Savitsky-Golay Filters

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References

1. Abraham Savitsky and Marcel J. E. Golay, "Smoothing and differentiation of data by simplified least squares procedures," Anal. Chem. **36**, 1627–1639 (1964).

2. Manfred U.A. Bromba and Horst Ziegler, "Application hint for Savitsky-Golay digital smoothing filters," Anal. Chem. **53**, 1583–1586 (1981).

3. Horst Ziegler, "Properties of digital smoothing Polynomial (DISPO) filters," Appl. Spec. **35**, 88–92 (1981).

Consider a dynamical variable as a set of readings $\mathbf{y}_i, i = 1...N$ measured at fixed time interval $t, t + \tau, t + 2\tau, ...$ Any point (not too near the beginning or end) can be taken as the origin of time $t = 0$ and its measurement relabelled y_0. This measurement, together with M additional measured y-values to each side will be used to determine best estimates of the y, dy/dt, and d^2y/dt^2 at $t = 0$. The set will be labeled by indices $m = -M, -M + 1, ..., -1, 0, 1, ..., M - 1, M$ for a total $2M + 1$ data points.

A polynomial fitting model is used $y(t) = \mathbf{a}_0 + \mathbf{a}_1 t + \mathbf{a}_2 t^2 + ...$ up to order R. That is,

$$y(t) = \sum_{r=0}^{R} \mathbf{a}_r t^r \tag{1}$$

The χ^2 is given by

$$\chi^2 = \frac{1}{\sigma_y^2} \sum_{m=-M}^{M} (y(t_m) - \mathbf{y}_m)^2 \tag{2}$$

where

$$t_m = -M\tau, ... - 3\tau, -2\tau, -\tau, 0, \tau, 2\tau, 3\tau..., M\tau \tag{3}$$

i.e., $t_m = m\tau$ and σ_y is the standard deviation of the measured $\mathbf{y}_m$, assumed to be constant. The best estimates of $\mathbf{a}_r$ are then determined by a least squares fit, and the sought-after nth derivatives at $t = 0$ are then given by

$$y^{[n]} = n!\mathbf{a}_n \tag{4}$$

The least squares equations $d\chi^2/d\mathbf{a}_n = 0$ can be rewritten in the vector-matrix form

$$\mathbf{Y} = [\mathbf{X}]\mathbf{a} \tag{5}$$

where the elements of the column vector $\mathbf{a}$ are the $R+1$ fitting coefficients $\mathbf{a}_r$, $\mathbf{Y}$ is another column vector of $R+1$ elements given by

$$\mathbf{Y}_r = \sum_{m=-M}^{M} \mathbf{y}_m t_m^r \tag{6}$$

and $[\mathbf{X}]$ is an $R+1$ by $R+1$ square matrix with elements

$$[\mathbf{X}]_{nr} = \sum_{m=-M}^{M} t_m^{n+r} \tag{7}$$

The vector $\mathbf{a}$ is then determined by finding $[\mathbf{X}]^{-1}$, the inverse of the matrix $[\mathbf{X}]$ so that

$$\mathbf{a} = [\mathbf{X}]^{-1}\mathbf{Y} \tag{8}$$

Moreover, the covariance matrix for the parameter estimates, $[\boldsymbol{\sigma}_a^2]$ is given in terms of this inverse matrix

$$[\boldsymbol{\sigma}_a^2] = \sigma_y^2[\mathbf{X}]^{-1} \tag{9}$$

Expressing all elements of Eq. 8 explicitly gives

$$\mathbf{a}_r = \sum_{n=0}^{R} [[\mathbf{X}]^{-1}]_{rn} \mathbf{Y}_n \tag{10}$$

and substituting Eq. 6 for $\mathbf{Y}_n$

$$\mathbf{a}_r = \sum_{n=0}^{R} \sum_{m=-M}^{M} [[\mathbf{X}]^{-1}]_{rn} \mathbf{y}_m t_m^n \tag{11}$$

Rearrange to get

$$\mathbf{a}_r = \sum_{m=-M}^{M} \left(\sum_{n=0}^{R} [[\mathbf{X}]^{-1}]_{nr} t_m^n \right) \mathbf{y}_m \tag{12}$$

Consider the $\mathbf{y}_m$-values as a column-vector $\mathbf{y}$ of $2M+1$ elements. The Savitsky-Golay filters can then be represented as a matrix $[\mathbf{c}]$ having $R+1$ rows and $2M+1$ columns with elements given by the term in enclosed in parentheses above

$$[\mathbf{c}]_{rm} = \sum_{n=0}^{R} [[\mathbf{X}]^{-1}]_{rn} t_m^n \tag{13}$$

so that Eq. 12 for the column vector $\mathbf{a}$ now becomes

$$\mathbf{a} = [\mathbf{c}]\mathbf{y} \tag{14}$$

The t_m are known ahead of time so the matrix $[\mathbf{c}]$ can be predetermined. To do so, first define $[\mathbf{m}]$ as a matrix of $R+1$ rows by $2M+1$ columns having elements

$$[\mathbf{m}]_{rm} = m^r \tag{15}$$

i.e., the explicit form

$$[\mathbf{m}] = \begin{bmatrix} 1 & 1 & ... & 1 & 1 & 1 & ... & 1 & 1 \\ -M & -M+1 & ... & -1 & 0 & 1 & ... & M-1 & M \\ \vdots & \vdots & ... & \vdots & \vdots & \vdots & ... & \vdots & \vdots \\ -M^R & -(M+1)^R & ... & -1 & 0 & 1 & ... & (M-1)^R & M^R \end{bmatrix} \tag{16}$$

With this matrix, it is then easy to show that the term t_m^n can be represented as the following matrix element

$$t_m^r = [[\mathbf{U}][\mathbf{m}]]_{rm} \tag{17}$$

where $[\mathbf{U}]$ is a square diagonal matrix representing the time units, i.e., having only nonzero elements for $[\mathbf{U}]_{nn} = \tau^n$, for $n = 0...R$.

Then Eq. 13 becomes

$$[\mathbf{c}] = [\mathbf{X}]^{-1}[\mathbf{U}][\mathbf{m}] \tag{18}$$

Furthermore, the square matrix $[\mathbf{X}]$ given by Eq. 7 can also be represented for computational purposes in terms of $[\mathbf{m}]$ and $[\mathbf{U}]$

$$[\mathbf{X}] = [\mathbf{U}][\mathbf{m}][\mathbf{m}]^T[\mathbf{U}]^T \tag{19}$$

where the superscript T indicates the transpose of the matrix. (Thus, $[\mathbf{m}]^T$ has $2M+1$ rows and $R+1$ columns with elements given by $[[\mathbf{m}]^T]_{mn} = [\mathbf{m}]_{nm}$, and $[\mathbf{U}]^T = [\mathbf{U}]$ because it is square diagonal.)

The inverse matrix $[\mathbf{X}]^{-1}$ can then be represented

$$[\mathbf{X}]^{-1} = [\mathbf{U}]^{-1}[[\mathbf{m}][\mathbf{m}]^T]^{-1}[\mathbf{U}]^{-1} \tag{20}$$

where the only nonzero elements of the inverse units matrix $[\mathbf{U}]^{-1}$ are on the diagonal and given by $[\mathbf{U}]^{-1}_{nn} = 1/\tau^n$.

Using this in Eqs. 18 and 9 gives the finished form for the filter coefficients

$$[\mathbf{c}] = [\mathbf{U}]^{-1}[[\mathbf{m}][\mathbf{m}]^T]^{-1}[\mathbf{m}] \tag{21}$$

and the covariance matrix

$$[\boldsymbol{\sigma}_a^2] = \sigma_y^2[\mathbf{U}]^{-1}[[\mathbf{m}][\mathbf{m}]^T]^{-1}[\mathbf{U}]^{-1} \tag{22}$$

For our rotary encoder, each y-count represents an angle of $\delta_y = 2\pi/1440$ rad. For determining y, dy/dt, and d^2y/dt^2, the filter coefficients can be made more efficient by applying the factor δ_y to all Savitsky-Golay coefficients, which can then be directly applied to the rotary encoder count. Also remember to apply a factor of 2 to the row of coefficients for $\mathbf{a}_2$ to take into account $d^2y/dt^2 = 2\mathbf{a}_2$.

If the measurement probability distribution for the rotary count is assumed uniform with a width of $\pm 1/2$ a count, the standard deviation is $\sqrt{1/12}$ counts or $\sigma_y = \delta_y/\sqrt{12}$. This is needed to determine the covariance matrix.

The LabVIEW programs for the Savitsky-Golay filtering are SavGolRaw.vi, which gives $[[\mathbf{m}][\mathbf{m}]^T]^{-1}[\mathbf{m}]$ and SavGolCoef.vi, which gives the zeroth, first, and second derivative coefficients, i.e., the first, second, and third row of $\delta_y[\mathbf{U}]^{-1}[[\mathbf{m}][\mathbf{m}]^T]^{-1}[\mathbf{m}]$, with the third row multiplied by 2. The Excel spreadsheet SG.xls shows graphs of the 33-point quartic polynomial filters. It also gives the covariance matrix for the filter coefficients and the uncertainties in the filtered y, dy/dt, and d^2y/dt^2.