ANALYSIS OF DECAY PROCESSES AND APPROXIMATION

BY EXPONENTIALS

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In several sciences, e.g. in physics, chemistry, biology, and medicine, often decay processes have to be analyzed. Then an empirical function \( f(t) \) is given, its domain may be an interval or a discrete point set; and a sum of exponentials of the form

\[
\sum_{v=1}^{n} \alpha_v e^{-\lambda_v t}
\]

is to be fitted to the function \( f \). Here, \( n \) is the given number of matters, while the \( \alpha_v \)'s are the concentrations and the \( \lambda_v \)'s are the decay constants. The latter \( 2n \) parameters are to be determined by the fit.

During the last decade an involved theory for the mathematical treatment of this problem has been developed, see e.g. [1,4,6]. In this talk, however, we will restrict our attention to those problems which arise when the theory is applied. Then the following question seems to be crucial: How sensitive are the different methods to the noise (pollution) of the empirical data? Although there is a certain connection with the numerical
stability [3], this problem must be considered separately.

Let us start our discussion with the "peeling-off-method" (German: Abschälmethode). It is one of the first effective methods. We do not know who has developed it. But it will not be discussed for historical reasons. At first glance the peeling-off-method seems to be a poor algorithm from the mathematical point of view. Yet it shows the limitation of any method, and therefore it is probably superior to a highly developed mathematical procedure which is used only in the black-box-manner.

The peeling-off-method proceeds in an inductive way. Note that the parameters of a single exponential term $a \cdot e^{-\lambda t}$ may be determined by a simple interpolation at two points $t_1$ and $t_2$:

$$\lambda = \frac{1}{t_2 - t_1} \cdot \log \frac{f(t_1)}{f(t_2)}, \quad a = f(t_1) e^{\lambda t_1}. \quad (1)$$

Moreover, if the decay constants are ordered: $\lambda_1 < \lambda_2 < \ldots < \lambda_m$, then all terms die away faster than the first one does. Therefore one gets a reasonable estimate for the first term by interpolating $f(t)$ at two large $t$'s. The result $a_1 e^{-\lambda_1 t}$ is peeled of the curve, i.e. it is subtracted from $f(t)$. Then the process is repeated.

Now, let us look for the conditions under which the peeling-off-method makes sense. They are obvious in the case when there is only one term and when $f$ is given at $m$ points $t_1 < t_2 < \ldots < t_m$. Then we require

$$\lambda_i \geq \frac{1}{5} \frac{1}{t_m - t_1}, \quad (2)$$

$$\lambda_i \leq \frac{1}{t_3 - t_1}. \quad (3)$$

The first condition says that the time must be so large that the decay causes an observable decrease of the amplitude. The second