Linear least squares problems and smoothing filters

Krystyna Ziętak (Wroclaw)

Iwona Wróbel (Warsaw)

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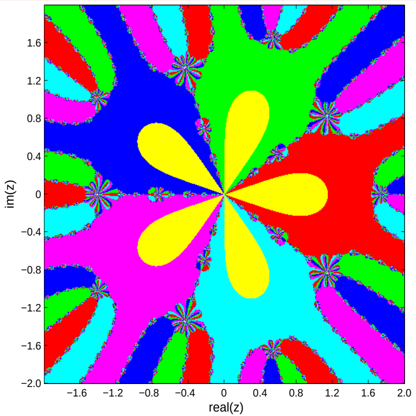
Outline

Goal of talk is to show that false formula can lead to better method.



Task

Given points $t_1 < \ldots < t_m$ and measured data corrupted by random noise

$$y_1, \ldots, y_m.$$

Compute smoothed value of y_i

$$\widetilde{y}_i = \sum_{j=-N_L}^{N_R} g_j y_{i+j}$$

where g_j are filter coefficients

Concept of Savitzky and Golay (1964)

interior point t_i: $1 + N_L \leq i \leq m - N_R$

polynomial $v(t)$ approximates data
over the set of points $\{t_{i-N_L}, \ldots, t_{i+N_R}\}$

in the least-squares sense

smoothed $\widetilde{y}_i = v(t_i)$

$N_L = N_R = N$

$$\widetilde{y}_i = v(t_i) = \sum_{j=-N}^{N} g_j y_{i+j} = g^T y$$

$$g = A_i (A_i^T A_i)^{-1} A_i^T e$$

A_i rectangular Vandermonde, $t_{i-N}, \ldots, t_{i+N}$

$$y = [y_{i-N}, \ldots, y_{i+N}]^T$$

$$e = [0, \ldots, 0, 1, 0, \ldots, 0]^T$$

Uniformly spaced data $t_{j+1} - t_j = \Delta$

new variable, $t \rightarrow h = (t - t_i)/\Delta$

new points $t_j \rightarrow h_j = j - i \quad t_i \rightarrow 0$

Savitzky-Golay filter coefficients

$$g^T = [g_{-N}, \dots g_N]$$

$$g = A_i(A_i^T A_i)^{-1} A_i^T e =$$
$$= B(B^T B)^{-1} B^T e = B(B^T B)^{-1} e_1$$

B rectangular Vandermonde, $-N, \dots, N$

$$e_1 = [1, 0, \dots, 0]^T, \quad e = [0, \dots, 0, 1, 0, \dots, 0]^T$$

$$B = \begin{bmatrix} 1 & -N & (-N)^2 & \cdots & (-N)^n \\ 1 & -N+1 & (-N+1)^2 & \cdots & (-N+1)^n \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & N & N^2 & \cdots & N^n \end{bmatrix}$$

$$C = \begin{bmatrix} (-N)^n & (-N)^{n-1} & \cdots & -N & 1 \\ (-N+1)^n & (-N+1)^{n-1} & \cdots & -N+1 & 1 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ N^n & N^{n-1} & \cdots & N & 1 \end{bmatrix}$$

How to compute $g = B(B^T B)^{-1} e_1$?

n degree of approx. polynomial

$$C = QR$$

$$g = \frac{1}{r_{n+1,n+1}} Q e_{n+1}$$

Gander, von Matt

Orthogonal (discrete) Gram polynomials

orthogonal over point set $\mathcal{S}_N = \{-N, \ldots, N\}$

$$q_j(h) = \sum_{k=0}^{j} (-1)^{k+j} \frac{(j+k)^{(2k)}(N+h)^{(k)}}{(k!)^2 (2N)^{(k)}}, \quad q_0(h) = 1,$$

$$a^{(0)} = 1$$
$$a^{(k)} = a(a-1)\cdots(a-k+1)$$

"discrete" Dirac delta

$$\delta_N = e = [0, \ldots, 0, 1, 0, \ldots, 0]^T \in \mathbb{R}^{n+1}$$

$$\mathcal{S}_N = \{-N, \ldots, N\}, \qquad n \quad \text{degree, even}$$

polynomial least-squares approximation over $\mathcal{S}_N$ to δ_N

$$q(h) = \frac{q_n(0) q_{n+1}(h)}{\xi \eta h}$$

ξ and η constant, depend on n and N

filter coefficients $g^T = [q(-N), \ldots, q(N)]$

orthogonal Legendre polynomials $[-1, 1]$

$$\langle P_i, P_j \rangle = \int_{-1}^{1} P_i(s) P_j(s) ds.$$

recurrence relation

$$P_k(s) = \frac{2k-1}{k} s P_{k-1}(s) - \frac{k-1}{k} P_{k-2}(s), \quad k = 1, 2, \ldots$$

$$P_0(s) = 1.$$

linear change of variable

$$[-1, 1] \to [-N, N]$$

Filter coefficients

Dirac delta $\delta(s)$

$$\delta(s) = 0 \quad \text{for } s \neq 0,$$
$$\delta(s) = \infty \quad \text{for } s = 0,$$

Persson-Strang

least-squares approximation to Dirac delta on interval $[-N, N]$ expressed by Legendre polynomials

Savitzky-Golay

least-squares approximation to vector
$e = [0, \ldots, 0, 1, 0, \ldots, 0]^T$
over the point set $\{-N, -N+1, \ldots, N\}$

Persson and Strang filter (2003)

degree of polynomial n even, $[-N, N]$

uniformly spaced data, filter coefficients $g_{-N}, \ldots, g_N$

Persson-Strang polynomial $g_j = L(j)$

$$L(h) = \frac{n+1}{2} P_n(0) \frac{P_{n+1}\left(\frac{2h}{2N+1}\right)}{h}$$

Optimal "Legendre" polynomial $g_j = K(j)$

$$K(h) = \frac{n+1}{2} P_n(0) \frac{P_{n+1}\left(\frac{h}{N}\right)}{h}$$

Examples of approximating polynomials $n = 2$

- Savitzky-Golay (Gram)

$$q(h) = \frac{-15h^2}{(2N-1)(2N+1)(2N+3)} + \frac{9N^2+9N-3}{(2N-1)(2N+1)(2N+3)}$$

- Persson-Strang

$$L(h) = \frac{-15h^2}{(2N+1)^3} + \frac{9}{4(2N+1)}$$

- optimal Legendre

$$K(h) = \frac{-15h^2}{8N^3} + \frac{9}{8N}$$

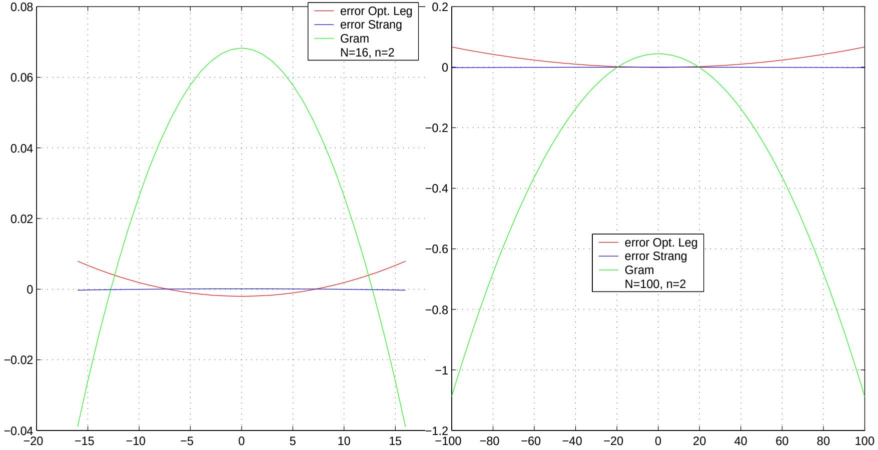


Figure : Savitzky-Golay polynomial $q(h)$ (green); differences $q(h) - L(h)$ and $q(h) - K(h)$; $N = 16$ (on left), $N = 100$ (on right); degree $n = 2$

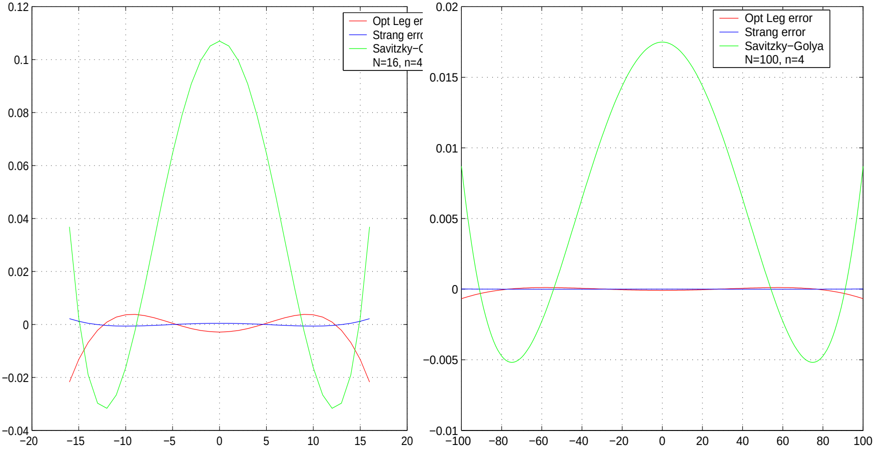


Figure : Savitzky-Golay polynomial $q(h)$ (green); differences $q(h) - L(h)$ and $q(h) - K(h)$; $N = 16$ (on left), $N = 100$ (on right); degree $n = 4$

Gander and von Matt test function on $[0, 1]$

$$F(t) = e^{-100(t-\frac{1}{5})^2} + e^{-500(t-\frac{2}{5})^2} + e^{-2500(t-\frac{3}{5})^2} + e^{-12500(t-\frac{4}{5})^2}$$

- uniform spaced data;
  $t_j = \frac{j-1}{m-1}$ for $j = 1, \ldots, m$, where $m = 1000$
- $y_j = F(t_j) + \varepsilon \times randn$, where $\varepsilon = 0.1$
- degree of polynomial $n = 4$
- window $N = 16$

Savitzky-Golay, Persson-Strang, optimal Legendre

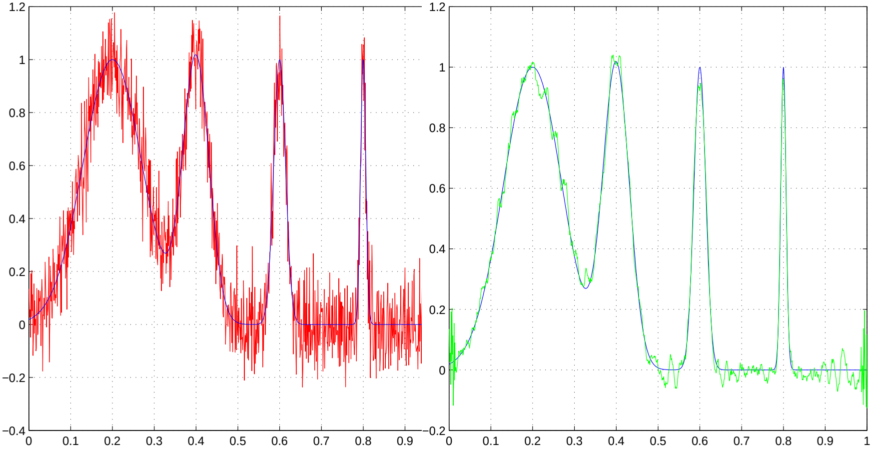


Figure : $F(t)$ exact and noise (on left); $F(t)$ exact and smoothed by Savitzky-Golay (on right)

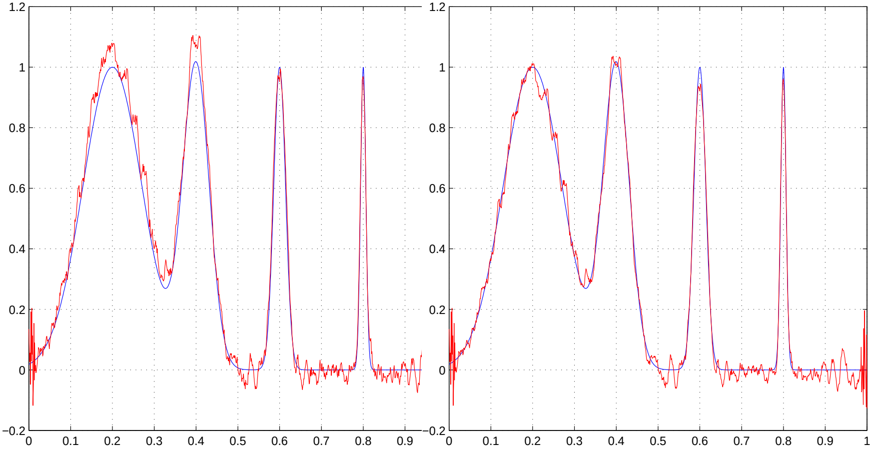


Figure : $F(t)$ exact and smoothed by optimal Legender (on left); $F(t)$ exact and smoothed by Persson-Strang (on right)

Errors: $F(t)$ exact – smoothed data (subtraction)

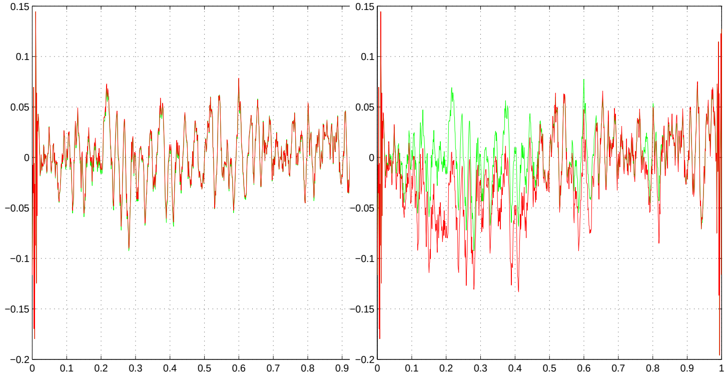


Figure : Savitzky-Golay (green) and Persson-Strang (red), (on left); Savitzky-Golay (green), optimal Legendre (red), (on right)

Gander-von Matt test function on $[0, 0.5]$

$$F(t) = e^{-100(t-\frac{1}{5})^2} + e^{-500(t-\frac{2}{5})^2} + e^{-2500(t-\frac{3}{5})^2} + e^{-12500(t-\frac{4}{5})^2}$$

- uniform spaced data;
  $t_j = \frac{j-1}{m-1}$ for $j = 1, \ldots, m$, where $m = 1000$
- $y_j = F(t_j) + \varepsilon \times randn$, where $\varepsilon = 0.1$
- degree of polynomial $n = 4$
- window $N = 32$

Savitzky-Golay, Persson-Strang, optimal Legendre

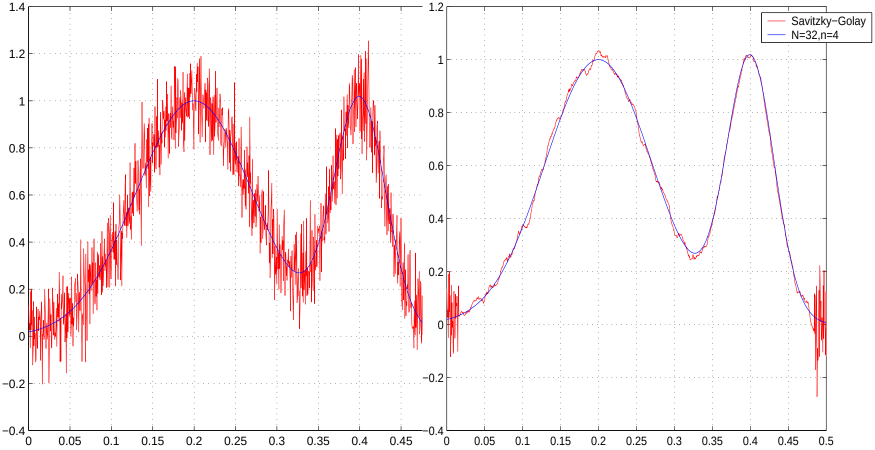


Figure : $F(t)$ exact and noise (on left); $F(t)$ exact and smoothed by Savitzky-Golay (on right); $N = 32, n = 4$

Errors: $F(t)$ exact – smoothed data (subtraction)

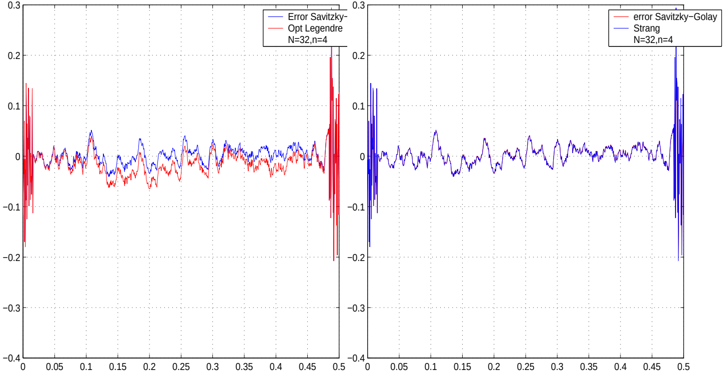


Figure : error Savitzky-Golay (blue), optim. Legendre (red), on left; error Savitzky-Golay (blue), Persson-Strang (red), on right, $N = 32, n = 4$

Persson and Strang write that the Legendre-based filters have extra advantages:

> “*in the case of irregularly spaced or missing data the polynomials stay the same and it is only the sampling points that change. (...)*
>
> The simplicity becomes especially valuable when the input no longer consists of uniformly spaced samples.
> The output from the new filter will be the natural non-uniform generalization of an ordinary convolution".

$$[t_{i-N}, t_{i+N}] \to [-N, N]$$

window $t_{i-N_L}, \ldots, t_{i+N_R}$

new variable

$$h = \frac{t - t_i}{\Delta t}, \qquad \Delta t = \frac{t_{i+N_R} - t_{i-N_L}}{N_L + N_R}$$

new points

$$h_j^{(i)} = \frac{t_j - t_i}{\Delta t} \quad \text{for } j = i - N_L, \ldots i + N_R.$$

$$\alpha_i = h_{i-N_L}^{(i)}, \qquad \beta_i = h_{i+N_R}^{(i)}$$

approximation of Dirac delta on $[\alpha_i, \beta_i]$

$P_k(t)$ Legendre polynomial

$[-1, 1] \to [\alpha_i, \beta_i]$

$$Z_k^{(i)}(h) = P_k\left(\frac{2}{\beta_i - \alpha_i}h + \frac{\alpha_i + \beta_i}{\alpha_i - \beta_i}\right)$$

$$K^{(i)}(h) = \frac{n+1}{2} \cdot \frac{Z_{n+1}^{(i)}(0)Z_n^{(i)}(h) - Z_n^{(i)}(0)Z_{n+1}^{(i)}(h)}{-h}$$

$$\tilde{y}_i = \sum_{j=i-N_L}^{i+N_R} g_j^{(i)} y_j, \quad \text{where } g_j^{(i)} = K^{(i)}(h_j^{(i)})$$

Bad news

A. Eisinberg, P. Pugliese, N. Salerno,
Numer. Math. 2001

Vandermonde matrices on integer nodes: the rectangular case

their case

$$1, 2, \ldots, N$$

- $B = V^T V$ Hankel matrix
- explicit Cholesky factor of B
- pseudo-inverse of V
- combinatorial identities

our case

$$-N, \ldots, N$$

References

Abraham Savitzky (1919–1999)
was an Americal analytical chemist. He specialized in the digital processing of infrared spectra.

Marcel J.E. Golay (1902–1989)
was a Swiss-born mathematician, physicst and information theorist.

Golay error-correcting codes

Savitzky coauthored with Marcel J.E. Golay an oft-cited paper describing the Savitzky-Golay smoothing filter.

THANK YOU FOR YOUR ATTENTION