First slide:

Heading: How to Use this Module

Text:

This module is for researchers already familiar with the basic concepts of curve fitting to a theoretical standard, but who would like to have a better understanding of what constitutes a "good" fit. The Artemis package (freely available here) is used for all examples, so it also helps to have some familiarity with it, although users of other analysis packages are also likely to find this material useful.

This module consists of:

- **Introductory videos.** These videos show a discussion between an expert in EXAFS analysis and a novice. They provide context and motivation for the screens that follow.
- **Demonstration videos.** These videos explain concepts of evaluating fits by showing examples from Artemis. During these videos, summaries of important points that have been stated by the narrator will appear in text at the bottom of the screen. These points will be included on a summary screen that follows the video. It is therefore not necessary to copy them down as you watch.
- **Applets.** Some videos are followed by applets which let you explore further what you have seen.

Second slide:

Heading: Introductory Video: "I Have No Idea When I'm Done"

Content: Introduction1.mov

Third slide:

Heading: Demonstration Video: Statistical Quality

Content: Demonstration1.mov

Fourth slide:

Heading: Summary Screen: Statistical Quality

Text:

- Statistical qualtiy can be measured by reduced chi-square
- Reduced chi-square works best for comparing fits on the same data
- When comparisons are valid, lower reduced chi-sqaure indicates a better fit
- Reduced chi-square should not be used for comparison of fits on data with different k-weights or k-ranges
- Reduced chi-square can be used to compare fits on different ranges in the Fourier transform, as long as the chi(k) data is the same

Fifth slide:

Heading: Demonstration Video: Closeness of Fit

Content: Demonstration2.m4v

Sixth slide:

Heading: Summary Screen: Closeness of Fit

Text:

- The EXAFS R-factor is a measure of the fractional mismatch between the fit and the data
- The closer the match between fit and data, the smaller the R-factor.
- A small R-factor does not necessarily mean the fit is “good,” but a large R-factor does mean the fit is “poor.”
- Low quality data will tend to have higher R-factors than high-quality data, even if the physical model is correct.
- R-factor is a simple measure of the mismatch between fit and data; reduced chi-square is an imperfect attempt at a statistically meaningful metric.
- Low R-factors are not the ultimate goal of fitting!

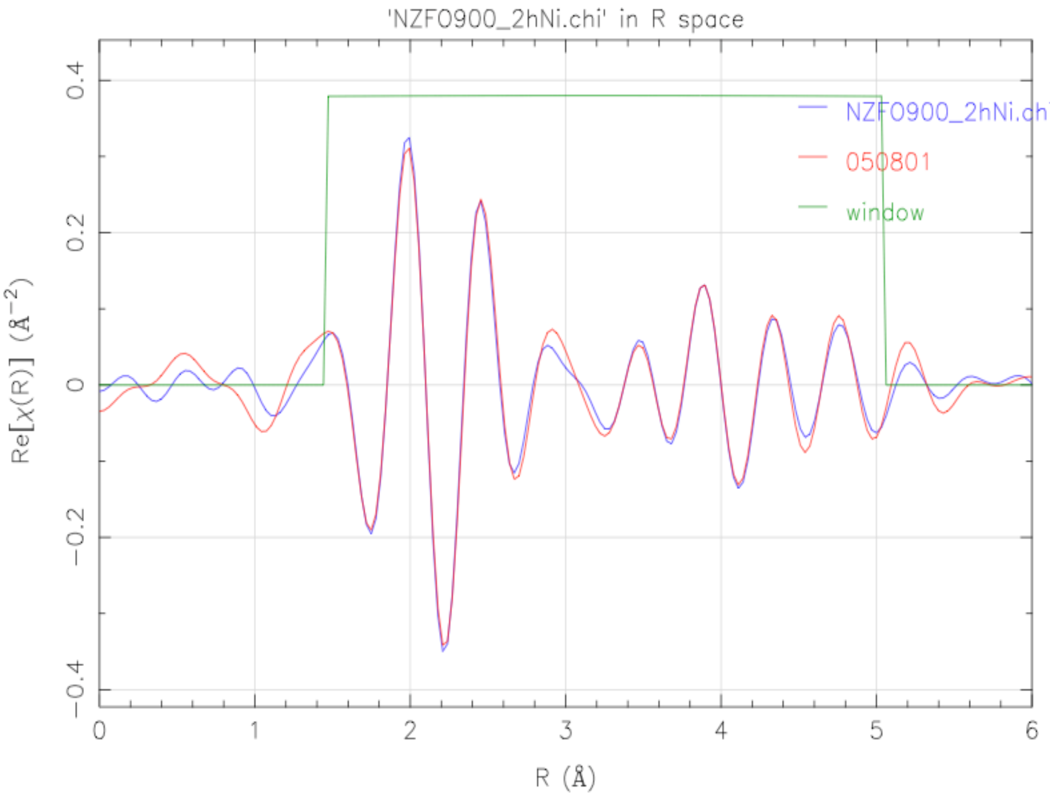
Seventh slide:

Heading: Applet: Closeness of Fit

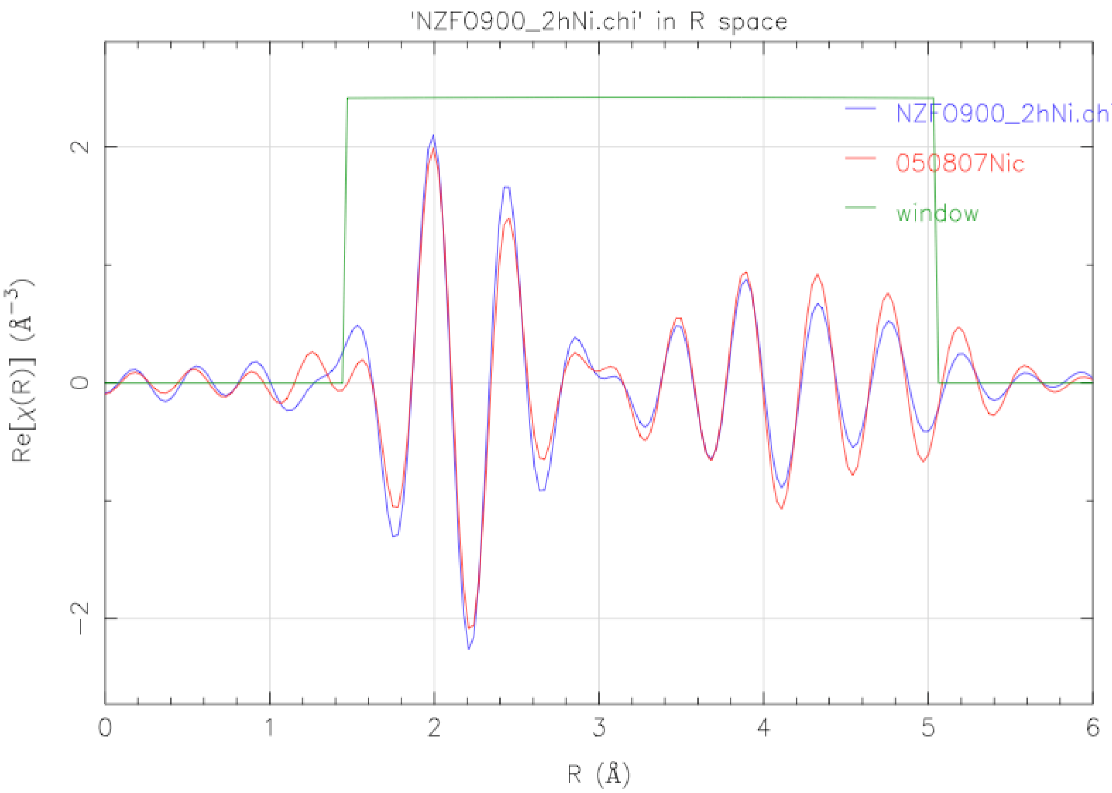
Content:

Some control that lets users pick between “R=0.01” “R=0.04” “R=0.09” “R=0.17”
The control could be buttons, radio buttons, a dial, a slider, or whatever you’d like.

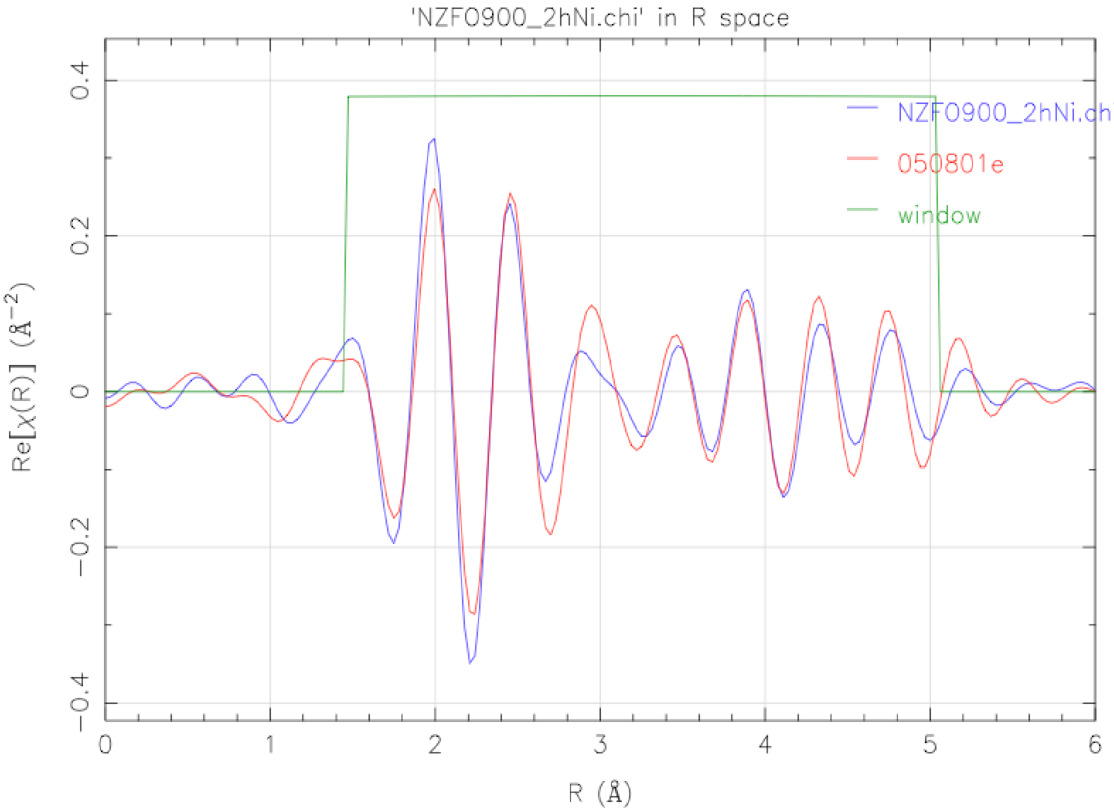
Choosing R = 0.01 yields this graph:



R = 0.04:

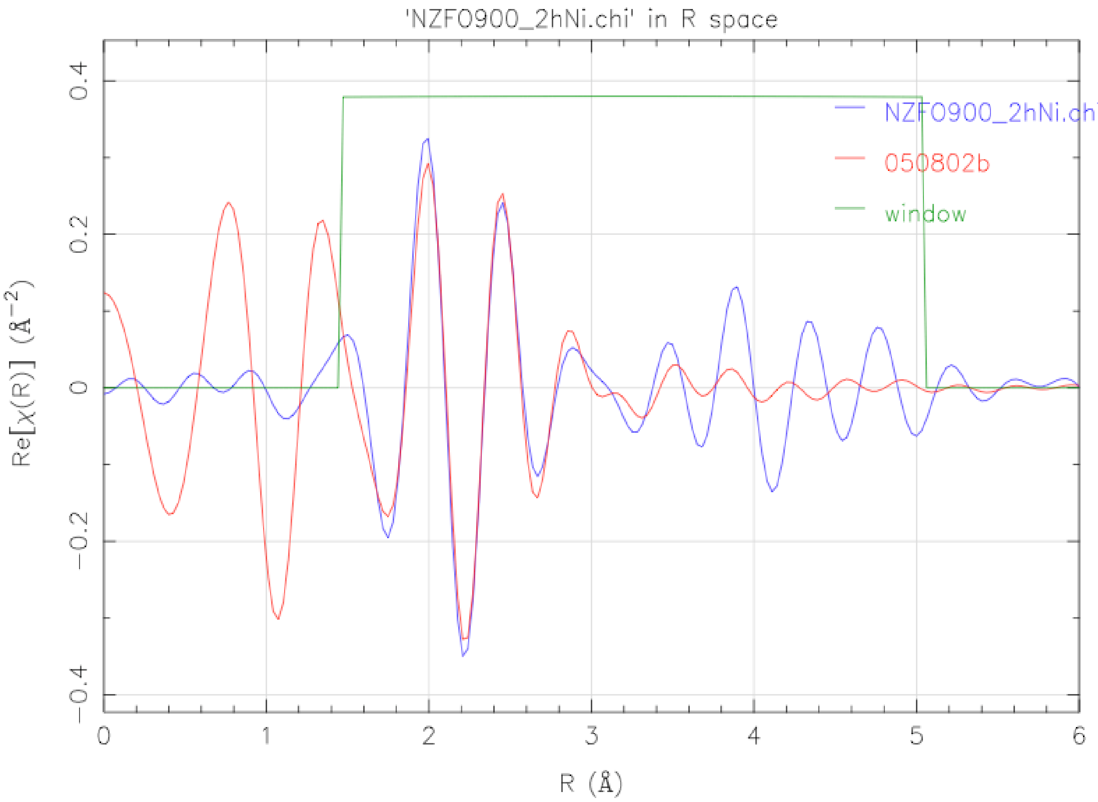

'NZFO900_2hNi.chi' in R space
NZFO900_2hNi.chi
050807Nic
window
Re[χ(R)] (Å⁻³)
R (Å)
2
0
−2
0
1
2
3
4
5
6

R = 0.09:



'NZFO900_2hNi.chi' in R space
NZFO900_2hNi.chi
050801e
window
Re[χ(R)] (Å^-2)
R (Å)
0.4
0.2
0
−0.2
−0.4
0
1
2
3
4
5
6

R = 0.17:



These options should appear in exactly the same place on the screen, with identical surroundings, so that the changes are clear. If it's possible to do a dissolve effect when switching, that's good.

Eighth Slide:

Heading: Introductory Video: "I Don't Think You're Done"

Content: Introduction2.m4v

Ninth Slide:

Heading: Demonstration Video: Are Parameter Values Physically Reasonable?

Content: Demonstration3.m4v

Tenth Slide:

Heading: Summary Slide: Are Parameter Values Physically Reasonable?

Text:

Parameter values that you would treat as ridiculous if provided to you by a person, you should treat as ridiculous if generated by a fit.

Some examples of ridiculous parameter values:

- Excessive coordination numbers. Caution: *Low* coordination numbers may be indicative of vacancies, a solution phase, nanoscale disorder, or other physical phenomena, and should not be rejected without careful consideration.
- Unheard of bond lengths for the species involved.
- Negative values of $sigma^2$
- Site occupancies of phase fractions that are negative or greater than one
- S_o^2 very small (say, less than 0.5) or very large (say, more than 1.2)
- E_o prior to the rising portion of the spectrum, or well past the white line region

Eleventh Slide:

Heading: Introductory Video: “Couldn’t the Fit Still Be Wrong?”

Content: Introduction3.m4v