NUMERICAL EXTREMAL METHODS AND BIOLOGICAL MODELS

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ABSTRACT. Discrete variable methods are given to find extremaloid solutions (extremals with corners) in the calculus of variations and optimal control theory for well defined mixtures of initial value problems and boundary value problems. Our methods are general, efficient, and accurate with a global a priori, pointwise error of $O(h^2)$ and a Richardson error of $O(h^4)$. Our methods are motivated by a generalization of Henrici's methods for ordinary differential equations and our discretized equations are tridiagonal, which is very important in practical applications.

1. Introduction. A major chapter in classical applied mathematics is to find the minimum of an integral of the form

(1)
$$I(x) = \int_a^b f(t, x, x') dt$$

subject to conditions which yield a unique solution. While there are many necessary and sufficient conditions, the first and major condition is that the minimizing solution x(t) satisfies the Euler-Lagrange equation

$$\frac{d}{dt}f_{x'} = f_x$$

between corners on [a, b]. In this case, x(t) is called an extremaloid solution (see [4, p. 60]). This equation follows from the first variational equation which requires that x(t) satisfy

(3)
$$I'(x,y) = \int_a^b [f_x y + f_{x'} y'] dt = 0$$

for all admissible variations y(t). Similarly, closely related problems (defined below) occur in the field of optimal control theory.

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 $[\]overline{\ }^{1}$ Supported in part by the Office of Naval Research, grant number N00014-88-K0081

The general setting and background of these problems is that given by Hestenes [4; pp. 57–62] or Leitmann [6; pp. 7–23]. In particular, we require $f_{x'x'} > 0$ and enough smoothness on f to yield unique piecewise smooth solutions x(t) for (2) or (3).

This paper has several purposes. The first purpose is to give efficient, stable and accurate algorithms for well defined combinations of the initial value problem and the boundary value problem associated with the numerical solution of (3) or the solution of (2) in integrated form. A global error estimate is given in §2 with similar results holding in §3 when x is an $m \ge 1$ dimensional dependent vector. In §4 we show how these results lead to numerical algorithms for the basic problems in optimal control theory. In §5 we consider some biological examples. Finally, in \(\)6 we present a nontrivial numerical example which agrees with our theoretical results.

The 1-Dimensional Problem. The purpose of this section is to motivate the derivation of our basic algorithm and to sketch a formal proof for the m=1 case.

We begin by choosing N to be a large positive integer, h = (b - a)/Nand a partition $\pi = (a = a_0 < a_1 < \cdots a_N = b)$ of the interval [a, b]where $a_k = a + kh$. We define the spline hat functions

(4)
$$z_k(t) = \begin{cases} (t - a_{k-1})/h, & \text{if } a_{k-1} < t < a_k, \\ (a_{k+1} - t)/h, & \text{if } a_k < t < a_{k+1}, \\ 0, & \text{otherwise} \end{cases}$$
(5)
$$x_h(t) = \sum_{k=0}^{N} c_k z_k(t) \quad \text{and} \quad y_h(t) = \sum_{k=0}^{N} d_l z_l(t).$$

(5)
$$x_h(t) = \sum_{k=0}^{N} c_k z_k(t)$$
 and $y_h(t) = \sum_{k=0}^{N} d_l z_l(t)$

For definitiveness, we assume that (1)–(3) are concerned with a boundary value problem. In this case, we assume that we require the conditions

(6)
$$x(a) = x_a \quad \text{and} \quad x(b) = x_b$$

to accompany (1)-(3). The function $x_h(t)$ is the numerical solution we seek while $y_h(t)$ is the numerical variation so that, associated with (6), we have

(7)
$$y_h(a) = d_0 = 0$$
 and $y_h(b) = d_N = 0$.

To motivate (2) or (3) as necessary conditions, we choose a variation y(t) of the extremal solution x(t) for the problem (1), (6). Letting $h(\epsilon) = I(x + \epsilon y)$ for ϵ in $|\epsilon| < \delta$ and, assuming the usual smoothness conditions as, for example, in Hestenes [4], we have

(8)
$$h(\epsilon) = h(0) + \epsilon h'(0) + \frac{1}{2} \epsilon^2 h''(0) + \cdots,$$

where h'(0) = I'(x, y) given in (3) and h''(0) is a quadratic form in y(t). The Euler-Lagrange equation (2) is obtained by integrating (3) by parts between corners of x(t).

The basis of our numerical methods is the equation (9) below, which is motivated by (3). Thus, on the subinterval $[a_{k-1}, a_{k+1}]$, we have a discretized form of (3) which is derived as follows:

$$0 = I'(x, z_k) = \int_{a_{k-1}}^{a_{k+1}} [f_x(t, x, x')z_k + f_{x'}(t, x, x')z'_k] dt$$

$$\cong \int_{a_{k-1}}^{a_k} [f_x(t, x_h(t), x'_h(t)) \cdot (t - a_{k-1})/h + f_{x'}(t, x_h(t), x'_h(t))/h] dt$$

$$+ \int_{a_k}^{a_{k+1}} [f_x(t, x_h(t), x'_h(t)) \cdot (a_{k+1} - t)/h + f_{x'}(t, x_h(t), x'_h(t))$$

$$(-1/h)] dt$$

$$\cong f_x \left(a^*_{k-1}, \frac{x_k + x_{k-1}}{2}, \frac{x_k - x_{k-1}}{h} \right) \cdot \frac{h^2}{2} \cdot \frac{1}{h}$$

$$+ f_{x'} \left(a^*_{k-1}, \frac{x_k + x_{k-1}}{2}, \frac{x_{k+1} - x_k}{h} \right) \cdot \frac{h^2}{2} \cdot \frac{1}{h}$$

$$+ f_{x'} \left(a^*_k, \frac{x_k + x_{k+1}}{2}, \frac{x_{k+1} - x_k}{h} \right) \cdot \left(-\frac{1}{h} \right) \cdot h$$
or
$$(9)$$

$$f_{x'} \left(a^*_{k-1}, \frac{x_k + x_{k-1}}{2}, \frac{x_k - x_{k-1}}{h} \right) + \frac{h}{2} f_x \left(a^*_{k-1}, \frac{x_k + x_{k-1}}{2}, \frac{x_k - x_{k-1}}{h} \right)$$

$$- f_{x'} \left(a^*_k, \frac{x_k + x_{k+1}}{2}, \frac{x_{k+1} - x_k}{h} \right) + \frac{h}{2} f_x \left(a^*_k, \frac{x_k + x_{k+1}}{2}, \frac{x_{k+1} - x_k}{h} \right) = 0$$
for $k = 1, 2, \dots, N - 1$.

In the above, $a_k^* = (a_k + a_{k+1})/2$ and $x_k = x_h(a_k)$ is the computed value of x(t) at a_k .

Note that (9) involves N-1 nonlinear equations in the N-1 unknowns $x_1, x_2, \ldots, x_{N-1}$. However, they are stable and in tridiagonal form so that our computations are relatively easy. In the important case where I(x) is quadratic, equation (9) is linear.

Our proof of Theorem 2 is in two steps. In Theorem 1 we show that (9) yields a local truncation error of $O(h^3)$. Then, in Theorem 2, we show that (9) gives a global error of $O(h^2)$. The first theorem is motivated by Henrici [3]. The second theorem involves new, more general a priori error methods than those in the current literature.

Thus, if

(10)
$$L(t,h) = f_{x'} \left(t - \frac{h}{2}, \frac{x(t) + x(t-h)}{2}, \frac{x(t) - x(t-h)}{h} \right) + \frac{h}{2} f_x \left(t - \frac{h}{2}, \frac{x(t) + x(t-h)}{2}, \frac{x(t) - x(t-h)}{h} \right) - f_{x'} \left(t + \frac{h}{2}, \frac{x(t) + x(t+h)}{2}, \frac{x(t+h) - x(t)}{h} \right) + \frac{h}{2} f_x \left(t + \frac{h}{2}, \frac{x(t) + x(t+h)}{2}, \frac{x(t+h) - x(t)}{h} \right),$$

then the Taylor series of x(t+h), x(t-h), and a function F(t, x, w) in the form

$$F(a+k_1,b+k_2,c+k_3) = \sum_{m=0}^{2} \frac{1}{m!} \left[k_1 \frac{\partial}{\partial t} + k_2 \frac{\partial}{\partial x} + k_3 \frac{\partial}{\partial w} \right]^m F \Big|_{(a,b,c)} + O(h^4)$$

are used to establish

THEOREM 1. If x(t) is the unique solution to (2) or (3) and (6), then, for h sufficiently small, we have

$$L(t,h) = q(t)h^3 + O(h^5),$$

where q(t) is a function only of the solution x(t), its derivatives, the function f and the partial derivatives of f evaluated along (t, x(t), x'(t)).

We note that the arguments are evaluated at the solution (t, x(t), x'(t)) and that, between corners, (2) holds which implies that $f_{x't} + f_{x'x}x' + f_{x'x}x'' = f_x$.

Our next task is to obtain an a priori, global error estimate for (9). We begin by defining $e_k = x_k - x(a_k)$ to be the difference between the computed value $x_k = x_h(a_k)$ and the actual value $x(a_k)$, and $\tau_k = L(a_k, h)$. We also define the quadratic form

(11)
$$I''(x,y) = \int_a^b \left[f_{x'x'} y'^2 + 2 f_{x'x} y' y + f_{xx} y^2 \right] dt,$$

where the coefficient functions $f_{x'x'}$, etc., are evaluated along a neighborhood of (t, x(t), x'(t)), with x(t) our solution.

We sketch a proof of Theorem 2 under the weak hypothesis that there are no conjugate points for I''(x;y) in (11). In this case, from [1] or [6], we have that there exists a $C_2 > 0$ such that the quadratic form $I''(x;y) \geq C_2 \bar{J}(y)$ on the space of variations y(t) on [a,b] where

$$\bar{J}(x,y) = \int_a^b x'(t)y'(t) dt$$
 and $\bar{J}(y) = \bar{J}(y,y)$.

We note that $\bar{J}(z_h, z_l) = j_{kl}/h$, where the matrix (j_{kl}) is the tridiagonal matrix J = diag (-1, 2, -1). Henrici shows that $||J^{-1}||_{\infty} \leq D/h^2$ for some positive constant D. The inequality $1/||A^{-1}|| \leq |\lambda|$ where A is any nonsingular matrix and λ is any eigenvalue of A shows that all eigenvalues of the positive definite matrix J satisfy $\lambda = |\lambda| \geq h^2/D$.

If $e = (e_1, \ldots, e_{N-1})^T$ and $\tau = (\tau_1, \ldots, \tau_{N-1})$, we may use an extension of the first author's quadratic form theory and the above ideas to show that there exist positive constants C_2, C_3 and C_4 independent of h, for small h > 0, such that

$$C_2 h \|e\|_2^2 \le C_3 h^3 \|e\|_2 \|\tau\|_2$$

or

$$||e||_{\infty} \le ||e||_2 \le C_4 h^{3/2}$$
.

Writing the difference between (9) and (11) in the form $A_h e = \tau$, it can be shown, using the above results, that A_h is invertible and the

elements of the inverse are bounded. Complete details of these results are too long to be given here and will be given in a later paper for the $m \geq 1$ case. From Theorem 1, we have $||e||_{\infty} \leq ||A_h||^{-1}C_1h^3 \leq C_1h^2$, and, hence,

THEOREM 2. If I''(x;y) > 0 in (11), or, equivalently, if there are no conjugate points in [a,b], then $|e_k| \leq C_1 h^2$ for some $C_1 > 0$ independent of h for h sufficiently small.

3. The m-Dimensional Problem. The purpose of this brief section is to indicate that the results in $\S 2$ hold with the obvious modifications in notation when x(t) is an m-vector, m > 1.

The major change will be in notation. Thus, we now have $x(t) = (x_1(t), x_2(t), \ldots, x_m(t))^T$; f_x and $f_{x'}$ in (2) and (3) are m-vectors; y(t) is an m-vector of variations; the integrand in (3) is replaced by $f_x^T y + f_{x'}^T y'$; etc. In particular, our basic algorithm is still (9) which is now a system of m(N-1) equations in m(N-1) unknowns for the two-point boundary value problem. Theorem 1 is as given except that L and q are m-vectors. A very long and difficult proof of Theorem 2 now follows, which will appear elsewhere.

To complete our error results, we define the Richardson value and error vectors by

$$x_h^R(a_k) = [4x_{h/2}(a_k) - x_h(a_k)]/3$$
 and $e_h^R(a_k) = x(a_k) - x_h^R(a_k)$

and note that each component e_{kJ}^R of $e_h^R(a_k)$ satisfies $|e_{kj}^R| \leq Ch^4$.

4. Optimal control problems. The purpose of this section is to show that numerical solutions for very general classes of optimal control problems can be obtained by converting these problems to the calculus of variations setting in $\S\S2$ and 3. For convenience of exposition we first summarize these problems in slightly different notation (our *m*-vector will become an *n*-vector), give a general theorem and describe the subproblems. We then give some specific example of how the actual conversion is accomplished.

Hestenes [4, pp. 346-351] shows that "A General Control Problem of Bolza" defined by the conditions

(12)
$$I_{\rho}(x) = g_{\rho}(b) + \int_{t^0}^{t^1} L_{\rho}(t, x(t), u(t)) dt, \qquad \rho = 0, 1, \dots, \bar{p},$$

(13)

$$\varphi_{\alpha}(t, x, u) \le 0, \quad 1 \le \alpha \le m', \qquad \varphi_{\alpha}(t, x, u) = 0, \quad m' < \alpha \le m,$$

$$\dot{x}^{i} = f^{i}(t, x, u),$$

and

(15)
$$t^s = T^s(b), \quad x^i(t^s) = X^{is}(b), \qquad i = 1, \dots, n, \ s = 0, 1,$$

(16)
$$I_{\gamma}(x) \leq 0, \quad 1 \leq \gamma \leq p', \qquad I_{\gamma}(x) = 0, \quad p' < \gamma \leq \bar{p},$$

has a minimizing solution for $I_0(x)$ of the form

(17)
$$x_0: x_0(t), b_0, u_0(t), t^0 \le t \le t^1,$$

if there exist multipliers

$$\lambda_0 \geq 0, \quad \lambda_{\gamma}, \quad p_i(t), \quad \mu_{\alpha}(t),$$

$$\gamma = 1, \dots, \bar{p}, \quad i = 1, \dots, n, \quad \alpha = 1, \dots, m,$$

not vanishing simultaneously, and functions

$$H(t, x, u, p, \mu) = p_i f^i - \lambda_\rho L_\rho - \mu_\alpha \varphi_\alpha, \quad G(b) = \lambda_\rho g_\rho,$$
$$\rho = 0, 1, \dots, \bar{p}$$

satisfying the usual, expected conditions (see [4, pp. 348–350]).

Finally, we claim

THEOREM 3. The definitions of $x^{n+1}(t), \ldots, x^{n+q+m}(t)$ given by

(18a)
$$\dot{x}^i = u^{i-n}, \quad x^i(a) = 0, \qquad i = n+1, \dots, n+q,$$

(18b)
$$\dot{x}^i = \mu_{\alpha}^{i-n-q}, \quad x^i(a) = 0, \qquad i = n+q+1, \dots, n+q+m,$$

allow us to convert the General Control Problem of Bolza to a problem of the form (1) and allows a numerical solution with errors described in Theorem 2 above.

In the above, (14) is the trajectory equation; (15) is the endpoint condition; (12) with $p \neq 0$, (13) and (16) are the constraints on our problem. The *problem* is to find the solution x_0 in (17) so that $I_0(x)$ in (12) is a minimum subject to the constraints, the endpoint conditions and the trajectory equation.

We now consider specific subproblems of the general problem discussed above. We begin with a basic problem characterized by (19)–(21). For convenience, we change our notation somewhat. Thus, let

(19)
$$J_1(x) = \int_1^b f(t, x, u) dt = \min,$$

$$(20) x'(t) = g(t, x, u)$$

$$(21a) x(1) = x_a, x(b) = x_b$$

or

(21b)
$$x(a) = x_a, \quad x(b) \text{ arbitrary},$$

where we assume x is an n-vector, u is an m vector, there exists a unique solution to our problem and that f and g are smooth enough to obtain the results given below.

The optimal control problem (19)–(21) is converted to an equivalent problem in the calculus of variations by defining

$$(22a) x_1(t) = x(t),$$

(22b)
$$x_2(t) = \int_a^t u(s) ds, \quad x_2(a) = 0,$$

and

(22c)
$$x_3(t) = \int_a^t \lambda(s) \, ds, \qquad x_3(a) = 0,$$

where $\lambda(t)$ is the Lagrange multiplier associated with $J_2(X)$ below.

Using (22) we define the 2n + m vector

(23)
$$X(t) = (x_1^T(t), x_2^T(t), x_3^T(t))^T$$

and

(24)
$$J_2(X) = \int_a^b \left\{ f(t, x_1, x_2') + x_3'^T [x_1' - g(t, x_1, x_2')] \right\} dt$$
$$= \int_a^b F(t, X, X') dt$$

We note that, except for the values $x_2(b)$, $x_3(b)$ considered below, the solution to (19)–(21) is equivalent to the minimizing solution of (24) which can be obtained by (9) with the accuracy in Theorem 2. We also note that (19)–(21) includes the well-known "linear regulator problem."

The class of basic problems (19)-(21) can be enlarged and is included in a class of problems where inequality constraints (13) are given. For strict equality, our results in (9) and Theorem 2 follow by use of auxiliary state vectors as we have done with x'_3 in (24) and (22c). Inequality constraints can be treated similarly by Kuhn-Tucker methods or by introducing a slack variable x'_4 , with $x'_4^T x'_4 + \varphi_{\alpha}(t, x, u) = 0$, and then a multiplier for this equality. These results will appear elsewhere.

Finally, we consider transversality conditions which are of the form (15) or which occur because of variables such as $x_2(t)$ and $x_3(t)$ in (22). For example, the optimal control u(t) is assumed to be unique but $x'_2(T) = u(t)$ is only unique up to a constant. The condition $x_2(a) = 0$ makes $x_2(t)$ unique, but, since $x_2(b)$ cannot be specified, there is a "natural" boundary condition and, hence, a further equation similar to (9) is required.

While (analytic) transversality conditions are known, they are not useful to us. Instead, motivated by the development leading to (9) for $m \geq 1$, extra equations can be derived when k = N to balance the components of $X(a_N)$ in (23) which are not explicitly specified. It can be shown that these equations have a local truncation error of $O(h^2)$ and that theorems similar to Theorem 2 hold.

To illustrate these ideas we will give four examples with the "same" solution. Let

(25)
$$I(x) = \frac{1}{2} \int_0^2 (x'^2 + 2xx' + 4x^2) dt = \min,$$
$$x(0) = 1, \quad x(2) \text{ arbitrary},$$

(26)
$$J(x,u) = \frac{1}{2} \int_0^2 (u^2 + 2xu + 4x^2) dt = \min x' = u,$$

$$x(0) = 1, \qquad x(2) \text{ arbitrary}$$

(27) same as (26) except that
$$x(2) = \frac{4}{3e^4 + e^{-4}} \doteq d_1$$

(28)
$$I_{1}(X) = \int_{0}^{2} \left[\frac{1}{2} (x_{2}^{\prime 2} + 2x_{1}x_{2}^{\prime} + 4x_{1}^{2}) + x_{3}^{\prime} (x_{1}^{\prime} - x_{2}^{\prime}) \right] dt$$

$$X(0) = \begin{pmatrix} 1\\0\\0 \end{pmatrix}, \qquad x(2) = \begin{pmatrix} d_{1}\\d_{2}\\d_{3} \end{pmatrix}$$

Example (25) is a one-dimensional calculus of variations problem which is solved by (9) when $k=1,\ldots,N-1$ and the transversality condition

(29)
$$f_{x'}\left(a_{N-1}^*, \frac{x_N + x_{N-1}}{2}, \frac{x_N - x_{N-1}}{h}\right) + \frac{h}{2} f_x\left(a_{N-1}^*, \frac{x_N + x_{N-1}}{2}, \frac{x_N - x_{N-1}}{h}\right) = 0$$

holds, where $f_{x'} = x' + x$, $f_x = x' + 4x$. We will not concern ourselves with the solution x(t) except to note that $x(2) = d_1$ is defined in (27).

Example (26) is an optimal control problem which becomes $I_1(X)$ in (28) with the definitions in (22). In this case,

(30)
$$f_{X'} = \begin{pmatrix} x_3' \\ x_2' + x_1 - x_3' \\ x_1' - x_2' \end{pmatrix}, \qquad f_X = \begin{pmatrix} x_2' + 4x_1 \\ 0 \\ 0 \end{pmatrix}$$

in (9) and (29). Thus, we have 3N equations in 3N unknowns X_1, X_2, \ldots, X_N .

Example (27) is the same as Example (26), except that (9) and the least two components of (29) are used since $x_1(b)$ is given, and, hence, we have 3N-1 equations in 3N-1 unknowns.

Example (28) is a three-dimensional calculus of variations problem with the 3(N-1) equations in (9) and (30) used along with the 3(N-1) unknowns $X_1, X_2, \ldots, X_{n-1}$.

We note the minimizing solutions in (25) and (26) lead to minimum values $I(x_0) = J(x_0, u_0)$ and that this value is not larger than the minimized integral in (27) which is equal to the minimized integral of $I(X_0)$ in (28) if d_2 and d_3 are fixed to be the same values as in (27).

5. Some biological examples. The theme of this brief section is to indicate that there are many important biological problem areas which can be successfully handled in a calculus of variations setting and efficiently solved using our methods. The hangup in these examples is almost always the lack of a good trajectory equation. Once this is obtained, many meaningful problems, including the minimal time problem (discussed below), immediately suggest themselves.

The first example was formulated with the help of Hugh Barclay. Thus, if we let F(t), N(t) and r(t) be, respectively the biomass of females, males, and the release rate of sterile males into a population of fruit-flies (for example) we have the trajectory equations

$$F'(t) = F \left[\frac{a_1 F}{F + N} - a_2 - b(F + N) \right]$$
$$N'(t) = r - a_2 N - bN(F + N),$$

where $(F(t), N(t))^T$ is the state vector and r(t) is the control vector. The values a_1, a_2 and b depend upon the particular population.

The objective functional to be minimized could be the integral from 0 to t^* (not necessarily fixed) with integrand r(t), F+N or 1. In this latter case, we would have a minimum time problem. An example of inequality constraints is that $0 \le r(t) \le r_{\text{max}}$, where r_{max} is a fixed constant. The reader can easily formulate other meaningful problems by using other meaningful integrands, boundary conditions and constraints.

The same general remarks hold for weight loss and gain problems. If x(t) and u(t) are, respectively, the weight and caloric intake of a person, a reasonable trajectory equation would immediately lead to a variety of important and interesting problems. A rough model can be formulated using the constant 3500 calories/lb.

6. A nontrivial example. To illustrate Theorem 2 we consider the case when m = 3 in §3 and the integrand in (1) is

$$f(t, x, x') = \frac{1}{3}e^{-t}x_1'^3 + \frac{1}{2}x_2'^2 + \frac{1}{4}x_3'^4 + \frac{1}{2}e^{-2t}x_1^4 + 48e^{6t}x_3$$
$$-e^{-t}x_3x_1 - tx_3' - x_2\sin t$$

subject to $x(0) = (1,0,1)^T$ and $x(1) = (e,\sin 1,e^2)^T$ on the interval [a,b] = [0,1]. The reader may verify that $x(t) = (e^t,\sin t,e^{2t})$ is the unique solution to this nonlinear problem on the interval [0,1].

Using (9), the nonlinear system of 3(N-1) equations in 3(N-1) unknowns was found using Newton's method. The initial guess for Newton's method was the linear values between x(0) and x(1).

To save space we only list the errors at t=.5. The complete run gives similar errors for t=k/8, $k=1,2,\ldots,9$. Note that each component ratio of e_{2h}/e_h below, is approximately four, while each component ratio of e_{2h}^R/e_h^R is approximately 16:

$$e_{1/8}(.5) = (-0.157D - 02, -0.383D - 04, -0.499D - 01)^{T},$$

$$e_{1/16}(.5) = (-0.401D - 03, -0.956D - 05, -0.127D - 01)^{T},$$

$$e_{1/32}(.5) = (-0.101D - 03, -0.239D - 05, -0.318D - 02)^{T},$$

$$e_{1/8}^{R}(.5) = (-0.100D - 04, 0.131D - 07, -0.255D - 03)^{T},$$

$$e_{1/16}^{R}(.5) = (-0.600D - 06, 0.816D - 09, -0.150D - 04)^{T},$$

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