Numerical methods: Runge-Kutta methods and the Simpson's rule

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- Some problems can not be solved analytically
  - Interpolation and extrapolation
  - Ordinary or partial differential equations
  - Integration
- One needs an appropriate numerical method to approximate the solution to the problem
- Example - Balitsky-Kovchegov evolution equation:

$$\frac{\partial N(r,Y)}{\partial Y} = \int \mathrm{d}\vec{r}_1 K(\vec{r},\vec{r}_1,\vec{r}_2)\left(N(r_1,Y)+N(r_2,Y)-N(r,Y)-N(r_1,Y)N(r_2,Y)\right). \quad (1)$$

$$N(r, Y=0) = 1 - \exp\left(-Ar^2\right) \quad (2)$$

Simpson's rule

- Integration over the closed interval $[a, b]$ spaced uniformly

$$x_i = a + ih, \quad i = 0, ..., n, \quad h = \frac{b-a}{n}$$

- Special case of *Newton-Cotes integration formulas*
- Replace the integrated function by an interpolating polynomial or order $n > 0$

$$\int_a^b f(x)\mathrm{d}x \approx \int_a^b P_n(x)\mathrm{d}x. \tag{3}$$

- Using Lagrange interpolation and integrating the interpolating polynomial:

$$\int_a^b P_n(x) = \sum_{i=0}^{n} f_i \int_a^b L_i(x)\mathrm{d}x = h \sum_{i=0}^{n} f_i \int_0^n \phi_i(t)\mathrm{d}t = h \sum_{i=0}^{n} f_i \alpha_i.$$

$$f_i = f(x_i) = f(a + ih) = P_n(x_i)$$

Simpson's rule

- For $n = 2$ (quadratic interpolation) we obtain the Simpson's 1/3 rule

$$\int_a^b f(x)\mathrm{d}x \approx \int_a^b P_2(x)\mathrm{d}x = h\left[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{1}{3}f_2\right] \tag{4}$$

- The above formula is applied directly to the entire interval $[a, b]$
- **Composite rule**
  - Integrating function is not smooth over the entire interval $[a, b]$
  - The interval $[a, b]$ is equidistantly divided into the set of N subintervals
  - The formula is applied in each of the subintervals
  - Total approximate value of the integral is given as a sum of theapproximations in each of subintervals

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{3}\left[f(a) + 2\sum_{i=1}^{\frac{N}{2}-1} f(x_{2i}) + 4\sum_{i=1}^{\frac{N}{2}} f(x_{2i-1}) + f(b)\right]. \tag{5}$$

  - N has to be an even number!

Application of the Simpson's rule

- Example of the code:

```
//simpson method for definite integrals
double simpson(double y[], int length, int n, double step){
  double sum = 0.;
  double Int;
  for(int i=1; i<n; i+=2){
    sum = sum+4.0*y[i];
  }
  for(int i=2; i<n-1; i+=2){
    sum = sum+2.0*y[i];
  }
  Int = step*(y[0]+y[n]+sum)/3.;
  return Int;
}
```

- Basic example provided in the attached file

- Approximation of the solution to the **Cauchy problem**
  - Differential equation of the 1^{st} order with an initial condition

$$y'(x) = f(x, y(x)), \qquad y(x_0) = y_0. \tag{6}$$

- Let η_n be the approximation at point x_n of the exact solution $y(x_n)$
- The approximation at point x_{n+1} is in general given as

$$\eta_{n+1} = \eta_n + h\Phi(x_n, \eta_n, h; f) \tag{7}$$

  - $\Phi(x_n, \eta_n, h; f)$ is the increment function and h is the step size

$$\Phi(x_n, \eta_n, h; f) = \sum_{i=1}^{s} b_i K_i, \quad K_i = f\left(x_n + c_i h, \eta_n + h \sum_{j=1}^{s} a_{ij} K_j\right). \tag{8}$$

- Single-point approximation methods
- Explicit method - η_{n+1} depends only on η_n

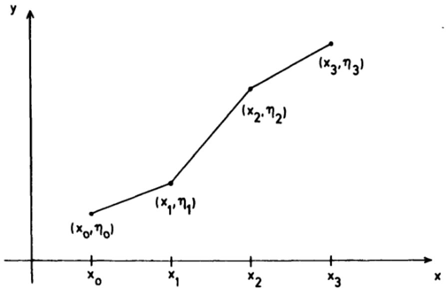
Forward Euler method

- RK method of the first order
- $f(x, y(x))$ in (6) is the slope of $y(x) \rightarrow$ for $h \neq 0$

$$y(x+h) = y(x) + hf(x, y(x)). \tag{9}$$

- In the limit of $h \rightarrow 0$ the approximation to (6) at point x_{n+1} is given as

$$\eta_{n+1} = \eta_n + hf(x_n, \eta_n), \qquad x_{n+1} = x_n + h. \tag{10}$$



Heun's method

- One of the two RK methods of the second order
- For $s = 2$ in (8) the approximation of the exact solution y_n at $(n+1)$-th step is

$$\eta_{n+1} = y_n + h\Phi(x_n, y_n, h; f) = y_n + h(b_1 K_1 + b_2 K_2)$$

using the expansion to the 2^{nd} order of the Taylor series:

$$\eta_{n+1} = y_n + hf_n(b_1 + b_2) + h^2 b_2 c_2 (f_{n,x} + f_n f_{n,y}) + \mathcal{O}(h^3)$$

- Compare it to the same expansion of the exact solution

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2} y_n'' + \mathcal{O}(h^3) = y_n + hf_n + \frac{h^2}{2}(f_{n,x} + f_n f_{n,y}) + \mathcal{O}(h^3)$$

- The resulting coefficents are

$$b_1 + b_2 = 1 \quad \text{and} \quad b_2 c_2 = \frac{1}{2} \rightarrow b_1 = \frac{1}{2}, \quad b_2 = \frac{1}{2} \quad \text{and} \quad c_2 = 1$$

- The resulting approximation prescription:

$$\eta_{n+1} = \eta_n + \frac{h}{2}\left[f(x_n, \eta_n) + f\left(x_n + h, \eta_n + hf(x_n, \eta_n)\right)\right]. \tag{11}$$

- RK method of the fourth order
- Analogical approach to its derivation as in Heun's method
  - Fourth order of the Taylor's expansion applied to the approximation and exact solution
  - The increment function is given as

$$\Phi(x_n, \eta_n, h; f) = \frac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$

where

$$K_1 = f(x_n, y(x_n))$$
$$K_2 = f\left(x_n + \frac{h}{2}, \eta_n + \frac{h}{2}K_1\right)$$
$$K_3 = f\left(x_n + \frac{h}{2}, \eta_n + \frac{h}{2}K_2\right)$$
$$K_4 = f\left(x_{n+1}, \eta_n + hK_3\right)$$

- The resulting prescription of the Classical method:

$$\eta_{n+1} = \eta_n + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4). \tag{12}$$

- Let us denote:

$$\frac{\partial N(r,Y)}{\partial Y} = \int \mathrm{d}\vec{r_1} K(\vec{r},\vec{r_1},\vec{r_2}) \left(N(r_1,Y) + N(r_2,Y) - N(r,Y) - N(r_1,Y)N(r_2,Y) \right)$$

$$N(r, Y=0) \equiv N_0(r)$$

$$I(r) \equiv \int \mathrm{d}\vec{r_1} K(\vec{r},\vec{r_1},\vec{r_2}) \left(N(r_1,Y) + N(r_2,Y) - N(r,Y) - N(r_1,Y)N(r_2,Y) \right)$$

$$f(r,r_1) \equiv K(r,r_1,r_2) \left(N(r_1,Y) + N(r_2,Y) - N(r,Y) - N(r_1,Y)N(r_2,Y) \right)$$

- r_2 is obtained from r and r_1
- Let's now apply the forward Euler method to the BK equation...

Application of the Runge-Kutta methods

- At $Y_0 = 0$ we define the values of $r[n]$ and therefore we obtain $N_0(r)$
- For each r we know $r_1[n]$ and therefpre we obtain $N_0(r_1)$
- Using values of $r[i]$ and $r_1[j]$ we obtain the values of r_2 and $N_0(r_2)$ and $K(r, r_1, r_2)$
- The integral is therefore $I(r) = \int \mathrm{d}\vec{r}_1 f(r, r_1)$
- Apply the Simpson's rule to the integral $I(r)$
- The approximation of N at rapidity $Y_1 = Y_0 + \Delta Y$ is then given as

$$N_1(r) = N_0(r) + \Delta Y I(r)$$

- The same procedure is applied at the next rapidity step
- The evolution of $N(r, Y)$ is possible to any desired rapidity Y
- For RK methods of higher order the evolution prescription is modified according to the given method

Thank you for your attention