^2 L}{\partial b \partial \mu} &= Nsgn(\mu-m)\left[-\frac{1}{b^2} - \left(e^{\frac{-|\mu-m|}{b}}\left(-\frac{1}{b^2}\right) + \frac{1}{b}e^{\frac{-|\mu-m|}{b}}\frac{|\mu-m|}{b^2}\right)\right] \\ &= -\frac{N}{b^2}sgn(\mu-m)(1-e^{-\frac{|\mu-m|}{b}}) - \frac{N}{b}.\frac{(\mu-m)}{b^2}.e^{-\frac{|\mu-m|}{b}}\end{aligned}$$

$$\text{Therefore,} \quad \mathrm{E}\left[\frac{\partial^2 L}{\partial b \partial \mu}\right] = -\frac{N}{b^2}(\mathrm{E}_1-\mathrm{E}_2) - \frac{N}{b^3}\mathrm{E}_3, \qquad \text{where}$$

$$\mathrm{E}_1 = \mathrm{E}[sgn(\mu - m)] = \int\limits_{m-\frac{\delta}{2}}^{m+\frac{\delta}{2}} sgn(\mu - m).\frac{1}{\delta}.d\mu = \frac{1}{\delta}\int\limits_{m-\frac{\delta}{2}}^{m+\frac{\delta}{2}} \frac{\mu - m}{|\mu - m|}d\mu$$

$$= \frac{1}{\delta}\int\limits_{-\frac{\delta}{2}}^{\frac{\delta}{2}} \frac{t}{|t|}dt = 0 \qquad \text{(as the integrand is an odd function)}$$

$$\mathrm{E}_2 = \mathrm{E}[sgn(\mu - m)e^{-\frac{|\mu-m|}{b}}] = \frac{1}{\delta}\int\limits_{m-\frac{\delta}{2}}^{m+\frac{\delta}{2}} \frac{\mu - m}{|\mu - m|}e^{-\frac{|\mu-m|}{b}}d\mu$$

$$= \frac{b}{\delta}\int\limits_{-\frac{\delta}{2}}^{\frac{\delta}{2}} \frac{t}{|t|}e^{-|t|}dt = 0 \qquad \text{(as the integrand is an odd function)}$$

$$\mathrm{E}_3 = \mathrm{E}[(\mu - m)e^{-\frac{|\mu-m|}{b}}] = \frac{1}{\delta}\int\limits_{m-\frac{\delta}{2}}^{m+\frac{\delta}{2}} (\mu - m)e^{-\frac{|\mu-m|}{b}}d\mu$$

$$= \frac{b^2}{\delta}\int\limits_{-\frac{\delta}{2}}^{\frac{\delta}{2}} te^{-|t|}dt = 0 \qquad \text{(as the integrand is an odd function)}$$

$$\text{Therefore,} \quad \mathrm{E}\left[\frac{\partial^2 L}{\partial b \partial \mu}\right] = 0 \tag{7}$$

Using (4), (6), (7),

$$\mathrm{F}(\mu, b) = \begin{pmatrix} \frac{N}{b^2} & 0 \\ 0 & \frac{N}{b^2} \end{pmatrix}$$

$$\text{Therefore,} \quad det(\mathrm{F}(\mu, b)) = \frac{N^2}{b^4} \tag{8}$$

### Priors on the parameters

A prior probability on $\mu$ and $b$ is assumed in accordance with the prior assumed in the case of Normal. The ranges from which $\mu$ and $\log b$ are drawn are prespecified as $\mathrm{R}_\mu$ and $\mathrm{R}_b$ respectively (Wallace, 2005).

$$\therefore h(\bar{\theta}) = h(\mu, b) = h(\mu)h(b)$$
$$= \frac{1}{\mathrm{R}_\mu}.\frac{1}{b\mathrm{R}_b} \tag{9}$$

Using (1), (8), (9),

$$I(\mu,b) = (\log\kappa_2 + \log(\mathrm{R}_\mu \mathrm{R}_\sigma) + \log N - \log b) + \left(N\log\left(\frac{2}{\epsilon}\right) + N\log b + \frac{1}{b}\sum_{n=1}^{N}|x_n-\mu| + 1\right)$$

To obtain the MML estimates $\hat{\mu}_{\mathrm{MML}}$ and $\hat{b}_{\mathrm{MML}}$ which results in minimum $I$, $\frac{\partial I}{\partial \mu} = 0$ and $\frac{\partial I}{\partial b} = 0$. The MML estimates are therefore, given by

$$\begin{aligned}\hat{\mu}_{\mathrm{MML}} &= \mathrm{median}\{x_n\}\\ \hat{b}_{\mathrm{MML}} &= \frac{1}{N-1}\sum_{n=1}^{N}|x_n - \hat{\mu}_{\mathrm{MML}}|\end{aligned} \tag{10}$$

The corresponding minimized message length is given as

$$\begin{aligned}\therefore I_{min} &= I(\hat{\mu}_{\mathrm{MML}}, \hat{b}_{\mathrm{MML}})\\ &= 1 + \log\kappa_2 + \log(\mathrm{R}_\mu \mathrm{R}_\sigma) + \log N + N\log\left(\frac{2}{\epsilon}\right)\\ &\quad + (N-1)\log\left(\frac{\sum_{n=1}^{N}|x_n-\hat{\mu}_{\mathrm{MML}}|}{N-1}\right) + (N-1)\end{aligned} \tag{11}$$

## 4. MML Inference for a Normal distribution

A Normal distribution whose density function (pdf) is given by (12)

$$\mathrm{pdf}(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{12}$$

is characterized by the mean $\mu$ and the standard deviation $\sigma$. The MML estimates for a Normal distribution is presented in Wallace (2005); Wallace and Freeman (1987) and are:

$$\begin{aligned}\hat{\mu}_{\mathrm{MML}} &= \frac{1}{N}\sum_{n=1}^{N}x_n\\ \hat{\sigma}^2_{\mathrm{MML}} &= \frac{\sum_{n=1}^{N}(x_n-\hat{\mu}_{\mathrm{MML}})^2}{N-1}\end{aligned}$$

The corresponding minimized message length is given as

$$\begin{aligned}\therefore I_{min} &= I(\hat{\mu}_{\mathrm{MML}}, \hat{\sigma}_{\mathrm{MML}})\\ &= 1 + \log\kappa_2 + \log(\mathrm{R}_\mu \mathrm{R}_\sigma) + \frac{1}{2}\log(2N^2)\\ &\quad + \frac{N}{2}\log\left(\frac{2\pi}{\epsilon^2}\right) + \frac{N-1}{2}\log\left(\frac{\sum_{n=1}^{N}(x_n-\hat{\mu}_{\mathrm{MML}})^2}{N-1}\right) + \frac{N-1}{2}\end{aligned} \tag{13}$$

As established in Wallace and Freeman (1987), the optimal precision to which the parameters need to be stated is given by: $AOPV \propto \frac{1}{\sqrt{det(F(\bar{\theta}))}}$. The Normal Fisher is $\frac{2N^2}{\sigma^4}$ (Wallace,

2005) and the Laplace Fisher as derived above is $\frac{N^2}{b^4}$. There is a marked difference in the optimal AOPVs computed in the two cases. For the same value of spread ($\sigma = b$), the uncertainty in the parameter values for a Laplace is $\sqrt{2}$ times that of Normal, which means that the parameters for a Laplace need to be stated less precisely when compared with the Normal.

## 5. Experiments

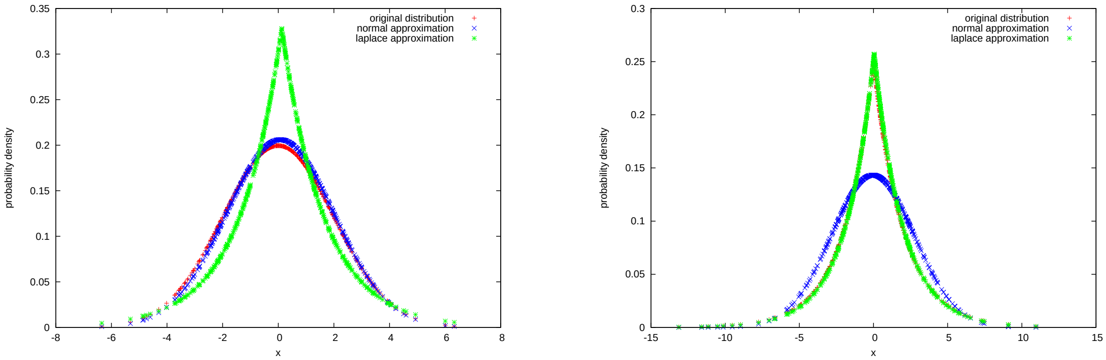
We demonstrate the use of Laplace estimates in two scenarios.

### 5.1. Data generation and modelling

In the first case, data is generated randomly from a distribution (Normal & Laplace) separately. This data is then modelled using the two distributions. It is observed that if the true distribution is a Laplace/Normal, then the compression in message length is better when it is modelled using a Laplace/Normal distribution. This is indeed expected and is done as a validation check to ensure that the derived MML formulation for the Laplace is consistent with the observation. (11) and (13) are used to determine the code length when the data is modelled using the Laplace and Normal distributions respectively.

As an example, 500 random samples are generated from each of the distributions. The mean of the true distribution is taken to be 0 and the spread (standard deviation $\sigma$ for a Normal and scale parameter $b$ for a Laplace) is chosen to be 2. Figure 1 shows the original distributions and the corresponding Normal and Laplace approximations. In 1($a$), the true distribution is normal (red curve). The Normal approximation (blue curve) overlaps almost entirely with the red curve which is an indication of a good fit. The Laplace approximation (green curve) significantly deviates from the original distribution. The same argument holds for 1($b$) where the underlying distribution of the data is Laplace, and hence, in this case, the Laplace seems to be a good fit.

Table 1 provides a comparison of the estimates of the two distributions. The message length (msglen) is computed in bits. It can be seen when the true distribution is Laplace, the message length corresponding to the Laplace estimate (6690.91 bits) is smaller compared to that of the Normal estimate (6755.68 bits).



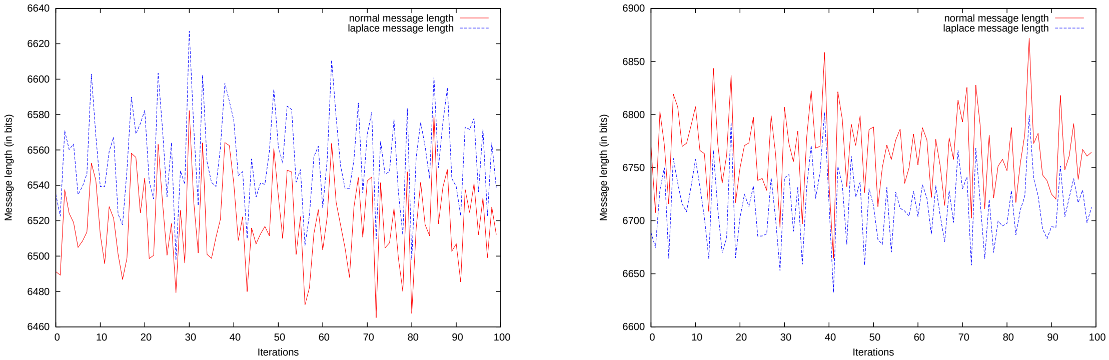
($a$) Original distribution: Normal

($b$) Original distribution: Laplace

Figure 1: Approximation of data using Normal & Laplace distributions

Table 1: Comparison of the estimates

| True distribution | True mean | True spread | Normal estimates | | | Laplace estimates | | |
|---|---|---|---|---|---|---|---|---|
| | | | mean | spread | msglen | mean | spread | msglen |
| Normal | 0 | 2 | 0.0722611 | 1.93638 | 6493.89 | 0.127191 | 1.52389 | 6518 |
| Laplace | 0 | 2 | -0.0455104 | 2.78563 | 6755.68 | 0.0471194 | 1.9376 | 6690.91 |



$(a)$ Original distribution: Normal

$(b)$ Original distribution: Laplace

Figure 2: Comparison of message lengths over many iterations

Figure 2 compares the message lengths over 100 iterations. In 2$(a)$, the original distribution is Normal and it is observed that over all the iterations, the message length for the Normal (red) is consistently less than that of the Laplace (blue). In 2$(b)$, the original distribution is Laplace and it is observed that over all the iterations, the message length for the Laplace (blue) is consistently less than that of the Normal (red).

### 5.2. Superposition of vector sets

Given any two vector sets $U = \{u_1, u_2, \ldots, u_m\}$ and $V = \{v_1, v_2, \ldots, v_m\}$ where each $u_i$ and $v_i$, $(i \in \{1, 2, \ldots, m\})$ is a vector in 3D space, the superpositioning problem refers to finding a suitable transformation on $U$ to align it with $V$ such that the deviations of each vector in $V$ with its counterpart in $U$ is minimum. Let the transformation be effected by a translation vector $t$ and a rotation matrix $R$. Let it result in an altered vector set $U' = \{u'_1, u'_2, \ldots, u'_m\}$, where $u'_i = R(u_i - t)$. The objective function corresponding to the sum of squares ($L^2$ norm) of all deviations:

$$\sum_{i=1}^{m} \|v_i - u'_i\|^2 = \sum_{i=1}^{m} \|v_i - R(u_i - t)\|^2 \tag{14}$$

and the objective function corresponding to the sum of absolute deviations ($L^1$ norm)

$$\sum_{i=1}^{m} \|v_i - u'_i\| = \sum_{i=1}^{m} \|v_i - R(u_i - t)\| \tag{15}$$

(where $\|.\|$ denotes the vector norm) needs to be minimized. The superposition problem can be formulated in the MML framework as finding the orientation of two proteins such that the deviations of each corresponding point are encoded in an effective manner. Superposition based on minimizing total least squares corresponds to stating the deviations using a Normal distribution. Superposition based on minimizing the absolute value of the deviations correspond to transmitting the deviations using a Laplace distribution. Keynes (1911) showed that the Laplace distribution minimized the absolute deviation from the median (which is also corroborated by the MML estimate of Laplace parameters (10)) and is, hence, pertinent for our current discussion.

Minimization of (14) yields $t = \left(\frac{\sum_{i=1}^{m} u_i}{m} - \frac{R\sum_{i=1}^{m} v_i}{m}\right)$. Substituting this value of $t$ in (14) results in the modified objective function:

$$\sum_{i=1}^{m} \left|\left| \left(v_i - \frac{\sum_{i=1}^{m} v_i}{m}\right) - R\left(u_i - \frac{\sum_{i=1}^{m} u_i}{m}\right) \right|\right|^2 \tag{16}$$

Kearsley (1989) provides a solution to (14) by resolving the transformation into translation and rotation. The centres of mass of the two vector sets are translated to the origin (16) and the problem then reduces to finding the rotation matrix which minimizes the total least squares. This involves respresenting the rotation matrix using a quaternion and then solving the resultant eigen value decomposition problem. As such, Kearsley (1989) offers an analytical way to solve the *least squares* superposition problem.

Minimizing (15), however, does not yield a closed form solution. Differentiating (15) with respect to $t$ and setting it to 0 yields

$$\sum_{i=1}^{m} \frac{Rv_i - (u_i - t)}{\|Rv_i - (u_i - t)\|} = 0 \tag{17}$$

In this case, $R$ and $t$ cannot be separated and hence, cannot be analytically solved for. As such, one needs to adopt approximate methods to find the best superposition corresponding to the $L^1$ norm. The one used in this paper is a version that uses Monte Carlo simulation. It is described below:

1. Apply Kearsley's transformation and find the superposition that corresponds to least sum of squares of the deviations. In this state, the value of the objective function (15) is computed.

2. From this orientation, the protein is perturbed randomly. If the new orientation results in a better value of the L1 norm (15), the new orientation is accepted. If however, the value of the objective function is less than the previous value, the new orientation is accepted with a minute probability.

3. This is repeated for many iterations. The process is expected to converge to the global minimum. As such, this would correspond to the optimal superposition which minimizes the sum of absolute deviations.

The two vector sets are first superposed using the Kearsley's method and the message length ($I_N$) computed through MML inference using a Normal distribution. Monte Carlo simulation is performed (as discussed above) from this stage and the final orientation is obtained. At this point, the message length ($I_L$) is computed through MML inference using a Laplace distribution. Two cases arise:-

- If $I_L < I_N$, then there exists a superposition which is optimal than the one resulting from minimizing the sum of squared deviations (14).
- If $I_N < I_L$, then the superposition obtained by minimizing (14) is better. Since the minimal L1 superposition is obtained using a Monte Carlo simulation (which is terminated after a certain number of iterations), it could also be possible that the optimal solution wasn't found.

The point of this exercise is to show that not all vector sets have their optimal superpositions dictated by minimizing sum of squared deviations. It also drives home the use of MML estimators in determining the kind of superposition to be considered.

### Results

We apply the problem of superposition to protein structures. The vector sets would correspond to the three dimensional coordinates of the $\alpha$-carbon atoms of amino acid residues constituting the proteins' backbone. We use SUPER (Collier et al., 2012) (which is an implementation of Kearsley's orthogonal superposition) to get all protein segments from the Protein Data Bank which fit to a Root Mean Squared Deviation (RMSD) of 5 Angstroms (Å). The protein segment corresponding to PDB ID 2IC7, chain A and residues 132-162 was randomly considered and there were ∼23000 segments which fit within a RMSD of 5 Å. The message length corresponding to this optimal $L^2$ superposition is calculated using (13). This orientation will also have a certain value for the sum of absolute deviations. The message length to encode these absolute differences is computed using (11). For these 23000 segments across several proteins, we determine the optimal $L^1$ superposition using Monte Carlo simulation. The superposition resulting after 1000 iterations is regarded as the optimal $L^1$ superposition. The message length to encode the absolute differences is computed. There were about ∼1700 instances where the optimal $L^1$ superposition is better than the $L^2$ equivalent. A few results are discussed in Table 2.

The 'moving structure' is the protein that is perturbed from its optimal $L^2$ superposition. Each segment is uniquely identified by its chain ID and residue span. These are obtained using SUPER. RMSD is the error of fit (in Å) of the $L^2$ superposition. The initial/final $L^1$ deviations correspond to the average of the absolute deviations (in Å) in both these orientations; msglen($L^2$) is the message length using a Normal distribution to encode the deviations in the optimal $L^2$ superposition; msglen (initial $L^1$) corresponds to the message length of encoding the absolute deviations before perturbations and msglen (final $L^1$) is the message length to encode the deviations after the Monte Carlo simulation. As expected, the final $L^1$ deviation is less than the initial one. It is observed this happens for most of

Table 2: Comparison of the minimum message lengths

| Moving structure | RMSD | initial $L^1$ deviation | Final $L^1$ deviation | msglen ($L^2$) | msglen (initial $L^1$) | msglen (final $L^1$) |
|---|---|---|---|---|---|---|
| 3IG7 [A:139-169] | 1.834 | 1.910 | 1.814 | 1134.82 | 1102.03 | 1096.32 |
| 4G87 [A:291-321] | 2.112 | 2.555 | 2.455 | 1153.54 | 1165.38 | 1145.22 |
| 3R8Y [A:105-135] | 0.479 | 0.673 | 0.666 | 956.711 | 1063.82 | 1059.25 |

the cases which suggest the presence of the $L^1$ optimal value somewhere close to the initial position.

For the discussion below, in Table 5.2, 4($a$), 4($b$), the red curve corresponds to the fixed protein; the blue curve is the optimal $L^2$ superposition, and the green curve corresponds to the optimal $L^1$ superposition.

The first row in Table 2 corresponds to Table 5.2. Its msglen(initial $L^1$) ¡ msglen($L^2$). This suggests that $L^1$ superposition supercedes the $L^2$ superposition, and it only gets better as the structure is perturbed as is evidenced by the msglen(final $L^1$), the message length after the Monte Carlo simulation. Here, it can be seen that the red curve (the fixed protein) is closer to the green curve ($L^1$ superposition) than to the blue curve ($L^2$ superposition) in the majority of the protein structure. The second row in Table 2 corresponds to the case where the final $L^1$ superposition (1145.22 bits) is optimal than the $L^2$ superposition (1153.54 bits). The initial $L^1$ superposition (1165.38 bits) is not the optimal one and hence, has to go through a series of iterations to reach the local optimum. In 4($a$), the green curve (final $L^1$) is better than $L^2$ superposition. The third row in Table 2 demonstrates the case where the $L^2$ superposition (956.711 bits) is optimal compared to the $L^1$ superposition (1059.25 bits). On careful inspection, one can see the red curve (in 4($b$)) is closer to the blue curve corresponding to the $L^2$ superposition than to the green curve ($L^1$ superposition).

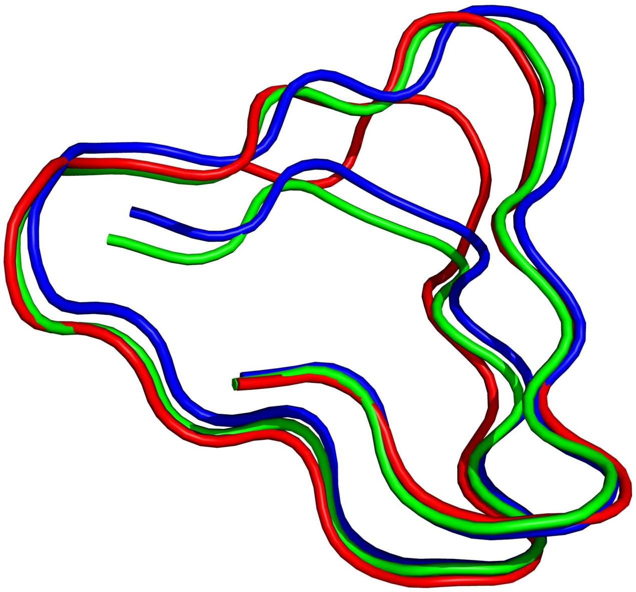
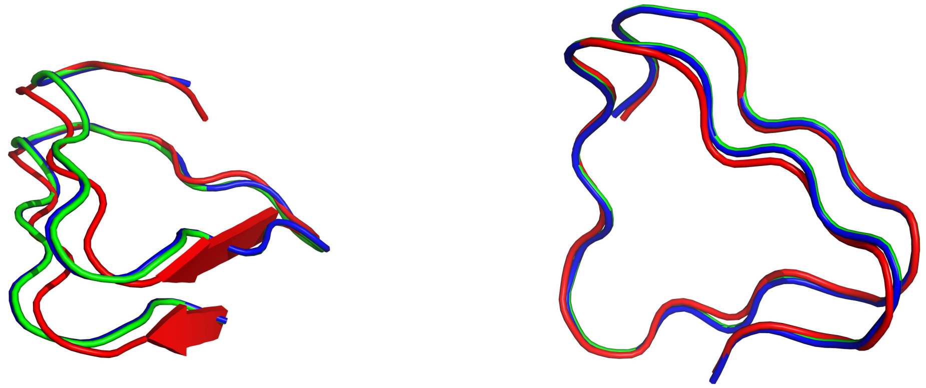


Figure 3: Initial & final $L^1$ superposition better than $L^2$ superposition



(*a*) Final $L^1$ superposition better than $L^2$ superposition

(*b*) $L^2$ superposition better than $L^1$ superposition

Figure 4: Comparing the protein superpositions with respect to $L^1$ and $L^2$ norm

## 6. Conclusion

We have derived the MML estimators for the Laplace distribution and applied it in the context of encoding the superposition of vector sets. This is used to distinguish the quality of superposition for any two vector sets. In general, if the objective function is formulated as the sum of absolute differences, we have a framework using MML to encode these values using a Laplace distribution. The quality of the overall fit can be evaluated using the MML inference technique and can be compared with other models. For the specific problem of superposition of two vector sets, the choice of $L^1$ or $L^2$ superposition is made by comparing the message lengths obtained by encoding deviations using $L^1$ and $L^2$ norm.

## Acknowledgments

TODO

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