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Dynamic Error-in-variables Models

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Abstract: Several environmental problems are described by models defined by systems of first order differential equations. Typically, the derivatives of concentrations are expressed as functions of independent variables such as temperature, pressure, pH, etc. However, the independent variables are generally known only through measurements made at discrete times. Thus we have to face two types of difficulties

1) estimate the errors in the measurements of the independent variables
2) assume suitable functional forms for them in the intervals between two successive measurements.

In analogy to the algebraic case, we have chosen to define this class of problems as "dynamic error-in-variables" models. Furthermore we have developed an algorithm to carry out the general estimation problem. An example is described in detail for illustration purposes.

Zusammenfassung: Viele Umweltprobleme können durch Systeme von Differentialgleichungen erster Ordnung beschrieben werden. Gewöhnlich werden Konzentrationsableitungen als Funktionen von unabhängigen Variablen (wie Temperatur, Druck, pH usw.) ausgedrückt. Die unabhängigen Variablen sind aber nur in einer begrenzten Anzahl von Zeitpunkten bekannt. Deswegen müssen zwei Probleme angeschnitten werden:

1) Die experimentellen Abweichungen abschätzen, die in den Abmessungen der unabhängigen Veränderlichen zustande kommen.
2) Die funktionelle Form dieser Variablen in den Zeitabständen vermuten, in denen sie nicht gemessen werden.

Analog zu dem rein algebraischen Fall hat man diese Probleme als dynamische error-in-variables Modelle definiert. Ein Algorithmus für die numerische Lösung dieses Problems wird vorgeschlagen. Weiters wird ein einfacher Fall vollkommen beschrieben.

Keywords: Error-in-variables, Bayesian Estimation, Dynamic Models.

1 Introduction

Several important models can be cast into the form

$$\frac{d\boldsymbol{w_1}}{dt} = f(\boldsymbol{w_1}, \boldsymbol{w_2}, \vartheta, t)$$
$$\boldsymbol{w_1}(0) = \boldsymbol{w_{10}} \qquad (1)$$

where ϑ are unknown parameters and $\mathbf{w}_1$ and $\mathbf{w}_2$ are the sets of variables that can be measured. According to the traditional classification, $\mathbf{w}_2$ can be regarded as independent variables and $\mathbf{w}_1$ as dependent variables.

If the set $\mathbf{w}_2$ were known over all the time interval in which the measurements of $\mathbf{w}_1$ are made, we could set up a suitable objective function Φ (such as the likelihood function) in terms of ($\mathbf{w}_1$-$\mathbf{w'}_1$), where $\mathbf{w}_1$ are the values predicted by the solution of system (1) and $\mathbf{w'}_1$ the corresponding measured values. If the derivatives of the objective function with respect to ϑ were required, the usual system of sensitivity equations could be set up. Unfortunately we only have a limited number of measurements of the set $\mathbf{w}_2$ carried out at discrete times. Thus, we have two types of difficulties.

- First of all the integration of the system of equations (1) requires the knowledge of $\mathbf{w}_2$ over all the time interval. It has been shown in a previous paper (Dovì, to be published) that deviations from interpolated values provided by "parsimony criteria" (typically linear interpolations) are to be taken into consideration for correct parameter estimation.

- Secondly we have to modify the likelihood function so as to include the experimental errors on $\mathbf{w}_2$. Since the methods that take into consideration errors on the independent variables are generally referred to as error-in-variables, we have chosen to define the algorithms capable of dealing with limited knowledge on the independent variables of differential models as dynamic error-in-variables models.

2 Theoretical Developments

Suppose the $\mathbf{w}_1$ variables are measured at N_1 time instants t_{1j}, whereas the $\mathbf{w}_2$ variables are measured at N_2 time instants t_{2j}, with N_1 not necessarily equal to N_2. If the measurements of $\mathbf{w}_1$ and $\mathbf{w}_2$ are statistically independent, with V_1 and V_2 being the two relevant variance-covariance matrices (assumed constant), the resulting likelihood function $\mathcal{L}$ can be written as

$$\mathbf{L} = \mathbf{L}_1 \cdot \mathbf{L}_2 = \frac{1}{\sqrt{2\pi^{(N_1N_2)}}} \frac{1}{\sqrt{(\det \mathbf{V}_1)^{N_1}}} e^{-\frac{1}{2}\sum_{i=1}^{N_1}(\mathbf{w}_{1,i}-\mathbf{w}'_{1,i})^T \mathbf{V}_1^{-1}(\mathbf{w}_{1,i}-\mathbf{w}'_{1,i})} \frac{1}{\sqrt{(\det \mathbf{V}_2)^{N_2}}} e^{-\frac{1}{2}\sum_{i=1}^{N_2}(\mathbf{w}_{2,i}-\mathbf{w}'_{2,i})^T \mathbf{V}_2^{-1}(\mathbf{w}_{2,i}-\mathbf{w}'_{2,i})}$$

According to the maximum likelihood method, we have to maximize $\mathcal{L}$ subject to the constraints (1). If, as usual, we maximize the logarithm of $\mathcal{L}$, we can write

$$-\ln \mathcal{L} = \Phi = \Phi_1 + \Phi_2 = \frac{N_1}{2} \ln \det \mathrm{V}_1 + \frac{1}{2}\sum_{i=1}^{N_1}(\mathbf{w}_{1,i} - \mathbf{w}'_{1,i})^T \mathbf{V}_1^{-1}(\mathbf{w}_{1,i} - \mathbf{w}'_{1,i}) +$$
$$\frac{N_2}{2} \ln \det \mathrm{V}_2 + \frac{1}{2}\sum_{i=1}^{N_2}(\mathbf{w}_{2,i} - \mathbf{w}'_{2,i})^T \mathbf{V}_2^{-1}(\mathbf{w}_{2,i} - \mathbf{w}'_{2,i}) = \min \qquad (2)$$

subject to

$$\frac{d\boldsymbol{w_1}}{dt} = f(\boldsymbol{w_1}, \boldsymbol{w_2}, \vartheta, t)$$
$$\boldsymbol{w_1}(0) = \boldsymbol{w_{10}}$$

Let us show first of all that the variance-covariance matrix $\mathbf{V}_2$ must be known for the function Φ to have a minimum. In fact, if $\mathbf{w}_2 = \mathbf{w}_2'$ and $\mathbf{V}_2 = \mathbf{I}\varepsilon$ (where I is the unit matrix), Φ tends to $-\infty$ as ε tends to zero. In other words there exists a perfectly legitimate solution which can assume arbitrarily large negative values. Of course the same demonstration is not valid for $\mathbf{w}_1$, because, unlike $\mathbf{w}_2$, it is a dependent variable so that the solution $\mathbf{w}_1 = \mathbf{w}_1'$ would not be consistent with the constraints.

Thus we can rewrite the optimization problem (2) as

$$\Phi = \frac{N_1}{2} \ln\det \mathrm{V}_1 + \frac{1}{2}\sum_{i=1}^{N_1} (\mathbf{w}_{10} + \int_0^{t_i} \mathbf{f}\, \mathrm{dt} - \mathbf{w}'_{1,\mathrm{i}})^T \mathbf{V_1}^{-1} (\mathbf{w}_{10} + \int_0^{t_i} \mathbf{f}\, \mathrm{dt} - \mathbf{w}'_{1,\mathrm{i}}) +$$
$$\frac{1}{2}\sum_{\mathrm{i}=1}^{\mathrm{N}_2} (\mathbf{w}_{2,\mathrm{i}} - \mathbf{w}'_{2,\mathrm{i}})^{\mathrm{T}} \mathbf{V_2}^{-1} (\mathbf{w}_{2,\mathrm{i}} - \mathbf{w}'_{2,\mathrm{i}}) = \min \tag{3}$$

This is the most general expression for maximum likelihood algorithms resulting from the model (1). It can be regarded as the maximum likelihood expression for error-in-variables models including differential equations. Hence the definition of dynamic error-in-variables models.

It was shown in a previous paper (Dovì, to be published) that if $\overline{\mathbf{w}}_2(\mathbf{t_j})$ are the reconstructed values of the vector $\mathbf{w}_2(\mathbf{t})$ at the times t_j,, the deviations $\overline{\mathbf{w}}_\mathbf{2}(\mathbf{t}) - \tilde{\mathbf{w}}_\mathbf{2}(\mathbf{t})$ from the function $\tilde{\mathbf{w}}_2(\mathbf{t})$ provided by the parsimony criterion

$$\tilde{\mathbf{w}}_\mathbf{2}(\mathbf{t}) = \overline{\mathbf{w}}_\mathbf{2}(\mathbf{t}_{\mathbf{j}-1}) + \frac{\overline{\mathbf{w}}_\mathbf{2}(\mathbf{t_j}) - \overline{\mathbf{w}}_\mathbf{2}(\mathbf{t}_{\mathbf{j}-1})}{\mathbf{t_j} - \mathbf{t}_{\mathbf{j}-1}} (\mathbf{t} - \mathbf{t}_{\mathbf{j}-1})$$

give rise to the following a-priori probability distribution.

$$\mathcal{L}_0 = \prod_{j=1}^{N_2} \frac{1}{t_j - t_{j-1}} \int_{t_{j-1}}^{t_j} \frac{1}{(2\pi)^{n_2/2} \xi^{n_2} \prod_{r=1}^{n_2} \mathrm{w}'_{2r,j-1}} e^{-\frac{1}{2\xi^2}\sum_{r=1}^{n_2}\left[\mathrm{w}_{2r}(t) - \tilde{\mathrm{w}}_{2r}(t)\right]^2 / \mathrm{w}'^2_{2r,j-1}} \mathrm{dt}$$

where n_2 is the dimension of the vector $\mathbf{w}_2$ and ξ a convenient weight factor.

Thus using a Bayesian regression method we can estimate the parameters ϑ by maximizing the a-posteriori likelihood function $\mathcal{L}_f = \mathcal{L} \bullet \mathcal{L}_0$ or by minimizing

$$-\ln \mathrm{L_f} = \Phi_\mathrm{f} = \frac{\mathrm{N}_1}{2} \ln \det \mathrm{V}_1 +$$

$$\frac{1}{2}\sum_{i=1}^{N_1}(\mathbf{w}_{10}+\int_0^{t_i}\mathbf{f}\left[\mathbf{w}_1(t),\mathbf{w}_2(\tilde{\mathbf{w}}_2,\gamma),t\right]\mathrm{dt}-\mathbf{w}'_{1,\mathrm{i}})^T\mathbf{V}_1^{-1}(\mathbf{w}_{10}+\int_0^{t_i}\mathbf{f}\left[\mathbf{w}_1(t),\mathbf{w}_2(\tilde{\mathbf{w}}_2,\gamma),t\right]\mathrm{dt}-\mathbf{w}'_{1,\mathrm{i}})+$$

$$\frac{1}{2}\sum_{i=1}^{N_2}(\mathbf{w}_{2,\mathrm{i}}-\mathbf{w}'_{2,\mathrm{i}})^T\mathbf{V}_2^{-1}(\mathbf{w}_{2,\mathrm{i}}-\mathbf{w}'_{2,\mathrm{i}})-\sum_{j=1}^{N_2}\ln\int_{t_{j-1}}^{t_j}\exp\left\{-\frac{1}{2\xi^2}\sum_{r=1}^{n_2}\gamma_{jr}^2(t-t_{j-1})^2(t-t_j)^2/w'^2_{2r,j-1}\right\}dt$$

$$= \quad \min \tag{4}$$

where $\mathrm{w}_{2\mathbf{r}}(\mathbf{t})-\tilde{\mathrm{w}}_{2\mathbf{r}}(\mathbf{t}))$ has been parametrized using the simplest one parameter relation

$$\mathbf{w}_{2\mathrm{r}}(\mathrm{t})-\tilde{\mathbf{w}}_{2\mathrm{r}}(\mathrm{t})=\gamma_{\mathrm{r,j}}(\mathrm{t}-\mathrm{t}_{\mathrm{j}})(\mathrm{t}-\mathrm{t}_{\mathrm{j-1}}) \qquad \mathrm{t}_{\mathrm{j\text{-}1}}\le\mathrm{t}\le\mathrm{t}_{\mathrm{j}} \qquad \mathrm{j}=1,.,\mathrm{N}_2 \tag{5}$$

The minimization procedure described above can be started only after the parameter ξ has been assigned a value. This value can be determined if we remember that

$$\chi^2=\sum_{\mathbf{i=1}}^{\mathbf{N_1}}(\overline{\mathbf{w}}_{\mathbf{1i}}-\mathbf{w}'_{\mathbf{1i}})^{\mathbf{T}}\mathbf{V}_{\mathbf{1}}^{-1}(\overline{\mathbf{w}}_{\mathbf{1i}}-\mathbf{w}'_{\mathbf{1i}})+\sum_{\mathbf{i=1}}^{\mathbf{N_2}}(\overline{\mathbf{w}}_{\mathbf{2i}}-\mathbf{w}'_{\mathbf{2i}})^{\mathbf{T}}\mathbf{V}_{\mathbf{2}}^{-1}(\overline{\mathbf{w}}_{\mathbf{2i}}-\mathbf{w}'_{\mathbf{2i}})$$

(where $\overline{\mathbf{w}}_{1i}$ are the final estimated values) follows the chi square distribution $\varphi(\chi^2)$ with $n_1 \bullet N_1 + n_2 \bullet N_2 - 1$ degrees of freedom.

In particular the minimization can be repeated until

$$\sum_{\mathbf{i=1}}^{\mathbf{N_1}}(\overline{\mathbf{w}}_{\mathbf{1i}}-\mathbf{w}'_{\mathbf{1i}})^{\mathbf{T}}\mathbf{V}_{\mathbf{1}}^{-1}(\overline{\mathbf{w}}_{\mathbf{1i}}-\mathbf{w}'_{\mathbf{1i}})+\sum_{\mathbf{i=1}}^{\mathbf{N_2}}(\overline{\mathbf{w}}_{\mathbf{2i}}-\mathbf{w}'_{\mathbf{2i}})^{\mathbf{T}}\mathbf{V}_{\mathbf{2}}^{-1}(\overline{\mathbf{w}}_{\mathbf{2i}}-\mathbf{w}'_{\mathbf{2i}})$$

attains the value that maximizes $\varphi(\chi^2)$.

In other words

$$\sum_{\mathbf{i=1}}^{\mathbf{N_1}}(\overline{\mathbf{w}}_{\mathbf{1i}}-\mathbf{w}'_{\mathbf{1i}})^{\mathbf{T}}\mathbf{V}_{\mathbf{1}}^{-1}(\overline{\mathbf{w}}_{\mathbf{1i}}-\mathbf{w}'_{\mathbf{1i}})+\sum_{\mathbf{i=1}}^{\mathbf{N_2}}(\overline{\mathbf{w}}_{\mathbf{2i}}-\mathbf{w}'_{\mathbf{2i}})^{\mathbf{T}}\mathbf{V}_{\mathbf{2}}^{-1}(\overline{\mathbf{w}}_{\mathbf{2i}}-\mathbf{w}'_{\mathbf{2i}})=\chi^2_{\max}$$

where $\chi^2_{\max}$ is given by $\varphi(\chi^2_{\max})=\max$.

A similar approach has been proposed for the estimation of parameters in approximate models (Dovì et al., 1996). On the other hand, the use of a predetermined functional form of $\mathbf{w}_2(t\ )$ (say $\tilde{\mathbf{w}}_2(t\ )$) can be regarded as a particular form of model approximation.

Clearly the optimization of $\mathcal{L}_f = \mathcal{L} \bullet \mathcal{L}_0$ will provide a value of χ^2 such that $\chi^2 \le \chi^2_s$, where χ^2_s is the value of χ^2 given by the solution of $\mathcal{L}$ =max, ({γ}≡0). In fact $\mathcal{L}_0(\gamma)$ has a maximum at {γ}≡0. Any decrease in $\mathcal{L}_0(\gamma)$ must be compensated by an increase in $\mathcal{L}(\gamma)$ and since $\mathcal{L}$ is a decreasing function of χ^2, it follows $\chi^2 \le \chi^2_s$.

In other words, an increase in the degrees of freedom resulting from the introduction of $\{\gamma\}$ leads to an improved fit of the original model.

As a consequence, the theory developed can be applied only if $\chi_s^2 \geq \chi_{\max}^2$. On the other hand a value of $\chi_s^2 \leq \chi_{\max}^2$ generally implies overparametrization of the original model or wrong values of the variance-covariance matrix V_1 (if known) and is therefore of limited interest.

Equation (6) can now be rewritten as

$$\frac{N_1}{2}\ln\det\ \mathrm{V}_1 - \sum_{j=1}^{N_2} \ln\int_{t_{j-1}}^{t_j} \exp\left\{-\frac{1}{2\xi^2}\sum_{r=1}^{n_2} \gamma_{jr}^2 (t-t_{j-1})^2 (t-t_j)^2 / w_{2r,j-1}'^2\right\} dt = \min$$

subject to (6)

$$\frac{1}{2}\sum_{i=1}^{N_1}(\mathbf{w}_{10} + \int_0^{t_i} \mathbf{f}\left[\mathbf{w}_1(t), \mathbf{w}_2(\tilde{\mathbf{w}}_2, \gamma), t\right] \mathrm{dt} - \mathbf{w}_{1,\mathrm{i}}')^T \mathbf{V}_1^{-1}(\mathbf{w}_{10} + \int_0^{t_i} \mathbf{f}\left[\mathbf{w}_1(t), \mathbf{w}_2(\tilde{\mathbf{w}}_2, \gamma), t\right]\mathrm{dt} - \mathbf{w}_{1,\mathrm{i}}') +$$
$$\frac{1}{2}\sum_{i=1}^{N_2}(\mathbf{w}_{2,\mathrm{i}} - \mathbf{w}_{2,\mathrm{i}}')^T \mathbf{V}_2^{-1}(\mathbf{w}_{2,\mathrm{i}} - \mathbf{w}_{2,\mathrm{i}}') = \chi_{\mathbf{max}}^2$$

In the presence of a high number of data points, additional constraints can be added, so as to constrain subsets of $\{\mathbf{w}_1 \oplus \mathbf{w}_2\}$ to satisfy relevant chi-square distributions.

The whole method has now been outlined.

3 Numerical Developments

The minimization problem described in the previous section is considerably difficult and special numerical techniques must be developed for the practical applicability of the method. This will be done in the next paragraph, which will be followed by the analysis of the results obtained in a special case.

3.1 Numerical Algorithms

It has been shown in a previous paper that the high number of parameters involved in the overall optimizaton requires the development of an ad-hoc algorithm for attaining convergence to the global optimum.

This can be realized by making use of the fact that $\delta \mathrm{w}_2$ is small and thus the overall problem can be linearized with respect to it.

Thus, if we set, for every value of $\{\vartheta, \mathrm{w}_{2\mathrm{k}}\}$

$$-\ln L\ [\gamma,\vartheta,\mathbf{w}_{1m}(\gamma,\vartheta),\mathbf{w}_{2k1}] \cong -\ln L\ [0,\vartheta,\mathbf{w}_{1m}(0,\vartheta),\mathbf{w}_{2k1}] - \sum_j \left.\frac{D\ln L}{D\gamma_j}\right|_{\gamma=0} \gamma_j$$

$$-\ln L_0\ [\gamma,\vartheta,\mathbf{w}_{1m}(\gamma,\vartheta),\mathbf{w}_{2k}] \cong -\ln L_0\ [0,\vartheta,\mathbf{w}_{1m}(0,\vartheta),\mathbf{w}_{2k}] - \sum_j \left.\frac{D\ln L_0}{D\gamma_j^2}\right|_{\gamma=0} \gamma_j^2$$

we can write equation (4) as

$$-\ln L_f\ [\gamma,\vartheta,\mathbf{w}_{1m}(\gamma,\vartheta),\mathbf{w}_{2k}] \cong -\ln L\ [0,\vartheta,\mathbf{w}_{1m}(0,\vartheta),\mathbf{w}_{2k}] - \sum_j \left.\frac{D\ln L_0}{D\gamma_j^2}\right|_{\gamma=0} \gamma_j^2 - \sum_j \left.\frac{D\ln L}{D\gamma_j}\right|_{\gamma=0} \gamma_j =$$

$$-\sum_j \left.\frac{D\ln L_0}{D\gamma_j^2}\right|_{\gamma=0} \gamma_j^2 - \sum_j \left[\sum_m \left(\frac{\partial \ln L}{\partial \mathbf{w}_{1m}}\right)\frac{\partial \mathbf{w}_{1m}}{\partial \gamma_j}\right]_{\gamma=0} \gamma_j = \Phi_f = \min \qquad (7)$$

In equation (7) all terms are readily available except $\frac{\partial \mathbf{w}_{1m}}{\partial \gamma_j}$. It can be evaluated using the system of sensitivity equations

$$\begin{aligned}
&\frac{d\mathbf{w}_{1m}}{dt} = f_m\ [\vartheta, \mathbf{w}_1, \mathbf{w}_2(\gamma = 0, t), t] \\
&\frac{d}{dt}\left.\frac{\partial \mathbf{w}_{1m}}{\partial \gamma_j}\right|_{\gamma=0} = \left.\frac{\partial f_m}{\partial \gamma_j}\right| + \sum_q \left(\frac{\partial f_m}{\partial \mathbf{w}_{1q}}\frac{\partial \mathbf{w}_{1q}}{\partial \gamma_j}\right) \\
&\mathbf{w}_{1m}(0) = \mathbf{w}_{1m0} \\
&\left.\frac{\partial \mathbf{w}_{1m}}{\partial \gamma_j}\right|_{\gamma=0} (0) = 0
\end{aligned} \qquad (8)$$

Thus for every value of the set $\{\vartheta,\ \mathbf{w}_2\}$ optimal values of γ can be computed by minimizing Φ_f with respect to it. This provides

$$\gamma_j = -\frac{1}{2}\left[\left.\frac{D\ln L_0}{D\gamma_j^2}\right|_{\gamma=0}\right]^{-1} \left[\sum_m \left(\frac{\partial \ln L}{\partial \mathbf{w}_{1m}} + \frac{\partial \ln L}{\partial V_1}\frac{\partial V_1}{\partial \mathbf{w}_{1m}}\right)\frac{\partial \mathbf{w}_{1m}}{\partial \gamma_j}\right]_{\gamma=0} \qquad (9)$$

By suitably changing the set $\{\vartheta, V_1, \mathbf{w}_2\}$ (using for instance the procedure described in Dovì et al., 1985) and computing the corresponding values of $\{\gamma\}$ from equation (9), we can attain the minimum of problem (7).

3.2 Numerical Results

The algorithm described has been applied to several examples resulting from simulated data and including up to six parameters.

The example chosen for this paper is intentionally simple, so that the integration can be carried out analytically and the general optimization task reduces to the minimization of an algebraic objective function with respect to two parameters. The model and the data considered are described in Bard (1974) and reported here for the reader's convenience.

The model is given by $\frac{dc}{dt} = -\vartheta_1 e^{-\vartheta_2/T} c$, where $c \equiv w_1$ and $T \equiv w_2$. The data are reported in Table 1.

Table 1 : Data for the numerical example

Run #	Experiment #	Time (hr)	Temperature (°K)	Molar Fractions
1	1	0.1	100	0.980
1	2	0.2	100	0.983
1	3	0.3	100	0.955
1	4	0.4	100	0.979
1	5	0.5	100	0.993
2	1	0.05	200	0.626
2	2	0.1	200	0.544
2	3	0.15	200	0.455
2	4	0.2	200	0.225
2	5	0.25	200	0.167
3	1	0.02	300	0.566
3	2	0.04	300	0.317
3	3	0.06	300	0.034
3	4	0.08	300	0.016
3	5	0.1	300	0.066

The values of T are assumed measured with a mean square error of 10^{-2} °C and the variance-covariance matrix of $\mathbf{w}_1$, which reduces to the variance of c, is supposed constant, its value ranging between 10^{-4} and $2.5\ 10^{-3}$.

It can be shown, using the demonstration provided in Dovì (to be published) that the objective function becomes

$$\Phi = \sum_{r=1}^{3}\sum_{j=1}^{q} \frac{\gamma_{jr}^2 (t_j - t_{j-1})^4}{60\xi^2 T_r^2} = \min$$

subject to

$$\sum_{r=1}^{3}\sum_{k=k'}^{q} \frac{\left(c'_{kr} - c_r^0 e^{-\vartheta_1 t_k e^{-\vartheta_2/T_r}}\right)^2}{\sigma^2} + \sum_{r=1}^{3}\sum_{k=k'}^{q} \frac{\left(T'_{kr} - \overline{T}_{kr}\right)^2}{10^{-4}} - \sum_{r=1}^{3}\sum_{j=1}^{q} \frac{\gamma_{jr}^2 (t_j - t_{j-1})^4}{60\xi^2 T_r^2} = \chi^2_{\max} \qquad (10)$$

Thus the general optimization process reduces to the minimization of an algebraic function with respect to two parameters. To this purpose a standard BFGS algorithm was used, in which the derivatives were computed using the relations

$$\frac{D\Phi}{DT} = \frac{\partial \Phi}{\partial T} + \frac{\partial \Phi}{\partial \xi}\frac{\partial \xi}{\partial T} \qquad \frac{D\Phi}{D\vartheta} = \frac{\partial \Phi}{\partial \vartheta} + \frac{\partial \Phi}{\partial \xi}\frac{\partial \xi}{\partial \vartheta}$$

The two terms $\frac{\partial \xi}{\partial \vartheta}, \frac{\partial \xi}{\partial T}$ were computed by differentiation of constraint (10).

In Table 2 the estimates of ϑ_1 and ϑ_2 computed according to traditional maximum likelihood algorithms (1st column) and those obtained with the algorithm described in this paper (2nd column) are displayed.

Table 2: Estimates of the kinetic parameters

	Maximum likelihood estimates	This work
ϑ_1	813.46	877.98
ϑ_2	960.90	1009.14

As can be seen, nontrivial differences appear in the estimates. These results show the importance of using error-in-variables algorithms in differential models.

4 Conclusions

We have described a new regression method, based on a Bayesian estimation analysis, capable of avoiding the usual assumption of constant independent variables in the system of differential equations that define dynamic models. The numerical results, if compared with those obtained using traditional techniques and/or allowing for fluctuations in the non monitored intervals (Dovì, to be published) indicate the importance of considering the experimental errors in the independent variables.

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