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Whittaker Smoother

Neal B. Gallagher

Key words: Data fitting, smoothing penalty

Introduction: Data are often fit to a curve such as a low order polynomial or other basis function. However, at times the fitting functions are too restrictive and don't provide a good representation of the original data. A more flexible approach was developed by Eilers[1] and is further modified to provide additional flexibility as demonstrated by the `wsmooth` function in PLS_Toolbox and Solo.[2]

The Whittaker Smoother: Eiler's paper[1] introduces the following objective function

$$O(\mathbf{z}) = (\mathbf{y} - \mathbf{z})^T \mathbf{W}_0 (\mathbf{y} - \mathbf{z}) + \lambda_s \mathbf{z}^T \mathbf{D}_s^T \mathbf{D}_s \mathbf{z}$$

where \mathbf{y} is a $N \times 1$ vector of measured data, \mathbf{z} is smooth curve to be fit to the data, \mathbf{W}_0 is a diagonal matrix of weights (typically $0 \leq w_{0,n} \leq 1$ for $n = 1, \dots, N$, \mathbf{D}_s is a second derivative operator (e.g., $\mathbf{D}_s \mathbf{z}$ is the second derivative of \mathbf{z}) and λ_s is a scalar penalty on the smoothing term. When data are missing, the corresponding weight, $w_{0,n}$, can be set to zero. Once that \mathbf{W}_0 and λ_s are given (set by default or provided by the user) the corresponding estimate of \mathbf{z} is given by

$$\hat{\mathbf{z}} = (\mathbf{W}_0 + \lambda_s \mathbf{D}_s^T \mathbf{D}_s)^{-1} \mathbf{W}_0 \mathbf{y}.$$

For example, an optical emission (OES) spectrum is plotted Figure 1 along with two smoothed versions shown for $\mathbf{W}_0 = \mathbf{I}$ and $\lambda_s = 0.1$ (low smoothing) and $\lambda_s = 10$ (stronger smoothing). The optical emission spectra are available at www.eigenvector.com and discussed in References [3,4]. The stronger smoothing (green curve) appears to suppress the noise better than the weak smoothing but it also suppresses the peaks more. With a slight modification to the objective function, the best of both worlds can be obtained.

The Modified Whittaker Smoother: The original smoother can be modified to allow for different smoothness weighting on each of the channels using

$$O(\mathbf{z}) = (\mathbf{y} - \mathbf{z})^T \mathbf{W}_0 (\mathbf{y} - \mathbf{z}) + \lambda_s \mathbf{z}^T \mathbf{D}_s^T \mathbf{W}_s \mathbf{D}_s \mathbf{z}$$

where \mathbf{W}_s is a diagonal matrix of weights with entries $0 \leq w_{s,n} \leq 1$ and corresponding estimator given by

$$\hat{\mathbf{z}} = (\mathbf{W}_0 + \lambda_s \mathbf{D}_s^T \mathbf{W}_s \mathbf{D}_s)^{-1} \mathbf{W}_0 \mathbf{y}.$$

For the example, lowering the weights in \mathbf{W}_s from 1 to 0.1 for the wavelengths (λ) with peaks corresponding to $258 < \lambda < 280$, $307 < \lambda < 311$ and $393 < \lambda < 397$, the smoother gives the final smoothed spectrum in Figure 2 (the black curve). The smooth black curve follows the green curve outside the peak ranges and the red curve with the peak ranges.

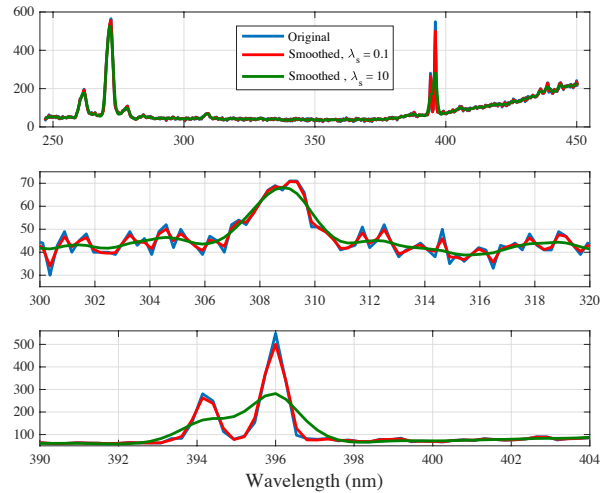


Figure 1: Uncorrected OES spectrum (blue), smoothed spectrum $\lambda_s = 0.1$ (red) and strongly smoothed spectrum $\lambda_s = 10$ (green). Zoom in on a small peak (middle) and significant sharp peaks (bottom).

A primary objective of smoothing, and preprocessing in general, is to increase the signal-to-noise (or more precisely signal-to-clutter). The eigenvalue distribution from PCA for a set of 46 OES spectra is

shown in Figure 3 for the original data and the three different smoothing approaches. The eigenvalue distribution for principal components (PCs) ≥ 6 are mostly attributable to noise. A proxy for S/N is the ratio of the sum of the eigenvalues 1 to 5 to the sum of eigenvalues ≥ 6 shown in the figure. The original spectra and the low smoothing appear to have the lowest S/N while the higher smoothing has the biggest S/N. Interestingly, relaxing the smoothing on the peaks appears to lower the S/N slightly compared to including smoothing over all the wavelengths.

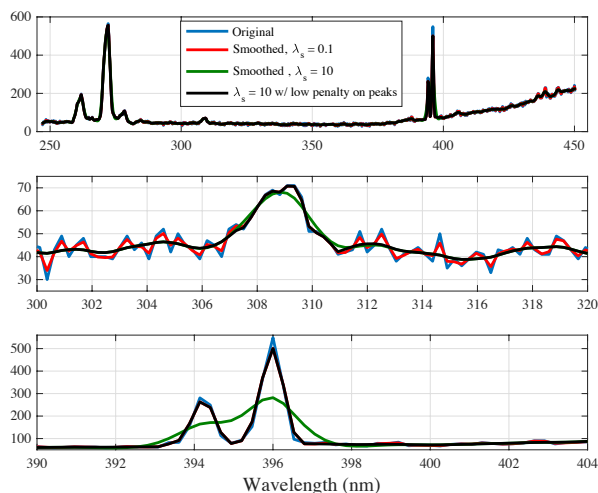


Figure 2: Uncorrected OES spectrum (blue), smoothed spectrum $\lambda_s = 0.1$ (red) and strongly smoothed spectrum $\lambda_s = 10$ (green). Strong smoothing except for the peaks (black) Zoom in on a small peak (middle) and significant sharp peaks (bottom).

Conclusions: Smoothing is a useful tool for providing interpretable trends given by the smoothed signal and has the potential to improve signal-to-noise.

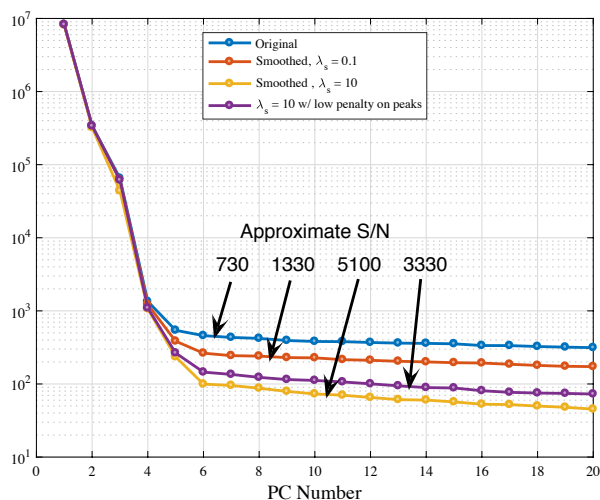


Figure 3: Eigenvalue distributions for the original signal and three versions of the smoothed signal for a set of 46 OES spectra.

References:

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