

# Improved Performance Baseline Correction Methods for Raman Spectroscopy

VTIP 20-065: “ISREA: An Efficient Peak-preserving Baseline Correction Algorithm for Raman Spectra”

## THE CHALLENGE

Raman spectroscopy is an established tool used for both qualitative and quantitative analyses of molecular composition of materials and biological systems. In Raman spectrum generation, a background signal generated by fluorescence or Rayleigh scattering can heavily interfere with analysis of underlying Raman spectrum. This background signal, commonly known as the baseline, often appears as a smooth curve in the raw spectrum. Currently used smooth functions and loss functions have limitations that can distort Raman spectroscopic data and methods with improved efficiency are needed.

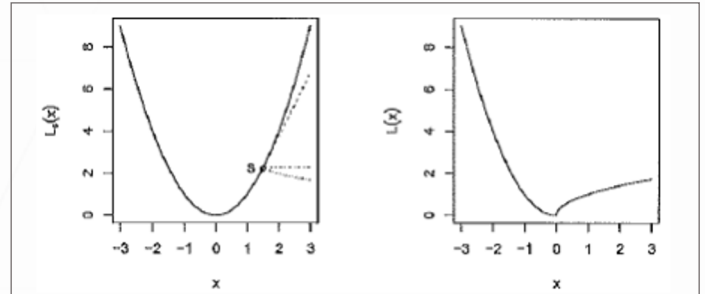
## OUR SOLUTION

Virginia Tech researchers have developed a baseline correction method called the Iterative Smoothing-splines with Root Error Adjustment (ISREA). ISREA is a statistically-based method for normalizing complex Raman spectroscopic data for analysis. Normally, Raman spectral data is collected across a wide band of wave numbers and some of this data is not meaningful due to artifacts of measurement and collection. The proposed invention will make more meaningful and rapid analysis of spectral data possible.



**CONTACT:**

**Grant Brewer**  
[grantb76@vt.edu](mailto:grantb76@vt.edu)  
 540-231-6648



Symmetric loss function compared with proposed asymmetric.

	Andersonite	Eastonite	Marialite	Parascholzite	Sugilite	Wadeite	
Goldindec	0.7822	0.8546	0.9878	0.9413	0.9598	0.8044	
ISREA	NK=5	0.8789	0.9479	0.9936	0.9740	0.9923	0.8910
	NK=10	0.9653	0.9484	<b>0.9966</b>	0.9806	<b>0.9913</b>	0.9055
	NK=15	<b>0.9872</b>	0.9818	0.9951	<b>0.9824</b>	0.9875	0.8938
	NK=20	0.9800	<b>0.9884</b>	0.9924	0.9814	0.9823	<b>0.9152</b>
	NK=25	0.9861	0.9805	0.9888	0.9717	0.9781	0.9140

Performance comparisons between Goldindec and ISREA for six minerals.

	Mean	Standard deviation
Goldindec	0.2559	0.2282
ISREA	NK=5	0.0446
	NK=10	0.1238

Similarity change comparisons of ISREA and Goldindec on dialysate spectra.

	1000 simulated spectra	50 dialysis spectra
Goldindec	885.36	38.54
ISREA	24.13	8.76

Computational time (in seconds) comparisons between Goldindec and ISREA.

