数值地球

舒乐乐，孟宪红

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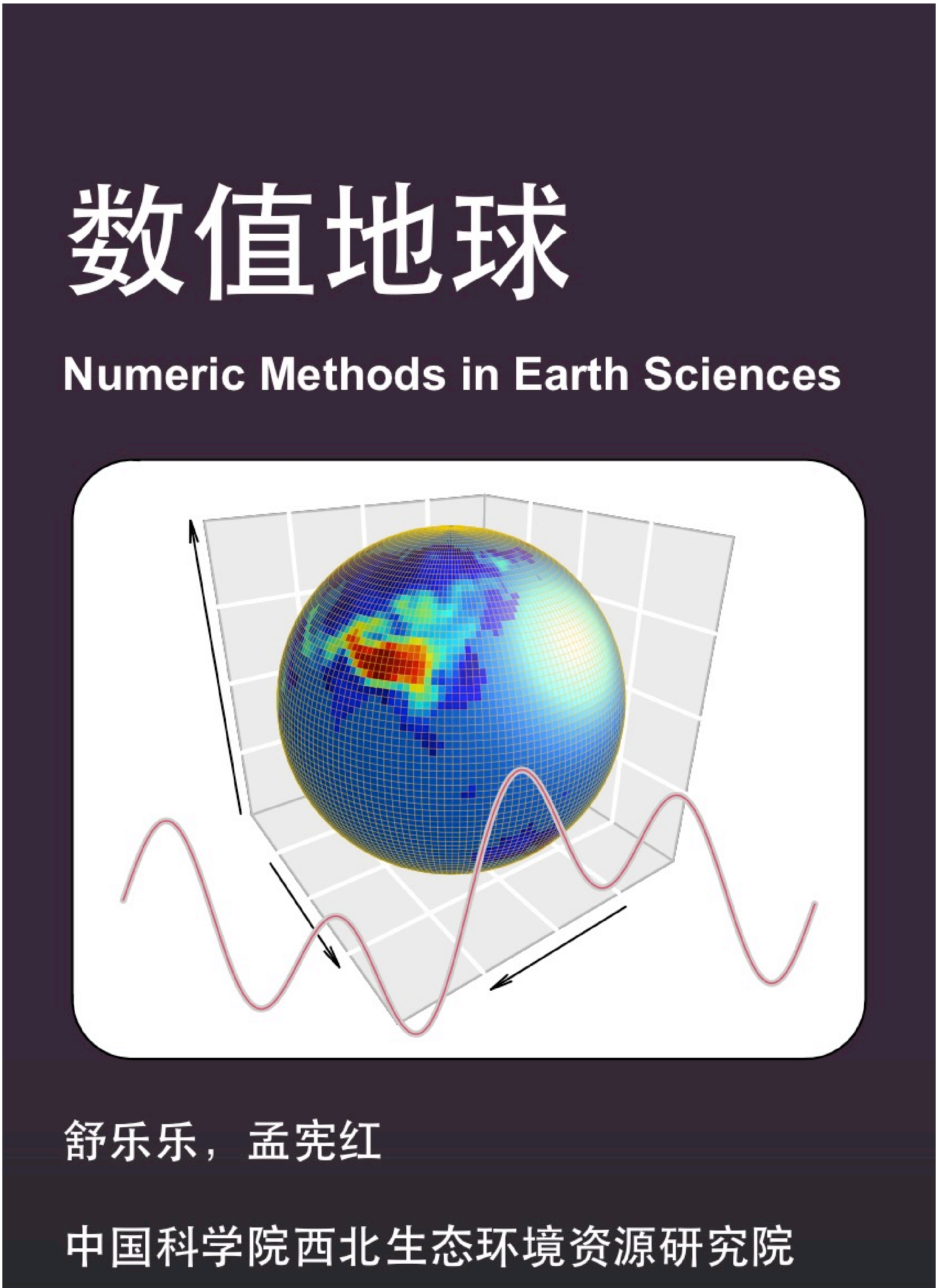
Contents

绪论


数值地球
Numeric Methods in Earth Sciences
舒乐乐，孟宪红
中国科学院西北生态环境资源研究院

这是一本有关数值方法在地球科学应用的书，可以作为数值方法在大气、水文、地貌、地址和环境科学等方面的应用的入门教科书。

主要面向对象是地球科学领域的学生（本科生、研究生)、科研人员，以及对数值方法感兴趣的读者。

书中会涉及以下内容：

1. 基础数值计算方法的概述。
2. 矩阵的求解方法。
3. 数值方法，包括简述有限差分、有限元和有限体积法。
4. 数值方法的特征要点，包括初始条件、边界条件和 CFL 条件。
5. 有限差分法求解方法，包括显式和隐式求解方法。
6. 有限元法求解方法，包括变分原理、形函数理论、单元矩阵的构造、全局矩阵的组装、边界条件施加、线性方程组求解。
7. 有限体积法求解方法，包括控制体积、通量计算、离散化方程、边界条件处理。
8. 数值方法的编程实现，包括 Python 和 R 语言的实现。
9. 数值方法在具体问题中的应用，包括大气、水文、水化学、地貌等学科的案例。
10. 数值计算方法的实践习题和练习项目。

第 1 章　建模基本方法论

本章极少数值方法建模的基本方法论，涉及一些基础的建模思路和数学基础。

1.1　建模基本思路

我称之为 CLAMS 方法，包含以下步骤：

1. **C**onceptual Model - 描述物理过程，形成概念模型（或认知模型）
2. **L**aws of Physics - 使用物理规律
3. **A**ssumptions - 列出合理假设，简化问题
4. **M**ath equations - 使用数学公式表达物理规律和假设
5. **S**olver - 求解数学公式

求解数学公式的过程，可以尝试寻找其解析解 (Analytical solution)，也可以使用数值方法求得数值解 (Numerical Solution)。

数值方法本质上是对离散（非连续）时空模型中因变量 (Dependant variable) 分布和变化的数学近似描述，从理论的解析解到数值解虽然损失了精度，但解析解通常无法求得，而数值方法可给出误差可接受的近似解。

案例：自由落体运动

描述问题描述下图。

问题：任意 $t > 0$ 时刻的速度，即 $v(t) = ?$。

建模步骤：

1. 认知模型：

   自由落体运动

2. 物理定律：

   牛顿定律：$F = ma$。

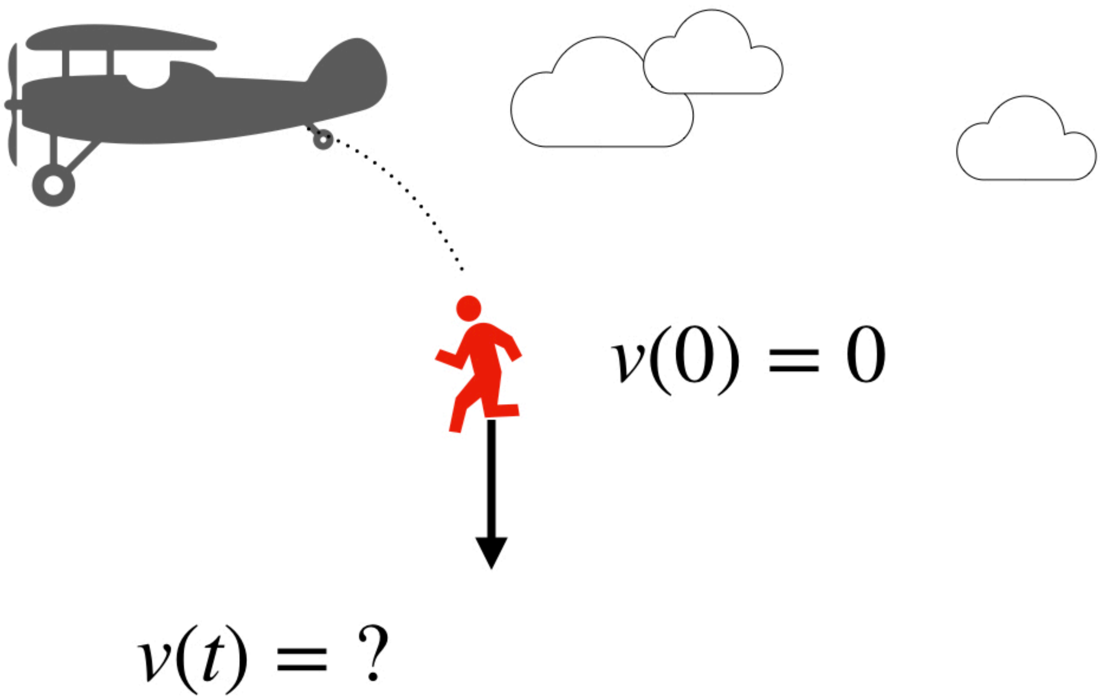


Figure 1.1: 自由落体运动示意图

3. 假设：

   $v(t=0)=0$

   且

   $F_{drag}(t) \propto v(t)$，即 $F_{drag}=cv$。

4. 数学公式：

   由 $F=ma$ 和 $\frac{dv}{dt}=a$ 可得：

$$\frac{dv}{dt}=a=\frac{F}{m} \tag{1}$$

   根据物体受力分析，其受到向下的重力 $F_g=mg$ 和向上的空气阻力 $F_{drag}=cv$，空气阻力在此假设与物体运动速度成正比关系。则其受力平衡公式为：

$$F=F_g-F_{drag}=mg-cv \tag{2}$$

   综合公式（1）和（2），则得到：

$$\frac{dv}{dt}=g-\frac{c}{m}v \tag{3}$$

5. 公式求解：

   初始条件：$v(0)=0$

   积分求解 (解析解)：

$$v(t)=\frac{mg}{c}\left[1-exp(-\frac{c}{m}t)\right]$$

6. 结果绘图：

```
c = 15 # drag coeefficient
g = 9.8 # Gravity
m = 150  # Mass in kg
x = seq(0,100, 1)  # Time
y = m*g/c *(1 - exp(-1 * c / m * x))  # Vecocity
plot(x, y, type='l', xlab='Time (s)', ylab='Velocity (m/s)', col=2, lwd=2);
grid()
```

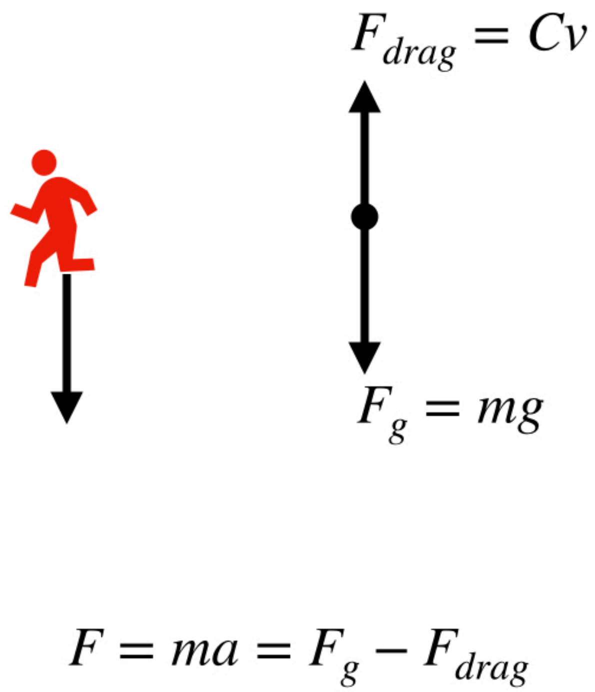
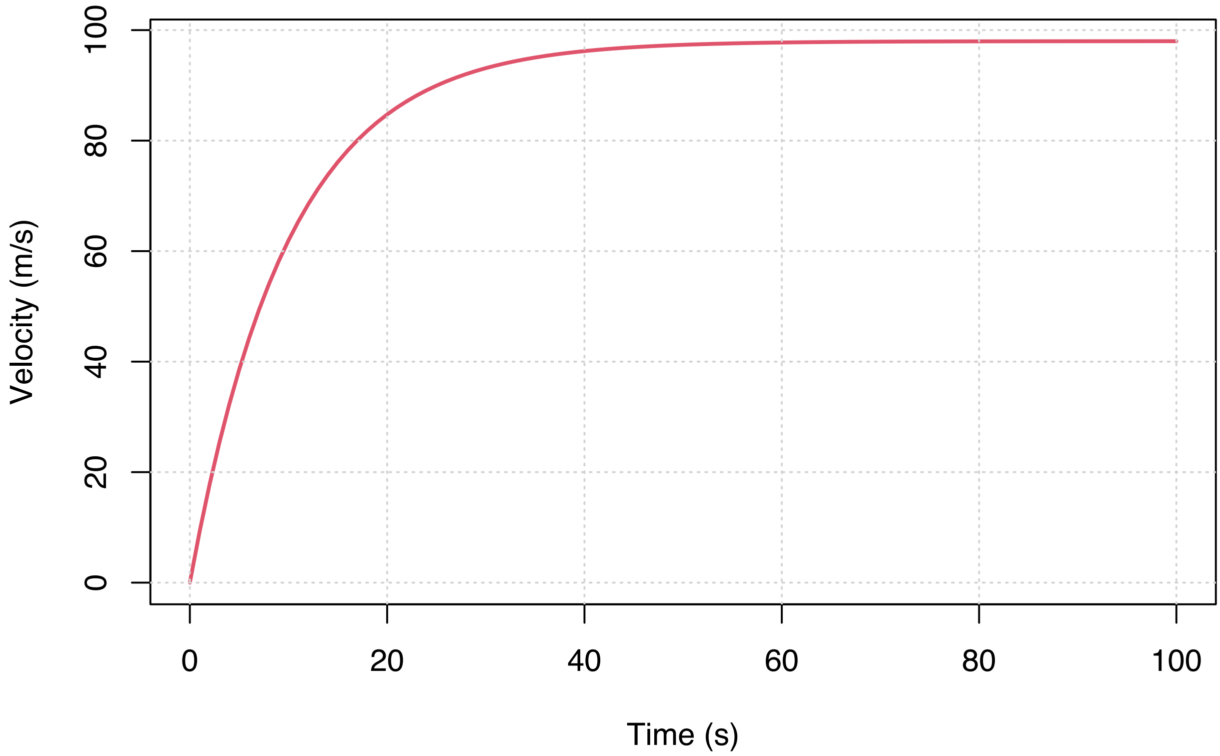


Figure 1.2: 自由落体运动的受力分析



变量表:

- $v(t)$ - 随时间变化的物体速度
- m - 物体质量
- g - 重力加速度
- a - 物体运动的加速度
- c - 空气阻力系数
- F - 物体所受的力
- F_g - 重力
- F_{drag} - 空气阻力

1.2 典型控制方程

1.2.1 一维承压地下水运动

Sure, let's derive the governing equation for one-dimensional confined aquifer groundwater flow step by step. We will use Darcy's Law and the principle of mass conservation.

1.2.1.1 Step 1: Darcy's Law

Darcy's Law describes the flow of groundwater through porous media. It states that the discharge per unit area (specific discharge or Darcy velocity, q) is proportional to the hydraulic gradient:

$$q = -K\frac{\partial h}{\partial x}$$

where: - q is the specific discharge (Darcy velocity) [L/T]. - K is the hydraulic conductivity of the aquifer [L/T]. - h is the hydraulic head [L]. - x is the spatial coordinate in the direction of flow [L].

1.2.1.2 Step 2: Conservation of Mass

Consider a control volume of length Δx, cross-sectional area A, and located at position x along the direction of flow within a confined aquifer.

1.2.1.2.1 Inflow and Outflow

- The rate of inflow at x: $q(x) \cdot A$.
- The rate of outflow at $ x + x $: $q(x + \Delta x) \cdot A$.

Using a Taylor series expansion for $q(x + \Delta x)$:

$$q(x + \Delta x) \approx q(x) + \left(\frac{\partial q}{\partial x}\right)\Delta x$$

1.2.1.2.2 Net Flow The net rate of flow into the control volume is:

$$q(x) \cdot A - \left(q(x) + \left(\frac{\partial q}{\partial x}\right)\Delta x\right) \cdot A$$

$$= -A\left(\frac{\partial q}{\partial x}\right)\Delta x$$

1.2.1.3 Step 3: Storage in the Aquifer

The change in storage within the control volume over a time interval Δt can be expressed using the specific storage S_s, which is the amount of water per unit volume of the aquifer that is stored or released from storage per unit change in hydraulic head:

$$\Delta S = S_s \cdot A \cdot \Delta x \cdot \frac{\partial h}{\partial t} \cdot \Delta t$$

1.2.1.4 Step 4: Applying Conservation of Mass

According to the conservation of mass principle, the rate of change of storage in the control volume must equal the net rate of flow into the control volume:

$$-A\left(\frac{\partial q}{\partial x}\right)\Delta x = S_s \cdot A \cdot \Delta x \cdot \frac{\partial h}{\partial t}$$

1.2.1.5 Step 5: Substituting Darcy's Law

Substitute $q = -K\frac{\partial h}{\partial x}$ into the equation:

$$-A\left(\frac{\partial}{\partial x}\left(-K\frac{\partial h}{\partial x}\right)\right)\Delta x = S_s \cdot A \cdot \Delta x \cdot \frac{\partial h}{\partial t}$$

Simplify the equation:

$$A\left(K\frac{\partial^2 h}{\partial x^2}\right)\Delta x = S_s \cdot A \cdot \Delta x \cdot \frac{\partial h}{\partial t}$$

Step 6: Simplifying and Rearranging Cancel out the common terms A and Δx:

$$K\frac{\partial^2 h}{\partial x^2} = S_s\frac{\partial h}{\partial t}$$

Final Governing Equation The one-dimensional groundwater flow equation for a confined aquifer is:

$$\frac{\partial h}{\partial t} = \frac{K}{S_s}\frac{\partial^2 h}{\partial x^2}$$

Define the hydraulic diffusivity D as:

$$D = \frac{K}{S_s}$$

Thus, the governing equation can also be written as:

$$\frac{\partial h}{\partial t} = D\frac{\partial^2 h}{\partial x^2}$$

This partial differential equation describes how the hydraulic head h varies with time t and position x within the confined aquifer.

1.2.2 二维承压地下水运动

Sure, let's derive the governing equation for two-dimensional confined aquifer groundwater flow step by step using Darcy's Law and the principle of mass conservation.

1.2.2.1 Step 1: Darcy's Law

In two dimensions, Darcy's Law describes the flow of groundwater through porous media. It states that the discharge per unit area (specific discharge or Darcy velocity, $\mathbf{q}$) is proportional to the hydraulic gradient:

$$\mathbf{q} = -K\nabla h$$

where: - $\mathbf{q}$ is the specific discharge (Darcy velocity) vector [L/T]. - K is the hydraulic conductivity of the aquifer [L/T]. - h is the hydraulic head [L]. - ∇h is the hydraulic gradient, which in two dimensions can be written as:

$$\nabla h = \left(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}\right)$$

1.2.2.2 Step 2: Conservation of Mass

Consider a differential control volume in the aquifer with dimensions dx by dy and thickness b.

1.2.2.2.1 Inflow and Outflow For simplicity, let's assume the flow is in the x- and y-directions.

- The rate of inflow in the x-direction at x: $ q_x(x) b dy $

  - The rate of inflow in the y-direction at y: $ q_y(y) b dx $

  The rate of outflow in the x-direction at $x + dx$:

  $$q_x(x + dx) \cdot b \cdot dy \approx \left(q_x(x) + \frac{\partial q_x}{\partial x}dx\right) \cdot b \cdot dy$$

  The rate of outflow in the y-direction at $y + dy$:

  $$q_y(y + dy) \cdot b \cdot dx \approx \left(q_y(y) + \frac{\partial q_y}{\partial y}dy\right) \cdot b \cdot dx$$

  1.2.2.2.2 Net Flow The net rate of flow into the control volume is:

  $$\text{Net inflow in } x\text{-direction} = [q_x(x) \cdot b \cdot dy] - \left[\left(q_x(x) + \frac{\partial q_x}{\partial x}dx\right) \cdot b \cdot dy\right]$$

  $$= -b \cdot dy \cdot \frac{\partial q_x}{\partial x}dx$$

$$\text{Net inflow in } y\text{-direction} = \left[q_y(y) \cdot b \cdot dx\right] - \left[\left(q_y(y) + \frac{\partial q_y}{\partial y} dy\right) \cdot b \cdot dx\right]$$
$$= -b \cdot dx \cdot \frac{\partial q_y}{\partial y} dy$$

The total net inflow into the control volume is:

$$-b\left(\frac{\partial q_x}{\partial x} dx \cdot dy + \frac{\partial q_y}{\partial y} dy \cdot dx\right)$$

$$= -b\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y}\right) dx \cdot dy$$

Step 3: Storage in the Aquifer The change in storage within the control volume over a time interval Δt can be expressed using the specific storage S_s:

$$\Delta S = S_s \cdot b \cdot dx \cdot dy \cdot \frac{\partial h}{\partial t} \cdot \Delta t$$

Step 4: Applying Conservation of Mass According to the conservation of mass principle, the rate of change of storage in the control volume must equal the net rate of flow into the control volume:

$$-b\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y}\right) dx \cdot dy = S_s \cdot b \cdot dx \cdot dy \cdot \frac{\partial h}{\partial t}$$

Step 5: Substituting Darcy's Law Substitute $q_x = -K\frac{\partial h}{\partial x}$ and $q_y = -K\frac{\partial h}{\partial y}$ into the equation:

$$-b\left(\frac{\partial}{\partial x}\left(-K\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K\frac{\partial h}{\partial y}\right)\right) dx \cdot dy = S_s \cdot b \cdot dx \cdot dy \cdot \frac{\partial h}{\partial t}$$

Simplify the equation:

$$b\left(K\frac{\partial^2 h}{\partial x^2} + K\frac{\partial^2 h}{\partial y^2}\right) dx \cdot dy = S_s \cdot b \cdot dx \cdot dy \cdot \frac{\partial h}{\partial t}$$

Step 6: Simplifying and Rearranging Cancel out the common terms b, dx, and dy:

$$K\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) = S_s \frac{\partial h}{\partial t}$$

Final Governing Equation The two-dimensional groundwater flow equation for a confined aquifer is:

$$\frac{\partial h}{\partial t} = \frac{K}{S_s}\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right)$$

Define the hydraulic diffusivity D as:

$$D = \frac{K}{S_s}$$

Thus, the governing equation can also be written as:

$$\frac{\partial h}{\partial t} = D\left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right)$$

This partial differential equation describes how the hydraulic head h varies with time t and position (x, y) within the confined aquifer.

1.2.3 一维非承压地下水运动

Let's go through the derivation for one-dimensional unconfined aquifer groundwater flow more carefully, considering the variation in aquifer thickness due to changes in the water table.

1.2.3.1 Step-by-Step Derivation for One-Dimensional Unconfined Aquifer

1.2.3.2 Step 1: Darcy's Law

For unconfined groundwater flow, Darcy's Law in one dimension is:

$$q = -K\frac{\partial h}{\partial x}$$

where: - q is the specific discharge (Darcy velocity) [L/T]. - K is the hydraulic conductivity of the aquifer [L/T]. - h is the hydraulic head [L]. - x is the spatial coordinate in the direction of flow [L].

1.2.3.3 Step 2: Volumetric Flow Rate

The volumetric flow rate Q at a point x for an unconfined aquifer with variable saturated thickness h is given by:

$$Q = q \cdot b \cdot h$$

where b is the aquifer width perpendicular to the flow direction. For simplicity, we assume $ b = 1 $ unit width, leading to:

$$Q = q \cdot h = -Kh\frac{\partial h}{\partial x}$$

1.2.3.4 Step 3: Conservation of Mass

Consider a differential control volume in the unconfined aquifer of width dx and saturated thickness \$ h(x) \$.

1.2.3.4.1 Inflow and Outflow

- Inflow at x: $Q(x) = -Kh\frac{\partial h}{\partial x}$
- Outflow at $x+dx$: $Q(x+dx) = -Kh\frac{\partial h}{\partial x} + \left(\frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)\right)dx$

1.2.3.4.2 Net Flow The net inflow into the control volume is:

$$\begin{aligned}
Q(x) - Q(x+dx) &= -Kh\frac{\partial h}{\partial x} - \left(-Kh\frac{\partial h}{\partial x} + \left(\frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)\right)dx\right) \\
&= -\frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)dx
\end{aligned}$$

1.2.3.5 Step 4: Change in Storage

The change in storage within the control volume \$ dx h \$ over a time interval \$ t \$ can be expressed using the specific yield S_y, which measures the volume of water released from storage per unit decline in the water table:

$$\Delta S = S_y \cdot dx \cdot \frac{\partial h}{\partial t} \cdot \Delta t$$

1.2.3.6 Step 5: Applying Conservation of Mass

According to the conservation of mass principle, the rate of change of storage in the control volume must equal the net rate of flow into the control volume:

$$-\frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)dx = S_y \cdot dx \cdot \frac{\partial h}{\partial t}$$

1.2.3.7 Step 6: Simplifying and Rearranging

Simplify the equation:

$$\frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right) = S_y\frac{\partial h}{\partial t}$$

1.2.3.8 Final Governing Equation

The one-dimensional groundwater flow equation for an unconfined aquifer is:

$$S_y \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right)$$

This is the governing equation for transient groundwater flow in an unconfined aquifer. It accounts for changes in the saturated thickness h due to fluctuations in the water table.

1.2.4 二维非承压地下水运动

Sure, let's derive the governing equation for two-dimensional unconfined aquifer groundwater flow step by step. We'll again use Darcy's Law, the principle of mass conservation, and the Dupuit assumption, which simplifies the analysis by assuming horizontal flow and a vertical hydraulic gradient.

1.2.4.1 Step-by-Step Derivation for Two-Dimensional Unconfined Aquifer

1.2.4.2 Step 1: Darcy's Law

In two dimensions, Darcy's Law for an unconfined aquifer can be written as:

$$\mathbf{q} = -K\nabla h$$

where: - $\mathbf{q}$ is the specific discharge (Darcy velocity) vector [L/T]. - K is the hydraulic conductivity of the aquifer [L/T]. - h is the hydraulic head [L]. - ∇h is the hydraulic gradient, which in two dimensions can be written as:

$$\nabla h = \left(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}\right)$$

1.2.4.3 Step 2: Volumetric Flow Rate

For a control volume in the unconfined aquifer, the volumetric flow rate Q at a point in two dimensions is given by:

$$Q_x = q_x \cdot h = -Kh\frac{\partial h}{\partial x}$$

$$Q_y = q_y \cdot h = -Kh\frac{\partial h}{\partial y}$$

where h is the saturated thickness of the aquifer.

1.2.4.4 Step 3: Conservation of Mass

Consider a differential control volume in the unconfined aquifer with dimensions dx by dy and saturated thickness h.

1.2.4.4.1 Inflow and Outflow

- Inflow in the x-direction at x: $Q_x(x) = -Kh\frac{\partial h}{\partial x}$
- Outflow in the x-direction at $x+dx$: $Q_x(x+dx) = -Kh\frac{\partial h}{\partial x} + \frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)dx$
- Inflow in the y-direction at y: $Q_y(y) = -Kh\frac{\partial h}{\partial y}$
- Outflow in the y-direction at $y+dy$: $Q_y(y+dy) = -Kh\frac{\partial h}{\partial y} + \frac{\partial}{\partial y}\left(-Kh\frac{\partial h}{\partial y}\right)dy$

1.2.4.4.2 Net Flow The net inflow into the control volume is:

$$\begin{aligned}\text{Net inflow in } x\text{-direction} &= Q_x(x) - Q_x(x+dx)\\ &= -Kh\frac{\partial h}{\partial x} - \left(-Kh\frac{\partial h}{\partial x} + \frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)dx\right)\\ &= -\frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)dx\end{aligned}$$

$$\begin{aligned}\text{Net inflow in } y\text{-direction} &= Q_y(y) - Q_y(y+dy)\\ &= -Kh\frac{\partial h}{\partial y} - \left(-Kh\frac{\partial h}{\partial y} + \frac{\partial}{\partial y}\left(-Kh\frac{\partial h}{\partial y}\right)dy\right)\\ &= -\frac{\partial}{\partial y}\left(-Kh\frac{\partial h}{\partial y}\right)dy\end{aligned}$$

The total net inflow into the control volume is:

$$\begin{aligned}\text{Net inflow} &= -\left(\frac{\partial}{\partial x}\left(-Kh\frac{\partial h}{\partial x}\right)dx + \frac{\partial}{\partial y}\left(-Kh\frac{\partial h}{\partial y}\right)dy\right)\\ &= \left(\frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right)dx + \frac{\partial}{\partial y}\left(Kh\frac{\partial h}{\partial y}\right)dy\right)\end{aligned}$$

1.2.4.5 Step 4: Change in Storage

The change in storage within the control volume over a time interval Δt can be expressed using the specific yield S_y, which is the volume of water released from storage per unit surface area per unit decline in the water table:

$$\Delta S = S_y \cdot dx \cdot dy \cdot \frac{\partial h}{\partial t} \cdot \Delta t$$

1.2.4.6 Step 5: Applying Conservation of Mass

According to the conservation of mass principle, the rate of change of storage in the control volume must equal the net rate of flow into the control volume:

$$\frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right)dx + \frac{\partial}{\partial y}\left(Kh\frac{\partial h}{\partial y}\right)dy = S_y \cdot dx \cdot dy \cdot \frac{\partial h}{\partial t}$$

1.2.4.7 Step 6: Simplifying and Rearranging

Divide through by \$ dx dy \$:

$$\frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Kh\frac{\partial h}{\partial y}\right) = S_y\frac{\partial h}{\partial t}$$

1.2.4.8 Final Governing Equation

The two-dimensional groundwater flow equation for an unconfined aquifer is:

$$S_y\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(Kh\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(Kh\frac{\partial h}{\partial y}\right)$$

This is the governing equation for transient groundwater flow in a two-dimensional unconfined aquifer. It accounts for the variation in the saturated thickness h due to fluctuations in the water table and assumes horizontal flow and a vertical hydraulic gradient, as per the Dupuit approximation.

1.2.5 三维非承压地下水运动

You are right. The Dupuit assumption is primarily applicable to simplifying two-dimensional flow problems in unconfined aquifers by assuming horizontal flow and neglecting vertical gradients. For a three-dimensional unconfined aquifer groundwater flow, we need to take a different approach that does not rely on the Dupuit assumption.

Let's derive the governing equation for three-dimensional unconfined aquifer groundwater flow without using the Dupuit assumption, considering the changes in storage and flow in all three dimensions properly.

1.2.5.1 Step-by-Step Derivation for Three-Dimensional Unconfined Aquifer

1.2.5.2 Step 1: Darcy's Law

In three dimensions, Darcy's Law for groundwater flow in an unconfined aquifer is given by:

$$\mathbf{q} = -K\nabla h$$

where: - $\mathbf{q}$ is the specific discharge (Darcy velocity) vector [L/T]. - K is the hydraulic conductivity of the aquifer [L/T]. - h is the hydraulic head [L]. - ∇h is the hydraulic gradient, which in three dimensions is written as:

$$\nabla h = \left(\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}, \frac{\partial h}{\partial z}\right)$$

1.2.5.3 Step 2: Conservation of Mass

Consider a differential control volume in the unconfined aquifer with dimensions dx, dy, and dz, where z is the vertical direction.

1.2.5.3.1 Inflow and Outflow

- Inflow in the x-direction at x: $Q_x(x) = q_x A_x = -K\frac{\partial h}{\partial x}A_x$, where $A_x = dy \cdot dz$ is the cross-sectional area perpendicular to the x-direction.
- Outflow in the x-direction at $x + dx$: $Q_x(x + dx) = \left(q_x + \frac{\partial q_x}{\partial x}dx\right) A_x$

Similarly, for the y- and z-directions:

- Inflow in the y-direction at y: $Q_y(y) = q_y A_y = -K\frac{\partial h}{\partial y}A_y$, where $A_y = dx \cdot dz$.
- Outflow in the y-direction at $y + dy$: $Q_y(y + dy) = \left(q_y + \frac{\partial q_y}{\partial y}dy\right) A_y$
- Inflow in the z-direction at z: $Q_z(z) = q_z A_z = -K\frac{\partial h}{\partial z}A_z$, where $A_z = dx \cdot dy$.
- Outflow in the z-direction at $z + dz$: $Q_z(z + dz) = \left(q_z + \frac{\partial q_z}{\partial z}dz\right) A_z$

1.2.5.3.2 Net Flow The net inflow into the control volume is the sum of the net inflows in each direction:

$$\text{Net inflow in } x\text{-direction} = Q_x(x) - Q_x(x + dx)$$

$$= \left(-K\frac{\partial h}{\partial x}\right)A_x - \left(-K\frac{\partial h}{\partial x} + \frac{\partial}{\partial x}\left(-K\frac{\partial h}{\partial x}\right)dx\right)A_x$$
$$= -A_x\frac{\partial}{\partial x}\left(-K\frac{\partial h}{\partial x}\right)dx$$

Similarly,

$$\text{Net inflow in } y\text{-direction} = -A_y\frac{\partial}{\partial y}\left(-K\frac{\partial h}{\partial y}\right)dy$$
$$\text{Net inflow in } z\text{-direction} = -A_z\frac{\partial}{\partial z}\left(-K\frac{\partial h}{\partial z}\right)dz$$

The total net inflow into the control volume is:

$$\text{Net inflow} = -\left(\frac{\partial}{\partial x}\left(-K\frac{\partial h}{\partial x}\right)dx\cdot dy\cdot dz + \frac{\partial}{\partial y}\left(-K\frac{\partial h}{\partial y}\right)dx\cdot dy\cdot dz + \frac{\partial}{\partial z}\left(-K\frac{\partial h}{\partial z}\right)dx\cdot dy\cdot dz\right)$$
$$= \left(\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right)\right)dx\cdot dy\cdot dz$$

1.2.5.4 Step 3: Change in Storage

The change in storage within the control volume over a time interval Δt can be expressed using the specific yield S_y, which is the volume of water released from storage per unit surface area per unit decline in the water table:

$$\Delta S = S_y\cdot dx\cdot dy\cdot dz\cdot\frac{\partial h}{\partial t}\cdot\Delta t$$

1.2.5.5 Step 4: Applying Conservation of Mass

According to the conservation of mass principle, the rate of change of storage in the control volume must equal the net rate of flow into the control volume:

$$S_y\frac{\partial h}{\partial t}\cdot dx\cdot dy\cdot dz = \left(\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right)\right)dx\cdot dy\cdot dz$$

1.2.5.6 Step 5: Simplifying and Rearranging

Divide through by \$ dx dy dz \$:

$$S_y\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right)$$

1.2.5.7 Final Governing Equation

The three-dimensional groundwater flow equation for an unconfined aquifer is:

$$S_y \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z}\right)$$

This equation describes the transient groundwater flow in a three-dimensional unconfined aquifer, accounting for variations in the hydraulic head in all three spatial dimensions. This derivation does not rely on the Dupuit assumption, making it suitable for three-dimensional flow problems.

1.2.6 一维热传导方程

Let's go through the step-by-step derivation of the one-dimensional heat conduction equation based on Fourier's law in a structured manner.

1.2.6.1 Step 1: Fourier's Law of Heat Conduction

Fourier's law states that the heat flux q (amount of heat per unit area per unit time) is proportional to the negative gradient of the temperature T:

$$q = -k\frac{\partial T}{\partial x}$$

where:

- $q$is the heat flux [W/m^2].
- $k$is the thermal conductivity of the material [W/(m $\cdot$ K)].
- $\frac{\partial T}{\partial x}$is the temperature gradient in the$x$-direction [K/m].

1.2.6.2 Step 2: Energy Conservation in a Differential Element

Consider a small differential control volume of lengthdx, cross-sectional area$A$, and located at position x along the rod's length.

1.2.6.2.1 Heat Entering and Leaving the Control Volume

- The rate of heat entering at x: $q(x) \cdot A$
- The rate of heat leaving at $x + dx$: $q(x + dx) \cdot A$

Using a Taylor series expansion for $q(x + dx)$:

$$q(x + dx) \approx q(x) + \left(\frac{\partial q}{\partial x}\right) dx$$

1.2.6.2.2 Net Heat Flow

The net rate of heat entering the differential element is:

$$q(x) \cdot A - \left(q(x) + \left(\frac{\partial q}{\partial x}\right) dx\right) \cdot A$$

$$= -A\left(\frac{\partial q}{\partial x}\right) dx$$

1.2.6.3 Step 3: Heat Storage in the Differential Element

The change in internal energy (ΔU) within the differential element over a time interval Δt can be expressed using the specific heat capacity c and density ρ of the material:

$$\Delta U = \rho \cdot c \cdot A \cdot dx \cdot \frac{\partial T}{\partial t} \cdot \Delta t$$

1.2.6.4 Step 4: Applying Conservation of Energy

Assuming no internal heat generation and applying the conservation of energy principle, the rate of heat entering the control volume must equal the rate of energy storage within the control volume:

$$-A\left(\frac{\partial q}{\partial x}\right) dx = \rho \cdot c \cdot A \cdot dx \cdot \frac{\partial T}{\partial t}$$

1.2.6.5 Step 5: Substituting Fourier's Law

Substitute$q = -k\frac{\partial T}{\partial x}$into the equation:

$$-A\left(\frac{\partial}{\partial x}\left(-k\frac{\partial T}{\partial x}\right)\right) dx = \rho \cdot c \cdot A \cdot dx \cdot \frac{\partial T}{\partial t}$$

Simplify the equation:

$$A\left(k\frac{\partial^2 T}{\partial x^2}\right) dx = \rho \cdot c \cdot A \cdot dx \cdot \frac{\partial T}{\partial t}$$

1.2.6.6 Step 6: Simplifying and Rearranging

Cancel out the common terms$A$anddx:

$$k\frac{\partial^2 T}{\partial x^2} = \rho c\frac{\partial T}{\partial t}$$

Divide both sides byρc:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\frac{\partial^2 T}{\partial x^2}$$

Define the thermal diffusivityαas:

$$\alpha = \frac{k}{\rho c}$$

1.2.6.7 Final Governing Equation

The one-dimensional heat conduction equation (also called the heat diffusion equation) is:

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2}$$

This partial differential equation describes how the temperature T varies with time t and position x within the material.

1.2.7 一维溶质运移-扩散方程

Sure, let's derive the governing equation for a one-dimensional solute advection-diffusion problem step by step. This equation describes how the solute concentration changes over time due to both advection (transport by the flow of the water) and diffusion (spreading due to concentration gradients).

1.2.7.1 Step-by-Step Derivation for One-Dimensional Solute Advection-Diffusion

1.2.7.2 Step 1: Define Variables

- $c(x, t)$: Solute concentration [M/L^3].
- u: Velocity of the fluid in the x-direction [L/T].
- D: Diffusion coefficient [L^2/T].
- x: Spatial coordinate in the x-direction [L].
- t: Time [T].

1.2.7.3 Step 2: Conservation of Mass (Continuity Equation)

Consider a differential control volume of length dx in the x-direction.

1.2.7.3.1 Inflow and Outflow by Advection

- Inflow of solute by advection at position x:

$$J_{\text{adv,in}} = uc(x,t)$$

- Outflow of solute by advection at position $ x + dx $:

$$J_{\text{adv,out}} = uc(x+dx,t) \approx u\left(c(x,t) + \frac{\partial c}{\partial x}dx\right)$$

1.2.7.3.2 Inflow and Outflow by Diffusion

- Inflow of solute by diffusion at position x:

$$J_{\text{diff,in}} = -D\frac{\partial c}{\partial x}$$

- Outflow of solute by diffusion at position $ x + dx $:

$$J_{\text{diff,out}} = -D\frac{\partial c}{\partial x}\bigg|_{x+dx} \approx -D\left(\frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right)dx\right)$$

1.2.7.4 Step 3: Net Flow

The net inflow of solute into the control volume is the difference between the inflow and outflow due to both advection and diffusion.

1.2.7.4.1 Net Advection Flow

$$\text{Net advective flow} = J_{\text{adv,in}} - J_{\text{adv,out}} = uc(x,t) - u\left(c(x,t) + \frac{\partial c}{\partial x}dx\right) = -u\frac{\partial c}{\partial x}dx$$

1.2.7.4.2 Net Diffusion Flow

$$\text{Net diffusive flow} = J_{\text{diff,in}} - J_{\text{diff,out}} = -D\frac{\partial c}{\partial x} - \left(-D\left(\frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right)dx\right)\right) = D\frac{\partial^2 c}{\partial x^2}dx$$

1.2.7.5 Step 4: Change in Storage

The change in solute mass within the control volume over a time interval Δt is:

$$\Delta S = \frac{\partial c}{\partial t} dx \Delta t$$

1.2.7.6 Step 5: Applying Conservation of Mass

According to the conservation of mass principle, the rate of change of solute storage in the control volume must equal the net rate of solute flow into the control volume:

$$\frac{\partial c}{\partial t} dx = -u \frac{\partial c}{\partial x} dx + D \frac{\partial^2 c}{\partial x^2} dx$$

1.2.7.7 Step 6: Simplifying and Rearranging

Divide through by dx:

$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2}$$

1.2.7.8 Final Governing Equation

The final governing equation for the one-dimensional solute advection-diffusion problem is:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2}$$

This partial differential equation describes how the solute concentration c varies with time t and position x due to advection by the flow field u and diffusion characterized by the diffusion coefficient D.

1.2.8 二维溶质运移-扩散方程

Let's derive the governing equation for a two-dimensional solute advection-diffusion problem step by step. This equation describes how a solute concentration changes over time due to both advection (transport by the flow of the water) and diffusion (spreading due to concentration gradients).

1.2.8.1 Step-by-Step Derivation for Two-Dimensional Solute Advection-Diffusion

1.2.8.2 Step 1: Define Variables

- $ c(x, y, t) $: solute concentration [M/L³].
- u: velocity component in the x-direction [L/T].
- v: velocity component in the y-direction [L/T].
- D_x: diffusion coefficient in the x-direction [L²/T].
- D_y: diffusion coefficient in the y-direction [L²/T].

1.2.8.3 Step 2: Conservation of Mass (Continuity Equation)

Consider a differential control volume in the x-y plane with dimensions dx and dy.

1.2.8.3.1 Inflow and Outflow

- Inflow of solute by advection in the x-direction at x:

$$u(x)c(x) \cdot dy$$

- Outflow of solute by advection in the x-direction at $ x + dx $:

$$u(x+dx)c(x+dx) \cdot dy \approx (u(x)c(x) + \frac{\partial}{\partial x}(uc)dx) \cdot dy$$

- Inflow of solute by advection in the y-direction at y:

$$v(y)c(y) \cdot dx$$

- Outflow of solute by advection in the y-direction at $ y + dy $:

$$v(y+dy)c(y+dy) \cdot dx \approx (v(y)c(y) + \frac{\partial}{\partial y}(vc)dy) \cdot dx$$

- Inflow of solute by diffusion in the x-direction at x:

$$-D_x \frac{\partial c}{\partial x} \cdot dy$$

- Outflow of solute by diffusion in the x-direction at $ x + dx $:

$$-D_x \frac{\partial c}{\partial x} \cdot dy - \frac{\partial}{\partial x}\left(-D_x \frac{\partial c}{\partial x}\right) dx \cdot dy$$

- Inflow of solute by diffusion in the y-direction at y:

$$-D_y \frac{\partial c}{\partial y} \cdot dx$$

- Outflow of solute by diffusion in the y-direction at $ y + dy $:

$$-D_y \frac{\partial c}{\partial y} \cdot dx - \frac{\partial}{\partial y} \left(-D_y \frac{\partial c}{\partial y} \right) dy \cdot dx$$

1.2.8.3.2 Net Flow The net inflow of solute into the control volume due to advection and diffusion is:

$$\text{Net inflow in } x\text{-direction} = (u(x)c(x) \cdot dy - (u(x+dx)c(x+dx) \cdot dy)) + \left(-D_x \frac{\partial c}{\partial x} \cdot dy - \left(-D_x \frac{\partial c}{\partial x} -\right.\right.$$

$$= -\frac{\partial}{\partial x} (uc)\, dx \cdot dy + \frac{\partial}{\partial x} \left(D_x \frac{\partial c}{\partial x} \right) dx \cdot dy$$

Similarly, for the y-direction:

$$\text{Net inflow in } y\text{-direction} = -\frac{\partial}{\partial y} (vc)\, dy \cdot dx + \frac{\partial}{\partial y} \left(D_y \frac{\partial c}{\partial y} \right) dy \cdot dx$$

The total net inflow of solute into the control volume is:

$$\text{Total net inflow} = \left(\frac{\partial}{\partial x} \left(D_x \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial x} (uc) \right) dx \cdot dy + \left(\frac{\partial}{\partial y} \left(D_y \frac{\partial c}{\partial y} \right) - \frac{\partial}{\partial y} (vc) \right) dy \cdot dx$$

1.2.8.4 Step 3: Change in Storage

The change in solute mass within the control volume over a time interval $ t $ is:

$$\Delta S = \frac{\partial c}{\partial t} \cdot dx \cdot dy \cdot \Delta t$$

1.2.8.5 Step 4: Applying Conservation of Mass

According to the conservation of mass principle, the rate of change of solute storage in the control volume must equal the net rate of solute flow into the control volume:

$$\frac{\partial c}{\partial t} = \left(\frac{\partial}{\partial x} \left(D_x \frac{\partial c}{\partial x} \right) - \frac{\partial}{\partial x} (uc) \right) + \left(\frac{\partial}{\partial y} \left(D_y \frac{\partial c}{\partial y} \right) - \frac{\partial}{\partial y} (vc) \right)$$

1.2.8.6 Step 5: Simplifying and Rearranging

Combine the terms and rearrange:

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} - \frac{\partial}{\partial x}\left(uc\right) - \frac{\partial}{\partial y}\left(vc\right)$$

1.2.8.7 Final Governing Equation

The final governing equation for the two-dimensional solute advection-diffusion problem is:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(uc) + \frac{\partial}{\partial y}(vc) = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2}$$

This partial differential equation describes how the solute concentration c varies with time t and position $ (x, y) $ due to advection by the flow field $ (u, v) $ and diffusion characterized by the diffusion coefficients D_x and D_y.

第 2 章　数值方法基础

2.1　隐式与显式求解法

数值方法可分为显式求解 (Explicit method) 与隐式求解 (Implicit method)：

定义 2.1 (显式求解法)**.** 当下一时刻变量由前一时刻变量直接计算得到的，称为显式求解法。数学表达可写为：

$$Y(t+\Delta t) = F(Y(t))$$

定义 2.2 (隐式求解法)**.** 当下一时刻变量由一系列公式、矩阵或者迭代算法计算得到，称为隐式求解法。数学表达可写为：

$$G(Y(t), Y(t+\Delta t)) = 0$$

相同时空分辨率条件下，显式求解法的计算速度显著高于隐式求解法，但是隐式求解法可以保证计算的稳定性，因此可采用较大时间步长进行计算，而显式求解法必须受制于 CFL 条件。

2.2　数值迭代方法

2.2.1　牛顿迭代 (Newton Iteration)

牛顿迭代法（Newton's method）又称为牛顿-拉夫逊（拉弗森）方法（Newton-Raphson method），是一种在实数域和复数域上近似求解方程的方法。方法使用函数 $f(x)$ 的泰勒级数的前面几项来寻找方程 $f(x)=0$ 的根。

以下我们将通过一个实例，展示如何使用 R 语言实现牛顿迭代法。

我们选取的方程是 $e^x - 3x = 0$，这是一个没有显式解的方程。我们的目标是找到这个方程的一个根。

牛顿迭代法的核心思想是利用函数在某点的切线来逼近函数的根。其迭代公式如下：

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

其中，x_n 是第 n 次迭代的近似值，$f(x)$ 是我们要解决的方程，$f'(x)$ 是 $f(x)$ 的导数。

下面是使用 R 语言实现牛顿迭代法求解 $e^x - 3x = 0$ 的代码：

```r
# 定义方程 f(x) 和它的导数 f_prime(x)
f <- function(x) {
  return(exp(x) - 3 * x)
}

f_prime <- function(x) {
  return(exp(x) - 3)
}

# 牛顿迭代法
newton_method <- function(f, f_prime, x0, tol = 1e-6, max_iter = 1000) {
  x <- x0
  for (i in 1:max_iter) {
    x_new <- x - f(x) / f_prime(x)
    if (abs(x_new - x) < tol) {
      return(x_new)
    }
    x <- x_new
  }
  warning("迭代未收敛")
  return(x)
}

# 初始猜测值
x0 <- 1.0

# 执行牛顿迭代
root <- newton_method(f, f_prime, x0)

# 输出结果
cat("方程 e^x - 3x = 0 的近似根为：", root, "\n")
```

```
## 方程 e^x - 3x = 0 的近似根为： 0.6190613
```

牛顿迭代法虽然是一种非常有效的数值方法，但它也存在一些局限性，以下是一些主要的局限性：

1. 初始猜测的重要性：牛顿迭代法的收敛速度和是否收敛很大程度上取决于初始猜测值。如果初始猜测远离实际根，迭代可能会发散，或者收敛到错误的根。
2. 导数的计算：牛顿迭代法需要计算函数的导数。对于一些复杂的函数，这可能非常困难或者计算成本很高。
3. 不可导函数：如果函数在某些点不可导，或者导数为零，牛顿迭代法可能无法应用或者失效。
4. 多根问题：对于具有多个根的方程，牛顿迭代法可能只收敛到其中的一个根，这取决于初始猜测值。它可能无法找到所有的根。
5. 奇点附近的问题：如果函数在根的附近有奇点（例如，函数值或导数趋向于无穷大），牛顿迭代法可能无法正确工作。
6. 全局收敛性：牛顿迭代法通常保证局部收敛，但不保证全局收敛。这意味着即使方程有多个根，迭代过程也可能只收敛到离初始猜测最近的根。
7. 数值稳定性：在某些情况下，由于浮点数的精度限制，牛顿迭代法可能产生数值不稳定。

以下是这些局限性的详细说明：

- 初始猜测的重要性
  - 收敛性：如果初始猜测接近实际根，牛顿迭代法通常能快速收敛。但如果初始猜测远离根，或者接近函数的拐点，迭代可能发散。
  - 根的选择：对于具有多个根的方程，迭代可能只收敛到某个特定的根，这取决于初始猜测。
- 导数的计算
  - 复杂性：对于复杂的函数，计算导数可能非常困难，尤其是当函数涉及多个变量或者嵌套的数学表达式时。
  - 成本：在某些情况下，导数的计算可能比函数本身的计算还要昂贵。-不可导函数
  - 应用限制：如果函数在某点不可导，或者导数为零，牛顿迭代法的迭代公式将无法应用。
- 多根问题
  - 局部收敛：牛顿迭代法可能只找到离初始猜测最近的根，而忽略了其他根。
- 奇点附近的问题
  - 发散：如果函数在根的附近有奇点，迭代过程可能会发散。
- 全局收敛性
  - 局限性：牛顿迭代法不保证找到方程的所有根，特别是当根分布复杂时。
- 数值稳定性

– 精度问题：由于计算机的有限精度，牛顿迭代法可能产生舍入误差，影响结果的准确性。了解这些局限性有助于我们更好地选择和使用牛顿迭代法，以及采取相应的策略来克服这些问题，例如使用更好的初始猜测，或者结合其他数值方法来提高解的可靠性。

2.2.2 欧拉方法 (Euler Method)

在数学和计算机科学中，欧拉方法，命名自它的发明者萊昂哈德·歐拉，是一种一阶数值方法，用以对给定初值的常微分方程（即初值問題）求解。它是常微分方程數值方法中最基本的显式方法（Explicit method）。

欧拉方法是一个一阶方法，意味着其局部截断误差（每步误差）正比于步长的平方，并且其全局截断误差正比于步长。欧拉方法经常应用于作为构建一些更复杂方法的基础，例如，预估-校正方法。

定义 **2.3** (欧拉方法)**.** 欧拉方法数学表达为:

$$y'(t) = f(t, y(t))$$

$$y(t_0) = y_0$$

求解时:

$$y_{n+1} = y_n + hf'(t_n, y_n)$$

其中 $t_n = t0 + nh$，h 即迭代步长，$h = t_{n+1} - t_n$。欧拉方法属于显式求解法。

例 **2.1.** 已知函数:

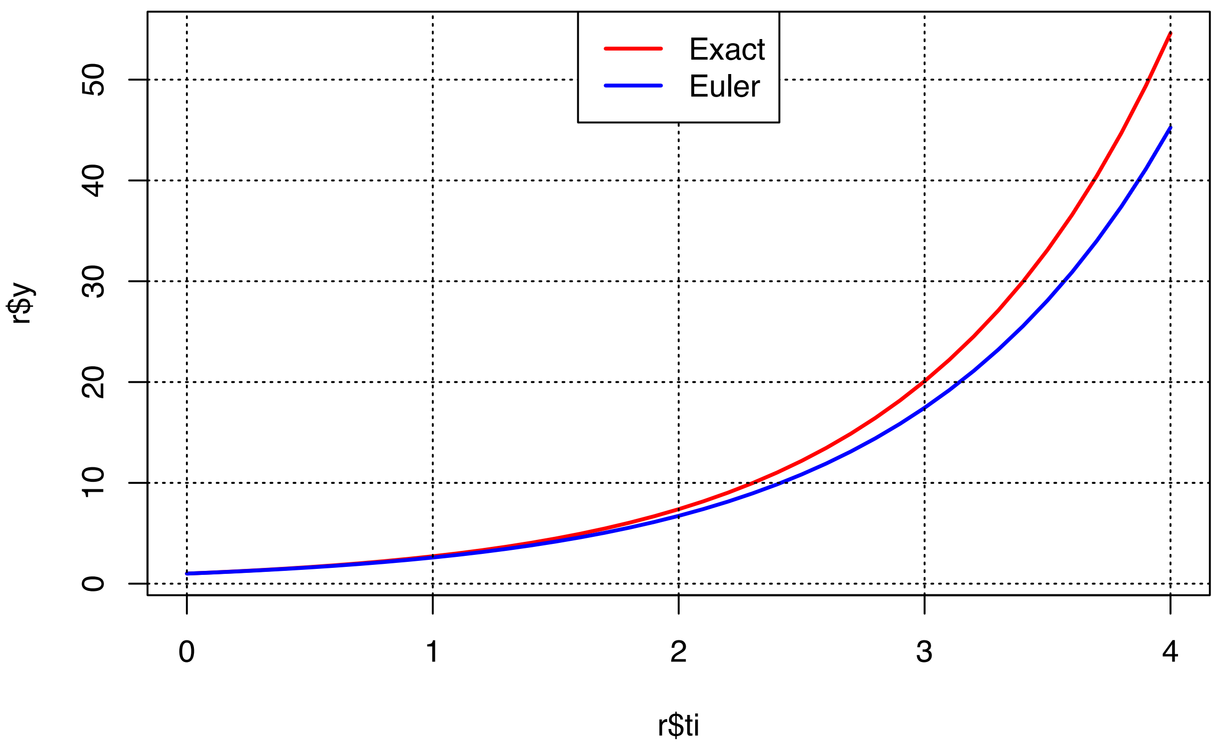
$$\frac{dy}{dt} = y$$
$$y(0) = 1$$

求:

$$y(4) = ?$$

```
# source: https://en.wikipedia.org/wiki/Euler_method
# ============
# SOLUTION to
#   y' = y,   where y' = f(t,y)
# then:
f <- function(ti,y) y
```

```
# INITIAL VALUES:
t0 <- 0
y0 <- 1
h  <- .1
tn <- 4

# Euler's method: function definition
Euler <- function(t0, y0, h, tn, dy.dt) {
  # dy.dt: derivative function

  # t sequence:
  tt <- seq(t0, tn, by=h)
  # table with as many rows as tt elements:
  tbl <- data.frame(ti=tt)
  tbl$yi <- y0 # Initializes yi with y0
  tbl$Dy.dt[1] <- dy.dt(tbl$ti[1],y0) # derivative
  for (i in 2:nrow(tbl)) {
    tbl$yi[i] <- tbl$yi[i-1] + h*tbl$Dy.dt[i-1]
    # For next iteration:
    tbl$Dy.dt[i] <- dy.dt(tbl$ti[i],tbl$yi[i])
  }
  return(tbl)
}

# Euler's method: function application
r <- Euler(t0, y0, h, tn, f)
rownames(r) <- 0:(nrow(r)-1) # to coincide with index n

# Exact solution for this case: y = exp(t)
#       added as an additional column to r
r$y <- exp(r$ti)

plot(r$ti, r$y, type="l", col="red", lwd=2)
lines(r$ti, r$yi, col="blue", lwd=2)
grid(col="black")
legend("top",  legend = c("Exact", "Euler"), lwd=2,  col = c("red", "blue"))
```




```r
# TABLE with results:
print(r)
```

```
##      ti       yi    Dy.dt        y
## 0   0.0 1.000000 1.000000 1.000000
## 1   0.1 1.100000 1.100000 1.105171
## 2   0.2 1.210000 1.210000 1.221403
## 3   0.3 1.331000 1.331000 1.349859
## 4   0.4 1.464100 1.464100 1.491825
## 5   0.5 1.610510 1.610510 1.648721
## 6   0.6 1.771561 1.771561 1.822119
## 7   0.7 1.948717 1.948717 2.013753
## 8   0.8 2.143589 2.143589 2.225541
## 9   0.9 2.357948 2.357948 2.459603
## 10  1.0 2.593742 2.593742 2.718282
## 11  1.1 2.853117 2.853117 3.004166
## 12  1.2 3.138428 3.138428 3.320117
## 13  1.3 3.452271 3.452271 3.669297
## 14  1.4 3.797498 3.797498 4.055200
## 15  1.5 4.177248 4.177248 4.481689
## 16  1.6 4.594973 4.594973 4.953032
## 17  1.7 5.054470 5.054470 5.473947
## 18  1.8 5.559917 5.559917 6.049647
```

```
## 19 1.9  6.115909  6.115909  6.685894
## 20 2.0  6.727500  6.727500  7.389056
## 21 2.1  7.400250  7.400250  8.166170
## 22 2.2  8.140275  8.140275  9.025013
## 23 2.3  8.954302  8.954302  9.974182
## 24 2.4  9.849733  9.849733 11.023176
## 25 2.5 10.834706 10.834706 12.182494
## 26 2.6 11.918177 11.918177 13.463738
## 27 2.7 13.109994 13.109994 14.879732
## 28 2.8 14.420994 14.420994 16.444647
## 29 2.9 15.863093 15.863093 18.174145
## 30 3.0 17.449402 17.449402 20.085537
## 31 3.1 19.194342 19.194342 22.197951
## 32 3.2 21.113777 21.113777 24.532530
## 33 3.3 23.225154 23.225154 27.112639
## 34 3.4 25.547670 25.547670 29.964100
## 35 3.5 28.102437 28.102437 33.115452
## 36 3.6 30.912681 30.912681 36.598234
## 37 3.7 34.003949 34.003949 40.447304
## 38 3.8 37.404343 37.404343 44.701184
## 39 3.9 41.144778 41.144778 49.402449
## 40 4.0 45.259256 45.259256 54.598150
```

2.2.3 龙格-库塔方法 (Runge-Kutta Method)

数值分析中，龙格-库塔方法（Runge-Kutta Methods）是用于非线性常微分方程的解的重要的一类隐式或显式迭代法。这些技术由数学家卡尔 · 龙格和马丁 · 威尔海姆 · 库塔于 1900 年左右发明。

定义 2.4 (4 阶 Runge-Kutta)**.** 4 阶 Runge-Kutta 方法的基本步骤如下：

1. 计算 $k_1 = f(x_n, y_n)$
2. 计算 $k_2 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_1)$
3. 计算 $k_3 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_2)$
4. 计算 $k_4 = f(x_n + h, y_n + hk_3)$
5. 更新 $y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$

例子 1: 考虑以下常微分方程初值问题:

$$y' = 1 + (y - x)^2, \quad y(0) = 0.5$$

我们需要使用 4 阶 Runge-Kutta 方法（RK4）来数值求解该微分方程在区间 $(0, 2)$ 上的解。

接下来我们将使用 R 语言实现该数值解法。

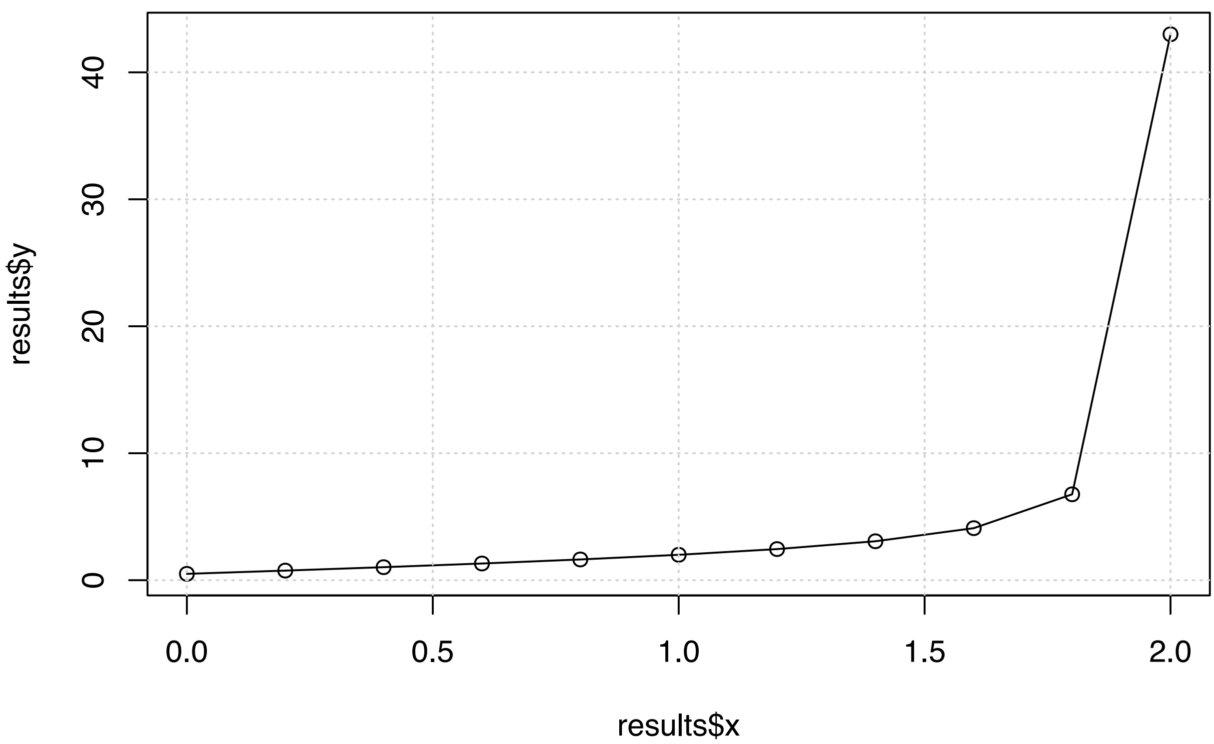
```
# 4 阶 Runge-Kutta 方法
rungeKutta4 <- function(func, x0, y0, x_end, n) {
  h <- (x_end - x0) / n
  x <- x0
  y <- y0
  results <- data.frame(x = x0, y = y0)

  for (i in 1:n) {
    k1 <- func(x, y)
    k2 <- func(x + 0.5 * h, y + 0.5 * h * k1)
    k3 <- func(x + 0.5 * h, y + 0.5 * h * k2)
    k4 <- func(x + h, y + h * k3)

    y <- y + h/6 * (k1 + 2*k2 + 2*k3 + k4)
    x <- x + h
    results <- rbind(results, data.frame(x = x, y = y))
  }

  return(results)
}
```

```
# 定义微分方程
dydx <- function(x, y) {
  return(1 + (y - x)^2)
}

# 初始条件
x0 <- 0
y0 <- 0.5
x_end <- 2
n <- 10  # 步数
```

```r
# 计算
results <- rungeKutta4(dydx, x0, y0, x_end, n)

# 打印结果
print(results)
```

```
##       x          y
## 1  0.0  0.5000000
## 2  0.2  0.7555552
## 3  0.4  1.0249990
## 4  0.6  1.3142831
## 5  0.8  1.6333266
## 6  1.0  1.9999816
## 7  1.2  2.4499414
## 8  1.4  3.0664221
## 9  1.6  4.0983141
## 10 1.8  6.7645620
## 11 2.0 42.9981995
```

```r
plot(results$x, results$y, type='o')
grid()
```



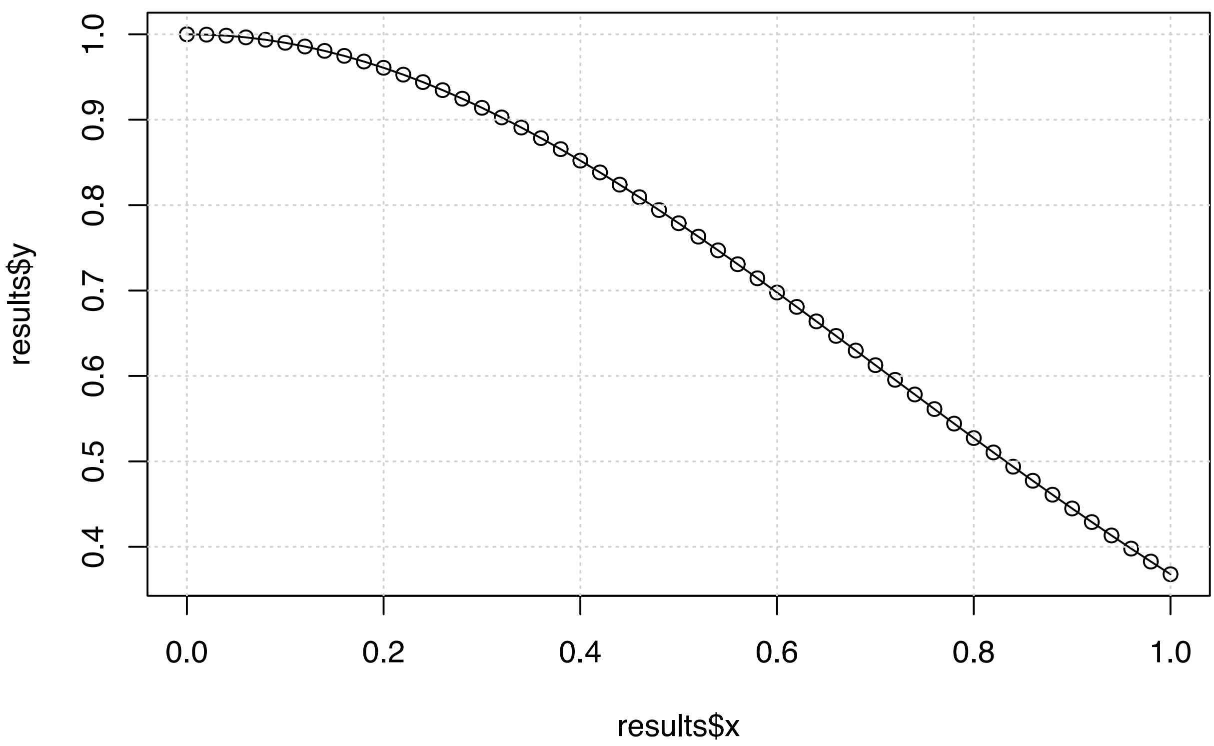
例子 2：考虑以下常微分方程初值问题：

$$y' = -2xy, \quad y(0) = 1$$

我们将使用 4 阶 Runge-Kutta 方法（RK4）来数值求解该微分方程在区间 $(0, 1)$ 上的解。

以下是 R 语言的实现代码：

```
# 定义微分方程
dydx <- function(x, y) {
  return(-2 * x * y)
}
# 初始条件
x0 <- 0
y0 <- 1
x_end <- 1
n <- 50  # 步数

# 计算
results <- rungeKutta4(dydx, x0, y0, x_end, n)

# 打印结果
plot(results$x, results$y, type='o')
grid()
```



2.2.4 皮卡法 (Picard Method)

皮卡逐次逼近法（Picard Successive Approximation Method）是常微分方程解的一种主要近似计算方法。皮卡 (Picard,(C.-)É) 最早在数学上完善处理这样的逐次逼近的函数序列，所以称为皮卡逐次逼近法。

2.3 有限元, 有限差分, 有限体积

数值方法中主要有有限差分（Finite Difference, FD）、有限元（Finite Element, FE）和有限体积（Finite Volume，FV）法三类。三类方法并无明显优劣之分，但其中各有特点。有限差分法方法简洁，物理意义清晰，编程容易，因而是水文/气象领域应用最多的方法。有限元法可以保证全局物质/能量守恒，但是无法保证局部守恒；有限体积法弥补了有限元这一缺陷，既可以保证全局守恒，也可以保证局部守恒。

三类方法的数学的意义略有不同：有限差分法计算为空间某一点的值，有限元法计算某一计算单元内的近似拟合曲线，有限体积法作为有限元法的特例，计算该计算单元内的均值。因此对于三种不同方法计算的结果的解读应当略有不同，但实际模型用户层面通常将其视为相同含义。

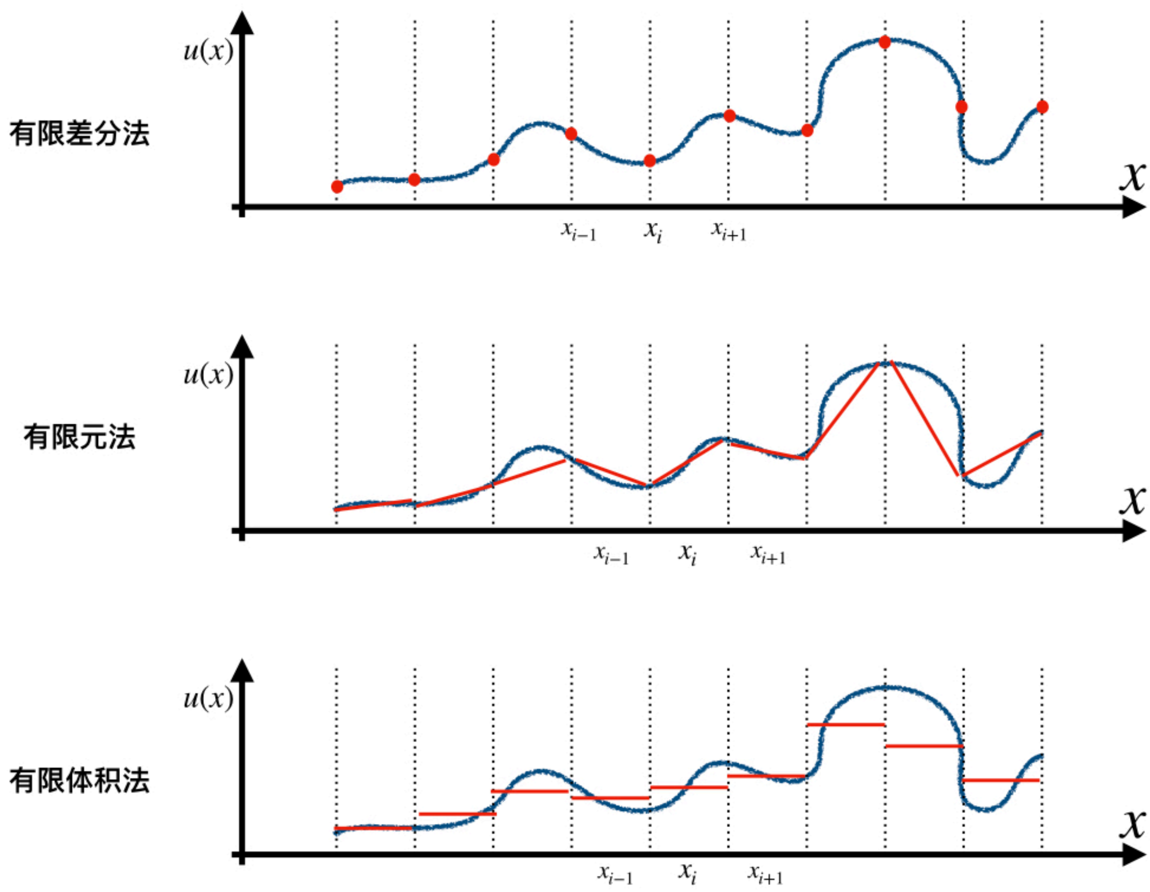


Figure 2.1: 三种数值方法对比

2.4 CFL 条件约束

CFL 条件是数值方法求解常/偏微分方程保证其收敛性和稳定性的必要条件，但不是充分条件；以 Courant，Fredrichs 和 Lewy 共同命名（cite）。CFL 条件即数值方法的时间步长要足够小，方能够保证计算精度，否则结果不收敛或者不稳定。

最简单可以理解为时间推进求解的速度必须大于物理扰动传播的速度，只有这样才能将物理上所有的扰动俘获到。

定义 **2.5** (CFL 条件)**.** CFL 条件数学表达形式为：

$$\frac{c\Delta t}{\Delta x^n} < C_{max}$$

其中 c 即为系统中变量的变化速率。C_{max} 是保持求解系统稳定和收敛的最大值，常见值为 0.5。有的系统中 $n = 1$，但有的科学问题中 $n > 1$。

2.5 时空离散化

空间离散化，即分割连续的空间称为空间若干子集的过程, 由一维 Δx, 二维 $(\Delta x, \Delta y)$, 或者三维 $(\Delta x, \Delta y, \Delta z)$ 构成的最小计算单元或质点。

时间离散化即模型时间步长，即 Δt。

时间步长和空间分辨率的组合关系，对于数值方法求解的稳定性和收敛性都有显著影响。CFL 条件是限制因素。为保证数值方法稳定性，空间分辨率越高，则要求时间分辨率也越高，时间分辨率与空间分辨率的（一次或多次）幂存在正比关系。

通常的空间离散化分为结构化 (Structured) 与非结构化 (Unstructured) 网格。

结构化网格主要是划分为形状和面积相同的计算单元。矩形规则化网格的好处是：求解过程直观易懂，编程实现简单，并且易于并行化；输入和输出数据都直接使用矩阵方式表达；数据制备、处理和可视化都直观且便捷。规则化网格常见矩形，也有正三角形和正六边形的方案。

非结构化网格的优势在于：（1）更好的表现不规则三维地形；（2）更好的表现不规则研究区 (流域）的边界，边界条件处理更合理，其边界条件控制也更符合数值理论；（3）计算单元的面积大小灵活可变，可以在保证整体边界条件情况下，对重点地区进行局部加密——亦或相反设置。非结构化网格既可以保证重点区域的高分辨率，在保证可靠的边界条件情况下，不显著增加计算单元数量，保证重点区域模拟精度和计算负担之间的平衡。非结构化网格的主要缺陷是：（1）计算过程相对复杂，仅支持有限元和有限体积法；（2）数据解读和可视化复杂，需要针对性的数据前处理和后处理软件。

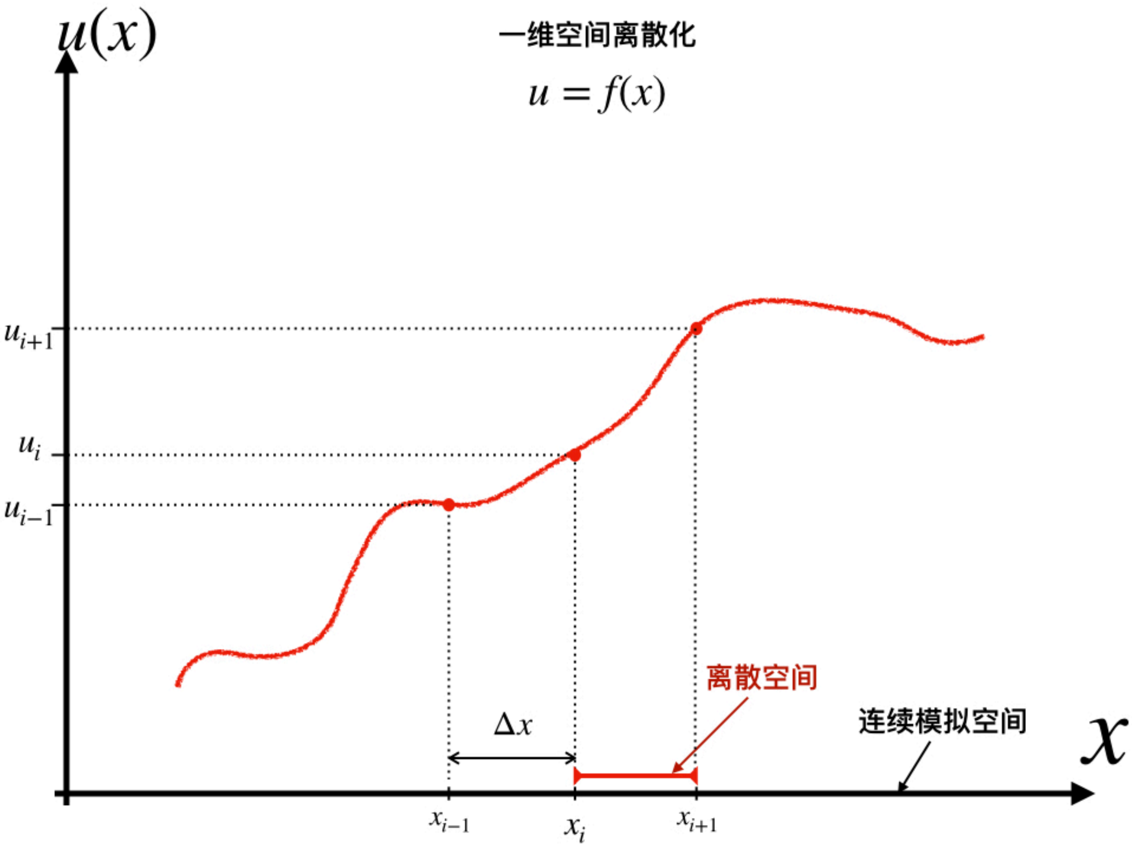


Figure 2.2: 一维空间离散化

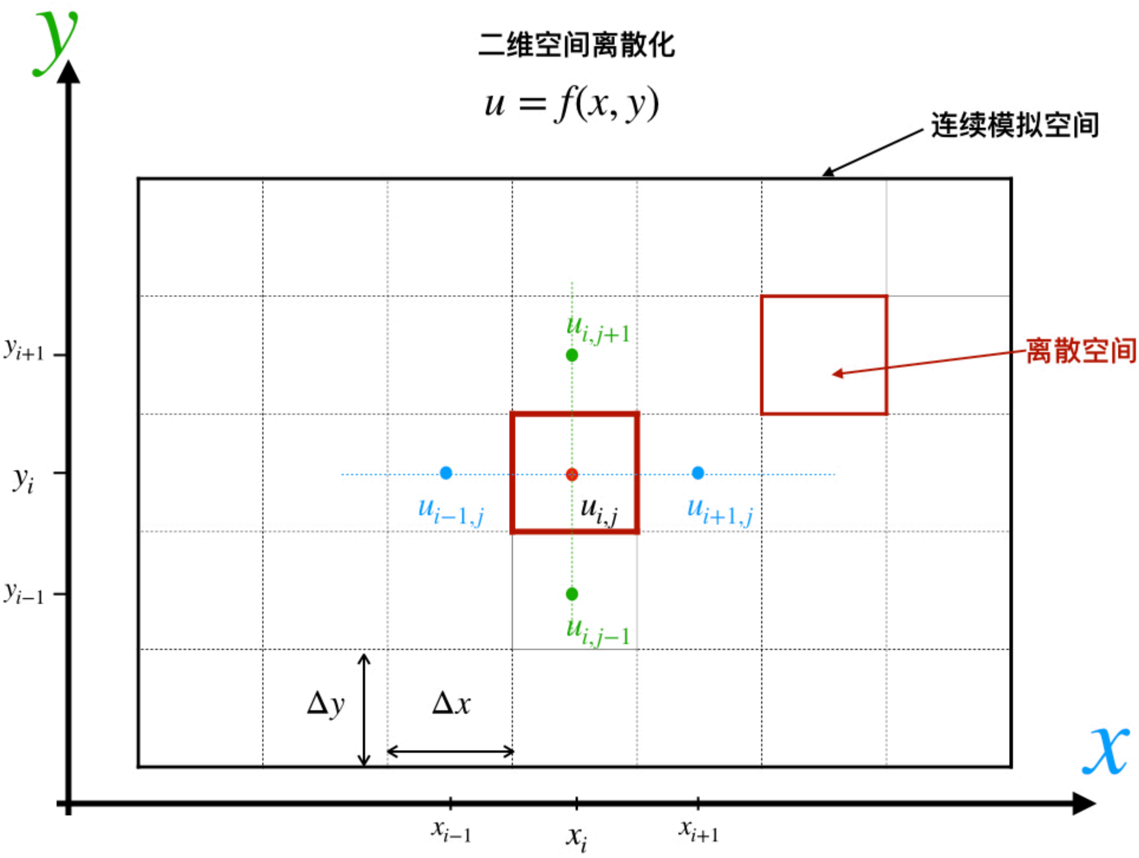


Figure 2.3: 二维空间离散化

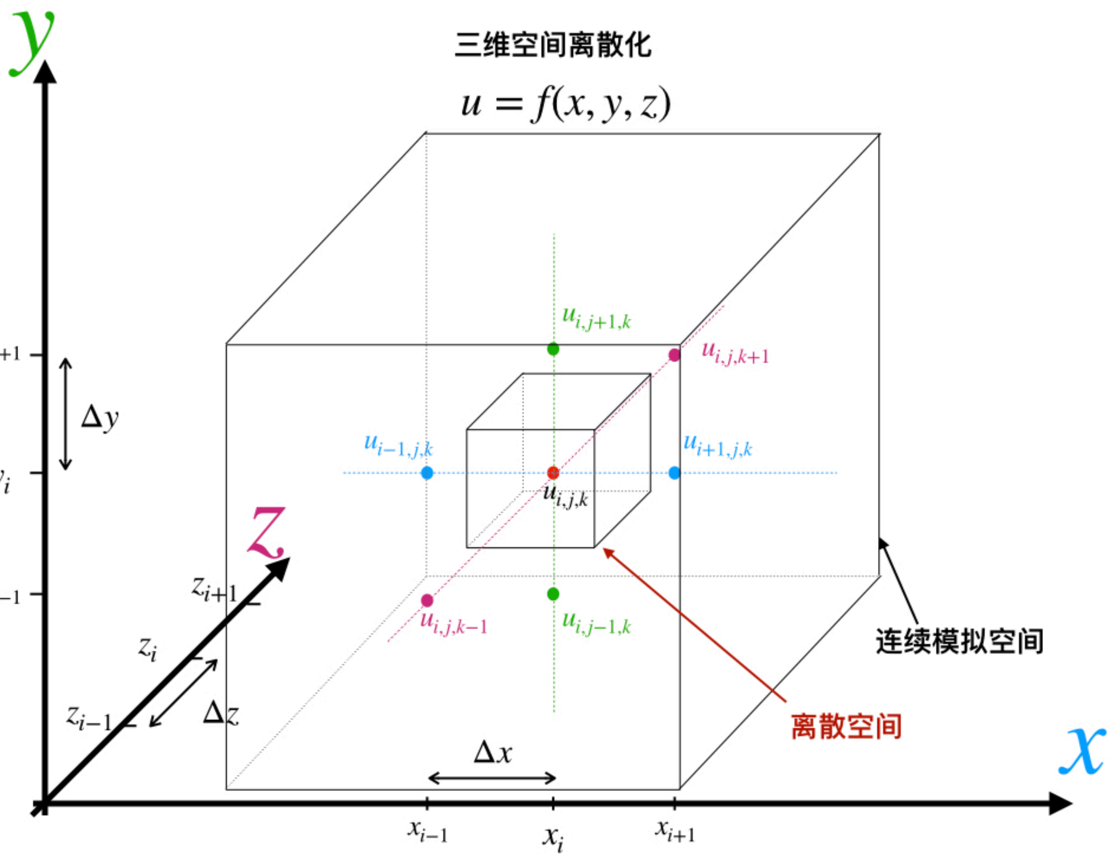
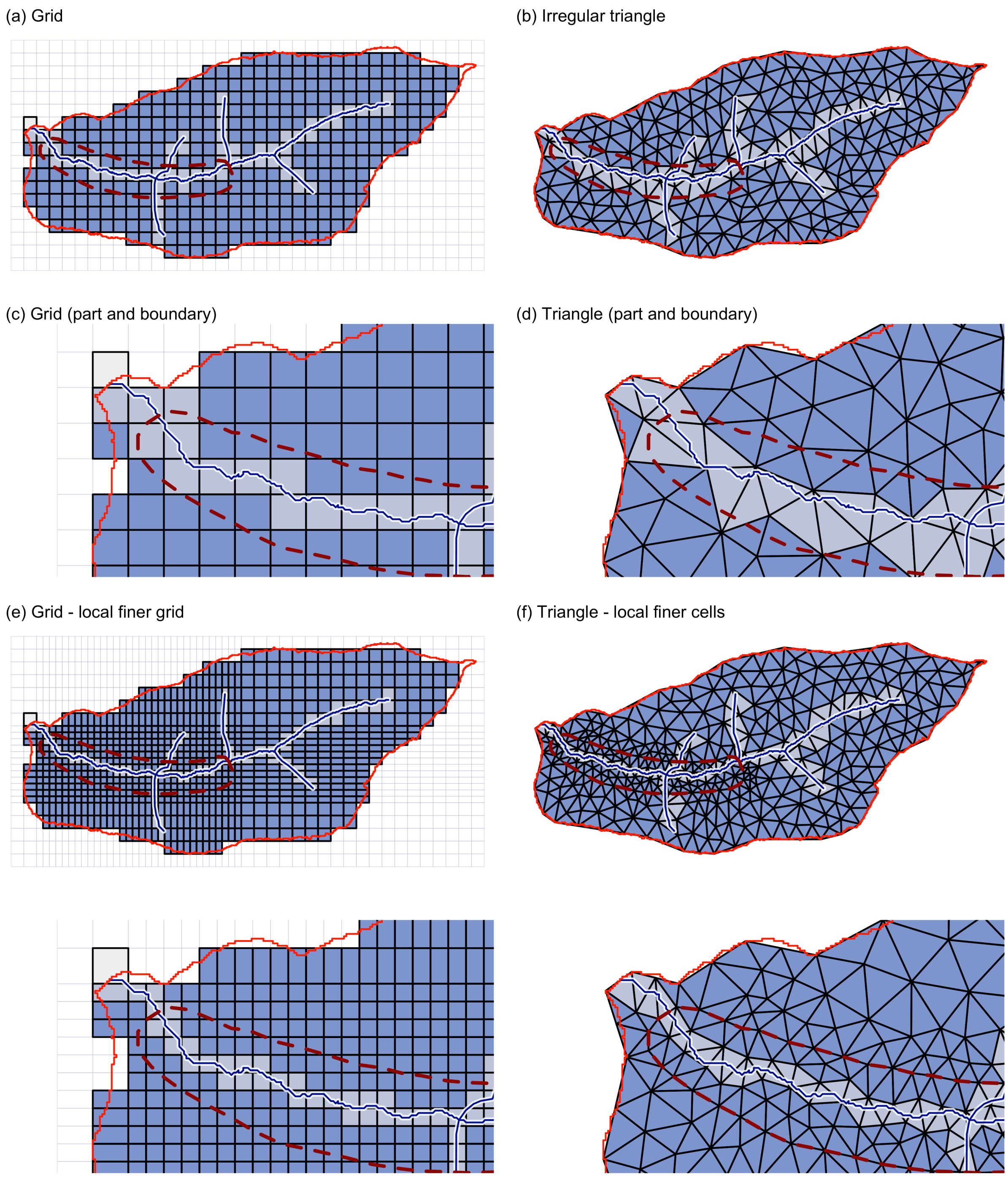


Figure 2.4: 三维空间离散化



2.6 初始条件

定义 2.6 (初始条件)**.** 初始条件定义为

$$y(t_0) = y_0$$

其中 t_0 为问题的初始时刻，y_0 为初始时刻包含目标变量值的向量。

数值方法研究中，模拟结果对初始条件具有一定敏感性。但是，初始条件的敏感性问题与

描述该系统的控制方程有关。部分问题的初始条件误差，可以通过一定时间的模型预热 (Spin-up) 消除；但另有一部分问题（例如 Lorenz System 为代表的混沌系统），初始条件敏感性极高。

2.7 边界条件

数值方法的边界条件通常分为 Dirichlet 和 Neumann 两类。

定义 **2.7** (第一类边界条件)**.** Dirichlet 边界条件 (Dirichlet Boundary Condition, DBC) 是常/偏微分方程的第一类边界条件，也称为固定边界条件，其指定了空间某点的固定值，比如在地下水中，Dirichlet 边界条件限定固定地下水水头高度。

定义 **2.8** (第二类边界条件)**.** 诺伊曼边界条件（Neumann boundary condition, NBC) 也被称为常/偏微分方程的 “第二类边界条件”，其给定空间特定位置上目标变量的一阶导数，在地下水问题中，通常某一点处固定的流量，如注水或者取水量。

作为三维的数值模型，两类边界条件都可以施加在空间任意位置的任意方向上。

第 3 章　有限差分法

3.1　泰勒级数 (Taylor Series)

泰勒级数（Taylor series）是数学中一个重要的概念，它提供了一种将函数表示为无限项的幂级数的方法。这种表示方法在微积分、复分析、数值分析以及物理学的许多领域中都有广泛的应用。泰勒级数是以于 1715 年发表了泰勒公式的英國数学家布魯克 · 泰勒（Sir Brook Taylor）来命名的。

以下是用学术语言对泰勒级数的介绍：

定义：设函数 $f(x)$ 在点 a 处无限次可微，则该函数在 a 点的泰勒级数展开式为：

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$

其中，$f^{(n)}(a)$ 表示函数 f 在点 a 处的第 n 阶导数，$n!$ 是 n 的阶乘。

收敛性：泰勒级数的收敛性取决于函数的性质和展开点的选择。根据泰勒定理，如果函数 $f(x)$ 在包含 a 的某个开区间内无限次可微，则对于该区间内的任意 x，泰勒级数都收敛于 $f(x)$。收敛区间可以通过比值判别法、根值判别法等方法确定。

余项：泰勒级数的余项（R remainder）是实际函数值与泰勒级数部分和之间的差值。根据泰勒定理，余项 $R_n(x)$ 可以表示为：

$$R_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!}(x-a)^{n+1}$$

其中 c 是 a 和 x 之间的某个点。余项的存在说明了泰勒级数近似的误差。

应用：泰勒级数在求解复杂函数的近似值、计算定积分、求解微分方程以及在物理学中分析波动和场的传播等方面都有重要应用。通过泰勒级数，可以将难以直接求解的问题转化为多项式问题，从而简化计算。

特殊情形：当展开点 $a = 0$ 时，泰勒级数称为麦克劳林级数（Maclaurin series），它是泰勒级数的一个特例。

泰勒级数的引入，不仅丰富了数学分析的内容，也为解决实际问题提供了强有力的工具。通过对函数的局部线性化，泰勒级数在理论和应用上都显示出了其独特的价值。

泰勒展开式的基本形式:

$$f(x)=\sum_{k=0}^{n}\frac{f^{(n)}(0)}{n!}(x)^n \tag{3.1}$$

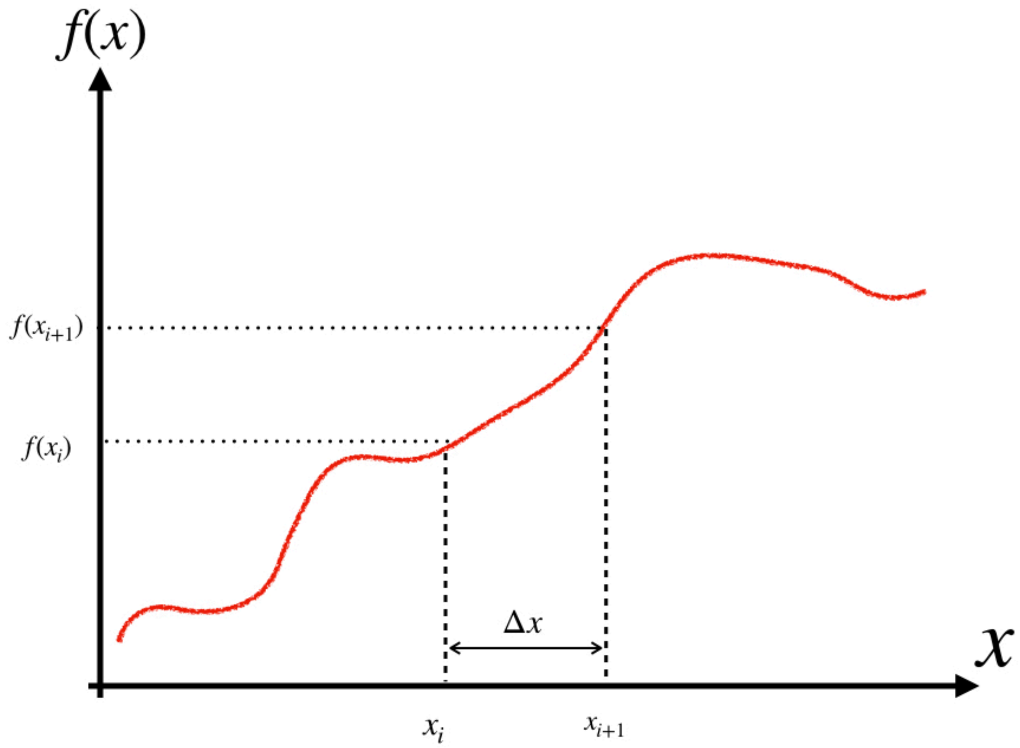


Figure 3.1: Taylor Series

根据泰勒展开式，通过 $f(x)$ 和其任意阶的导数，可以获得任意 Δx 值下的函数值 $f(x+\Delta x)$ ，即:

$$f(x+\Delta x)=f(x)+\frac{f'(x)}{1!}\Delta x+\frac{f''(x)}{2!}\Delta x^2+\frac{f'''(x)}{3!}\Delta x^3+\cdots+\frac{f^{(n)}(x)}{n!}(\Delta x)^n \tag{3.2}$$

或者在 $-\Delta x$ 位置，可写为:

$$f(x-\Delta x)=f(x)-\frac{f'(x)}{1!}\Delta x+\frac{f''(x)}{2!}\Delta x^2-\frac{f'''(x)}{3!}\Delta x^3+\cdots+\frac{f^{(n)}(x)}{n!}(-\Delta x)^n \tag{3.3}$$

以上公式也可以写为:

$$u_{i+1} = u_i + \frac{u_i^{'}}{1!}\Delta x + \frac{u_i^{''}}{2!}\Delta x^2 + \frac{u_i^{'''}}{3!}\Delta x^3 + \cdots + \frac{u_i^{(n)}}{n!}(\Delta x)^n \tag{3.4}$$

$$u_{i-1} = u_i - \frac{u_i^{'}}{1!}\Delta x + \frac{u_i^{''}}{2!}\Delta x^2 - \frac{u_i^{'''}}{3!}\Delta x^3 + \cdots + \frac{u_i^{(n)}}{n!}(-\Delta x)^n \tag{3.5}$$

3.1.1 截断误差

在泰勒级数的应用中，截断误差（truncation error）是一个重要的概念，它描述了当我们使用有限项的泰勒级数来近似一个函数时所产生的误差。

定义：截断误差是指在泰勒级数展开中，由于只取有限项而忽略剩余无限项所引起的误差，数学表达为 $O()$。具体来说，如果我们对函数 $f(x)$ 在点 a 处进行泰勒级数展开，并只取前 n 项，那么截断误差就是函数在 x 处的真实值与这 n 项部分和之间的差值。

$O(2)$ 和 $O(3)$ 分别表示为在泰勒展开式上的二阶和三阶导数上的误差。截取误差的阶数越高，误差越小。

数学表达：如果 $f(x)$ 在 a 处的泰勒级数为:

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(a)}{k!}(x-a)^k$$

那么，当我们取前 n 项时，截断误差 $T_n(x)$ 可以表示为:

$$O(n) = f(x) - \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k$$

余项的另一种形式：在泰勒定理中，余项 $R_n(x)$ 也可以用来描述截断误差。对于拉格朗日形式的余项，我们有:

$$R_n(x) = \frac{f^{(n+1)}(c)}{(n+1)!}(x-a)^{n+1}$$

其中 c 是 a 和 x 之间的某个点。这个余项提供了截断误差的一个上界，即:

$$|O(x)| \leq |R_n(x)|$$

$$O(1) = \frac{u_i^{''}}{2!}\Delta x^2 + \frac{u_i^{'''}}{3!}\Delta x^3 + \frac{u_i^{(4)}}{4!}\Delta x^4 + \cdots + \frac{u_i^{(n)}}{n!}(\Delta x)^n$$

$$O(2) = \frac{u_i^{'''}}{3!}\Delta x^3 + \cdots + \frac{u_i^{(n)}}{n!}(\Delta x)^n$$

$$O(3) = \frac{u_i^{(4)}}{4!}\Delta x^4 + \cdots + \frac{u_i^{(n)}}{n!}(\Delta x)^n$$

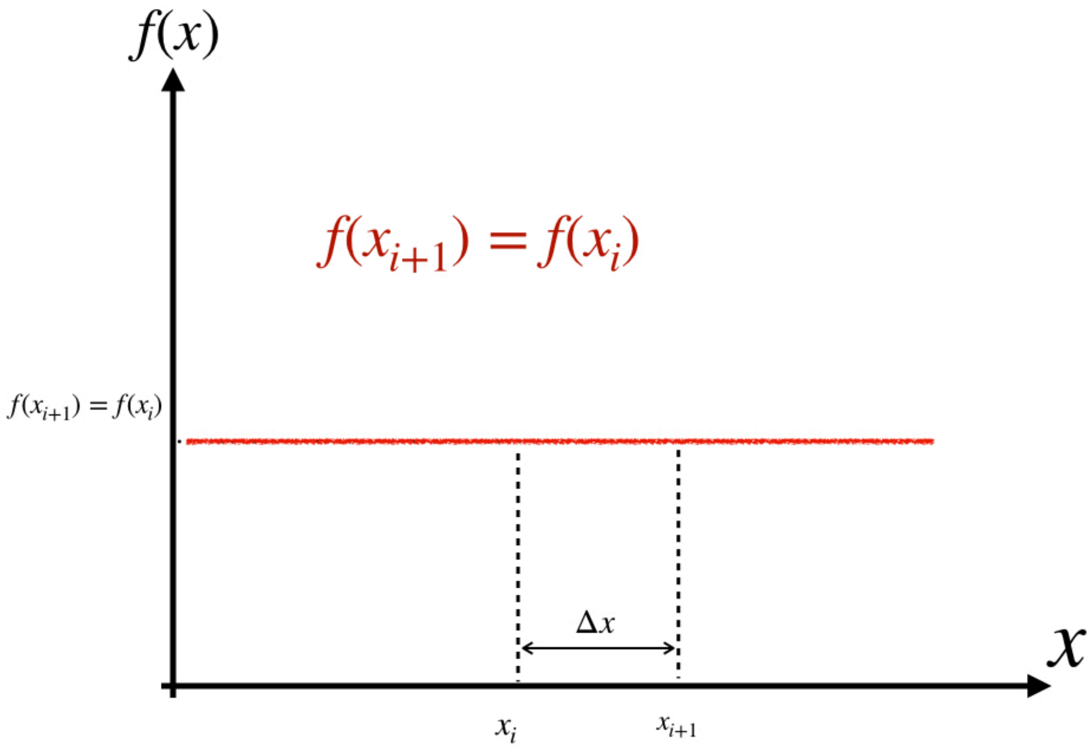
影响因素：截断误差的大小受到多个因素的影响，包括：1. 函数 $f(x)$ 在 a 附近的平滑性。2. 点 x 与展开点 a 之间的距离。3. 所取泰勒级数项数 n 的大小。

减小截断误差：为了减小截断误差，可以采取以下措施：1. 增加泰勒级数的项数 n。2. 选择更接近 x 的展开点 a。3. 选择一个更平滑的函数或者在更平滑的区间内进行展开。

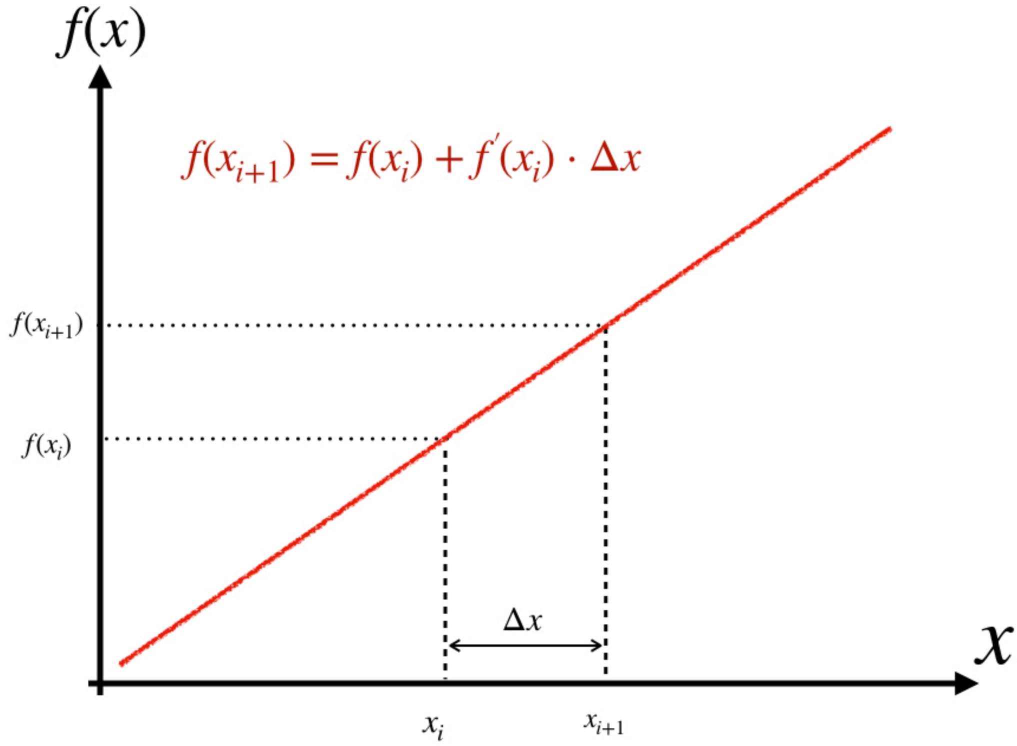
截断误差是评估泰勒级数近似效果的重要指标，对于数值计算和函数逼近的准确性具有重要意义。在实际应用中，理解和控制截断误差对于提高计算结果的可靠性至关重要。

何种情况下，泰勒展开式的截断误差为 **0**?

- $O(0) = 0$ 时，意味着：$f(x+\Delta x) = f(x)$。则该函数为 $f(x) = C$, C 为常数。如图：



- $O(1) = 0$ 时，意味着：$f(x+\Delta x) = f(x) + f^{'}(x)\cdot\Delta x$。则该函数为 $f(x) = ax + b$。如图：



如何依据泰勒级数，得到函数的一阶和二阶导数?

3.1.2 一阶导数

3.1.2.1 向前估计 (Forward Approximation)

采纳一阶截断误差，我们可将公式(3.2)写为:

$$f(x+\Delta x) = f(x) + \frac{f'(x)}{1!}\Delta x + O(1) \tag{3.6}$$

则:

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} \tag{3.7}$$

或者

$$u_i' = \frac{u_{i+1} - u_i}{\Delta x} \tag{3.8}$$

注：公式(3.8)隐含了 $O(1)$ 的误差。

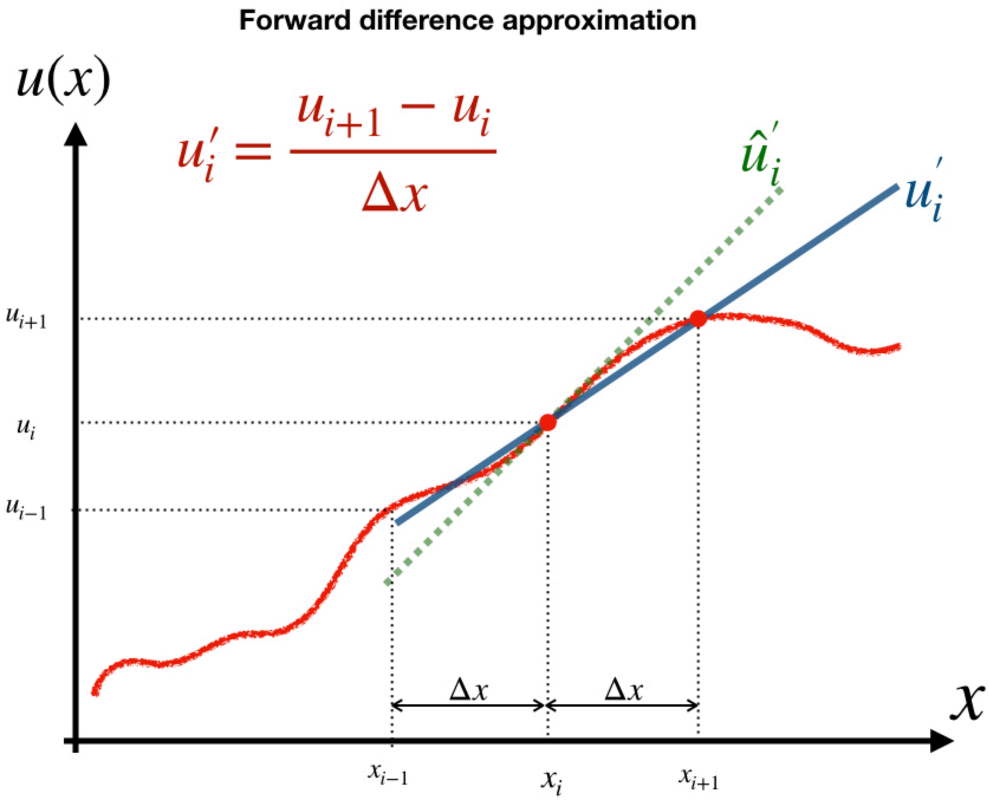


Figure 3.2: 向前估计

3.1.2.2 向后估计 (Backward Approximation)

采纳一阶截断误差，我们可将公式(3.3)写为：

$$f(x-\Delta x)=f(x)-\frac{f'(x)}{1!}\Delta x+O(1) \tag{3.9}$$

则：

$$f'(x)=\frac{f(x)-f(x+\Delta x)}{\Delta x} \tag{3.10}$$

或者

$$u_i'=\frac{u_i-u_{i+1}}{\Delta x} \tag{3.11}$$

注：公式(3.11)隐含了 $O(1)$ 的误差。

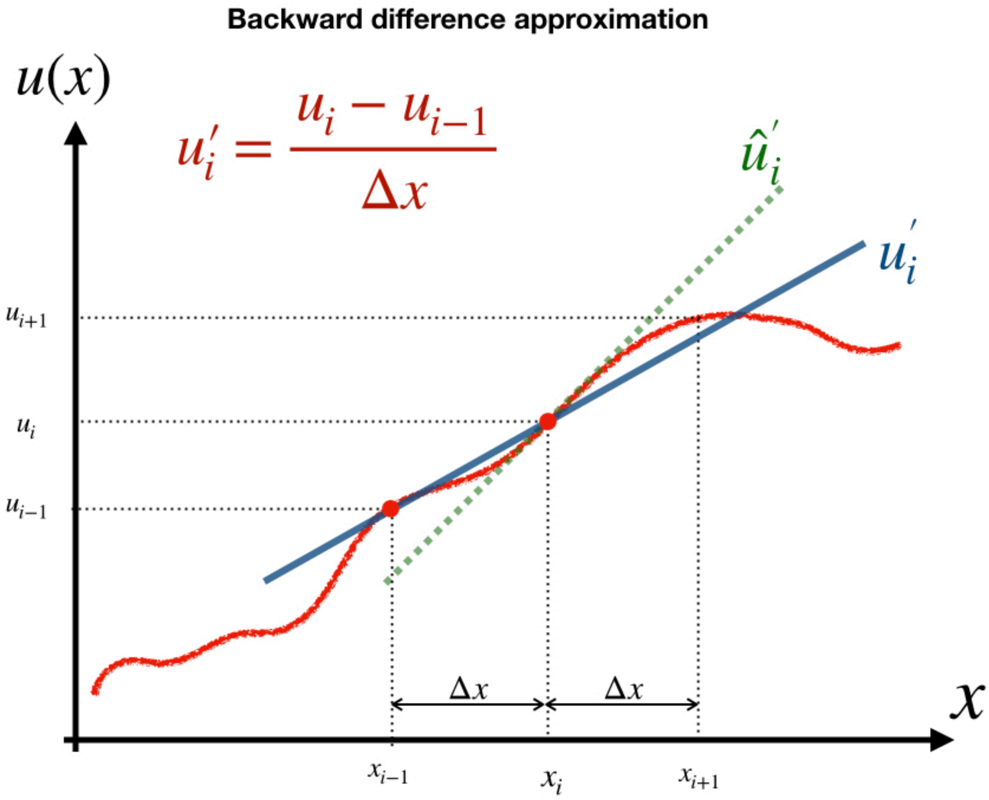


Figure 3.3: 向后估计

3.1.2.3 中心估计 (Central Approximation)

中心估计算法中，我们将从公式(3.2)减去公式(3.3)，得到：

$$f(x+\Delta x)-f(x-\Delta x)=0+2*\frac{f'(x)}{1!}\Delta x+0+2*\frac{f'''(x)}{3!}+\ldots$$

截断误差由以上公式右边的第四项（三阶导数）开始，则该公式的截取误差为 $O(2)$，即二阶精度的截取误差，公式表达为：

$$f(x+\Delta x)-f(x-\Delta x)=0+2*\frac{f'(x)}{1!}\Delta x+0+O(2)$$

可得到二阶精度的一阶导数的中心估计：

$$f'(x)=\frac{f(x+\Delta x)-f(x-\Delta x)}{2\Delta x} \tag{3.12}$$

或者

$$u_i'=\frac{u_{i+1}-u_{i21}}{2\Delta x} \tag{3.13}$$

公式(3.13)隐含了 $O(2)$ 的误差，同时(3.8)和(3.11)都隐含了 $O(1)$ 的误差。

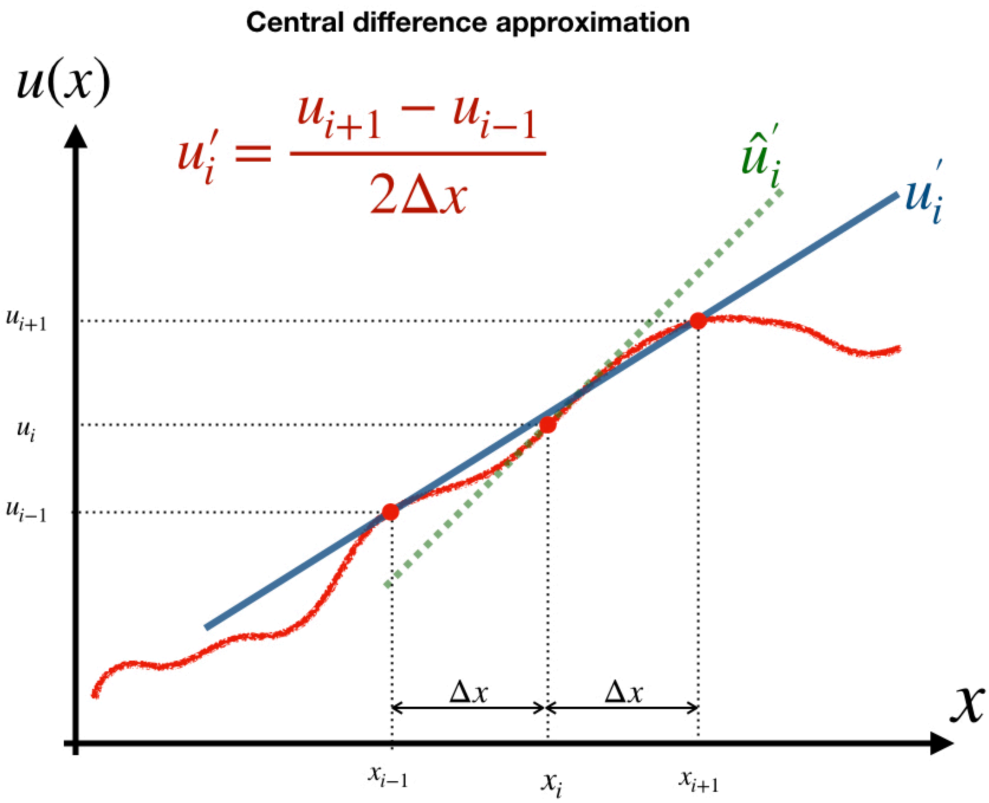


Figure 3.4: 中心估计

3.1.3 二阶导数

我们将公式 (3.2)和(3.3)相加，可得到：

$$f(x+\Delta x)+f(x-\Delta x)=2\cdot f(x)+0+2\cdot\frac{f^{''}(x)}{2!}\Delta x^2+0+2\cdot\frac{f^{(4)}(x)}{4!}\Delta x^4+\cdots \tag{3.14}$$

公式(3.14)来自公式 (3.2)和(3.3)的相加，三阶导数项在相加过程中为零，因此我们截取其三阶截取误差，则公式(3.14)可写为：

$$f(x+\Delta x)+f(x-\Delta x)=2f(x)+f^{''}(x)\Delta x^2+O(3) \tag{3.15}$$

根据公式(3.15)，我们可获得函数 $f(x)$ 在 x 位置的二阶导数为：

$$f^{''}(x)=\frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{\Delta x^2}+O(3) \tag{3.16}$$

当移除其三阶截断误差 $O(3)$ 后，我们得到近似的二阶导数：

$$\begin{align} f^{''}(x) &\approx \frac{1}{\Delta x}\left(\frac{f(x+\Delta x)-f(x)}{\Delta x}+\frac{f(x)-f(x-\Delta x)}{\Delta x}\right) \tag{3.17}\\ &\approx \frac{f(x+\Delta x)-2f(x)+f(x-\Delta x)}{\Delta x^2} \tag{3.18}\end{align}$$

将公式一般化，我们可写为以下形式：

$$\begin{align} u_i^{''} &\approx \frac{1}{\Delta x}\left(\frac{u_{i+1}-u_i}{\Delta x}-\frac{u_i-u_{i-1}}{\Delta x}\right) \tag{3.19}\\ &\approx \frac{u_{i+1}-2u_i+u_{i-1}}{\Delta x^2} \tag{3.20}\\ & \tag{3.21}\end{align}$$

3.2 构建数值方法

例 **3.1.** 一根 100cm 长的铁棍，初始温度 25 °C，在其左右两边分别持续施加 100°C 和 50°C 的温度。求解：任意时刻铁棍的温度分布。

参考信息：

- wiki:Thermal_diffusivity
- wiki:Heat_equation

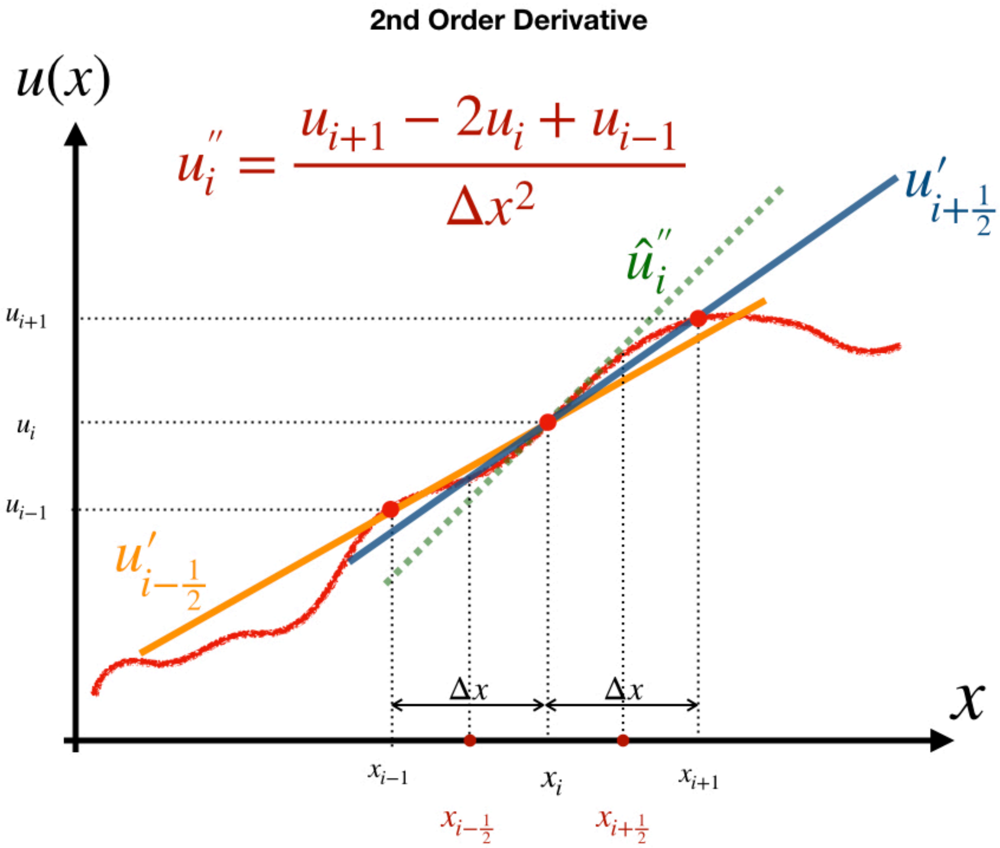
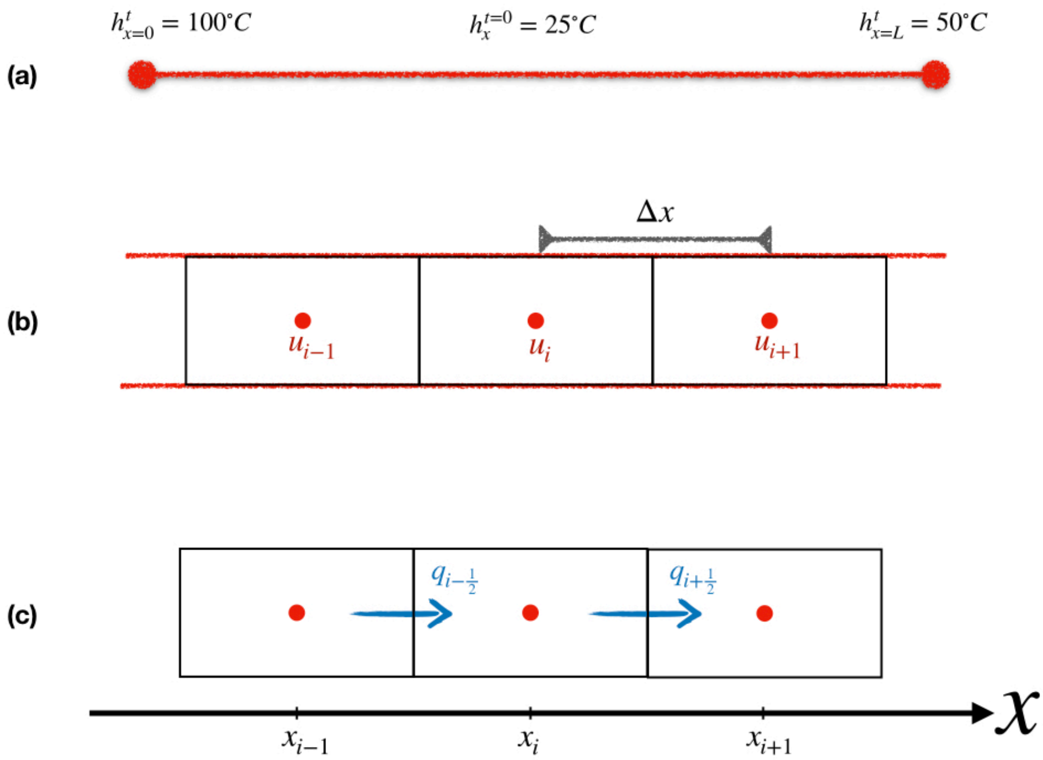


Figure 3.5: 二阶导数估计

为求解这个铁棍中的温度变化问题， @ref{modeling} 当中的方法，该方法总结为 CLAMS 方法：概念描述 (Conceptual model)、物理定律 (physic Laws)、假设 (Assumptions)、数学推导 (Math derivation)、求解 (Solver)。

1. 概念描述



   空间微分，如图。

2. 物理定律

   能量守恒：
   能量变化 = 能量流入 - 能量流出

$$\Delta E = Q_{in} - Q_{out}$$

3. 假设此问题的假设包括：

   1. 铁棍绝热，即两端之外的部分并不存在热传递作用。
   2. 忽略热辐射作用。
   3. 铁棍的介质/物理属性均一。

4. 数学推导

$$= \frac{}{}.$$

   - k - 热传导率 $[Wm^{-1}K^{-1}]$。

- c - 比热容 (specific heat capacity)$[Jkg^{-1}K^{-1}]$。
- ρ - 密度 $[kgm^{-3}]$。
- A - 截面积 $[m^2]$。
- D - 热力学扩散度（Thermal diffusivity）$D = \frac{k}{\rho c}$ $[m^2 s^{-1}]$。

$$\rho * c * \Delta x * A * \Delta u = q_{in} * A * \Delta t - q_{out} * A * \Delta t$$

两边同时除以 $\rho c \Delta x A$，得到

$$\frac{\Delta u}{\Delta t} = \frac{1}{\rho c} \frac{q_{in} - q_{out}}{\Delta x}$$

以上公式当 Δx 趋近与 0，Δt 趋近于 0 时，得到微分形式：

$$\frac{\partial u}{\partial t} = \frac{1}{\rho c} \frac{\partial q}{\partial x}$$

$$q = k \frac{\partial u}{\partial x}$$

则得到其控制方程：

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{1}{\rho c} \frac{\partial q}{\partial x} \\ &= \frac{1}{\rho c} \frac{k \frac{\partial u}{\partial x}}{\partial x} \\ &= D \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) \end{aligned} \tag{3.22}$$

令 $D = \frac{k}{\rho c}$，单位 $[ms^{-2}]$，则最终控制方程 (Governing Equation) 写为

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \tag{3.23}$$

控制方程，通常是我们关键数学/数值求解的核心对象，控制方程也是我们对问题最重要的描述，其中已经包含了问题的概念描述、假设、物理定律等信息。

5. 求解

这里我们使用数值方法对本问题进行求解。

由一阶泰勒级数可知，控制方程(3.23)左边 (Left Hand Side, LHS) 可写为：

$$\frac{\partial u}{\partial t} = D \frac{u_i^t - u_i^{t-1}}{\Delta t} + O(1)$$

控制方程(3.23)右边 (Right Hand Side, RHS) 可写为:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^{t-1} - 2u_i^{t-1} + u_{i-1}^{t-1}}{\Delta x} + O(2) \tag{3.24}$$

或者

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^{t} - 2u_i^{t} + u_{i-1}^{t}}{\Delta x} + O(2) \tag{3.25}$$

此时，方程左边在时间尺度上具有一阶截取误差，方程右边在空间尺度上具有二阶截断误差。省去误差项，离散化后控制方程写为:

$$\frac{u_i^t - u_i^{t-1}}{\Delta t} = D\frac{u_{i+1}^{t-1} - 2u_i^{t-1} + u_{i-1}^{t-1}}{\Delta x^2} \tag{3.26}$$

或者

$$\frac{u_i^t - u_i^{t-1}}{\Delta t} = D\frac{u_{i+1}^{t} - 2u_i^{t} + u_{i-1}^{t}}{\Delta x^2} \tag{3.27}$$

3.3 显式求解法

显式求解法以公式(3.26)作为起点，该公式可变形为:

$$u_i^t - u_i^{t-1} = \frac{D\Delta t}{\Delta x^2}\left(u_{i+1}^{t-1} - 2u_i^{t-1} + u_{i-1}^{t-1}\right)$$

令 $\alpha = \frac{D\Delta t}{\Delta x^2}$, $\beta = 1 - 2\alpha$，整理以上公式可得:

$$\begin{aligned} u_i^t - u_i^{t-1} &= \alpha\left(u_{i+1}^{t-1} - 2u_i^{t-1} + u_{i-1}^{t-1}\right) \\ u_i^t &= \alpha u_{i+1}^{t-1} + (1-2\alpha)u_i^{t-1} + \alpha u_{i-1}^{t-1} \\ u_i^t &= \alpha u_{i+1}^{t-1} + \beta u_i^{t-1} + \alpha u_{i-1}^{t-1} \end{aligned} \tag{3.28}$$

将以上公式应用于离散点上，

点号 i	公式
1	边界条件: $u_1^t = U_0$
2	$u_2^t = \alpha u_3^{t-1} + \beta u_2^{t-1} + \alpha u_1^{t-1}$
3	$u_3^t = \alpha u_4^{t-1} + \beta u_3^{t-1} + \alpha u_2^{t-1}$
4	$u_4^t = \alpha u_5^{t-1} + \beta u_4^{t-1} + \alpha u_3^{t-1}$
5	$u_5^t = \alpha u_6^{t-1} + \beta u_5^{t-1} + \alpha u_4^{t-1}$
...	...