Optimum Choice of Weights in Slope Calculation

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1 Introduction.

We address the question of what is the optimal weighted linear least squares estimate of the slope of an assumed linear function which is the output of a differential system corrupted by noise that is only partially damped from step to step. We will take the definition of "optimal" to mean that the variance of the estimate is minimal. We assume that the integrator provides an approximation to the solution at a series of points (typically equally spaced, although that is not essential), that the solution at the n-th output point contains an error r_n, and that there is the relation

$$r_n = \rho r_{n-1} + \eta_n \tag{1}$$

where the η_n are independent random variables. Without loss of generality we can assume that the slope is zero so that the integrator gives r_n as the output. For this report we will assume that the η_n are independent random variables with mean zero and variances σ_n^2. (If the output points are evenly spaced, it is likely that the variances would be equal, while is they are unevenly spaced, it is likely that they would be proportional to the corresponding integration step sizes.) We are going to assume that $r_0 = 0$ and fit to the output points r_1 through r_N. Two extremes of eq. (1) are the case when there is no damping ($\rho = 1$) so the output is a random walk, and the case $\rho = 0$ so the output is a set of independent random variables.

We want to estimate the slope, s, of a straight line though the points (t_n, r_n) using linear least squares with weights w_n and would like to choose the w_n so that the variance of s is minimal. Since the time origin is arbitrary, we will assume that it has been set so that

$$\sum_{n=1}^{N} w_n t_n = 0 \tag{2}$$

In that case, the slope is given by

$$s = \frac{\sum_{n=1}^{N} w_n t_n r_n}{\sum_{n=1}^{N} w_n t_n^2} \tag{3}$$

From eq. (1) we have

$$r_n = \sum_{j=1}^{n} \rho^{n-j} \eta_j \tag{4}$$

Substituting this into eq. (3) we get

$$\begin{aligned} s &= \frac{\sum_{n=1}^{N} w_n t_n \sum_{j=1}^{n} \rho^{n-j} \eta_j}{\sum_{n=1}^{N} w_n t_n^2} \\ &= \frac{\sum_{j=1}^{N} \eta_j \sum_{n=j}^{N} \rho^{n-j} w_n t_n}{\sum_{n=1}^{N} w_n t_n^2} \end{aligned} \tag{5}$$

Since this now is a weighted sum of independent random variables with mean zero and variances σ_j^2 the variance of s is given by

$$\mathrm{Var}(s) = \frac{\sum_{j=1}^{N} \sigma_j^2 (\sum_{n=j}^{N} \rho^{n-j} w_n t_n)^2}{(\sum_{n=1}^{N} w_n t_n^2)^2} \tag{6}$$

We want to find the weights that minimize this subject to eq. (2) so we want

$$0 = \frac{\partial}{\partial w_k} \left[\mathrm{Var}(s) + \lambda \sum_{n=1}^{N} w_n t_n \right] \tag{7}$$

or

$$0 = 2 \frac{\sum_{j=1}^{k} \sigma_j^2 (\sum_{n=j}^{N} \rho^{n-j} w_n t_n) \rho^{k-j}}{D^2} t_k - 2 \frac{\mathrm{Var}(s)}{D} t_k^2 + \lambda t_k$$

where

$$D = \sum_{n=1}^{N} w_n t_n^2$$

Setting

$$W_j = \sum_{n=j}^{N} \rho^{n-j} w_n t_n, \tag{8}$$

$$Z_k = \sum_{j=1}^{k} \sigma_j^2 W_j \rho^{k-j}, \tag{9}$$

$$\beta = \mathrm{Var}(s) D,$$

and

$$\mu = -\frac{\lambda D^2}{2\beta}$$

we get

$$Z_k = \beta(t_k + \mu) \tag{10}$$

Note that from eq. (8) and eq. (9)

$$\begin{aligned} W_N &= w_N t_N \\ W_j &= w_j t_j + \rho W_{j+1}, \quad j < N \end{aligned} \tag{11}$$

$$\begin{aligned} Z_1 &= \sigma_1^2 W_1 \\ Z_k &= \sigma_k^2 W_k + \rho Z_{k-1}, \quad k > 1 \end{aligned} \tag{12}$$

Hence

$$\begin{aligned} W_1 &= \beta \frac{t_1 + \mu}{\sigma_1^2} \\ W_k &= \beta \frac{t_k - \rho t_{k-1} + (1-\rho)\mu}{\sigma_k^2}, \quad k > 1 \\ w_1 t_1 &= \beta \left[\frac{t_1 + \mu}{\sigma_1^2} - \rho \frac{t_2 - \rho t_1 + (1-\rho)\mu}{\sigma_2^2} \right] \\ w_k t_k &= \beta \left[\frac{t_k - \rho t_{k-1} + (1-\rho)\mu}{\sigma_k^2} - \rho \frac{t_{k+1} - \rho t_k + (1-\rho)\mu}{\sigma_{k+1}^2} \right], \quad 1 < k < N \\ w_N t_N &= \beta \frac{t_N - \rho t_{N-1} + (1-\rho)\mu}{\sigma_N^2} \end{aligned}$$

It is clear that β is an arbitrary scale factor that can be taken as 1. The condition in eq. (2) determines the value of μ.

In the case $\rho = 1$ eq. (2) implies $\mu = -t_1$. If in this case $\sigma_k^2 = \gamma(t_k - t_{k-1})$ (which is plausible for a random walk) and we find that $w_1 t_1 = -1, \quad w_k t_k = 0,\ 1 < k < N$, and $w_N t_N = 1$ so that

$$s = \frac{r_N - r_1}{T_N - t_1},$$

that is, it is the slope of a line between the two end points. Note that this is not true if the variances of the noise are not proportional to the step length.

When $\rho = 0$ eq. (2) implies

$$\mu = -\frac{\sum_{j=1}^N t_j / \sigma_j^2}{\sum_{j=1}^N 1/\sigma_j^2}$$

Note that μ acts as a shift of the t_k (through eq. (10). It does not change the values of $w_k t_k$ which are the only way in which the weights enter into the calculation of s by eq. (3). If we choose the origin for t so that $\mu = 0$ we find that

$$w_k = 1/\sigma_k^2$$

meaning all points are treated equally after factoring out the different variances. This statement is independent of the integration intervals.

If all of the variances σ_i^2 are the same, say 1, then, after shifting the time origin so that

$$\mu = \frac{\rho^2 t_N - (1-\rho)^2 \sum_{k=1}^{N} t_k - \rho(t_1 + t_N)}{1 + (N-1)(1-\rho)^2}$$

is zero, we find that

$$\begin{aligned} w_1 t_1 &= (1+\rho^2) t_1 - \rho t_2 \\ w_k t_k &= (1-\rho)^2 t_k \\ w_N t_N &= t_N - \rho t_{N-1} \end{aligned}$$