Computational Physics – Lecture 18

(22 April 2020)

Recap

In the previous class, we acquired the capability of numerically computing the Fourier Transform of a function.

Recap

The FT of a function $f(x)$, given by

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \cdot f(x) \cdot \exp(-ikx), \tag{1}$$

can be computed at $k_q = 2\pi q / n\Delta$, for $q = 0, \ldots, n-1$, by choosing some x_{min}, x_{max} and Δ, and computing

$$\tilde{f}(k_q) = \Delta \cdot \sqrt{\frac{n}{2\pi}} \cdot \exp\left(-ik_q \cdot x_{\mathrm{min}}\right) \cdot \mathrm{DFT}\left[\{f(x_p)\}\right], \tag{2}$$

where $x_p = x_{\mathrm{min}} + p\Delta$ for $p = 0, \ldots, n-1$, the number n is given by

$$n = \frac{x_{\mathrm{max}} - x_{\mathrm{min}}}{\Delta} + 1, \tag{3}$$

and $\{f(x_p)\}$ is the set of numbers

$$\left\{ f(x_p) \;\middle|\; p = 0, \ldots, n-1 \right\}. \tag{4}$$

Recap

Excellent libraries for computing the FT are commercially available. For example, Numpy, GSL, and FFTW.

But before using these libraries we should always read their documentation and check

- The DFT formula used by the library, and
- The frequency ordering assumed by the library.

Today's plan

In today's class, we want to understand how to convolve two functions numerically.

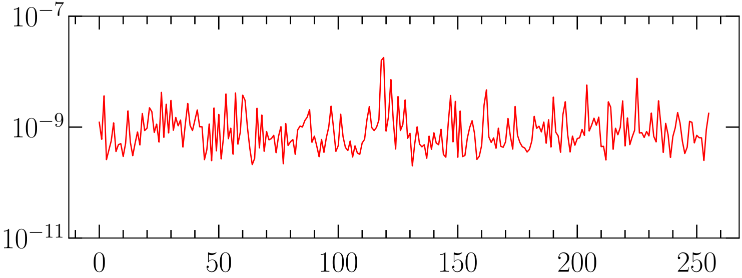
Convolution

The convolution of two functions $g(x)$ and $h(x)$ is defined as

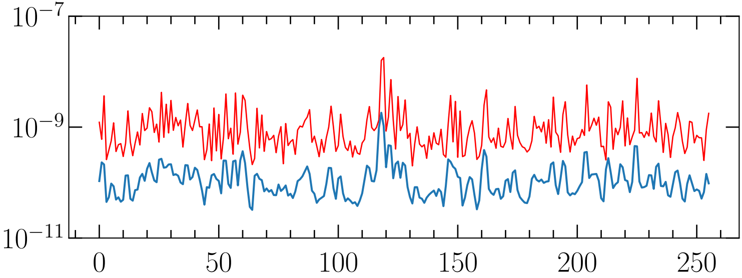
$$f(x) \equiv [g \otimes h](x) = \int_{-\infty}^{\infty} dr \cdot g(r) \cdot h(x-r). \tag{5}$$

This *smears* one function by another.

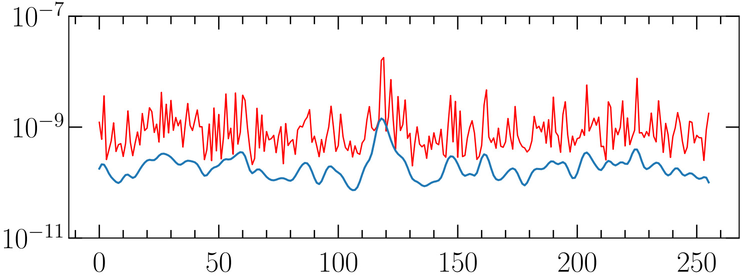
Convolution



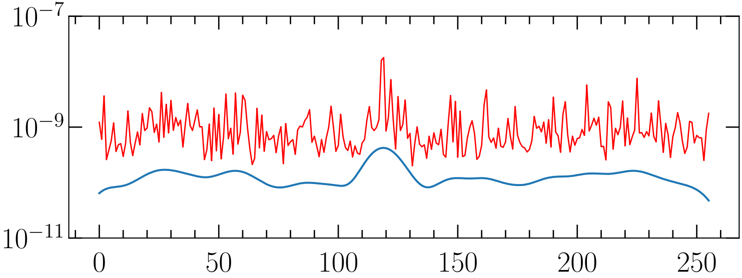
Convolution



Convolution



Convolution



Convolution Theorem

The *convolution theorem* says that

$$\tilde{f}(k) = \sqrt{2\pi} \cdot \tilde{g}(k) \cdot \tilde{h}(k). \tag{6}$$

The Fourier Transform of the convolution of two functions is equal to the product of the individual Fourier Transforms of the two functions.

Convolution Theorem

$$\begin{aligned}\tilde{f}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x \cdot f(x) \cdot \exp(-ikx) \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x \cdot \left[\int_{-\infty}^{\infty} dr \cdot g(r) \cdot h(x-r)\right] \cdot \exp(-ikx)\end{aligned}$$

Change variable from x to $u = x - r$.

$$\begin{aligned}\tilde{f}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} drg(r)h(u)\ \exp(-ik[u+r]) \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} drg(r)h(u)\ \exp(-iku)\exp(-ikr)\end{aligned}$$

Convolution Theorem

$$
\begin{aligned}
\tilde{f}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}u \int_{-\infty}^{\infty} dr g(r) h(u) \; \exp(-iku) \exp(-ikr) \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}u \, h(u) \exp(-iku) \int_{-\infty}^{\infty} dr g(r) \exp(-ikr) \\
&= \tilde{h}(k) \cdot \sqrt{2\pi} \, \tilde{g}(k) \\
&= \sqrt{2\pi} \cdot \tilde{h}(k) \cdot \tilde{g}(k) \qquad (7)
\end{aligned}
$$

Discrete convolution

To do convolution on computers, we have discretise the above relations by sampling all the functions.

Let g_p be a sample of $g(x)$ and h_p be a sample of $h(x)$, where $p = 0, \ldots, n-1$.

Then we can define the discrete convolution of these samples such that the convolution theorem holds for them.

In other words, we define the discrete convolution as

$$f_p = \sum_{r=0}^{n-1} g_r h_{p-r}. \tag{8}$$

Discrete convolution theorem

When the discrete convolution is defined this way, we have

$$\tilde{f}_q = \sqrt{n} \cdot \tilde{h}_q \cdot \tilde{g}_q. \tag{9}$$

It is easier to see this using the unscaled expressions:

$$\tilde{w}_q = \frac{1}{\sqrt{n}} \sum_{p=0}^{n-1} w_p \cdot \exp\left(\frac{-i2\pi qp}{n}\right), \tag{10}$$

and the inverse is

$$w_p = \frac{1}{\sqrt{n}} \sum_{q=0}^{n-1} \tilde{w}_q \cdot \exp\left(\frac{i2\pi qp}{n}\right). \tag{11}$$

Discrete convolution theorem

We have

$$
\begin{aligned}
\tilde{f}_q &= \frac{1}{\sqrt{n}} \sum_{p=0}^{n-1} f_p \cdot \exp\left(\frac{-i2\pi qp}{n}\right) \\
&= \frac{1}{\sqrt{n}} \sum_{p=0}^{n-1} \sum_{r=0}^{n-1} g_r h_{p-r} \cdot \exp\left(\frac{-i2\pi qp}{n}\right) \\
&= \frac{1}{\sqrt{n}} \sum_{p=0}^{n-1} \sum_{r=0}^{n-1} g_r h_{p-r} \cdot \exp\left(\frac{-i2\pi q[p-r]}{n}\right) \exp\left(\frac{-i2\pi qr}{n}\right) \\
&= \frac{1}{\sqrt{n}} \sum_{u=0}^{n-1} h_u \exp\left(\frac{-i2\pi qu}{n}\right) \sum_{r=0}^{n-1} g_r \exp\left(\frac{-i2\pi qr}{n}\right) \\
&= \sqrt{n} \cdot \tilde{h}_q \cdot \tilde{g}_q.
\end{aligned}
$$

(We have assumed than h is n-periodic.)

Consistency between DFT and FT

Is the above discrete convolution consistent with the continuous convolution?

Let us assume $x_{\min} = 0$ and write

$$\tilde{g}(k_q) = \Delta \cdot \sqrt{\frac{n}{2\pi}} \cdot \mathrm{DFT}\left[\{g(x_p)\}\right], \tag{12}$$

and

$$\tilde{h}(k_q) = \Delta \cdot \sqrt{\frac{n}{2\pi}} \cdot \mathrm{DFT}\left[\{h(x_p)\}\right]. \tag{13}$$

Consistency between DFT and FT

Now expect that the inverse DFT of

$$\sqrt{2\pi} \cdot \tilde{h}(k_q) \cdot \tilde{g}(k_q) \tag{14}$$

should be $f(x_p)$.

We have

$$\begin{aligned} &\sqrt{2\pi} \cdot \tilde{h}(k_q) \cdot \tilde{g}(k_q) && (15) \\ &= \sqrt{2\pi} \cdot \Delta^2 \cdot \frac{n}{2\pi} \cdot \mathrm{DFT}\left[\{g(x_p)\}\right] \cdot \mathrm{DFT}\left[\{h(x_p)\}\right] && (16) \end{aligned}$$

What is the IDFT of this?

Consistency between DFT and FT

The IDFT is

$$\frac{1}{\sqrt{n}}\sum_{q=0}^{n-1}\sqrt{2\pi}\cdot\Delta^2\cdot\frac{n}{2\pi}\cdot\mathrm{DFT}\left[\{g(x_p)\}\right]_q\cdot\mathrm{DFT}\left[\{h(x_p)\}\right]_q\cdot\exp\left(ik_q x_p\right)$$

$$=\Delta^2\cdot\sqrt{\frac{n}{2\pi}}\cdot\sum_{q=0}^{n-1}\mathrm{DFT}\left[\{g(x_p)\}\right]_q\cdot\mathrm{DFT}\left[\{h(x_p)\}\right]_q\cdot\exp\left(ik_q x_p\right)$$

$$=\Delta^2\sqrt{\frac{n}{2\pi}}\sum_{q=0}^{n-1}\left\{\left[\sum_{p'=0}^{n-1}\frac{g(x_{p'})}{\sqrt{n}}\exp\left(-ik_q x_{p'}\right)\right]\right.$$

$$\left.\times\left[\sum_{p''=0}^{n-1}\frac{h(x_{p''})}{\sqrt{n}}\exp\left(-ik_q x_{p''}\right)\right]\cdot\exp\left(ik_q x_p\right)\right\}$$

Consistency between DFT and FT

$$= \frac{\Delta^2}{\sqrt{2\pi n}} \sum_{q=0}^{n-1} \sum_{p'=0}^{n-1} \sum_{p''=0}^{n-1} g(x_{p'}) h(x_{p''}) \exp\left(-ik_q \left[x_{p'} + x_{p''} - x_p\right]\right)$$

$$= \frac{\Delta^2}{\sqrt{2\pi n}} \cdot n \sum_{p'=0}^{n-1} \sum_{p''=0}^{n-1} g(x_{p'}) h(x_{p''}) \delta_{p,p'+p''}$$

$$= \Delta^2 \sqrt{\frac{n}{2\pi}} \sum_{p'=0}^{n-1} \sum_{p''=0}^{n-1} g(x_{p'}) h(x_{p''}) \delta_{p,p'+p''}$$

$$= \Delta^2 \sqrt{\frac{n}{2\pi}} \sum_{p'=0}^{n-1} g(x_{p'}) h(x_{p-p'}).$$

Consistency between DFT and FT

Or, to simplify the argument a bit, the IDFT of

$$\mathrm{DFT}\left[\{g(x_p)\}\right] \cdot \mathrm{DFT}\left[\{h(x_p)\}\right] \tag{17}$$

is

$$\frac{\Delta^2 \sqrt{\frac{n}{2\pi}} \sum_{p'=0}^{n-1} g(x_{p'}) h(x_{p-p'})}{\sqrt{2\pi} \cdot \Delta^2 \cdot \frac{n}{2\pi}} \tag{18}$$

which is just

$$\frac{1}{\sqrt{n}} \sum_{p'=0}^{n-1} g(x_{p'}) h(x_{p-p'}). \tag{19}$$

Is this related to $f(x_p)$?

Consistency between DFT and FT

Recall

$$f(x_p) = \int_{-\infty}^{\infty} dr \cdot g(r) \cdot h(x_p - r). \tag{20}$$

If we discretise this, we get

$$\begin{aligned} f(x_p) &= \sum_{p'=0}^{n-1} g(x_{p'}) h(x_{p-p'}) && (21) \\ &= \Delta \cdot \sum_{p'=0}^{n-1} g(x_{p'}) h(x_{p-p'}) && (22) \\ &= \Delta \cdot \sqrt{n} \cdot \mathrm{IDFT}\Big(\mathrm{DFT}\left[\{g(x_p)\}\right] \cdot \mathrm{DFT}\left[\{h(x_p)\}\right] \Big) && (23) \end{aligned}$$

Consistency between DFT and FT

So our definitions of continuous and discrete convolution are consistent.

To compute the convolution of two functions,

- Sample them and take their discrete Fourier transforms
- Multiply the Fourier transforms
- Take the inverse discrete Fourier transform of the result
- Multiply the result by $\Delta \cdot \sqrt{n}$

Example

Let us consider the two functions

$$g(x) = \exp\left(-x^2\right) \tag{24}$$

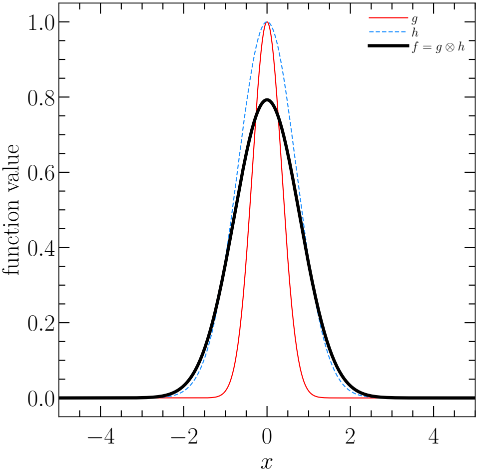
and

$$h(x) = \exp\left(-4x^2\right). \tag{25}$$

The convolution of these two functions can be calculated analytically, and is given by

$$f(x) = \sqrt{\frac{\pi}{5}} \exp\left(\frac{-4x^2}{5}\right) \tag{26}$$

Example



(Convolution of two Gaussians is a Gaussian.)

Example

We can calculate the Fourier transforms of $f(x)$, $g(x)$, and $h(x)$ analytically and confirm the convolution theorem.

We have

$$\tilde{g}(k) = \frac{1}{\sqrt{2}} \exp\left(\frac{-k^2}{4}\right), \tag{27}$$

and

$$\tilde{h}(k) = \frac{1}{2\sqrt{2}} \exp\left(\frac{-k^2}{16}\right), \tag{28}$$

and

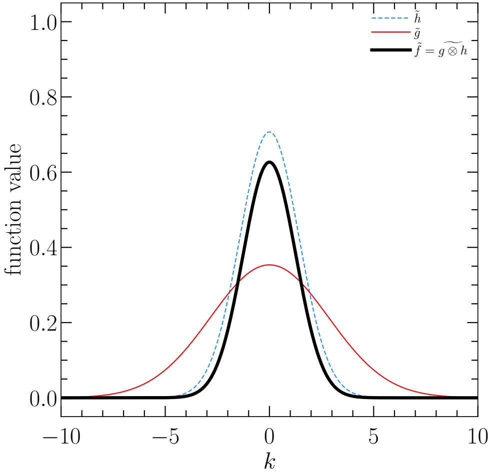
$$\tilde{f}(k) = \frac{1}{2}\sqrt{\frac{\pi}{2}} \exp\left(\frac{-5k^2}{16}\right). \tag{29}$$

Example

So the convolution theorem holds.

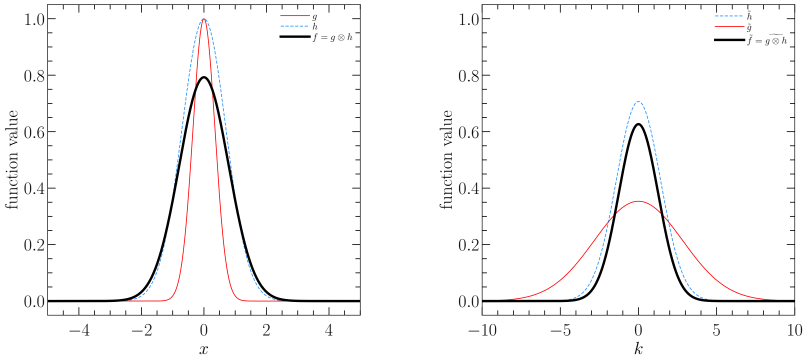
$$
\begin{aligned}
&\sqrt{2\pi} \cdot \tilde{g}(k) \cdot \tilde{h}(k) \\
&= \sqrt{2\pi} \cdot \left[\frac{1}{\sqrt{2}} \exp\left(\frac{-k^2}{4} \right) \right] \cdot \left[\frac{1}{2\sqrt{2}} \exp\left(\frac{-k^2}{16} \right) \right] \\
&= \frac{1}{2} \sqrt{\frac{\pi}{2}} \exp\left(\frac{-5k^2}{16} \right) \\
&= \tilde{f}(k).
\end{aligned}
$$

Example



$\tilde{h}$
$\tilde{g}$
$\tilde{f} = \widetilde{g \otimes h}$
function value
1.0
0.8
0.6
0.4
0.2
0.0
−10
−5
0
5
10
k

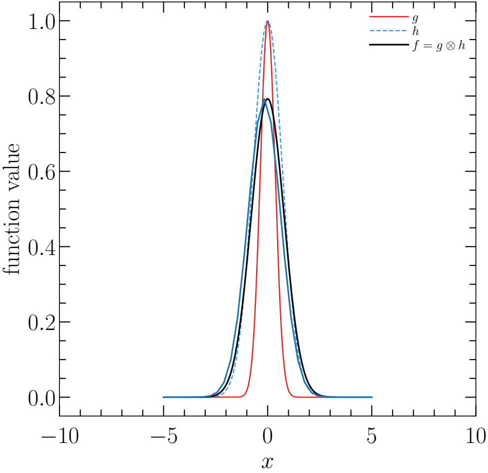
Example



function value
g
h
$f = g \otimes h$
x
$\tilde{h}$
$\tilde{g}$
$\tilde{f} = \widetilde{g \otimes h}$
k

Example

However, when we compute the convolution using our new method we find



(I used $x_{\text{min}} = -5$, $x_{\text{max}} = 5$, and $n = 32$.)

Zero padding

The result is not accurate because the discrete convolution assumes that our function $h(x_p)$ is periodic, but it is not.

We can avoid this problem by means of zero padding.

Consider the simple case of $n = 4$, in which we have

$$f_p = \sum_{r=0}^{3} g_r h_{p-r}. \tag{30}$$

Zero padding

We expect

$$f_0 = g_0 h_0 + g_1 h_{-1} + g_2 h_{-2} + g_3 h_{-3} \tag{31}$$
$$= g_0 h_0, \tag{32}$$

but due to periodicity we get

$$f_0 = g_0 h_0 + g_1 h_{-1} + g_2 h_{-2} + g_3 h_{-3} \tag{33}$$
$$= g_0 h_0 + g_1 h_3 + g_2 h_2 + g_3 h_1, \tag{34}$$

which is wrong.

Zero padding

Now suppose we expand our $n = 4$ array to an $n = 8$ array for which the last four elements are zero.

Now we will have

$$f_p = \sum_{r=0}^{7} g_r h_{p-r}. \tag{35}$$

which will give us

$$\begin{aligned} f_0 &= g_0 h_0 + g_1 h_{-1} + g_2 h_{-2} + g_3 h_{-3} + g_4 h_{-4} \\ &\quad + g_5 h_{-5} + g_6 h_{-6} + g_7 h_{-7} && (36) \\ &= g_0 h_0 + g_1 h_{-1} + g_2 h_{-2} + g_3 h_{-3} && (37) \\ &= g_0 h_0 + g_1 h_7 + g_2 h_6 + g_3 h_5 && (38) \\ &= g_0 h_0, && (39) \end{aligned}$$

which is now the correct answer.

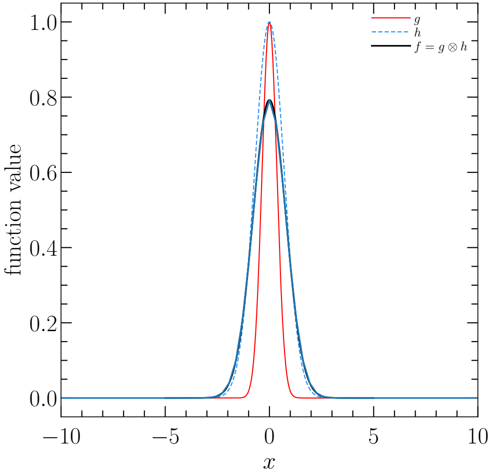
Zero padding

With zero padding, to compute the convolution of two functions we do the following:

- Sample the functions *and zero pad them*
- Take their discrete Fourier transforms
- Multiply the Fourier transforms
- Take the inverse discrete Fourier transform of the result
- Multiply the result by $\Delta \cdot \sqrt{n}$

Example

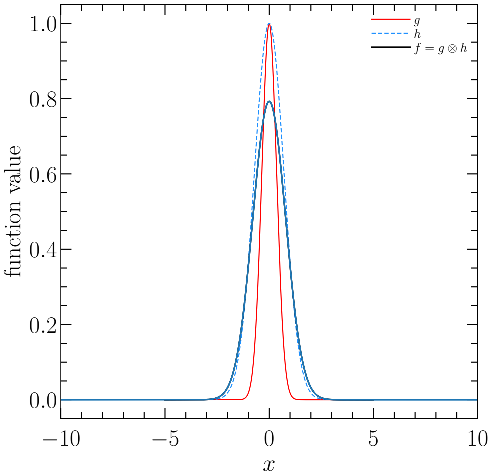
With zero padding in our example, we get



($x_{\text{min}} = -5$, $x_{\text{max}} = 5$, and $n = 32$.)

Example

We can increase the resolution for a better result:



($x_{\min} = -5$, $x_{\max} = 5$, and $n = 1024$.)

Deconvolution

We now know how to numerically compute the convolution $g \otimes h$ of two functions g and h.

But if we are given $g \otimes h$ and g, we can then also compute h by simply dividing the Fourier transforms.

This is called deconvolution.

We can think of this as "removing instrumental response".

Optimal filtering

Suppose we want to measure an uncorrupted signal $u(t)$ but an experiment as produced a corrupted signal $c(t)$, given by

$$c(t) = s(t) + n(t) \tag{40}$$

where

$$s(t) = \int_{-\infty}^{\infty} r(t-\tau) \cdot u(\tau) d\tau \tag{41}$$

If there was not noise, we can solve this problem by deconvolution.

Optimal filtering

In presence of noise, we try to find the *optimal filter* $\phi(t)$ such that when this is applied to $c(t)$, and the result is deconvolved by $r(t)$, we get something, say $u'(t)$, that is as close as possible to $u(t)$.

So we will calculate

$$\tilde{u}'(k) = \frac{\tilde{c}(k)\tilde{\phi}(k)}{\tilde{r}(k)} \tag{42}$$

and solve this for ϕ such that

$$\int_{-\infty}^{\infty} |u'(t) - u(t)|^2 dt$$

is minimised.

Optimal filtering

But this is equal to the condition that

$$\int_{-\infty}^{\infty} |\tilde{u}'(k) - \tilde{u}(k)|^2 dk$$

is minimised.

Or

$$\int_{-\infty}^{\infty} \left| \frac{[\tilde{s}(k) + \tilde{n}(k)]\,\tilde{\phi}'(k)}{\tilde{r}'(k)} - \frac{\tilde{s}(k)}{\tilde{r}(k)} \right|^2 dk$$
$$= \int_{-\infty}^{\infty} |\tilde{r}(k)|^{-2} \left\{ |\tilde{s}(k)|^2 |1 - \tilde{\phi}(k)|^2 + |\tilde{n}(k)|^2 |\tilde{\phi}(k)|^2 \right\} dk$$

is minimised. (Cross terms integrate to zero.)

Optimal filtering

Differentiating by ϕ and setting the result to zero gives

$$\tilde{\phi}(k) = \frac{|\tilde{s}(k)|^2}{|\tilde{s}(k)|^2 + |\tilde{n}(k)|^2}. \tag{43}$$

This is called the Optimal Filter, or the Wiener Filter.

It requires us to know $|\tilde{s}(k)|^2$ and $|\tilde{n}(k)|^2$.

You can make this process more sophisticated by using better optimisation ideas.