Improving the accuracy of the discrete gradient scheme

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Main topics of the talk

1. Exact discretization.
2. Discrete gradient method.
3. Locally exact discrete gradient schemes: LEX and SLEX.
4. Discrete gradient schemes of Nth order: GRAD(N).
5. Locally exact modifications of numerical integrators.
6. Applications.

Notation

t-derivative is denoted by dot, x-derivative by prime:

$$\dot{x} := \frac{dx}{dt}, \quad V'(x) := \frac{dV(x)}{dx}, \quad \ddot{x} := \frac{d^2x}{dt^2}.$$

$$V_x := \frac{dV(x)}{dx}\ , \quad V_{xx} = \frac{d^2V(x)}{dx^2}\ , \quad V_{jx} := \frac{d^jV(x)}{dx^j}\ .$$

Time step is denoted by h.

Exact discretizations.

We consider an ODE with a general solution $\mathbf{x}(t)$ (satisfying the initial condition $\mathbf{x}(t_0) = \mathbf{x}_0$), and a difference equation with the general solution $\mathbf{x}_n$. The difference equation is the exact discretization of the ODE if $\mathbf{x}_n = \mathbf{x}(t_n)$.

Theorem. All linear ODE's admit explicit exact discretizations.

R.B.Potts: "Differential and difference equations", *Am. Math. Monthly* **89** (1982) 402-7.

Simple example: $\dot{x} = ax, \quad x(0) = x_0$.

$$x_n = x(nh) = e^{ahn} x_0 \quad \Rightarrow \quad x_{n+1} = e^{ah} x_n \ ,$$

Exact discretization: $\dfrac{x_{n+1} - x_n}{\frac{e^{ah}-1}{a}} = a x_n$. Note: $\lim\limits_{a \to 0} \dfrac{e^{ah} - 1}{a} = h$.

Example: harmonic oscillator

$$\ddot{x} + \omega^2 x = 0, \quad p = \dot{x}$$

Exact discretization (i.e., $x_n = x(nh)$, $p_n = p(nh)$):

$$x_{n+1} - 2\cos(\omega h) x_n + x_{n-1} = 0 \ , \quad p_n = \frac{x_{n+1} - \cos(\omega h) x_n}{\sin(\omega h)}$$

Equivalent form: $$\frac{x_{n+1} - 2x_n + x_{n-1}}{\left(2 \sin \frac{\omega h}{2}\right)^2} + \omega^2 x_n + 0$$

Details, generalizations, applications:

J.L.Cieśliński, "On the exact discretization of the classical harmonic oscillator equation", preprint **arXiv: 0911.3672 (2009)**; *J. Difference Equ. Appl.*, in press.

Discrete gradient method (GRAD)

As an illustrative example we consider the system

$$\dot{p} = -V'(x) \; , \quad p = \dot{x} \; . \qquad \text{(Newton)}$$

The discrete gradient method (shortly: GRAD) applied to (Newton), yields [LaBudde, Greenspan (1974)]:

$$\frac{p_{n+1} - p_n}{h} = -\frac{V(x_{n+1}) - V(x_n)}{x_{n+1} - x_n} \; ,$$

$$\frac{1}{2}(p_{n+1} + p_n) = \frac{x_{n+1} - x_n}{h} \; . \qquad \text{GRAD}$$

Theorem. GRAD preserves the energy integral exactly (up to round-off errors). Indeed, $\frac{1}{2}p_n^2 + V(x_n) = \frac{1}{2}p_{n+1}^2 + V(x_{n+1})$.

LOCALLY EXACT MODIFICATION OF THE DISCRETE GRADIENT SCHEME (GRAD-LEX AND GRAD-SLEX)

We consider the following extension of the discrete gradient scheme:

$$\frac{p_{n+1}-p_n}{\delta_n} = -\frac{V(x_{n+1})-V(x_n)}{x_{n+1}-x_n} \ ,$$
$$\frac{1}{2}(p_{n+1}+p_n) = \frac{x_{n+1}-x_n}{\delta_n} \ , \qquad \text{GRAD-DEL}$$

where δ_n is an arbitrary positive function of $h, x_n, p_n, x_{n+1}, p_{n+1}$ etc. The system GRAD-DEL is a consistent approximation of (Newton) if we add the condition $\lim_{h\to 0}\frac{\delta_n}{h} = 1$.

THEOREM. Any numerical scheme of the form GRAD-DEL preserves exactly the energy integral (for any positive function δ_n).

PROOF: Multiplying side by side both equations of (GRAD-DEL) we obtain: $$\frac{1}{2}p_{n+1}^2 + V(x_{n+1}) = \frac{1}{2}p_n^2 + V(x_n).$$

In order to get locally exact gradient schemes (GRAD-LEX and GRAD-SLEX) we linearize GRAD-DEL around $x = \bar{x}$:

$$\begin{aligned} \frac{\xi_{n+1} - \xi_n}{\delta_n} &= \frac{1}{2}\left(p_{n+1} + p_n\right) \ , \\ \frac{p_{n+1} - p_n}{\delta_n} &= -V'(\bar{x}) - \frac{1}{2}V''(\bar{x})\left(\xi_n + \xi_{n+1}\right) \ . \end{aligned} \qquad \text{(LIN)}$$

where $\xi_n := x_n - \bar{x}$ and $\xi_{n+1} = x_{n+1} - \bar{x}$.

THEOREM. The system (LIN) is the EXACT discretization of the harmonic oscillator equation with a constant driving force: $\ddot{x} + \omega^2 x = g$, $p = \dot{x}$, provided that

$$g = -V'(\bar{x}) \ , \quad \omega^2 = V''(\bar{x}) \ , \quad \delta_n = \frac{2}{\omega} \tan \frac{\omega h}{2} \ .$$

The simplest choice is $\bar{x} = 0$ (small oscillations around the equilibrium), then $\delta = \mathrm{const}$, and we get MOD-GRAD scheme.

J.L.Cieśliński, B.Ratkiewicz: *J. Phys. A: Math. Theor.* **42** (2009) 105204.

Choosing $\bar{x} = x_n$ we get GRAD-LEX scheme. The symmetric (time-reversible) choice $\bar{x} = \frac{1}{2}(x_n + x_{n+1})$ yields GRAD-SLEX scheme (note that in both cases we change $\bar{x}$ at every step).

J.L.Cieśliński, B.Ratkiewicz: *Physical Review* **E 81** (2010) 016704.

Locally exact discretizations (LEX). Main idea

1. Take a numerical scheme (applied to a nonlinear system).
2. Modify the scheme by introducing h-dependent parameters (e.g., $\delta(h)$) in place of h. It is of advantage to preserve geometric properties of the original scheme.
3. Apply the modified scheme to the LINEARIZATION of the nonlinear system and require that the obtained discretization is EXACT.
4. Either the resulting conditions on $\delta(h)$ are contradictory (then one may try another modification, perhaps with larger number of parameters), or we get LOCALLY EXACT MODIFIACTION OF THE ORIGINAL SCHEME.

Gradient schemes

GRAD is of 2nd order,
GRAD-LEX of 3rd order,
GRAD-SLEX of 4th order

All these schemes are extremaly stable.
They have very high accuracy in the region of small oscillations.

However, it is possible to constuct gradient schemes of higher orders, GRAD(N), without the loss of excellent qualitative properties of the gradient method.

Taylor expansion of the exact solution

We expand $x(t+h)$ and $p(t+h)$ in Taylor series:

$$x(t+h) = \sum_{k=0}^{\infty} \frac{h^k}{k!} \frac{d^k x(t)}{dt^k} \ ,$$

$$p(t+h) = \sum_{k=0}^{\infty} \frac{h^k}{k!} \frac{d^k p(t)}{dt^k} \ ,$$

where all derivatives can be replaced by functions of x, p using (Newton) and its differential consequences, e.g.,

$$\ddot{p} \equiv \frac{d^2 p}{dt^2} = -V''(x)\dot{x} = -V''(x)p.$$

The Taylor expansion can be represented in the form

$$x(t+h) = \sum_{k=0}^{\infty} \frac{h^k}{k!}\, b_k(x,p)\ , \qquad p(t+h) = \sum_{k=0}^{\infty} \frac{h^k}{k!}\, c_k(x,p)\ ,$$

where $c_k = b_{k+1}$, $b_0 = 0$, and

$$b_{k+1} = \frac{d}{dt} b_k = \frac{\partial b_k}{\partial x}\dot{x} + \frac{\partial b_k}{\partial p}\dot{p} = p\frac{\partial b_k}{\partial x} - V'(x)\frac{\partial b_k}{\partial p}\ .$$

Corollary. The Taylor series of the exact solution:

$$\begin{aligned} x(t+h) &= x + ph - \tfrac{1}{2}V'h^2 - \tfrac{1}{6}pV''h^3 \\ &\quad + \tfrac{1}{24}\left(V'V'' - V'''p^2\right)h^4 + \dots \\ p(t+h) &= p - V'h - \tfrac{1}{2}pV''h^2 + \tfrac{1}{6}\left(V'V'' - V'''p^2\right)h^3 \\ &\quad + \tfrac{1}{24}\left(3pV'V''' + p(V'')^2 - p^3V^{(4)}\right)h^4 + \dots \end{aligned} \qquad \text{(Taylor)}$$

Discrete gradient schemes of Nth order

We proceed to consider the family GRAD-DEL of numerical schemes (parameterized by a single function δ):

$$\frac{x_{n+1}-x_n}{\delta}=\frac{1}{2}\left(p_{n+1}+p_n\right) \ .$$

$$\frac{p_{n+1}-p_n}{\delta}=-\frac{V(x_{n+1})-V(x_n)}{x_{n+1}-x_n} \ , \qquad \text{GRAD-DEL}$$

where δ can depend on h, x_n, p_n, x_{n+1}, p_{n+1}.

This family contains GRAD (2nd order), GRAD-LEX (3rd order) and GRAD-SLEX (4th order) schemes. We are able to construct discrete gradient schemes of any order: GRAD(N).

The system GRAD-DEL (where $x_n \equiv x$, $p_n \equiv p$ are given and δ is a small parameter) implicitly defines x_{n+1} and p_{n+1}. Using implicit differentiation, we write down the Taylor series:

$$x_{n+1} = x + p\delta - \tfrac{1}{2}V_x\delta^2 - \tfrac{1}{4}pV_{xx}\delta^3 + \tfrac{1}{24}\left(3V_xV_{xx} - 2p^2V_{3x}\right)\delta^4 + \dots\ ,$$

$$p_{n+1} = p - V_x\delta - \tfrac{1}{2}pV_{xx}\delta^2 + \tfrac{1}{12}\left(3V_xV_{xx} - 2V_{3x}p^2\right)\delta^3$$
$$-\tfrac{1}{24}\left(4pV_xV_{3x} + 3pV_{xx}^2 - p^3V_{4x}\right)\delta^4 + \dots\ .$$

We assume that x_{n+1} and p_{n+1} are of Nth order, i.e., their Taylor expansions have at least N first terms identical with (Taylor).

This assumption fix first N terms of $\delta \equiv \dfrac{2(x_{n+1} - x_n)}{p_{n+1} + p_n}$.

The first N terms of δ form a polynomial δ_N

$$\delta_N = \delta_N(x,p,h) = h + \sum_{k=2}^{N} a_k(x,p) h^k$$

where few first coefficients a_k read

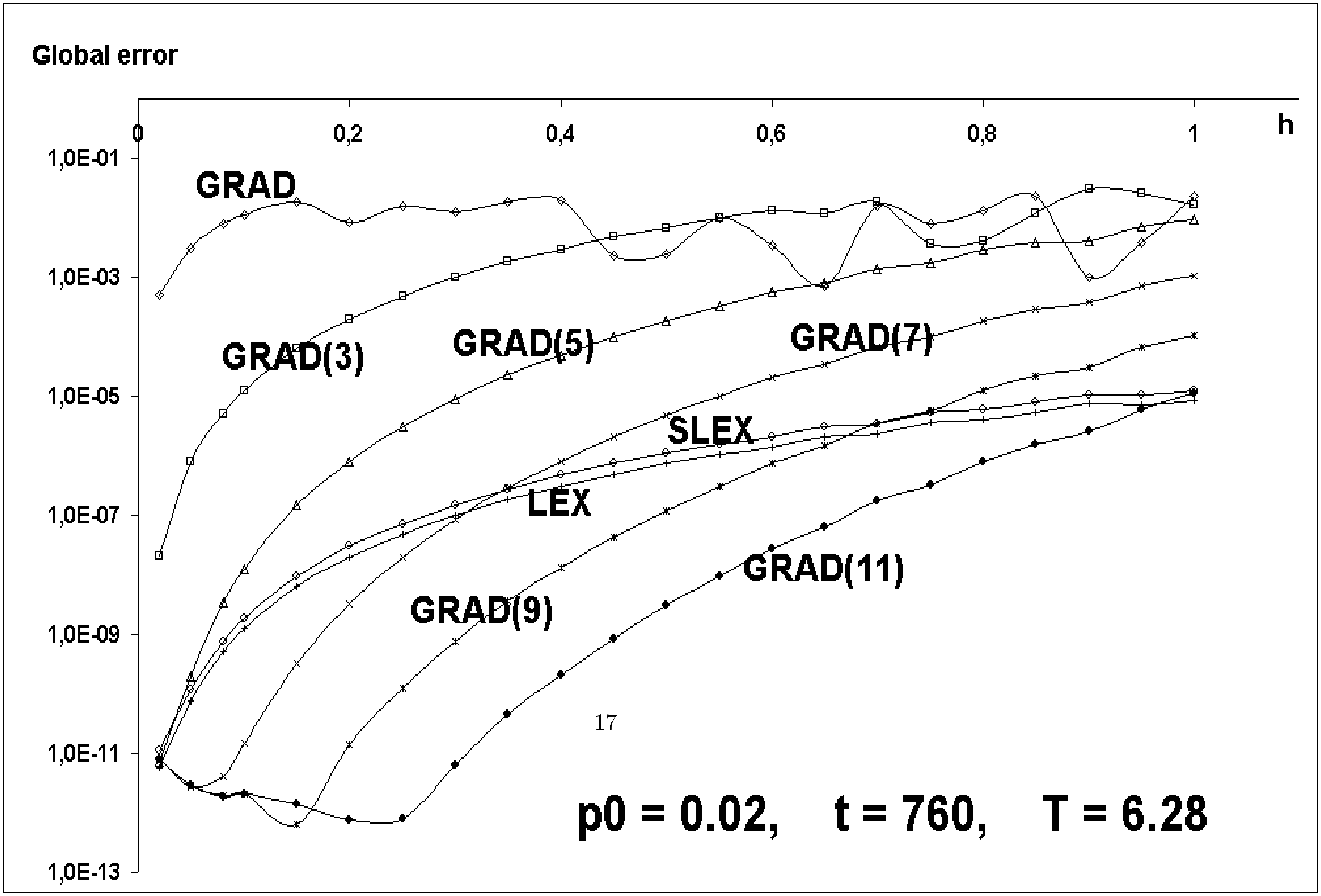
$$a_2 = 0 \ , \qquad a_3 = \frac{1}{12} V_{xx} \ , \qquad a_4 = \frac{1}{24} p V_{xxx} \ ,$$

$$a_5 = \frac{1}{240}\left(2V_{xx}^2 - 4V_x V_{xxx} + 3p^2 V_{4x}\right) \ ,$$

$$a_6 = \frac{1}{1440}\left((5V_{xx}V_{xxx} - 15V_x V_{4x})p + 4V_{5x}p^3\right) \ ,$$

The gradient scheme GRAD-DEL with $\delta = \delta_N$ is called GRAD(N). Its order is at least N, sometimes higher (e.g., the order of GRAD(1) is 2, actually: GRAD(1) $=$ GRAD(2)$=$GRAD).

Figure 1: Simple pendulum. Discrete gradient schemes of high accuracy



Extensions and generalizations

1. One-dimensional Hamiltonian systems

$$\frac{1}{2}p^2 + V(x) \quad \longrightarrow \quad T(p) + V(x)$$

A family of discrete gradient integrators (GRAD-DEL) preserving exactly all trajectories of the Lotka-Volterra system.

2. Multidimensional Hamiltonian systems.

δ is a matrix! To be published soon.

3. ODE with integrals of motion

$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x}), \qquad I_1, I_2, \ldots, I_k \ - \text{integrals of motion}$$

Generalized discrete gradient method (McLachlan, Quispel, Robidoux) preserves all integrals of motion. GRAD-DEL type integrators: in preparation.

Conclusion.

Modified gradient schemes GRAD-LEX, GRAD-SLEX, GRAD(N) have important advantages:

- conservation of the energy integral (up to round-off errors)
- high stability, exact trajectories in the phase space,
- high accuracy (third, fourth and Nth order, respectively), ,
- very good long-time behaviour of numerical solutions.

Future directions

- multi-dimensional cases
- locally exact modification of the implicit midpoint rule and some other numerical schemes
- locally exact variable time-step integrators
- PDE's (e.g., wave equation and Fourier transform)

Figure 2: Simple pendulum. Relative error of the period T as a function of p_0 for $\varepsilon = 0.02$. White triangles: LEAP-FROG, white diamonds: GRAD, black diamonds: MOD-GRAD ($\delta = \text{const}$), black squares: GRAD-LEX, grey squares: GRAD-SLEX.

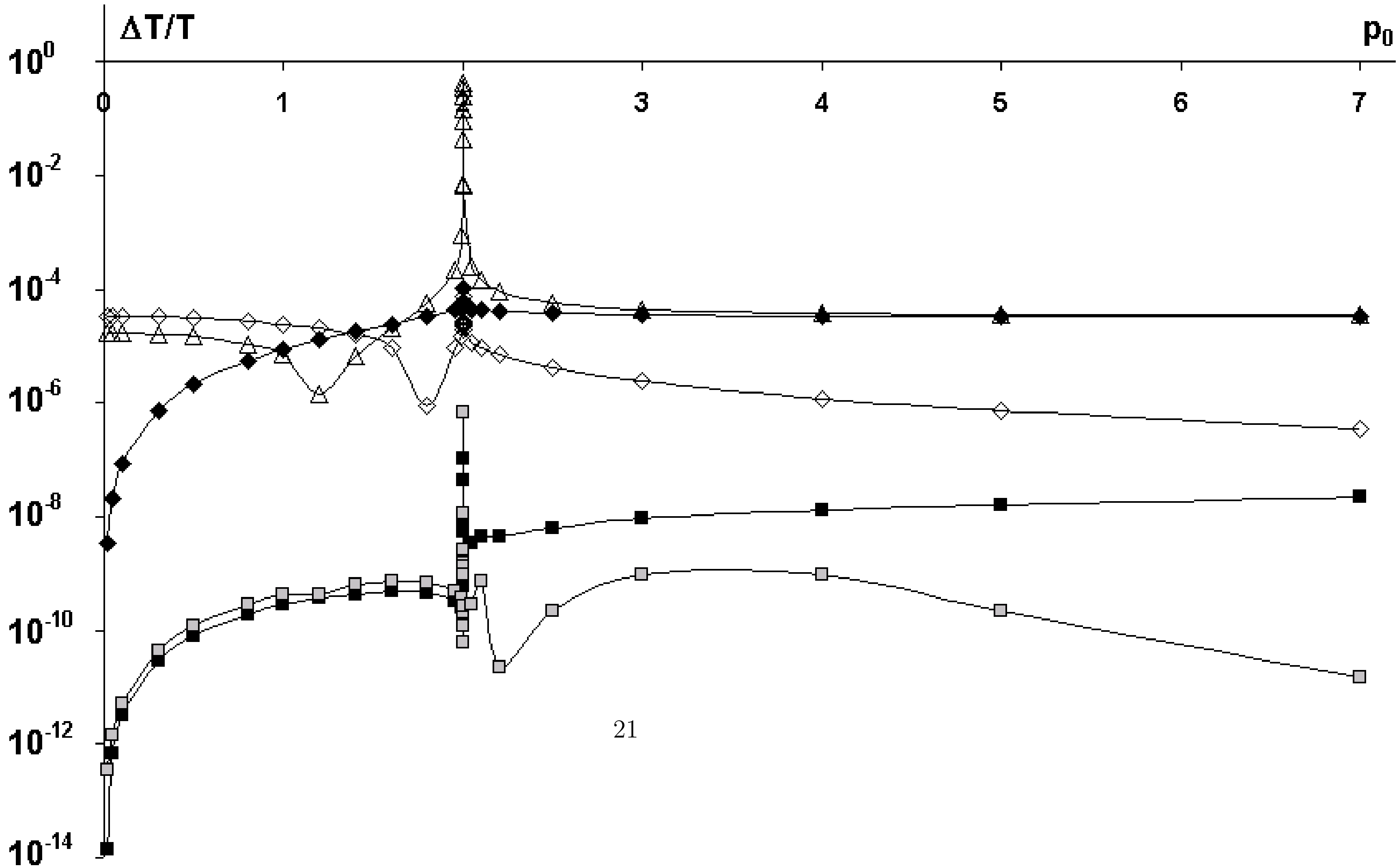


Figure 3: Relative error of the period T as a function of ε for $p_0 = 1.8$. Symbols: see figure ??.

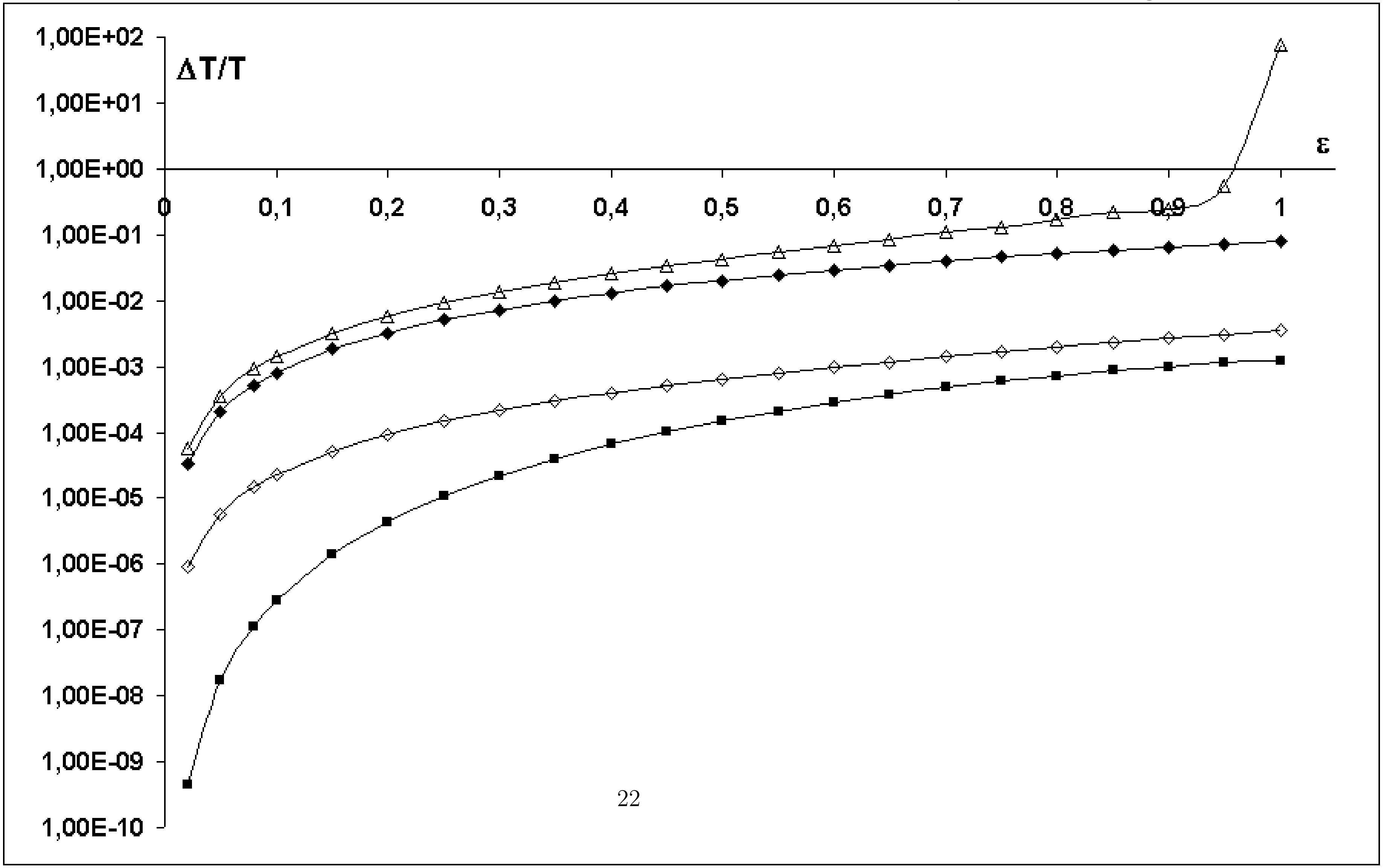


Figure 4: x_n as a function of n, very near the separatrix ($p_0 = 1.9999999999$), for $\varepsilon = 0.9$. Symbols: see figure **??**. The solid line corresponds to the exact (continuous) solution.