On Kutta-Merson Process and its Allied Processes

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1. *Preface*

In this paper, we'll describe some trials to give Runge-Kutta methods the ability of error estimation taking up as our object only single-stage method. R. Merson, F. Ceschino and R. E. Scraton have already made researches of the same kind, the one by the last author being too complicated though. (See [1], [2] and [3].) Those by the first two will be explained in this paper. The difference that lies between the methods by these pioneers and those proposed by us is this: the former consumes the freedom of conditional equations for the purpose of simplifying the procedure, while the latter uses the same freedom to highten the accuracy both of estimated value of truncation error and of the formula to search for the numerical solution. (Henceforth on account of space consideration the following abbreviations will be used; t. e. for truncation error, ac. for accuracy and e. v. for estimated value.)

2. *Preparation*

We let the given differential equation be

$$\frac{dy}{dx}=f(x, y),\ y(x_0)=y_0. \tag{2. 1}$$

Then we set a Runge-Kutta formula using five functional values as follows:

$$k_i=hf(x_0+\alpha_i h,\ y_0+\sum_{j=1}^{i-1}\beta_{ij}k_i) \qquad (i=1, 2, 3, 4, 5, \quad \alpha_1=\beta_{10}=0) \tag{2. 2}$$

$$y_1=y_0+\sum_{i=1}^{5}\nu_i k_i, \tag{2. 3}$$

where α_i, β_{ij} and ν_i are constants, h is the pitch of the integration and y_1 is the approximate solution at $x=x_0+h$.

If $y(x)$ is the true solution of (2. 1),

$$\begin{aligned} y_1-y(x_0+h)=[&a_1hf+a_2h^2Df+h^3(a_3D^2f+a_4f_yDf)+h^4(b_1D^3f\\ &+b_2f_yD^2f+b_3f_y^2Df+b_4DfDf_y)+h^5(c_1D^4f\\ &+c_2DfD^2f_y+c_3D^3ff_y+c_4D^2fDf_y+c_5D^2ff_y^2\\ &+c_6(Df)^2f_{yy}+c_7f_yDfDf_y+c_8Dff_y^3)+\cdots\cdots]. \end{aligned} \tag{2. 4}$$

where $D=\frac{\partial}{\partial x}+f_0\frac{\partial}{\partial y}$ and also where a_i, b_i, $i=1, 2, 3, 4$ and c_j, $j=1, 2, \cdots, 8$ are the functions of coefficients to characterize the formula. (Concerning to the details of these fuctions, see the original paper [4].) $_0$ at the end of the parentheses shows that the functions in them

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are estimated at the point (x_0, y_0). The other $_0$'s in later expressions have the same meaning.

3. *The measurement of ac. of t. e.*

To acquire ac. of third and fourth order Runge-kutta formulae, we use three kinds of measures with almost the same property.

If formula (2. 3) is a third order method, its t. e. E is obtained in (2. 4) when $a_i=0$ and $i=1, 2, 3, 4$. The following measures are used to know ac. of t. e. of the formula (2. 3).

$$A_4=8|b_1|+|b_2|+|2b_2+b_4|+|b_2+b_4|+2|b_3|+2|b_4| \tag{3. 1}$$

$$B_4=\sum_{i=1}^{4}|b_i| \tag{3. 2}$$

$$C_4=\sum_{i=1}^{4}b_i^2 \tag{3. 3}$$

$$\begin{aligned}A_5=16|c_1|+4|c_2|+|c_2+3c_3|+|2c_2+3c_3|+|c_2+c_3|+|c_3|\\+8|c_4|+|c_5|+|2c_5+c_7|+|c_5+c_6+c_7|+|c_6|+|2c_6+c_7|\\+|c_7|+2|c_8|\end{aligned} \tag{3. 4}$$

$$B_5=\sum_{i=1}^{8}|c_i| \tag{3. 5}$$

$$C_5=\sum_{i=1}^{8}c_i^2 \tag{3. 6}$$

A_i, B_i and C_i are the criteria of ac. of t. e., the first used by A. Ralston and the last two by T. E. Hull and R. L. Johnston. (see [5], [6].) These measures reflect rather precisely ac. of t. e. of the formula. For the later convenience sake the above quantities concerning to the typical Runge-Kutta formulae are given in Table 1.

Table 1. Ac. of t. e. of the typical Runge-Kutta formulae.

Method	Order	i	A_i	B_i	C_i
Classical Runge-Kutta method	4	5	1.01×10^{-1}	2.67×10^{-2}	1.41×10^{-4}
Runge-Kutta-Gill method	4	5	8.41×10^{-2}	2.24×10^{-2}	1.06×10^{-4}
Ralston's method with the highest ac. of t. e.	4	5	5.46×10^{-2}	1.67×10^{-2}	8.76×10^{-5}
Heun's method	3	4	2.31×10^{-1}	7.41×10^{-2}	2.14×10^{-3}
Kutta's method	3	4	2.50×10^{-1}	8.33×10^{-2}	3.47×10^{-3}
Ralston's method with the highest ac. of t. e.	3	4	1.11×10^{-1}	4.51×10^{-2}	1.75×10^{-3}

4. *Kutta-Merson Process and Ceschino's Method*

Concerning to Kutta-Merson Process, we use the same symbols and so on with those in the original paper. (see [1]) Now we set $T=\frac{1}{5}(y_4-y_5)$. As is shown in the original paper, y_5 is a fourth order method and T is so made as to give e. v. of t. e. of y_5 when $f(x, y)$ is a liner expression of x, y. However, Merson insists that when the pitch h is small enough, T can give a good e. v. of t. e. even if $f(x, y)$ is a non-linear function of x, y.

Concerning to Ceschino's method, we use the same symbols and so on with those in the original paper. (See the case of rank 5 pp. 227–229 in [2].) Now we set $T=y_{i+1}-y_{i+1}^*$. In his method y_{i+1}, y_{i+1}^* and T are a third order formula, a fourth order formula and e. v. of t. e. of y_{i+1}, respectively.

The measured quantities of ac. of t. e. concerning to the two methods above mentioned are given in Table 2.

Table 2. Ac. of Kutta-Merson process and Ceschino's method.

method \ integral formula \ Criterion		A_4	B_4	C_4	A_5	B_5	C_5
Kutta-Merson procees	y_5	(2.73×10^{-10})	(7.16×10^{-11})	(2.10×10^{-21})	4.65×10^{-2}	1.18×10^{-2}	2.09×10^{-5}
	y_5-T	4.81×10^{-2}	1.01×10^{-2}	4.20×10^{-5}	1.33×10^{-1}	2.04×10^{-2}	9.59×10^{-5}
	y_5+T	4.81×10^{-2}	1.01×10^{-2}	4.20×10^{-5}	1.13×10^{-1}	2.06×10^{-2}	7.94×10^{-5}
	y_4	2.41×10^{-1}	5.09×10^{-2}	1.05×10^{-3}	5.92×10^{-1}	9.47×10^{-2}	1.65×10^{-3}
Ceschino	y_{i+1}	3.51×10^{-1}	7.69×10^{-2}	3.38×10^{-3}	6.92×10^{-1}	1.10×10^{-1}	3.10×10^{-3}
	y_{i+1}^*	(7.55×10^{-8})	(2.27×10^{-8})	(1.68×10^{-16})	2.89×10^{-2}	6.17×10^{-3}	6.54×10^{-6}

The values in round parentheses are 0 by nature, though they ceased to be because of the computations done in finite digits.

Through the close observation of Table 1 and 2, we can see many facts, one of which is, for instance, as follows. If $f(x, y)$ is a non-linear function of x and y, the estimated error T in Kutta-Merson Process is e. v. of t. e. of y_5+T with the ac. of third order, but not of y_5 which has *a* fourth order ac. In other word, Kutta-Merson process is a method in which t. e. of y_5 which is the sum of all the error terms with degrees larger than 5 concerning to h, is replaced by the t. e. term of degrees four concerning to h which are in another integral formula with ac. of third order. Here T has no logical relation to t. e. of y_5. However, T will generally give too large value for t. e. of y_5 in those problems of good sort, and where the t. e. term of order h^4 in the formula to search for the numerical solution is excessively large compared with that of order h^5, and accordingly the convergence of Taylor's expansion of the solution goes rapidly. When the assumption above is satisfied, Ceschino's Method becomes effective, too. These facts will be affirmed when the quantities representing ac. of t. e. of order h^5 in the formula to search for the numerical solution are compared with those in the formula which seeks for t. e. of the formula firstly mentioned.

By Ceschino's method, we get the ac. of the integral formula y_{i+1} which is not so good as a third order one, but the ac. of the formula y_{i+1}^*, which is for the error estimation, is comparatively desirable as a fourth order one, so that e. v. brought out as the difference between y_{i+1} and y_{i+1}^* is correct to a considerable degree. On the other hand, Kutta-Merson Process is inferior in its ac. of e. v. of t. e. to that by Ceschino when y_5+T is used as a formula to obtain numerical solutions. It is clear in the Table, too.

Table 3 shows the true error and e. v. of t. e. when a differential equation $\frac{dy}{dx}=\frac{1}{y}$, $y(1)=2$ is integrated one step using Kutta-Merson Process and Ceschino's Method. E. V. of t. e. in Kutta-Merson Process is excessively large because of the assumption of non-linearity, while that in Ceschino's method is very correct.

Table 3. The Error of the numerical solution when $\frac{dy}{dx}=\frac{1}{y}$, $y(1)=2$ is intergrated from $x=0.0$ to $x=0.1$ by the pitch of 0.1.

method	actual error	estimated error
Kutta-Merson Process	72×10^{-9}	2089×10^{-9}
Ceschino's method	15125×10^{-9}	15099×10^{-9}

5. *Similar Methods*

5. 1. *Methods using three functional values*

The general form of the formula is

$$k_i=hf(x_0+\alpha_i h, y_0+\sum_{j=1}^{i-1}\beta_{ij}k_j) \quad (i=1, 2, 3, \ \alpha_1=\beta_{10}=0) \tag{5.1.1}$$

$$y_1=y_0+\sum_{i=1}^{3}\mu_i k_i \tag{5.1.2}$$

$$T=\sum_{i=1}^{3}\nu_i k_i \tag{5.1.3}$$

where α_i, β_{ij}, μ_i and ν_i are constants, y_1 is an integral formula and T stands for e. v. of t. e. of y_1. The conditions for T to express t. e. of y_1 and those by which y_1 is made a second order method are solved using α_2 and α_3 as parameters. (Details are in [4].) Two examples are given below.

(1) The case where $\alpha_2=\frac{1}{2}$, $\alpha_3=1.0$

Formula I: $\alpha_2=\beta_{21}=\frac{1}{2}$, $\alpha_3=1.0$, $\beta_{31}=-1.0$, $\beta_{32}=2.0$, $\mu_1=0.0$, $\mu_2=1.0$, $\nu_1=-\frac{1}{6}$, $\nu_2=\frac{1}{3}$, $\nu_3=-\frac{1}{6}$.

(2) The case where $\alpha_2=1$, $\alpha_3=\frac{1}{2}$

Formula II: $\alpha_2=\beta_{21}=1.0$, $\alpha_3=\frac{1}{2}$, $\beta_{31}=\frac{1}{4}$, $\beta_{32}=\frac{1}{4}$, $\mu_1=\mu_2=\frac{1}{2}$, $\nu_1=\nu_2=\frac{1}{3}$, $\nu_3=-\frac{2}{3}$.

5. 2. *The methods using four functional values*

The general formula is

$$\begin{cases} k_i = hf(x_0+\alpha_i h,\ y_0+\sum_{j=1}^{i-1}\beta_{ij}k_i) \quad (i=1,2,3,4,\ \ \alpha_1=\beta_{10}=0) & (5.2.1) \\ y_1 = y_0+\sum_{i=1}^{3}\mu_i k_i & (5.2.2) \\ y_2 = y_0+\sum_{i=1}^{4}\nu_i k_i & (5.2.3) \\ T = y_1 - y_2, & (5.2.4) \end{cases}$$

where α_i, β_{ij}, μ_i and ν_i are constants, y_1 and y_2 are respectively an integral formula and a formula with higher ac., which is necessary for error estimation, and T stands for e. v. of t. e. concerning to y_1. The two systems of conditional equations for y_1 and y_2 to be respectively a third and a fourth order method have not any solutions. However, it is possible to obtain as good an approximate solution as we desire.

Taking off the two conditional equations

$$\nu_2\alpha_2^2\beta_{32}+\nu_4(\sum_{i=2}^{3}\alpha_i^2\beta_{4i})=\frac{1}{12} \tag{5.2.5}$$

and

$$\nu_3\alpha_2\alpha_3\beta_{32}+\nu_4(\sum_{i=2}^{3}\alpha_i\beta_{4i})\alpha_4=\frac{1}{8} \tag{5.2.6}$$

from the system of y_2, we solve the rest and the system of y_1 using α_2, α_3 and α_4 as parameters. (Details are in [4].) If the solution is substituted for (5. 2. 5) and (5. 2. 6) both of these two become

$$\frac{3-4\alpha_2}{6-9\alpha_2}=\frac{1}{2}. \tag{5.2.7}$$

Accordingly, when α_2 converges to 0, the equations (5. 2. 5) and (5. 2. 6) are satisfied. If α_2 is set small enough when we choose free parameters α_2, α_3 and α_4, we can make y_1 and y_2 formulae each with ac. of a third order method and with that of almost a fourth order one. For instance, if we set $\alpha_2=\frac{1}{60}$, $\alpha_3=\frac{1}{2}$ and $\alpha_4=1$ we can get the following Formula III.

Formula III: $\alpha_2=\beta_{21}=\frac{1}{60}$, $\alpha_3=\frac{1}{2}$, $\beta_{31}=-\frac{541}{78}$, $\beta_{32}=\frac{290}{39}$, $\alpha_4=1.0$,

$\beta_{41}=\frac{1918321}{65598}$, $\beta_{42}=-\frac{34225}{1131}$, $\beta_{43}=\frac{117}{58}$, $\mu_1=10$, $\mu_2=-\frac{300}{29}$,

$\mu_3=\frac{39}{29}$, $\nu_1=\nu_4=\frac{1}{6}$, $\nu_3=\frac{2}{3}$.

Next, we try to optimize the coefficients from the standpoint of t. e. so as to higher ac. of error estimation. In this case, we use the criteria of ac. of t. e. explained in 3.

Henceforth, A_{ij}, B_{ij} and C_{ij} stand for the criteria of the t. e. at jth degrees concerning to h in the integral formula $y_i (i=1, 2)$.

It is rather a hard requirement for a third order formula y_1 to have the ability of error estimation through four computations of function. So we'll try to minimize the t. e. terms of order h^4, and h^5 in y_2 giving attention not to make the t. e. term of order h^4 in y_1 excessively small. One of the formulae obtained thus will be given below.

Formula IV: $\alpha_2=\beta_{21}=0.001$, $\alpha_3=0.7$, $\beta_{31}=-244.3175262$, $\beta_{32}=245.0175262$,
$\alpha_4=0.8$, $\beta_{41}=136.1510201$, $\beta_{42}=-136.0025668$, $\beta_{43}=0.6515466956$,
$\mu_1=-23.52380952$, $\mu_2=23.84358607$, $\mu_3=0.6802234484$,
$\nu_1=-53.31547619$, $\nu_2=53.71521268$, $\nu_3=0.3392601675$,
$\nu_4=0.2610033375$,

where

$$A_{14}=3.05\times10^{-1},\ B_{14}=9.44\times10^{-2},\ C_{14}=3.54\times10^{-3},\ B_{24}=6.25\times10^{-5},$$
$$A_{25}=7.52\times10^{-2},\ B_{25}=2.70\times10^{-2},\ C_{25}=1.69\times10^{-4}.$$

Table 4 shows the following things: firstly the numerical solution y_1, which was attained when the ordinary difierential equation

$$\frac{dy}{dx}=\frac{5y}{1+x},\ y(0)=1$$

was integrated using Formula IV from $x=0$ to $x=0.1$ by the pitch of 0.1, secondly its true error ε, and thirdly T which is e. v. of t. e., and lastly the ratio of T to ε.

Table 4. The numerical solution at $x=0.1$ in $\frac{dy}{dx}=\frac{5y}{1+x}$, $y(0)=1$.

y_1(numerical solution)	ε(actual error)	T(e. v. of t. e.)	T/ε
1.6093414971	−0.0011685030	−0.0010419490	0.892

5.3. *The methods using five functional values*

The general form of the formula is

$$k_i=hf(x_0+\alpha_i h,\ y_0+\sum_{j=1}^{i-1}\beta_{ij}k_j)\quad (i=1,2,3,4,5,\ \alpha_1=\beta_{10}=0) \tag{5.3.1}$$

$$y_1=y_0+\sum_{i=2}^{5}\mu_i k_i \tag{5.3.2}$$

$$y_2=y_0+\sum_{i=1}^{5}\nu_i k_i \tag{5.3.3}$$

$$T=y_1-y_2, \tag{5.3.4}$$

where α_i, β_{ij}, μ_i and ν_i are constants, y_1 and y_2 are each an integral formula and a formula with higher ac., which is necessary for error estimation, and T stands for e. v. of t. e. in y_1. The condition for y_2 to be a fifth order method is that a_i, b_i $i=1,2,3,4$ and c_j, $j=1,2,\cdots\cdots,8$ in (2.4), where y_1 is replaced by y_2, become all 0. As the impossibility of such a condition has been already proved [7], we take out of the above conditional equations

$$a_i=b_i=0\quad (i=1,2,3,4)$$

and also

$$c_i=0\quad (i=1,2,5)$$

and then solve them together with conditional equations for y_1 to be a third order method using α_2, α_3, α_4 and α_5 as parameters. (See the details in [4].)

The search of coefficients has been made in the following way.

(1) We decide all of the lattice points of four dimensions which are gained when each of α_2, α_3, α_4 and α_5 in the set of parameters are moved at a fixed interval within a certain region.

(2) By dint of the solution, we compute all the coefficients of y_2 and A_{25}, B_{25} and C_{25} for each of the above sets of parameters, α_2, α_3, α_4 and α_5, in which case, for these coeffieints, y_2 naturally becomes a fourth order mechod with rather high ac.

(3) Out of the innumerable sets of parameters in (1), we take up the set of parameters which makes A_{25}, B_{25} and C_{25} sufficiently small and consequently lets y_2 be endowed with ac. nearly of the fifth order.

(4) For each set of parameters contained in the group of coefficients obtained in (3), we compute all the coefficients in y_1 and A_{1j}, B_{1j} and $C_{1j}(j=4, 5)$. In this case, y_1 is of course a third order method.

(5) Out of groups of coefficients gained in (4), we choose firstly the group where A_{15}, B_{15} and C_{15} are not so small, and then out of this group, the following three coefficients are chosen.

(a) A type whose A_{14}, B_{14} and C_{14} are small enough.

(b) A type whose A_{14}, B_{14} and C_{14} are considerably small.

(c) A type whose A_{14}, B_{14} and C_{14} are small.

The following Formula V, VI and VII correspond respectively with (a), (b) and (c) above stated.

Formula V: $\alpha_2=\beta_{21}=0.0031$, $\alpha_3=0.402$, $\beta_{31}=-25.66412331$, $\beta_{32}=26.06612331$, $\alpha_4=1.0005$, $\beta_{41}=321.3722438$, $\beta_{42}=-324.1161348$, $\beta_{43}=3.744391046$, $\alpha_5=1.0$, $\beta_{51}=319.9266520$, $\beta_{52}=-322.6578129$, $\beta_{53}=3.730663566$, $\beta_{54}=0.0004973349184$, $\mu_2=0.1276529869$, $\mu_3=0.5774104702$, $\mu_4=-54.90255223$, $\mu_5=55.19748877$, $\nu_1=-0.001106906558$, $\nu_2=0.1289088032$, $\nu_3=0.5770159269$, $\nu_4=-55.08439267$, $\nu_5=55.37957484$.

Formula VI: $\alpha_2=\beta_{21}=-0.0025$, $\alpha_3=0.3985$, $\beta_{31}=32.15974180$, $\beta_{32}=-31.76124180$, $\alpha_4=1.0005$, $\beta_{41}=-402.9114034$, $\beta_{42}=400.1456441$, $\beta_{43}=3.766259273$, $\alpha_5=1.0$, $\beta_{51}=-401.1095721$, $\beta_{52}=398.3565430$, $\beta_{53}=3.752531702$, $\beta_{54}=0.0004973503641$, $\mu_2=0.1216605083$, $\mu_3=0.5834052183$, $\mu_4=-54.23420321$, $\mu_5=54.52913749$, $\nu_1=-0.009699144572$, $\nu_2=0.1323963467$, $\nu_3=0.5803923412$, $\nu_4=-55.73162758$, $\nu_5=56.02853803$.

Formula VII: $\alpha_2=\beta_{21}=-0.0023$, $\alpha_3=0.401$, $\beta_{31}=35.35729065$, $\beta_{32}=-34.95629065$, $\alpha_4=1.0005$, $\beta_{41}=-439.0806052$, $\beta_{42}=436.3303196$, $\beta_{43}=3.750785679$, $\alpha_5=1.0$, $\beta_{51}=-437.1081827$, $\beta_{52}=434.3706279$, $\beta_{53}=3.737057439$, $\beta_{54}=0.0004973393253$, $\mu_2=0.09505105246$, $\mu_3=0.6628977358$,

$\mu_4 = -15.30917274$, $\mu_5 = 15.55122395$, $\nu_1 = 0.2068670840$,
$\nu_2 = -0.08053328809$, $\nu_3 = 0.5779923511$, $\nu_4 = -55.26802466$,
$\nu_5 = 55.56369851$.

Table 5 shows ac.'s of Formula V, Formula VI and Formula VII which have been measured using the criteria stated before. Formula V has high ac. of the integral formula, but is inferior in the ability of error estimation, while Formula VII has good ability of error estimation but its ac. of the integral formula is inferior. Formula VI, being the medium of the above two, seems to be fairly desirable.

Table 5. The ac. of t. e. of Formula V, VI and VII.

method	i	A_{i4}	B_{i4}	C_{i4}	A_{i5}	B_{i5}	C_{i5}
Formula V	1	6.67×10^{-4}	1.99×10^{-4}	1.41×10^{-8}	1.76×10^{-3}	3.35×10^{-4}	2.81×10^{-8}
	2	——	——	——	9.76×10^{-8}	3.25×10^{-8}	5.28×10^{-16}
Formula VI	1	5.58×10^{-3}	1.65×10^{-3}	9.65×10^{-7}	1.45×10^{-2}	2.76×10^{-3}	1.88×10^{-6}
	2	——	——	——	7.76×10^{-8}	2.58×10^{-8}	3.34×10^{-16}
Formula VII	1	1.48×10^{-1}	4.41×10^{-2}	6.94×10^{-4}	3.89×10^{-1}	1.37×10^{-1}	7.39×10^{-2}
	2	——	——		7.14×10^{-8}	2.38×10^{-8}	2.83×10^{-16}

We'll give an example showing Table 6 in which the case when the ordinary differential equation $\frac{dy}{dx} = -\frac{1}{3}x^2y^2$, $y(2)=1$
is integrated from $x=2.0$ to $x=2.1$ by the pitch of $h=0.1$ is displayed. The second line of the table presents numerical solution y_1, the third line presents the true error, and the last, e. v. of t. e. The columns from the second to the sixth give the results obtained each by Formula V, VI, VII, Kutta-Merson Process and Ceschino's method.

Table 6. The Numerical solution at $x=2.1$ in $\frac{dy}{dx} = -\frac{1}{3}x^2y^2$, $y(2)=1$.

method	Formula V	Formula VI	Formula VII	Kutta-Merson	Ceschino
y_1(numerical solution)	0.87710757	0.87710823	0.87712818	0.87710774	0.87711650
(true error)$\times10^8$	8	74	2069	25	901
(error estimate)$\times10^8$	10	77	2075	217	860

5. *Conclusion*

Our methods are basically different from that of Cheschino and from Kutta-Merson Process in this point: while the latter two consume the degrees of freedom of conditional equations, in order to take away the procedure of making the integral formula, the former makes use of the same degrees of it for the improvement of ac. of the integral formula and also of the ability of error estimation.

Our methods will increase the utility as a system of functions grows more complicated, and the procedure of making the integral formula has smaller and smaller ratio to the amount of all the computations. The formulae we gave here are not necessarily the best one. Especially the formula proposed in 4 has still room for examination. However, the method we used, being effective, seems to be capable of obtaining fairly good formulae. Though we were forced to omit many of the important items here as space was limited, more details will be found in the Japanese issue of the same paper.

6. *Acknowledgement*

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