Estimation of the parameters of the particular solution of a partial differential equation through Cramer Rao

F Mesa¹, D M Devia¹, and R Ospina²
¹ Departamento de Matemáticas, Universidad Tecnológica de Pereira, Pereira, Colombia
² Escuela de Física, Universidad Industrial de Santander, Bucaramanga, Colombia

E-mail: femesa@utp.du.co

Abstract. The parameter estimation task is given by statistical exploration of probability density functions. The volume of samples and characteristics of a database is an advantage to solve the problem of parameter estimation but finding a function that models the behavior of a database or its distribution is complex and without this step it is not possible to use advanced statistical techniques. This document solves the problem of parameter estimation of a particular solution of a partial differential diffusion equation, the parameters found are suitable for the distribution in a domain of the amount of concentration of a material by means of the Cramer Rao limit and the value expected coefficients. With the non-linear technique used to find the optimal value of the constants, it was possible to observe the convergence of the coefficients at a given value thanks to the performance of this technique and the intrinsic characteristics of the database combined with a Gaussian normal distribution.

1. Introduction
Recently, progress has been made in various fields such as image reconstruction, information restoration and segmentation through non-linear filtering. Since the objective of this type of filtering techniques is usually the extraction of information in the presence of noise, with its own pro ballistics interpretation, that is, the use of various techniques such as Cramer Rao elevation calculation, or filtering with active noise of samples from a database to solve the task of parameter estimation or problem detection. An answer could be given to the task of parameter estimation through the use of classical detection techniques and estimation theory to characterize a set of samples and a model that converges to a desirable performance given the noise probability function of either the samples themselves or an induced noise in the database. Given the measurements of the inputs and outputs it is necessary to know the parameters that model a phenomenon from a database, such as evaluating the aerodynamics of a ship from the flight measurements, these measurements contain the coefficients that describe the behavior of a differential equation that relates the variables of entry and exit of a ship's flight. The calculation of these parameters varies from non-linear methods of estimating coefficients to linear methods from various assumptions, relaxations and approximations by means of probability density functions and optimality criteria determined by a cost function as proposed in [1]. The minimization of these cost functions requires the minimization of the sum of squares or the deviation between the samples that refer to the output.

On the other hand, the estimation by maximum probability is a method that consists in the maximization of a probability density function that must be adjusted to the dynamics of the problem.
that you want to solve, as presented in [2] the probability density function it involves modeling the flow of a fluid in porous media considering the existence of filtration in the outer layers and that the fluid flows freely in the inner layers and is described by a stochastic partial differential equation [3,4]. Otherwise, the stochastic processes for the solution of differential equations have the property of convergence with probability equal to 1 for the occurrence of the process (or coefficient) x, between normalized random variables [5].

Finally, this document statistically explores the variability and expected value of the parameters that describe a particular solution of a partial differential equation that models the concentration of a material in a specific area, that is, according to the location, the coefficients of a function of two variables \((x,y) \in \mathbb{R}^2\) that allow the coordinates to be related to the material exposure, using a linear approximation with the Cramer Rao method and an approximation with the estimation maximization to determine the convergence of the parameters.

2. Mathematical concepts
Once a minimum level given by the samples of a database Equation (1) is estimated, the variance of an estimator does not exceed these limits for an unbiased estimation model. This is achieved with the correctness of the parameters compared to the probability of the expected value,

\[ x[n] = F[n] + \omega[n]. \tag{1} \]

Equation describes the path of each of the nth samples of a database X, where F is the output or characteristic and \(\omega\) is an induced noise to separate the correlated measurements. On the other hand, a probability density function that depends on an unknown parameter is given by Equation (2).

\[ p(x[n], A) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x[n] - A)^2}. \tag{2} \]

When the probability density function is seen as a function of unknown parameters it is known as the likelihood function, this function accommodates the unknown parameters according to the minimization of Equation (2) as shown in [6] Equation (3).

\[ \ln(p(x[n], A)) = -\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}(x[n] - A)^2. \tag{3} \]

The first derivative with respect to the unknown parameter is Equation (4).

\[ \frac{\partial \ln(p(x[n], A))}{\partial A} = \frac{1}{\sigma^2}(x[n] - A), \tag{4} \]

and the second derivative becomes Equation (5).

\[ x \frac{\partial^2 \ln(p(x[n], A))}{\partial A^2} = -\frac{1}{\sigma^2}. \tag{5} \]

With the previous calculations it is necessary that Equation (5) the curvature increases as \(\sigma^2\), therefore the variance and the expected value of the unknown parameter are given by Equation (6) and Equation (7).

\[ \text{var}(\hat{A}) = \frac{1}{\frac{\partial^2 \ln(p(x[n], A))}{\partial A^2}}, \tag{6} \]

\[ \hat{A} = -\varepsilon \left[ \frac{\partial^2 \ln(p(x[n], A))}{\partial A^2} \right]. \tag{7} \]
3. Application

The results obtained in [7] combine the Gaussian processes applied to the databases of three problems: Computational biology, motion capture and geostatistics. The main idea is to mix the measures obtained in each of the problems with the solution of the models obtained by means of differential equations. From the partial differential equation
\[
\frac{\partial y_{q}(X,t)}{\partial t} = \sum_{k=1}^{K} k_{q} \frac{\partial^{2} y_{q}(X,t)}{\partial x_{j}^{2}},
\]
the parameter \(k_{q}\) which refers to the material diffusion constant is unknown. The measurement of concentration of polluting materials in space and in time comes from \(y_{q}(X,t)\), the concentration measures of the following materials (cadmium (Cd), copper (Cu), cobalt (Co), chrome (Cr), nickel (Ni), lead (Pb), and zinc (Zn)) and the localization in a certain area (Table 1).

**Table 1. Database under study.**

| Xloc | yloc | Cd   | Co   | Cr   | Cu   | Ni   | Pb   | Zn   |
|------|------|------|------|------|------|------|------|------|
| 2.386| 3.077| 1.740| 9.320| 38.320| 25.720| 21.320| 77.360| 92.560|
| 2.544| 1.972| 1.335| 10.000| 40.200| 24.760| 29.720| 77.880| 73.560|

The model and strategy are given by the covariance function that relates the solution of the partial differential equation to the concentration of material and the latent force function is given by Equation (8).

\[
k_{y_{q}f}(X, X', t) = \frac{S_{q}[L_{r}^{-1}]^{1/2}}{|L_{r}^{-1}+L_{f}^{-1}|^{1/2}} \left[ -\frac{(x-x')^{T}[L_{q}+L_{f}]^{-1}(x-x')}{} \right].
\]

With the isotropic matrices \(L_{r}, L_{f}\) with inputs \(2k_{R}, 1/ L_{f}^{2}\) respectively. This model seeks to predict the concentration of material by defining the concentration of Cd, Cu, and Co as the primary variable, and conditioning the secondary variables Zn-Cu, Ni-Zn. By means of Gaussian processes, the average and standard deviation values for the material concentration were obtained for 10 repetitions as shown in the following Table 2.

**Table 2. Concentration of material.**

| Material | IGP       |
|----------|-----------|
| Cd       | 0.5823±0.0133 |
| Cu       | 15.9357±0.0907 |
| Pb       | 22.9141±0.6076 |
| Co       | 2.0735±0.1070 |

3.1. Proposed solution

The partial differential Equation (9).

\[
\frac{\partial y_{q}(X,t)}{\partial t} = \sum_{j=1}^{2} k_{q} \frac{\partial^{2} y_{q}(X,t)}{\partial x_{j}^{2}}.
\]

Has a solution given by the function Equation (10).

\[
F(x,y) = Axy + c_{1}x + c_{2}y + c_{3},
\]

where the parameters \([A, c_{1}, c_{2}, c_{3}]\) but the coordinates \((x, y)\) and the material concentration \(F(x, y)\) of the database are found.
3.2. Algorithm

Extract the coordinates \((x, y)\) and the concentration of material from the database, each column represents coordinates and material concentration, respectively. Add Gaussian white noise \(\omega_n = \sigma^2 \text{rand}(N, 1)\), \(\sigma = 1/4\) to the material concentration \(F_{\text{on}} = F + \omega_n\). The addition of Gaussian white noise allows separating the correlation of the samples. Define the problem linearly as:

\[
F_{\text{on}} = H\theta + \omega_n
\]

With \(H = [xy x \text{ and } I_{nx1}]\) and \(\theta = [A \ C_1 \ C_2 \ C_3]^T\); estimate the parameters \(\theta\) with the estimation model \(\theta = (H^T H)^{-1} H^T F_{\text{on}}\).

### Table 3. Cramer Rao dimensions.

| \(\theta\) CRLB | Estimate |
|-----------------|----------|
| A               | 0.2208   |
| C1              | -0.3471  |
| C2              | -0.6379  |
| C3              | 2.2344   |

Figure 1. EDP solution (Black color), Cd samples (red color).

The results obtained Figure 1, above will be used as initial values to estimate the optimal values by means of the Newton Raphson method Equation (11) to Equation (15).

\[
\theta^{k+1} = \theta^k - I(\theta)^{-1} g(F_{\text{on}}),
\]

\[
I(\theta) = \frac{H^T H}{\sigma^2},
\]

\[
g(F_{\text{on}}) = (H^T H)^{-1} H^T F_{\text{on}},
\]

\[
g_k = (H^T H)^{-1} H^T (H\theta_k + \omega_n),
\]

\[
\theta^0 = [0.2208 \ -0.3471 \ -0.6379 \ 2.2344].
\]

4. Analysis and results

The partial differential equation to be solved is \(\frac{\partial f}{\partial t} = k \left( \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} \right)\) with a particular solution \(F(x, y) = Axy + c_1x + c_2y + c_3\). For each value of \((x, y)\) \(\exists F(x, y)\) that determines the concentration of material. The database has the following configuration: \(\text{Datos} = [x \ y \ F(x, y)_{\text{sln}}]\) where \(F(x, y)_{\text{sln}}\) is the numerical solution of the partial differential equation \(\gamma(x, y) = \mathbb{R}^2\). For the multiparametric case \([8, 9]\) it has to: \(\omega_n = F - H\theta \sim \mathcal{N}(\bar{0}, \sigma^2\mathbb{I})\), the noise follows a normal multivariate Gaussian distribution (Equation (16) to Equation (18)).
The expected value of noise comes as follows Equation (19) to Equation (22).

\[
\bar{\mu} = \bar{\mu} \Sigma^{-1} = \frac{1}{\sigma^2},
\]

\[
\text{Ln}(p(\omega_n, \theta)) = \text{Ln}(1) - \text{Ln}\left(\frac{N^2}{(2\pi\sigma^2)^N}\right) - \left(\frac{(F-H\theta)^i(F-H\theta)}{2\sigma^2}\right),
\]

\[
\frac{\partial \text{Ln}(p(\omega_n, \theta))}{\partial \theta} = -\frac{1}{2\sigma^2} (-2F^iH + 2H^iH\theta),
\]

\[
\frac{\partial \text{Ln}(p(\omega_n, \theta))}{\partial \theta} = \frac{1}{\sigma^2} H^iH((H^iH)^{-1}H^iF - \theta).
\]

Fisher's information matrix is given by Equation (23) to Equation (25).

\[
\Gamma(\theta) = \frac{1}{\sigma^2} H^iH,
\]

\[
\hat{\theta} = g(F) = (H^iH)^{-1}H^iF,
\]

\[
\frac{\partial \text{Ln}(p(\omega_n, \theta))}{\partial \theta} = \Gamma(\theta)(\hat{\theta} - \theta).
\]

The calculation of the covariance comes as follows Equation (26) to Equation (30).

\[
\varepsilon\{g(F)\} = \varepsilon\{\hat{\theta}\} = \theta,
\]

\[
\varepsilon\{g(F)\} = \varepsilon\{(H^iH)^{-1}H^iF\},
\]

\[
\varepsilon\{g(F)\} = (H^iH)^{-1}H^i\varepsilon\{F\},
\]

\[
\varepsilon\{g(F)\} = (H^iH)^{-1}H^i\varepsilon(\theta + \omega_n),
\]

\[
\varepsilon\{g(F)\} = (H^iH)^{-1}H^iH\theta + \varepsilon(\omega_n).
\]

The expected value of noise \(\omega_n\) is associated with the average of this, that is: \(\varepsilon(\omega_n) = 0\), Equation (31).

\[
\varepsilon\{g(F)\} = (H^iH)^{-1}H^iH\theta = \mathbb{I} \theta,
\]
The hope of the parameters becomes the expected value or the minimum level of Cramer Rao [10]. The average results and standard deviation for Cd are given in Table 4.

|     | CRLB±NR | Σ   |
|-----|---------|-----|
| Cd  | 1.5123±0.1597 | 0.0255 |
| Cd  | 1.3091±0.9152  | 0.8376 |

The Figure 2 show us the minimum bound of variance of the constants A, c1, c2 and c3 of the particular solution, Equation (10), proposed. The minimum bound of variance of the constant A is presented in Figure 2(a), this value sets the expected value of this constant through the samples obtained from the numerical solution with a trend of -0.0671.

![Figure 2](image)

**Figure 2.** Constants of $F(x,y)$, (a) constant A, (b) constant c1, (c) constant c2, and (d) constant c3.

The efficient value for the particular solution gives as a result the variation bound for the constant c1 shown in the graph of Figure 2(b), where it is observed that it takes the trend of 0.3414. Given that each of the constants that multiply the particular solution should not take random values due to the nature of the data, with the bound of the constant c2 shown in the graph of Figure 2(c) it takes the trend of 0.2731. From Figure 2(d) it can be seen that the minimum Cramer Rao bound obtained for the constant c3 takes the trend at 0.2608.

Due to the samples in the database [11], with the Cramer Rao minimum bound obtained for each of the constants A, c1, c2 and c3, it is possible to configure the particular solution using the samples taken from the numerical solution [12]. The parameters $\theta$ with the estimation model are given by Equation (32).

$$\theta^{500} = [-0.0671 \ 0.3414 \ 0.2731 \ 0.2608].$$
5. Conclusions
The minimum variance can be reached by means of the Cramer Rao calculation as shown in the graphs of Figure 2. Since the multivariate data are Gaussian trend or identically distributed as those treated in this document, it was possible to find the convergence of the dimensions lastly, the estimates obtained in the results are efficient since they reach the minimum levels of Cramer Rao as shown in the results section. The statistical exploration proposed in this document allowed to find the coefficients of the particular solution of a partial differential equation by means of the combination of the Cramer Rao technique to know the expected value. With the non-linear technique used to find the optimal value of the constants, the convergence of the coefficients at a given value could be observed thanks to the performance of this technique and the intrinsic characteristics of the database combined with a normal Gaussian distribution.

Among the most important applications of statistical exploration for the estimation of parameters from a database is computational statistics in the estimation of probability density functions due to the volume of samples and characteristics of the databases, which in this document it was treated as the numerical solution of a partial differential equation. The estimation of parameters by means of the probability function induced by the Gaussian white noise allowed to model the equation proposed for the particular solution of this.

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