

## DERIVATIVE SPECTROSCOPY—AN ENHANCED ROLE FOR NUMERICAL DIFFERENTIATION

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ABSTRACT. In many areas of science, through the use of modern computer-controlled instrumentation, highly accurate indirect measurements of the phenomenon/process of interest are being generated on a (very) fine spatial and/or temporal grid. Consequently, this is creating new opportunities for the enhanced recovery of information about the underlying phenomenon/process being studied. In particular, an enhanced role for numerical differentiation is emerging in the application of *derivative spectroscopy*, which has its origins in the analysis of various forms of spectroscopic data. For example, through its use, information about the molecular components in plant material, such as barley seeds, is being recovered by comparing the fourth derivatives of their measured near infra-red (NIR) spectroscopic responses. As well as practical matters that arise with the utilization of derivative spectroscopy in the recovery of information, there are theoretical questions that require investigation about the choice of the numerical differentiator, the interpretation of the fourth derivative and an assessment of how high a level of differentiation that given data will support. Such matters have already been investigated in considerable detail except for the question of estimating the maximum level of differentiation that given data can support before the onset of instability. This is the focus of the current paper, which highlights how published results can be reinterpreted to answer this question. In particular, it will be shown that, if circumstances are such that, for a particular numerical differentiator, an accurate approximation to the first derivative of the available observational data can be guaranteed, then it is highly likely that it can be utilized to generate good approximations to second, third and fourth derivatives. Interestingly, this runs contrary to the historical view that, as the order  $k$  of the differentiation of observational data increases, the onset of instability increases rapidly.

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