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# Chapter 3 – The Bane of the “Inverse” Problem

In science, an “inverse” problem is using observations to try to calculate the factors that caused them. This is distinct from the forward problem, which starts from causes and then calculates the effects. Inverse problems are often termed “ill-posed”, which means they either (1) don’t have a solution, (2) the solution is not unique, or (3) the solution’s behavior does not change continuously with the initial conditions. In X-ray spectroscopy, the “inverse” problem – going from spectra to structure – often runs into problems with both (2) and (3).

## Lossy information

### Quantum mechanics creates uncertainty

Because of the Heisenberg uncertainty principle, you cannot know exactly both momentum and position, or energy and time. Because excited states have inherent lifetimes, electronic transitions are broadened in energy. Moreover, limits on experiment apparati, such as the resolution of your monochromator, have inherent resolution. Thus, any transition too close in energy will be smoothed out and indistinguishable from each other. Other types of spectral broadening can occur from more classical phenomena, such as plasmons and thermal vibrations.

### Transforms lose phase information

In addition to information loss due to quantum mechanics, there is also loss of phase information. This issue is particularly prominent in the interpretation of EXAFS.

* More here

## Workarounds to the “inverse” problem

### Repeat the forward problem

This is what theorists did to improve quantum chemistry codes and theoretically calculated spectra. [cite]

### Bayesian approach

Discuss the Rehr, Kas, Vila papers(s) and why it is very inaccessible and intensive. [cite]

### Linear Combination Fitting (LCF) to references

This method propagates any errors in theory and is especially unreliable if your references have different second or third coordination shells. [cite]

### Machine Learning

* Cite Nascimento and Govind, 2022 on TD-DFT providing good enough training data for ML studies

## References