Model selection for inverse problems: 
Best choice of basis function and model order selection

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Abstract. A complete solution for an inverse problem needs five main steps: choice of basis functions for discretization, determination of the order of the model, estimation of the hyperparameters, estimation of the solution, and finally, characterisation of the proposed solution. Many works have been done for the last three steps. The two first have been neglected for a while, in part due to the complexity of the problem. However, in many inverse problems, particularly when the number of data is very low, a good choice of the basis functions and a good selection of the order become primordial. In this paper, we first propose a complete solution within a Bayesian framework. Then, we apply the proposed method to an inverse elastic electron scattering problem.

1. Introduction
In a very general linear inverse problem, the relation between the data \( y = [y_1, \cdots, y_m]^T \) and the unknown function \( f(.) \) is
\[
y_i = \int h_i(r) f(r) \, dr, \quad i = 1, \cdots, m, \tag{1}
\]
where \( h_i(r) \) is the system response for the data \( y_i \). We assume here that \( h_i(r) \) are known perfectly. The first step for any numerical processing is the choice of a basis function \( b_j(r) \) and an order \( k \), in such a way to be able to write
\[
f(r) = \sum_{j=1}^{k} x_j b_j(r). \tag{2}
\]
This leads to
\[
y = Ax + \epsilon \tag{3}
\]
with \( y = [y_1, \cdots, y_m]^T \), \( x = [x_1, \cdots, x_k]^T \) and
\[
A_{i,j} = \int h_i(r) b_j(r) \, dr, \quad i = 1, \cdots, m, \quad j = 1, \cdots, k \tag{4}
\]
where $\epsilon = [\epsilon_1, \ldots, \epsilon_m]^T$ represents the errors (both the measurement noise and the modeling and the approximation related to the numerical computation of matrix elements $A_{i,j}$). Even, when the choice of the basis functions $b_i(r)$ and the model order $k$ is fixed, obtaining a good estimate for $x$ needs other assumptions about the noise $\epsilon$ and about $x$ itself. The Bayesian approach provides a coherent and complete framework to handle the random nature of $\epsilon$ and the a priori incomplete knowledge of $x$.

The first step in a Bayesian approach is to assign the prior probability laws

$$p(y|x, \phi, \psi, k, l) = p(y - Ax | \phi, k, l), p(x | \psi, k, l), p(\phi | k, l) \text{ and } p(\psi | k, l),$$

where $p_e(y - Ax | \phi, k, l)$ is the probability law of the noise, and $(\phi, \psi)$ the hyperparameters of the problem. Note that $x$ represents the unknown parameters, $k = \text{dim}(x)$ is the order of the model, $m = \text{dim}(y)$ is the number of the data and $l$ is an index to a particular choice of basis functions. Note that the elements of the matrix $A$ depend on the choice of the basis functions. However, to simplify the notations, we do not write this dependance explicitly. We assume that we have to select one set $l$ of basis functions among a finite set (indexed by $[1 : l_{max}]$) of them. Thus, for a given $l \in [1, l_{max}]$ and a given model order $k \in [1, k_{max}]$, and using the mentioned prior laws, we define the joint probability law

$$p(y, x, \phi, \psi | k, l) = p(y | x, \phi, \psi, k, l) p(x | \psi, k, l) p(\phi | k, l) p(\psi | k, l).$$

From this probability law, we obtain, either by integration or by summation, any marginal law, and any a posteriori probability law using the Bayes rule.

What we propose in this paper is to consider the following problems:

- Parameter estimation:
  $$\hat{x} = \text{arg max}_x \left\{ p(x | y, \hat{\phi}, \hat{\psi}, \hat{k}, \hat{l}) \right\}$$

  where
  $$p(x | y, \phi, \psi, k, l) = p(y, x | \phi, \psi, k, l) / p(y | \phi, \psi, k, l),$$
  $$p(y, x | \phi, \psi, k, l) = p(y | x, \phi, k, l) p(x | \psi, k, l)$$

  and
  $$p(y | \phi, \psi, k, l) = \int p(y, x | \phi, \psi, k, l) \, dx.$$  

- Hyperparameter estimation:
  $$(\hat{\phi}, \hat{\psi}) = \text{arg max}_{(\phi, \psi)} \left\{ p(\phi, \psi | y, \hat{k}, \hat{l}) \right\}$$

  where
  $$p(\phi, \psi | y, k, l) = p(y, \phi, \psi | k, l) / p(y | k, l)$$

  and
  $$p(y | k, l) = \int \int p(y, \phi, \psi | k, l) \, d\phi \, d\psi.$$
- Model order selection:

\[
\hat{k} = \arg \max_k \left\{ p(k | y, l) \right\} \tag{13}
\]

where

\[
p(k | y, l) = p(y | k, l) p(k) / p(y | l) \tag{14}
\]

and

\[
p(y | l) = \sum_{k=1}^{k_{\text{max}}} p(y | k; l) p(k). \tag{15}\]

- Basis function selection:

\[
\hat{l} = \arg \max_l \left\{ p(l | y) \right\} \tag{16}
\]

where

\[
p(l | y) = p(y | l) p(l) / p(y) \tag{17}
\]

and

\[
p(y) = \sum_{l=1}^{l_{\text{max}}} p(y | l) p(l). \tag{18}\]

- Joint parameter, hyperparameter, model order and basis function estimation:

\[
(\hat{x}, \hat{\phi}, \hat{\psi}, \hat{k}, \hat{l}) = \arg \max_{(x, \phi, \psi, k, l)} \left\{ p(y, x, \phi, \psi | k, l) p(k) p(l) \right\}. \tag{19}
\]

As it can be easily seen, the first problem is, in general, a well posed problem and the solution can be computed, either analytically or numerically. The others (excepted the last) need integrations. These integrals can be done analytically only in the case of Gaussian laws. In other cases, one can either use a numerical integration (either deterministic or stochastic) or to resort to approximations such as the Laplace’s method which allows to obtain a closed-form expression for the criterion to optimise.

Here, we consider these problems for the particular case of Gaussian prior laws:

\[
p(y | x, \phi, k, l) = \mathcal{N} \left( Ax, \frac{1}{\phi} I \right) = (2\pi/\phi)^{-m/2} \exp \left[ -\frac{1}{2\phi} \| y - Ax \|^2 \right] \tag{20}
\]

\[
p(x | \psi, k, l) = \mathcal{N} \left( 0, \frac{1}{\psi} I \right) = (2\pi/\psi)^{-k/2} \exp \left[ -\frac{1}{2\psi} \| x \|^2 \right] \tag{21}
\]

where \( \frac{1}{\phi} \) and \( \frac{1}{\psi} \) are respectively the variance of the noise and the parameters.
2. Parameter estimation

First note that in this special case we have

\[ p(y, x | \phi, \psi, k, l) = (2\pi/\phi)^{-m/2} (2\pi/\psi)^{-k/2} \exp \left[ -\frac{1}{2\phi} \|y - Ax\|^2 - \frac{1}{2\psi} \|x\|^2 \right]. \]

Integration with respect to \( x \) can be done analytically and we have:

\[ p(y | \phi, \psi, k, l) = \int p(y, x | \phi, \psi, k, l) \, dx = N(\mathbf{0}, P_y), \]

with

\[ P_y = \frac{1}{\psi} AA^t + \frac{1}{\phi} I = \frac{1}{\psi}(AA^t + \lambda I) \quad \text{and} \quad \lambda = \frac{\psi}{\phi}. \]

It is then easy to see that the \textit{a posteriori} law of \( x \) is also Gaussian:

\[ p(x | y, \phi, \psi, k, l) = N(\hat{x}, \hat{P}) \quad \text{with} \quad \hat{P} = \frac{1}{\phi}(A^tA + \lambda I)^{-1} \quad \text{and} \quad \hat{x} = \phi\hat{P}A^ty. \]

Thus the parameter estimation in this case is straightforward:

\[ \hat{x} = \text{arg max}_x \{ p(x | y, \phi, \psi, k, l) \} = \text{arg min}_x \{ J_1(x) \}, \]

with

\[ J_1(x) = \|y - Ax\|^2 + \lambda\|x\|^2, \]

which is a quadratic function of \( x \). The solution is then a linear function of the data \( y \) and is given by

\[ \hat{x} = K(\lambda) y \quad \text{with} \quad K(\lambda) = (A^tA + \lambda I)^{-1}A^t. \]

3. Hyperparameter estimation

For the hyperparameter estimation problem we note that:

\[ p(\phi, \psi | y, k, l) = \frac{p(\phi | k, l) p(\psi | k, l)}{p(y | k, l)} \frac{p(y | \phi, \psi, k, l)}{p(y | k, l)} = \frac{p(\phi | k, l) p(\psi | k, l)}{p(y | k, l)} (2\pi)^{-m/2} |P_y|^{-1/2} \exp \left[ -\frac{1}{2} y^t P_y^{-1} y \right]. \]

Thus, the hyperparameter estimation problem becomes:

\[ (\hat{\phi}, \hat{\psi}) = \text{arg max}_{(\phi, \psi)} \left\{ p(\phi, \psi | y, \hat{k}, \hat{l}) \right\} = \text{arg min}_{(\phi, \psi)} \{ J_2(\phi, \psi) \} \]

where

\[ J_2(\phi, \psi) = -\ln p(\phi | k, l) - \ln p(\psi | k, l) + \frac{1}{2} \ln |P_y| + \frac{1}{2} y^t P_y^{-1} y. \]
Unfortunately, in general, there is not an analytical expression for the solution, but this optimization can be done numerically. Many works have been investigated to perform this optimization appropriately for particular choices of \( p(\phi \mid k, l) \) and \( p(\psi \mid k, l) \). Among the others, we may note the choice of improper prior laws such as Jeffry’s prior \( p(\phi \mid k, l) \propto \frac{1}{\phi} \) and \( p(\psi \mid k, l) \propto \frac{1}{\psi} \) or proper prior laws of uniform \( p(\phi \mid k, l) = \frac{1}{\phi_{\text{max}} - \phi_{\text{min}}} \) and \( p(\psi \mid k, l) = \frac{1}{\psi_{\text{max}} - \psi_{\text{min}}} \) or still the proper Gamma prior laws.

One main issue with improper prior laws is the existence of the solution, because \( p(\phi, \psi \mid y, k, l) \) may even not have a maximum or its maximum can be located at the border of the domain of variation of \((\phi, \psi)\). Here, we propose to use the following proper Gamma priors:

\[
p(\phi) = G(\alpha_1, \beta_1) \propto \phi^{(\alpha_1 - 1)} \exp[-\beta_1 \phi] \rightarrow E\{\phi\} = \alpha_1 / \beta_1 \tag{32}
\]

\[
p(\psi) = G(\alpha_2, \beta_2) \propto \psi^{(\alpha_2 - 1)} \exp[-\beta_2 \psi] \rightarrow E\{\psi\} = \alpha_2 / \beta_2. \tag{33}
\]

With these priors, we have

\[
J_2(\phi, \psi) = (1 - \alpha_1) \ln \phi + (1 - \alpha_2) \ln \psi + \beta_1 \phi + \beta_2 \psi + \frac{1}{2} \ln |P_y| + \frac{1}{2} y^t P_y^{-1} y. \tag{34}
\]

The second main issue is the numerical optimization. Many works have been done on this subject. Among the others we can mention those who try to integrate out one of the two parameters directly or after some transformation. For example transforming \((\phi, \psi) \rightarrow (\phi, \lambda)\) and using the identities

\[
 |AA^t + \lambda I| = \lambda^{m-k} |A^t A + \lambda I| \tag{35}
\]

and

\[
 (AA^t + \lambda I)^{-1} = \frac{1}{\lambda} (I - AK(\lambda)) \tag{36}
\]

we have

\[
 \ln |P_y| = -m \ln \phi - k \ln \lambda + \ln |A^t A + \lambda I| \tag{37}
\]

and

\[
y^t P_y^{-1} y = \phi y^t (I - AK(\lambda))y = \phi y^t (y - A\hat{x}) = \phi y^t (y - \hat{y}). \tag{38}
\]

Then, we obtain

\[
J_2(\phi, \psi) = (1 - \alpha_1 - \frac{m-k}{2} \ln \phi + (1 - \alpha_2 - \frac{k}{2} \ln \psi + \beta_1 \phi + \beta_2 \psi \tag{39}
\]

\[
+ \frac{1}{2} \ln |A^t A + \frac{\lambda}{\psi} I| + \frac{\phi}{2} y^t (y - \hat{y}).
\]

or

\[
J_2(\phi, \lambda) = (2 - \alpha_1 - \alpha_2 - \frac{m-k}{2} \ln \phi + (1 - \alpha_2 - \frac{k}{2} \ln \lambda + \beta_1 \phi + \beta_2 \phi \lambda \tag{40}
\]

\[
+ \frac{1}{2} \ln |A^t A + \lambda I| + \frac{\phi}{2} y^t (y - \hat{y}).
\]

For fixed \( \lambda \), equating to zero the derivative of this expression with respect to \( \phi \) has an explicit solution which is

\[
\frac{\partial J_2(\phi, \lambda)}{\partial \phi} = 0 \rightarrow \phi = \left( \frac{m}{2} + \alpha_1 + \alpha_2 - 2 \right) / \left[ \beta_1 + \beta_2 + \frac{1}{2} y^t (y - \hat{y}) \right] \tag{41}
\]
Putting this expression into \( J_2 \) we obtain a criterion depending only on \( \lambda \) which can be optimized numerically. In addition, it is possible to integrate out \( \phi \) to obtain \( p(\lambda | y, k, l) \), but the expression is too complex to write.

4. Joint estimation

One may try to estimate all the unknowns simultaneously by

\[
(\hat{x}, \hat{\phi}, \hat{\psi}, \hat{k}, \hat{l}) = \arg \max_{(x, \phi, \psi, k, l)} \{ p(x, \phi, \psi, k, l | y) \} = \arg \min_{(x, \phi, \psi, k, l)} \{ J_3(x, \phi, \psi, k, l) \} \tag{42}
\]

where

\[
J_3(x, \phi, \psi, k, l) = -\ln p(k) - \ln p(l) - (m^2 + \alpha - 1) \ln \phi - (\beta_1 + \frac{1}{2} \| y - A \hat{x} \|^2) + \psi (\beta_2 + \frac{1}{2} \| x \|^2) \tag{43}
\]

The main advantage of this criterion is that we obtain explicit solutions for \( x, \phi \) and \( \psi \) by equating to zero the derivatives of \( J_3(x, \phi, \psi, k, l) \) with respect to them:

\[
\begin{align*}
\hat{x} &= (A^t A + \lambda I)^{-1} A^t y, \quad \text{with} \quad \lambda = \phi/\psi; \\
\hat{\phi} &= (m^2 + \alpha - 1)/ (\beta_1 + \frac{1}{2} \| y - A \hat{x} \|^2); \\
\hat{\psi} &= (k^2 + \alpha - 1)/ (\beta_2 + \frac{1}{2} \| \hat{x} \|^2). \tag{44}
\end{align*}
\]

We can not obtain closed form expressions for \( \hat{k} \) and \( \hat{l} \) which depend on the particular choice for \( p(k) \) and \( p(l) \). These relations suggest an iterative algorithm such as:

```
Joint MAP estimation algorithm 1

for \( l = 1: l_{\text{max}} \)
    for \( k = 1: k_{\text{max}} \)
        compute the elements of the matrix \( A \);
        initialize \( \lambda = \lambda_0 \);
        repeat until convergency:
            \[
            \begin{align*}
            \hat{x} &= (A^t A + \lambda I)^{-1} A^t y; \\
            \hat{\phi} &= (m^2 + \alpha - 1)/ (\beta_1 + \frac{1}{2} \| y - A \hat{x} \|^2); \\
            \hat{\psi} &= (k^2 + \alpha - 1)/ (\beta_2 + \frac{1}{2} \| \hat{x} \|^2)
            \end{align*}
            \]
        \rightarrow \lambda = \hat{\phi}/\hat{\psi}
        compute \( J(k, l) = J_3(\hat{x}, \hat{\phi}, \hat{\psi}, k, l) \);
    end
end
choose the best model and the best order by
\[
(\hat{l}, \hat{k}) = \arg \min_{(k, l)} \{ J(k, l) \}
\]
```

Note however that, for fixed \( x, \phi \) and \( \psi \), the criteria \( J_3 \) in (43) or \( J_5 \) in (47) are mainly linear functions of \( k \) if we choose a uniform law for \( p(k) \). This means
that we may not have a minimum for these criteria as a function of \( k \). The choice of the prior \( p(k) \) is then important. One possible is the following:

\[
p(k) = \begin{cases} 
\frac{2(k_{\text{max}} - k)}{k_{\text{max}}(k_{\text{max}} - 1)} & 1 \leq k < k_{\text{max}} \\
0 & k > k_{\text{max}} 
\end{cases}
\]  

(45)

which is a decreasing function of \( k \) in the range \( k \in [1, k_{\text{max}}] \) and zero elsewhere. This choice may insure the existence of a minimum if \( k_{\text{max}} \) is chosen appropriately.

For \( p(l) \) we propose to choose a uniform law, because we do not want to give any favor to any model.

Another algorithm can be obtained if we replace the expression of \( \hat{x} \) into \( J_3 \) to obtain a criterion depending only on \((\phi, \psi)\):

\[
J_4(\phi, \psi, k, l) = -\ln p(k) - \ln p(l) - (\frac{m+k}{2} + \alpha_1 - 1) \ln \phi - (\frac{k}{2} + \alpha_2 - 1) \ln \psi + \psi \left( \beta_2 + \frac{1}{2} \| \hat{\phi}(\lambda) \|^2 \right)
\]

(46)

or on \((\phi, \lambda)\):

\[
J_5(\phi, \lambda, k, l) = -\ln p(k) - \ln p(l) - (\frac{m+k}{2} + \alpha_1 + \alpha_2 - 2) \ln \phi - (\frac{k}{2} + \alpha_2 - 1) \ln \lambda + \phi \left( \beta_1 + \frac{1}{2} \| y - \hat{y}(\lambda) \|^2 \right) + \lambda \phi \left( \beta_2 + \frac{1}{2} \| \hat{x}(\lambda) \|^2 \right)
\]

(47)

and then optimize it with respect to them. In the second case, we can again obtain first \( \phi \) and put its expression

\[
\hat{\phi} = \left( \frac{m+k}{2} + \alpha_1 + \alpha_2 - 2 \right) / \left( \beta_1 + \frac{1}{2} \| y - \hat{y}(\lambda) \|^2 \right)
\]

(48)
in the criterion to obtain another criterion depending only on \( \lambda \) and optimize it numerically. This gives the following algorithm:

```
Joint MAP estimation algorithm 2

for \( l = 1 : l_{\text{max}} \)
    for \( k = 1 : k_{\text{max}} \)
        compute the elements of the matrix \( A \);
        for \( \lambda \in 10^{-8:1:4} \)
            compute \( \hat{x} = (A^tA + \lambda I)^{-1}A^ty \) and \( \hat{y} = A\hat{x} \)
            compute \( \hat{\phi} \) using (eq. 48)
            compute \( J(\lambda) = J_5(\hat{\phi}, \lambda, k, l) \) (eq. 47)
        end
        choose \( \hat{\lambda} = \arg\min_{\lambda} \{ J(\lambda) \} \)
        compute \( \hat{x} = (A^tA + \hat{\lambda} I)^{-1}A^ty \);
        compute \( \hat{\phi} \) using (eq. 48);
        compute \( J(k, l) = J_5(\hat{\phi}, \hat{\lambda}, k, l) \) (eq. 47)
    end
end
choose the best model and the best order by \( (\hat{l}, \hat{k}) = \arg\min_{(l,k)} \{ J(l,k) \} \)
```
5. Model order selection

The model order selection

\[
\hat{k} = \arg \max_k \{ p(k | y, l) \} = \arg \min_k \{ J_6(k) \}
\]

(49)

with

\[
J_6(k) = - \ln p(k) - \ln p(y | k, l)
\]

(50)

needs one more integration

\[
p(y | k, l) = \int \int p(y, \phi, \psi | k, l) \, d\phi \, d\psi.
\]

(51)
or

\[
p(y | k, l) = \int \int p(y, \phi, \lambda | k, l) \, d\phi \, d\lambda.
\]

(52)

where \( p(y, \phi, \lambda | k, l) \propto \exp \left[ -J_2(\phi, \lambda) \right] \) given by (41). As we mentioned in preceding section, these integrations can only be done numerically. A good approximation can be obtained using the following:

\[
p(y | k, l) = \int \int p(y, \phi, \psi | k, l) \, d\phi \, d\psi \simeq \sum_i \sum_j p(y | \phi_j, \psi_i, k, l)
\]

(53)

where \( \{ \phi_j \} \) and \( \{ \psi_i \} \) are samples generated using the prior laws \( p(\phi) \) and \( p(\psi) \).

6. Best basis or model selection

The model selection

\[
\hat{l} = \arg \max_l \{ p(l | y) \} = \arg \min_l \{ J_7(l) \}
\]

(54)

with

\[
J_7(l) = - \ln p(l) - \ln p(y | l)
\]

(55)

does not need any more integration, but only one summation. Choosing \( p(l) \) uniform and making the same previous approximations we have

\[
J_7(l) = - \ln \sum_{k=1}^{k_{\text{max}}} p(y | k, l) p(k).
\]

(56)

7. Proposed algorithms

Based on the equations (55), (53), (50), (39) and (40) we propose the following algorithm:
Marginal MAP estimation algorithm 2

Generate a set of samples \{\phi_j\} drawn from \(p(\phi)\)
Generate a set of samples \{\psi_i\} drawn from \(p(\psi)\)

for \(l = 1 : l_{\text{max}}\)
    for \(k = 1 : k_{\text{max}}\)
        compute the elements of the matrix \(A\);
        for \(\phi \in \{\phi_j\}\)
            for \(\psi \in \{\psi_i\}\)
                compute \(\lambda = \phi/\psi\), \(\hat{x} = (A^tA + \lambda I)^{-1}A^ty\) and \(\hat{y} = A\hat{x}\)
                compute \(p_\psi(i,j,k,l) = \exp[-J_2(\phi_j, \psi_i)]\) (eq. 39)
            end
            normalize \(p_\psi(i,j,k,l) = p_\psi(i,j,k,l) / \sum_i p_\psi(i,j,k,l)\)
        end
        normalize \(p_\phi(j,k,l) = p_\phi(j,k,l) / \sum_j p_\phi(j,k,l)\)
    end
    normalize \(p_k(k,l) = p_k(k,l) / \sum_k p_k(k,l)\)
    compute \(p_l(l) = \sum_k p_k(k,l)\)
end
normalize \(p_l(l) = p_l(l) / \sum_l p(l)\)

choose the best model by \(\hat{l} = \arg\max_l \{p_l(l)\}\)
choose the best model order by \(\hat{k} = \arg\max_k \{p_k(k, \hat{l})\}\)
choose the best value for \(\phi = \phi_{\hat{j}}\) with \(\hat{j} = \arg\max_j \{p_\phi(j, \hat{l}, \hat{k})\}\)
choose the best value for \(\psi = \psi_{\hat{i}}\) with \(\hat{i} = \arg\max_i \{p_\psi(i, \hat{j}, \hat{l}, \hat{k})\}\)
compute \(\hat{\lambda} = \hat{\phi}/\hat{\psi}\)
compute the elements of the matrix \(A\) for \(l = \hat{l}\) and \(k = \hat{k}\)
compute \(\hat{x} = (A^tA + \hat{\lambda} I)^{-1}A^ty\).

8. Application: Electron scattering data inversion

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

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

(57)

where \(J_0\) is the spherical Bessel function of zero order and \(q\) is the absolute value of the three momentum transfer.

We applied the proposed method with the following usual discretization pro-
We chose the following basis functions:

$$\rho(r) = \begin{cases} \sum_{j=1}^{k} x_j b_j(r) & r \leq R_c \\ 0 & r > R_c \end{cases}$$

which results in

$$F(q) = 4\pi \sum_{j=1}^{k} x_j \int_{0}^{R_c} r^2 J_0(qr) b_j(r) \, dr$$

and

$$\mathbf{y} = A\mathbf{x} + \mathbf{\epsilon}$$

where $\mathbf{x}$ is a vector containing the coefficients $\{x_j, j = 1, \cdots, k\}$, $\mathbf{y}$ is a vector containing the form factor data $\{F(q_i), i = 1, \cdots, m\}$ and $A$ an $(m \times k)$ matrix containing the coefficients $A_{i,j}$ given by

$$A_{i,j} = 4\pi \int_{0}^{R_c} r^2 J_0(q_i r) b_j(r) \, dr.$$  

To compute $A_{i,j}$ we define a discretization step $\Delta r = R_c/N$, a vector $\mathbf{r} = \{r_n = (n-1)\Delta r, n = 1, \cdots, N\}$, a $(N \times k)$ matrix $\mathbf{B}$ with elements $B_{n,j} = b_j(r_n)$, a $(m \times N)$ matrix $\mathbf{C}$ with elements $C_{i,n} = (4\pi \Delta r) r_n^2 J_0(q_i r_n)$ such that we have $A = CB$. Note also that when the vector $\mathbf{x}$ is determined, we can compute $\mathbf{\rho} = \{\rho(r_n), n = 1, \cdots, N\}$ by $\mathbf{\rho} = B\mathbf{x}$.

To test the proposed methods, we used the following simulation procedure:

- Select a model type $l$ and an order $k$ and generate the matrixes $B$, $C$ and $A$, and for a random set of parameters $\mathbf{x}$ generate the data $\mathbf{y} = A\mathbf{x}$.
- Add some noise $\mathbf{\epsilon}$ on $\mathbf{y}$ to obtain $\mathbf{y} = A\mathbf{x} + \mathbf{\epsilon}$.
- Compute the estimates $\hat{l}$, $\hat{k}$, $\hat{\mathbf{x}}$, $\hat{\mathbf{y}} = A\hat{\mathbf{x}}$ and $\hat{\mathbf{\rho}} = B\hat{\mathbf{x}}$ and compare them with $\mathbf{l}$, $\mathbf{k}$, $\mathbf{x}$, $\mathbf{y} = A\mathbf{x}$ and $\mathbf{\rho} = B\mathbf{x}$.

We chose the following basis functions:

- $l = 1$: $b_j(r) = J_0(q_j r)$ — This is a natural choice due to the integral kernel and the orthogonality property of the bessel functions.
- $l = 2$: $b_j(r) = \text{sinc}(q_j r)$ — This choice is also natural due to the orthogonality and the limited support hypothesis for the function $\rho(r)$.
- $l = 3$: $b_j(r) = \exp\left[-\frac{1}{2}(q_j r)^2\right]$ — This choice can account for the positivity of the function $\rho(r)$ if $\{x_j\}$ are constrained to be positive.
- $l = 4$: $b_j(r) = \exp\left[-\frac{1}{2}(q_j r)^2\right] J_0(q_j r)$ — This choice combines the first and the third properties.
- $l = 5$: $b_j(r) = 1/(\cosh(q_j r))$ — This choice has the same properties of the third one.
- $l = 6$: $b_j(r) = 1/(1 + (q_j r)^2)$ — This choice has the same properties of the third one.

In all these experiments we chose $k = 6$, $m = 20$, $N = 100$, $R_c = 8$ and $q_i = i\pi/R_c$. The following figures show typical solutions. Figures 1 and 2 show the details of the procedure for the case $l = 1$. Figures 3, 4 and 5 show the results for the cases $l = 1$ to $l = 6$. 
\[ b_j(r) \quad j = 1, \ldots, k = 6 \]

\[ \rho(r) = \sum_{j=1}^{k} x_j b_j(r) \]

with
\[ x_1 = x_2 = \cdots = x_6 = 1 \]

\[ F(q_i) = \sum_{j=1}^{k} A_{ij} x_j \]

\[ A_{ij} = \int r^2 J_0(q_i r) b_j(r) \, dr \]

\[ i = 1, \ldots, m = 14 \]
\[ j = 1, \ldots, k = 6 \]

Fig. 1: a) basis functions \( b_j(r) \), b) \( \rho(r) \), c) data \( F(q_i) \) in a logarithmic scale.
Fig. 2: a) $p(k, l|y)$, $p(l|y)$ and $p(k|y, \hat{l})$,  b) original $\rho(r)$ and estimated $\hat{\rho}(r)$,  c) original $F(q_i)$ and estimated $\hat{F}(q_i)$. 

$p(k, l)$

$p(l)$ and $p(k|\hat{l})$

$\hat{\rho}(r) = \sum_{j=1}^{k} \hat{x}_j b_j(r)$
and
$\rho(r) = \sum_{j=1}^{k} x_j b_j(r)$

$\hat{F}(q_i) = \sum_{j=1}^{k} A_{ij} \hat{x}_j$
and
$F(q_i) = \sum_{j=1}^{k} A_{ij} x_j$
Fig. 3:  
Left: $l = 1$  
  a) basis functions $b_j(r)$;  
  b) $p(k,l|y)$;  
  c) $p(k|y)$ and $p(k|y,\hat{l})$;  
  d) $\rho(r)$ and $\hat{\rho}(r)$;  
  e) $F(q_k)$ and $\hat{F}(q_k)$.  
Right: $l = 2$
Fig. 4: Left: $l = 3$
- a) basis functions $b_j(r)$;
- b) $p(k, l|y)$;
- c) $p(k|y)$ and $p(k|y, \hat{l})$;
- d) $\rho(r)$ and $\hat{\rho}(r)$;
- e) $F(q_i)$ and $\hat{F}(q_i)$.

Right: $l = 4$
Fig. 5: Left: $l = 5$
   a) basis functions $b_j(r)$;
   b) $p(k, l|y)$;
   c) $p(k|y)$ and $p(k|y, \hat{l})$;
   d) $\rho(r)$ and $\hat{\rho}(r)$;
   e) $F(q_i)$ and $\hat{F}(q_i)$.

Right: $l = 6$
Note that in these tests, we know perfectly the model and generated the data according to our hypothesis. To test the method to a more realistic case, we chose a model for which we can have an exact analytic expression for the integrals. For example, if we choose 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:

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

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

$$4\pi \int r^2 \rho(r) \, dr = Z.$$  \hfill (64)

Figure 6 shows the theoretical charge density $\rho(r)$ of $^{12}\text{C}$ ($Z=6$) obtained from (62) for $r \in [0,8] \text{ fm}$ with $R = 1.1 \text{ A}$ and $d = 0.626 \text{ fm}$ and the theoretical charge form factor $F(q)$ obtained by (63) for $q \in [0,8] \text{ fm}^{-1}$ and the 15 simulated data:

$$q = [0.001, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0] \text{ fm}^{-1}$$

which are used as inputs to the inversion method.

![Fig. 6: Theoretical charge density $\rho(r)$, charge form factor $\log|F(q)|$ and the data [stars] used for numerical experiments [right].](image)

First note that, even with the exact data, there are an infinite number of solutions which fits exactly the data. The following figure shows a few set of these solutions.
9. Conclusions

We discussed the different steps for a complete resolution of an inverse problem and focused on the choice of a basis function selection and the order of the model. An algorithm based on Bayesian estimation is proposed and tested on simulated data.
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