Fitting a Sum of Exponentials to Numerical Data

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Abstract

A finite sum of exponential functions may be expressed by a linear combination of powers of the independent variable and by successive integrals of the sum. This is proved for the general case and the connection between the parameters in the sum and the coefficients in the linear combination is highlighted. The fitting of exponential functions to a given data- set is therefore reduced to a multilinear approximation procedure. The results of this approximation do not only provide the necessary information to compute the factors in the exponents and the weights of the exponential terms but also they are used to estimate the errors in the factors.

1 Introduction

From time to time the need arises to fit a sum of exponentials to numerical data. That means to approximate a given data- set consisting of pairs of real numbers (x_j, y_j) by the following expression:

$$y(x) = a_0 + \sum_{i=1}^{N} a_i e^{-b_i x}$$
 (1)

where $x, x_j \in \mathbb{R}^+, y_j \in \mathbb{R}$, $N \in \mathbb{N}^+$ and a_i, b_i are unknown real numbers which have to be chosen so that the fit becomes optimal.

If the b_i were known, the task usually would be a well posed linear problem, but if the b_i are unknown too, it turns out to be ill conditioned. The hopelessness of efforts dealing with this kind of problem has been described drastically by F.S. Acton [1] in a chapter entitled "What not to compute".

At first sight, fitting equation 1 to a given data- set inevitably seems to be a nonlinear problem. However it has been noted [2], [3] that equation 1 may be expressed as a linear combination of powers of x and successive integrals of y(x), reducing the problem to a multilinear fitting procedure. This method is based on the fact that y(x) can be shown to satisfy an ordinary linear differential equation of N-th order with constant coefficients. The roots of the characteristic

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polynomial of this equation give the b_i and the a_i are identified as solutions to linear equations involving the b_i and the derivatives of y(x) at x=0. However, derivatives of experimental data- sets enhance the errors in the data, therefore it is desirable to eliminate them. Actually, [3] shows already the way to do this, but only for the case N=2 and $a_0=0$, the general case not really being obvious. In the present paper, this method of linearizing the fitting procedure is revived and without referring to differential equations and without using derivatives, the general case is derived. Additionally, a method for estimating the errors in the exponential factors is presented. Of course, the problem remains ill posed, but linear fitting offers computational advantages over nonlinear approximation and also supplies estimates of the errors in the computed coefficients, which may be used to predict the errors in the exponential coefficients.

2 Results

The functions used to construct a linear approximation problem are powers of x and successive integrals of y(x). Before the announced relation can be asserted, some definitions are required.

Definition: The k-th integral of y(x) is defined recursively:

$$I_0(x) = y(x)$$

 $I_k(x) = \int_0^x I_{k-1}(t)dt \qquad k > 0$ (2)

Definition: β_{Nij} , α_{Nij} . Given the set $B = \{b_1, \dots, b_N\}$ of N exponential factors b_k in equation 1 we consider the products of i different elements of B. Each of these products corresponds to a combination of i elements out of B, the number of these products therefore is

$$C(N,i) = \frac{N!}{(N-i)!i!} = \binom{N}{i}$$
(3)

as is proved in combinatorics. We assume that the products are ordered in some way. β_{Nij} then is the j-th of these products. Additionally, we define $\beta_{N01}=1$. α_{Nij} is the sum of all a_k in equation 1 excluding those whose index is equal to that of one of the b's in β_{Nij} . By definition, $\alpha_{N01}=\sum_{k=0}^{N}a_k$. Obviously, each α_{Nij} contains at least a_0 .

Example: N=3

With these definitions, the central statement of this article now may be asserted:

$$a_0 + \sum_{i=1}^{N} a_i e^{-b_i x} = -\sum_{i=1}^{N} I_i(x) \sum_{j=1}^{C(N,i)} \beta_{Nij} + \sum_{i=0}^{N} \frac{x^i}{i!} \sum_{j=1}^{C(N,i)} \beta_{Nij} \alpha_{Nij}$$
(4)

Assuming the validity of equation 4 the task now consists in approximating the data- set $\{(x_j, y_j)\}$ by a linear combination of the 2N functions $(I_1, \ldots, I_N, x, \ldots, x^N)$ plus a constant. By standard linear approximation techniques the coefficients $(c_1, \ldots, c_N, d_1, \ldots, d_N)$ and the intercept d_0 may be determined together with their errors $(\Delta c_1, \ldots, \Delta c_N, \Delta d_1, \ldots, \Delta d_N)$ and Δd_0 . It follows that

$$c_i = -\sum_{j=1}^{C(N,i)} \beta_{Nij} \qquad i = 1, \dots, N$$
 (5)

$$d_i = \sum_{j=1}^{C(N,i)} \frac{\beta_{Nij}\alpha_{Nij}}{i!} \qquad i = 1, \dots, N$$
 (6)

$$d_0 = \alpha_{N01} = \sum_{k=0}^{N} a_k \tag{7}$$

Given the c_i in 5 Vieta's root theorem asserts that the b_i are the N roots of the polynomial

$$P(x) = x^{N} + \sum_{i=1}^{N} (-1)^{i+1} c_{i} x^{N-i}$$
(8)

As soon as the b_i are known, the expressions 6 and 7 represent a system of N+1 linear equations for the N+1 coefficients a_i .

If the Δc_i are small, the relation between the errors may be approximated by the linear terms of the Taylor- series for P(x).

$$\Delta P(x) = \frac{\partial P(x)}{\partial x} \Delta x + \sum_{i=1}^{N} \frac{\partial P(x)}{\partial c_i} \Delta c_i$$
 (9)

As the b_k are roots of P, ΔP should be zero and therefore, inserting b_k for x, we get:

$$\Delta b_k = -\frac{1}{\frac{\partial P(b_k)}{\partial x}} \sum_{i=1}^N \frac{\partial P(b_k)}{\partial c_i} \Delta c_i$$
 (10)

Treating the c_i and b_k as probability variables with standard deviations s_{ci} and s_{bk} , the standard deviation and therefore the estimated error of b_k is given by

$$s_{bk} = \frac{1}{\left|\frac{\partial P(b_k)}{\partial x}\right|} \sqrt{\sum_{i=1}^{N} b_k^{2(N-i)} s_{ci}^2 + 2\sum_{i=1}^{N} \sum_{j=i+1}^{N} (-1)^{i+j} b_k^{2N-i-j} Cov(c_i, c_j)}$$
(11)

As usual, $Cov(c_i, c_j)$ means the covariance between c_i and c_j .

It remains to show that equation 4 is valid. For this purpose it is useful to state some properties of the coefficients β .

For any l with $1 \le l < N$ and any $i \le N$ the sum of all β_{Nlm} may be divided into the sum of all β_{Nlm} containing b_i and those not containing b_i :

$$\sum_{m=1}^{C(N,l)} \beta_{Nlm} = b_i \sum_{i=1}^{C(N-1,l-1)} \beta_{(N-1)(l-1)j}^{(-i)} + \sum_{i=1}^{C(N-1,l)} \beta_{N-1,l,j}^{(-i)}.$$
(12)

With $\beta_{(N-1)lj}^{(-i)}$ we denote the products not containing b_i that is, which are chosen from the set $\{b1,\ldots,b_{i-1},b_{i+1},\ldots,b_N\}$ containing N-1 elements and not containing b_i . For $l \leq 0$ we define $\beta_{(N-1)lm}^{(-i)} = 1$.

An important special case of 12 results if i = N. Then $\beta_{(N-1)lm}^{(-N)} = \beta_{(N-1)lm}$ and the following expression results:

$$\sum_{m=1}^{C(N,l)} \beta_{Nljm} = \sum_{j=1}^{C(N-1,l)} \beta_{(N-1)lj} + b_N \sum_{j=1}^{C(N-1,l-1)} \beta_{(N-1)(l-1)j}$$
 (13)

For a proof of equation 4 consider the following system of equations:

$$I_0(x) = a_0 + \sum_{i=1}^{N} a_i e^{-b_i x}$$

$$I_k(x) = a_0 \frac{x^k}{k!} + \sum_{i=1}^{N} a_i \left[\left(\frac{-1}{b_i} \right)^k e^{-b_i x} - \sum_{j=0}^{k-1} \left(\frac{-1}{b_i} \right)^{k-j} \frac{x^j}{j!} \right]$$
(14)

The validity of 14 is easily seen by performing the integrals in equation 2 analytically.

Now consider the following linear transformations defined recursively on the set of equations 14:

$$I_k^{(1)} = I_k + b_1 I_{k+1}$$

$$I_k^{(h)} = I_k^{(h-1)} + b_h I_{k+1}^{(h-1)} \qquad h > 1$$
(15)

For this kind of transformation a rather general relationship holds:

$$I_k^{(h)} = I_k + \sum_{l=1}^h \sum_{m=1}^{C(h,l)} \beta_{hlm} I_{k+l}$$
 (16)

Proof: Induction for h. For h=1, proposition 16 just repeats the definition of $I_k^{(1)}$. Now assume that 16 holds for $I_k^{(h)}$. Then

$$\begin{split} I_k^{(h+1)} &= I_k^{(h)} + b_{h+1} I_{k+1}^{(h)} = \\ I_k + \sum_{l=1}^h \sum_{m=1}^{C(h,l)} \beta_{hlm} I_{k+l} + b_{h+1} I_{k+1} + \sum_{l=1}^h \sum_{m=1}^{C(h,l)} b_{h+1} \beta_{hlm} I_{k+l+1} = \\ I_k + \sum_{l=1}^h \sum_{m=1}^{C(h,l)} \beta_{hlm} I_{k+l} + b_{h+1} I_{k+1} + \sum_{l=2}^{h+1} \sum_{m=1}^{C(h,l-1)} b_{h+1} \beta_{h(l-1)m} I_{k+l} = \\ I_k + \sum_{m=1}^{C(h+1,1)} \beta_{(h+1)1m} I_{k+1} + \sum_{l=2}^h \sum_{m=1}^{C(h+1,l)} \beta_{(h+1)lm} I_{k+l} + b_{h+1} \beta_{hh1} I_{k+h+1} \end{split}$$

where 13 has been used in order to obtain the last line. Obviously, this result may be converted into

$$I_k^{(h+1)} = I_k + \sum_{l=1}^{h+1} \sum_{m=1}^{C(h+1,l)} \beta_{(h+1)lm} I_{k+l}$$

whereby the proof of 16 is completed. Consider now $I_0^{(N)}$. By 16

$$I_0^{(N)} = y + \sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} I_l$$
 (17)

Inserting 14 this expands into

$$y + \sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} I_l =$$

$$a_0 + \sum_{i=1}^{N} a_i e^{-b_i x} \left[1 + \sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} \left(\frac{-1}{b_i} \right)^l \right] +$$

$$\sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} \left[a_0 \frac{x^l}{l!} - \sum_{i=1}^{N} a_i \sum_{j=0}^{l-1} (-b_i)^{j-l} \frac{x^j}{j!} \right]$$
 (18)

The motive for applying transform 15 to I_0 was to get rid of the exponential terms. The following proposition asserts that equation 18 is actually free of exponential terms:

$$\sum_{l=1}^{h} \sum_{m=1}^{C(h,l)} \beta_{hlm} \left(\frac{-1}{b_i}\right)^l = -1 \qquad 1 \le i \le h$$
 (19)

Proof:

For h = 1 the assertion is trivial. Now assume that 19 is valid for h. Then the following calculations prove the truth for h+1 and therefore for all h:

$$\sum_{l=1}^{h+1} \sum_{m=1}^{C(h+1,l)} \beta_{(h+1)lm} \left(\frac{-1}{b_i}\right)^l =$$

$$\begin{split} \sum_{l=1}^{h} \left(\frac{-1}{b_{i}}\right)^{l} \left[\sum_{m=1}^{C(h,l)} \beta_{hlm} + b_{h+1} \sum_{m=1}^{C(h,l-1)} \beta_{h(l-1)m}\right] + \left(\frac{-1}{b_{i}}\right)^{h+1} \beta_{(h+1)(h+1)1} = \\ -1 - \frac{b_{h+1}}{b_{i}} + b_{h+1} \sum_{l=1}^{h-1} \sum_{m=1}^{C(h,l)} \beta_{hlm} \left(\frac{-1}{b_{i}}\right)^{l+1} + \left(\frac{-1}{b_{i}}\right)^{h+1} \beta_{(h+1)(h+1)1} = \\ -1 - \frac{b_{h+1}}{b_{i}} - \frac{b_{h+1}}{b_{i}} \sum_{l=1}^{h} \sum_{m=1}^{C(h,l)} \beta_{hlm} \left(\frac{-1}{b_{i}}\right)^{l} + \frac{b_{h+1}}{b_{i}} \left(\frac{-1}{b_{i}}\right)^{h} \beta_{hh1} + \\ \left(\frac{-1}{b_{i}}\right)^{h+1} \beta_{(h+1)(h+1)1} \end{split}$$

Using equation 19 for and collecting all terms the last expression evaluates to -1.

To complete the proof of equation 4 some more transformations on formula 18 are required:

$$y + \sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} I_l = a_0 + \sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} \left[a_0 \frac{x^l}{l!} - \sum_{i=1}^{N} a_i \sum_{j=0}^{l-1} (-b_i)^{j-l} \frac{x^j}{j!} \right] = \sum_{i=0}^{N} a_i + \sum_{l=1}^{N} \frac{x^l}{l!} \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,j)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{l=1}^{N} a_l \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 - \sum_{j=l+1}^{N} \sum_{m$$

$$\sum_{i=0}^{N} a_i + \sum_{l=1}^{N} \frac{x^l}{l!} \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} a_0 + \sum_{i=1}^{N} a_i (-b_i)^l + \sum_{j=1}^{l} \sum_{m=1}^{C(N,j)} \beta_{Njm} \sum_{i=1}^{N} a_i (-b_i)^{l-j} \right] = \sum_{i=0}^{N} a_i + \sum_{l=1}^{N} \frac{x^l}{l!} \left[\sum_{m=1}^{C(N,l)} \beta_{Nlm} \sum_{i=0}^{N} a_i + \sum_{i=1}^{N} a_i S_{il} \right]$$
(20)

where

$$S_{il} = \sum_{p=1}^{l-1} \sum_{m=1}^{C(N,l-p)} \beta_{N(l-p)m}(-b_i)^p + (-b_i)^l \quad \text{for } l > 1$$

and

$$S_{i1} = -b_i$$
 for $l = 1$

Using 12, for l > 1 S_{il} transforms into

$$S_{il} =$$

$$\sum_{p=1}^{l-1} \left(\sum_{m=1}^{C(N-1,l-p)} \beta_{(N-1)(l-p)m}^{(-i)} + b_i \sum_{m=1}^{C(N-1,l-p-1)} \beta_{(N-1)(l-p-1)m}^{(-i)} \right) (-b_i)^p + (-b_i)^l$$

Substituting in the second part of this sum q for p+1 this expression transforms into

$$S_{il} = -\sum_{m=1}^{C(N-1,l-1)} \beta_{(N-1)(l-1)m}^{(-i)} b_i + \sum_{p=2}^{l-1} \sum_{m=1}^{C(N-1,l-p)} \beta_{(N-1)(l-p)m}^{(-i)} (-b_i)^p$$

$$-\sum_{q=2}^{l-1} \sum_{m=1}^{C(N-1,l-q)} \beta_{(N-1)(l-q)m}^{(-i)} (-b_i)^q - (-b_i)^l + (-b_i)^l =$$

$$-\sum_{m=1}^{C(N-1,l-1)} \beta_{(N-1)(l-1)m}^{(-i)} b_i$$

Therefore S_{il} is the negative sum of all β_{Nlm} which contain b_i . Consequently, in expression 20 only those a_i are not cancelled for which β_{Nlm} does not contain b_i . For that, 20 may be written as

$$y + \sum_{l=1}^{N} \sum_{m=1}^{C(N,l)} \beta_{Nlm} I_{l} = \sum_{l=0}^{N} \frac{x^{l}}{l!} \sum_{m=1}^{C(N,l)} \beta_{Nlm} \alpha_{Nlm}$$

which proves equation 4.

Example: Consider this sum of two exponentials and a constant:

$$y(x) = 0.3 + exp(-0.7x) + 0.4exp(-0.3x)$$

The function is evaluated in in the interval $0 \le x \le 6$ at Np equally spaced points. The discrete function values are multiplied by one plus a gaussian distributed random variable so that the relative error has the standard deviation σ . I1 and I2 are calculated using the trapezoidal method. For different settings of Np and σ the coefficients c1 and c2, d0 (the intercept), d1 and d2 and the corresponding errors of c1 and c2 as well as the covariance between these two factors are determined by the commercial statistics program STATISTICA® and are listed in table 1. The parameters b1, b2, a0, a1, a2 and the errors Δb_1 and Δb_2 are calculated from these coefficients as described above and are listed in table 2.

Table 1: Statistically determined coefficients

Id	Np	σ	c_1	Δc_1	c_2	Δc_2	Cov	d_0	d_1	d_2
1	601	0.0000	-1.0000	10^{-6}	-0.2100	10^{-6}	0	1.7000	0.8800	0.0315
2	601	0.0001	-1.0054	0.0024	-0.2130	0.0014	3.10^{-6}	1.7001	0.8890	0.0320
3	601	0.001	-1.0358	0.0253	-0.2300	0.0146	0.000343	1.7008	0.9396	0.0349
4	601	0.01	-1.0842	0.2954	-0.2615	0.1700	0.0502	1.7006	1.0249	0.0408
5	2001	0.01	-0.9155	0.1190	-0.1603	0.0685	0.00815	1.6999	0.7369	0.0228

Table 2: Parameter estimates based on the coefficients in table 1

Id	b_1	Δb_1	b_2	Δb_2	a_0	a_1	a_2
1	0.7000	3.10^{-6}	0.3000	3.10^{-6}	0.30	1.00	0.40
2	0.7020	0.0019	0.3034	0.0021	0.30	0.99	0.41
3	0.7134	0.0180	0.3224	0.0196	0.30	0.95	0.45
4	0.7220	0.1211	0.3622	0.1754	0.31	0.88	0.51
5	0.6796	0.0281	0.2359	0.0911	0.28	1.09	0.32

The results show that for small errors in the coefficients the estimated variance of b_1 and b_2 is also small and the estimate is realistic. The first case was computed without artificial noise, in this case the accuracy seems to be determined mainly by the statistics program. Adding noise deteriorates the accuracy of the results rapidly. While a relative error of 0.0001 (case 2) still leads to a reasonable result, the tenfold relative error (case 3) already means that the calculated uncertainty of b_2 is about 7%. A one- percent inaccuracy in the data (case 4) gives a result even with the first digit uncertain. As case 5 where the number of data- points is raised to 2001 shows, increasing the size of the data-set may at least partially compensate for noise.

References

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