Proceeding Series of the Brazilian Society of Computational and Applied Mathematics, v. 8, n. 1, 2021.

Trabalho apresentado no XL CNMAC, Evento Virtual - Co-organizado pela Universidade do Mato Grosso do Sul (UFMS).

Proceeding Series of the Brazilian Society of Computational and Applied Mathematics

Applications of nonlinear and fractional diffusion processes to signal processing in Raman spectroscopy

André Persechino[1]
CBPF, Rio de Janeiro, RJ

Raman Spectroscopy (RS) is a powerful analytical technique, based on the inelastic scattering of light by the analyte. Its versatility lies on the fact that a wide range of materials can be analyzed in a non-destructive testing (NDT) fashion, ranging from bulk mineralogy to characterization of highly sensitive biological samples [6]. Despite such "universality", Raman scattering cross-section is quite small, in such a manner signals are very often observed in noisy environments, accounting different contributions, e.g. from fluorescence and CCD shot noise.

To extract both qualitative and quantitative information, signal undergoes noise suppression processes. This suppression is often achieved through signal smoothing with linear low-pass (LP) filters. However, linear shift-invariant (LSI) filters are isotropic, which means that the signal relevant features (peaks, steps, backgrounds etc.) are suppressed by LP filters in the same way noise itself is.

Preserving peaks while one suppresses random noise is a contradiction, in the classical sense. However, embedding the signal into a scale-space representation [2] allows one to separate features according their hierarchical position, given a set of chosen requisites. It is possible to show that a scale-space representation which ensures linearity, homogeneity and minimum-maximum principles is completely equivalent to evolve the signal through a linear diffusion process. It is well known, however, that such evolution leads to a complete degradation of the signal, since the solution of the initial value problem in question is given by a convolution between initial datum and a Gaussian kernel with variance dependent on t, $\sigma^2 = 2t$. Since Gaussian kernels are zero-phase, oscillation-free isotropic LP filters, as t (the scale-parameter) increases, the signal tends to a constant representation, in which all information is lost. To circumvent such condition, Perona and Malik [4] proposed a nonlinear diffusion process, ruled by

$$\begin{cases} \partial_t u = \nabla \cdot \left[f\left(|\nabla u| \right) \nabla u \right] \\ u(x,0) = u_0(x), \end{cases} \tag{1}$$

in which $f(\xi)$ is a positive monotonically decreasing function for $\xi > 0$. Its role is to regulate the diffusion strength according signal variations, detected by $|\nabla u|$.

Despite its importance in image processing theory, Perona-Malik Equation (PME), given by Eq.(1) does not play a major role in spectroscopy. In fact, up to our knowledge, PME first appearance took place in 2016, when Li, Ding and Li [3] used nonlinear diffusion in nuclear magnetic resonance (NMR) signal enhancement. In this sense, we present a formal introduction of the PME framework in RS signal processing, since the latter constitutes an appropriate object to application of robust noise suppression procedures. In fact, our goal is twofold:

1. understand whether the PME is in fact an adequate resource to enhance and preserve peaks in RS; and

[1]aamerico@cbpf.br

2. investigate possible alternatives in the diffusion process, such as a generalization to derivatives of fractional order.

Concerning with the first item, we carry out massive numerical experiments on simulated and real data, varying PME many parameters in order to check their influence on the global performance of the technique, mainly determined by its capability to suppress noise in such a manner peaks remain as unchanged as possible. We observe that – to some extent – PME filter leads to a robust noise reduction, preserving peaks position more efficiently than filters based on Continuous Wavelet Transform (CWT), such as the one introduced by Du *et al.* [1]. In this sense, we advocate the use of PME as a tool for peak detection, another crucial step in RS. However, due the strong dependence of the PME on its parameters, we are investigating in which conditions it supersedes CWT-based filters, since numerical methods for nonlinear diffusion can be computationally expensive.

On other hand, we seek extensions to diffusion processes in RS signal processing. The motivation to carry out such investigation lies on the fact that scale-space representations are built on an axiomatic basis, allowing one to insert additional criteria to improve/suppress a set of attributes on the final representation. In the present context, we look for theoretical backgrounds which take into account non-local correlations among signal components. Fractional calculus (FC) machinery seems to constitute a well-suited framework to this kind of analysis, demanding the use of complex numerical methods [5] to approximate temporal and/or spatial derivatives in the fractional diffusion equation:

$$\begin{cases} D_t^{\alpha} u = D_x^{2\beta} u \\ u(x,0) = u_0(x) \end{cases} \qquad \text{with } \alpha, \beta > 0, \tag{2}$$

in which D stands for derivative operator.

As a final goal, we intend to benchmark PME against fractional diffusion, in order to acquire some basis on the real need into adopting more complex evolution processes, or whether a consistent parameter adaptation suffices to enhance RS signal, allowing efficient extraction of information.

References

[1] Du, P., Kibbe, W. A., Lin, S. M. Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching. *Bioinformatics*, 22:2059–2065, 2006. DOI: 10.1093/bioinformatics/btl355.

[2] Duits, R., Florack, L., de Graaf, J., Romeny, B. ter Haar. On the Axioms of Scale Space Theory. *Journal of Mathematical Imaging and Vision*, 20:267–298, 2004. DOI: https://doi.org/10.1023/B:JMIV.0000024043.96722.aa.

[3] Li, Y., Ding, Y., Li, T. Nonlinear diffusion filtering for peak-preserving smoothing of a spectrum signal. *Chemometrics and Intelligent Laboratory Systems*, 156:157–165, 2016. DOI: http://dx.doi.org/10.1016/j.chemolab.2016.06.007.

[4] Perona, P., Malik, J. Scale-space and edge detection using anisotropic diffusion. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 12:629–639, 1990. DOI: 10.1109/34.56205

[5] Persechino, A. Introduction to fractional calculus: Numerical methods and application to HF dielectric response. *Advanced Electromagnetics*, 9:19–30, 2020. DOI: https://doi.org/10.7716/aem.v9i1.1192

[6] Turrell, G., Corset, J. (Edits.). *Raman Microscopy: developments and applications, 1st ed.* Elsevier Academic Press, Oxford, 1996.