A Bayesian Approach for the Determination of the Charge Density from Elastic Electron Scattering Data

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Abstract. The problem of the determination of the charge density from limited information about the charge form factor is an ill-posed inverse problem. A Bayesian probabilistic approach to this problem which permits to take into account both errors and prior information about the solution is presented. We will show that many classical methods can be considered as special cases of the proposed approach. We address also the problem of the basis function choice for the discretization and the uncertainty of the solution. Some numerical results for an analytical model are presented to show the performance of the proposed method.

1. Introduction
Elastic electron scattering provides a mean of determining the charge density of a nucleus, \( \rho(r) \), from the experimentally determined charge form factor, \( F(q) \). The connection between the charge density and the cross section is well understood and in plane wave Born approximation \( F(q) \) is just the Fourier transform of \( \rho(r) \) which for the case of even-even nuclei, which we shall consider, is simply given by

\[
F(q) = 4\pi \int_0^\infty r^2 J_0(qr) \rho(r) \, dr
\]

where \( J_0 \) is the spherical Bessel function of zero order and \( q \) is the absolute value of the three momentum transfer. Given that the experimental measurements are performed over a limited range at a finite number of values of the momentum transfer \( q \), a unique determination of \( \rho(r) \) is not possible since the resulting inverse problem is ill posed.

One of the generally accepted procedures for determining \( \rho(r) \) is to expand it in a basis and then determine the expansion coefficients from a least squares (LS) fit to the experimentally measured values of \( F(q) \) \cite{1,2,3,14,18}. The following questions then arise: how to choose a basis and how to determine the order of the expansion? Another problem with the LS methods is that increasing the number of terms in the expansion generally leads to non physical oscillations in the charge density in spite of the fact that the charge form factor is well reproduced at the experimentally determined values of \( q \) \cite{4,13}. Finally, due to the fact that the
problem is inherently ill posed, a small error in the data (experimental errors
or measurement noise) will produce large variations in the solution which is not
acceptable in practical situations.

What we are going to do is to show how a Bayesian approach can be helpful to
give both correct and reasonable answers to the aforementioned questions and to
propose new methods which are more stable with respect to the errors and finally
to give procedures to put the correct error bars on the proposed solutions.

2. Fundamentals of the Bayesian approach
Let us start by discretizing the problem in the usual manner by expanding \( \rho(r) \) in
a basis \( \phi_n(r) \):

\[
\rho(r) = \begin{cases} 
\sum_{n=1}^{N} a_n \phi_n(r) & r \leq R_c \\
0 & r > R_c 
\end{cases}
\]  

(2)

and substituting it in (1) yields

\[
F(q) = 4\pi \int_0^{R_c} r^2 J_0(qr) \sum_{n=1}^{N} a_n \phi_n(r) \, dr \\
= 4\pi \sum_{n=1}^{N} a_n \int_0^{R_c} r^2 J_0(qr) \phi_n(r) \, dr 
\]  

(3)

Now, defining

\[
A_{m,n} = 4\pi \int_0^{R_c} r^2 J_0(q_m r) \phi_n(r) \, dr
\]  

(4)

we obtain

\[
F_c = A a + \epsilon
\]  

(5)

where \( a \) is a vector containing the coefficients \( \{a_n, n = 1, \cdots, N\} \), \( F_c \) is a vector containing the form factor data \( \{F_c(q_m), m = 1, \cdots, M\} \) and \( A \) an \((M \times N)\) matrix containing the coefficients \( A_{m,n} \) given by (4). Note also that when the vector \( a \) is
determined, we can calculate \( \rho = \{\rho(r_k), k = 1, \cdots, K\} \) by

\[
\rho = \Phi a
\]  

(6)

where \( \Phi \) is a \( K \times N \) matrix with the elements \( \Phi_{kn} = \phi_n(r_k) \).

The vector \( \epsilon \) is added to take account of the errors in both measurement noise
and due to discretization. We assume that the components \( \{\epsilon_m, m = 1, \cdots, M\} \)
are additive, zero mean (no systematic error), mutually independent (no correlation)
and independent of \( a \), and they can only be characterized by their common variance \( \sigma^2_\epsilon \). This hypothesis is reasonable unless we know more about its characteristics.

Note that we have not yet discussed the choice of the basis functions \( \phi_n \) and
the determination of the expansion order, \( N \). We will come back to these questions
later. Let us now see how the Bayesian estimation approach works.
The main idea behind the Bayesian probabilistic approach is to represent the uncertainty or any lack of knowledge or any diffuse prior knowledge about a quantity by a probability law. For example, the knowledge (or the hypothesis) that \( \{\epsilon_m, m = 1, \cdots, M\} \) are zero mean, mutually independent and that they are only characterized by their common variance \( \sigma^2 \) can be described by choosing a Gaussian probability distribution for them. One may also use the Maximum Entropy Principle to enforce this choice. This means that we can write

\[
p(\epsilon_m) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp \left\{ -\frac{1}{2\sigma^2} \epsilon_m^2 \right\}
\]

or \( p(\epsilon_m) = \mathcal{N}(0, \sigma^2) \) and

\[
p(\epsilon) = \prod_{m=1}^{M} p(\epsilon_m) = \frac{1}{(2\pi\sigma^2)^{M/2}} \exp \left\{ -\frac{1}{2\sigma^2} \|\epsilon\|^2 \right\}
\]

or simply \( p(\epsilon) = \mathcal{N}(0, \sigma^2 I) \) where \( I \) is the \((M \times M)\) unitary matrix and \( \sigma^2 \) is the common variance of \( \epsilon_m \) for all \( m \). Now, using this model \( (5) \), we can define the conditional probability law

\[
p(F_c|a) = \frac{1}{(2\pi\sigma^2)^{M/2}} \exp \left\{ -\frac{1}{2\sigma^2} \|F_c - Aa\|^2 \right\}
\]

or \( p(F_c|a) = \mathcal{N}(Aa, \sigma^2 I) \). It is usual to call \( p(F_c|a) \) or its logarithm, considered as a function of \( a \), the Likelihood.

One can stop here and define the solution of the problem \( (5) \) as the vector \( \hat{a} \), which maximizes the likelihood (ML):

\[
\hat{a} = \arg \max_a \{ p(F_c|a) \}
\]

or equivalently

\[
\hat{a} = \arg \min_a \{ -\ln p(F_c|a) \}
\]

which, in the case of a Gaussian distribution \( (8) \) becomes

\[
\hat{a} = \arg \min_a \{ \|F_c - Aa\|^2 \}
\]

and we find here the LS solutions given by:

\[
(A^t A) \hat{a} = A^t F_c
\]

The main problem with these solutions is that, very often, the matrix \( A^t A \) is either singular or at least ill-conditioned, so that the solutions are very sensitive to the errors in the data or even on the round-off errors during the numerical calculation.

The Bayesian approach can do better. In fact, before looking at the data, we may have some prior knowledge about \( a \). For example, we know that \( a \in \mathbb{R}^N \) and
that we might prefer those vectors which have a minimal norm \( \| \mathbf{a} \| \). To translate this prior knowledge and this preference, we may assign a Gaussian probability distribution to the vector \( \mathbf{a} \):

\[
p(\mathbf{a}) = \frac{1}{(2\pi \sigma_a^2)^{M/2}} \exp \left\{ -\frac{1}{2\sigma_a^2} \| \mathbf{a} \|^2 \right\}
\]

where \( \sigma_a^2 \) gives an idea about the scale of the norm of the vector \( \mathbf{a} \). Now, using the Bayes rule we can calculate the posterior probability law

\[
p(\mathbf{a}|F_c) = \frac{p(F_c|\mathbf{a})p(\mathbf{a})}{p(F_c)}
\]

where the denominator

\[
p(F_c) = \int \int p(F_c|\mathbf{a})p(\mathbf{a}) \, d\mathbf{a}
\]

is the normalization constant (called sometimes the Evidence).

This posterior law contains all the information we may wish about the solution. For example, we may want to know what is the probability that \( \underline{\mathbf{a}} < \mathbf{a} \leq \overline{\mathbf{a}} \). This can be calculated by

\[
P(\underline{\mathbf{a}} < \mathbf{a} \leq \overline{\mathbf{a}}) = \int_{\underline{\mathbf{a}}}^{\overline{\mathbf{a}}} p(\mathbf{a}|F_c) \, d\mathbf{a}
\]

Or, we may be interested only in one of these parameters \( a_n \) and want to know what is the probability that \( \underline{a}_n < a_n \leq \overline{a}_n \). This can be calculated by

\[
P(\underline{a}_n < a_n \leq \overline{a}_n) = \int_{\underline{a}_n}^{\overline{a}_n} p(a_n|F_c) \, da_n
\]

where the marginal posterior law \( p(a_n|F_c) \) can be calculated by

\[
p(a_n|F_c) = \int \cdots \int p(\mathbf{a}|F_c) \, da_1 \cdots da_{n-1} \, da_{n+1} \cdots da_N.
\]

We can also simply define as the solution the vector \( \hat{\mathbf{a}} \) which corresponds to the mean value of the posterior law—called Posterior mean (PM) estimator:

\[
\hat{\mathbf{a}} = \int \mathbf{a} \, p(\mathbf{a}|F_c) \, d\mathbf{a}
\]

or the vector \( \hat{\mathbf{a}} \) which maximizes this posterior distribution—called Maximum a posteriori (MAP) estimator:

\[
\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} \{ p(\mathbf{a}|F_c) \} = \arg \min_{\mathbf{a}} \{ -\ln p(\mathbf{a}|F_c) \}
\]
or even the vector $\hat{a}$ whose components $\hat{a}_n$ correspond to the maximizer of the marginal posterior law (19) —called Marginal MAP estimator:

$$\hat{a}_n = \arg \max_{a_n} \{ p(a_n|F_c) \} = \arg \min_{a_n} \{- \ln p(a_n|F_c) \}.$$  

(22)

In the following we consider only the MAP estimator (21). Using the probability distributions (9) and (14) in (15), the MAP solution is given by:

$$\hat{a} = \arg \min_{a} \{ \| F_c - a \|^2 + \lambda \| a \|^2 \}.$$  

(23)

where $\lambda = (\sigma_x/\sigma_a)^2$ and we find the minimum norm least squares (MNLS) solution which is given explicitly by

$$\hat{a} = (A^tA + \lambda I)^{-1} A^tF_c.$$  

(24)

Comparing (13) and (24) we see that, for a given $N$, the matrix $(A^tA + \lambda I)$ is always better conditioned than the matrix $(A^tA)$ and so the solution (24) always is more stable than the solution (13).

We may also want some information about the uncertainty of this solution. For this we can use the posterior law $p(a|F_c)$. For example, using the likelihood (9) and the prior law (14), it is easy to show that the posterior law is Gaussian, i.e. $p(a|F_c) = N(\hat{a}, \hat{P})$ with $\hat{a}$ given by (24) and $\hat{P} = (A^tA + \lambda I)^{-1}$. We can then use the diagonal elements of the posterior covariance matrix $\hat{P}$ to calculate the posterior variances of the estimates, i.e. $\text{Var}(a_n) = \hat{P}_{nn}$ and so put the error bars on the solution. When the posterior law is not Gaussian, we can always calculate

$$E(a_n) = \int a_n p(a_n|F_c) da_n$$  

(25)

and

$$\text{Var}(a_n) = \int (a_n - E(a_n))^2 p(a_n|F_c) da_n$$  

(26)

but in general we may not have explicit expressions for these integrals. We can however do numerical calculation either by approximating the posterior law by a Gaussian law or by a stochastic integral calculation.

One question still remains: how to determine $\lambda$ and $N$? Three approaches are possible:

1. Assign them experimentally from the data using some knowledge on the physics of the problem. For example, the Parseval-type relation between $\rho(r)$ and $F_c(q)$:

$$\int 4\pi r^2 \rho^2(r) dr = \frac{1}{(2\pi)^3} \int 4\pi q^2 F_c(q) dq$$  

(27)

can be used to estimate $\sigma_a^2$ by:

$$\sigma_a^2 = \frac{1}{N} \sum_{n=1}^{N} a_n^2 = \frac{1}{M} \sum_{m=1}^{M} F_{cm}^2$$  

(28)

and having an estimate of the noise variance $\sigma_e^2$ we can determine $\lambda$.  

5
2. Consider $\lambda$ and $N$ as two extra parameters (hyper parameters) to estimate jointly with the unknown parameter $a$. We can then assign a prior law for them. For example Jeffrey’s priors $p(\lambda) = \frac{1}{\lambda}$ for $\lambda$ and a uniform $p(N) = 1/N_{\text{max}}$ for $N$. (Other choices are possible, for example a Gamma prior $\lambda$ which eliminates $\lambda = 0$ and $\lambda = \infty$ and a binomial prior for $N$ which eliminates $N = 0$ and $N = N_{\text{max}}$.)

Finally, we can estimate them jointly with $a$ by

$$\hat{a}, \hat{\lambda}, \hat{N} = \arg \max_{(\hat{a}, \hat{\lambda}, \hat{N})} \{ p(\hat{a}, \hat{\lambda}, \hat{N}|F_c) \}$$

(29)

where

$$p(\hat{a}, \hat{\lambda}, \hat{N}|F_c) \propto p(F_c|\hat{a}, \hat{\lambda}, \hat{N}) p(\hat{a}|\hat{\lambda}, \hat{N}) p(\hat{\lambda}) p(\hat{N}).$$

(30)

We must however be careful to verify that this joint criterion has at least a local optimum.

3. Consider $\lambda$ and $N$ as two extra parameters as in the precedent case but not on the same level. This means that we can try to estimate them first by

$$(\hat{\lambda}, \hat{N}) = \arg \max_{(\lambda, N)} \{ p(\lambda, N|F_c) \}$$

(31)

where

$$p(\lambda, N|F_c) = \int \int p(\lambda, N|F_c) d\lambda dN$$

(32)

and then use them in (21). Note, however that finding an analytical expression for $p(\lambda, N|F_c)$ is not always possible and its numerical calculation may be very costly.

4. Consider $\lambda$ and $N$ as two nuisance parameters, integrate them out and estimate $a$ directly by

$$\hat{a} = \arg \max_a \{ p(a|F_c) \} = \arg \max_a \left\{ \sum_{n=1}^{N} \int p(a, \lambda, n|F_c) d\lambda \right\}$$

(33)

(For more details on these methods, their relative characteristics, their practical implementations and their relatives performances see [20, 17, 19, 16]).

Still one question remains: the choice of the basis-functions.

3. Choice of the basis-functions

Two approaches are used to select the basis functions. We call them the operator based parametric approach and the non parametric approach and we will discuss both in detail in the following sections. We propose then a new third approach which tries to eliminate the limitations and to keep the advantages of the previous approaches. We call this third approach physically based parametric.
3.1. Operator based parametric approach

The first approach is to choose special purpose basis functions based on the properties of the operator linking the data to the unknowns. For example in our case, due to the fact that the kernel of the integral operator of the direct problem is a Bessel function, we may also use the Bessel functions as the basis functions for $\rho(r)$$

$$
\rho(r) = \begin{cases} 
\sum_{n=1}^{N} a_n j_0(q_n r) & r \leq R_c \\
0 & r > R_c 
\end{cases}
$$

(34)

This will permit us, using the orthogonality relation

$$
\int_0^{R_c} r^2 J_l(q_n r) J_l(q_m r) \, dr = \frac{R_c^3}{2} J_{l+1}^2(q_n R_c) \delta_{n,m},
$$

(35)

to find an explicit expression for the charge form factor as a function of the coefficients $a_n$:

$$
F(q) = \frac{4\pi R_c^2}{q} \sum_{n=1}^{N} a_n \frac{(-1)^n}{(q R_c)^2 - (n\pi)^2} \sin(q R).
$$

(36)

With this choice, note also that, if the form factor $F(q)$ was known exactly at $q_n = \frac{n\pi}{R_c}$ then the coefficients $a_n$ could be calculated analytically by

$$
a_n = \frac{F(q_n)}{2\pi R_c^2 [J_1(q_n R)]^2}.
$$

(37)

In general, however, the cross section is measured at momentum transfers different from $q_n = \frac{n\pi}{R_c}$.

Now, assume that we are given $M$ measurements at arbitrary momentum transfers $q = \{q_1, q_2, \ldots, q_M\}$ and we wish to determine the $N$ expansion coefficients $\mathbf{a} = \{a_1, a_2, \ldots, a_N\}$. In this case Eq. (36) leads to

$$
F_c = \mathbf{Aa} + \epsilon
$$

(38)

as in (3).

The main advantage of this approach is the fact that $\mathbf{a}$ is a small dimension vector and so is the matrix $\mathbf{A}$ and we have an explicit analytical expression for calculating its elements.

But at least one main disadvantage to such a choice is that our prior knowledge on $\mathbf{a}$ may be limited. For example, if we know that $\rho(r)$ is a positive function we cannot easily incorporate this information in the parameters, $\mathbf{a}$.

3.2. Non parametric approach

The second approach is to choose the basis-functions as general as possible and independently of the direct problem operator, for example, either:

$$
\phi_n(r) = \delta(r - n\Delta)
$$

(39)
or
\[
\phi_n(r) = \begin{cases} 
1 & \text{if } (n-1)\Delta < r \leq n\Delta \\
0 & \text{elsewhere}
\end{cases}
\]  
(40)

with \(\Delta\) chosen appropriately small (maximum needed resolution) to be certain we are able to approximate any function \(\rho(r)\) as precisely as desired. But, this means that \(N\) will probably be large. This is a disadvantage, but this can be compensated, as we will see further, by the fact that the coefficients \(a_n\) now have a direct physical meaning: the samples of \(\rho(r)\) in the first case and the mean values of \(\rho(r)\) in the intervals \((n-1)\Delta < r \leq n\Delta\) in the second case. This means, for example, that the prior knowledge such as the smoothness or the positivity of the function \(\rho(r)\) can be transmitted to the coefficients \(a_n\) easily.

Let us choose (39) and go further into the details. Replacing (2) with the basis-functions (39) in (1) we obtain:
\[
F(q) = \sum_{n=1}^{N} a_n \int_{0}^{R_c} dr \, 4\pi r^2 J_0(qr) \delta(r - n\Delta) = 4\pi \sum_{n=1}^{N} a_n \Delta (n\Delta)^2 J_0(n\Delta q) 
\]  
(41)

Denoting by
\[
A_{m,n} = 4\pi \Delta (n\Delta)^2 J_0(n\Delta q_m) 
\]  
(42)

we obtain \(F_c = Aa + \epsilon\) as in (38). If we use (40) in place of (39), the only change will be in the expression of the Matrix elements \(A_{m,n}\) which become
\[
A_{m,n} = 4\pi \int_{(n-1)\Delta}^{n\Delta} r^2 J_0(qm r) dr. 
\]  
(43)

To make a distinction between this approach and the preceding one, let us denote \(a\) by \(\rho\) and \(A\) by \(B\):
\[
F_c = B\rho + \epsilon 
\]  
(44)

Let us now compare (44) and (38): \(a\) in (38) is a vector of small dimension while \(\rho\) in (44) is a vector of much larger dimension.

Here we can also define either the LS solution:
\[
\hat{\rho} = \arg \min_{\rho} \left\{ \|F_c - B\rho\|^2 \right\} = (B^tB)^{-1}B^tF_c 
\]  
(45)
or the MNLS solution:
\[
\hat{\rho} = \arg \min_{\rho} \left\{ \|F_c - B\rho\|^2 + \lambda \|\rho\|^2 \right\} = (B^tB + \lambda I)^{-1}B^tF_c 
\]  
(46)

but neither of these solutions may be satisfactory.

In (44) it is possible to incorporate the smoothness and the positivity of the function \(\rho(r)\) into a more appropriate prior distribution for the components \(\rho_n\).

For example, to enforce the smoothness of \(\rho(r)\) we can assign
\[
p(\rho) = p(\rho_1) \prod_{n=2}^{N} p(\rho_n|\rho_{n-1}) = N(\rho_{n-1}, \sigma_0^2) 
\]  
(47)
with
\[ p(\rho_1) = \mathcal{N}(\rho_0, \sigma_0^2) \propto \exp \left[ -\frac{1}{2\sigma_0^2}(\rho_1 - \rho_0)^2 \right] \] (48)
and
\[ p(\rho_n|\rho) = p(\rho_n|\rho_{n-1}) = \mathcal{N}(\rho_{n-1}, \sigma_0^2) \propto \exp \left[ -\frac{1}{2\sigma_0^2}(\rho_n - \rho_{n-1})^2 \right] \] (49)
which leads to
\[ p(\rho) \propto \exp \left[ -\frac{1}{2\sigma_0^2} \sum_{n=1}^{N} (\rho_n - \rho_{n-1})^2 \right] \] (50)
Using this prior distribution in (15), the MAP estimator becomes
\[ \hat{\rho} = \arg \max_{\rho} \{p(\rho|F_c)\} = \arg \min_{\rho} \{J(\rho)\} \] (51)
with
\[ J(\rho) = \|F_c - B\rho\|^2 + \lambda \sum_{n=1}^{N} (\rho_n - \rho_{n-1})^2 \] (52)
Defining the matrix
\[ D = \begin{pmatrix} 1 & -1 & \cdots & -1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \] (53)
it is easy to show that
\[ J(\rho) = \|F_c - B\rho\|^2 + \lambda \|D\rho\|^2 + \lambda (\rho_1 - \rho_0)^2 \] (54)
Let us temporarily assume that \( \rho_1 = \rho_0 \). We then have an explicit solution for the
minimizer of (54) which is given by:
\[ \hat{\rho} = (B^t B + \lambda D^t D)^{-1} B^t F_c \] (55)
Comparing this solution with the MNLS solution (46) gives us the possibility to see the difference in which the term \( D^t D \) is used in place of \( I \). Indeed, due
to the fact that \( D \) corresponds to a first order derivative, we may designate the
MNLS solution as the zero order regularized solution in contrast to the first order
regularized solution. It is possible to extend this to more general regularized
solutions by an appropriate choice of the matrix \( D \).
Now, let us go back to (54), \( \rho_0 \) is now a new extra hyper-parameter which
may play a great role in the solution of our inverse problem where the data do not
contain information about the DC level of the function \( \rho(r) \).
One way to enforce the positivity of the solution is to choose a prior distribution
such as :
\[ p(\rho) = \sum_{n=1}^{N} p(\rho_n) = \sum_{n=1}^{N} \frac{\beta^\alpha}{\Gamma(\alpha)} \rho_n^{\alpha-1} \exp[-\beta \rho_n] \] (56)
which can also be written as:

\[ p(\rho) \propto \exp \left[ - \sum_{n=1}^{N} (1 - \alpha) \ln \rho_n + \beta \rho_n \right] \]  

and which is called an Entropic prior in [20]. Using this prior law in (15), the MAP estimator becomes

\[ \hat{\rho} = \arg \max_{\rho} \{ p(\rho | F_c) \} = \arg \min_{\rho} \{ J(\rho) \} \]  

with

\[ J(\rho) = \| F_c - B\rho \|^2 + \lambda_1 \sum_{n=1}^{N} \ln \rho_n + \lambda_2 \sum_{n=1}^{N} \rho_n \]  

where \( \lambda_1 \) and \( \lambda_2 \) are related to \( \alpha, \beta \) and \( \sigma^2 \). Other choices are possible [20].

To enforce both positivity and the smoothness we propose here to choose

\[ p(\rho) \propto \exp \left[ - \lambda_1 \sum_{n=1}^{N} (\rho_n - \rho_{n-1})^2 - \lambda_2 \sum_{n=1}^{N} \ln \rho_n - \lambda_3 \sum_{n=1}^{N} \rho_n \right] \]  

which leads to

\[ \hat{\rho} = \arg \min_{\rho > 0} \{ J(\rho) \} \]  

with

\[ J(\rho) = \| F_c - B\rho \|^2 + \sum_{n=1}^{N} \lambda_1 (\rho_n - \rho_{n-1})^2 + \lambda_2 \ln \rho_n + \lambda_3 \rho_n \]  

### 3.3. Physically Based Parametric Approach

In this approach we choose special purpose basis functions based on the physics of the problem. For example, in our case, since the charge density is a single-valued function defined in a finite domain, the Fourier-Bessel (FB) basis functions which satisfy both the orthogonality and the concentration property conditions, can be used for expansion:

\[ \rho(r) = \begin{cases} \sum_{n=1}^{N} a_n j_0(q_n r) & \text{if } r \leq R_c \\ 0 & \text{if } r > R_c \end{cases} \]  

where \( q_n = \frac{n \pi}{R_c} \). Excepted the original motivation, this choice is exactly the same as in the first approach and all the relations developed and discussed there can be used.

We may choose other basis functions which are more appropriate to translate our prior knowledge on the desired solution. For example, in our case, we know a priori that, the solution is smooth, positive and a decreasing function. Then we can choose the following function:

\[ \rho(r) = \begin{cases} \sum_{n=1}^{N} a_n \exp(-q_n r^2) & \text{if } r \leq R_c \\ 0 & \text{if } r > R_c \end{cases} \]
Using this expansion in eq. (1) we find $F_c = Aa + \epsilon$ as in (5) or in (38), where
\[ A_{m,n} = 4\pi \int_0^{R_c} dr r^2 J_0(q_m r) \exp(-q_n r^2). \] (65)

With this choice we keep the main advantage of the first approach which is the small dimension of the vector $a$ and the main advantages of the second approach which is the translation of our prior knowledge of the positivity of the function $\rho(r)$. This is due to the fact that if we impose the positivity constraint on the coefficients $a_n$ we insure that the solution remains always positive.

In the next section we will illustrate the performance of these different solutions for the estimation of the charge density from elastic electron scattering data.

4. Issues on the uncertainty of the solution

In any scientific problem solving, a proposed solution should be given in any way with a measure of its uncertainty or confidence. In Bayesian approach, the posterior probability gives us naturally the necessary tool. To see this, let come back to our problem and make a summary. We have a set of data $F$ and we want to estimate $\rho(r)$ or more precisely $\rho_{i}$ for some locations $r_{i}$. Let assume that we have chosen a constant discretization step and so, we want to estimate a vector $\rho = \{\rho_{i} \}_{i=1}^{K}$.

We presented two approaches: parametric and non-parametric. In the first approach, we have
\[ F = Aa + \epsilon \] (66)
\[ \rho = \Phi a \] (67)
and in the second
\[ F = B\rho + \epsilon \] (68)

In both cases, we are interested to $\rho$. In the first approach, we assigned $p(a)$ and $p(F|a)$, calculated the posterior $p(a|F)$, defined a solution $\hat{a}$ for the parameters $a$, and finally, a solution $\hat{\rho} = \Phi \hat{a}$ for $\rho$. In the second, we assigned directly $p(\rho)$ and $p(F|\rho)$, calculated the posterior $p(\rho|F)$, and finally defined a solution $\hat{\rho}$. In both cases, we can use the posterior laws to quantify the uncertainty of the solutions.

There are, at least, three approaches:

- Simply generate samples from the posterior law $p(\rho|F)$ using for example a monte carlo method, and show all these samples to see the distribution of the proposed solution.
- Calculate the posterior mean and the posterior variance of the solution at each point either analytically (when possible) or numerically using for example the samples generated by a monte carlo method.
- Calculate the posterior mean and covariance of the solution either analytically (when possible) or approximate it numerically by any quadrature algorithm.
To illustrate this, let consider the cases where all the probability laws are Gaussian. Then, all the calculations can be done analytically. The following summarizes all the steps for the calculation of the solutions and their posterior covariances in the above-mentioned two cases:

| Non-parametric | Parametric |
|----------------|------------|
| $F = \mathbf{B}\mathbf{\rho} + \epsilon$ | $F = \mathbf{Aa} + \epsilon$ |
| $p(\mathbf{\rho}) = \mathcal{N}(\mathbf{\rho}_0, \sigma^2_{\mathbf{\rho}}\mathbf{P}_0)$ | $p(\mathbf{a}) = \mathcal{N}(\mathbf{a}_0, \sigma^2_{\mathbf{a}}\mathbf{I})$ |
| $p(F|\mathbf{\rho}) = \mathcal{N}(\mathbf{B}\mathbf{\rho}, \sigma^2_{\epsilon}\mathbf{I})$ | $p(F|\mathbf{a}) = \mathcal{N}(\mathbf{Aa}, \sigma^2_{\mathbf{a}}\mathbf{I})$ |
| $p(\mathbf{\rho}|F) = \mathcal{N}(\mathbf{\hat{\rho}}, \mathbf{P}_F)$ | $p(\mathbf{a}|F) = \mathcal{N}(\mathbf{\hat{a}}, \mathbf{P}_F\mathbf{P}_F^t)$ |
| $\hat{\mathbf{\rho}} = \left[\mathbf{B}^t\mathbf{B} + \lambda\mathbf{P}_0^{-1}\right]^{-1}\mathbf{B}^t(F - \mathbf{B}\mathbf{\rho}_0)$ | $\hat{\mathbf{a}} = \left[\mathbf{A}^t\mathbf{A} + \lambda\mathbf{I}\right]^{-1}\mathbf{A}^t(F - \mathbf{A}\mathbf{a}_0)$ |
| $\mathbf{P}_F = \left[\mathbf{B}^t\mathbf{B} + \lambda\mathbf{P}_0^{-1}\right]^{-1}$ | $\mathbf{P}_a = \left[\mathbf{A}^t\mathbf{A} + \lambda\mathbf{P}_0^{-1}\right]^{-1}$ |
| with $\lambda = \sigma^2_{\epsilon}/\sigma^2_{\mathbf{\rho}}$ | with $\lambda = \sigma^2_{\mathbf{a}}/\sigma^2_{\mathbf{a}}$ |
| Special cases | Special cases |
| $\sigma_{\epsilon} \rightarrow 0$ | $\sigma_{\epsilon} \rightarrow 0$ |
| \[
\begin{align*}
\hat{\mathbf{\rho}} &= \left[\mathbf{B}^t\mathbf{B}\right]^{-1}\mathbf{B}^tF \\
\mathbf{P}_F &= \mathbf{0}
\end{align*}
| \[
\begin{align*}
\hat{\mathbf{\rho}} &= \mathcal{N}(\mathbf{A}^t\mathbf{A})^{-1}\mathbf{A}^tF \\
\mathbf{P}_F &= \mathbf{0}
\end{align*}
|
| $\sigma_{\mathbf{\rho}} \rightarrow 0$ | $\sigma_{\mathbf{a}} \rightarrow 0$ |
| \[
\begin{align*}
\hat{\mathbf{\rho}} &= \mathbf{\rho}_0 \\
\mathbf{P}_F &= \mathbf{0}
\end{align*}
| \[
\begin{align*}
\hat{\mathbf{a}} &= \mathbf{\Phi}\mathbf{a}_0 \\
\mathbf{P}_a &= \mathbf{0}
\end{align*}
|
| $\sigma_{\epsilon} \rightarrow \infty$ | $\sigma_{\epsilon} \rightarrow \infty$ |
| \[
\begin{align*}
\hat{\mathbf{\rho}} &= \mathbf{\rho}_0 \\
\mathbf{P}_F &= \sigma^2_{\epsilon}\mathbf{P}_0
\end{align*}
| \[
\begin{align*}
\hat{\mathbf{a}} &= \mathbf{\Phi}\mathbf{a}_0 \\
\mathbf{P}_a &= \sigma^2_{\mathbf{a}}\mathbf{P}_F\mathbf{P}_F^t
\end{align*}
|
| $\sigma_{\mathbf{\rho}} \rightarrow \infty$ | $\sigma_{\mathbf{a}} \rightarrow \infty$ |
| \[
\begin{align*}
\hat{\mathbf{\rho}} &= \left[\mathbf{B}^t\mathbf{B}\right]^{-1}\mathbf{B}^tF \\
\mathbf{P}_F &= \sigma^2_{\epsilon}\left[\mathbf{B}^t\mathbf{B}\right]^{-1}
\end{align*}
| \[
\begin{align*}
\hat{\mathbf{a}} &= \mathcal{N}(\mathbf{A}^t\mathbf{A})^{-1}\mathbf{A}^tF \\
\mathbf{P}_a &= \sigma^2_{\mathbf{a}}\left[\mathbf{A}^t\mathbf{A}\right]^{-1}\mathbf{F}
\end{align*}
|

Table 1: A comparison between parametric and non-parametric approaches.
When the posterior covariance matrix $P_\rho$ is calculated, we can use it to give some information about the uncertainty of the solution. For example, we can use its diagonal elements to calculate $\sigma_k = \sqrt{P_{kk}}$ and use it to error bars on the solution.

5. Numerical experiments

In order to demonstrate the preceding considerations we make use of the following analytical model. For a charge density given by a symmetric Fermi distribution

$$\rho(r) = \alpha \frac{\cosh(R/d)}{\cosh(R/d) + \cosh(r/d)}$$

an analytical expression for the corresponding charge form factor can easily be obtained:

$$F(q) = -\frac{4\pi^2 \alpha d}{q} \cosh(R/d) \left[ \frac{R \cos(qR)}{\sinh(\pi qd)} - \frac{\pi d \sin(qR) \cosh(\pi qd)}{\sinh^2(\pi qd)} \right].$$

Only two of the parameters $\alpha$, $R$ and $d$ are independent since the charge density must fulfill the normalization condition

$$4\pi \int r^2 \rho(r) \, dr = Z.$$  

Figure 1 shows the theoretical charge density $\rho(r)$ of $^{12}\text{C}$ ($Z=6$) obtained from (69) for $r \in [0, 0.8]$ with $R = 1.1$ A$^+$ and $d = 0.626$ fm and the theoretical charge form factor $F_c(q)$ obtained by (70) for $q \in [0, 8]$ fm$^{-1}$ and the nine simulated experimental data:

$q = [0.001, 0.5, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]$ fm$^{-1}$

![Figure 1. Theoretical charge density $\rho(r)$ [left], charge form factor log $\|F_c(q)\|$ and the data [stars] used for numerical experiments [right].](image-url)
5.1. Experiments with operator based parametric models

We use these data in the parametric model (34) with $R_c = 8$ fm and estimate the coefficients $a$ by

$$
\text{LS} : \quad \hat{a} = (A^t A)^{-1} A^t F_c \\
\text{MNLS} : \quad \hat{a} = (A^t A + \lambda I)^{-1} A^t F_c \\
\text{MAP} : \quad \hat{a} = (A^t A + \lambda D^t D)^{-1} A^t F_c
$$

Then using these coefficients we calculate $\rho(r)$ by (34) and $F_c(q)$ by (36).

Figure 2 and Figure 3 show the reconstructed charge densities $\hat{\rho}$ and the corresponding charge form factors $\hat{F}_c$ obtained by LS and by MNLS for $N = 5$ and $N = 10$.

Figure 4 shows the reconstructed charge densities by LS and by MNLS for different expansion order $N$ from 5 to 10. Note that the LS solutions are very sensitive and vary greatly with $N$, but the MNLS solution stays more stable with respect to $N$.

Figure 5 shows the reconstructed charge densities and the corresponding charge form factors obtained by MNLS and MAP for $N = 30$.

Figure 2. Parametric reconstruction of $\hat{\rho}(r)$ obtained by LS (point) and by MNLS (dotted) for $N = 5$ [left] and the corresponding reconstructed charge form factors $\log \| \hat{F}_c(q) \|$ [right]. Two solutions are practically indistinguishable and both not very satisfactory due to a large bias of the solution for small radius $r$. Note also that both solutions fit well the data.
Figure 3. Parametric reconstruction of \( \hat{\rho}(r) \) obtained by LS (point) and by MNLS (dotted) for \( N = 10 \) [left] and the corresponding reconstructed charge form factors \( \log || F_{\rho}(q) || \) [right]. Note that the LS solution fits very well the data but is very unstable but the MNLS solution, which does not fit perfectly the data, is at least more stable.

Figure 4. Parametric reconstruction of \( \hat{\rho}(r) \) obtained by LS (left) and by MNLS (right) for different values of \( N := 5 : 1 : 10 \). Note that the LS solutions vary greatly with \( N \), but the MNLS solutions stay more stable with respect to \( N \).
Figure 5. Parametric reconstruction of $\hat{\rho}(r)$ obtained by MNLS (point) and by MAP (dotted) for $N = 30$ [left] and the corresponding reconstructed charge form factors $\log \| \hat{F}_c(q) \|$ [right]. In this case the LS solution is completely unrealistic and is not presented. The MNLS solution has a large bias for small radius. The MAP solution is very satisfactory. Note also that both solutions satisfy the data constraint practically in the same way.

5.2. Experiments with non parametric models

The same data are then used with the non parametric model (44) with $N = 100$ and $R_c = 8$ fm and $\hat{\rho}$ is calculated by

- LS : $\hat{\rho} = (B^tB)^{-1}B^tF_c$
- MNLS : $\hat{\rho} = (B^tB + \lambda I)^{-1}B^tF_c$
- MAP1 : $\hat{\rho} = (B^tB + \lambda D^tD)^{-1}B^tF_c$

Figure 6 shows the estimated $\hat{\rho}$ and the corresponding $\hat{F}_c$ by MNLS and by MAP.

Figure 7 shows two solutions obtained by a parametric and a non-parametric method and their associated error bars.
Figure 6. Non parametric reconstruction of $\hat{\rho}(r)$ obtained by MNLS (point) and MAP1 (dotted) for $N = 100$ [left] and the corresponding reconstructed charge form factors $\log ||\hat{F}_c(q)||$ [right].

Figure 8. Uncertainty in parametric and non parametric methods:
Left: Parametric reconstruction of $\hat{\rho}(r)$ obtained by MAP1
Right: Non-parametric reconstruction of $\hat{\rho}(r)$ obtained by MAP1
6. Conclusion
We considered the problem of the determination of the charge density from a limited number of charge form factor measures as an ill-posed inverse problem. We proposed a Bayesian probabilistic approach to this problem and showed how many classical methods can be considered as special cases of the proposed approach. We addressed also the problem of the basis function choice for the discretization and the uncertainty of the solution. We illustrated the performances of the proposed methods by some numerical results.

References
1. J. L. Friar and J. W. Negele, Nucl. Phys. A 212, 93 (1973).
2. B. Dreher et al., Nucl. Phys. A 235, 219 (1974).
3. J. Heisenberg and H. P. Blöck, Ann. Rev. Nucl. Part. Sc. 33, 569 (1983).
4. D. S. Watkins, Fundamentals of Matrix Computations (Wiley, New York, 1991).
5. M. E. Grypeos, G. A. Lalazissis, S. E. Massen, and C. P. Panos, J. Phys. G 17, 1093 (1991).
6. R. E. Kozak, Am. J. Phys. 59, 74 (1991).
7. R. Anni, G. Co', and P. Pellegrino, preprint (1994).
8. C. R. Rao and S. K. Mitra, Generalized Inverse of Matrices and its Applications (Wiley, New York, 1971).
9. J. Baker-Jarvis, J. Math. Phys. 30, 302 (1989).
10. J. Baker-Jarvis, M. Racine, and J. Alameddine, J. Math. Phys. 30, 1459 (1989).
11. N. Canosa, H. G. Miller, A. Plastino and R. Rossignoli, Physica A 220, 611 (1995).
12. S. F. Gull and G.J. Daniell, Nature 272, 686 (1978).
13. H.G. Miller, Y. Tzeng, G.D. Yen, N. Canosa, R. Rossignoli and A. Plastino, to be published.
14. Buck and Macaulay, “Linear inversion by the method of maximum entropy,” in Maximum Entropy and Bayesian Methods 89, (J. Skilling, ed.), Kluwer Academic Publishers, 1990.
15. J. Skilling, “Classical maximum entropy” in Maximum Entropy and Bayesian Methods 89, (J. Skilling, ed.), pp. 45–52, Kluwer Academic Publishers, 1989.
16. A. Mohammad-Djafari, “A full Bayesian approach for inverse problems,” in Maximum Entropy and Bayesian Methods 95, (K. Hanson and R. Silver, ed.), Kluwer Academic Publishers, 1996.
17. D.J.C. MacKay, “Hyperparameters: Optimize or integrate out?” in Maximum Entropy and Bayesian Methods 93, (G. Heidbreder, ed.), pp. 43–59, Kluwer Academic Publishers, 1996.
18. V.A. Macaulay and B. Buck, “A fresh look at model selection in inverse scattering,” in Maximum Entropy and Bayesian Methods 94, (J. Skilling and S. Sibisi ed.), Kluwer Academic Publishers, 1996.
19. A. Mohammad-Djafari and J. Idier, “A scale invariant Bayesian method to solve linear inverse problems”, pp. 121–134, in Maximum Entropy and Bayesian Methods 94, (G. Heidbreder, ed.), Kluwer Academic Publishers, 1996.
20. A. Mohammad-Djafari and J. Idier, “Maximum entropy prior laws of images and estimation of their parameters,” pp. 285–293, in Maximum Entropy and Bayesian Methods 90, (T. Grandy, ed.), Kluwer Academic Publishers, 1991.