示踪实验确定河流纵向离散系数的单纯形加速法

张江山

（福建师范大学环境科学研究所，福州　350007）

摘要　应用单纯形加速法结合实例求出福建闽江干流富屯溪洋口段纵向离散系数 $D_L=2.62\mathrm{m^2/s}$。研究结果表明，该法用于估计非线性模型参数优于"非线性逼近法"。由于单纯形法寻优过程不需要计算目标函数的偏导数，不受模型复杂程度的限制，因而计算简便，可广泛应用于环境、生态模型的拟合和参数估计。

关键词　河流水质模型，参数估计，纵向离散系数，单纯形加速法。

天然河流的纵向离散系数和横向混合系数是反映河流混合输移过程特性的2个主要参数。研究和确定它们的数值是建立河流水质模型，进行水质预测和水环境规划等必不可少的关键步骤。关于河流纵向离散系数的识别，清华大学等单位在《沱江水环境容量研究》(国家"六五"科技攻关项目)中所推荐的方法——非线性逼近法，是利用示踪研究数据估算河流纵向离散系数的一种好方法[1]。笔者曾应用该方法计算闽江干流富屯溪洋口段的纵向离散系数 $D_L=2.641\mathrm{m^2/s}$[2]，本文用单纯形加速法求得该河段纵向离散 $D_L=2.622\mathrm{m^2/s}$，两者颇为接近。相比之下，单纯形加速法的优点是：①不必计算目标函数的偏导数，只需计算目标函数的函数值，计算较为简便；②对于各种模型，不论是单参数还是多参数模型，不论其复杂程度如何，其计算过程十分相似，可以编制通用计算程序。因此可以预料，单纯形加速法对于生态、环境科学中非线性模型的拟合和模型参数的识别具有广泛的适用性。

1　单纯形加速法基本原理和计算方法

单纯形加速法是一种优化方法，它是由Nalder和Mead(1964)首先提出，被认为是优秀的非线性优化技术之一[3,4]。其突出的优点是优化过程不必计算函数的偏导数，仅需计算函数值，而且收敛性好。

所谓单纯形是指 n 维空间 E^n 中具有 $n+1$ 个顶点的凸多面体。设 $X_0,X_1,\cdots\cdots,X_n$ 为 E^n 中的 $n+1$ 个点，若 n 个向量 $X_1-X_0,X_2-X_0,\cdots\cdots X_n-X_0$ 线性无关，则这 $n+1$ 个点可取为 E^n 中一个单纯形的顶点。单纯形加速法寻优的基本思想是：对 n 维空间中 $n+1$ 个点(它们构成单纯形的顶点)的函数值进行比较，去掉其中最坏的点，代之以新的点，构成新的单纯形，反复迭代逐步逼近目标函数极小值点，具体步骤如下：

(1)给定初始单纯形，其顶点：

$$X_i\in E^n,\qquad i=0,1,2,\ldots,n$$

计算目标函数值：

$$f(x_i),\qquad i=0,1,2,\ldots,n$$

(2)确定最高点 X_h，次高点 X_g，最低点 X_l，使得：

$$f(X_h)=\max\{f(X_0),f(X_1),\ldots,f(X_n)\}$$

$$f(X_g)=\max\{f(X_i)\mid X_i\neq X_h\}$$

$$f(X_l)=\min\{f(X_0),f(X_1),\ldots,f(X_n)\}$$

计算除 X_h 外 n 个点的形心 $\overline{X}$，令：

$$\overline{X}=\frac{1}{n}\Big[\sum_{i=0}^{n}X_i-X_h\Big]$$

计算 $f(\overline{X})$。

(3)进行反射，令：

$$X_{n+1}=\overline{X}+\alpha(\overline{X}-X_h)$$

其中，$\alpha>0$ 为给定的反射系数，X_{n+1} 是 X_h 关于 $\overline{X}$ 的反射点。计算 $f(X_{n+1})$。

(4)若 $f(X_{n+1})<f(X_l)$，则进行扩展，令：

$$X_{n+2}=\overline{X}+\gamma(X_{n+1}-\overline{X})$$

其中，$\gamma>1$ 为给定的扩展系数，计算 $f(X_{n+2})$，转步(5)；若：

$$f(X_l)\leqslant f(X_{n+1})\leqslant f(X_g)$$

则置 $X_h=X_{n+1}$，$f(X_h)=f(X_{n+1})$，转步(7)；若：

1993年7月26日收到修改稿

$$f(X_{n+1}) > f(X_g)$$

则进行压缩，记：

$$f(X_{h'}) = \min\{f(X_h), f(X_{n+1})\}, h' \in \{h, n+1\}$$

并令：

$$X_{n+3} = \bar{X} + \beta(X_{h'} - \bar{X})$$

其中，$0<\beta<1$ 为给定的压缩系数，计算 $f(X_{n+3})$，转步(6)。

(5)若 $f(X_{n+2})<f(X_{n+1})$，则置 $X_h=X_{n+2}$，$f(X_h)=f(X_{n+2})$，转步(7)；否则置 $X_h=X_{n+1}$，$f(X_h)=f(X_{n+1})$，转步(7)。

(6)若 $f(X_{n+3})\leqslant f(X_{h'})$，则置 $X_h=X_{n+3}$，$f(X_h)=f(X_{n+3})$；否则进行收缩，令：

$$X_i = X_i + \frac{1}{2}(X_l - X_i), i = 0,1,2,\ldots,n$$

计算 $f(X_i)$，$i=0,1,2,\cdots\cdots,n$，转向步(7)。

(7)检验是否满足收敛准则。设 $\varepsilon>0$ 为给定的控制误差，若：

$$\left\{\frac{1}{n+1}\sum_{i=0}^{n}[f(X_i) - f(\bar{X})]^2\right\}^{\frac{1}{2}} < \varepsilon$$

则停止计算，现行最好点可作为极小点的近似；否则返回步(2)。

2 单纯形加速法识别河流纵向离散系数

河流纵向离散系数的示踪实验，示踪剂溶液采用瞬时源投放方式。假定 $c(x,t_i)$ 为某断面示踪剂实测浓度，断面与投放断面的距离为 x，从投放到采样的时间为 $t_i(i=1,2,\ldots m)$，则断面示踪剂浓度随时间的变化规律可用如下函数来拟合：

$$\tilde{c}(x,t) = \frac{M}{\sqrt{4\pi D_L t}}\exp\left[-\frac{(x-ut)^2}{4D_L t}\right] \quad (1)$$

式中，$\tilde{c}$ 为采样断面处理论示踪剂浓度；M 为单位面积示踪物质投放量；x 为投放断面与采样断面的距离；u 为示踪实验河段平均纵向流速；D_L 为示踪实验河段纵向离散系数，令：

$$\frac{M}{\sqrt{4\pi D_L}} = A \quad (2)$$

$$\frac{u^2}{4D_L} = B \quad (3)$$

$$\frac{x}{u} = T \quad (4)$$

代入(1)式便得：

$$\tilde{c}(x,t) = \frac{A}{\sqrt{t}} - \exp\left[-\frac{B(T-t)^2}{t}\right] \quad (5)$$

将 A、B 和 T 视作待定参数，目的是寻找最佳的参数向量(A、B、T)，使实测浓度系列 $c(X,t_i)$ 与理论浓度系列 $\tilde{c}(x,t_i)$ 差的平方和最小，即使得目标函数为最小。

$$E = \sum_{i=1}^{m}(c_i - \tilde{c}_i)^2 = \sum_{i=1}^{m}\left\{c_i - \frac{A}{\sqrt{t_i}}\exp\left[-\frac{B(T-t_i)^2}{t_i}\right]\right\}^2 \quad (6)$$

一旦确定出最佳参数向量(A、B、T)，则由(3)和(4)两式即可推算出河段的纵向离散系数 D_L。

下面根据单纯形加速法来计算河流纵向离散系数，并与非线性逼近法的计算结果加以对照。

1987年1月13日笔者在闽江干流富屯溪洋口段进行玫瑰精投放示踪实验。示踪剂瞬时投放量为11kg，投放断面设在石溪，采样断面设在将军阁，两断面相距2000m，实测纵向平均流速0.16m/s。采样时间间隔为7.5min，高浓度染团经过时段改为每隔5min取样一次，不同时刻示踪剂实测浓度列于表1。

确定河流纵向离散系数的单纯形法的目标函数 $E(t;A,B,T)$ 的表达式如(6)式所示，实测浓度 c_i 见表1。

表1 不同时刻示踪剂实测浓度

t_i(min)	150	157.5	165	172.5	180	185	190	195	200	205	
$c_i(10^{-6})$	0.13	0.27	1.20	5.06	5.19	17.74	17.61	19.40	16.42	16.16	
t_i(min)	210	217.5	225	232.5	240	247.5	255	262.5	270	277.5	285
$c_i(10^{-6})$	14.27	11.30	10.37	8.51	6.11	5.06	7.05	6.91	4.79	3.06	2.93

为了给单纯形法提供初值(A_0,B_0,T_0),以加速运算收敛速度。将(5)式两边同乘 $\sqrt{t}$,取对数后进行多元线性回归,可求得:

$\theta_0=(A_0,B_0,T_0)=(252.2323,\ 0.1477,\ 219.6137)$,再取三维参数空间的另外3个点:

$$\theta_1=(A_0+4a,B_0+a,T_0+a)$$
$$\theta_2=(A_0+a,B_0+4a,T_0+a)$$
$$\theta_3=(A_0+a,B_0+a,T_0+4a)$$

其中,a 的值视具体问题而定,本计算取 $a=0.1$。以 $\theta_0,\theta_1,\theta_2$ 和 θ_3 作为初始单纯形的顶点,取反射系数 $\alpha=1$,扩展系数 $\gamma=2$,压缩系数 $\beta=1/2$,误差控制 $\varepsilon=0.0001$。按单纯形法计算步骤编成计算程序。经128次迭代计算,最终求得最佳参数值:$A=237.3612,B=0.1509,T=205.2412$。由(4)式得:

$$u=\frac{x}{T}=\frac{2000}{205.2412}=9.7446(\mathrm{m/min})=0.1624(\mathrm{m/s})$$

由(3)式得:

$$D_L=\frac{u^2}{4B}=\frac{(0.1624\times60)^2}{4\times0.1509}=157.319(\mathrm{m^2/min})=2.622(\mathrm{m/s})$$

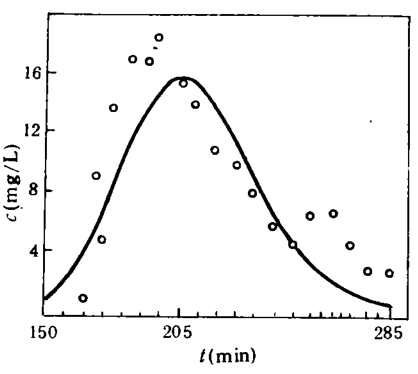

图1 实测浓度与数字模拟曲线

本文用单纯形加速法求得富屯溪洋口段平均流速0.1624m/s,与当时实测流速0.16m/s基本符合。而单纯形法计算得到该河段纵向离散系数 $D_L=2.622\mathrm{m^2/s}$,与非线性逼近法计算结果[2] $D_L=2.641\mathrm{m^2/s}$ 颇为接近,两者相对误差不超过1%。

经验证,本方法确定的示踪剂浓度随时间变化模拟曲线与实测浓度值拟合较好(见图1),相关系数达0.93,说明用单纯形加速法求得的纵向离散系数基本符合实际情况。

3 结语

本文阐述了应用单纯形加速法计算河流纵向离散系数的原理、方法、步骤,并用实例加以验证,结果令人满意。实践证明,单纯形优化方法的精度优于人们常用的对原模型先线性化后拟合的方法。与其它一些优化方法相比,它具有计算简便,收敛性好,适用性广等优点。由于单纯形法只需计算目标函数的函数值而不必计算其偏导数,从而避免了繁琐计算。而且,对各种模型寻优过程十分相似,便于编制统一的计算程序。可以断言,单纯形加速法不仅可用于确定河流混合输移参数,它在环境、生态模型的参数识别,非线性解析模型的拟合等方面都将有广泛的应用。

但需要指出的是,在单纯形法计算中,初始单纯形的选择是十分重要的,选择不当,可能使迭代过程发散,关于初始单纯形的选择,最保守,也是最可靠的方法是用"线性化"模型拟合所取得的参数向量粗估值作为初始单纯形的一个顶点,其余的顶点可参考文献[5]的方法来确定。

参考文献

1 清华大学等. 中国环境科学. 1986,6(3):8

2 方秋贤,张江山. 福建师大学报. 1987,3(4):83

3 范鸣玉. 最优化技术基础. 北京:清华大学出版社,1982

4 Nelder J A & R Mead. The computer Journal. 1975,7:308

5 席少霖,赵风治. 最优化计算方法. 上海:科学技术出版社,1983:178

An anomalous phenomenon was discussed, in which it was found from a calculation of the allowable discharge levels of water pollutants in the Huainan reaches of the Huaihe River that there was a large flow of water with a small allowable capacity of pollutant discharge. A quantitative analysis for the causes of this problem was made, based on the mechanism of forming the capacity of the river to receive pollutants and on the equations for calculating the discharge of pollutants. Finally, the reaches of the Huaihe River in Huainan city were taken as an example to preliminarily study how can identify and determine the design flow of a river.
Key words: allowable discharge level, water pollutants, design flow.

Grey Systems Analysis of the Factors Affecting the Efficiency of Wastewater Treatment in Anearobic Reactors. Guo Jingsong, Long Tengrui (Dept. of Urban Construction, Chongqing Institute of Architecture and Engineering, Chongqing 630045): *Chin. J. Environ. Sci.*, **15** (4), 1994, pp. 62—65
The methods for grey systems analysis have been applied to studying the significance of each of major factors that would affect the efficiency of anearobic reactors in treating wastewater. The data from the experiments in an anearobic fluidized bed reactor were taken as an example to make a calculation analysis, resulting in a conclusion which was consistent with that based on a theoretical analysis. The results show that the use of a grey systems analysis for the factors affecting the efficiency of a biological reactor has the advantage of requiring relatively less data, as compared with other methods.
Key words: grey system, interference analysis, efficiency of wastewater treatment, anaerobic reactor, fluidized bed.

Accelerated Simplex Algorithm to Determine the Longitudinal Dispersion Coefficient in a River by Tracer Test. Zhang Jiangshan (Institute of Environmental Science, Fujian Normal University, Fuzhou 350007): *Chin. J. Environ. Sci.*, **15** (4), 1994, pp. 66—68
The accelerated simplex algorithm has been used to calculate the longitudinal dispersion coefficient in a river, as an example for which the Ynagkou reaches of the Futunxi River, a mainstream of the Minjiang River in Fujian province, was found to have a longitudinal dispersion coefficient D_2 of 2.62 m^2/s. The results show that the accelerated simplex algorithm was more effective to be used for evaluating the parameters for a nonlinear model than the nonlinear approach algorithm. This was simply because the accelerated simplex algorithm had a process of optimization in which it was not necessary to calculate the partial derivative of the goal function and was not limited by the complexity of a model so that it was easy to be calculated and widely applicable. This algorithm could be widely used to fit environmental and ecological models and to make parameters evaluation.
Key words: river water quality model, parameter estimation, longitudinal dispersion coefficient, accelerated simplex algorithm.

Effects of Fumigation with sulfur Dioxide, Nitrogen Dioxide, Ozone and Mixtures Thereof on Ethylene Emissions from Rice. Yu Fei et al. (Nanjing Institute of Environmental Sciences, NEPA, Nanjing 210042): *Chin. J. Environ. Sci.*, 15 (4), 1993, **pp.** 69—71
A study was carried out on the effects of fumigation with sulfur dioxide (SO_2), nitrogen dioxide (NO_2), ozone (O_3) and mixtures thereof on the release of ethylene from rice plant being fumigated. It was found that the emission of ethylene as an internal hormone of plant increases when the crop rice is fumigated with SO_2, NO_2, O_3, or mixtures thereof. This can be considered as an indicator for the level of environmental pollution. If the O_3 level is constant, the emission of ethylene from rice is directly proportional to the levels of SO_2 and NO_2 in fumigating gases, where $O_3 + SO_2$ have a greater effect on the emission of ethylene from rice than $O_3 + NO_2$. If the total level of both SO_2 and NO_2 altogether is kept constant, an increased level of SO_2 can lead to a higher emission of ethylene than an increased level of NO_2. A fumigation with NO_2 at a concentration of 4 ppm for 2 hours has caused the leaves of rice to have bleached or yellow spots when ethylene and ethane are released at 7.70 and 2.30 nl/g • F • W • h, respectively.
Key words: rice, sulfur dioxide, nitrogen dioxide, ozone, fumigation, ethylene, ethane, release.

Watercolumn Barometer without Mercury Contamination. Zhang Xiong (Dept. of Physics, Yunnan Normal University, Kunming 650092): *Chin. J. Environ. Sci.*, **15**(4), 1994, pp. 72—74
A miniatured (1.2 m long) watercolumn barometer has been developed to solve the environmental problem of mercury pollution resulted from the production and opreation of a mercury column barometer. The working principles, use methods and measurement errors of the watercolumn barometer were discussed and some aspects of its application were briefly described. This barometer can work well at 0—3 km above sea level and at an ambient temperature in the range of 6—40℃. The results from its measurement have a standard error of less than ±0.9 mmHg and it can detecct a change in atmospheric pressure of ±0.1 mmHg. This newly developed barometer is applicable to measure the atmospheric pressure in a room where there will be a less change in ambient temperature. A conventional watercolumn barometer is very difficult to be used to measure the atmospheric pressure because the pressure of saturated water vapor varies largely with a change in room temperature. The use of this new barometer can also solve this problem.