

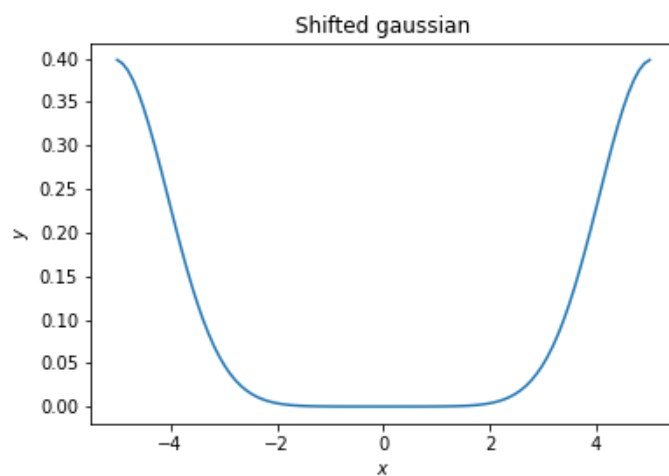
Assignment 5

Phys 512 Computational Physics

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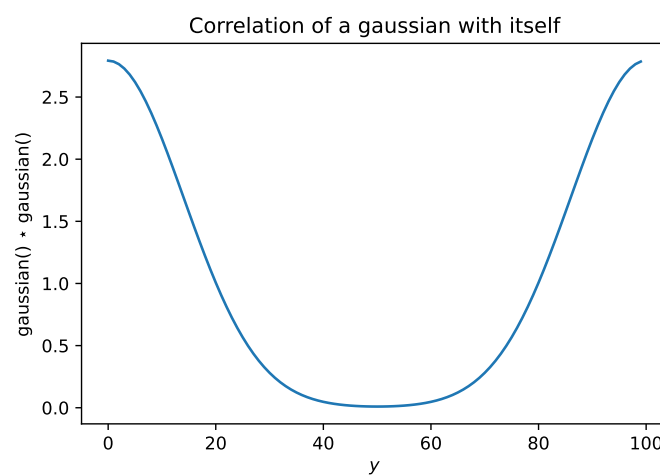
Q1:

The resulting plot is this:



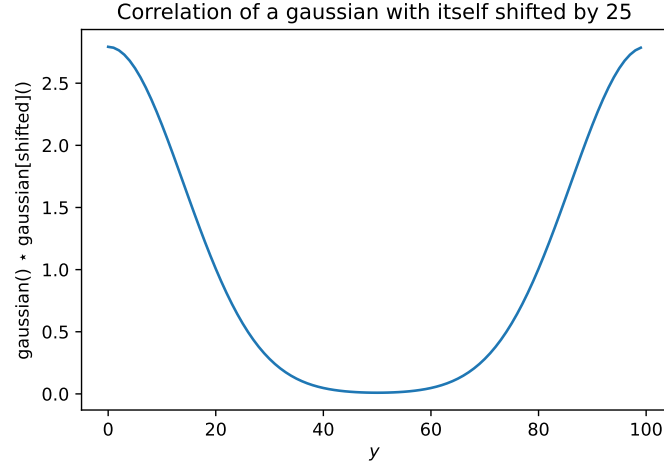
Q2:

The resulting plot is this:



Q3:

I tried shifting by different amounts and always got the same output:



To explain, let's say we're shifting array f by m amount. Let g be the zero array but with 1 in the m th place. The equation we used for shifting is:

$$\begin{aligned}
 \text{shift}(f) &= f * g \\
 &= \text{idft}(\text{dft}(f)\text{dft}(g)) \\
 &= \text{idft}(\text{dft}(f) \exp(-2\pi i m k / N)) \\
 &= \text{idft} \left(\sum_{n=0}^{N-1} f[n] \exp(-2\pi i n k / N) \exp(-2\pi i m k / N) \right) \\
 &= \text{idft} \left(\sum_{n=0}^{N-1} f[n] \exp(-2\pi i (n + m) k / N) \right)
 \end{aligned}$$

(I didn't actually use it; I just did a direct convolution, but it's equivalent.)

Meanwhile for correlation we use

$$f \star h = \text{idft}(\text{dft}(f) \text{conj}(\text{dft}(h)))$$

If we let $h = \text{shift}(f)$ we get:

$$\begin{aligned}
 f \star \text{shift}(f) &= \text{idft}(\text{dft}(f) \text{conj}(\text{dft}(\text{shift}(f)))) \\
 &= \text{idft} \left(\text{dft}(f) \text{conj} \left(\sum_{n=0}^{N-1} f[n] \exp(-2\pi i (n + m) k / N) \right) \right) \\
 &= \text{idft} \left(\text{dft}(f) \left(\sum_{n=0}^{N-1} \text{conj}(f[n]) \exp(2\pi i (n + m) k / N) \right) \right) \\
 &= \text{idft} \left(\left(\sum_{n=0}^{N-1} f[n] \exp(-2\pi i n k / N) \right) \left(\sum_{n=0}^{N-1} \text{conj}(f[n]) \exp(2\pi i (n + m) k / N) \right) \right) \\
 &= \frac{1}{N} \sum_{k=0}^{N-1} \left(\left(\sum_{n=0}^{N-1} f[n] \exp(-2\pi i n k / N) \right) \left(\sum_{n=0}^{N-1} \text{conj}(f[n]) \exp(2\pi i (n + m) k / N) \right) \right) \exp(2\pi i m k / N)
 \end{aligned}$$

The part that the shift amount m affects is in the exponent in the second sum. $(n + m)k$. But notice that every value of n and k are getting summed over anyway, so the m is just changing the order of terms in the sum. (This is also because everything is mod N , so mk will wrap around.) That's why we don't expect the shift amount to change anything.

Q4:

The way I'll do it is to start the g array shifted almost entirely to the left, so that only the last element of g and the first element of f multiply, then gradually shift over g until only the first element of g and the last element of f multiply.

If N is the length of the f array and M is the length of the g array, my output array will be $N + M - 1$ long.

The code is in A5.Q4.py

Q5:

a)

Let $\alpha = \exp(-2\pi i k/N)$. This gives

$$\begin{aligned} \sum_{x=0}^{N-1} \exp(-2\pi i k x/N) &= \sum_{x=0}^N \alpha^x \\ &= \frac{1 - \alpha^N}{1 - \alpha} && \text{geometric sum} \\ &= \frac{1 - \exp(-2\pi i k)}{1 - \exp(-2\pi i k/N)} \end{aligned}$$

b) At $k = 0$, this is $\frac{0}{0}$, so we can use l'Hopital (treating k as nondiscrete variable):

$$\begin{aligned} \lim_{k \rightarrow 0} \frac{1 - \exp(-2\pi i k)}{1 - \exp(-2\pi i k/N)} &= \lim_{k \rightarrow 0} \frac{2\pi i \exp(-2\pi i k)}{\frac{2\pi i}{N} \exp(-2\pi i k/N)} \\ &= N \lim_{k \rightarrow 0} \exp(-2\pi i k(1 + 1/N)) \\ &= N \end{aligned}$$

This is true when k is continuous, so it must also be true when k is discrete by limit properties.

Proving it's always equal to 0 if k isn't a multiple of N :

Since k is an integer, the numerator $1 - \exp(-2\pi i k) = 1 - 1$ is always 0. The denominator $1 - \exp(-2\pi i k/N)$ is always nonzero since k/N isn't an integer. Dividing 0 by nonzero always gives 0.

c)

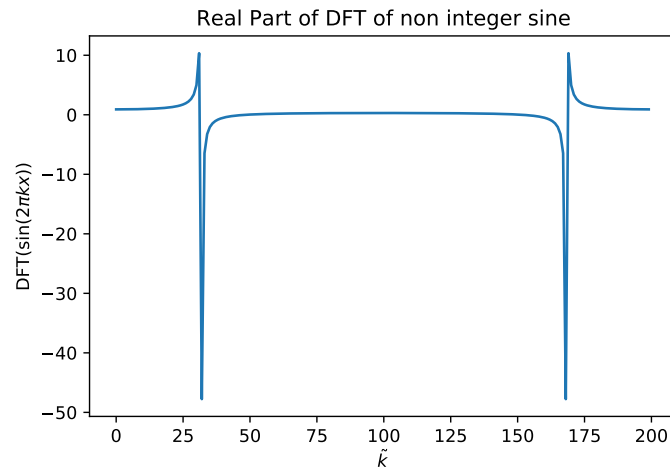
Choose k to be a non integer. Then the non integer sine wave is

$$\sin(2\pi k x) = \frac{\exp(2\pi i k x) - \exp(-2\pi i k x)}{2i}$$

Let $F(\tilde{k})$ be the dft, where \tilde{k} is an integer. We write that out as:

$$\begin{aligned} F(\tilde{k}) &= \sum_{x=0}^{N-1} \left(\frac{\exp(2\pi i k x) - \exp(-2\pi i k x)}{2i} \right) \exp(-2\pi i \tilde{k} x/N) \\ &= \frac{1}{2i} \sum_{x=0}^{N-1} \exp(2\pi i (k - \tilde{k}/N)x) - \frac{1}{2i} \sum_{x=0}^{N-1} \exp(2\pi i (-k - \tilde{k}/N)x) \\ &= \frac{1}{2i} \frac{1 - \exp(2\pi i (kN - \tilde{k}))}{1 - \exp(2\pi i (k - \tilde{k}/N))} - \frac{1}{2i} \frac{1 - \exp(2\pi i (-kN - \tilde{k}))}{1 - \exp(2\pi i (-k - \tilde{k}/N))} \end{aligned}$$

This is the resulting plot: (k is chosen to be $\frac{1}{2\pi}$ and it's plotting 200 points.)

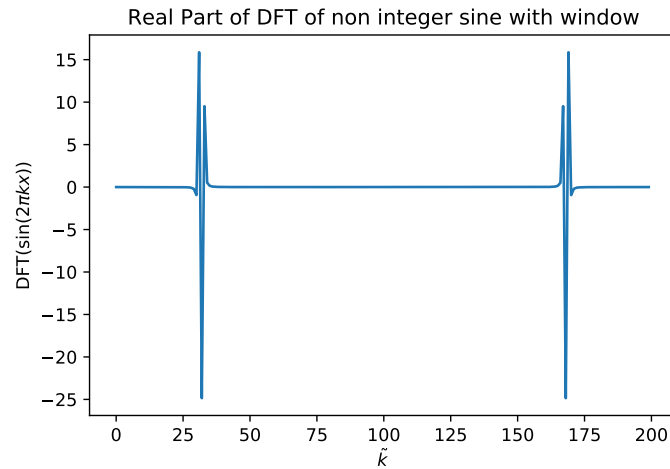


The maximum absolute value of the difference between the analytic points and the numpy fft points is about 10^{-12} , but this goes down when testing fewer points. It's probably just caused by the ringing. With 100 points, it's down to 10^{-13} . With 10 points it's at 10^{-14} .

It's not really a delta function. It's a negative delta function and then a tiny positive delta function beside it. Also the delta spike has a wide base instead of a narrow base.

d)

This is the resulting plot (for same k and N values)



Well the base of the spike is a lot narrower, which is good, but it's still not just one spike.

But maybe this makes sense. The spike is centered around 30, and $\frac{200}{2\pi} \approx 31.83$. So maybe those spikes are like $\tilde{k} = 31$ and $\tilde{k} = 32$, and it needs a linear combination for the two to produce the original sine function.

e) The Fourier transform of the window is

$$\begin{aligned}
W(k) &= \sum_{x=0}^{N-1} w(x) \exp(-2\pi i k x / N) \\
&= \sum_{x=0}^{N-1} \left(\frac{1}{2} - \frac{1}{2} \left(\frac{\exp(2\pi i x / N) + \exp(-2\pi i x / N)}{2} \right) \right) \exp(-2\pi i k x / N) \\
&= \sum_{x=0}^{N-1} \left(\frac{1}{2} \exp(-2\pi i k x / N) - \frac{1}{4} (\exp(2\pi i (1-k)x / N) + \exp(-2\pi i (1+k)x / N)) \right) \\
&= \frac{1}{2} \left(\frac{1 - \exp(-2\pi i k)}{1 - \exp(-2\pi i k / N)} \right) - \frac{1}{4} \left(\frac{1 - \exp(2\pi i (1-k))}{1 - \exp(2\pi i (1-k) / N)} \right) - \frac{1}{4} \left(\frac{1 - \exp(-2\pi i (1+k))}{1 - \exp(-2\pi i (1+k) / N)} \right)
\end{aligned}$$

The first term goes to $\frac{N}{2}$ (proved earlier) only when $k = 0$, and it's 0 otherwise. The second term is 0 unless $k = 1$, in which case it takes the value $-\frac{N}{4}$. The final term is 0 unless $k = -1$, which is the same as saying $k = N-1$. It also takes the value of $-\frac{N}{4}$.

The resulting array looks like $[\frac{N}{2}, -\frac{N}{4}, 0, \dots, 0, -\frac{N}{4}]$.

Let the unwrapped Fourier transform array look like $[F[0], F[1], \dots, F[N-1]]$. We're taking a convolution of this and the above array, which we'll call $G = [\frac{N}{2}, -\frac{N}{4}, 0, \dots, 0, -\frac{N}{4}]$.

Let D be the convolution array. Then $D[i]$ is:

$$D[i] = \sum_{j=0}^{N-1} F[j] G[i-j]$$

The only nonzero terms are $j = i$, $j = i+1$, and $j = i-1$.

$$\begin{aligned}
D[i] &= F[i-1]G[-1] + F[i]G[0] + F[i+1]G[1] \\
&= -\frac{N}{4}F[i-1] + \frac{N}{2}F[i] - \frac{N}{4}F[i+1]
\end{aligned}$$

And this $D[i]$ should be the exact same thing we get by multiplying in real space and then taking the Fourier transform.

Q6:

a) From the Wiener-Khinchin Theorem, we get that the power spectrum is the Fourier transform of the correlation function.

The correlation function we found is $g(\delta) = c - |\delta|$. Then the Fourier transform is

$$\begin{aligned} G(k) &= \sum_{\delta=0}^{N-1} (c - \delta) e^{-2\pi i k \delta / N} \\ &= c \sum_{\delta=0}^{N-1} e^{-2\pi i k \delta / N} - \sum_{\delta=0}^{N-1} \delta e^{-2\pi i k \delta / N} \end{aligned}$$

Using partial sum identities, we can write

$$\begin{aligned} \sum_{\delta=0}^{N-1} e^{-2\pi i k \delta / N} &= \frac{1 - \exp(-2\pi i k)}{1 - \exp(-2\pi i k / N)} \\ \sum_{\delta=0}^{N-1} \delta e^{-2\pi i k \delta / N} &= \frac{\exp(2\pi i k / N) - N \exp(-2\pi i k) + (N-1) \exp(-2\pi i k \frac{N+1}{N})}{(1 - \exp(-2\pi i k / N))^2} \end{aligned}$$

So we subtract the two fractions:

$$G(k) = \frac{c - c \exp(-2\pi i k)}{1 - \exp(-2\pi i k / N)} - \frac{\exp(2\pi i k / N) - N \exp(-2\pi i k) + (N-1) \exp(-2\pi i k \frac{N+1}{N})}{(1 - \exp(-2\pi i k / N))^2}$$

Putting them over the same common denominator means we need to multiply out the numerator of the first fraction:

$$(c - c \exp(-2\pi i k))(1 - \exp(-2\pi i k / N)) = c - c \exp(-2\pi i k) - c \exp(-2\pi i k / N) + c \exp(-2\pi i k \frac{N+1}{N})$$

Adding those terms into the rest gives:

$$G(k) = \frac{c - (c+1) \exp(2\pi i k / N) + (N-c) \exp(-2\pi i k) - (N-1-c) \exp(-2\pi i k \frac{N+1}{N})}{(1 - \exp(-2\pi i k / N))^2}$$

Now we're going into approximation land. We'll take N to be large, so $\frac{N+1}{N} \rightarrow 1$.

$$G(k) = \frac{c - (c+1) \exp(2\pi i k / N) + (N-c) \exp(-2\pi i k) - (N-1-c) \exp(-2\pi i k)}{(1 - \exp(-2\pi i k / N))^2}$$

So we can subtract off the $(N-c)$ multiple.

$$G(k) = \frac{c - (c+1) \exp(2\pi i k / N) + \exp(-2\pi i k)}{(1 - \exp(-2\pi i k / N))^2}$$

And actually $\exp(-2\pi i k)$ is always 1 since k is an integer.

$$\begin{aligned} G(k) &= \frac{c - (c+1) \exp(2\pi i k / N) + 1}{(1 - \exp(-2\pi i k / N))^2} \\ &= (c+1) \frac{1 - \exp(2\pi i k / N)}{(1 - \exp(-2\pi i k / N))^2} \\ &= (c+1) \frac{1}{1 - \exp(-2\pi i k / N)} \\ &= \frac{c}{1 - \exp(-2\pi i k / N)} \end{aligned}$$

In the last line, we redefined c as $c+1$ since it's nothing but a constant multiple anyway.

Now we use the fact that $g(\delta) = c - |\delta| = c - |-\delta| = g(-\delta)$ to conclude that the Fourier transform $G(k)$ is real. The easiest way to find the real part of this is to find the absolute value squared and then square root.

$$\begin{aligned} |G(\delta)|^2 &= \left(\frac{c}{1 - \exp(-2\pi i k/N)} \right) \left(\frac{c}{1 - \exp(2\pi i k/N)} \right) \\ &= \frac{c^2}{1 - \exp(2\pi i k/N) - \exp(-2\pi i k/N) + 1} \\ &= \frac{c^2}{2 - 2\cos(2\pi k/N)} \end{aligned}$$

This concludes the part of the math where I know what's happening.

If we assume k is small relative to N , then we can Taylor expand \cos around k/N .

$$\cos(2\pi i k/N) \approx 1 - 2\pi^2 \frac{k^2}{N^2}$$

Plugging this in gives:

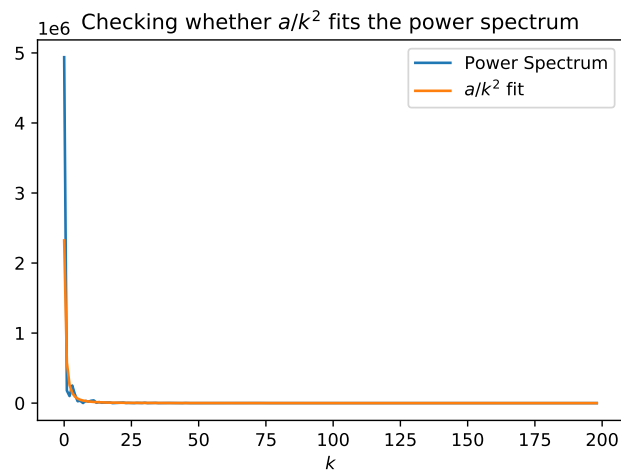
$$\begin{aligned} |G(\delta)|^2 &= \frac{c^2}{2 - 2(1 - 2\pi^2 \frac{k^2}{N^2})} \\ &= \frac{c^2 N^2}{4\pi^2 k^2} \end{aligned}$$

This *does* go like k^{-2} , but the power spectrum is supposed to be the square root of this.

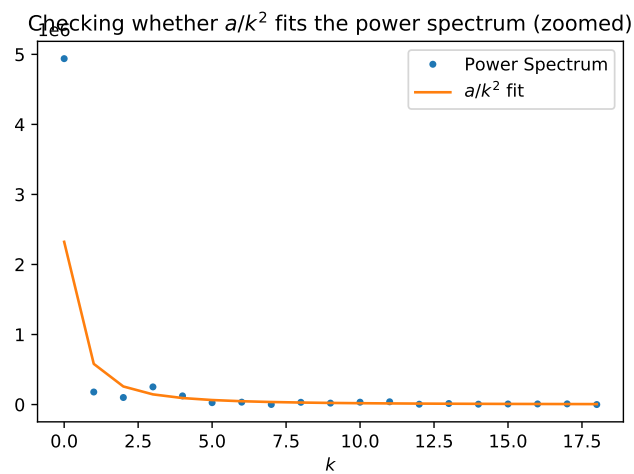
$$G(\delta) = \frac{cN}{2\pi k}$$

Which goes like k^{-1} . Apparently I dropped a power of 2 somewhere.

b) Using an example random walk, we can plot the power spectrum and compare it to an $\frac{a}{k^2}$ function:



And zoomed-in on the interesting part:



We can see that the fit is pretty good.