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RECIPROCAL POLYNOMIAL EXTRAPOLATION *[1)]

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Abstract

An alternative to the classical extrapolations is proposed. The stability and the accuracy are studied. The new extrapolation behaves better than the classical ones when there are problems of stability. This technique will be useful in those problems where the region of stability is very small and it forces to work with too fine scales.

Key words: Extrapolation, Stability, ODE's.

1. Introduction

In order to improve the accuracy of a numerical method to approximate any quantity, several strategies are used, in most cases increasing its computational cost. Thus, reducing the discretization parameters, or obtaining higher order methods get better resolution, but the number of arithmetic computations to do is drastically increased. One of the best known strategies to get higher order methods based on a given one is extrapolation.

The discretization in space of PDE's leads to stiff systems of ODE's. When we apply the classical Runge-Kutta methods to these systems an order reduction takes place. A possibility is to use extrapolation methods in order to increase the final order. Moreover, we need to have a method with good stability properties. We are going to present a new extrapolation verifying these properties.

Let X and Y Banach spaces and $A : D(A) \subset X \to Y$ a linear operator. We consider the problem:

$$\frac{d}{dt}x(t) = Ax(t) + f(t),\ 0 \le t \le T, \tag{1}$$

$$x(0) = u_0 \in X, \tag{2}$$

where $T > 0$.

If we use a Runge-Kutta method to solve this problem we will have an approximation in the way:

$$S(h) = a_0 + a_1 h^p + \dots \tag{3}$$

where a_0 is the exact solution. Then considering, for example, two different discretizations h and $2h$, an extrapolation methods make a new approximation with error $O(h^r),\ r > p$.

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In this paper we carry out a theoretical study (analyzing the errors, the regions of stability...) and later, one practical. We will present a comparison with the classical rational and polynomial extrapolations.

The structure of the paper is the following: In section two we introduce the extrapolation concept, in section three we present the reciprocal polynomial extrapolation, the error and the stability are analyzed in section four, finally, we present some numerical results and conclusions in section five.

2. The Extrapolation Concept

Usually, if we assume we are approximating a value a_0 by means of a numerical method, we get the approximation $S(h)$, where

$$\lim_{h\to 0} S(h) = a_0. \tag{4}$$

The error of classical methods can be expressed as a Taylor series:

$$S(h) = a_0 + a_1 h^{\gamma_1} + a_2 h^{\gamma_2} + \dots \tag{5}$$

The most classical extrapolation method consists of successive elimination of the terms $a_i h^{\gamma_i}$ by linear combinations of approximations $S(h)$ for different h (Richardson's extrapolation). This can be viewed as the value of the only polynomial $P(x)$ interpolating those chosen $S(h)$ in $h = 0$.

Nevertheless, we can consider not only linear but also nonlinear strategies. We say $\phi(h, h^{'})$ is an extrapolation of (5) if

$$\phi(h, h^{'}) = a_0 + a_2^{'} h^{\hat{\gamma}_1} + \dots \tag{6}$$

with $\hat{\gamma}_1 > \gamma_1$.

It is clear, the order of accuracy is the same both cases. Our goal is to analyze the stability concept (in stiff problem nonlinear extrapolation obtain better practical results). The most used nonlinear extrapolation is a special class of rational one, in which the degrees of the polynomials in the rational function follow a special sequence. This extrapolation can be use when the exponents of the error expansion follow an arithmetic sequence only (see [7] for more details). On the other hand, in stiff problems, implicit methods are used, because they have better properties of stability. In this case we have to solve a nonlinear equation associated to the implicit method. The nonlinear equation can be to solve with an error $O(h^{p+1})$, where p is the order of the original methods. Thus, if we consider a coarser discretization, like extrapolation methods, then we can solve the equation with a bigger error.

In this paper we will study the behavior of $\frac{1}{P(x)}$ (reciprocal polynomial extrapolation). We will see all the classical methods can be extrapolated by this technique, and it will have better stability properties than usual rational and polynomial extrapolations.

3. Interpretation of the Reciprocal Polynomial Extrapolation

Richardson's extrapolation is equivalent to extrapolate by couples with functions of type $ax^p + b$ (p =order of the method in each step). In our case, it will be equivalent to consider the extrapolator function $R(x) = \frac{1}{P(x)}$ than considering extrapolations by couples with functions of the type $\frac{1}{dx^p+e}$.

Notice you in first place that for the construction of $\frac{1}{dx^p+e}$, one has to suppose that S_{h_i} and $S_{h_{i+1}}$ have the same sign. If $S_{h_i} S_{h_{i+1}} \leq 0$, then, to find the rational function, first we would make a translation of the axis, we would build then $\frac{1}{dx^p+e}$ and we would make the inverse translation lastly.

Let us see the previously equivalence. Let us suppose we have:

$$S(h_1), S(h_2), \ldots, S(h_k)$$

with the same sign and $h_1 > h_2 > \ldots > h_k > 0$.

To find an interpolator function $\frac{1}{P(x)}$ is equivalent to find a polynomial $P(x)$ that interpolates to:

$$\frac{1}{S(h_1)}, \frac{1}{S(h_2)}, \ldots, \frac{1}{S(h_k)}$$

we know this is equivalent to extrapolate by couples with functions of the type $ax^p + b$ and for construction, this is equivalent to consider the inverse of the data, that is to say $\frac{1}{\frac{1}{S(h_i)}} = S(h_i)$; and to extrapolate by couples with functions of the type $\frac{1}{dx^p+e}$.

This way, we conclude that to extrapolate with functions of the type $\frac{1}{P(x)}$ is equivalent to extrapolate by couples with functions $\frac{1}{ax^p+b}$.

Remark 1. Moreover, it is deduced to extrapolate by the reciprocal polynomial method with the previous data is equivalent to take the inverse data, to extrapolate by the polynomial method (Richardson) with them and to consider the inverse of the result.

In practice, we use a more stable direct algorithm for the implementation of the reciprocal polynomial extrapolation. Applying induction the following algorithm is obtained:

for $l = 1, 2, 3, \ldots, n$

$$b_{(0,l)} = S(2^{l-1}h)$$

for $j = 1$ up to $r = n - 1$ and **for** $l = 1$ up to k where $k = r - j + 1$

$$b_{(j,l)} = \frac{2^p - 1}{\frac{2^p}{b_{(j-1,l)}} - \frac{1}{b_{(j-1,l+1)}}} = \frac{(2^p - 1)b_{(j-1,l)}b_{(j-1,l+1)}}{2^p b_{(j-1,l+1)} - b_{(j-1,l)}}$$

where p is the first power of the error in each step.

4. Accuracy and Stability

Given (h, S_1), $(2h, S_2)$, and imposing the interpolation conditions, we obtain:

$$R(x) = \frac{1}{(\frac{S_2 - S_1}{S_1 S_2 h^{p_1}(1-2^{p_1})})x^{p_1} + (\frac{S_1 - 2^{p_1} S_2}{S_1 S_2 (1-2^{p_1})})}$$

reciprocal polynomial extrapolation, and

$$P(x) = (\frac{2^{p_1} S_1 - S_2}{2_1^p - 1}) + (\frac{S_2 - S_1}{h^{p_1}(2^{p_1} - 1)})x^{p_1}$$

polynomial extrapolation.

If we consider $\frac{1}{dx^{p_1}+e}$ and $ax^{p_1} + b$, we will have that $\frac{1}{e}$ and b they will be the approaches to a_0.

Proposition 1. *The first terms of the error in the reciprocal polynomial extrapolation and in the polynomial extrapolation are respectively:*

$$\frac{{a_1}^2(1 - 2^{2p_1})h^{2p_1} + (2^{p_2} - 2^{p_1})a_0 a_2 h^{p_2}}{a_0(1 - 2^{p_1})}$$

and

$$(1+\frac{1-2^{p_2}}{2^{p_1}-1})a_2h^{p_2}$$

Proof. It is gotten easily by algebraic manipulations and Taylor series.

Remark 2. In the usual methods, $2p_1 \geq p_2$ (thus, these methods can be extrapolated by this technique), even in most of them, $2p_1 > p_2$, in which case, the first term of the error in the reciprocal polynomial extrapolation approximately is $(\frac{2^{p_2}-2^{p_1}}{1-2^{p_1}})a_2h^{p_2}$, the same as the polynomial extrapolation.

On the other hand, $|1+\frac{1-2^{p_2}}{2^{p_1}-1}| \geq 1$, since $p_2 \geq p_1+1$, then the coefficient of the first power of the error goes increasing in module in each extrapolation, the idea is consider not much extrapolations.

If we only have two nodes both rational extrapolations are the same function:

$$\frac{1}{dx^p+e}$$

Let us see that it happens if we have three.

Proposition 2. *Supposing that:*

$$\begin{aligned} S_0 &= S(\frac{h}{2}) = a_0 + a_1(\frac{h}{2})^{p_1} + a_2(\frac{h}{2})^{2p_1} + \ldots \\ S_1 &= S(h) = a_0 + a_1(h)^{p_1} + a_2(h)^{2p_1} + \ldots \\ S_2 &= S(2h) = a_0 + a_1(2h)^{p_1} + a_2(2h)^{2p_1} + \ldots \end{aligned}$$

and considering the rational function $\frac{x^{p_1}+c}{dx^{p_1}+e}$.

The error in the rational extrapolation is:

$$(a_3 - \frac{{a_2}^2}{a_1})h^{3p_1}$$

Proof. It is straightforward.

As we see, the first terms of the errors, of the different extrapolations, depend on $a_0,\ a_1,\ \ldots$and, so the approach not only depends on the extrapolation, but of the own original method.

4.1. Analysis of the Stability

In this section we will see the reciprocal polynomial extrapolation conserves the properties of stability better than the classical polynomial extrapolation.

We will study the linear test equation:

$$y' = \lambda y$$

When we use Runge-Kutta methods, the following expression is obtained:

$$y_n = T(h\lambda)y_0 = T(z)y_0$$

the function $T(z)$ will give us the region of stability.

In the case of polynomial extrapolation, if we denote $T_{i,0},\ (i = 0, 1, \dots)$ the stability functions from different discretizations $(\dots,\ 2h,\ h)$ of some method, then the stability function for the extrapolation method will be

$$T_{i,k} = T_{i,k-1} + \frac{T_{i,k-1} - T_{i-1,k-1}}{2^{p_i} - 1}$$

Similarly for the reciprocal polynomial extrapolation we will have

$$T_{i,k} = \frac{2^{p_i} - 1}{\frac{2^{p_i}}{T_{i,k-1}} - \frac{1}{T_{i-1,k-1}}}$$

where p_j are the different orders. And for the rational extrapolation.

$$T_{i,k} = T_{i,k-1} + \frac{T_{i,k-1} - T_{i-1,k-1}}{(\frac{h_{i-k}}{h_i})^{p_1} K - 1} \tag{7}$$

where $K = 1 - \frac{T_{i,k-1} - T_{i-1,k-1}}{T_{i,k-1} - T_{i-1,k-2}}$.

The region of stability is:

$$\{z \in \mathcal{C} : |T(z)| \leq 1\}$$

According to the regions of the negative semiplane

$$\mathcal{C}^- = \{z \in \mathcal{C} : Re(z) \leq 0\}$$

that the region of stability contains, the method is said A-stable, A(α)-stable,... see[6].

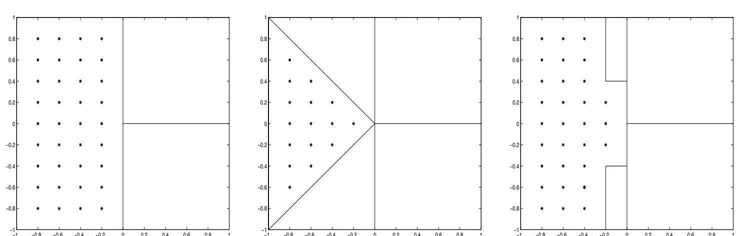

Figure 1: A-stability, A(α)-stability, Stiff stability

We want to analyze the region associated to the extrapolations, we will suppose that we are in the extreme case that $|T_{i,0}(z)| = 1$. In this case, it is clear that the polynomial extrapolation can have problems (to consider for instance $p = 1$, $T_{1,0} = (1, 0)$ and $T_{0,0} = (0.9, \sqrt{1 - (0.9)^2})$ then $|T_{1,1}| > 1$). In next section, we will see these type of stability problems (for the rational extrapolation also). Now, we analyze the reciprocal extrapolation

$$T_{1,1} = \frac{2^p - 1}{\frac{2^p T_{1,0} - T_{0,0}}{T_{1,0}\ T_{0,0}}} = \frac{(2^p - 1)(T_{1,0}\ T_{0,0})}{2^p T_{1,0} - T_{0,0}}$$

Let $I_j = Im(T_{j,0})$ and $R_j = Re(T_{j,0})$, $j = 0, 1$. Then

$$T_{1,1} = \frac{(2^p - 1)([R_1\ R_0 - I_1\ I_0] + i[R_1\ I_0 + I_1\ R_0])}{[2^p R_1 - R_0] + i[2^p I_1 - I_0]}$$

So,

$$
\begin{aligned}
|T_{1,1}|^2 &= \frac{(2^p-1)^2[{R_1}^2\ {R_0}^2+{I_1}^2\ {I_0}^2+{R_1}^2\ {I_0}^2+{I_1}^2\ {R_0}^2]}{2^{2p}\ {R_1}^2-2^{p+1}\ R_1\ R_0+{R_0}^2+2^{2p}\ {I_1}^2-2^{p+1}\ I_1\ I_0+{I_0}^2} \\
&= \frac{(2^p-1)^2({R_0}^2+{I_0}^2)\ ({R_1}^2+{I_1}^2)}{2^{2p}\ ({R_1}^2+I_1^2)-2^{p+1}(R_1\ R_0+\ I_1\ I_0)+(R_0^2+{I_0}^2)} \\
&= \frac{(2^p-1)^2}{2^{2p}+1-2^{p+1}\ (R_1R_0+I_1I_0)}
\end{aligned}
$$

Since $R_1R_0+I_1I_0 \leq 1$, we obtain

$$|T_{1,1}| \leq 1$$

and we have stability.

Remark 3. This extrapolation works by couples.

Now we compute numerical stability regions. We use two nodes to compare the polynomial extrapolation and the reciprocal polynomial extrapolation, and three to compare both rational.

We will use the following acronyms: P.E.= Richardson's extrapolation, R.P.E.= Reciprocal polynomial extrapolation, R.E.=Rational extrapolation.

Remark 4. In [4] you can see the details of the ordinary differential methods that we use in this paper.

First we applied extrapolation (polynomial and reciprocal polynomial) to Euler implicit method and to Randau IA-3 method. Both extrapolations are L-stable but the region of stability is bigger when the reciprocal polynomial extrapolation is applied (see remark 5 and figure 2).

Next we consider the Gauss-2 and trapezoidal methods (they give the same approximation when they are applied to the test equation). We observe reciprocal polynomial extrapolation is A(α)-stability for everything $\alpha \in (0, \frac{\pi}{2})$, in fact, contains the whole half-plane except the segments $(0, 0.2i)$; $(-2i, 0)$. For the polynomial extrapolation we obtain A(α)-stability with $\alpha < 86^o$.

Moreover we compared the reciprocal polynomial extrapolation and the rational extrapolation. Both extrapolations improve the region of the Euler (explicit) method considerably, and as in previous cases, the reciprocal polynomial extrapolation obtains a bigger region (see remark 5 and figure 2).

Remark 5. The regions of stability are symmetric respect to x-axis, then we have plotted one part only. The regions of Euler and Gauss methods are bounded and non-bounded respectively, because these methods are explicit and implicit respectively.

To conclude the section, we have studied the case of Gauss-2 with three nodes. In this case, the reciprocal polynomial extrapolation is A(89.88^o)-stable, the rational extrapolation is A(89.59^o)-stable and the polynomial one is A(76.50^o)-stable.

Therefore, the reciprocal polynomial extrapolation obtains better properties of stability than the classical extrapolations, improving the stability when the method it is explicit and maintaining good properties of stability in the implicit schemes.

5. Numerical Analysis and Conclusions

In order to show the performance of the different extrapolation methods, we have tested them on the results obtained for the numerical solution of the first order linear differential equation with constant coefficients,

$$y' = \lambda y$$

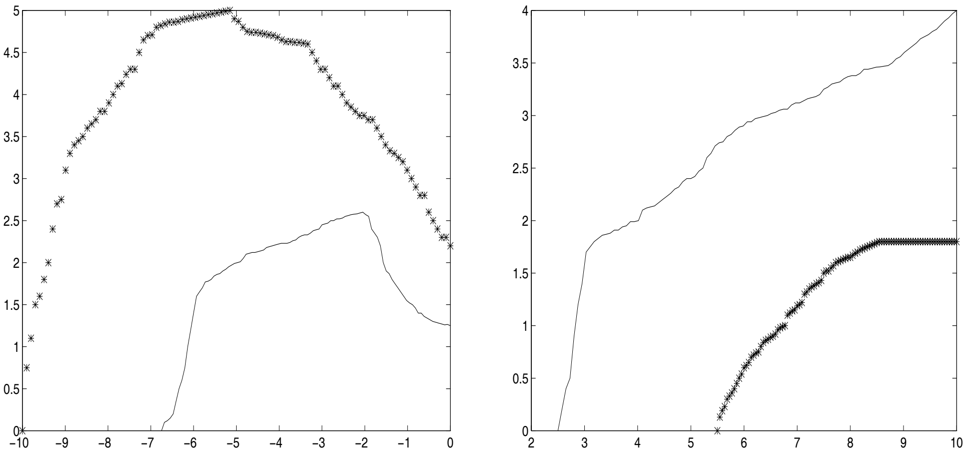

Figure 2: Boundary bounds of the numerical stability region, Left: Explicit Euler (*=R.P.E, -=P.E.), Right: Randau IA-3 (*= R.P.E, -=R.E.).

$$y(0) = 1$$

We solve this equation by means of some usual Runge-Kutta methods in $t = 1$, and we extrapolate the results for discretizations of size h, $2h$ (denoted by nd=2) and, eventually, $4h$ (we denote it by nd=3). The extrapolation we use is the passive one (we only extrapolate the final results), in order not to modify the original stability of the method. We will make it for different values of lambda and for different discretizations.

The three extrapolations obtain comparable results when the discretizations is within the stability region. However, when problems of stability exist, the reciprocal polynomial extrapolation obtains better results (see tables 1-2).

Table 1: Error in explicit Euler's method, test equation, t=1, nd=3

Input Data	R.P.E.	R.E.	P.E.
$\lambda = -1, h = 0.1$	$3.69e-01$	$1.64e-02$	$2.65e-02$
$\lambda = -1, h = 0.01$	$1.37e-06$	$5.27e-08$	$3.18e-07$
$\lambda = -6, h = 0.01$	$1.09e-04$	$1.24e-05$	$6.86e-07$
$\lambda = -10, h = 0.01$	$3.24e-05$	$8.73e-06$	$2.16e-06$
$\lambda = -12, h = 0.01$	$5.84e-06$	$1.08e-05$	$8.28e-07$
$\lambda = -15, h = 0.01$	$3.05e-07$	$3.98e-07$	$1.08e-07$
$\lambda = -40, h = 0.01$	$4.24e-18$	$4.24e-18$	$9.47e-07$
$\lambda = -40, h = 0.04$	$4.24e-18$	$2.89e+0.4$	$1.74e+04$

In the case we introduced here, it can said that the unstable approximation does not *contaminate* the stable one. Also, we observe that when the reciprocal polynomial extrapolation is used the region of stability is bigger taking place the jump of the error later (see tables 3-4 and figure 3).

The nature of the test problem and the accuracy of the obtained results are the reasons that we have not tried higher order extrapolations (more than three nodes). In the worst shown case,

Table 2: Error in Gauss-2, test equation, t=1, nd=3

Input Data	R.P.E.	R.E.	P.E.
$\lambda=-1, h=0.1$	$2.42e-02$	$1.47e-04$	$2.71e-03$
$\lambda=-1, h=0.2$	$8.62e-02$	$4.21e-02$	$1.36e-01$
$\lambda=-10, h=0.02$	$7.45e-06$	$1.40e-05$	$5.26e-06$
$\lambda=-10, h=0.08$	$5.23e-06$	$2.51e-07$	$6.22e-06$
$\lambda=-20, h=0.01$	$4.88e-10$	$1.71e-10$	$1.52e-10$
$\lambda=-20, h=0.04$	$2.06e-09$	$1.11e-09$	$5.03e-05$
$\lambda=-30, h=0.1$	$3.83e-08$	$1.43e-02$	$2.32e-01$

Table 3: Error in explicit Euler's method, test equation $\lambda=-40$, t=1, nd=3

Input Data	R.P.E.	R.E.	P.E.
$h=0.06$	$8.15e+01$	$2.12e+03$	$8.45e+04$
$h=0.05$	$3.75e-01$	$4.70e+03$	$1.23e+05$
$h=0.04$	$1.06e-06$	$2.89e+04$	$1.74e+04$
$h=0.03$	$4.24e-18$	$1.02e+02$	$1.40e+04$
$h=0.02$	$4.24e-18$	$1.42e-06$	$4.28e+03$
$h=0.01$	$4.24e-18$	$4.24e-18$	$9.47e-07$
$h=0.009$	$4.24e-18$	$4.24e-18$	$7.87e-11$
$h=0.008$	$4.24e-18$	$4.24e-18$	$6.67e-18$

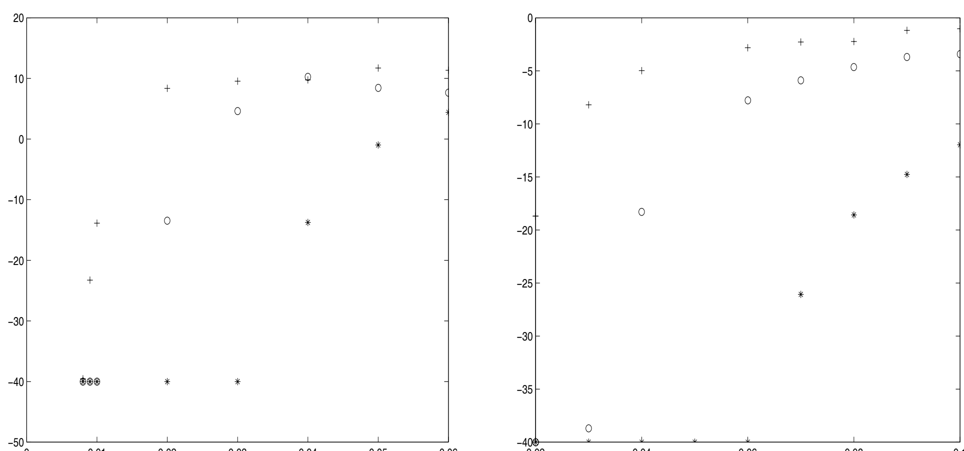

Figure 3: *=R.P.E., o=R.E. , +=P.E., Left: Euler, Right: Gauss-2, Error-log_{10}

the rational and polynomial extrapolations are affected with the third unstable approximation (see table 5).

In this paper we have studied a nonlinear extrapolation technique. Nonlinearity is important in case we have stability problems. Reciprocal polynomial extrapolation behaves better than classical ones when the discretization is close to the unstable region. On the other side, the

Table 4: Error in Gauss-2, test equation $\lambda = -40$, t=1, nd=3

Input Data	R.P.E.	R.E.	P.E.
$h = 0.1$	$6.34e-06$	$3.26e-02$	$3.57e-01$
$h = 0.09$	$3.88e-07$	$2.50e-02$	$3.05e-01$
$h = 0.08$	$8.55e-08$	$9.56e-03$	$1.07e-01$
$h = 0.07$	$4.78e-12$	$2.74e-03$	$1.02e-01$
$h = 0.06$	$4.24e-18$	$4.16e-04$	$5.97e-02$
$h = 0.04$	$4.24e-18$	$1.14e-08$	$6.68e-03$
$h = 0.03$	$4.24e-18$	$1.57e-17$	$2.75e-04$
$h = 0.02$	$4.24e-18$	$4.24e-18$	$7.60e-09$

Table 5: Error with different numbers of nodes, t=1

Input Data	R.P.	R.P.	R.P.	R.	R.	P.	P.	P.
	Euler	RK-4	GS-2	Euler	GS-2	Euler	RK-4	GS-2
$\lambda = -20, h = 0.0001, nd = 2$	$e-13$	$e-23$	$e-19$	$e-13$	$e-19$	$e-13$	$e-23$	$e-19$
$\lambda = -20, h = 0.0001, nd = 3$	$e-14$	$e-24$	$e-23$	$e-14$	$e-23$	$e-14$	$e-24$	$e-19$
$\lambda = -20, h = 0.001, nd = 2$	$e-10$	$e-18$	$e-15$	$e-10$	$e-15$	$e-11$	$e-18$	$e-15$
$\lambda = -20, h = 0.001, nd = 3$	$e-11$	$e-20$	$e-17$	$e-11$	$e-18$	$e-11$	$e-20$	$e-15$
$\lambda = -20, h = 0.01, nd = 2$	$e-09$	$e-13$	$e-11$	$e-09$	$e-11$	$e-09$	$e-13$	$e-11$
$\lambda = -20, h = 0.01, nd = 3$	$e-09$	$e-15$	$e-11$	$e-09$	$e-12$	$e-09$	$e-14$	$e-11$
$\lambda = -20, h = 0.02, nd = 2$	$e-09$	$e-12$	$e-09$	$e-09$	$e-09$	$e-04$	$e-12$	$e-10$
$\lambda = -20, h = 0.02, nd = 3$	$e-09$	$e-12$	$e-09$	$e-09$	$e-10$	$e-04$	$e-10$	$e-10$
$\lambda = -40, h = 0.0001, nd = 2$	$e-20$	$e-30$	$e-26$	$e-20$	$e-26$	$e-20$	$e-30$	$e-19$
$\lambda = -40, h = 0.0001, nd = 3$	$e-21$	$e-32$	$e-30$	$e-21$	$e-30$	$e-21$	$e-32$	$e-19$
$\lambda = -40, h = 0.001, nd = 2$	$e-18$	$e-25$	$e-22$	$e-18$	$e-22$	$e-18$	$e-25$	$e-15$
$\lambda = -40, h = 0.001, nd = 3$	$e-18$	$e-27$	$e-24$	$e-18$	$e-24$	$e-19$	$e-27$	$e-15$
$\lambda = -40, h = 0.01, nd = 2$	$e-18$	$e-20$	$e-18$	$e-18$	$e-18$	$e-18$	$e-20$	$e-11$
$\lambda = -40, h = 0.01, nd = 3$	$e-18$	$e-20$	$e-18$	$e-18$	$e-17$	$e-07$	$e-19$	$e-11$
$\lambda = -40, h = 0.02, nd = 2$	$e-18$	$e-19$	$e-18$	$e-18$	$e-18$	$e-18$	$e-19$	$e-10$
$\lambda = -40, h = 0.02, nd = 3$	$e-18$	$e-19$	$e-18$	$e-06$	$e-18$	$e+03$	$e+00$	$e-10$

introduced extrapolation has a computational cost similar than the linear case.

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