11. 1stOpt 复合数据微分方程拟合求解

对一般微分方程拟合求解，1stOpt 有非常好的表现，不论在易用性还是效果方面，但如果拟合数据不是针对各特定微分项，而是不同微分项的组合，即复合数据，此时该如何处理呢？下面以实际案例进行求解演示。

11.1 一般微分方程拟合

有如下微分方程组及对应的数据，试通过微分方程拟合求解参数 k1，k2 及 k3.

$$
\begin{cases}
\dfrac{dy_1}{dx} = k_1 \cdot y_1 \\
\dfrac{dy_2}{dx} = k_1 \cdot y_1 - k_2 \cdot y_2 \\
\dfrac{dy_3}{dx} = k_2 \cdot y_2 - k_3 \cdot y_3 \\
\dfrac{dy_4}{dx} = k_1 \cdot y_1 + k_2 \cdot y_2 + k_3 \cdot y_3
\end{cases}
\tag{11-1}
$$

表 11.1. 数据一

x	0,3,28,53,78,103,183,303,463,603
y1	0.9922,0.9602,0.8352,0.5316,0.2798,0.1241,0.0175,0.0000,0.0000,0.0000
y4	0.0000,0.0169,0.0746,0.2409,0.4348,0.6058,0.7922,0.8666,0.8777,0.8799

这是非常一般的微分方程拟合问题，1stOpt 的求解代码、结果及计算对比图如下。

求解代码 11-1

```
Parameter k1,k2,k3 ;
Variable x,y1,y4;
ODEFunction y1'=k1*y1;
                y2'=k1*y1-k2*y2;
                y3'=k2*y2-k3*y3;
                y4'=k1*y1+k2*y2+k3*y3;
Data;
x=0,3,28,53,78,103,183,303,463,603;
y1=0.9922,0.9602,0.8352,0.5316,0.2798,0.1241,0.0175,0.0000,0.0000,0.0000;
y4=0.0000,0.0169,0.0746,0.2409,0.4348,0.6058,0.7922,0.8666,0.8777,0.8799;
```

结果：

```
Root of Mean Square Error (RMSE): 0.0534684363911388
Sum of Squared Residual: 0.0514597264220387
```

Correlation Coef. (R): 0.99123884813378
R-Square: 0.982554454049584
Adjusted R-Square: 0.972185194193075
Determination Coef. (DC): 0.977613829576524
F-Statistic: 18.3132100973571

Parameter   Best Estimate
-------------------- -------------
k1   -0.0141381652046682
k2   0.0362911502939322
k3   0.0109004605986451
y2 Initial Value   -2.22151839040572
y3 Initial Value   8.29247048065614

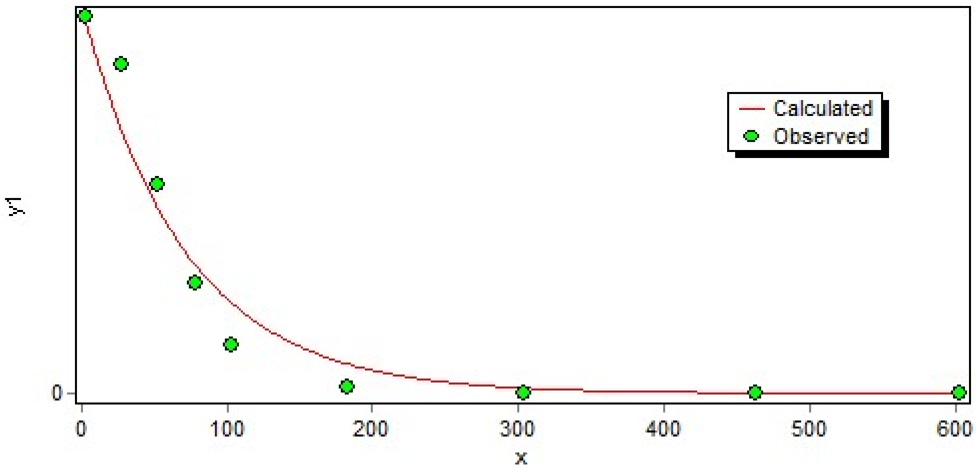

图 11.1 微分方程 y1 拟合计算对比图

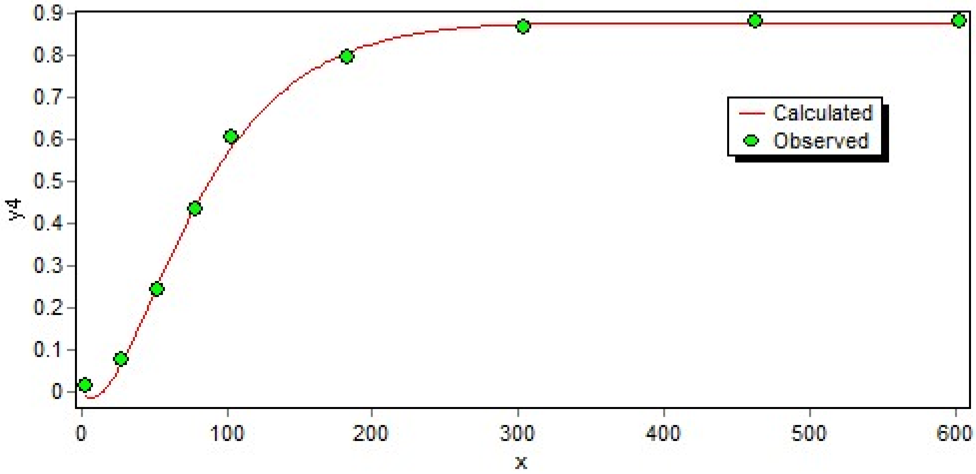

图 11.2 微分方程 y4 拟合计算对比图

11.2 复合数据微分方程拟合

假如微分方程组形式与前相同而数据只知道 y1 与 y4 之和，如下，同时已知 y1 和 y4 的初值分别为 0.9922 和 0.0.

表 11.2. 数据二

x	0,3,28,53,78,103,183,303,463,603
y1+y4	0.9922,0.9771,0.9098,0.7725,0.7146,0.7299,0.8097,0.8666,0.8777,0.8799

因为 y1+y4 的数据无法分拆成独立的 y1 和 y4 数据，因此不可能像前节按一般微分方程拟合那样计算，这种问题该如何处理呢？此时可引入一个新的变量 y5。

令：

$$y_5 = y_1 + y_4 \tag{11-2}$$

两边求导，有：

$$y_5' = y_1' + y_4' \tag{11-3}$$

此时微分方程组变为：

$$\begin{cases} \dfrac{dy_1}{dx} = k_1 \cdot y_1 \\ \dfrac{dy_2}{dx} = k_1 \cdot y_1 - k_2 \cdot y_2 \\ \dfrac{dy_3}{dx} = k_2 \cdot y_2 - k_3 \cdot y_3 \\ \dfrac{dy_4}{dx} = k_1 \cdot y_1 + k_2 \cdot y_2 + k_3 \cdot y_3 \\ \dfrac{dy_5}{dx} = \dfrac{dy_1}{dx} + \dfrac{dy_4}{dx} \end{cases} \tag{11-4}$$

这样就可以按照一般微分方程拟合去计算了。

求解代码 11-2

```
Parameter k1,k2,k3;
InitialODEValue x=0,y1=0.9922,y4=0,y5=0.9922;
Variable x,y5;
ODEFunction y1'=k1*y1;
            y2'=k1*y1-k2*y2;
            y3'=k2*y2-k3*y3;
            y4'=k1*y1+k2*y2+k3*y3;
            y5'=y1'+y4';
Data;
x=0,3,28,53,78,103,183,303,463,603;
y5=0.9922,0.9771,0.9098,0.7725,0.7146,0.7299,0.8097,0.8666,0.8777,0.8799;
```

注意上述代码中的“InitialODEValue x=0,y1=0.9922,y4=0,y5=0.9922;”，是给已

知起始值的微分项赋值，如果不用该句，也可用如下代码，效果一样，即用“Variable”定义“x,y1,y4,y5”四个变量，对应的数据跟在“Data;”后，已知数据给出，未知数据用“NAN”表示。

求解代码 11-3

```
Parameter k1,k2,k3;
Variable x,y1,y4,y5;
ODEFunction y1'=k1*y1;
            y2'=k1*y1-k2*y2;
            y3'=k2*y2-k3*y3;
            y4'=k1*y1+k2*y2+k3*y3;
            y5'=y1'+y4';
Data;
x=0,3,28,53,78,103,183,303,463,603;
y1=0.9922,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN;
y4=0,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN;
y5=0.9922,0.9771,0.9098,0.7725,0.7146,0.7299,0.8097,0.8666,0.8777,0.8799;
```

结果：

```
Root of Mean Square Error (RMSE): 0.00940056092631382
Sum of Squared Residual: 0.000883705457293381
Correlation Coef. (R): 0.894478947584556
R-Square: 0.800092587671975
Adjusted R-Square: 0.88532235210663
Determination Coef. (DC): 0.886887791400166
F-Statistic: 73.6570830923427

Parameter            Best Estimate
-------------------- -------------
k1      -0.0329169165549509
k2      0.046121173464352
k3      0.0132797805608404
y2 Initial Value    0.951345175784998
y3 Initial Value    1.95592365106421
```

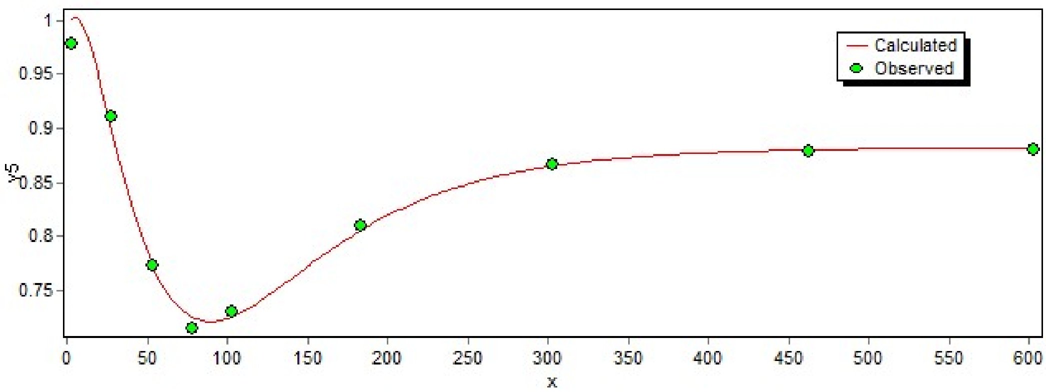

图 11.3 微分方程复合数据 y5 拟合计算对比图

11.3 乘法组合数据微分方程拟合

上节中已知数据是 y1 和 y2 之和，如下，假如数据是 y1 和 y4 的乘积，y1 和 y4 的初值仍分别为 0.9922 和 0.0，此时又该如何处理呢？

表 11.3. 数据三

x	0,3,28,53,78,103,183,303,463,603
y1*y4	0,0.01622738,0.06230592,0.12806244,0.12165704,0.07517978,0.0138635,0,0,0

同样，令：

$$y_5 = y_1 \cdot y_4 \tag{11-5}$$

两边求导，有：

$$y_5' = y_1' \cdot y_4 + y_1 \cdot y_4' \tag{11-6}$$

此时微分方程组就变为：

$$\begin{cases} \dfrac{dy_1}{dx} = k_1 \cdot y_1 \\ \dfrac{dy_2}{dx} = k_1 \cdot y_1 - k_2 \cdot y_2 \\ \dfrac{dy_3}{dx} = k_2 \cdot y_2 - k_3 \cdot y_3 \\ \dfrac{dy_4}{dx} = k_1 \cdot y_1 + k_2 \cdot y_2 + k_3 \cdot y_3 \\ \dfrac{dy_5}{dx} = \dfrac{dy_1}{dx} \cdot y_4 + y_1 \dfrac{dy_4}{dx} \end{cases} \tag{11-7}$$

可按一般微分方程拟合处理，求解代码 11-4

```
Parameter k1,k2,k3;
InitialODEValue x=0,y1=0.9922,y4=0,y5=0;
Variable x,y5;
ODEFunction y1'=k1*y1;
            y2'=k1*y1-k2*y2;
            y3'=k2*y2-k3*y3;
            y4'=k1*y1+k2*y2+k3*y3;
            y5'=y1'*y4+y1*y4';
Data;
x=0,3,28,53,78,103,183,303,463,603;
y5=0,0.01622738,0.06230592,0.12806244,0.12165704,0.07517978,0.0138635,0,0,0;
```

或者：

```
Title "myfunction";
Parameter k1,k2,k3;
Variable x,y1,y4,y5;
ODEFunction y1'=k1*y1;
            y2'=k1*y1-k2*y2;
            y3'=k2*y2-k3*y3;
            y4'=k1*y1+k2*y2+k3*y3;
            y5'=y1'*y4+y1*y4';
Data;
x=0,3,28,53,78,103,183,303,463,603;
y1=0.9922,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN;
y4=0,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN,NAN;
y5=0,0.01622738,0.06230592,0.12806244,0.12165704,0.07517978,0.0138635,0,0,0;
```

结果：

```
Root of Mean Square Error (RMSE): 0.00197456241518077
Sum of Squared Residual: 3.89889673144451E-5
Correlation Coef. (R): 0.899198226284822
R-Square: 0.80855745015377
Adjusted R-Square: 0.897862889116697
Determination Coef. (DC): 0.898393424391681
F-Statistic: 560.626035977376

Parameter            Best Estimate
-------------------- -------------
k1     -0.0425380414381262
k2     0.0694441191380877
k3     -0.0135577622298462
y2 Initial Value   0.281158268089891
y3 Initial Value   -2.34689476605199
```

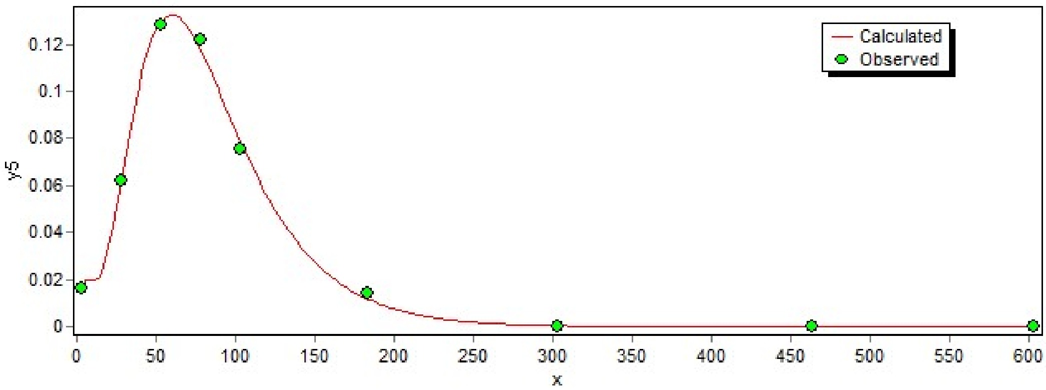

图 11.4 微分方程复合数据 y5 拟合计算对比图

11.4 任意形式的复合数据

上面给出了复合数据为“和”及“乘积”两种情景的处理方式，实际上，任

何其它形式的复合数据都可以按类似方式处理，唯一要注意的就是新增变量（如y5）的复合函数的求导过程。

比如如果复合数据形式为：

$$y_5 = y_1 \cdot y_4^2 \tag{11-8}$$

两边求导，有：

$$y_5' = y_1' \cdot y_4^2 + y_1 \cdot 2 \cdot y_4 \cdot y_4' \tag{11-9}$$

又如复合数据形式为：

$$y_5 = \ln(y_1) + y_1 \cdot y_4 \tag{11-10}$$

两边求导，有：

$$y_5' = \frac{1}{y_1} + y_1' \cdot y_4 + y_1 \cdot y_4' \tag{11-11}$$

遵循数学基本求导规则，以此类推即可处理不同形式的复合数据微分方程拟合问题。

11.5 小结

通过引入新的变量及实施复合函数的求导变换，1stOpt 可方便处理不同复合数据的微分方程拟合问题。