算法简化描述

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List of Algorithms

Chapter 1

微分方程数值解

Problem 1 (带初值常微分方程)

$$\begin{cases} \frac{dy}{dx} = f(x, y) \\ y(0) = y_0 \end{cases} \tag{1.1}$$

1.1 龙格库塔 (Runge Kutta)

1.1.1 四阶龙格库塔

Algorithm 1 四阶龙格库塔

Require: f, y_0, h, n

for $i = 0, 1, \ldots$ **do**

  $k_1 = f(x_i, y_i)$

  $k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$

  $k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h)$

  $k_4 = f(x_i + h, y_i + k_3 h)$

  $y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$

end for

求解微分方程组.

Chapter 2

最优化算法

Problem 2 (无约束极小化)

$$\min_x f(x) \tag{2.1}$$

2.1 停止准则

2.2 步长

2.2.1 Backtracking Search

2.3 直接搜索

指无需对目标函数求导的搜索方法, 比如文献 [4] 中的方法.

2.3.1 单纯形法 (Simplex Search Method)

2.4 梯度法 (Gradient Method)

2.4.1 梯度法 (Gradient Descent Method)

梯度法或称梯度下降法.

2.4.2 加速邻近梯度法 (Accelerated Proximal Gradient Method)

此方法由 Nesterov[2] 首先提出. 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.

Algorithm 2 梯度法

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

1: **for** $k = 0, 1, \ldots$ **do**

2: $\quad x_{k+1} = y_k - t_k \nabla f(y_k)$

3: **end for**

Algorithm 3 加速邻近梯度法 [2, 1](APG)

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

1: **for** $k = 0, 1, \ldots$ **do**

2: $\quad x_{k+1} = y_k - t_k \nabla f(y_k)$

3: $\quad \theta_{k+1}^2 = (1 - \theta_{k+1})\theta_k^2 + q\theta_{k+1}, \theta_{k+1} \in (0, 1)$, 求解 θ_{k+1}

4: $\quad \beta_{k+1} = \theta_k(1 - \theta_k)/(\theta_k^2 + \theta_{k+1})$

5: $\quad y_{k+1} = x_{k+1} + \beta_{k+1}(x_{k+1} - x_k)$

6: **end for**

2.4.3 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 (算法2). 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** $j = 0, 1, \ldots$ **do**

2: $\quad$ 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: $\quad x_0 = x_k, y_0 = x_k, \theta_0 = 1$

4: **end for**

2.5 牛顿法及拟牛顿法

2.5.1 Broyden–Fletcher–Goldfarb–Shanno Algorithm(BFGS)

Bibliography

[1] Yu Nesterov. Introductory lectures on convex programming volume i: Basic course. *Lecture notes*, 1998.

[2] Yurii Nesterov. A method of solving a convex programming problem with convergence rate O(1/k2). In *Soviet Mathematics Doklady*, volume 27, pages 372–376, 1983.

[3] Brendan O'Donoghue and Emmanuel Candès. Adaptive restart for accelerated gradient schemes. *Foundations of computational mathematics*, 15(3):715–732, 2015.

[4] Oliver Schütze, Adriana Lara, and CA Coello Coello. The directed search method for unconstrained multi-objective optimization problems. *Proceedings of the EVOLVE–A Bridge Between Probability, Set Oriented Numerics, and Evolutionary Computation*, pages 1–4, 2011.