算法简化描述

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非线性方程求根

线性方程组求解

微分方程数值解

- 3.1 龙格库塔 (Runge Kutta)
- 四阶龙格库塔 3.1.1

$$\frac{dy}{dx} = f(x,y), y(0) = y_0$$
 (3.1)

Algorithm 1 四阶龙格库塔

Require: f, y_0, h, n

- 1: **for** $i = 0, 1, \dots$ **do**

- $k_1 = f(x_i, y_i)$ $k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1h)$ $k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2h)$
- $k_4 = f(x_i + \bar{h}, y_i + k_3\bar{h})$
- $y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$

求解微分方程组.

最优化算法

4.1 直接搜索

指无需对目标函数求导的搜索方法, 比如 [4].

- 4.1.1 单纯形法 (Simplex Search Method)
- 4.2 梯度法 (Gradient Method)
- 4.2.1 梯度法 (Gradient Descent Method)

梯度法或称梯度下降法.

Algorithm 2 梯度法

Require: $x_0 \in \mathbf{R}^n$

- 1: **for** $k = 0, 1, \dots$ **do**
- $2: x_{k+1} = y_k t_k \nabla f(y_k)$

4.2.2 加速邻近梯度法 (Accelerated Proximal Gradient Method, APG)

此方法由 Nesterov[2] 首先提出.

Algorithm 3 加速邻近梯度法 [2, 1]

Require: $x_0 \in \mathbb{R}^n, y_0 = x_0, \theta_0 = 1, q \in [0, 1]$

- 1: **for** $k = 0, 1, \dots$ **do**
- $2: x_{k+1} = y_k t_k \nabla f(y_k)$
- 3: $\theta_{k+1}^2 = (1 \theta_{k+1})\theta_k^2 + q\theta_{k+1}, \theta_{k+1} \in (0,1), \ \Re \theta_{k+1}$
- 4: $\beta_{k+1} = \theta_k (1 \theta_k) / (\theta_k^2 + \theta_{k+1})$
- 5: $y_{k+1} = x_{k+1} + \beta_{k+1}(x_{k+1} x_k)$

其中, $\theta_{k+1} \in (0,1)$ 见文献 [1] 91 页. 当 q=1 时, 该算法为梯度法.

4.2.3 自适应重启加速梯度法

加速邻近梯度法 (算法3) 迭代到一定程度时, 外推系数 β_k 趋于 0, 算法退化成梯度法. 使用该算法自适应的重置参数, 能够保持加速邻近梯度法的快速收敛.

Algorithm 4 自适应重启加速梯度法 [3]

Require: $x_0 \in \mathbf{R}^n, y_0 = x_0, \theta_0 = 1$

- 1: **for** $j = 0, 1, \dots$ **do**
- 2: 取 q = 0 执行算法3, 直到 $f(x_k) > f(x_{k+1})$ 时停止 (或可以在 $\nabla f(y_{k-1})^T(x_k x_{k-1})$ 时停止, 两者选其中一种)
- 3: $x_0 = x_k, y_0 = x_k, \theta_0 = 1$

随机搜索

- 5.1 遗传算法 (Genetic Algorithm, GA)
- 5.2 粒子群算法 (Particle Swarm Optimization, PSO)

数据分析

6.1 聚类

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