Differentiation and Integration

You think you know when you learn, are more sure when you can write,
even more when you can teach, but certain when you can program.

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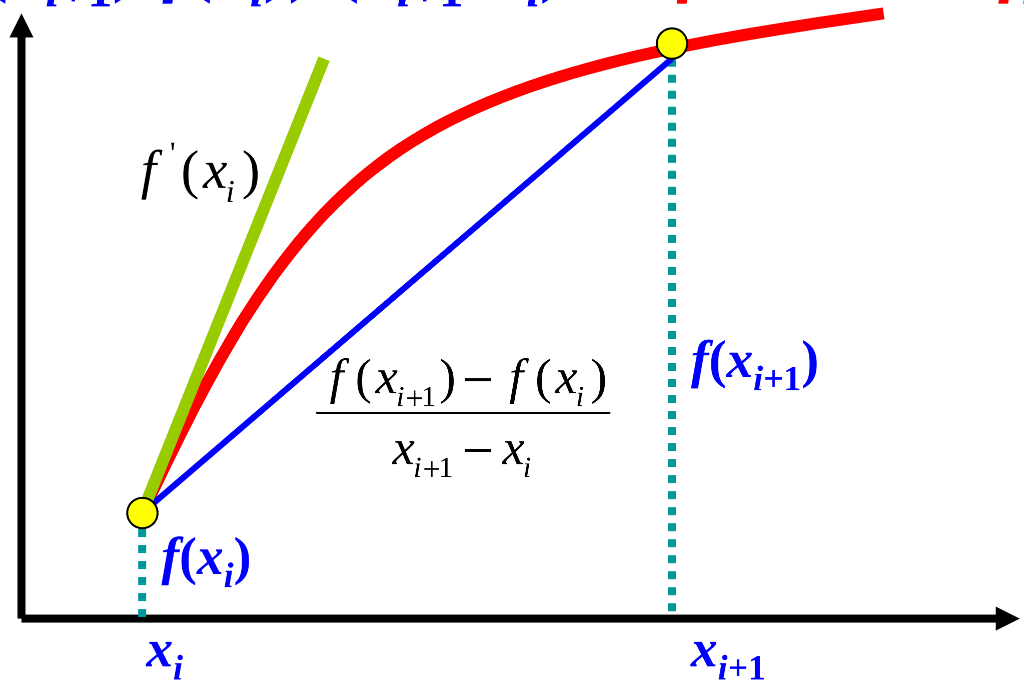
Topics to Be Discussed

- This unit requires the knowledge of differentiation and integration in calculus.
- The following topics will be presented:
  - Forward difference, backward difference and central difference methods for differentiation.
  - Richardson extrapolation technique
  - Trapezoid, Simpson's 3-point and iterative methods for numerical integration
  - Romberg's method for numerical integration.

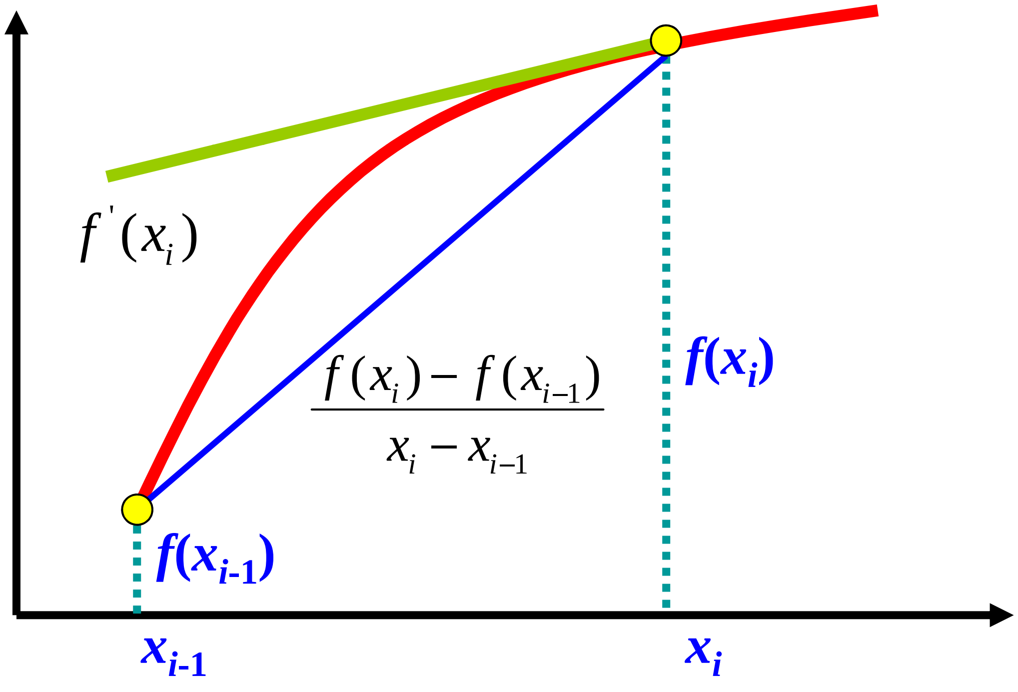
Numerical Differentiation: 1/14

- **If function $f(x)$ is complex, computing $f'(x)$ is difficult and approximation may be needed.**
- **Suppose we wish to compute $f'(x_i)$. We may choose a $x_{i+1} > x_i$ and approximate $f'(x_i)$ by the slope $(f(x_{i+1})-f(x_i))/(x_{i+1}-x_i)$ — *forward difference*.**



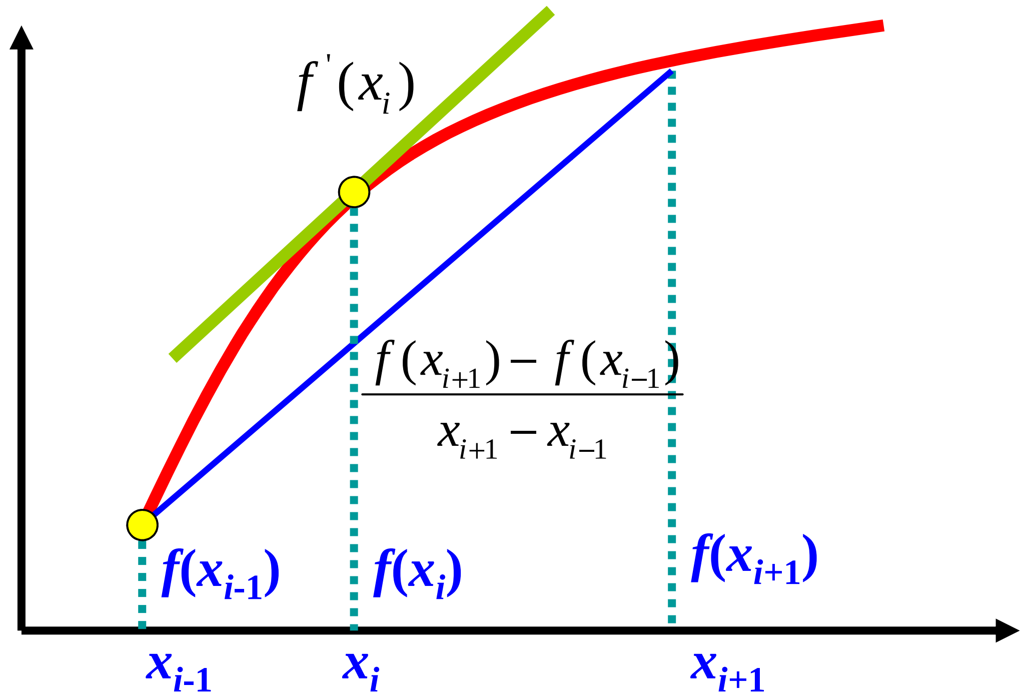
Numerical Differentiation: 2/14

- **Or, we may choose a $x_{i-1} < x_i$ and use the slope $(f(x_i)-f(x_{i-1}))/(x_i-x_{i-1})$ as an approximation of $f'(x_i)$ — *backward difference*.**



Numerical Differentiation: 3/14

- **Or, we may choose $x_{i-1} < x_i$ and $x_{i+1} > x_i$, both close to x_i, and use slope $(f(x_{i+1})-f(x_{i-1}))/(x_{i+1}-x_{i-1})$ as an approximation of $f'(x_i)$ — *central difference*.**



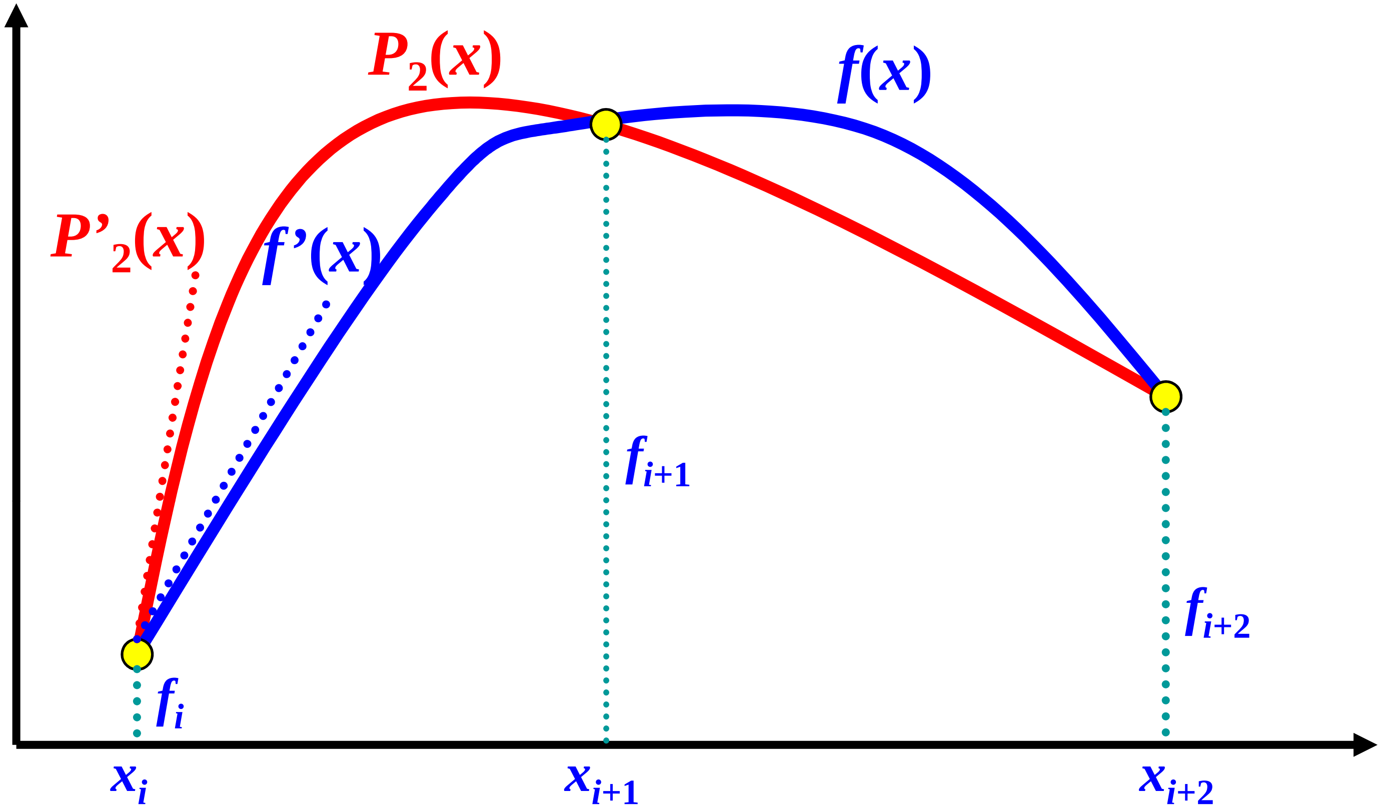
Numerical Differentiation: 4/14

- **Forward difference, backward difference and central difference methods can be viewed as the use of an *interpolating polynomial of degree 1* that interpolates two chosen points and uses its slope for the derivative of *f*(*x*) .**
- **If we can use interpolating polynomial of degree 1, *why don't we use degree* 2, degree 3, etc?**
- **Yes, of course we can. But, higher degree means more points. Normally, three (*i.e.*, degree 2) may be sufficient.**

Numerical Differentiation: 5/14

- **Suppose we wish to compute $f'(x_i)$. We may choose x_{i+1} and x_{i+2}, both close to x_i, and evaluate f_i, f_{i+1} and f_{i+2}.**
- **Then, we have three points (x_i, f_i), (x_{i+1}, f_{i+1}) and (x_{i+2}, f_{i+2}).**
- **An interpolating polynomial of degree 2, $P_2(x)$, can be found, and, use $P_2'(x_i)$ as an approximation of $f'(x_i)$. See next slide.**
- **Newton divided difference is a simple tool for this purpose.**

Numerical Differentiation: 6/14



Numerical Differentiation: 7/14

- **Given $x_i < x_{i+1} < x_{i+2}$, divided difference yields $P_2(x)$ as follows:**

$$P_2(x) = f[x_i] + f[x_i, x_{i+1}](x - x_i) + f[x_i, x_{i+1}, x_{i+2}](x - x_i)(x - x_{i+1})$$

- **Differentiating $P_2(x)$ yields:**

$$P_2^{'}(x) = f[x_i, x_{i+1}] + f[x_i, x_{i+1}, x_{i+2}](2x - (x_i + x_{i+1}))$$

- **Plugging x_i into $P_2'(x)$ as an approximation of $f'(x_i)$ yields:**

$$P_2^{'}(x_i) = f[x_i, x_{i+1}] + f[x_i, x_{i+1}, x_{i+2}](x_i - x_{i+1})$$

Numerical Differentiation: 8/14

- **Normally, x_i, x_{i+1} and x_{i+2} are *equally spaced* (*i.e.*, $x_{i+1} - x_i = x_{i+2} - x_{i+1} = \Delta$). This condition makes computation easier.**
- **Note that $f[x_i, x_{i+1}]$ and $f[x_{i+1}, x_{i+2}]$ are computed as follows:**

$$f[x_i, x_{i+1}] = \frac{f(x_{i+1}) - f(x_i)}{\Delta} \qquad f[x_{i+1}, x_{i+2}] = \frac{f(x_{i+2}) - f(x_{i+1})}{\Delta}$$

- **As a result, $f[x_i, x_{i+1}, x_{i+2}]$ is**

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i} = \frac{f_{i+2} - 2f_{i+1} + f_i}{2\Delta^2}$$

Numerical Differentiation: 9/14

- **Recall that $P_2'(x)$ is**

$$P_2'(x_i) = f[x_i, x_{i+1}] + f[x_i, x_{i+1}, x_{i+2}](x_i - x_{i+1})$$

- **Plugging $f[x_i,x_{i+1}]$, $f[x_i,x_{i+1},x_{i+2}]$ and $x_i - x_{i+1} = -\Delta$ into $P_2'(x)$, we have**

$$\boxed{P_2'(x_i) = \frac{1}{2\Delta}\left(-3f_i + 4f_{i+1} - f_{i+2}\right)}$$

- **This is the *three-point forward difference*.**

Numerical Differentiation: 10/14

- **If the three chosen points are $x_{i-2} < x_{i-1} < x_i$, the interpolating polynomial of degree 2, $P_2(x)$, is**

$$P_2(x) = f[x_{i-2}] + f[x_{i-2}, x_{i-1}](x - x_{i-2}) + f[x_{i-2}, x_{i-1}, x_i](x - x_{i-2})(x - x_{i-1})$$

- **Differentiating $P_2(x)$ yields:**

$$P_2'(x) = f[x_{i-2}, x_{i-1}] + f[x_{i-2}, x_{i-1}, x_i](2x - (x_{i-2} + x_{i-1}))$$

- **Plugging x_i into $P_2'(x)$ yields**

$$P_2'(x_i) = f[x_{i-2}, x_{i-1}] + f[x_{i-2}, x_{i-1}, x_i](2x_i - (x_{i-2} + x_{i-1}))$$

Numerical Differentiation: 11/14

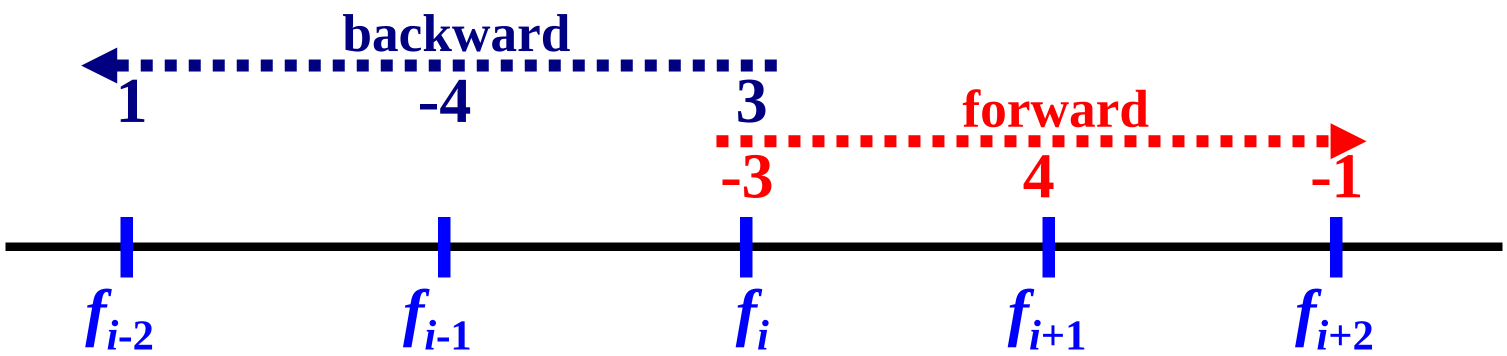
- **If x_{i-2}, x_{i-1} and x_i are equally spaced (*i.e.*, $x_{i-1} - x_{i-2} = \Delta$ and $x_i - x_{i-1} = \Delta$), we have**

$$2x_i - (x_{i-2} + x_{i-1}) = (x_i - x_{i-1}) + (x_i - x_{i-2}) = \Delta + 2\Delta = 3\Delta$$

- **$P_2'(x)$ becomes:**

$$\boxed{P_2'(x_i) = \frac{1}{2\Delta}\left(f_{i-2} - 4 f_{i-1} + 3 f_i \right)}$$

- **This is the *three-point backward difference*.**



Numerical Differentiation: 12/14

- **Forward difference uses $x_i < x_{i+1} < x_{i+2}$, and backward difference uses $x_{i-2} < x_{i-1} < x_i$. Is there a "central" difference that uses $x_{i-1} < x_i < x_{i+1}$?**
- **You certainly can do this because the $P_2(x)$ is:**

$$P_2(x) = f[x_{i-1}] + f[x_{i-1}, x_i](x - x_{i-1}) + f[x_{i-1}, x_i, x_{i+1}](x - x_{i-1})(x - x_i)$$

- **Some calculations yield the following (exercise):**

$$P_2^{'}(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta}$$

- **This does not involve f_i and is the same as the 2-point central difference.**

Numerical Differentiation: 13/14

- Exercises:
  - **If the equally spaced data points are $x_{i-1} < x_i < x_{i+1}$, show that $P_2'(x_i)$ is the following:**

$$P_2'(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta}$$

  - **Given a parabola $f(x)=ax^2+bx+c$ and three points $s-\Delta$, s and $s+\Delta$, show that**

$$f'(s) = \frac{f(s+\Delta) - f(s-\Delta)}{2\Delta}$$

Now we know that the three-point central difference does not make much sense for equally spaced data points.

Numerical Differentiation: 14/14

- Examples:
  - $f(x) = e^x$, $x = 1$ and $\Delta = 0.001$
  - $f'(x) = e^x$ and $f'(1) = e^1 = 2.718281828$

Method	*Result*
Forward Difference	**2.71964142**
Backward Difference	**2.71962268**
Central Difference	**2.71828228**
3-point Forward	**2.71828091**
3-point Backward	**2.71828091**

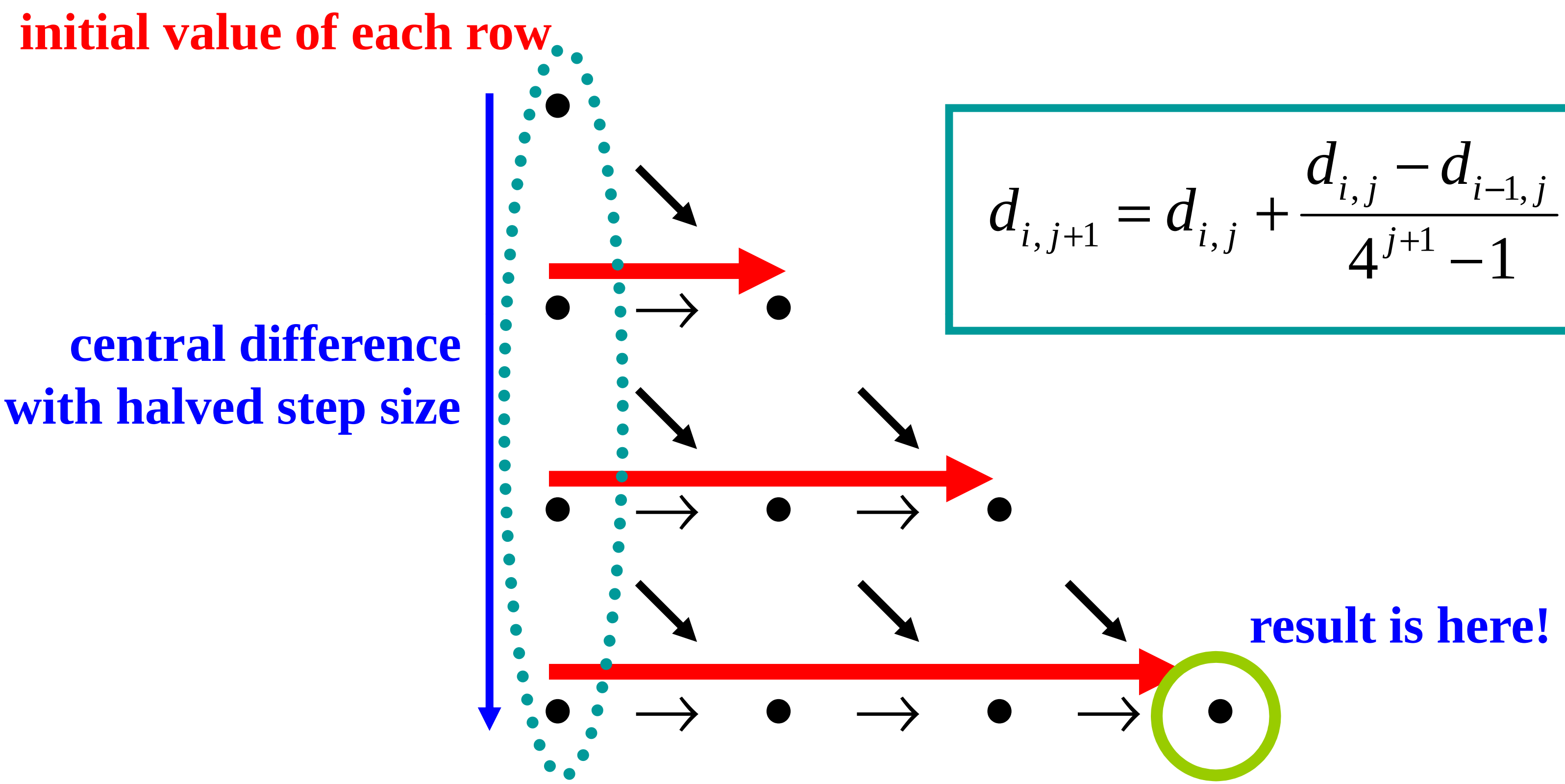
Richardson Extrapolation: 1/4

- Richardson has an *extrapolation* scheme that can make the central different method more accurate.
- This extrapolation scheme is very similar to the divided difference scheme:

$$
\begin{array}{ccc}
d_{i-1,j} & & \\
& \searrow & \\
d_{i,j} & \rightarrow & d_{i,j+1} = d_{i,j} + \dfrac{d_{i,j} - d_{i-1,j}}{4^{j+1} - 1} \\
\text{col } j & & \text{col } j+1
\end{array}
$$

Richardson Extrapolation: 2/4

- **Richardson extrapolation is computed row-by-row. The 0-th entry is a central difference with reduced step size.**



$$d_{i,j+1} = d_{i,j} + \frac{d_{i,j} - d_{i-1,j}}{4^{j+1} - 1}$$

Richardson Extrapolation: 3/4

- Here is the algorithm of Richardson's method.
- ***x***: input, ***n***: number of rows, and **Δ**: initial step size that will be halved for each row.

```
DO i = 0, n                                ! compute row-by-row
    d_{i,0} = (f(x+Δ) - f(x-Δ)) / (2Δ)     ! central difference
    DO j = 0, i-1                          ! on row i, ……
        d_{i,j+1} = d_{i,j} + (d_{i,j} - d_{i-1,j}) / (4^{j+1} - 1)   ! obtain d_{i,j+1} on next col
    END DO
    Δ = Δ/2                                ! reduce step size
END DO
```

where

$$d_{i,0} = \frac{f(x+\Delta) - f(x-\Delta)}{2\Delta}$$

$$d_{i,j+1} = d_{i,j} + \frac{d_{i,j} - d_{i-1,j}}{4^{j+1} - 1}$$

Richardson Extrapolation: 4/4

- Let $f(x)=e^x$. Compute $f'(x)$ at $x=1$ with $n=3$ (3 rows) and $\Delta=1$ (initial step size=1).

$$\boxed{d_{i,j+1} = d_{i,j} + \frac{d_{i,j} - d_{i-1,j}}{4^{j+1}-1}}$$

	col 0	col 1	col 2	col 3
row 0 (Δ=1)	3.194528			
row 1 (Δ=.5)	2.8329677	2.7124476		
row 2 (Δ=.25)	2.7466855	2.7179248	2.71829	
row 3 (Δ=.125)	2.7253665	2.7182602	2.7182826	2.7182826

Numerical Integration: 1/4

- **Numerical integration means computing the following in a numerical way (*i.e.*, a value rather than a closed form formula).**

$$\int_a^b f(x)dx$$

- **In fact, the above cannot be integrated precisely in closed form for most functions *f*(*x*). As a result, numerical integration is needed.**

Numerical Integration: 2/4

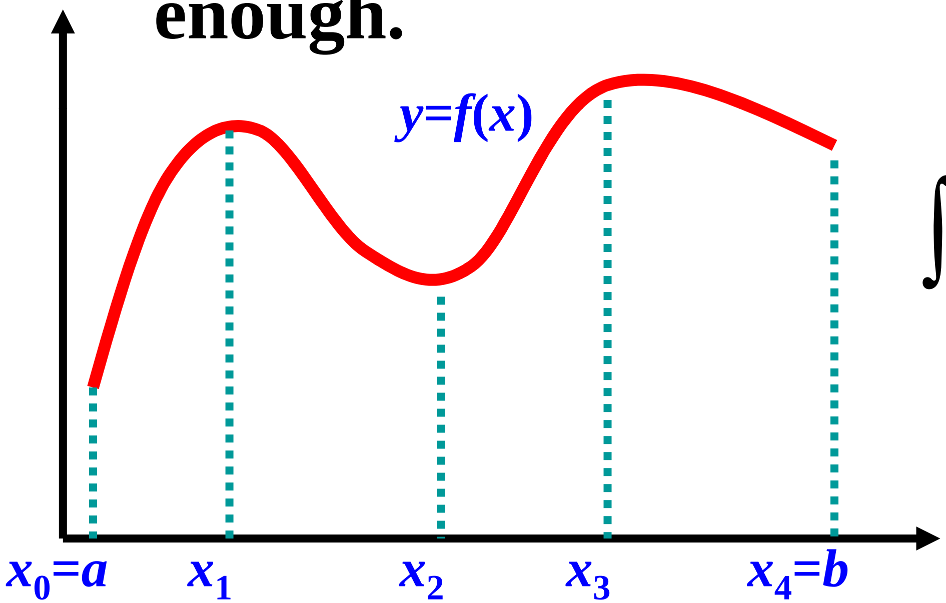
- **One way to compute the integration is to (1) choose a number of data points ($x_0=a$, f_0), (x_1, f_1), …, ($x_n=b$, f_n) and (2) find an interpolating polynomial of degree n, $P_n(x)$.**
- **Then, we use $P_n(x)$ to replace $f(x)$:**

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx$$

- **Since $P_n(x)$ is a polynomial, its integration is easy to compute. But, this is a tedious and inefficient procedure.**

Numerical Integration: 3/4

- **In fact, one may divide the interval [*a*,*b*] into subintervals for better approximation instead of using the whole interval [*a*,*b*].**
- **If the subintervals are small enough, degree 1 or 2 interpolating polynomials may be good enough.**



$$\int_{a=x_0}^{b=x_4} f(x)dx = \sum_{i=0}^{3} \int_{x_i}^{x_{i+1}} f(x)dx$$

Numerical Integration: 4/4

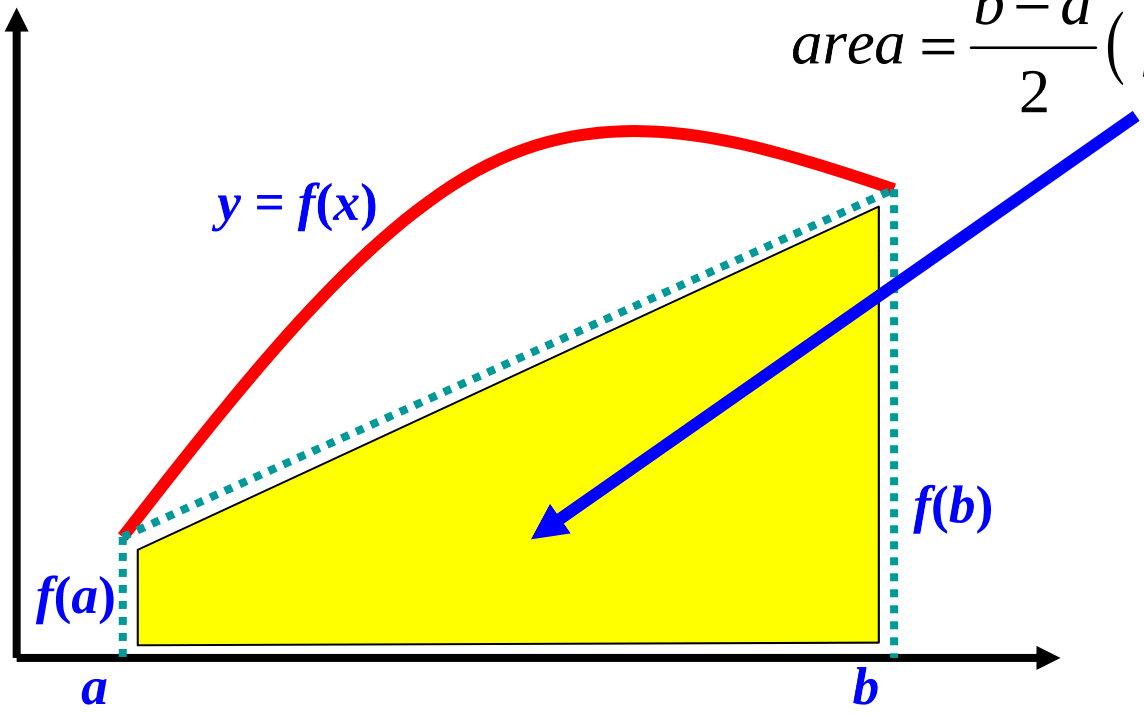
- **While the subintervals do not have to be of equal length, equally spaced points do make computation easier.**
- **Therefore, if we choose to divide the interval $[a,b]$ into n subintervals, each of which has length $\Delta=(b-a)/n$, the division points are $x_0 = a$, $x_1 = x_0+\Delta$, $x_2 = x_0+2\Delta$ …, $x_i = x_0+i\Delta$, .., $x_n = x_0+n\Delta=b$.**
- **The integration becomes:**

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_i+\Delta} f(x)dx$$

Trapezoid Rule: 1/5

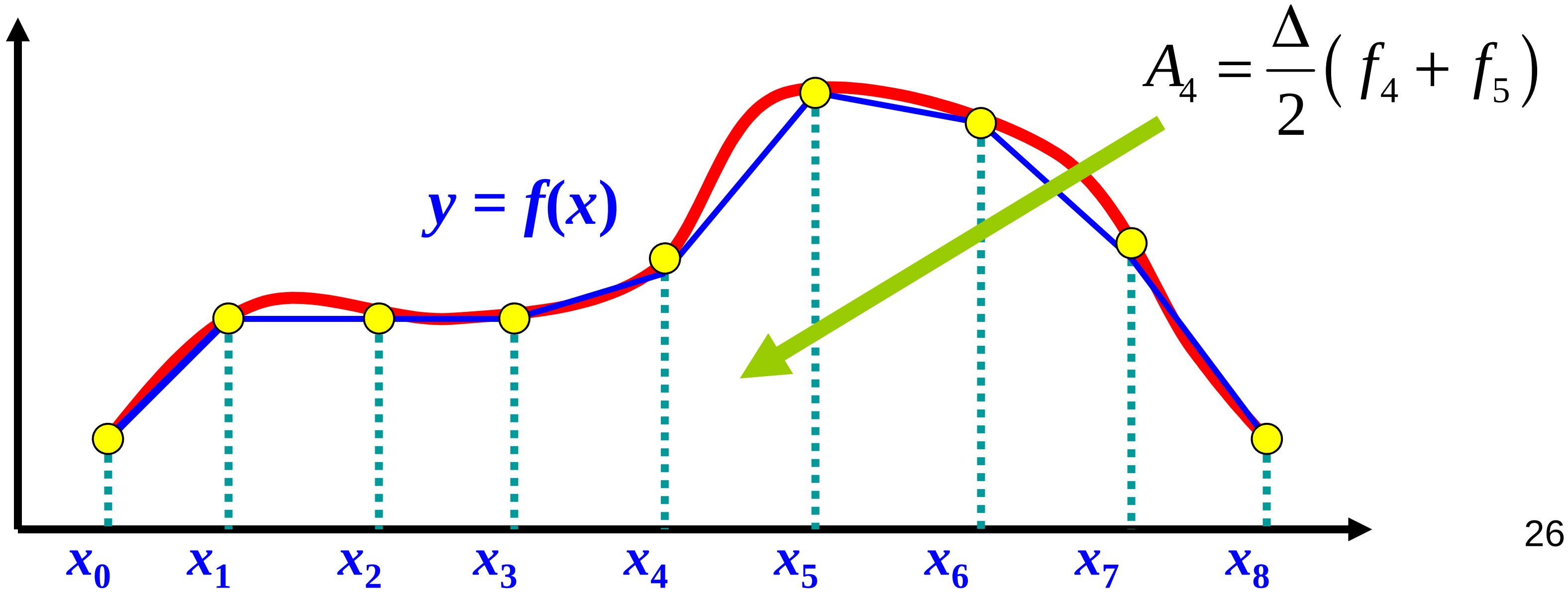
- **The trapezoid bounded by *(a,0)*, *(a, f(a))*, *(b, f(b))* and *(b,0)* has an area close to the area below *y=f(x)* bounded by *x=a* and *x=b*.**

$$area = \frac{b-a}{2}\left(f(a) + f(b) \right)$$



Trapezoid Rule: 2/5

- **If $[a,b]$ is divided into n equally spaced intervals with length $\Delta=(b-a)/n$. Then, $x_i = x_0+i\Delta$.**
- **The area A_i of the i-th ($0 \le i \le n-1$) trapezoid is $(f_i+f_{i+1})\Delta/2$.**
- **The approximation is the sum of all A_i's.**



Trapezoid Rule: 3/5

- **Therefore, the sum of all areas A_0, A_1, …, A_{n-1} as an approximation of the integration is easy to compute.**

$$
\begin{aligned}
\int_a^b f(x)dx &\approx A_0 + A_1 + \cdots + A_{n-1} \\
&= \frac{\Delta}{2}(f_0 + f_1) + \frac{\Delta}{2}(f_1 + f_2) + \cdots + \frac{\Delta}{2}(f_{n-1} + f_n) \\
&= \frac{\Delta}{2}\left[f_0 + 2(f_1 + f_2 + \cdots + f_{n-1}) + f_n \right] \\
&= \Delta \left[\frac{f_0 + f_n}{2} + \sum_{i=1}^{n-1} f_i \right]
\end{aligned}
$$

Trapezoid Rule: 4/5

- **Recall the following trapezoid rule:**

$$\int_a^b f(x)dx \approx \Delta\left[\frac{f_0 + f_n}{2} + \sum_{i=1}^{n-1} f_i\right]$$

- **The following is a possible implementation:**

```
! INPUT: a, b, n
Δ = (b-a)/n       ! step size
x = a + Δ         ! x1 here
s = 0.0           ! sum of f(x1) to f(xn-1)
DO i = 1, n-1     ! cumulate each term
  s = s + f(x)
  x = x + Δ
END DO
Result = ((f(a)+f(b))/2+s)*Δ
```

Trapezoid Rule: 5/5

- **Consider the integration of e^x from 0 to 1. The correct result is $e^1 - e^0 = 1.718282$.**
- **If [0,1] is divided into 4 subintervals, we have $n=4$ and $\Delta=0.25$.**

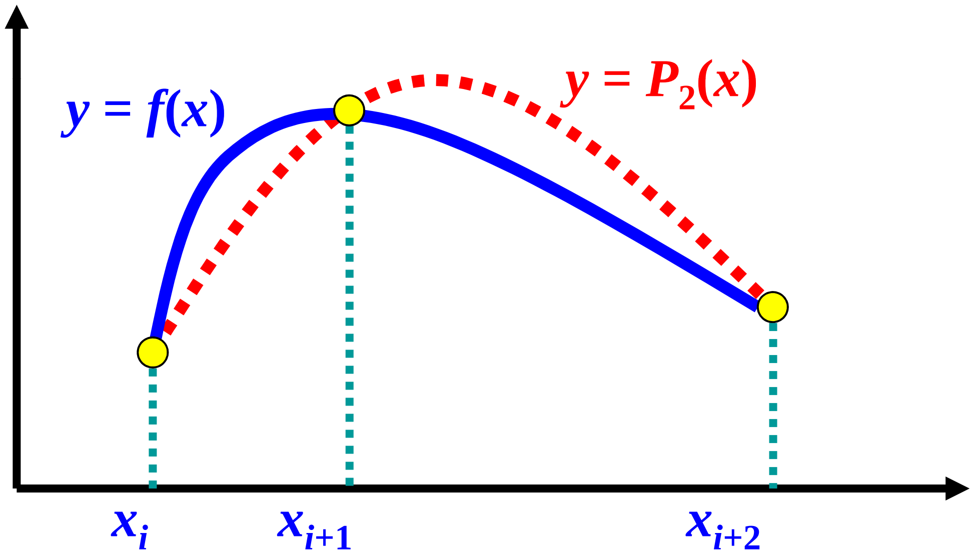
x_i	EXP(x_i)
0	**1**
0.25	**1.284025**
0.5	**1.648721**
0.75	**2.117000**
1.0	**2.718282**

Sum = 5.049747

$$\int_0^1 e^x dx \approx 0.25\left[\frac{1+2.718182}{2}+5.049747\right] \approx 1.7272095$$

Simpson's 3-Point Rule: 1/12

- Trapezoid rule is an approximation of $f(x)$ on $[x_i, x_{i+1}]$ with a line (*i.e.*, degree 1 polynomial).
- Simpson's 3-point rule approximates $f(x)$ on $[x_i, x_{i+2}]$ with a parabola (*i.e.*, degree 2 polynomial) that interpolates (x_i, f_i), (x_{i+1}, f_{i+1}) and (x_{i+2}, f_{i+2}).



Simpson’s 3-Point Rule: 2/12

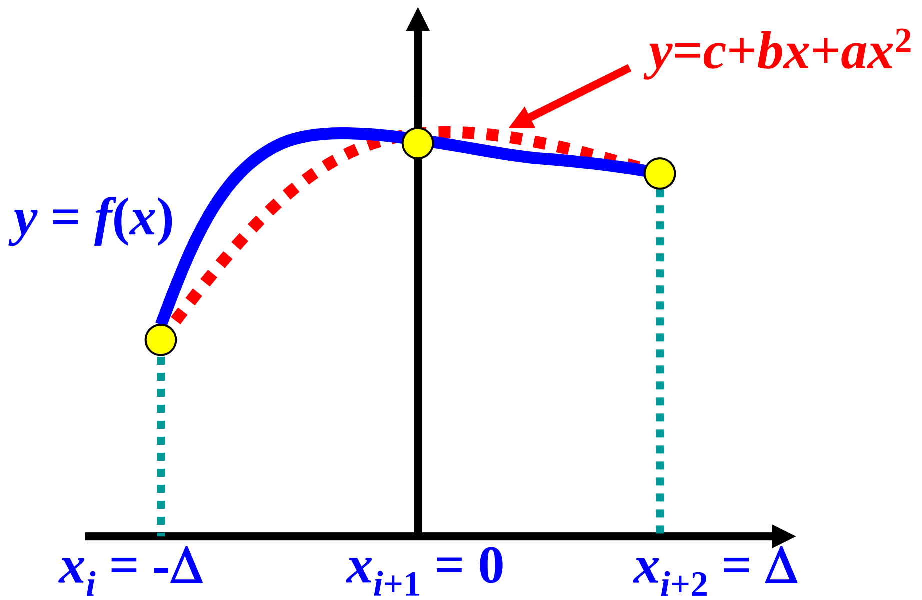
- Since the $P_2(x)$ that interpolates (x_i, f_i), (x_{i+1}, f_{i+1}) and (x_{i+2}, f_{i+2}) can easily be found, we have

$$\int_{x_i}^{x_{i+2}} f(x)dx \approx \int_{x_i}^{x_{i+2}} P_2(x)dx$$

- Since $P_2(x)$ is a degree 2 polynomial, its integration is very easy.
- How do we find this $P_2(x)$? Should we use Lagrange or Newton divided difference?
- It turns out we don’t need these tools!

Simpson's 3-Point Rule: 3/12

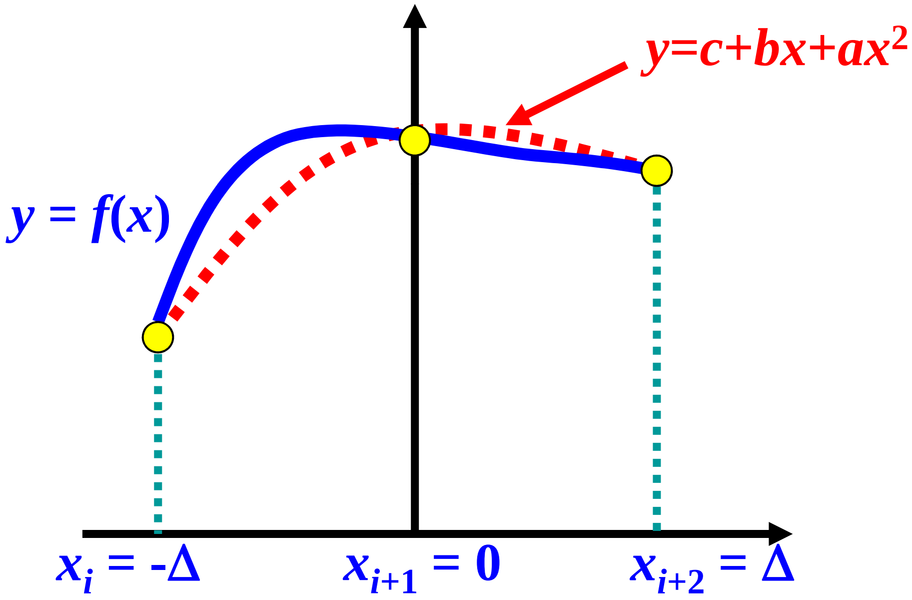
- **We still use equally spaced subintervals.**
- **Since translation does not change integration result, we translate x_{i+1} to 0 so that $x_i=-\Delta$ and $x_{i+2}=\Delta$. This will simplify our calculation.**
- **Let the interpolating polynomial be $c+bx+ax^2$**



Simpson's 3-Point Rule: 4/12

- **The integration of the polynomial $c+bx+ax^2$ from $-\Delta$ to Δ is easy to compute as follows:**

$$\int_{-\Delta}^{\Delta}(c+bx+ax^2)dx = cx\,\Big|_{-\Delta}^{\Delta} + \frac{b}{2}x^2\,\Big|_{-\Delta}^{\Delta} + \frac{a}{3}x^3\,\Big|_{-\Delta}^{\Delta} = (2\Delta)\left[c+\frac{a}{3}\Delta^2\right]$$



***b* is not used!**

Simpson's 3-Point Rule: 5/12

- **How to compute c and a in $P_2(x) = c+bx+ax^2$?**
- **From the setup, we have**

$$
\begin{aligned}
f_i &= P_2(-\Delta) = c - b\Delta + a\Delta^2 \\
\boxed{f_{i+1} = P_2(0) = c} \\
f_{i+2} &= P_2(\Delta) = c + b\Delta + a\Delta^2
\end{aligned}
$$

c is known!

- **Adding the first and the third equations together and solving for a yield the following:**

$$a = \frac{1}{2\Delta^2}\left(f_i - 2 f_{i+1} + f_{i+2} \right)$$

Simpson's 3-Point Rule: 6/12

- **What do we have now?**

$$\begin{aligned} \int_{-\Delta}^{\Delta} f(x)dx &\approx (2\Delta)\left[c + \frac{a}{3}\Delta^2\right] \\ c &= f_{i+1} \\ a &= \frac{1}{2\Delta^2}\left(f_i - 2f_{i+1} + f_{i+2}\right) \end{aligned}$$

- **Plugging *a* and *c* into the integration yields:**

$$\int_{-\Delta}^{\Delta} f(x)dx \approx \frac{\Delta}{3}\left[f_i + 4f_{i+1} + f_{i+2}\right]$$

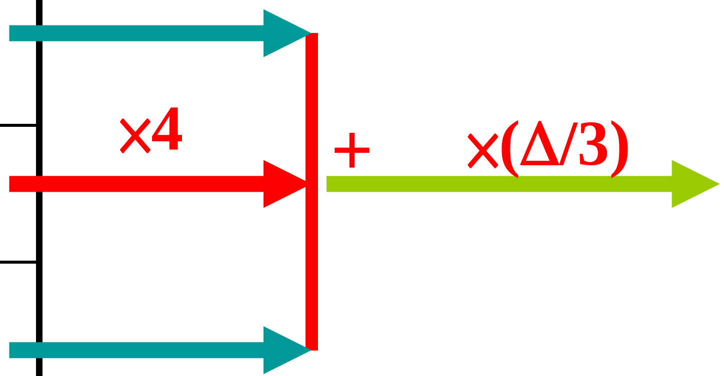
- **Note that this result does not depend on the x_i's!**

Simpson's 3-Point Rule: 7/12

- Compute $\int_0^1 e^x dx = e^1 - e^0 = 1.718281828\ldots$
- We need 3 equally spaced points $x_0=0$, $x_1=0.5$ and $x_2=1$. Thus, $\Delta=0.5$.

$$\boxed{\int_{x_i}^{x_{i+2}} f(x)dx \approx \frac{\Delta}{3}\left[f_i + 4f_{i+1} + f_{i+2} \right]}$$

x_i	f_i
0.	1
0.5	1.648721271
1.	2.718281828



1.718861152

Simpson's 3-Point Rule: 8/12

- **For a general integration problem, we need to divide $[a,b]$ into an *even number* of subintervals, and apply Simpson's 3-point rule to two consecutive ones.**
- **More precisely, apply Simpson's 3-point rule to $[x_0,x_1,x_2]$, $[x_2,x_3,x_4]$, $[x_4,x_5,x_6]$, …, $[x_{n-2},x_{n-1},x_n]$.**
- **Note that Simpson's 3-point rule only depends on the f_i's and the length of subinterval Δ.**
- **For convenience, we shall use $n = 2m$, where n is the number of subintervals, and $\Delta=(b-a)/n$.**

Simpson's 3-Point Rule: 9/12

- **Consider the following results from integrating two consecutive subintervals.**

Odd indices f_i's have coefficient 4

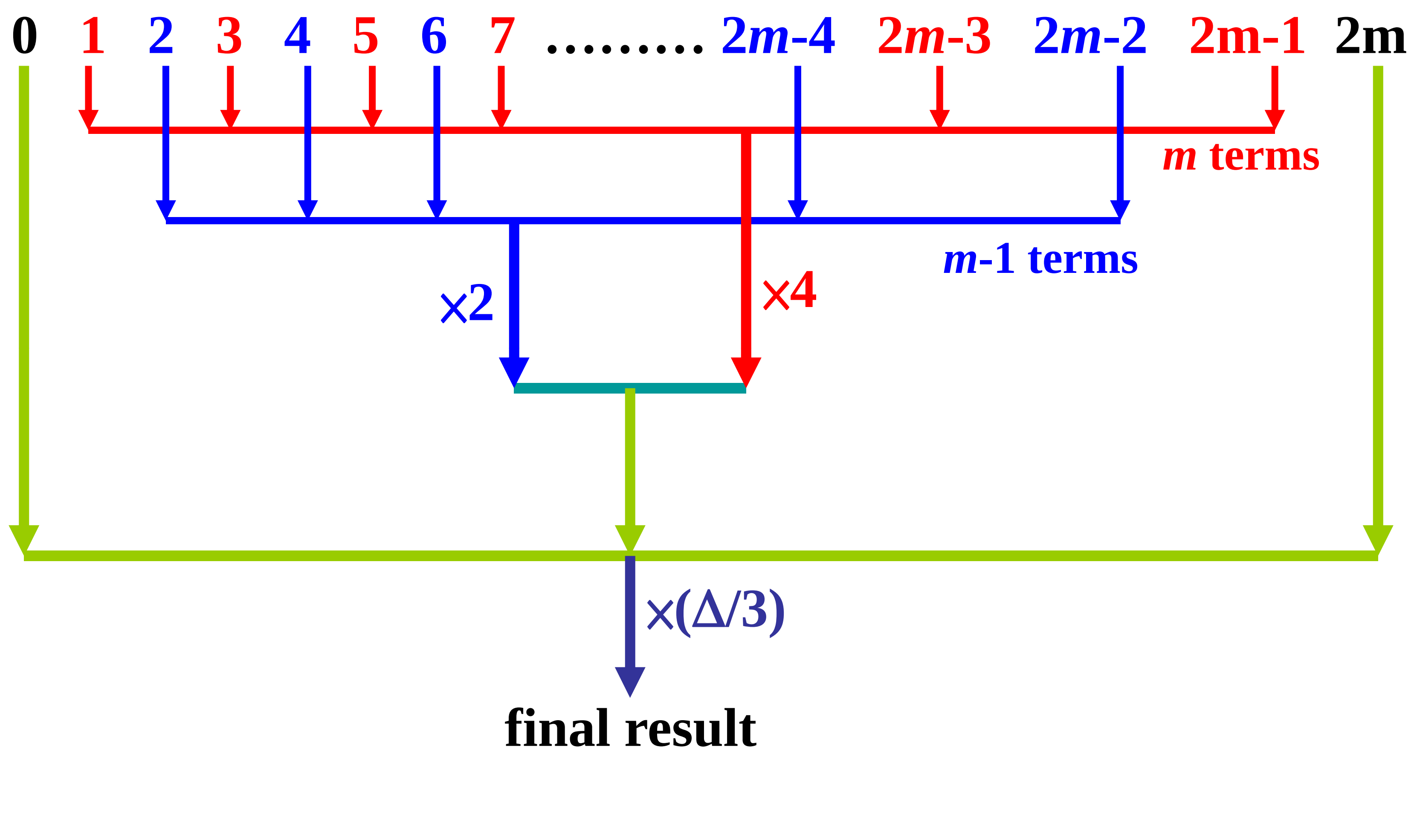
even indices f_i's have coefficient 2

f_0 and f_{2m} appear exactly once

$$
\begin{array}{ll}
[x_0, x_1, x_2] & \dfrac{\Delta}{3}[f_0 + 4f_1 + f_2] \\
[x_2, x_3, x_4] & \dfrac{\Delta}{3}[f_2 + 4f_3 + f_4] \\
[x_4, x_5, x_6] & \dfrac{\Delta}{3}[f_4 + 4f_5 + f_6] \\
\vdots & \vdots \\
[x_{2m-4}, x_{2m-3}, x_{2m-2}] & \dfrac{\Delta}{3}[f_{2m-4} + 4f_{2m-3} + f_{m-2}] \\
[x_{2m-2}, x_{2m-1}, x_{2m}] & \dfrac{\Delta}{3}[f_{2m-2} + 4f_{2m-1} + f_{2m}]
\end{array}
$$

Simpson's 3-Point Rule: 10/12

- **The following is a computation scheme:**



Simpson's 3-Point Rule: 11/12

- In summary, the sum is the following:

$$\frac{\Delta}{3}\left[(f_0 + f_{2m}) + 4\sum_{i=1}^{m} f_{2i-1} + 2\sum_{i=1}^{m-1} f_{2i}\right]$$

- Input:
  - interval: *[a,b]*
  - *n=2m*: # of divisions
  - Output in `Result`

```
Δ = (b-a)/n
step = Δ+Δ
m = n/2
odd = 0.0
x = a + Δ
DO i = 1, m, 2
   odd = odd + f(x)
   x = x + step
END DO
even = 0.0
x = a + Δ+Δ
DO i = 2, m-1, 2
   even = even + f(x)
   x = x + step
END DO
Result = (f(a)+f(b)+4*odd
           + 2*even)*Δ/3
```

odd terms

even terms

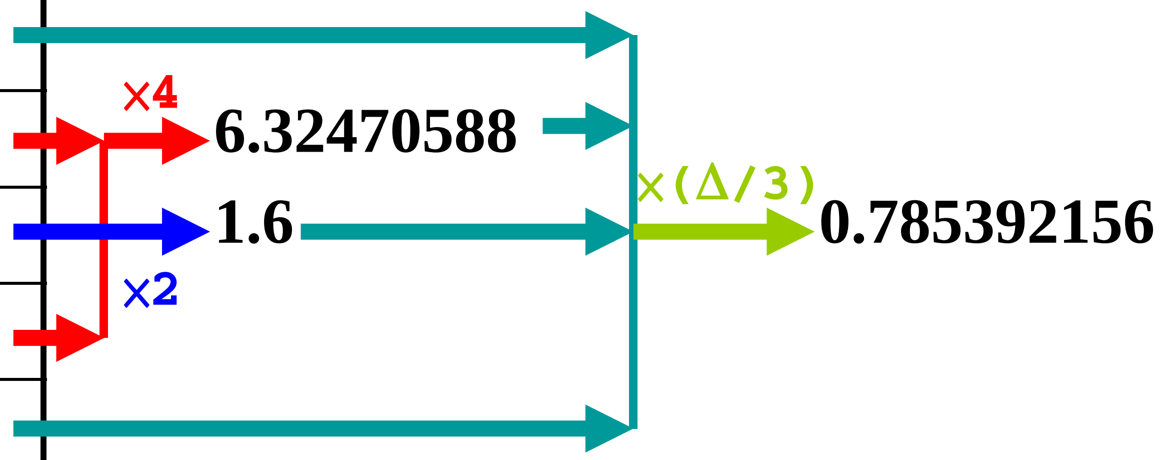
Simpson’s 3-Point Rule: 12/12

- Integrate $1/(1+x^2)$ from 0 to 1. The answer is 0.78539816…

$$\int_0^1 \frac{1}{1+x^2}\,dx = \tan^{-1}(1) - \tan^{-1}(0) = \frac{\pi}{4} = 0.785398163...$$

$\Delta=0.25$

index	x_i	f_i
0	0	1
1	0.25	0.94117647
2	0.5	0.8
3	0.75	0.64
4	1	0.5



Iterative Methods

- **An iterative method increases the number of subdivisions until the process converges.**
- **Since trapezoid and Simpson 3-point rules are simple, we shall look at how they can be modified to become "*iterative*."**
- **We may start with a coarse subdivision of [a,b], and compute the integration.**
- **If two successive integration results are close to each other, stop.**
- **Otherwise, refine the subdivision and do again!**

Iterative Trapezoid Method: 1/4

- **Initially, we have one subinterval $[a,b]$, and $\Delta = b - a$.**
- **The integration is $I_0 = \Delta \times (f(a)+f(b))/2$**
- **In the next iteration, the length of each subinterval is halved (*i.e.*, $\Delta = \Delta/2$) and the number of subintervals is doubled.**
- **Thus, if the previously computed result I_n with n subintervals is not very different from the newly computed result I_{2n} with $2n$ subintervals, then stop. Otherwise, start the next iteration.**

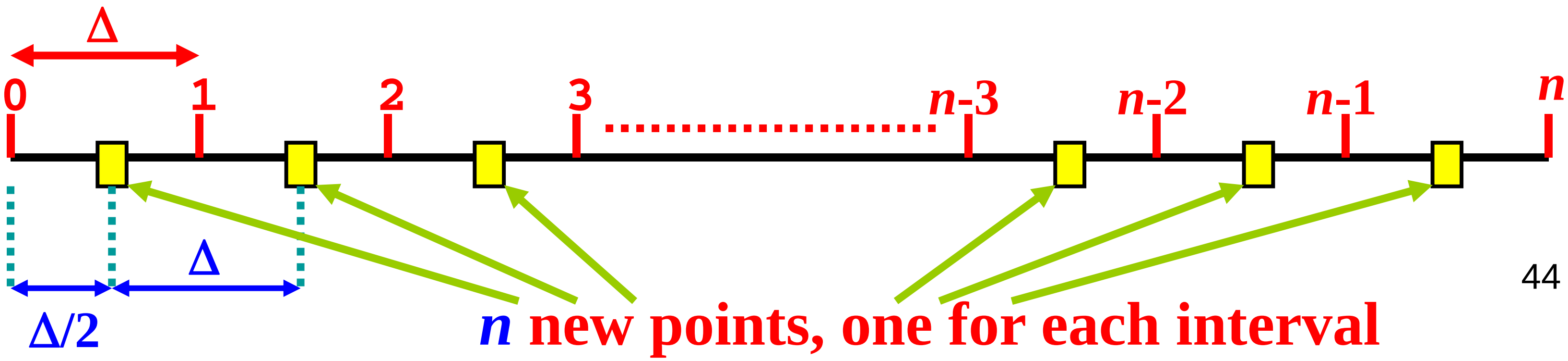
Iterative Trapezoid Method: 2/4

- Trapezoid method has a simple relationship between I_n and I_{2n}.
- It uses the following formula:

Only need to update this sum!

$$\int_a^b f(x)dx \approx \Delta\left[\frac{f_0+f_n}{2}+\boxed{\sum_{i=1}^{n-1} f_i}\right]$$

- Let K_n be the previous sum, then K_{2n} can be obtained by adding new values.



Iterative Trapezoid Method: 3/4

$$\int_0^1 \frac{1}{1+x^2}\,dx \approx \frac{\pi}{4}$$

$$\pi/4 \approx 0.785398163$$

	Δ=0.5	Δ=0.25	Δ=0.125
0	**1**		
0.125			**0.984615384**
0.25		**0.94117647**	
0.375			**0.876712328**
0.5	**0.8**		
0.625			**0.719101123**
0.75		**0.64**	
0.875			**0.566371681**
1	**0.5**		
Prev. Sum	**0**	**0.8**	**2.381176471**
New Sum	**0.8**	**1.581176471**	**3.146800518**
This Sum	**0.8**	**2.381176471**	**5.527976989**
Integration	**0.775**	**0.782794117**	**0.784747123**

$$\frac{f(0)+f(1)}{2} = 0.75$$

Iterative Trapezoid Method: 4/4

- **The following is a possible algorithm:**

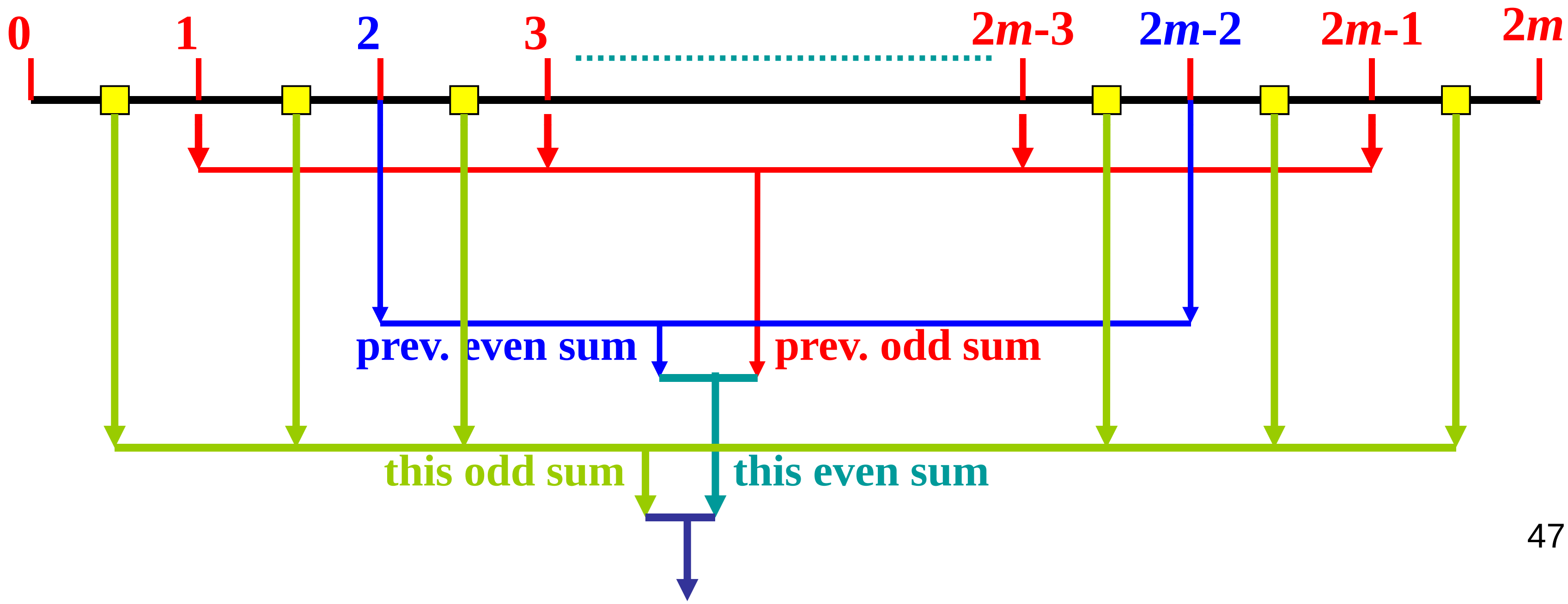
```
! Initialization
! Int  - integration
! This - new integration
! Prev - previous sum
! Next - new sum

Fixed = (f(a) + f(b))/2
Int   = Fixed
Prev  = 0
Δ = b-a
Intervals = 1
```

```
DO
  Δ2 = Δ/2
  x  = a + Δ2
  Next = 0
  DO i = 1, Intervals
    Next = Next + f(x)
    x    = x + Δ
  END DO
  This = (Fixed+Prev+Next)*Δ2
  IF (|This - Int| < ε) EXIT
  Prev = Next
  Int  = This
  Δ    = Δ2
  Intervals = Intervals*2
END DO
```

Iterative Simpson Method: 1/3

- **Simpson method can also be made iterative.**
- **All newly added points have *odd* indices!**
- **All original points have *even* indices!**

$$\int_{a=x_0}^{b=x_{2m}} f(x) = \frac{\Delta}{3}\left[(f_0 + f_{2m}) + 4\sum_{i=1}^{m} f_{2i-1} + 2\sum_{i=1}^{m-1} f_{2i} \right]$$



Iterative Simpson Method: 2/3

$$\int_0^1 \frac{1}{1+x^2}dx \approx \frac{\pi}{4}$$

$$f(0)+f(1)=1.5$$

$$\pi/4 \approx 0.785398163$$

	Δ=0.5	Δ=0.25	Δ=0.125
0	**0**		
0.125			**0.984615384**
0.25		**0.94117647**	
0.375			**0.876712328**
0.5	**0.8**		
0.625			**0.719101123**
0.75		**0.64**	
0.875			**0.566371681**
1	**0.5**		
Previous	**0**	**0.8**	**2.38117647**
This Odd	**0.8**	**1.58117647**	**3.146800516**
Integration	**0.78333…**	**0.785392156**	**0.785398125**

$\times 2$

$\times 4$

$+$

$\times \Delta/3$

Iterative Simpson Method: 3/3

```
! Initialization
! Integrate over [a,b]
! Extra = f(a)+f(b)

Δ      = (b-a)/2
Fixed = f(a)+f(b)
Even  = 0
Odd   = f(a+Δ)
Int = (Fixed+4*Odd)*Δ/3
Intervals = 2
```

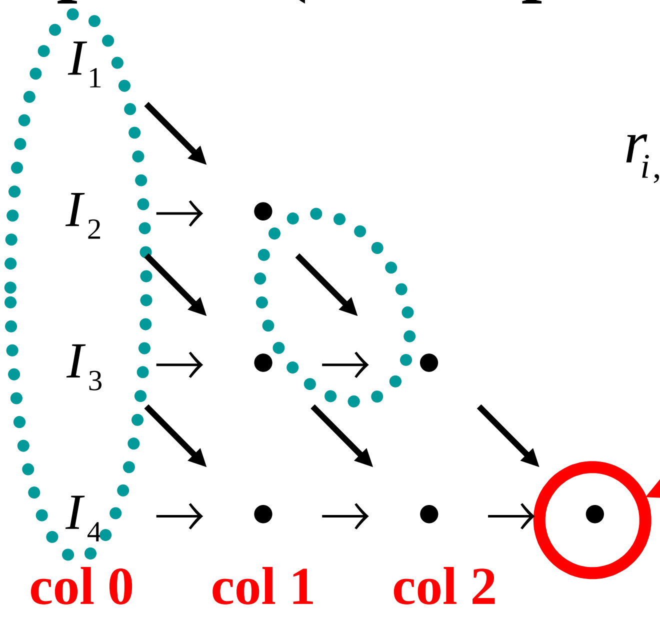
```
DO
  New_Even = Even + Odd
  New_Odd  = 0
  Δ2 = Δ/2
  x  = a + Δ2
  DO i = 1, Intervals
    New_Odd = New_Odd + f(x)
    x       = x + Δ
  END DO
  New_Int = (Fixed+4*New_Odd+
                2*New_Even)*Δ2/3
  IF (|New_Int - Int| < ε) EXIT
  Even = New_Even
  Odd  = New_Odd
  Int  = New_Int
  Intervals=Intervals+Intervals
  Δ    = Δ2
END DO
```

Romberg's Method: 1/4

- Romberg's method for integration is similar to Richardson's method for differentiation.
- Romberg's method extrapolates the results from two successive values computed with the iterative trapezoid (or Simpson) method.

$$r_{i,j+1} = r_{i,j} + \frac{r_{i,j} - r_{i-1,j}}{4^{j+1} - 1}$$

I_n: trapezoid method using n subintervals



use Richardson's formula

Romberg's Method: 2/4

- Romberg's method requires an update from I_n to I_{2n}, where I_k is the integration from k intervals.
- I_n is computed as follows:

$$I_n = \Delta_n \left[\frac{f_0 + f_n}{2} + \sum_{i=1}^{n-1} f_i \right]$$

- I_{2n} is computed as

$$I_{2n} = \Delta_{2n} \left[\frac{f_0 + f_1}{2} + \boxed{(original)} + (new) \right]$$

- Since $\Delta_{2n} = \Delta_n/2$, we have

$$I_{2n} = I_n / 2 + \Delta_{2n} \times (new)$$

Romberg Method: 3/4

- The left is Romberg's method
- ***n***: number of rows
- Result is in $r_{n,n}$

```
Δ = b-a
r0,0 = (f(a) + f(b))*Δ/2
intervals = 1
DO i = 1, n
  Δ2 = Δ/2
  x  = a + Δ
  sum = 0
  DO k = 1, intervals
    sum = sum + f(x)
    x   = x + Δ
  END DO
  ri,0 = ri-1,0/2 + Δ2*sum
  DO j = 0, i-1
```

$$r_{i,j+1} = r_{i,j} + \frac{r_{i,j} - r_{i-1,j}}{4^{j+1} - 1}$$

```
  END DO
  Δ = Δ2
  intervals = intervals*2
END DO
```

trapezoid rule

Richardson extrapolation

Romberg Method: 4/4

- **The following is an example:**

$$\int_0^1 \frac{1}{1+x^2}\,dx = \tan^{-1}(1) - \tan^{-1}(0) = \frac{\pi}{4} = 0.785398163\ldots$$

$$
\begin{array}{ccccccccc}
0.75 & & & & & & & & \\
 & \searrow & & & & & & & \\
0.775 & \rightarrow & 0.7833333 & & & & & & \\
 & \searrow & & \searrow & & & & & \\
0.7827941 & \rightarrow & 0.78539216 & \rightarrow & 0.78552943 & & & & \\
 & \searrow & & \searrow & & \searrow & & & \\
0.7847471 & \rightarrow & 0.7853981 & \rightarrow & 0.78539854 & \rightarrow & 0.78539645 & & \\
 & \searrow & & \searrow & & \searrow & & \searrow & \\
0.7852354 & \rightarrow & 0.7853982 & \rightarrow & 0.7853982 & \rightarrow & 0.7853982 & \rightarrow & 0.7853982
\end{array}
$$

The End