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Innovations in Modelling Spectral Data

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Spectroscopy and chromatography data - from methods such as FTIR, NMR, mass spectroscopy, and HPLC - are ubiquitous in chemical, pharmaceutical, biotech and other process industries. Until now, scientists didn't have good ways to use this data as part of designed experiments or machine learning applications. They were required to 'extract features' such as the mean, peak height, or a threshold crossing point. Summarising and approximating the spectral data in this way meant that models were less accurate and difficult to interpret.

Now you can directly model these data types in designed experiments and machine learning applications with Functional Data Explorer in JMP Pro. Wavelet analysis is a new capability in the platform that make it easier than ever to build models that treat spectral data as first-class citizens in their own right.

Keywords

Spectroscopy, DOE, Machine Learning

Classification

Both methodology and application

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Session Classification: INVITED Software

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