

# Topic Outline

## 3b2a. Background Subtraction

### Objective

### Classifications

Empirical

Semi-empirical

Analytical

### Methodology

Determining the Range

Determining the Endpoint Values

Determining the Shape

Algorithm

### Shapes

Constant

Polynomial

Linear

Higher Order Polynomial

Special Functions

Step

Cosine

Shirley (Integrated)

XPS Analytical

### Problems

### Example Shapes

# Objective

The objective of background subtraction is to remove

- a constant offset from the signal
- an underlying spectral feature

In this process, we want to

- be consistent in our approach
- be accurate in our methodology
- avoid altering the true character of the spectrum

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# Empirical

Empirical backgrounds arise with no consideration to the theoretical rationale behind them.

Few if any background shapes used in AES and XPS are purely empirical in nature.

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# Semi-empirical

Semi-empirical backgrounds arise from some consideration of the underlying principles that give rise to a background signal in the spectrum.

Most background shapes used in AES and XPS are semi-empirical in nature.

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# Analytical

Analytical backgrounds arise from direct consideration of the underlying principles that give rise to a background signal in the spectrum.

Few background shapes used in AES and XPS are analytical in nature.

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# Determining the Range

One of the first considerations is to determine the range over which the background will be fit.

## The Entire Spectrum

This is the usual choice when we have only one feature of interest (a peak) in the entire spectrum.

## A Portion of the Spectrum

This choice is made because we have a) multiple features in the spectrum, b) abrupt changes in background shape, or c) both

# Determining the Endpoint Values

At the endpoints (where the background meets the data), we will typically want to decide whether to have the background

- a) match the values of the data points exactly
- b) be the expected value of the signal at those points

For any data outside of the chosen range, we will typically want to decide whether to

- a) use the raw data values
- b) set everything to a pre-determined value
- c) extrapolate the behavior of the background

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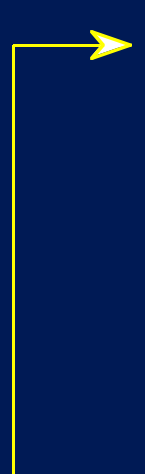
# Determining the Shape

The background shape will typically be determined by

- a) how easy it is to apply
- b) how close it is to theoretical principles

# Algorithm

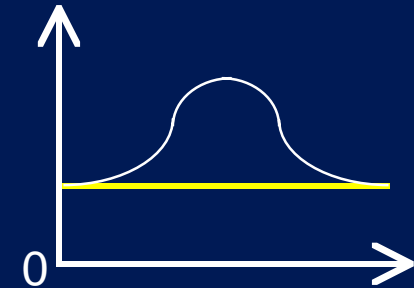
A typical algorithm for background subtraction might be

- 
1. determine the range
  2. determine the shape
  3. determine the endpoint values
  4. apply the background
  5. consider whether your choices where suitable

Background subtraction can be an iterative process.

# Constant

A constant background removes a constant value from the spectrum in the selected range.



## Application Note

This can be used in all cases.

### pros

all spectra typically have a constant underlying offset in the signal throughout their range

easy to apply

### cons

not always the end of the story (further background subtraction is typically needed)

# Linear

A linear background removes a sloped line from the spectrum in the selected range.

## pros

easy to apply

## cons

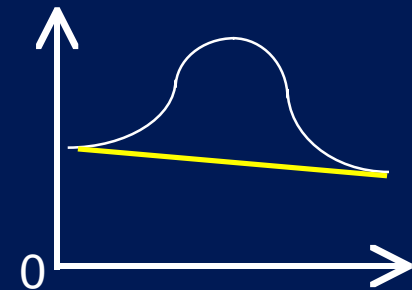
not always rigorous (theoretically sound)

requires careful selection of range and endpoint behavior

can alter the shape of spectral features

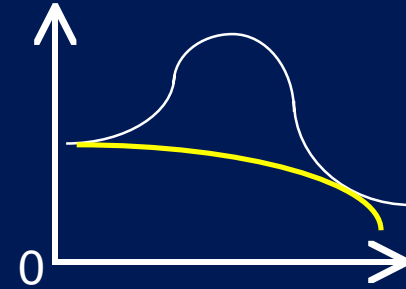
## Application Note

This is very often the best “first guess” for the background shape.



# Higher Order Polynomial

A polynomial background removes a curved line from the spectrum in the selected range.



**pros** not really

**cons**

generally never rigorous  
(theoretically sound)

requires extreme care in selecting range and  
endpoint behavior

requires extreme care in selecting the order of the  
polynomial and the fitting method  
will alter the shape of spectral features

Application Note

You better know what you  
are doing with this and why!

# Step

A step background removes a constant step from the spectrum in the selected range.

## Application Note

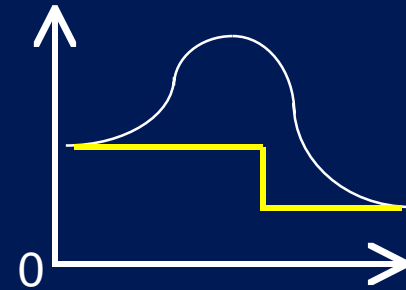
This is used to fit the Fermi edge in valence band spectra.

### pros

easy to apply

### cons

will change peak parameters



# Cosine

This removes a cosine shaped curve from the spectrum in the selected range.

## Application Note

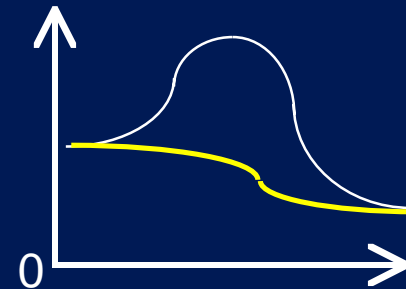
This is used to fit spectra from synchrotron radiation sources.

### pros

relatively easy to apply

### cons

will change peak parameters

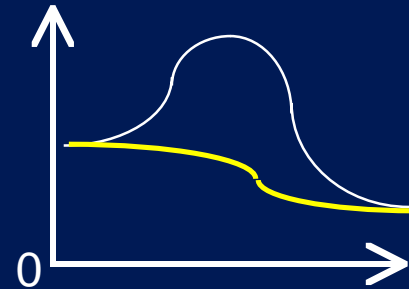


# Shirley (Integrated)

This removes an integrated shape curve from the spectrum in the selected range.

## Application Note

This is used with XPS spectra.



## pros

some basis in theory

## cons

requires numerical integration of spectrum

will change peak parameters

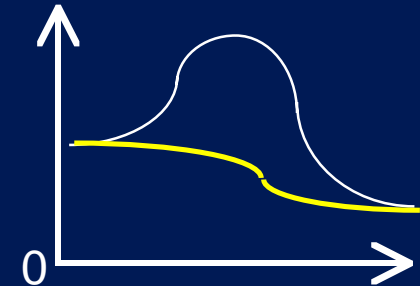
The height of the background is proportional to the area under the spectrum up to that channel.

# XPS Analytical

This removes a curve that has an analytical form.

## Application Note

This is used with XPS spectra.



## pros

basis in theory

## cons

requires numerical integration of spectrum

requires a recursive, iterative fitting algorithm

will change peak parameters

The height of the background is calculated by a recursive formulation based on the remaining area up to the channel and the value at the channel.

# Problems

Background subtraction will change peak parameters.

## peak position

will shift in all cases but the constant background

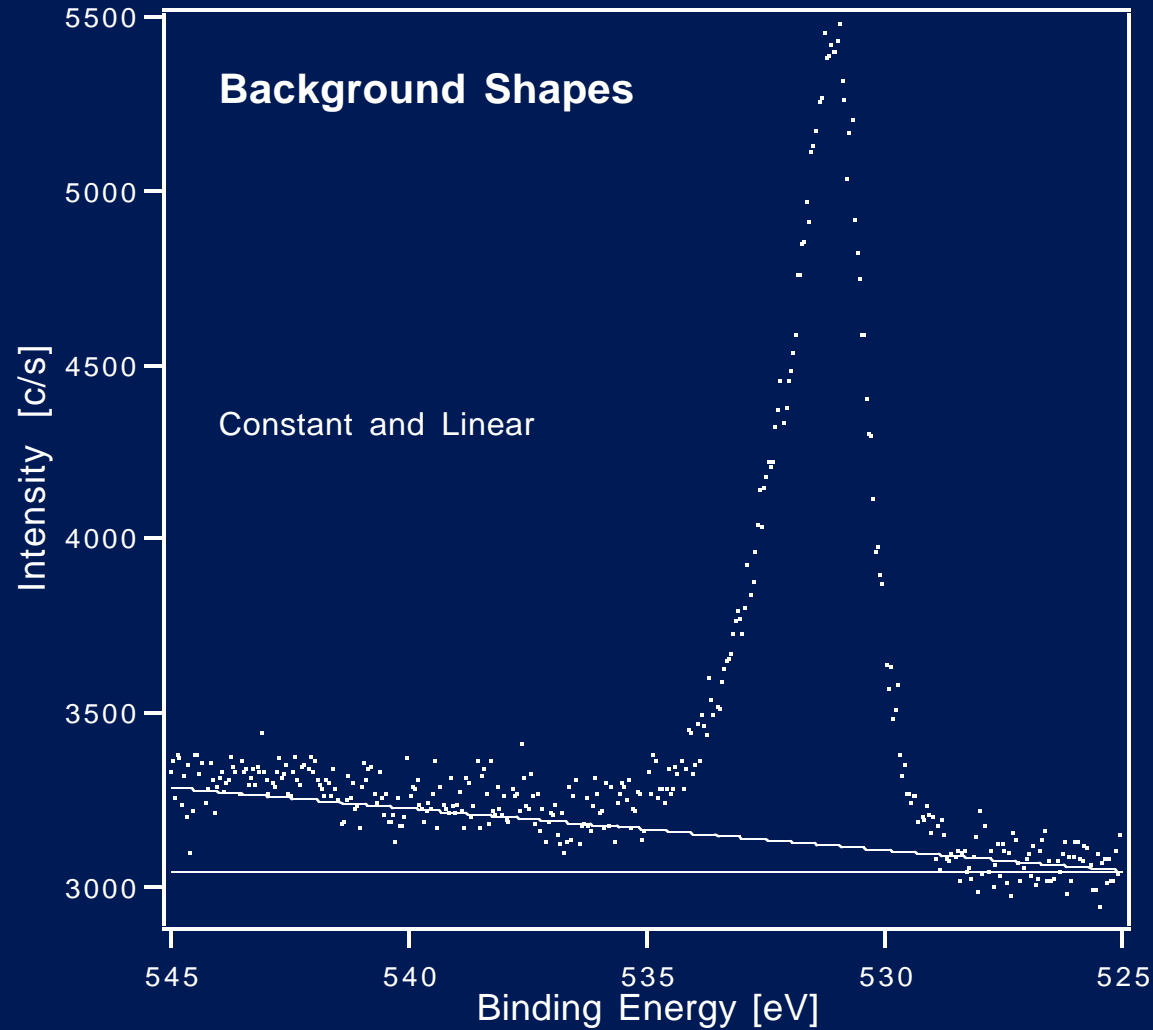
## peak half-width

will cause or remove asymmetric shape of peak

## peak height/area

will depend on the type of background removed

# Constant and Linear



# Shirley and Cosine

