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ESTIMATION OF PERTURBATIONS WITHOUT MODELING ASSUMPTIONS IN SECOND-ORDER ODEs.

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ESTIMATION OF PERTURBATIONS WITHOUT MODELING ASSUMPTIONS IN SECOND-ORDER ORDINARY DIFFERENTIAL EQUATIONS

By Rodolfo Rodriguez

Abstract. This paper is concerned with the estimation of ^a small perturbing function affecting a system of second-order ODEs, in order to get a solution of it fitting ^a given set of measurements. The classical approach consist of perturbation modeling and least-squares parameter specification. Alternative procedures are needed when no a-priori adequate perturbation model is at disposal. ^A general scheme for methods needing no modeling assumption is introduced and ^a complete error analysis of them is obtained. Tills error characterisation allows to determine methods minimising the effect of each error source; therefore, optimal schemes under different restrictions are deduced.

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I. Introduction. The aim of this work is to study the problem of how to determine numerical values of a small perturbing function p(t) , which affects ^a system of second-order ordinary differential equations of the form

$$
\ddot{y}(t) = f(t,y(t)) + p(t),
$$

where f(t,y) is ^a known function and the data consist of measured values of the system solution y(t) and of its first derivative y(t) .

On having ^a perturbation model, the standard aproach consist of leastsquares adjusting its free parameters in order to get ^a system solution fitting the given measurements. Sometimes, either no a-priori modeling is posible, or parameter specification for an actual physical model is an ill-posed problem. In both cases, it is useful to have perturbation estimators not depending on previous modeling assumptions.

The ''obvious" deterministical method of approximating the second-order derivatives y(t) in the equations by using any of the usual difference schemes, would not be ^a good one. For instance if we consider the standard discretisation

$$
\ddot{y}(t) = \frac{y(t-h) - 2y(t) + y(t+h)}{h^2} - \frac{h^2}{12} \bar{y}^{\text{iv}}(t,h)
$$

(where. $\overline{y}_i^{iv}(t, h) = y_i^{iv}(t + \theta_i h)$, $|\theta_i| < 1$) and replace y-values by their **measurements y , we get as an approximation of p(t) :**

$$
\frac{\gamma(t+h)}{p(t,h)} = \frac{\gamma(t-h) - 2\gamma(t) + \gamma(t+h)}{h^2} - f(t,\gamma(t))
$$

For the error in this estimation we have:

$$
p(t) - \tilde{p}(t, h) = -h^2 \bar{y}^T(t, h) + \frac{\delta y(t-h) - 2\delta y(t) + \delta y(t+h)}{h^2} + [f(t, y(t)) - f(t, \tilde{y}(t))],
$$

where jy(s) are the measurement errors of the used y(s)-values.

This characterisation shows that, truncation errors appearing in the determination of small p-values in this way, would be proportional to ² iv ^h and to not-small ^y -values. On the other hand, the measurement 2 error component is O(l/h); so, it is not possible to use an excesively small stepsize h in order to leave the error under a prescribed tolerance.

In some recent papers [5], [6], P. E. Zadunaisky developed ^a class of methods to estimate those perturbations, with truncation errors proportional to higher order derivatives of the small perturbing function. **without modeling assumptions. These methods have been successfully used in several applications: the estimation of non gravitational forces affecting ^a comet's trajectory near the perihelion [5], the modeling of dissipative forces affecting an inertial sensor [7], the localisation of an unknown celestial body detected from the deviations produced in the trajectories of other observable bodies [8]. On the other hand, a variant of these methods has been developed [4] in order to estimate the perturbations in those problems where the measurable data consist of y-values only (and not of y-values).**

The object of the present work is to introduce ^a new approach to this kind of methods in order to get a general scheme of them and a complete error analysis separating its components according to the different error sources. This analysis will allow us to get optimal schemes under several different restrictions. Finally, the obtained optimal schemes will be used in ^a classical problem of Celestial Mechanics in order to show their efficiency.

2. General Scheme. Although the methods we are going to describe are applicable to a set of second-order ODEs, for the sake of simplicity we shall consider a single equation of the form

(2.1)
$$
\ddot{y}(t) = f(t, y(t)) + p(t)
$$
,

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where ^p is an unknown perturbation depending on t .

To study this problem we shall assume that ^p and f are sufficiently regular functions and we particularly suppose that the unknown perturbation and its derivatives are small in relation to the corresponding values of the solution y .

Let t_0 be a point where we are going to compute the perturbation **value and let us assume that it is possible to measure y- and y-values d .d on a mesh centered on ίθ with stepsize h . Let y^ and y^ be the measurements** of $y_k \equiv y(t_k)$ and $\dot{y}_k \equiv \dot{y}(t_k)$ respectively, affected by **small random errors** δy_k and $\delta \dot{y}_k$; **i.e.**, **for** $k = -m, ..., m$ (m2l):

$$
y_k = y_k^d + \delta y_k,
$$

(2.2)

$$
\dot{y}_k = \dot{y}_k^d + \delta \dot{y}_k.
$$

The basic idea of our methods is to compare these measured values with those of the solutions of certain initial value problems "neighbouring" to the original one. These, which will be called reference problems, are obtained from equation (2.1) by dropping the unknown perturbation and by using as initial values the measured data at any of the nodes. (k) That is, for ^k ■ -m,...,m , let ^y (t) be the solution of the reference problem:

(2.3)
$$
\begin{cases} \ddot{y}^{(k)}(t) = f(t, y^{(k)}(t)), \\ y^{(k)}(t_k) = y_k^d, \quad \dot{y}^{(k)}(t_k) = y_k^d \end{cases}
$$

(k) Subtracting Taylor's formulae for ^y and ^y we can write:

$$
(2.4) \t r_k^{\pm} \t s (y_{k\pm 1}^d - y_{k\pm 1}^{(k)}) = (\delta y_k - \delta y_{k\pm 1}) \pm h \delta \dot{y}_k + I_k^{\pm} {\{\Delta^{(k)}(t)\} + I_k^{\pm} {p(t)\}}
$$

where

(2.5)
$$
I_{k}^{\dagger}(g(t)) = \int_{t_{k}}^{t_{k}+1} g(t) (t_{k+1}^{-t}) dt
$$

and

(2.6)
$$
\Delta^{(k)} f(t) \equiv f(t, y(t)) - f(t, y^{(k)}(t)) .
$$

Expresion (2.4) shows that **Taylor integrals** $I_{k} (p(t))$ **can be written in terms** of <u>residuals</u> r_k^{\dagger} (which are differences of known measured values **d (k) ^y . and computable values ^y .), measurement errors and Taylor inte-k±l k±l grais of i^')f(t) which will be shown to be easily computable. So, our next step is to show how to approximate** $p(t_n)$ **by means** of **linear** $\texttt{combinations of} \quad \mathbf{I}^{\pm}_{\cdot\cdot} \{ \mathbf{p}(\mathbf{t}) \} \quad \texttt{terms}.$

Let us consider a set of coefficients

$$
A = \{a_k^+, k = -m, ..., m-1; a_k^-, k = -m+1, ..., m\}.
$$

We shall look for conditions over these coefficients in order to get a linear combination

$$
-\frac{1}{h^{2}}\left[\begin{matrix} m-1 & m \\ \sum a_{k}^{+} 1^{+}_{k} \{p(t)\} + \sum a_{k}^{-} 1^{+}_{k} \{p(t)\} \\ k=-m+1 \end{matrix}\right]
$$

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approximating $P_0 \equiv p(t_0)$. To study this we can integrate Taylor series **for p to get:**

(2.7)
$$
I_{k}^{\pm}{p(t)} = h^{2} \sum_{r=0}^{\infty} \beta_{r}^{(k)} \frac{(\pm h)^{r} p_{0}^{(r)}}{(r+2)!}
$$

where

(2.8)
$$
\beta_{r}^{(k)} = [(k+1)^{r+2} - k^{r+2} - (r+2)k^{r+1}],
$$

(Because of notational simplicity we use Taylor series; notwithstanding our results remain valid provided the perturbation ^p admits (R+l) continuous derivatives, being ^R the order of the approximation),

In particular $\beta_0^{(k)} = 1$ and so our approximation error is:

$$
P_0 - \frac{1}{h^2} \begin{bmatrix} m-1 & m \\ \sum a_i I_k(p(t)) + \sum a_i I_k(p(t)) \end{bmatrix}
$$

\n
$$
= \begin{bmatrix} m-1 & m \\ k=-m+1 & k \end{bmatrix} \frac{P_0}{2!} - \sum_{r=1}^{\infty} \begin{bmatrix} m-1 & m \\ \sum a_i I_k(-1)^r a_{-k} B_r(p(t)) \end{bmatrix} \frac{h P_0}{(r+2)!}.
$$

So, to have a linear expresion approximating p_0 when **h** \rightarrow 0, the **+ 'coefficients a, have to verify the compati billty condition:**

(2.9)
$$
\sum_{k=-m}^{m-1} \binom{+}{k} = 2.
$$

Assuming such a condition, we can write for the truncation error σ(Α) of this approximation:

(2.10)
$$
\sigma(A) = p_0 - \frac{1}{h^2} \begin{bmatrix} m-1 & m \\ \sum a_i I_i(p(t)) + \sum a_i I_i(p(t)) \\ k=-m+1 \end{bmatrix}
$$

$$
= \sum_{r=1}^{\infty} \gamma_r(A) \frac{h^{\Gamma}(r)}{(r+2)!},
$$

where the factors γ^(Α) depend on the particular set ^A of coefficients; that is:

(2.11)
$$
\gamma_{r}(A) = \sum_{k=-m}^{m-1} [a_{k}^{+}(-1)^{r} a_{-k}^{-}] \beta_{r}^{(k)}
$$

Now in order to get an effectively computable expresion for p_0 **we shall (k) use (2.4), where the Taylor integrals Ι^{Δ f(t)} will be calculated (k) by discretising them with approximated ^Δ f-values:**

(2.12)
$$
\Delta^{(k)} f_j^d = f(t_j, y_j^d) - f(t_j, y_j^{(k)})
$$

+ By the moment, let us merely call ^r^ to the computed integrals and + e^ to the corresponding errors; that is:

(2.13)
$$
I_{k}^{\pm} \{ \Delta^{(k)} f(t) \} = \delta r_{k}^{\pm} + e_{k}^{\pm}.
$$

+ Later, we shall show that it is possible to get approximations ir^ such + that the errors e^ be negligible if ^a stepsize ^h small enough is used.

By using expresions (2.4) and (2.10), and dropping all the error terms, we get an estimated p_0 -value:

(2.14)
$$
\begin{array}{ccc} \n\gamma & = & \frac{1}{\sqrt{2}} \left[\sum_{k=-m}^{m-1} \frac{1}{k} (r_k^+ - \delta r_k^+) + \sum_{k=-m+1}^{m} a_k^-(r_k^- - \delta r_k^-) \right]. \n\end{array}
$$

The error $δp_0$ of this estimation can be written

(2.15)
$$
\delta_{P_0} = p_0 - \gamma_0 - N(A) + M(A) + \sigma(A) + E(A),
$$

where each component in this expresión takes account of a different error source; that is:

(2.16)
$$
N(A) = \frac{1}{h^2} \left[\sum_{k=-m}^{m-1} a_k^+(\delta y_{k+1} - \delta y_k) + \sum_{k=-m+1}^{m} a_k^-(\delta y_{k-1} - \delta y_k) \right],
$$

which comes from the measurement errors in the determination of y—valuesj

(2.17)
$$
M(A) = \frac{1}{h} \left[\sum_{k=-m+1}^{m} a_k^T \delta \dot{y}_k - \sum_{k=-m}^{m-1} a_k^T \delta \dot{y}_k \right],
$$

which comes from the measurement errors in the determination of y-values; σ(Α) is the truncation error of expresión (2.10), and,

(2.18)
$$
E(A) = -\frac{1}{h^2} \begin{bmatrix} m-1 & m \\ \sum a^+e^+ & \sum a^-e^- \\ k^-=m \end{bmatrix},
$$

which comes from the errors in the numerical computation of the integral terms $I_k^{\pm} \{\Delta^{(k)} f(t)\}$.

3. Optimal schemes. Our next step is to study the possibility of determining values of the coefficients in ^A in order to get optimal schemes in the sense of minimising the error δp_0 in the estimation of the pertur**bation. To do this, it is necessary to consider bounds of the components N(A) and M(A) , not depending on the particular set of measurement errors Sy^ and δγ^ respectively.**

Let δΥ be an upper bound of measurement errors dy^ ; e< g.;

(3.1)
$$
\delta Y = \max_{-\text{m}\leq k\leq \text{m}} |\delta y_k|.
$$

Then, arranging the terms in (2.16) It is possible to write:

$$
N(A) \leq \nu(A) \frac{\delta Y}{h},
$$

where

(3.3)
$$
v(A) = \left| -a_{-m}^{+} + a_{-m+1}^{-} \right| + \sum_{k=-m+1}^{m-1} \left| a_{k-1}^{+} - a_{k}^{-} + a_{k+1}^{-} - a_{k}^{-} \right| + \left| a_{m-1}^{+} - a_{m}^{-} \right|.
$$

The estimation (3.2) is optimal and it is the unique that can be done in absence of any hypothesis about dy^-errors distribution.

Analogously, if we define

(3.4)
$$
\delta \dot{Y} = \max_{-m \le k \le m} |\delta y_k|,
$$

we can write the optimal bound

$$
M(A) \leq \mu(A) \frac{\delta \tilde{Y}}{h},
$$

where

(3.6)
$$
\mu(A) = |a_{-m}^{+}| + \sum_{k=-m+1}^{m-1} |a_{k}^{+} - a_{-k}^{-}| + |a_{m}^{-}|.
$$

The error component E(A) could be bounded in ^a similar way but it will not be described because we shall show later that its effect is negligible if an adequate quadrature formula and ^a sufficiently small stepsize h are used. So, neglecting this component, we can write:

(3.7)
$$
|\delta p_0| \le v(A) \frac{\delta Y}{h} + \mu(A) \frac{Y}{h} + \sum_{r=1}^{\infty} |\gamma_r(A)| \frac{h^r| p_0^{(r)}}{(r+2)!} \equiv \epsilon(A, h) .
$$

By means of convexity arguments it is easy to show that to get ^a minimum of e(A,h) it is sufficient to consider symmetric sets ^A of coefficients in the sense of verifying:

(3.8)
$$
a_k^+ = a_{-k}^-, k^{=-m}, \ldots, m-1
$$

In such a case, each set of coefficients is determined by the a, s ^a k k values, and, the characterisations (2,16), (2.17), (2.18), the bounds (3.3), (3,6) and the compatibility condition (2.9), can be rewritten in terms of the a, 's. Moreover, from (2.11) we have for r odd k

$$
\gamma_{r}(\mathbf{A}) = 0 ,
$$

and, therefore, the truncation error can he rewritten

(3.9)
$$
\sigma(A) = \sum_{s=1}^{\infty} \gamma_{2s}(A) \frac{h^{2s}(2s)}{(2s+2)!}
$$

with

(3.10)
$$
\gamma_{2s}(A) = -2 \sum_{k=-m}^{m-1} a_k \beta_{2s}^{(k)}.
$$

At this point, the problem of finding optimal schemes can be formulated in the foliowig terms: given realistic bounds for the measurement errors 6Y and δΥ , and estimations of the even order derivatives of the unknown perturbation, to determine the number mtN , the set of coefficients ^a ,...^s^a , satisfying the compatibility condition (2.9) and, eventually, the step size h>0 , lit such a way that the error bound e(A.,h) attains its minimum.

Because of the impossibility of a theoretical solution for this optimisation problem, we made an exhaustive numerical experimentation with different values for the needed bounds. This experimentation shows that in most of cases, e(A,h) takes its minimum when one of both components **coming from measurement errors -that is N(A) or M(A)- vanishes. (Let us remark, that there is no set of coefficients verifying the compatibility condition and such that both components vanish simultaneously).**

So, we decided to study each case separately in order to get optimal schemes under two different restrictions:

Case ¹ : N(A) ⁼ 0, for those problems whose main error source is the determination of solution values;

Case 2: M(A) ⁼ ⁰ , for those problems whose main error source is the determination of derivative values.

It is necessary to remark that in each case, the effect of the corresponding measurement errors does not disappear, because of the neglected component E(A) . Later on studying this component, we shall show that 6y^ and 6y^ errors appear there but not affected by amplifying factors $O(1/h)$ or $O(1/h^2)$.

In the two following sections we shall describe the main results which can be obtained under each restriction. For the sake of brevity, we shall not give In this paper the proofs of some assertions. These proofs are straightforward (see reference [3]) and, in our opinion, they are not relevant for the comprehension of the main ideas introduced in this work.

4. Robust methods under solution measurement errors. In this section we shall describe methods whose main part of the error is not affected

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by measurement errors Cy in the DDEs solution; namely methods with ^a vanishing M(A) component. The coefficients defining such a scheme must verify (see (3.2), (3.3) and (3.8)):

$$
a_{k-1} = a_{k-1}, \quad k=1, \ldots, m
$$

and in this case the set ^A of coefficients is determined by the values of a_0, \ldots, a_{m-1} .

In order to simplify the error analysis of these methods it is convenient to make ^a change of coefficients. Let

$$
b_k = a_{k-1} - a_k, \text{ for } k=1,...,m-1 ,
$$

(4.2)
$$
b_m = a_{m-1} .
$$

The remaining error components can be written in terms of the new coefficients. The component which takes account of 6y^ errors is

(4.3)
$$
M(A) = \frac{1}{h} \sum_{k=1}^{m} b_k (\delta \dot{y}_k - \delta \dot{y}_{-k})
$$

and then, the bound (3.5) , $K(A) \leq \mu(A)\delta Y/h$, is valid with

$$
\mu(A) = 2 \sum_{k=1}^{m} |b_k|.
$$

For the coefficients of the. truncation error (3.9) w may write:

(4.5)
$$
\gamma_{2s}(A) = -2 \sum_{k=1}^{m} k^{2s+1} b_k
$$

On the other hand the compatibility condition cu the b, *s is now: ^k

$$
\begin{array}{c}\n\mathbf{m} \\
\sum k \, b_k = \frac{1}{2} \, .\n\end{array}
$$

At this point, the number m«N and the corfftciente b,,...,b satisfying (4.C)^f can be chosen in ^a free way. Sc. it 1ε yet possible to impose additional restrictions. We shall study how to get optimal schemes under two different criteria.,

Each criterion is an attempt to minimise the effect of each remaining error source. The two additional requirements are:

a) to have derivative measurement error' bound p(A) attaining its minimum.

b) to have truncation error σ(Α) of maximal order in terms of the stepsize ^h ,

and we shall analise each case separately.

Case l.a. In this case it is easy to show that under the restriction imposed by the compatibility condition, ^μ(A) attains its minimum at the set of coefficients corresponding to:

 \bullet

(4.7)
$$
b_k = \begin{cases} 0, & \text{if } k=1,...,m-1 \\ 1/2m, & \text{if } k=m. \end{cases}
$$

The error in the estimation of the perturbation obtained with these coefficients is

(4.8)
$$
\delta p_0 = \frac{\delta \dot{y}_n - \delta \dot{y}_m}{2mh} - \sum_{s=1}^{\infty} \frac{(\text{mh})^2 s_0 (2s)}{(2s+1)!} - \frac{1}{2m} \sum_{k=-m}^{m-1} (\mathbf{e}_k^+ \mathbf{e}_k^-)
$$

which depends on (mh) but not on ^m or ^h separately, in an essential way.

If we neglect the 0(h)-terms in the truncation error, we get as an approximate bound:

(4.9)
$$
|\delta p_0| \leq \frac{\delta \dot{Y}}{\min} + \frac{(\min)^2 |p_0\|^2}{6} + 2 \max_{-\text{m} \leq k \leq m-1} |\epsilon_{\pm k}^{\pm}|,
$$

(we also assume ρθ/Ο). So, the best procedure is to use. m=l (in order to reduce computational cost) and a stepsize h (eventually a multiple of the original one) which minimise the previous bound. An actual computation of such an ^h is usually not possible because of the necessity of having ^a good estimate for ρθ . In spite of this, the previous analysis shows the existence of an optimal stepsize and it suggests the convenience of experimentation with different ones.

The optimal scheme corresponding to m=l , will be described at the end of this section.

Case l.b. In this case, it is easy to show that for every value of m<N , the set of coefficients corresponding to

(4.10)
$$
b_k = \frac{(-1)^{k+1} (\frac{m!}{m!})^2}{k (\frac{m+k}{m-k})^2}, \quad k=1,...,m
$$

satisfies γ_{2s}^{\bullet} (A) = 0, for $s=1,\ldots,n-1$, and the compatiblity condition **(4.6). So, it defines ^a method with truncation error of maximal order, that is** $\sigma(A) = O(h^{2m})$.

2m+2 Once more, neglecting rhe O(h)-terms in the truncation error and the component coming from the computation of $I^{\pm}_k(\Delta^{(k)}f(t))$ **too, we** get **ⁱ ^z (2m). _ . as an approximate bound (assuming ρθ):**

(4.11)
$$
|\delta p_0| \lesssim 2(m!)^2 S_m \frac{\delta \dot{Y}}{h} + \frac{(m!)^2}{(2m+1)!} h^{2m} |p_0^{(2m)}|,
$$

where

(4.12)
$$
S_{m} = \sum_{k=1}^{m} \frac{1}{k (m+k)!(m-k)!}.
$$

From ^a theoretical point of view, it would be posible to determine an optimal stepsize

$$
h_{\text{opt}} = \left[\frac{(2m+1)!}{m} S_m \frac{\delta \dot{\gamma}}{\left|P_0^{(2m)}\right|}\right]^{\frac{1}{2m+1}}
$$

and by using this stepsize we would get as an optimal bound of (4.11)

$$
(2m+1)(m!)^2 \left[\frac{s^{2m}}{\sqrt{\frac{2m}{m}}(2m+1)!} \frac{|p_0^{(2m)}|}{\delta \dot{Y}}\right]^{\frac{1}{2m+1}} \delta \dot{Y}.
$$

As the factor

$$
(2m+1)(m!)^{2}\left[\frac{s_{m}^{2m}}{m^{2m}(2m+1)!}\right]^{\frac{1}{2m+1}}
$$

grows with ^m , whenever the involved perturbation derivatives are smaller than δΥ , the optimal value of that bound will be attained at m=¹ .

If that is not the case, it is not possible to do ^a theoretical comparison among methods of different orders. Notwithstanding, numerical experience did not show any adventage for higher order methods, when a near optimal stepsize was used. Therefore, lower order methods will be preferable because of computational effort.

2 Example 1. For m=l , the optimal 0(h)-method is exactly the same that was obtained under the previous restriction in case ¹ .a. For this method, the estimation of the perturbation is

(4.13)
$$
\begin{array}{rcl}\n\gamma_0 &=& \frac{1}{2h^2} (\gamma_1^+ + \gamma_0^+ + \gamma_0^- + \gamma_1^-) \\
\gamma_1^+ &=& \frac{1}{2h^2} (\gamma_1^- + \gamma_0^- + \gamma_0^- + \gamma_1^-)\n\end{array}
$$

where

 \hat{r}_k^{\pm} = r_k^{\pm} - δr_k^{\pm} , **(4.14)**

 $\frac{1}{r}$ = $\begin{pmatrix} y' & -y' \\ y' & -y' \end{pmatrix}$ are the previously defined residuals and $\delta r^{\frac{1}{r}}$ are the $k \times k$ ¹ k ¹ **following numerical approximations** of $I_{k}^{t}(\Delta^{(k)}f(t))$ ($\Delta^{(k)}f_{1}^{d}$ are the **approximate evaluations** of $\Delta^{(k)}f$ **defined in** (2.12)):

$$
\delta r_{-1}^{+} = \frac{h^{2}}{24} (6\Delta^{(-1)} f_{0}^{d} - \Delta^{(-1)} f_{1}^{d}), \qquad \delta r_{0}^{+} = \frac{h^{2}}{24} (-\Delta^{(0)} f_{-1}^{d} + 3\Delta^{(0)} f_{1}^{d}),
$$
\n(4.15)\n
$$
\delta r_{0}^{-} = \frac{h^{2}}{24} (3\Delta^{(0)} f_{-1}^{d} - \Delta^{(0)} f_{1}^{d}), \qquad \delta r_{1}^{-} = \frac{h^{2}}{24} (-\Delta^{(1)} f_{-1}^{d} + 6\Delta^{(1)} f_{0}^{d}).
$$

The error in this **estimation** of *p***₀ is:**

(4.16)
$$
\delta p_0 = \frac{\delta \dot{y}_1 - \delta \dot{y}_1}{2h} - \sum_{s=1}^{\infty} \frac{h^2 s_0^{(2s)}}{(2s+1)!} + E(A) ,
$$

where the component E(A) , coming from the errors in the numerical computation of $I_{k}^{\pm}(\Delta^{(k)}f(t))$, can be splitted in two terms:

(4.17)
$$
E(A) = \frac{\delta f_{-1} + 4 \delta f_0 + \delta f_1}{6} + \tau.
$$

The first one involves the differences

(4.18)
$$
\hat{f}_j = f(t_j, y_j) - f(t_j, y_j^d)
$$

which can be bounded by means of ^a Lipschitz constant ^L cf f and d measurement errors in ^y ; 1.e.:

$$
|\delta f_j| \leq L \delta y_j.
$$

powers of h ; in particular: (k) The second one can be written in terms of ^Δ f derivative values and

(4.20)
$$
\tau = \frac{\Delta^{(-1)} f_0^{111} - \Delta^{(1)} f_0^{111}}{45} h^3 + \frac{1}{\sum_{k=1}^{\infty} c_k \Delta^{(k)} f^{1v} (\xi_k) h^4},
$$

.where $\mathbf{F_k}(\mathbf{t}_{-1}, \mathbf{t}_1)$ and \mathbf{c}_k are numerical constants.

i^^f- derivatives will be shown (see the appendix) to be bounded by measurement errors and perturbation derivatives. Therefore, both truncation errors in this method are actually proportional to perturbation derivatives instead of y-derivatives.

Finally, we must remark that in E(A) there appears the influence 2 of óy^ errors but, as it was previously stated, not affected by 0(1/h) factors.

5. Robust methods under derivative measurement errors. Now we shall look for optimal schemes, such that its main part of the error be not affected

by measurement errors ¿y. in the ODE solution derivative. We shall k proceed in an analogous way to that of the previous section. To get a vanishing $M(A)$ component for any particular errors $\delta \dot{y}_k$, it is necessary **to consider coefficients satisfying (see (3.5), (3.6) and (3.8)):**

(5.1)
$$
a_{-k} = a_{k}, \quad k=1,...,m-1,
$$

$$
a_{-m} = 0.
$$

The set A is again determined by the values a_0, \ldots, a_{m-1} . The adequate **change of coefficients is in this case:**

(5.2)
$$
c_k = a_{k-1} - 2a_k + a_{k+1}, \quad k = 1,...,m-1,
$$

$$
c_m = a_{m-1},
$$

(where we are considering 3^=0) and we may write the remaining error components in terms of the c^'s . Namely:

(5.3)
$$
N(A) = \frac{1}{h^2} \left[\sum_{k=1}^{m} c_k (\delta y_k + \delta y_{-k}) - 2(\sum_{k=1}^{m} c_k) \delta y_0 \right],
$$

and so, the inequality (3.2), $N(A) \le v(A)\delta Y/h^2$, is satisfied with

(5.4)
$$
v(A) = 2 \sum_{k=1}^{m} |c_k| + 2 |\sum_{k=1}^{m} c_k|.
$$

For the truncation error coefficients we may write

(5.5)
$$
\gamma_{2s}(A) = -2 \sum_{k=1}^{m} k^{2s+1} c_k
$$

and the compatibility condition is now

$$
\sum_{k=1}^{m} k^2 c_k = 1.
$$

As in the last section, it is possible to choose arbitrary values for the number meN and the coefficients c,,...,c satisfying this ¹ tn compatibility condition. Once again, we shall study two cases in order to minimise the effect of each remaining error source:

a) methods with ^a measurement error bound v(A) attaining its minimum,

b) methods with truncation error σ(Α) of maximal order in terms of the stepsize h .

Case 2.a. In this case, it is easy to show that ^V(A) attains its minimum, under the restriction (5.6), for the set of coefficients corresponding to:

(5.7)
$$
c_k = \begin{cases} 0, & \text{if } k=1,...,m-1 \\ 1/m^2, & \text{if } k=m \end{cases}
$$

The error in the estimation of the perturbation obtained with these coefficients is:

(5.8)

which again depends on (mh) but not on ^m or h in an essential way. 4 Keglecting the 0(h)-terms in the truncation error we have the approximate bound:

$$
(5.9) \t\t\t\t |\delta p_0| \leq \frac{4\delta Y}{(mh)^2} + \frac{(mh)^2|p_0^n|}{12} + \max_{-h \neq 1 \leq k \leq m-1} |e_k^+ + e_k^-|,
$$

(we have assumed $p_0^{\text{H}} \neq 0$). Just as in the previous section, the best proce**dure is to use 8=1 and ^a stepsize ^h (eventually ^a multiple of the original one) which minimise the previous bound. Usually it is not possible to have a theoretical a-priori estimation of the optimal stepsize (because of the necessity of ρθ-estimates), but the previous analysis suggest the convenience of trying with different ones.**

The optimal scheme corresponding to hf^I **, will be described at the end of this section.**

Case 2,b. In this case it is easy to show that for every value of m*N , the set of coefficients corresponding to

(5.10)
$$
c_k = \frac{2(-1)^{k-1} (m!)^2}{k^2 (m+k)!(m-k)!}, \quad k=1,...,m
$$

satisfies $Y_{2a}(A) = 0$, for $s=1,...,m-1$ and the compatibility condition **(5.6). So, it defines ^a method with truncation error of optimal order,** $name{1y}$ $\sigma(A) = O(h^{2m})$ **.**

Neglecting again the 0(h^^m ^)-terms in σ(Α) and the component arising from the computation of $I^{\pm}_k\{\Delta^{(k)}f(t)\}$, we get as an approximate error **bound (assuming** $P_0^{(2m)} \neq 0$):

(5.11)
$$
|\delta_{P_0}| \leq 8(m!)^2 T_m \frac{\delta Y}{h^2} + \frac{2(m!)^2}{(2m)!} h^{2m} |p_0^{(2m)}|,
$$

where

(5.12)
$$
T_m = \sum_{k=1}^{m} \frac{1}{k^2 (m+k)!(m-k)!}
$$

From ^a theoretical point ci view, it would be possible to determine cn optimal stepsit.e

$$
h_{opt} = \left(\frac{(2m+2)!}{m} 4T_m \frac{\delta Y}{\left[p_0^{(2m)} \right]} \right)^{\frac{1}{2m+2}}
$$

and by using, it, the optimal value of bound (5.12) would be:

$$
8(\pi+1)(\pi!)^{2}\left[\frac{T_{m}^{m}}{2(\pi^{m}(2\pi+2))!}-\frac{p_{0}^{(2m)}\pi^{m}}{(\pi+1)(\pi+1)}\right]\pi+1}.
$$

Δε the factor

$$
B(\mathbf{m}^{t+1})(\mathbf{m}^{t})^2 \left[\frac{\mathbf{T}^{\mathbf{m}}}{4\mathbf{m}^{\mathbf{m}}(2\mathbf{m}^{t}2)!}\right]^{\frac{1}{\mathbf{m}^{t}1}}
$$

grows with ^m , whenever the involved perturbation deiivativcc are smaller then ίϊ , the optimal value of that bound attains at m-1 .

If that is not the case, it is not possible to do ^a theoretical comparison. among methods of different orders. Once again, numerical experiments did not show any adventage for methods of higher order. If ^a near optimal stepsize were used. So, lower order methods will be preferable.

For m=l , the optimal 0(h)-method is exactly the same that was obtained under the previous restriction in case 2.a. It is interesting to remark. that the method developed in reference [8] by quite a different way, 4 coincides with the optimal 0(h)-scheme of case 2.b (see reference [3]).

2 Example 2. We shall describe now the optimal 0(h)-method. The perturbation estimation is in this case:

(5.13)
$$
\int_{0}^{\infty} = \frac{1}{h^2} (r_0^+ + r_0^- - \delta r_0) ,
$$

where $r_0^{\pm} = (y_{\pm 1}^d - y_{\pm 1}^{(0)})$ are the standard residuals and δr_0 is the follow**ing numerical approximation** of $I_0^{\dagger}(\Delta^{(0)}f(t)) + I_0^{\dagger}(\Delta^{(0)}f(t))$:

(5.14)
$$
\delta r_0 = \frac{h^2}{12} \left(\Delta^{(0)} f_{-1}^d + \Delta^{(0)} f_1^d \right) .
$$

The error in this estimation of p_0 is

(5.15)
$$
\delta p_0 = \frac{\delta y_{-1} - 2\delta y_0 + \delta y_1}{h^2} - 2 \sum_{s=1}^{\infty} \frac{h^{2s} p_0^{(2s)}}{(2s+2)!} - e_0,
$$

where the component e_0 , coming from the numerical computation (5.14), **can be written**

$$
(5.16) \qquad e_0 = \frac{\delta f_{-1} + 10 \delta f_0 + \delta f_1}{12} - \frac{\Delta^{(0)} f^{iv} h^4}{240} + C \Delta^{(0)} f^{v1}(\xi) h^6
$$

with $\xi \in (t_{1}, t_{1})$ and C being a numerical constant.

Let us recall that 6f -values defined in (4.18), can be bounded in j terms of **a** Lipschitz constant of **f** and δy ⁻values (form. (4.19)) and **(0) that ^Δ f-derivatives will be shown in the appendix to be bounded by measurement errors and perturbation derivatives.**

6. Numerical experiments. In order to show the efficiency of the optimal schemes developed in the previous sections, we applied them to a classical problem of Celestial Mechanics: the localisation of an unknown massiv body whose presence is presumed because of the gravitational perturbative forces affecting other observable celestial bodies.

The particular problem we use to test our methods is the "discovery" of Neptune from the deviations that it causes in Saturn's and UranUs* orbits. Neptune was actually discovered at the end of the last century by Leverrier and Adams by means of perturbational methods of analytical nature.

We made a numerical simmulation with a simplified "solar system" composed only by the Sun and the three involved planets. To get the "true" positions and velocities of both observable planets -Saturn and Uranus-, the classical

motion equations in heliocentric coordinates for this four bodies problem were integrated to ^a high precision with true initial conditions. This and all the numerical integrations needed for this experiment were made by using a subroutine based on the well-known Bulirsch-Stoer extrapolation method [1].

The "measured" positions and velocities were got by adding to the "true" values, "measurement errors" taken from a zero mean normal random sequence scaled to specific realistic variances obtained from reference [2]. See Table 6.1.

TABLE 6.1

Variances of "measured" positions and velocities

With this measured data we tried to estimate the perturbatory gravitational forces owing to Neptune and affecting the motion equations of the other two planets; i.e.:

(6.1)
$$
\begin{cases} \bar{y}_{U} = G[(m_{\theta} + m_{U})\nabla_{U}(\mathbf{N}y_{U} + \mathbf{N}^{T}) - m_{S}\nabla_{S}(\mathbf{N}y_{S} - \mathbf{y}_{U} + \mathbf{N}^{T}) + \mathbf{p}_{U}, \\ \bar{y}_{S} = G[(m_{\theta} + m_{S})\nabla_{S}(\mathbf{N}y_{S} + \mathbf{N}^{T}) - m_{U}\nabla_{U}(\mathbf{N}y_{U} - \mathbf{y}_{S} + \mathbf{N}^{T}) + \mathbf{p}_{S} \end{cases}
$$

where the indexes means: ^Θ Sun, ^U Uranus, ^S Saturn, (and, later on, N Neptune); $\mathbf{m}_{\mathbf{A}}$ is the mass of body **A** ; $\nabla_{\mathbf{A}}$ is the gradient respect **the variables** y^{\prime} **;** $\|\cdot\|$ **is the usual euclidean norm; G** is the **universal gravitational constant, and, p^ and p\$ are the ''unknown*' gravitational forces affecting Uranus' and Saturn's orbits respectively.**

To estimate this gravitational perturbations we used both optimal 2 0(h)-schemes described in sections ⁴ and 5; let us call each procedure PERT-1 and PERT-2 respectively. We experimented too with the higher order optimal schemes obtained in the same sections, but these results will not be described, because they are more or less of the same quality than those of PERT-1 and PERT-2 (and more expensive in computational cost).

In order to get an idea of the quality of this estimations we used them for the inverse problem of determining the position and mass of the "unknown" planet -Neptune- by solving in the least square sense the rectangular system of non linear algebraic equations

(6.2)
$$
\begin{cases} P_{U} = -G \mathbb{m}_{N} \mathbb{V}_{N} (\|\mathbf{y}_{N} - \mathbf{y}_{U}\|^{-1} - \|\mathbf{y}_{N}\|^{-1}) , \\ P_{S} = -G \mathbb{m}_{N} \mathbb{V}_{N} (\|\mathbf{y}_{N} - \mathbf{y}_{S}\|^{-1} - \|\mathbf{y}_{N}\|^{-1}) , \end{cases}
$$

defining the perturbative forces. To solve this system, with the "treasured" positions of Uranus and Saturn and the obtained estimations of the perturbative forces, we used Newton's method with the "true" Neptune's position and mass as initial guess.

Finally we computed Neptune's spherical coordinates -right ascension and declination- from its cartesian ones. The error in the estimation of these magnitudes is what determines the possibility of visual localisation of the "unknown" planet.

Each procedure, PERT-1 and PERT-2, was accomplished with different stepsizes in order to find an optimal one. The obtained results showed for both schemes that the optimal stepsize is such that measurement and truncation errors are approximately of the same magnitude. For PERT-1 it is between ⁸⁰⁰ and ²⁰⁰⁰ days and for PERT-2 between ²⁰⁰⁰ and ³⁰⁰⁰ days. The amplitude of these intervals shows a big robustness of our methods under the choice of stepsize.

Table 6.2 summarise the results obtained with each scheme at different dates. The efficiency of each computed magnitude has been estimated by means of the expression

$$
(6.3) \qquad \qquad \mathbf{eff}(\stackrel{\sim}{\mathbf{q}}) = -\log_{10}(\frac{\stackrel{\sim}{\mathbf{q}}-\mathbf{q}}{\stackrel{\sim}{\mathbf{q}}})
$$

where ^q is the approximation of ^q . When this efficiency is positive,

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it roughly counts the number of significant decimal digits correctly calculated.

The estimation of the unknown Neptune's mass and coordinates strongly depends on the particular measurement errors of the data. In order tr be able to appreciate the general behaviour of each method. Table 6.2 shows the averages of absolute value of errors and of the efficiencies for each computed magnitude, over three experiments carried out with different particular measurements.

TABLE 6.2

Errors and efficiencies for PERT-1 and PERT-2

PERT-1 PERT-2

Comparing the results of each method in Table 6.2, a better performance of PERT-1 can be observed. Such a behaviour could be predicted attending to the previously made error analysis and to the lower variances of velocity data. Table 6.1 shows that data errors in planet's position are greater than those in planet's velocities. So, ^a method with ^a vanishing N(A) component -like PERT-1- should be preferable to ^a method with ^a vanishing M(A) component -like PERT-2-, since N(A) takes care of position errors and M(A) of velocity ones. In fact, it explains too that optimal stepsizes for PERT-2 are bigger than those for PERT-1, since measurement and truncation errors must be approximately of the same magnitude when using such optimal stepsize.

Finally, we must remark that Neptune's angular coordinates predicted by using PERT-1 are sensibly more precise than those obtained with the $O(h^2)$ **0(h) optimal method of case 2.b, which essentially is the same that was used in reference [8].**

7. Concluding remarks. Every method introduced in references [4], [5], [6], [7] and [8] to estimate perturbations in ODEs without modeling assumptions and with truncation errors proportional to its small derivatives, are based on ^a same idea: to get ^a computable expresión of perturbation values in terms of residuals (i.e. differences between ODE-solution measured values and non perturbed ODE-solution values). The way used in those works to get such expresions consist of discretising integrals

involving the perturbation by means of its unknown nodal values and, then, solving the resultant equations.

An alternative way to get such expresión was introduced in this paper. It consist of a direct approximation of the unknown perturbation-values by means of arbitrary linear combinations of those integrals. By this way, a general scheme for this kind of methods was studied, obtaining a complete error analysis of them. This analysis can be applied to methods in previous works since they are particular cases of this general scheme.

The obtained error characterisation allowed us to determine the coefficients in the linear combinations in order to be used to minimise the influence of each error source; therefore, optimal schemes under different restrictions were deduced. In particular, one of this optimal schemes proved to be more adequate to solve a Celestial Mechanics problem than those, previously used.

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Appendix. In sections ⁴ and ⁵ we have shown how to numerically integrate (k) Ι^{Δ f(t)} with negligible errors in relation to the remaining error components of the perturbation estimation (formulae (4.15) and (5.14)).

In both cases, truncation errors of these numerical integrations involve (k) ^Δ f-derivatives (formulae (4.15) and (5.16)). The following lemma shows that these derivatives are actually bounded by perturbation derivatives and by measurement errors, if the stepsize is sufficiently small. Therefore, it is proved that all truncation errors in our methods are indeed proportional to small perturbation derivatives.

Lemma. Let **y** and \overrightarrow{y} : $[a,b] \longrightarrow [c,d]$ be the solutions of the following **initial value problems:**

$$
\begin{cases}\n\ddot{y}(t) = f(t, y(t)) + p(t), \\
y(a) = y_0, \quad \dot{y}(a) = \dot{y}_0; \n\end{cases}
$$

$$
\begin{cases} \n\ddot{\tilde{y}}(t) = f(t, \tilde{y}(t)), \\ \n\ddot{\tilde{y}}(a) = \tilde{y}_0 + \delta \tilde{y}_0, \quad \dot{\tilde{y}}(a) = \dot{\tilde{y}}_0 + \delta \dot{\tilde{y}}_0. \n\end{cases}
$$

Let $\Delta f(t) = f(t,y(t)) - f(t,y(t))$, for $t \in [a,b]$. For every $h \ge 0$ and **every** continuous function g , let $\|\ddot{g}\|_{h}$ = $\max_{f \in \text{Aut}(h)} |g(f)|$. Given any **aStSa+h integer kiO , if f has (k+1) continuous derivatives on the rectangle** $R = [a,b] \times [c,d]$, if p is a continuous function with $(k-2)$ continuous **derivatives on [a,b] (if ki2), and, if the interval [a,b] is small 2 Example 1 EXPLENEEF E EXPLENEEF 1 CONFIDE**

constant for f , then, for any h£0 such that a+hSb , the following inequalities hold;

(A.1)
$$
\|y - y\|_{h} \leq C_0 \left(|\delta y_0| + h |\delta y_0| + \frac{h^2}{2} \|p\|_{h} \right) ,
$$

(A.2)
$$
\|f\|_{h} \leq C_0' \left(|\delta y_0| + h |\delta \dot{y}_0| + \frac{h^2}{2} \|p\|_{h} \right) ,
$$

if kil , then:

(A.3)
$$
\|\dot{y} - \dot{y}\|_{h} \leq C_1 (|\delta y_0| + |\delta \dot{y}_0| + h \|p\|_{h}),
$$

$$
|f|_{h} \leq C_{1}^{'} (|\delta y_{0}| + |\delta \dot{y}_{0}| + h||p||_{h}),
$$

and, if k¿j¿2 , then:

(A.5)
$$
\|y^{(1)} - y^{(j)}\|_{h} \leq C_{j} (|\delta y_{0}| + |\delta \dot{y}_{0}| + \sum_{i=0}^{j-2} \|p^{(i)}\|_{h}),
$$

(A.6)

where C **and** C^{\dagger} **,** $j=0,\ldots,k$, are constants not depending on h **.**

Proof. Subtracting the Taylor formulae for y and y , we can write for every te[a,b] :

(A.7)
$$
y(t)-y'(t) = \delta y_0 + (t-a)\delta y_0 + \int_a^t \Delta f(\tau) (t-\tau) d\tau + \int_a^t p(\tau) (t-\tau) d\tau
$$

On the other hand, as $(\tau, y(\tau))$ and $(\tau, y'(\tau))$ belong to R for **every T<.[a,a+h] , we have the following bound:**

$$
|\Delta f(\tau)| \le L \|y - \tilde{y}\|_{L^2}
$$

By using this bound in (A.7) it fallows for every t<[a,a+h] :

$$
|\mathbf{y}(t)-\hat{\mathbf{y}}(t)| \leq |\delta y_0| + h |\delta \hat{y}_0| + \frac{L(b-a)^2}{2} ||y - \hat{y}||_h + \frac{h^2}{2} ||p||_h
$$

ż

and, as $L(b-a)^2/2 < 1$, we get the bound (4.1) with $C_0 = [1-L(b-a)^2/2]^{-1}$, **and,** by replacing this bound in $(A.8)$, we get $(A.2)$ with C_0^* \bullet C_0L .

To prove the remaining bounds, it is necessary to have analogous estimates to $(A, 7)$ and $(A, 8)$ for $(y-y)$ and Δf -derivatives. For $(y-y)$ we can **write:**

$$
(A.9) \t\t\t\t\t\dot{y}(t)-y(t) = \delta \dot{y}_0 + \int_a^t \Delta f(\tau) d\tau + \int_a^t p(\tau) d\tau,
$$

and, for j=2,...,k ,

(A.10)
$$
y^{(j)}(t)-y^{(j)}(t) = \Delta f^{(j-2)}(t) + p^{(j-2)}(t)
$$
.

On the other hand, it is easy to show that for $j=1,\ldots,k$ and for $t\in [a,b]$

(A.11)
$$
|\Delta f^{(j)}(t)| \leq \frac{1}{\sum_{i=0}^{j} A_{ij}} |y^{(1)}(t) - \hat{y}^{(1)}(t)|,
$$

where A^ are constants not depending on t .

Now from (A.9), (A.8) and (A.l), it follows bound (A.3) with C_1 = $\max\{C_0^1(b-a)$, $1+C_0^1(b-a)^2\}$ which do not depend on h; and, therefore, **from (A.11), (A.l) and (A.3) we get bound (A.4) with other constant 'C' not depending on h .**

Finally, proceeding in a recursive way, we can prove the remaining bounds (A.5) and (A.6) for J«2,...,k .

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