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NUMERICAL DIFFERENTIATION AND INTEGRATION THROUGH AITKEN-NEVILLE SCHEMES

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Abstract. Some new formulas are given to approximate higher order derivatives and integrals through Aitken-Neville iterative schemes for arbitrary spaced grids. An algorithm is given in MATLAB for numerical differentiation. Also, numerical examples are provided to study error analysis of new formulas for numerical differentiation and integration.

1. Introduction.

The problem of numerical differentiation is a long-standing issue. There are plenty of published works devoted to estimate derivatives of a function numerically for arbitrary spaced grids. Some of them are polynomial interpolation type [5, 9], finite difference formulas [2, 4, 6] and Richardson extrapolation [2]. Most of them do not aim to iterate derivatives upto k^{th} order per addition of a new grid. The finite difference formulas for the calculation of any order derivative in a one dimensional grid with arbitrary spacing are discussed in Ref[4] (algorithm given in Fortran) with the cost of $O(kn^2)$ operations. It also generates sequence of approximate derivatives upto order k per addition of a new grid. It should be noted that there exists a great deal of formulas and techniques of numerical integration. But, they have been of considerable complexity and often been limited to lower order formulas on equidistantly spaced grids.

Aitken-Neville schemes [5, 7, 8] are popular interpolation methods to iterate interpolation when a new grid is added. An obvious advantage of these schemes is that it gives a good idea of the accuracy of the result at any stage [8]. In the present study we describe new formulas to approximate numerical derivatives and integrals through Aitken-Neville iterative schemes for arbitrary spaced grids. Also, we provide an efficient algorithm in MATLAB to iterate numerical differentiation (upto k^{th} order) per addition of a new grid with cost of $O(k^2n)$ operations.

2. Numerical differentiation

2.1. Formulae for numerical differentiation.

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Definition 2.1. Define $N_j^{(r)}[x] = \frac{1}{(x_j - x)^r}$ and

$$N^{(r)}_{j,j+1,\ldots,j+i}[x] = \frac{1}{x_{i+j} - x_j} \begin{vmatrix} N^{(r)}_{j,j+1,\ldots,j+i-1}[x] & x_j - x \\ N^{(r)}_{j+1,j+2,\ldots,j+i}[x] & x_{i+j} - x \end{vmatrix}. \tag{2.1}$$

Also, define $\tilde{N}_j^{(r)}[x] = \frac{f(x_j)}{(x_j - x)^r}$ and

$$\tilde{N}^{(r)}_{j,j+1,\ldots,j+i}[x] = \frac{1}{x_{i+j} - x_j} \begin{vmatrix} \tilde{N}^{(r)}_{j,j+1,\ldots,j+i-1}[x] & x_j - x \\ \tilde{N}^{(r)}_{j+1,j+2,\ldots,j+i}[x] & x_{i+j} - x \end{vmatrix}. \tag{2.2}$$

Where $N^{(r)}_{j,j+1,j+2,\ldots,j+i}[x]$ and $\tilde{N}^{(r)}_{j,j+1,j+2,\ldots,j+i}[x]$ are constructed by Neville scheme of interpolation, $i = 1, 2, \ldots, n$ and $j = 0, 1, 2, 3 \ldots n - i$. At the n^{th} iteration, assume that $N^{(r)}_{0,1,2,\ldots,n}[x] = N^{(r)}(x)$, $r = 0, 1, 2, \ldots k$.

Definition 2.2. Define $A^{(r)}_{0,j}[x] = \frac{1}{x_j - x_0} \begin{vmatrix} \frac{1}{(x_0 - x)^r} & x_0 - x \\ \frac{1}{(x_j - x)^r} & x_j - x \end{vmatrix}$ and

$$A^{(r)}_{0,1,2,\ldots,i-1,i,j}[x] = \frac{1}{x_j - x_0} \begin{vmatrix} A^{(r)}_{0,1,\ldots,i-1,i}[x] & x_i - x \\ A^{(r)}_{0,1,\ldots,i-1,j}[x] & x_j - x \end{vmatrix}. \tag{2.3}$$

Also, define $\tilde{A}^{(r)}_{0,j}[x] = \frac{1}{x_j - x_0} \begin{vmatrix} \frac{f(x_0)}{(x_0 - x)^r} & x_0 - x \\ \frac{f(x_j)}{(x_j - x)^r} & x_j - x \end{vmatrix}$ and

$$\tilde{A}^{(r)}_{0,1,2,\ldots,i,j}[x] = \frac{1}{x_j - x_i} \begin{vmatrix} \tilde{A}^{(r)}_{0,1,\ldots,i-1,i}[x] & x_i - x \\ \tilde{A}^{(r)}_{0,1,\ldots,i-1,j}[x] & x_j - x \end{vmatrix}. \tag{2.4}$$

Where $A^{(r)}_{0,1,2,\ldots,i-1,i,j}[x]$ and $\tilde{A}^{(r)}_{0,1,2,\ldots,i-1,i,j}[x]$ are constructed by Aitken's scheme of interpolation, $i = 1, 2, \ldots, n$ and $j = i + 1, i + 2, \ldots, n$. At the n^{th} iteration, assume that $A^{(r)}_{0,1,2,\ldots,n}[x] = A^{(r)}(x)$, $r = 1, 2, \ldots k$.

The following theorem gives recursive formulas for numerical differentiation through Aitken-Neville schemes.

Theorem 2.3. *Let $x, x_0, x_1, x_2, \ldots x_n$ are $n + 1$ distinct numbers on the interval $[a, b]$, $k \in W$ and $f \in C^{n+k+1}[a, b]$. Then*

$$\sum_{i=0}^{k} \frac{f^{(i)}(x)}{i!} N^{(k-i)}(x) = \tilde{N}^{(k)}_{0,1,\ldots,n}[x] + E(x). \tag{2.5}$$

and

$$\sum_{i=0}^{k} \frac{f^{(i)}(x)}{i!} A^{(k-i)}(x) = \tilde{A}^{(k)}_{0,1,\ldots,n}[x] + E(x). \tag{2.6}$$

Where $E(x) = \frac{f^{(n+k+1)}(\xi)}{(n+k+1)!} \prod_{i=0}^{n} (x - x_i)$ *and for* $\min\{x, x_0, \ldots, x_n\} < \xi < \max\{x, x_0, \ldots, x_n\}$.

Proof. Let $P_n(x)$ is a polynomial of degree $\leq n$ in x that approximates the function f. Using equation (2.7), gives

$$f[\underbrace{x, \ldots, x}_{k+1 \text{ times}}] = D_{0,1,2,\ldots,n}[x] + l(x) \frac{f^{(n+k+1)}(\xi)}{(n+k+1)!}.$$

Where $P_n[\underbrace{x,\dots,x}_{k+1 \text{ times}}/x_0,x_1,\dots x_n] = D_{0,1,2,\dots,n}[x]$ and $l(x) = \prod_{i=0}^{n}(x-x_i)$ and $\min\{x,x_0,\dots,x_n\} < \xi < \max\{x,x_0,\dots,x_n\}$. Expand $P_n[\underbrace{x,\dots,x}_{k \text{ times}},x_j]$ repeatedly, using the recursive formula of divided difference [2, p-41] to get

$$P_n[\underbrace{x,\dots,x}_{k \text{ times}},x_j] = -\sum_{r=0}^{k-1}\frac{P_n^{(r)}(x)}{r!}\frac{1}{(x_j-x)^{k-r}} + \frac{P_n(x_j)}{0!(x_j-x)^k}. \tag{2.7}$$

Applying equation (2.7) for two consecutive data x_j, x_{j+1}

$$P_n[\underbrace{x,\dots,x}_{k+1 \text{ times}}/x_j,x_{j+1}] = \frac{1}{x_{j+1}-x_j}\begin{vmatrix} P_n[\underbrace{x,\dots,x}_{k \text{ times}}/x_j] & x_j - x \\ P_n[\underbrace{x,\dots,x}_{k \text{ times}}/x_{j+1}] & x_{j+1}-x \end{vmatrix}.$$

Using (2.7) and properties of determinants, finds that

$$P_n[\underbrace{x,\dots,x}_{k+1 \text{ times}}/x_j,x_{j+1}] = -\sum_{r=0}^{k-1}\frac{P_n^{(r)}(x)}{r!}N_{j,j+1}^{(k-r)}[x] + \tilde{N}_{j,j+1}^{(k)}[x].$$

Proceeding this for some i,

$$\begin{aligned} &P_n[\underbrace{x,\dots,x}_{k+1 \text{ times}}/x_j,x_{j+1},\dots,x_{j+i}] \\ &\qquad = -\sum_{r=0}^{k-1}\frac{P_n^{(r)}(x)}{r!}N_{j,j+1,\dots,j+i}^{(k-r)}[x] + \tilde{N}_{j,j+1,\dots,j+i}^{(k)}[x]. \end{aligned}$$

Putting $i = n$ and $j = 0$,(i.e at n^{th} iteration)

$$P_n[\underbrace{x,\dots,x}_{k+1 \text{ times}}/x_0,x_1,\dots,x_n] = -\sum_{r=0}^{k-1}\frac{P_n^{(r)}(x)}{r!}N_{0,1,\dots,n}^{(k-r)}[x] + \tilde{N}_{0,1,\dots,n}^{(k)}[x].$$

Since P_n approximates f and $N_{0,1,\dots n}^{(r)}[x] = N^{(r)}(x)$. Then

$$f[\underbrace{x,\dots,x}_{k+1 \text{ times}}] - l(x)\frac{f^{(n+k+1)}(\xi)}{(n+k+1)!} = -\sum_{r=0}^{k-1}\frac{f^{(r)}(x)}{r!}N^{(k-r)}(x) + \tilde{N}_{0,1,\dots,n}^{(k)}[x].$$

Since $f[\underbrace{x,\dots,x}_{k+1 \text{ times}}] = \frac{f^{(k)}(x)}{r!}$ and after simplification gives (2.5). Similar manner using Definition 2.2, yields (2.6). □

Theorem 2.4. *Let $x, x_0, x_1, x_2, \dots x_n$ are $n+1$ distinct numbers on the interval $[a,b]$, $k \in W$ and $f \in C^{n+k+1}[a,b]$. Then direct formula for numerical differentiation through Neville scheme as follows*

$$\frac{f^{(t)}(x)}{t!} = a_t f(x)\chi + \sum_{k=\chi}^{t} a_{t-k}\tilde{N}_{0,1,2,\dots n}^{(k)}[x] + E_D(a;x). \tag{2.8}$$

and

$$a_0 = 1, \quad a_t = -\sum_{k=0}^{t-1} a_k N^{(t-k)}(x), \qquad t = 1, 2, 3, \ldots. \tag{2.9}$$

The direct formula for numerical differentiation through Aitken scheme as follows

$$\frac{f^{(t)}(x)}{t!} = b_t f(x)\chi + \sum_{k=\chi}^{t} b_{t-k}\tilde{A}^{(k)}_{0,1,2,\ldots n}[x] + E_D(b;x). \tag{2.10}$$

and

$$b_0 = 1, \quad b_t = -\sum_{k=0}^{t-1} b_k A^{(t-k)}(x), \qquad t = 1, 2, 3, \ldots. \tag{2.11}$$

Where

$$\chi = \begin{cases} 1 & \text{if } x = x_i \\ 0 & \text{if } x \neq x_i, \end{cases}$$

$$E_D(y;x) = l(x)\sum_{m=\chi}^{t} y_{t-m}\frac{f^{(n+m+1)}(\xi_m)}{(n+m+1)!}.$$

and $y = \begin{bmatrix} y_0 & y_1 & \ldots & y_t \end{bmatrix}$ *is an one dimensional array of length* $t+1$.

Proof. If one use equation (2.5) recursively to derive direct formulas for k^{th} order differentiation, then we obtain the following form, for some $t = 0, 1, 2, 3\ldots$

$$\frac{f^{(t)}(x)}{t!} = a_t f(x)\chi + \sum_{k=\chi}^{t} a_{t-k}\tilde{N}^{(k)}_{0,1,2,\ldots n}[x] + E_D(a;x).$$

To evaluate these unknown $a's$, set $f(x) = 1$ in the above equation, gives $a_0 = 1$ when $t = 0$ and for $t = 1, 2, 3, \ldots$ gives

$$\sum_{k=1}^{t-1} a_{t-k} N^{(k)}(x) + a_t = 0.$$

This gives (2.9). Similarly, from (2.6), it can be easily find (2.10). □

2.2. **Numerical experiment.** In this subsection, we present algorithm (coded in MATLAB) and numerical result to illustrate the performance of the new formulas given in (2.9) and (2.10) for arbitrary spaced grids.

Algorithm 2.5. Numerical differentiation through Neville scheme

```
function [d]=differentiation(x,y,k,s)
%    Input parameters
%    s          location where approximations are to be accurate
%    x(1:n)     grid point locations, found in x(1:n)
%    y(1:n)     functional value locations, found in y(1:n)
%    k          highest derivatives are sought at 's'
%     Output parameters
%   d(1:k+1,1:n)   sequence of approximate derivatives of order 0:k
n=length(x);
% Check whether 's' coincide with any one of 'x'. (i.e) functional value
% of 's' is known or not.
```

```
xs=x-s*ones(1,n);
pos=find(~(xs&xs));
chi=~all(xs);
% If chi=1 (functional value at 's' is known), then swap respective
% position of s and its functional value with first element of x and y.
if chi==1;
x([1 pos])=x([pos 1]);
y([1 pos])=y([pos 1]);
nevy(1,1:n)=y(1);
nev(1,1:n)=1;
end
f=1+chi;
```

% Determine the value of $N^{(r)}(s)$ and $\tilde{N}^{(r)}_{0,1,2,\ldots,n}[s]$ by Neville scheme and store %it in 'nev' and 'nevy' respectively

```
for ij=f:k+1
        yy(f:n)=1./(x(f:n)-s).^(ij-1);
        yy1=y.*yy;
        nev(ij,f)=yy(f);
        nevy(ij,f)=yy1(f);
        for i= f:n
            yy(f:n+f-i-1)=(yy(f+1:n+f-i).*(s-x(f:n+f-i-1))-yy (f:n+f-i-1)
                .*(s-x(i+1:n)))./(x(i+1:n)-x(f:n+f-i-1));
            yy1(f:n+f-i-1)=(yy1(f+1:n+f-i).*(s-x(f:n+f-i-1))- yy1(f:n+f-i-1)
                .*(s-x(i+1:n)))./(x(i+1:n)-x(f:n+f-i-1));
            nev(ij,i)=yy(f);
            nevy(ij,i)=yy1(f);
        end
end
```

% Find the value of a's and store them in a two dimensional array 'b'

```
for m=1:n
        b(1,m)=1;
        mn=min(m,k+1);
        a(1,1)=1;
        FACT(mn)=1;
        for i=2:mn
             b(i,m)=0;
             for j=1:i-1
             b(i,m)=b(i,m)-b(j,m)*nev(i-j+1,m);
             end
             a(i,i:-1:1)=b(1:i,m)';
             FACT(mn+1-i)=factorial(i-1);
        end
% Evaluate sequence of approximate derivatives up to order 'k'
        Diff=(a(mn:-1:1,:)*nevy(1:mn,m)).*FACT';
        d(1:mn,m)=Diff(mn:-1:1);
end
```

The algorithm for numerical differentiation through Aitken scheme is similar to the algorithm 2.5. The following are some notes regarding the implementation of the algorithm:

- A call to `differentiation` to obtain value of m^{th} derivative returns also value of k^{th} derivative, $k = 0, 1, 2, \ldots, m$ with no additional costs.
- The code returns all the data above also for points which extend only over $x_0, x_1, \ldots, x_j$, $j = 0, 1, 2, \ldots, n$, still no additional costs.
- It requires $O\left(k^2 n\right)$ operations. Also, the maximum size of array used is $(k+1) \times n$.

In the following example, we have taken 20 Chebyshev first kind of points on [-1,1] of function $f(x) = e^x$. We evaluate the first order derivatives at 100 equally spaced points on $[-1+h, 1-h]$, where $h = 2/101$. Figure 1 plots the errors for numerical

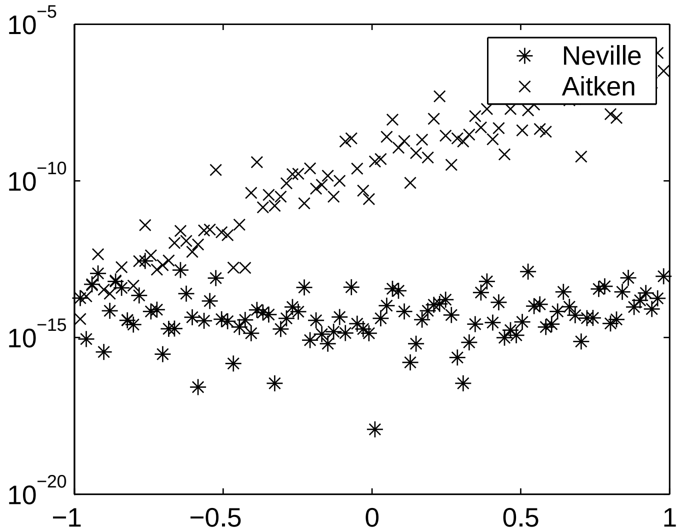

FIGURE 1. Relative errors in computed $f'(x)$ for 20 Chebyshev first kind of points of $f(x) = e^x$.

differentiation through Aitken-Neville schemes. We see that the Neville scheme performs stably and Aitken scheme becomes very unstable as x approaches one end of the interval.

3. NUMERICAL INTEGRATION.

3.1. **Formulae for Numerical integration.** In this section, we derive numerical integration formulas for arbitrary spaced grids to any order of accuracy. Let $x, x_0, x_1, x_2, \ldots, x_n$ are distinct numbers on the closed interval $[a, b]$ and $f \in C^{(n+1)}[a, b]$. To derive an expression for the definite integral $\int_x^{x+h} f(x)dx$, $(h \neq 0)$ expanding through Taylor series, yields

$$\int_x^{x+h} f(x)dx = \sum_{k=0}^{n} \frac{f^{(k)}(x)}{(k+1)!} h^{k+1} + O\left(h^{n+2}\right). \tag{3.1}$$

Using (2.8), gives

$$\int_{x}^{x+h} f(x)dx = \sum_{k=0}^{n} \frac{h^{k+1}}{k+1} \left(a_k f(x)\chi + \sum_{m=\chi}^{k} a_{k-m} \tilde{N}^{(m)}_{0,1,2,\dots n}[x] \right.$$
$$\left. + l(x) \sum_{m=\chi}^{k} a_{k-m} \frac{f^{(n+m+1)}(\xi_m)}{(n+m+1)!} \right) + O\left(h^{n+2}\right).$$

Setting $\gamma_k = \sum_{m=0}^{n-k} a_m \frac{h^{m+k+1}}{m+k+1}$, $k = 0,1,2,\dots n$ and rearranging above equation, yields

$$\int_{x}^{x+h} f(x)dx = \gamma_0 f(x)\chi + \sum_{k=\chi}^{n} \gamma_k \tilde{N}^{(k)}_{0,1,2,\dots,n}[x] + E_I(\gamma; x). \tag{3.2}$$

Where

$$E_I(\gamma; x) = l(x) \sum_{m=\chi}^{n} \gamma_m \frac{f^{(n+1+m)}(\xi_m)}{(n+1+m)!} + O\left(h^{n+2}\right). \tag{3.3}$$

Similarly, numerical integration formula through Aitken scheme can be easily found from (2.1) as follows

$$\int_{x}^{x+h} f(x)dx = \gamma'_0 f(x)\chi + \sum_{k=\chi}^{n} \gamma'_k \tilde{A}^{(k)}_{0,1,2,\dots,n}[x] + E_I(\gamma'; x). \tag{3.4}$$

Where $\gamma'_k = \sum_{m=0}^{n-k} b_m \frac{h^{m+k+1}}{m+k+1}$, $\qquad k = 0,1,2,\dots n$

3.2. **Numerical Experiment.** We evaluate the integral $\int_{-1}^{1} e^x dx$ on Chebyshev and other point distributions. The exact value of the integral is $e - e^{-1}$. Table

It	Equally spaced points		Chebyshev first kind		Chebyshev second kind	
	Aitken	Neville	Aitken	Neville	Aitken	Neville
1	6.8696e-01	6.8696e-01	1.2962e+00	1.2962e+00	6.8696e-01	6.8696e-01
2	3.4633e-01	3.4633e-01	9.1875e-01	9.1875e-01	2.9095e-01	2.9095e-01
3	1.3011e-01	1.3011e-01	4.2473e-01	4.2473e-01	9.8765e-02	9.8765e-02
4	3.6744e-02	3.6744e-02	1.3578e-01	1.3578e-01	2.4775e-02	2.4775e-02
5	7.8565e-03	7.8565e-03	3.0515e-02	3.0515e-02	4.4655e-03	4.4655e-03
6	1.2724e-03	1.2724e-03	4.7856e-03	4.7856e-03	5.5864e-04	5.5864e-04
7	1.5482e-04	1.5484e-04	5.1025e-04	5.1025e-04	4.6114e-05	4.6114e-05
8	1.3890e-05	1.3899e-05	3.5295e-05	3.5295e-05	2.3236e-06	2.3236e-06
9	1.2211e-05	7.2372e-07	1.4669e-06	1.4670e-06	6.3110e-08	6.3209e-08
10	3.3453e-04	1.0280e-06	2.1951e-09	3.7429e-08	4.2184e-08	4.1447e-09
11	2.2040e-02	2.9403e-05	1.9287e-05	4.6798e-06	2.5779e-05	1.1667e-04
12	1.0882e+00	5.4514e-04	1.9782e+00	1.0000e+00	1.5238e+03	2.1884e+02
13	2.9428e+01	6.3104e-03	1.8712e+12	4.6780e+12	1.1153e+05	8.6310e+08

TABLE 1. Comparisons between relative errors of computation of $\int_{-1}^{1} e^x dx$ on various point distributions through Aitken-Neville schemes

1 shows the comparisons between relative errors of computation of the required integral through (3.2) and (3.4) on 13 grids of various point distributions (equally spaced and Chebyshev grids). We observe that the relative errors of both schemes converge up to 9^{th} iteration on equally spaced grids and converge up to 10^{th} iteration for Chebyshev grids, after that, diverge rapidly in all point distributions. Also, it gives an idea of the accuracy of the result per addition of a new grid. It is observed that the new formulas give greater accuracy on Chebyshev point distributions than evenly spaced grids.

4. Conclusion.

The formulas for approximating derivatives and integrals for arbitrary spaced grids through Aitken-Neville schemes have been developed in this article. We have provided an efficient algorithm (in MATLAB) to iterate numerical differentiation with cost of $O(k^2n)$ operations. Also, the numerical result shows that the numerical differentiation through Neville scheme is stable than Aitken scheme. All available numerical integration formulas do not iterate integral values per addition of a new grid to any degree of accuracy. But the new formulas for integration described in section 3, will do this with cost of $O(n^3)$ operations. Also, an interesting advantage is that they are also applicable to unevenly grids.

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