
Learning to Read Spectra: Teaching Decomposition with Excel in a Scientific Writing Course

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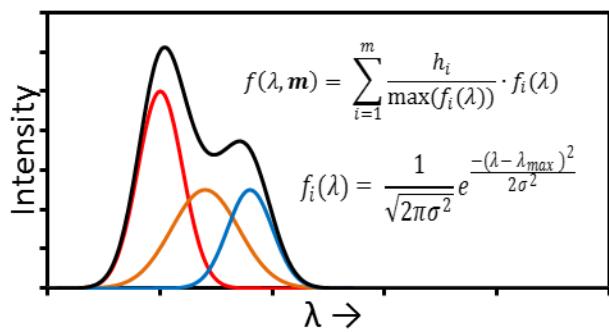
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ABSTRACT

Literacy requires reading comprehension and fostering reading skills is an essential prerequisite to and a synergistic enabler of the development of writing skills. Reading comprehension in the chemical sciences not only consists in the understanding of text but also includes the reading and processing of data tables, schemes, and graphs. Thus, education in *Scientific Writing in Chemistry* cannot focus on writing alone, but such efforts must aim both at the development of higher level skills in reading and writing and, moreover, the reading instruction ought to occur concurrently with or precede the writing exercise. In this context, a computer laboratory experiment is described which develops students' *Learning to Read Spectra*. The computer laboratory experiment cultivates students' Excel skills with the specific objective of teaching them how individual transitions overlap in spectra. Qualitative decomposition and an automated *Solver* extension method are discussed. Qualitative decomposition is best suited to develop students' understanding of overlapping transitions and spectra and to advance their conceptual knowledge. Learning to use *Solver* is a valuable *additional* skill, but the automated process is no substitute for the learning experience provided by the qualitative decomposition.

GRAPHICAL ABSTRACT



KEYWORDS

25 Upper-Division Undergraduate; Curriculum; Laboratory Instruction; Analytical Chemistry; Collaborative / Cooperative Learning; Communication / Writing; Computer-Based Learning; Problem Solving / Decision Making; Applications of Chemistry; Constructivism; Laboratory Computing / Interfacing; Spectroscopy.

INTRODUCTION

There is general agreement that chemistry students need to develop their skills to analyze data, solve complex problems, and clearly communicate their findings. All of these skills are taught in the writing-intensive *Undergraduate Seminar in Chemistry* (CHEM 3700W) for upper division chemistry majors at the University of Missouri, Columbia. An assignment-based curriculum *Scientific Writing in Chemistry* was developed to teach scientific writing and peer review. The curriculum consists of a framework of assignments and the theme changes with every implementation.¹ All tasks are performed in pairs and students are asked to complete eleven assignments including one oral presentation. The submissions are peer-reviewed using criteria-based rubrics and the students need to prepare and submit revisions in response to the peer reviews. Assignments A01 – A07 focus on the development of specific skills (writing, graphing, image art, tables, information access & data mining, quantitative data analysis) and assignments A08 - A11 engage the students in a near-authentic exercise of scientific writing and of the science publication process: Syllabi, schedules, assignments and rubrics are available at the CHEM 3700W course web sites which are accessible to the public, and we refer here especially to the web sites of the courses taught in spring semester of 2016 (SP16) and 2017 (SP17).²

Microsoft Excel is a common program used to automate calculations, analyze data, and create graphs. Textbooks are available that focus on applications of Excel in chemistry^{3,4} and teach Excel functions and techniques directly alongside the chemical theory.⁵ Several articles in the *Journal* describe exercises to develop Excel skills with applications ranging from elementary quantitative analysis,⁶ to FTIR spectroscopy,⁷ and the deconvolution⁸ of gas chromatograms.⁹

Spectra show the envelope resulting from the superposition of all individual peaks of a molecule or a mixture of molecules. Decomposition consists in the resolution of a complex spectrum into these discrete bands. Methods for computational decomposition have been described in the literature since the 1970s, and they usually employ Gaussian curves to approximate absorption bands.¹⁰⁻¹³ Solution state ultraviolet/visible (UV/Vis) spectra are well known to have broad peaks because of the vast number of vibrational and rotational microstates and the Doppler and lifetime broadening.^{14,15} While not to the same extent, infrared (IR) peaks are widened by rotational microstates as well as Doppler

and lifetime broadening.¹⁶ Peak broadening leads to overlap and decomposition can determine the approximate centers, heights, and widths of each of the underlying bands.¹⁷

60 Here we describe a computer lab experiment to teach the qualitative decomposition of an authentic spectrum published in the contemporary research literature. This activity is a major part of assignment A04 and builds on skills acquired in assignment A03: an introduction to Excel tables, graphs, statistics, and the normal curve. Both A03 and A04 have been included in the CHEM 3700W curriculum in every implementation since 2010. In this spectrum simulation, students predict the 65 parameters for the primitive Gaussian curves that make up the overall spectrum. The parameters of each primitive Gaussian are iteratively adjusted until the superposition of the primitives closely resembles the experimental spectrum. This computer simulation serves three main objectives. First, it builds spreadsheet skills that are important for analyzing and presenting large data sets for professional scientists. Second, this activity helps students to realize the effect of overlapping peaks 70 and prepare them to interpret spectra they will encounter in the future. Third, the activity can easily be extended to replace the manual adjustment process to obtain the best fit with an automated iterative nonlinear regression. Hence, this part provides an opportunity to introduce Excel's *Solver* add-in.

75 **METHODS**

Our discussion focuses on spectral simulations assigned in SP16 and SP17. The UV/Vis spectra to be simulated in SP16 are shown in Figure 1 and were reported in an article¹⁸ published in *RSC Advances* by Sarkar et al. In SP17, the students simulated IR spectra published in an article¹⁹ by Weinstein, Hartl, et al. in *Inorganic Chemistry* just a few months earlier. Assignments A03 and A04 80 and the associated rubrics employed in SP16 and SP17 are included in the Supporting Information together with Excel workbooks for assignment A04 of both semesters.

Below the original spectra in Figures 1 and 2, the simulations are shown resulting by qualitative decomposition and by nonlinear regression. The first proposed method is a qualitative decomposition by estimation of the parameters of a set of primitive Gaussians that make up the overall spectra. A 85 fairly high level of accuracy can be achieved and, along the way to finding that perfect match, students

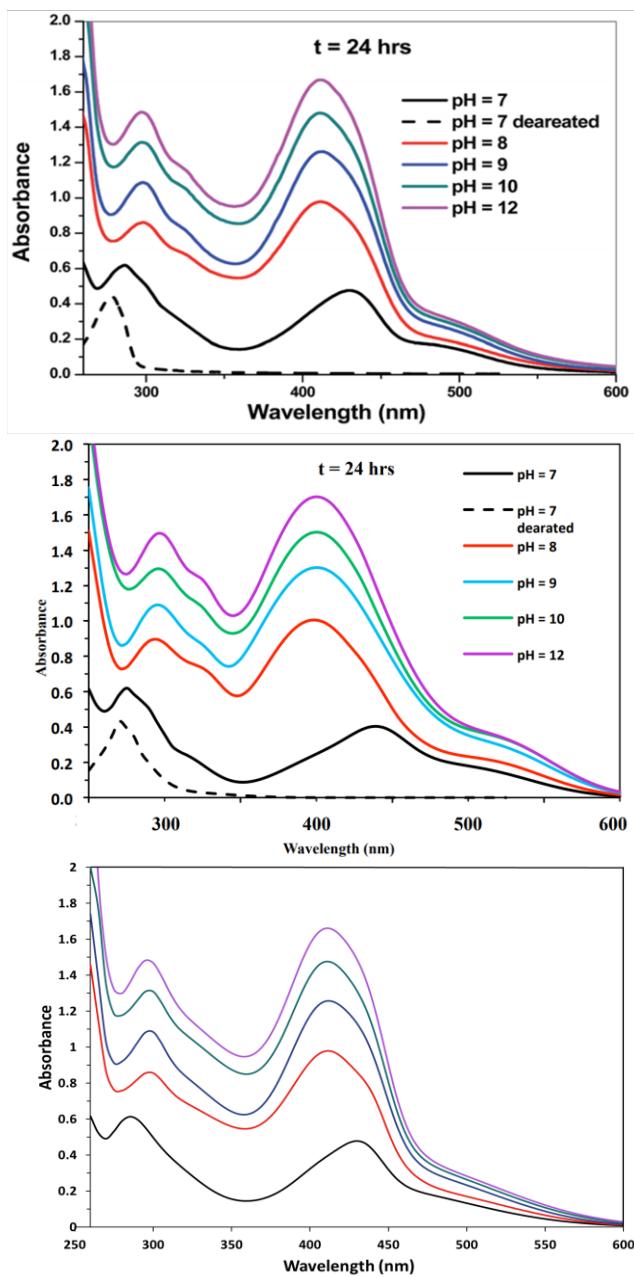


Figure 1. The top panel shows the reported UV/Vis spectra that are to be simulated (Fig. 1b in ref.

18, reproduced by permission of *The Royal Society of Chemistry*). The simulation shown in the middle panel is the result of a qualitative decomposition performed by students in SP16 with $n = 7$ primitive Gaussians (presented with permission). The simulation shown in the bottom panel was prepared by the authors by decomposition using the *Solver* extension method and $n = 6$ primitive Gaussians.

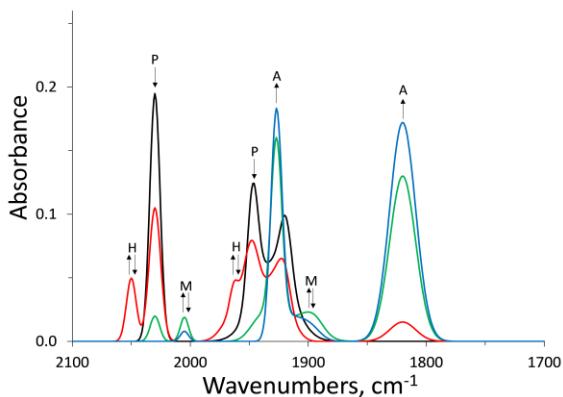
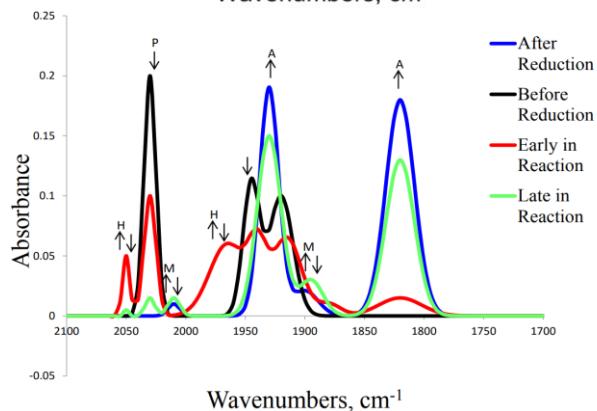
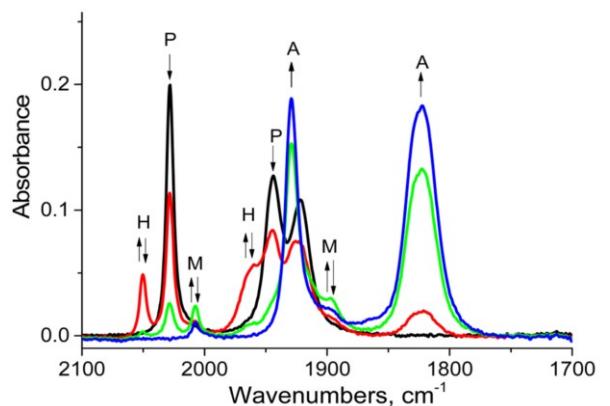


Figure 2. The top panel shows the reported IR spectra that are to be simulated (Fig. 9, bottom in ref. 19, reproduced by permission of *The American Chemical Society*). Letters refer to various compounds discussed in ref. 19 and arrows indicate decreasing (\downarrow) or increasing (\uparrow) concentration of substrate and products, respectively, and bands for intermediates first increase and then decrease ($\uparrow\downarrow$) in the course of the reaction. The simulation in the middle panel is the result of a qualitative decomposition performed by students in SP17 (presented with permission). The simulation in the bottom panel is the result of a decomposition performed using the *Solver* extension method.

will learn how the addition of primitive Gaussians can create shoulders and other heterogeneous features of a spectra. For ambitious students, or in a course that places more importance on the use of Excel, a more numerical method is also presented. A plot digitizer (software that transforms the image of a spectrum into a set of (x, y) coordinates that can be employed in computer processing) is used to replicate the measured spectrum to a high degree of precision and then *Solver* is employed to minimize the error between the digitized points and the sum of the primitives.

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	A	B	C
1	λ_{\max} (Center)	255	
2	Height	0.4	
3	Width (std. dev.)	7.9	
4			
5	λ (nm)	Normal Curve	Normed Gaussian
6	260	=NORM.DIST(A6 , B\$1 , B\$3 , FALSE)	= (B6/B\$76)*B\$2
7	= A6 + 5	=NORM.DIST(A7 , B\$1 , B\$3 , FALSE)	= (B7/B\$76)*B\$2
8	= A7 + 5	=NORM.DIST(A8 , B\$1 , B\$3 , FALSE)	= (B8/B\$76)*B\$2
...
74	600	=NORM.DIST(A74 , B\$1 , B\$3 , FALSE)	= (B74/B\$76)*B\$2
75			
76		=MAX(B6:B74)	

Figure 3. Layout of spreadsheet formulas for one Gaussian primitive in the simulation of one measured spectrum in Figure 1. The value in cell **A6** is the left bound of the wavelength and cell **A74** is the right bound. The “5” in cells **A7** through **A73** represents the selected step size.

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Qualitative Decomposition

To begin the decomposition, one should first consider the number of primitive Gaussians necessary. For the simulation of the IR spectra in Figure 2, the number of primitive Gaussians can be determined with some confidence. For example, it is highly probable that the blue spectrum is best described by four peaks, and the red line requires seven bands. For the spectra in Figure 1, on the other hand, an approach might require anywhere from five to seven Gaussians.

The basic layout of the data sheet is exemplified in Figure 3. For each Gaussian primitive curve, three parameters must be specified: the center of the curve, $\lambda_{\max,i}$, the width of the curve for which the

standard deviation (σ_i) will be used, and the height of the curve, h_i , and these three parameters should
120 be present at the top of the sheet (rows **1 – 3**). Below each set of parameters should be three columns
that contain respectively: wavelength (column **A**), normal curve (**B**), and a normed Gaussian (**C**). The
cells of the wavelength column should contain discrete values that cover the range of the measured
spectrum with a reasonable step size. Based on experience, it is recommended that a step size is
chosen such that there are 50 – 100 points between the left and right bounds. The cells of column **B**
125 contain a function which calculates the value of the normal curve at a given wavelength using the
center of the curve λ_{max} and the standard deviation σ . The normal curve is defined by Equation 1 and
this is a built-in function in Excel.

$$f_i(\lambda) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(\frac{-(\lambda - \lambda_{max,i})^2}{2\sigma_i^2}\right) \quad (1)$$

The height at the center of the normal curve is a function of the standard deviation because of its
130 normalization of the area integral to unity. To set the maximum of the curve to unity we divide the $f_i(\lambda)$
value by the maximum value $\max(f_i(\lambda))$ in column **B**. The value of the normed Gaussian in column **C** is
then obtained by multiplication by the height parameter h_i chosen as described in Equation 2.

$$n_i(\lambda) = \frac{h_i}{\max(f_i(\lambda))} f_i(\lambda) \quad (2)$$

Once one set has been created with properly defined references, this columns can be copied
135 directly to create data for as many primitives as necessary. This is exemplified by the A04 workbook
for SP16. The sheet labelled “pH 7” contains the equivalent of columns **A – C** of Figure 3 for the first
primitive in columns **B - D**, for the second primitive in columns **F - H**, for the third primitive in
columns **J - L**,....

The values in each normed Gaussian column for each wavelength are summed using Equation 3
140 and the sum is placed in another column, which creates the values of the simulated spectrum $g(\lambda)$. In
the sheet “pH 7” of the SP16 Excel A04 workbook, these values are contained in column **Z**. Plotting
the values of this set of cells **Z8:Z76** as a scatter plot with smooth lines as a function of the
wavelengths **B8:B76** generates the black spectrum curve in the bottom panel of Figure 1.

With the Excel sheet setup as described, the students are able to improve their simulation by
145 varying the initial parameters ($\lambda_{\max,i}$, σ_i , h_i) selected for each primitive. As one varies each primitive,

$$g(\lambda) = \sum_{i=1}^m n_i(\lambda) \quad (3)$$

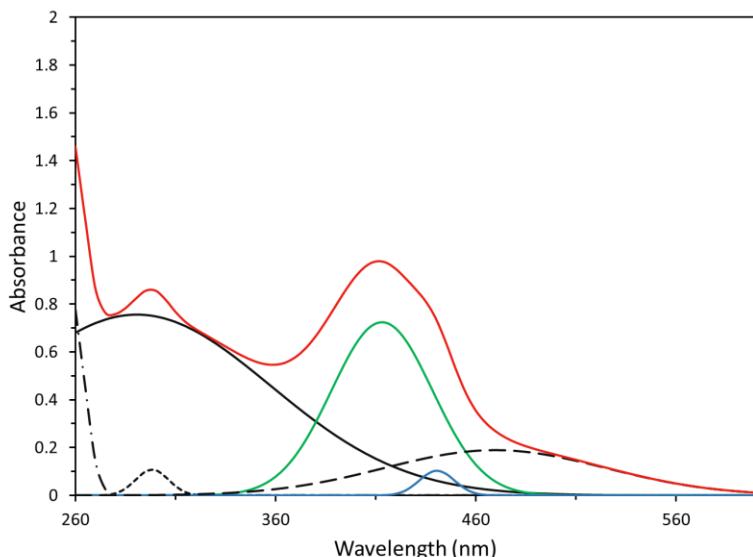
the sheet will automatically update the values for that primitive and anything linked to these values, including the values of the column in which primitives are summed and any charts referencing either set of cells. A video of this process is provided as part of Supporting Information. The stepwise
150 approach of Figure 3 is advantageous for the instruction of an audience with varying mathematical skills. Of course, this is not the only way to approach the problem, and some alternatives are described in Supporting Information.

For spectra with isolated bands (i.e., rightmost band in Fig. 2), the initial parameter selection is relatively straightforward. The initial λ_{\max} value of a primitive can be estimated to a certain degree of
155 accuracy just by finding the location of the band's maximum in the measured spectrum. The estimations of the width and height are slightly more complicated. For peaks that are clearly distinct from others, the full width at half maximum (FWHM) is about 2.355σ .²⁰ Therefore, the width parameter σ of the primitive can be approximated by selecting a value slightly lower ($\approx 18\%$) than half of the FWHM. The height parameter h is selected simply by measuring the height of the distinct peak.

160 The simulation of spectra with overlapping bands presents a much greater challenge both with regard to the initial choices of the parameters ($\lambda_{\max,i}$, σ_i , h_i) and their iterative optimization. In fact, in such cases it is not even clear at the beginning how many primitives will be needed for a successful simulation. The graphical abstract to this article shows how three primitives (shown in color) superimpose to an overall spectrum (black) that on first inspection might suggest the presence of just
165 two transitions. It takes some time for students to realize that the superposition of any two Gaussians will never quite fit the overall spectrum and that an additional transition must be present.

In Figure 1, the region $360 \text{ nm} < \lambda < 460 \text{ nm}$ contains one prominent band at about *ca.* 410 nm and the decomposition of this feature provides an authentic illustration that such asymmetric band shapes require at least two primitives. Figure 4 shows the spectrum for $\text{pH} = 8$ (red curve) together
170 with the primitives and the two primitives characterized by the parameter sets ($\lambda_{\max} = 413.07$, $\sigma =$

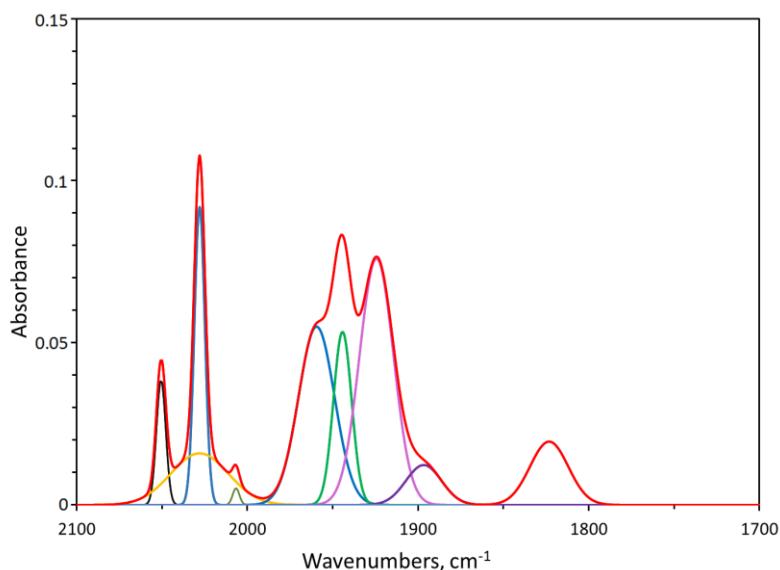
25.20, $h = 0.72$) and ($\lambda_{\max} = 440.49$, $\sigma = 8.75$, $h = 0.10$) result in the observed shape of the 410 nm feature. The approximation of parameters in this case must be performed iteratively and there might be many options. Generally, one wants to use $\lambda_{\max,i}$ values that are below and above the apparent λ_{\max} of the feature. For overlapping peaks, $\lambda_{\max,i}$ will be close to the observed maximum, though they will be skewed slightly away from the center of the overlapping bands and in opposite directions. There is no straightforward way to select initial values for the heights (h_i) and widths (σ_i) but rather the values must be discovered by trial and error.



180 **Figure 4.** Simulation of the spectrum measured at pH = 8 (cf. Figure 1). The simulated spectrum is shown in red and the result of superposition of the primitives shown in other colors. The primitives shown in blue and green result in the asymmetry of the feature at 410 nm.

185 Peaks with shoulders generally arise not from a large difference in the heights of the underlying bands, but rather a significant difference in their widths. Figure 5 illustrates this phenomenon by showing the primitive Gaussians that superimpose to form the red spectrum in Figure 2. As one can see in Figure 5, the left shoulder at ca. 1960 cm^{-1} is the result of the addition of a broader primitive at ca. 1960 cm^{-1} and a narrow primitive at ca. 1945 cm^{-1} which have nearly identical heights. Peaks with shoulders generally arise not from a large difference in the heights of the underlying bands, but

190 rather a significant difference in their widths. Figure 5 illustrates this phenomenon by showing the primitive Gaussians that superimpose to form the red spectrum in Figure 2. As one can see in Figure 5, the left shoulder at *ca.* 1960 cm^{-1} is the result of the addition of a broader primitive at *ca.* 1960 cm^{-1} and a narrow primitive at *ca.* 1945 cm^{-1} which have nearly identical heights. The addition of the tail of the broader peak with the narrow peak forms the highest peak of that feature (red, *ca.* 1945 cm^{-1}),
195 while the center of the broader peak does not overlap the tail of the thinner peak, and therefore creates a local maximum or shoulder.



200 **Figure 5.** Simulation of the red IR spectrum (cf. Figure 2). The simulated spectrum is shown in red and the result of superposition of the primitives shown in other colors. The primitives in blue and green result in a shouldered peak at 1960 cm^{-1} due to the difference in widths between the two.

Nonlinear Regression Using *Solver* Extension

Solver is an optimization add-in in Excel. It iteratively adjusts selected “variable” cells to optimize 205 the value in an “objective” cell. This follows the same logical process as adjusting the parameters to a desired fit in the qualitative decomposition. Instead of performing the iterations based on a qualitative evaluation of the match, *Solver* minimizes an error function automatically. The error function used is the sum of the squared error between the simulated and measured spectra in a least-squares method.

	Z	AA	AB		AD
5	Sum of Normed	Digitized	Error Squared		Sum of Error Squared
6	=SUM($n_i(\lambda)$, i=1,2,...,n)	from digitizer	= (Z6 - AA6)^2		=SUM(AB6:AB74)
7	=SUM($n_i(\lambda)$, i=1,2,...,n)	...	= (Z7 - AA7)^2		
...		
73	=SUM($n_i(\lambda)$, i=1,2,...,n)	...	= (Z73 - AA73)^2		
74	=SUM($n_i(\lambda)$, i=1,2,...,n)	...	= (Z74 - AA74)^2		

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Figure 6. Spreadsheet columns needed to optimize fit using *Solver*. The values in column **Z** are obtained by summing each cell in a normed Gaussian column in the given row, using Equation 3. Digitized points in column **AA** must be obtained using a plot digitizer. Cell **AD6** is the error function minimized by *Solver*. This figure is indexed to match the SP16 workbook.

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Performing this task in *Solver* requires the measured spectrum to be digitized and some additions to the workbook used in the Qualitative Decomposition. A plot digitizer²¹ is employed to collect coordinates at discrete points of the measured spectrum and their x-values must match the simulated points in the workbook. The digitized coordinates are saved to a CSV file and the y-coordinates are imported into the Excel sheet. Conveniently, we placed the imported data directly beside the column of the summed normed Gaussians in the rows corresponding to the proper discrete x-values (Figure 6). A new column was created for the squared error in each row and, finally, the error function was defined in cell **AD6**, which is the objective cell for *Solver* (Figure 6).

To initialize the optimization, one opens the *Solver* window and specifies the error cell as the objective for minimization and one or more parameters as variables. Experts have the opportunity to adjust several *Solver* options (see Supporting Information) and the defaults usually can produce satisfactory results. The *Solver* process requires carefully selected initial parameters, that is, it needs to be preceded by a qualitative decomposition.

STUDENT RESPONSE

230 Students in SP16 and SP17 were asked to complete a survey about the effectiveness of A04 and the results are reported in Table 1. The data were similar for both cohorts and reveal a few important

results. This is a rather work intensive project (average *ca.* 9 hours). The standard deviations are very large because a handful of students reported much longer completion times (30 – 40 hours).

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Table 1. Student Responses to a Survey Judging the Effectiveness of A04

Survey Questions	Spring 2016 n = 15		Spring 2017 n = 23	
	Mean	Std. Dev.	Mean	Std. Dev.
Total hours to complete? ^a	10.2	9.2	8.6	7.3
Challenging in regard to:	Interpreting spectra ^b	5.4	2.4	5.2
	Working in Excel ^b	6.2	2.5	5.7
	Organizing data ^b	5.7	2.8	5.2
Beneficial in developing:	Understanding of chemical spectra ^b	5.5	2.9	6.5
	Excel Skills ^b	7.8	1.9	7.6
Was A03 helpful in completing A04? ^c	86.7		91.3	
Did A04 give you greater confidence in completing subsequent assignments? ^c	71.4		82.6	
Have you used the skills learned in A04 since? ^c	42.9		34.8	

(a) In hours.

(b) Responses to a 10 point Lickert scale (1 – low, 10 – high).

(c) Responses to yes/no questions in percent of yes responses.

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This project seems best suited to develop Excel skills and also to foster a deeper understanding of chemical spectra. The assignment is well designed for rigor and a proper balance of challenge in each of its competencies: interpreting spectra, working in Excel, and organizing data. The assignment is clearly assisted by assignment A03, with almost 90% of students responding that A03 had helped them complete A04.

CONCLUSION

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The main objectives of this assignment are to cultivate students' Excel skills (general) and to teach the students to recognize how individual transitions overlap in spectra (specific). Qualitative decomposition and the *Solver* extension method were discussed and illustrated by specific student-created examples. The qualitative decomposition requires manual iterative adjustment and is best suited to develop students' understanding of overlapping transitions and spectra and to advance their

250 conceptual knowledge. With the optimization of the parameters largely automated in the *Solver* extension method, however, students tend to focus on the mathematics of the minimization problem to achieve the best fit and less on the chemical concept of overlapping transitions. Learning to use *Solver* is a valuable *additional* skill, but the automated process is no substitute for the learning experience provided by the qualitative decomposition.

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ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI:

A03 Handouts for students used in SP16 (PDF, DOC) and SP17 (PDF, DOC)

260 A03 Rubrics for students used in SP16 (PDF, DOC) and SP17 (PDF, DOC)

A04 Handouts for students used in SP16 (PDF, DOC) and SP17 (PDF, DOC)

A04 Rubrics for students used in SP16 (PDF, DOC) and SP17 (PDF, DOC)

Excel workbooks for A04 in SP16 (XLSX) and SP17 (XLSX)

Animation (MOV, AVI) to demonstrate the organization and functionality of the XLSX workbook

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270 Notes

The authors declare no competing financial interest.

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