Topic Outline

IIIB2b. Smoothing

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Simple n Point

Weighted n Point

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General

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- Principles
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- Ideal Filter Design

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Objective

The objective of smoothing is to increase the S/N at each channel in a spectrum by utilizing the trends in the signal over the entire spectrum.

Goal

A “noise free” spectrum where $S_{channel} = \overline{S}_{channel}$ and therefore $(S/N)_{channel}$ -> infinity

In this process, we want to

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

General

Sliding Point Algorithms

- Simple n Point Averaging
- Weighted n Point Averaging

Curve Fitting Algorithms

- Polynomial/Spline Curve Fitting
- Peak Fitting (to be discussed separately)

Noise Reduction Algorithms

- Fast Fourier Transform (FFT) Filtering
- Wavelet Filtering

Simple n Point Averaging

$$\hat{S}_j = \sum_{j-(p-1)/2}^{j+(p-1)/2} S_i \,/\, p$$

where

$\hat{S}_j$ the new value of signal at channel j

S_i the original value of signal at channel i

p the number of smoothing points (an odd number)

We must calculate the new value $\hat{S}_j$ based on the old values S_i, then substitute the new for the old.

General

$$\hat{S}_j = \sum_{j-(p-1)/2}^{j+(p-1)/2} w_i \, S_i$$

where

w_i the weighting factor at channel i
$\Sigma\, w_i$ cannot be greater than 1

The weighting factor has a defined functional form that is designed to account for the significance of signals in channel i as a function of their distance from the central channel j.

Types

Binomial

The values of w_i form a binomial distribution (Gaussian curve) derived from Pascal's triangle.

1
1 1
1 2 1
1 3 3 1
1 4 6 4 1
....

P. Marchard and L. Marmet, Rev. Sci. Instrum. 54(8) (1983) 1034.

Savitzky-Golay

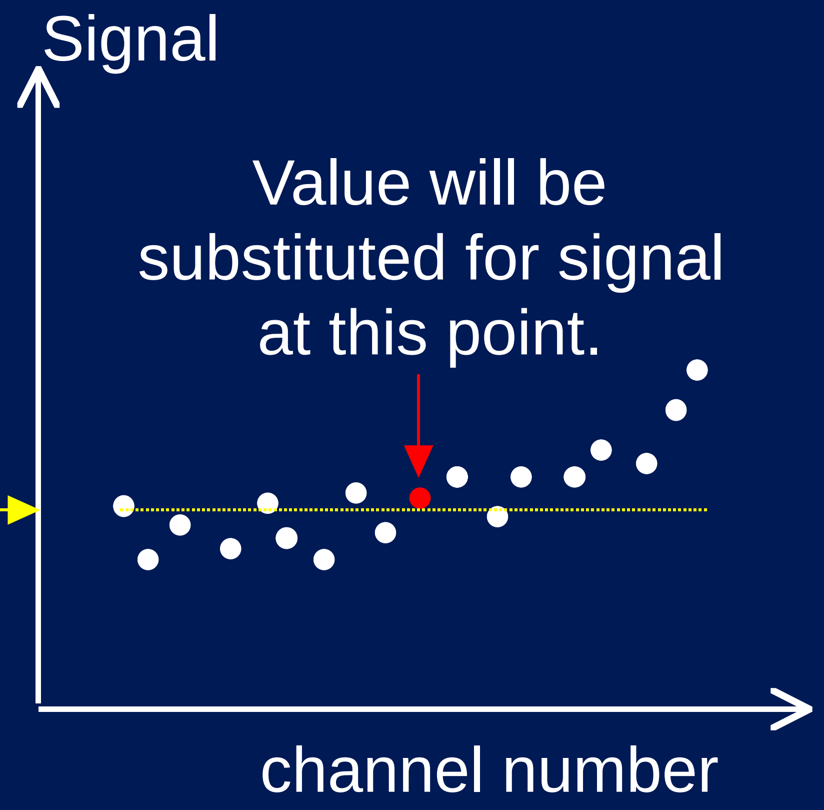
The values of w_i are determined by a type of least squares polynomial with relevance to chemistry.

H. Madden, Anal. Chem. 50 (1978) 1383.

Example

$$\hat{S}_j = \sum_{j-(p-1)/2}^{j+(p-1)/2} S_i \,/\, n$$

Value of simple 17 point smoothing algorithm calculated at central point.



Artifacts

n point smoothing algorithms ALWAYS alter the shape of peaks in a spectrum

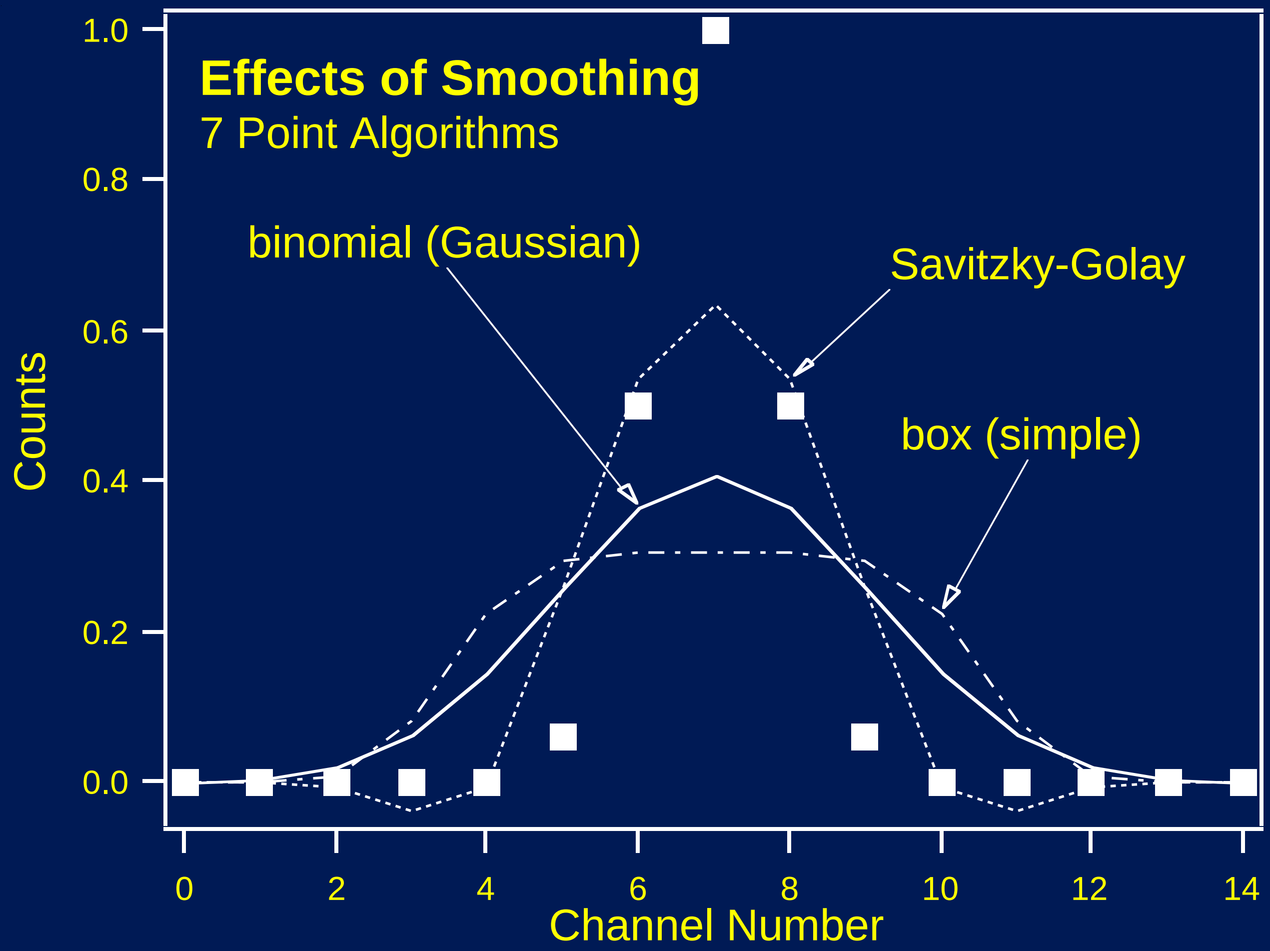
increase peak half-width

decrease peak height

shift peak positions on assymetric peaks

The extent of these changes may be insignificant, but they are NOT non-existent.

Examples



Effects of Smoothing
7 Point Algorithms
binomial (Gaussian)
Savitzky-Golay
box (simple)
Counts
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
12
14
Channel Number

End Effects

We have to consider how to handle the values that extend beyond the ends of a spectrum.

Method	S_{-i}	$S_{(n-1)+i}$
Bounce	S_i	$S_{(n-1)-i}$
Wrap	$S_{(n-1)-i}$	S_i
Zero	0	0
Fill	S_o	$S_{(n-1)}$

$$\hat{S}_j = \sum_{j-(p-1)/2}^{j+(p-1)/2} S_i \,/\, p$$

n total number of points in spectrum

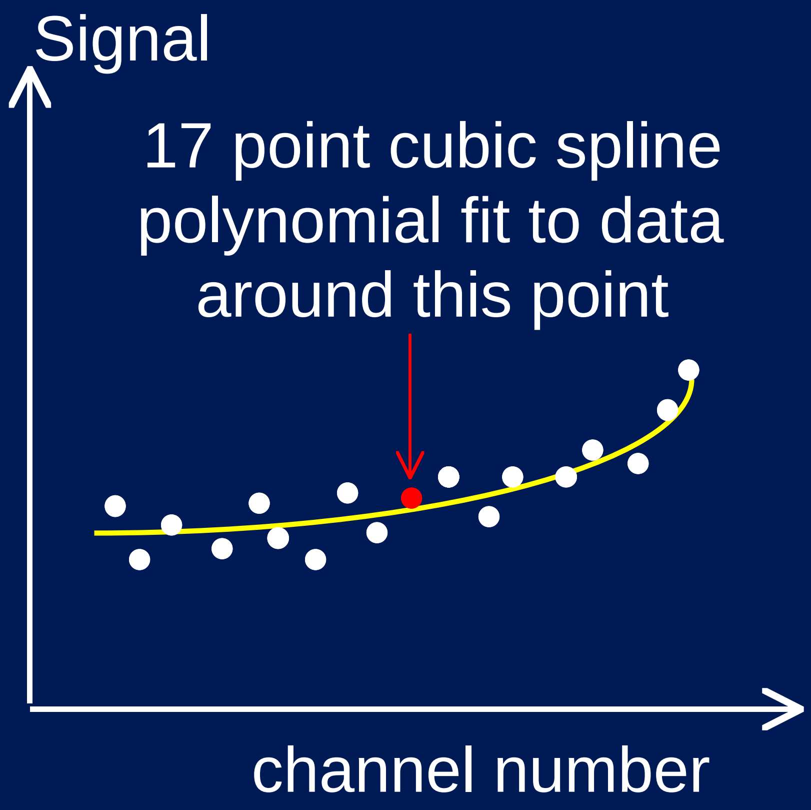
i counting index (from 0 to n-1)

Polynomial/Spline Curve Fitting

The data is fit over a given range (of n) by regression analysis to a polynomial curve of a given order.

The value of the fit curve is substituted for the original value.

We calculate the new values without changing the old ones.



Peak Fitting

Peak fitting is a sophisticated form of smoothing.

We will cover the details later.

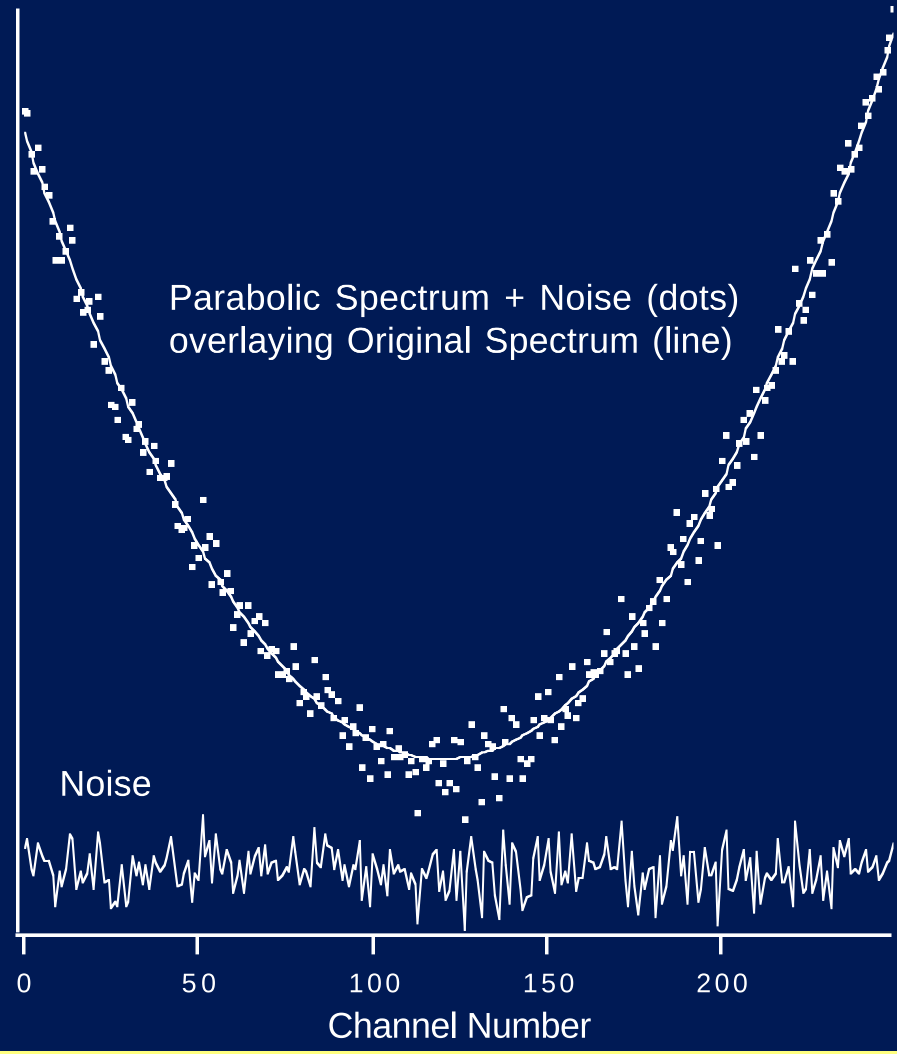
Problems

The spline fitting routines have the same problems as the n point smoothing algorithms.

They introduce artifacts into peak shapes.

General

The assumption behind noise reduction algorithms is that the signal and the noise can be cleanly separated over the entire spectrum, for example by simple mathematical subtraction.



Principles

The objective of FFT filtering is to remove noise N(E) from an ideal signal S*(E) by working in Fourier space.

$$S(E) = S^*(E) + N(E) \qquad \text{in real space}$$

$$S(f) = S^*(f) + N(f) \qquad \text{in Fourier space}$$

Our goal is to find a filter f(f) to multiply to the signal in Fourier space such that

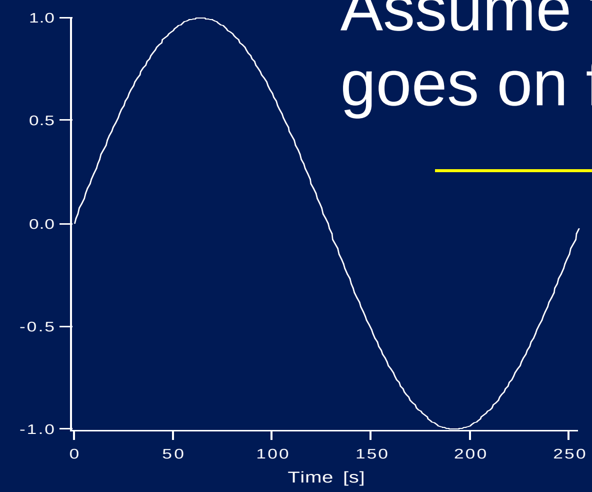
$$S^*(f) = S(f) \bullet f(f)$$

(multiplication in Fourier space is convolution in real space)

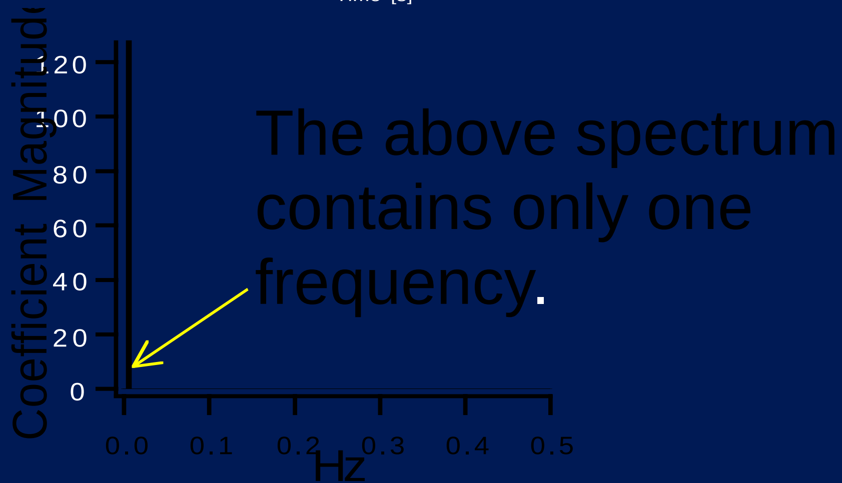
General

A Fourier transform puts a signal measured with time into an amplitude versus frequency domain.

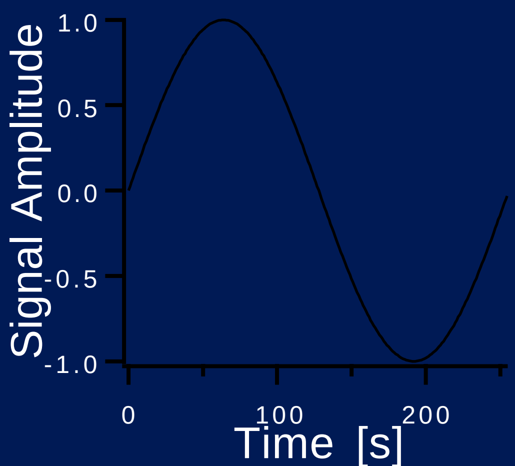
To make further considerations easier, consider channel number as a measure of time.

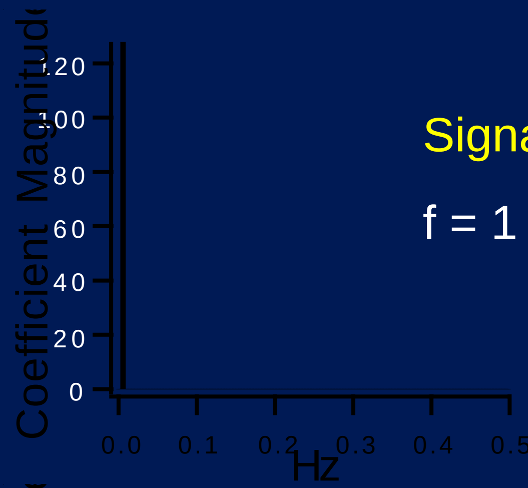


Assume this goes on forever



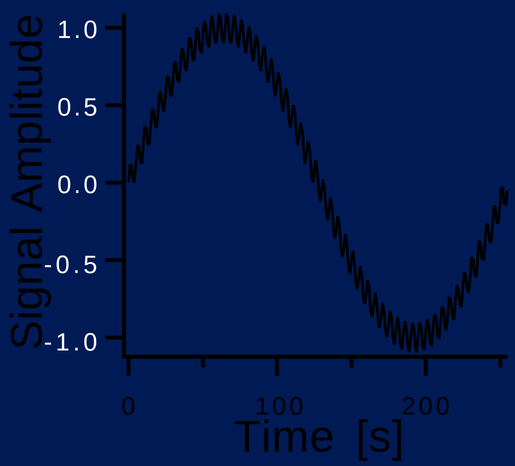
Samples

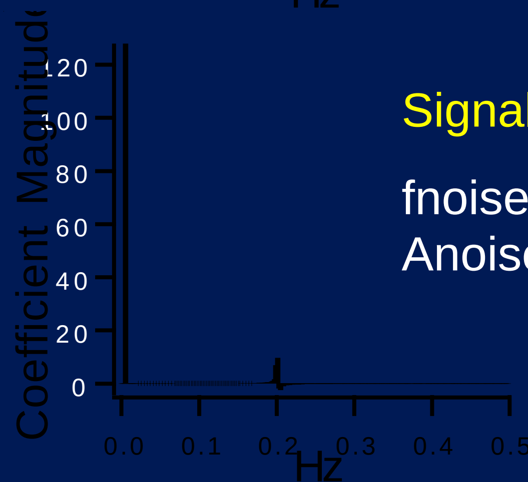




Signal

f = 1 cycle/256 s



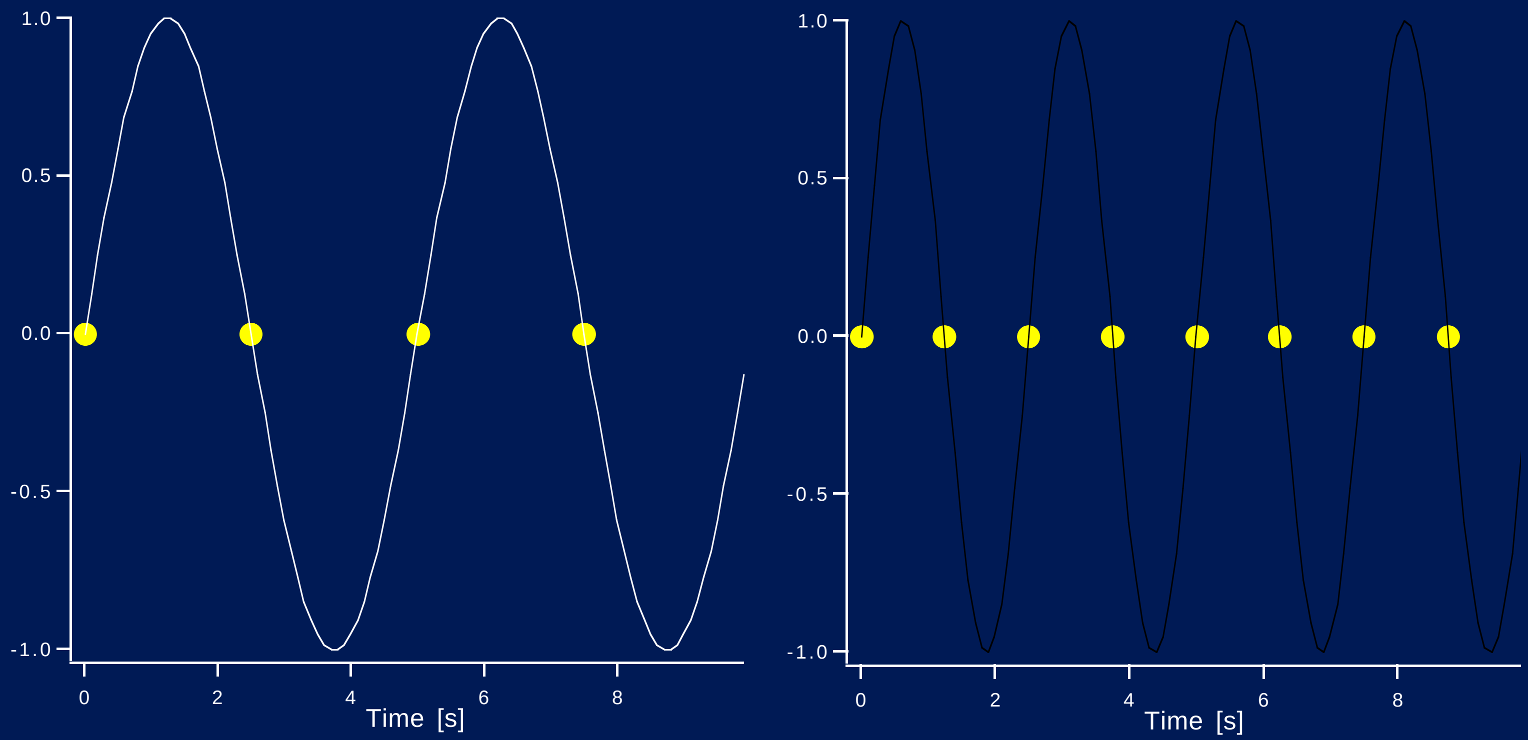


Signal + Noise

fnoise = 1 cycle/50 s
Anoise = Asignal/10

Nyquist Sampling Theorem

With digital data, the maximum frequency spectrum that can fit the data is limited by the sampling rate.



These both show the maximum frequency sine wave that fits to the measured signals. Doubling the sampling rate doubles this frequency.

Frequency Limit

The maximum “frequency” in Fourier space that will fit digital data sampled at a rate r is defined by the Nyquist limit.

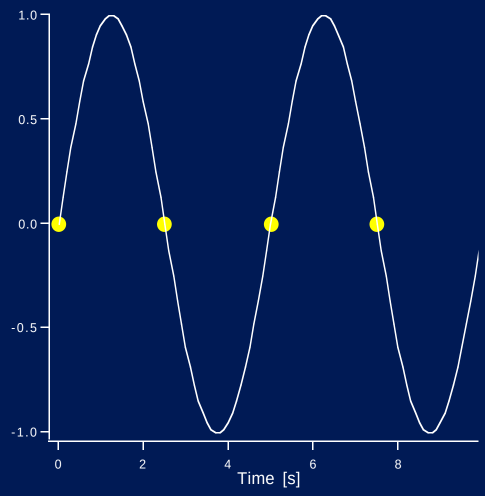
$$f_{max} = \frac{r}{2}$$

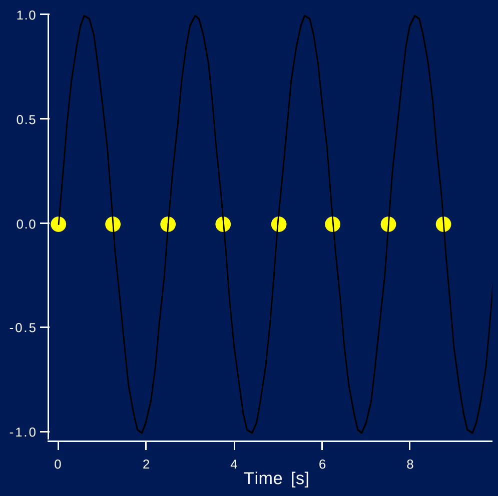
r is number of points per “time”
(or number of points per unit interval)

The minimum “frequency” in Fourier space that will fit digital data containing n points in real space is just one half of a sine wave over all the points.

Example

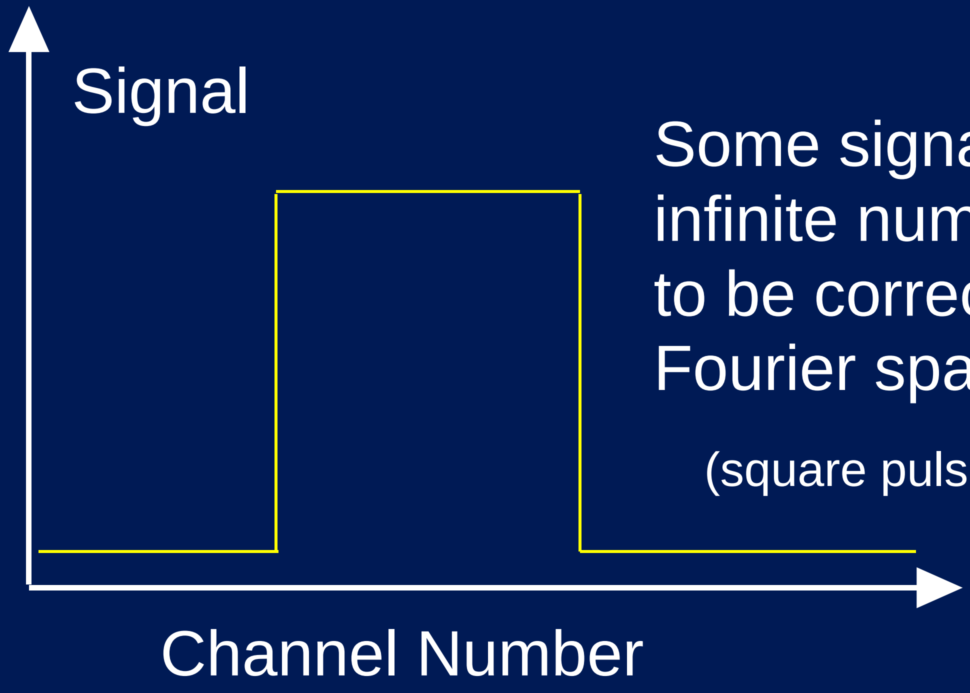
Sampling Rate (points per second)	fmax (Hz)	Sampling Rate (points per second)	fmax (Hz)
1/2	1/4	1	1/2





In AES or XPS, you can consider sampling rate as the number of "points per eV" or the inverse of step size between channels (in eV).

Series Truncation



Some signals may require an infinite number of coefficients to be correctly represented in Fourier space.

(square pulses are an example)

Use of a finite number of Fourier coefficients will cause “ringing” or so-called “Gibb’s oscillations” at the points of abrupt change in slope.

Pros and Cons

Pros

We expect to be able to use Fourier space to remove noise easily because the noise coefficients should appear mostly at higher frequencies.

Cons

The signal coefficients are distributed throughout the entire frequency range.

The noise coefficients are distributed throughout the entire frequency range.

Cutting off some of the coefficients could lead to artifacts (Gibb's oscillations).

Objective

The objective of FFT transform filtering is to remove noise from a spectrum by selectively removing the coefficients associated with noise.

Restrictions

FFT must be done on a spectrum with 2n points
(2, 4, 8, 16, ... 128, 256, 512, 1024 ...)

filter design must consider the “type” of coefficients used to represent the FFT spectrum
(they are typically a real + imaginary pair or an amplitude + phase pair)

Basic Types

Low Pass

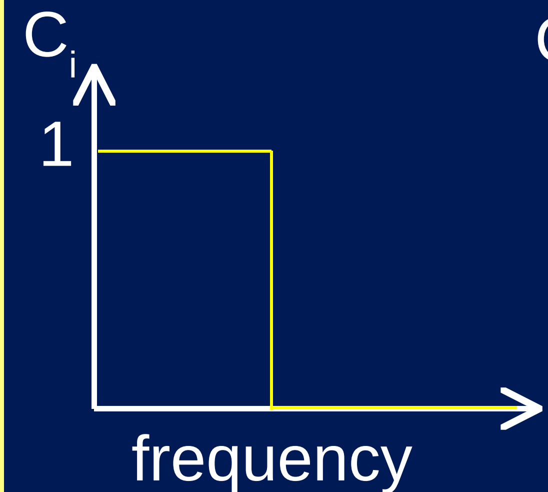
All coefficients below a cutoff frequency are used. The others are zero.

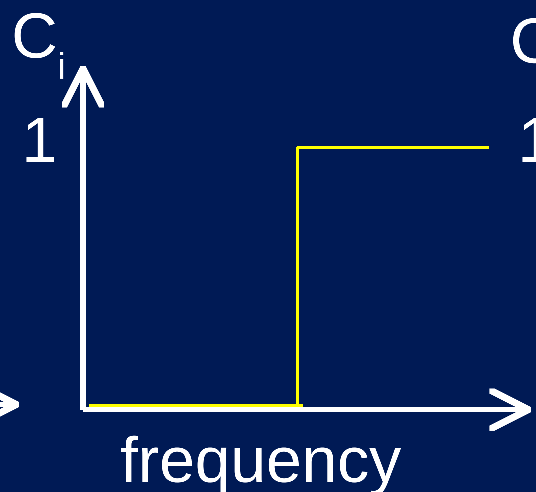
High Pass

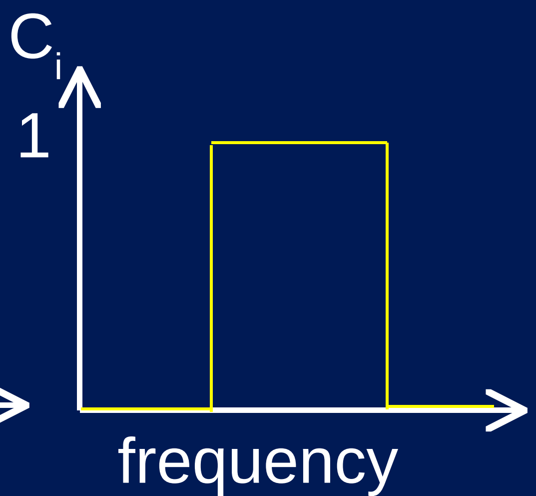
All coefficients above a cutoff frequency are used. The others are zero.

Band Pass

All coefficients between two cutoff frequencies are used. The others are zero.







The low pass filter has the most utilty for removing noise from a signal.

Low Pass Limitations

- we cannot filter out all the noise
- we loose some of the signal coefficients
- we produce Gibb's oscillations (especially at the endpoints of the spectrum)
- it is not the optimal filter when the shape of the signal is known

The balance between loss of spectral features and amount of noise removed is determined by the placement of the cutoff frequency

Use of an FFT low pass filter does not distort peak parameters as drastically as n-point smoothing algorithms do.

Principle

The objective is to find the optimal filter f*(f) that can separate the signal S*(f) from the noise N(f) in Fourier space based on *a priori* knowledge about the shape of the “ideal” signal in real space S*(E).

$$F(f) = f^*(f) \cdot S(f) \quad \text{when transformed } F(f) \rightarrow S^*(E)$$

Goal

Minimize the residual r^2 between the filtered signal F(E) and the “ideal” signal S*(E).

$$\langle r^2 \rangle = \int | F(E) - S^*(E) |^2 \, dE$$

Formulation

The optimal filter (the Wiener filter) is designed according to

$$f^*(f) = \frac{|\,S^*(f)\,|^2}{|\,S^*(f)\,|^2 + <|\,N(f)\,|^2>}$$

RMS noise

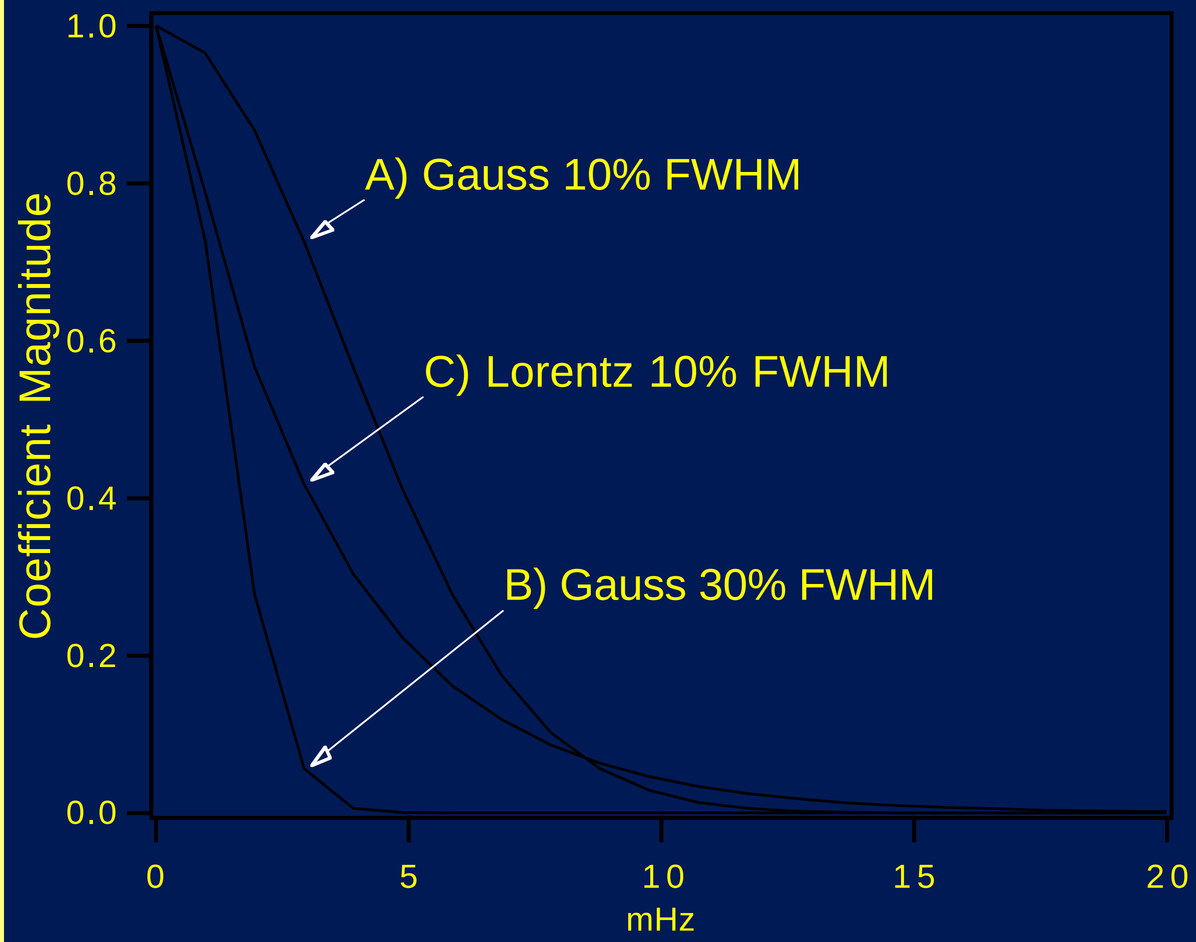
We must have

the shape of the ideal signal S*(E)

the magnitude of the RMS noise in Fourier space

The former is a guess, and the latter is measured from the spectrum in some manner, typically by looking at high frequency in the FFT coefficients.

Samples



As the FWHM of a peak widens, the filter narrows.

A Lorentzian filter is narrower at low frequency than a Gaussian.

Wavelet Filtering

Wavelet analysis applies FFT filtering to a higher level of sophistication. It breaks the spectrum into "time slices" and analyzes for the frequencies that best fit within the given time slice. In other words, it does some of the separation of low and high frequency information in the time domain before going to the Fourier domain.

Wavelet analysis may be an option for smoothing spectra (as well as images) at some point in your future career.

Sample Smoothed Curves