

# Computational Physics

## Lecture 4

[sieversj@ukzn.ac.za](mailto:sieversj@ukzn.ac.za)

git clone [https://github.com/ukzncompphys/lecture4\\_2015.git](https://github.com/ukzncompphys/lecture4_2015.git)

# Tutorial Problems

- How can you list all files in a directory, with the most recent one displayed last? (5)
- How can you display the first 25 lines of a file? How can you display just lines 16 through 25? (5)
- How can you search for all commands relating to python? Hint - it will be a use of “man”. (5)
- Make a new text file with your name, email address, what you’re working on for your honours project, plus a few things you’d like to learn in the course. Initialize a git repository and commit this file. (5)
- Put your answers to the other tutorial questions into another text file. Add this to the repository also. (5)
- Make a github account and push the repository onto github. Email me your github name so I can have a look at your file/answers. (10)

# Fourier Transforms

- Functions can be represented in many different ways
- We normally use “real” space -  $f(x)$
- Generally, arbitrarily many transforms exist to represent functions in different spaces -  $F(y)=Af(x)$  for some matrix  $A$  and some new variable  $y$ .  
Iff  $A$  is invertible,  $f(x)=A^{-1}F(y)$
- One important basis nature has picked out is complex exponentials/sines and cosines. Fundamental across physics, particularly quantum mechanics.

# Fundamental Definition

- $F(k) = \int f(x) \exp(2\pi i k x) dx$  (where  $k = 1/\omega$ )
- Integral gets rid of  $x$ , replaces with  $k$ . New function has amplitude and phase as a function of  $k$ .
- Quantum mechanics - de Broglie says  $p = \hbar k$ . So, Fourier transform position to get momentum.
- Fourier transform electric field  $E(t)$  to get frequency spectrum.
- Fourier transform to get fast correlations, convolutions, many other things.

# DFT (Discrete FT)

- Computers don't do continuous. Not enough RAM for starters...
- Function exists over finite range in  $x$  at finite number of points.
- If input function has  $n$  points, output can only have  $n$   $k$ 's.
- Gives rise to discrete Fourier Transform (DFT)
- $F(k) = \sum f(x) \exp(2\pi i k x / N)$  for  $N$  points and  $0 \leq k < N$
- What would DFT of  $f(0)=1$ , otherwise  $f(x)=0$  look like?
- What would DFT of  $f(x)=1$  look like?
- DFTs have subtle behaviours not seen in continuous, infinite FTs.

# Inverse

- One way to think about DFT is as a matrix multiply.
- $F(k) = Af$ ,  $A_{mn} = \exp(2\pi i mn/N)$
- But look -  $A_{mn} = A_{nm}$ , so matrix is symmetric.
- Also, columns are orthogonal under conjugation:  
 $\sum \exp(-2\pi i kx) \exp(2\pi i k'x) = \sum \exp(2\pi i (k' - k)x)$ .  $N$  if  $k' = k$ , otherwise  $0$ .
- So,  $A^{-1} = 1/N \cdot \text{conj}(A)$ .  $\text{IFT} = 1/N \sum F(k) \exp(-2\pi i kx)$ .
- Get back to where we started by just doing another DFT with a sign flip, then divide by # of data points.
- Alternative: divide by  $\sqrt{N}$  in both DFT and IFT, (not standard computationally)

# Numpy Complex

```
import numpy
def exp_prod(m,n,N):
    #define imaginary unity
    J=numpy.complex(0,1)
    #now rest of code is just like for real numbers
    x=numpy.arange(0.0,N)*2*J*numpy.pi/N
    return numpy.sum(numpy.exp(-1*x*m)*numpy.exp(x*n))
if __name__=="__main__":
    print exp_prod(0,0,8)
    print exp_prod(2,4,8)
    print exp_prod(3,3,8)
    print exp_prod(0,7,8)
```

```
Jonathans-MacBook-Pro:lecture4 sievers$ python dft_columns.py
(8+0j)
(-4.28626379702e-16+4.4408920985e-16j)
(8+0j)
(3.44169137634e-15-1.11022302463e-15j)
Jonathans-MacBook-Pro:lecture4 sievers$
```

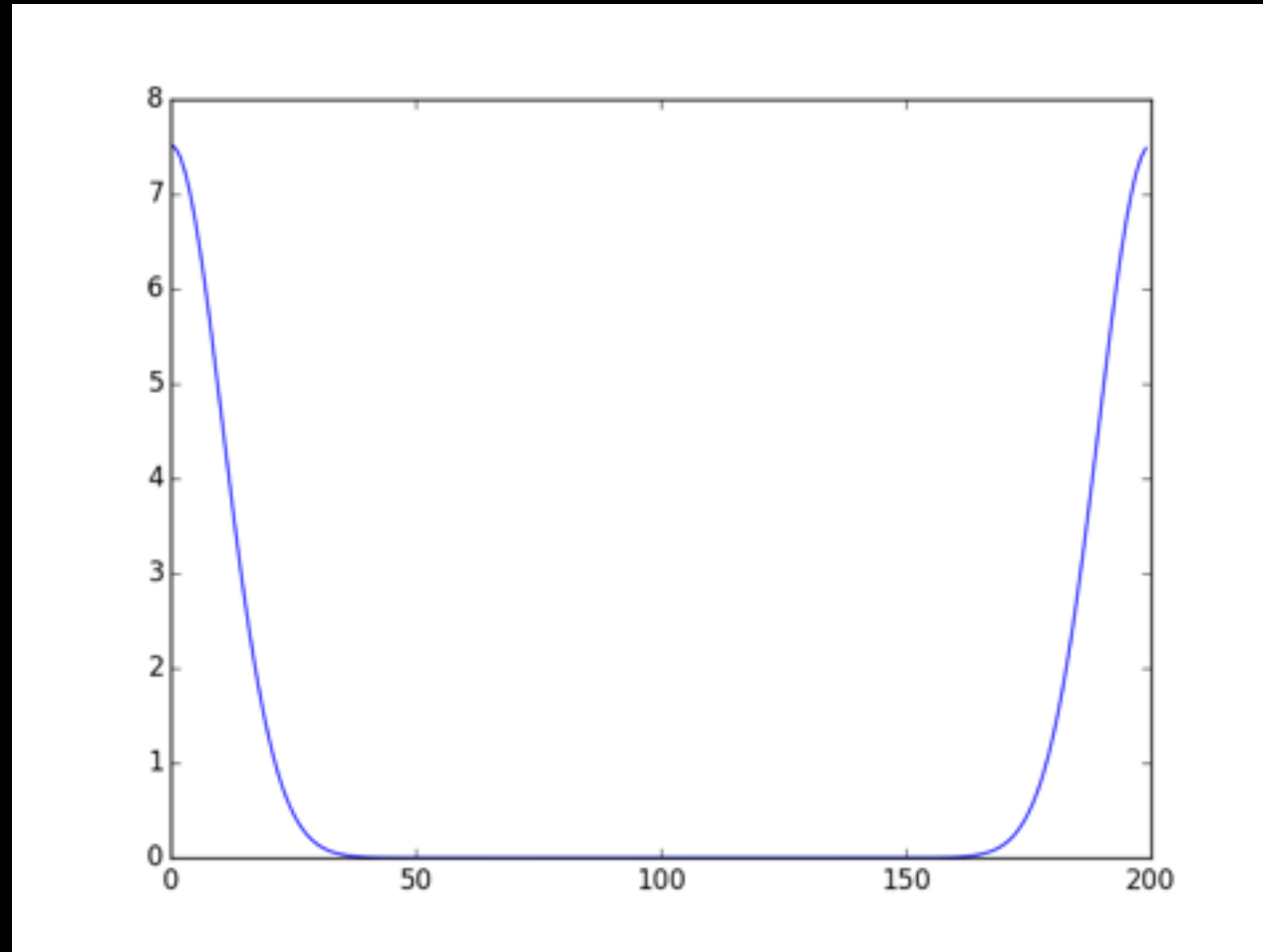
- Let's check orthogonality, need complex #'s.
- `numpy.complex(re,im)` will make a complex #
- numpy functions usually defined for complex #'s.

# DFTs with Numpy

- Numpy has many Fourier Transform operations
- (for reasons to be seen) they are called *Fast* Fourier Transforms - FFT is one way of implementing DFTs.
- FFT's live in a submodule of numpy called FFT
- `xft=numpy.fft.fft(x)` takes DFT
- `x=numpy.fft.ifft(x)` takes inverse DFT
- Numpy normalizes such that  $f = \text{fft}(\text{ifft}(f)) = \text{ifft}(\text{fft}(f))$

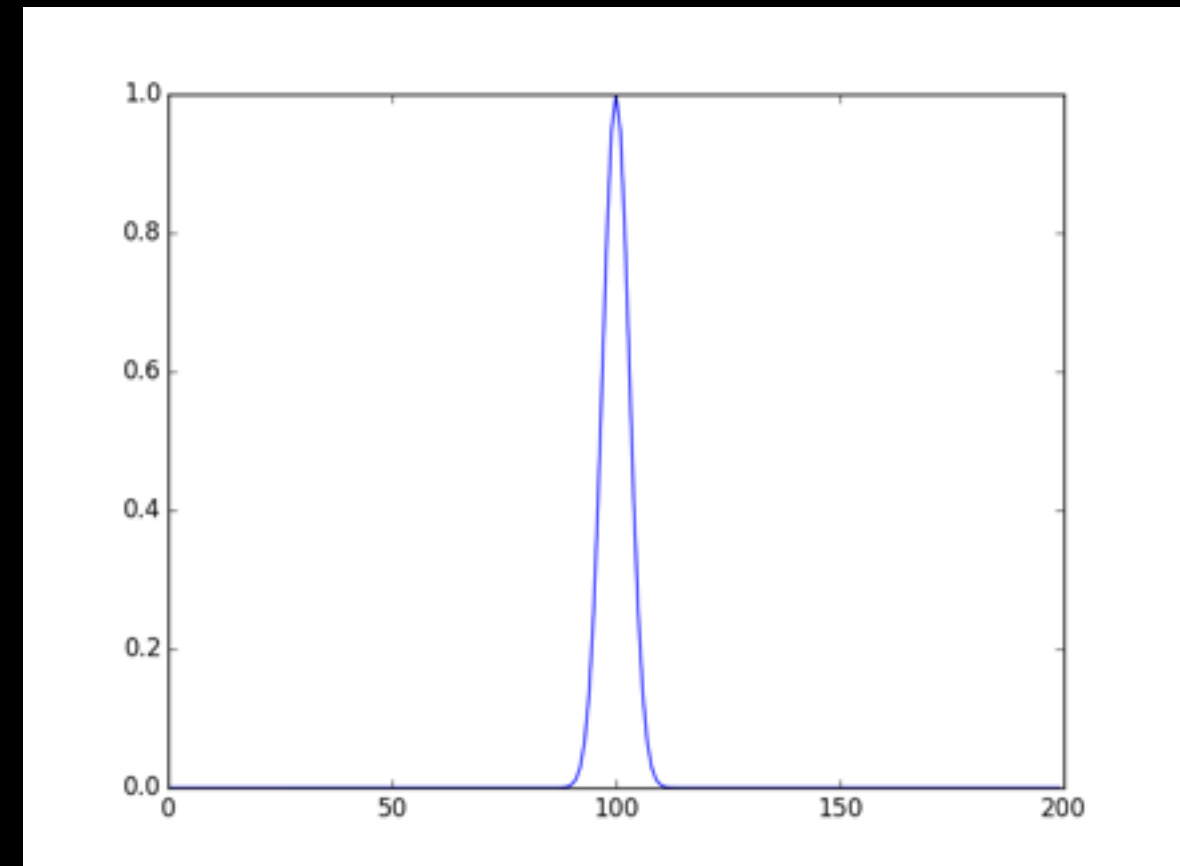


# DFT in Action



```
import numpy
from matplotlib import pyplot as plt

x=numpy.arange(-10,10,0.1)
y=numpy.exp(-0.5*x**2/(0.3**2))
yft=numpy.fft.fft(y)
plt.plot(numpy.abs(yft))
plt.savefig('gauss_dft')
plt.show()
```



- Left: input Gaussian
- Top: DFT of the Gaussian

# Periodicity

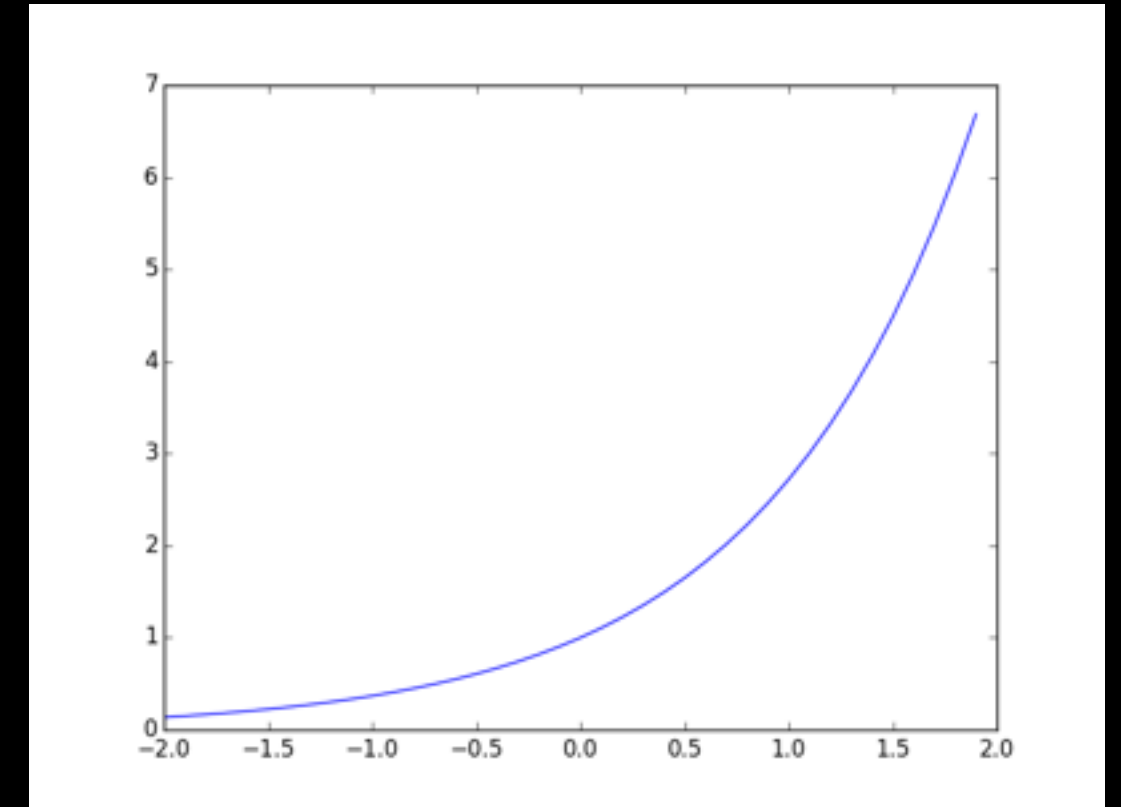
- $f(x) = \sum F(k) \exp(2\pi i k x / N)$
- What is  $f(x+N)$ ?  $\sum F(k) \exp(2\pi i k (x+N) / N)$
- $= \sum F(k) \exp(2\pi i k) \exp(2\pi i k x / N)$ .
- $\exp(2\pi i k) = 1$  for integer  $k$ , so  $f(x+N) = f(x)$
- DFT's are periodic - they just repeat themselves ad infinitum.

# Periodicity

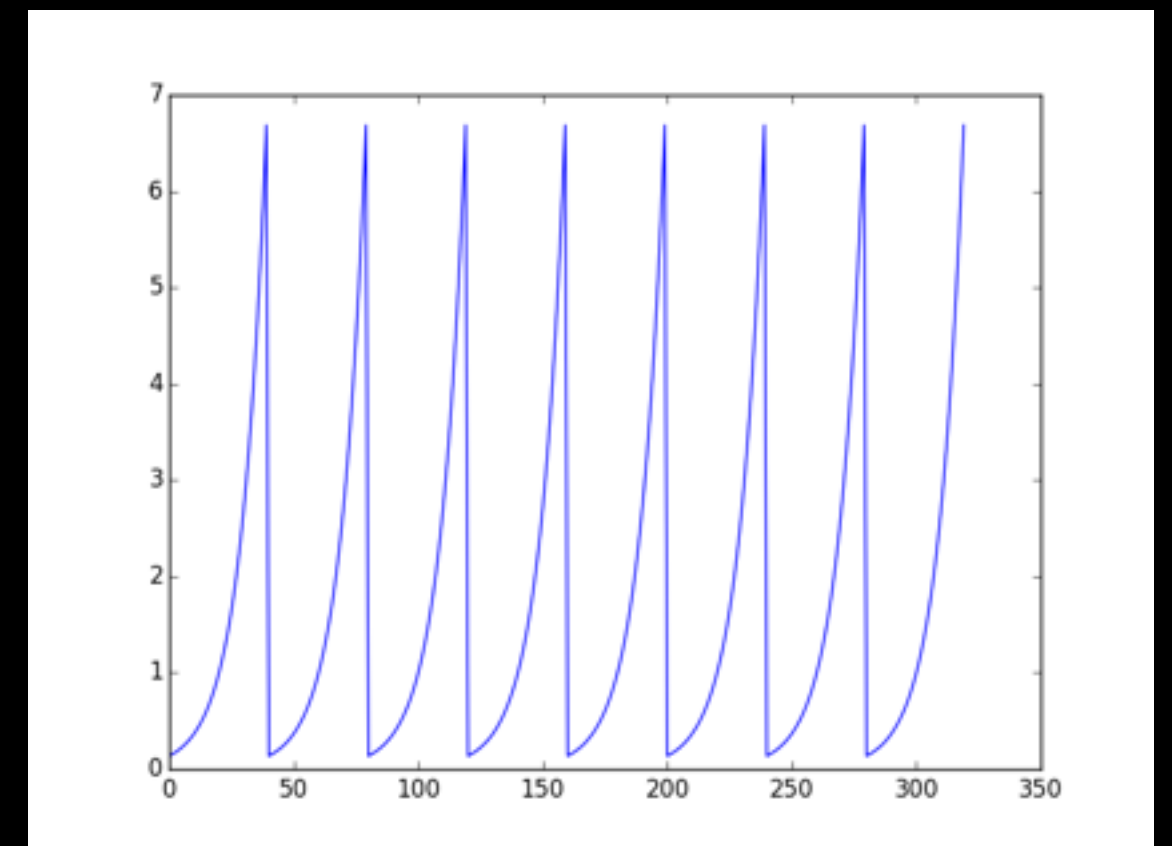
```
import numpy
from matplotlib import pyplot as plt

x=numpy.arange(-2,2,0.1)
y=numpy.exp(x)
plt.plot(x,y)
plt.savefig('fft_exp')
plt.show()

yy=numpy.concatenate((y,y))
yy=numpy.concatenate((yy,yy))
yy=numpy.concatenate((yy,yy))
plt.plot(yy)
plt.savefig('fft_exp_repeating')
plt.show()
```



- You may think you're taking top transform. You're not - you're taking the bottom one.
- In particular, jumps from right edge to left will strongly affect DFT



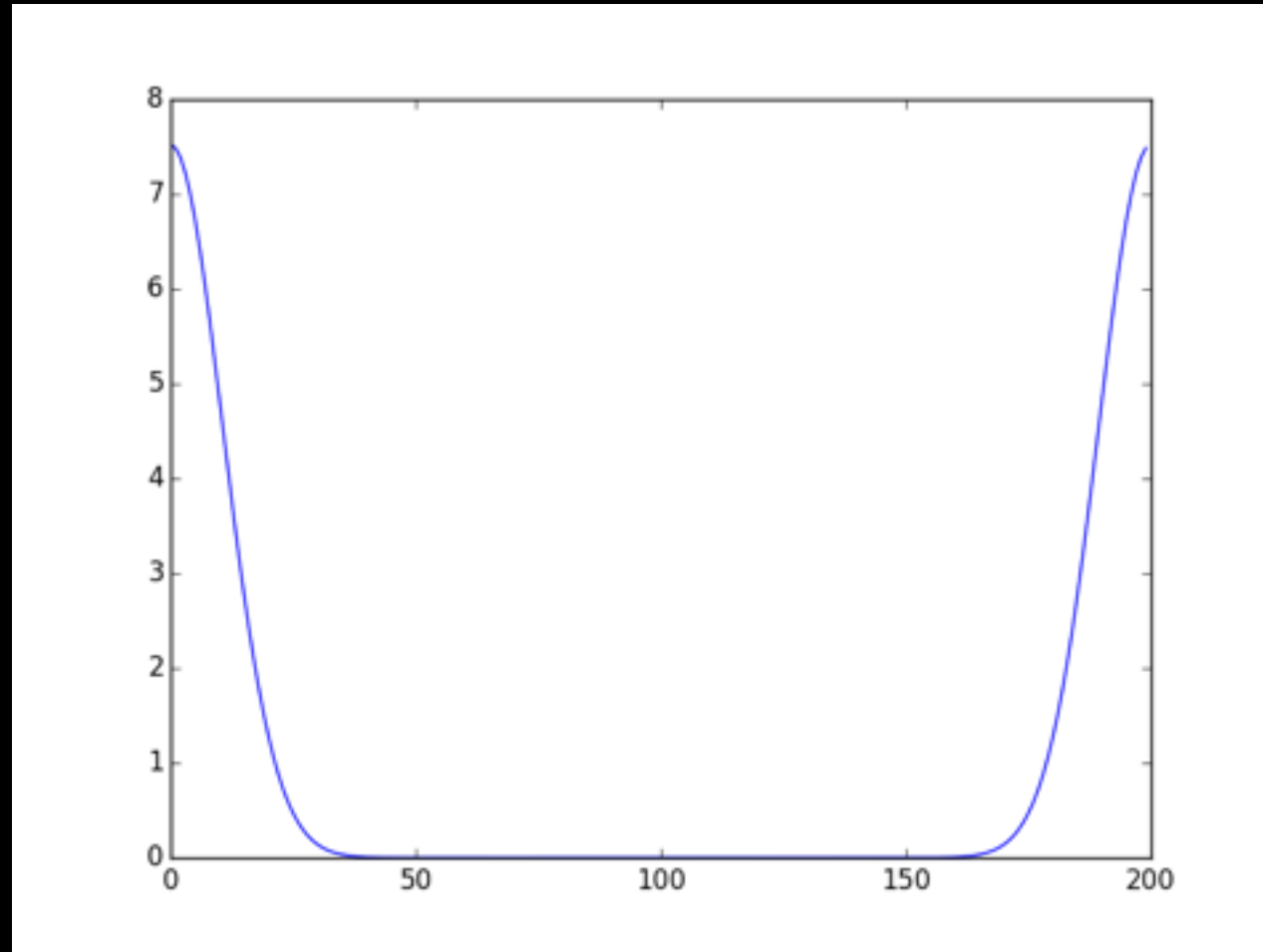
# Aliasing

- $f(x) = \sum F(k) \exp(-2\pi i k x / N)$
- What if I had higher frequency,  $k > N$ ? let  $k^* = k - N$  (i.e.  $k^*$  low freq.)
- $f(x) = \sum F(k) \exp(-2\pi i (k^* + N)x / N) = \sum F(k) \exp(-2\pi i x) \exp(-2\pi i k^* x / N)$
- for  $x$  integer, middle term goes away:  $\sum F(k^* + N) \exp(-2\pi i k^* x / N)$
- High frequencies behave exactly like low frequencies - power has been *aliased* into main frequencies of DFT.
- Always keep this in mind! Make sure samples are fine enough to prevent aliasing.

# Negative Frequencies

- All frequencies that are  $N$  apart behave identically
- DFT has frequencies up to  $(N-1)$ .
- Frequency  $(N-1)$  equivalent to frequency  $(-1)$ . You will do better to think of DFT as giving frequencies  $(-N/2, N/2)$  than frequencies  $(0, N-1)$
- *Sampling theorem*: if function is band-limited - highest frequency is  $\nu$  - then I get full information if I sample *twice* per frequency,  $\Delta t = 1/(2\nu)$ . Factor of 2 comes from aliasing.

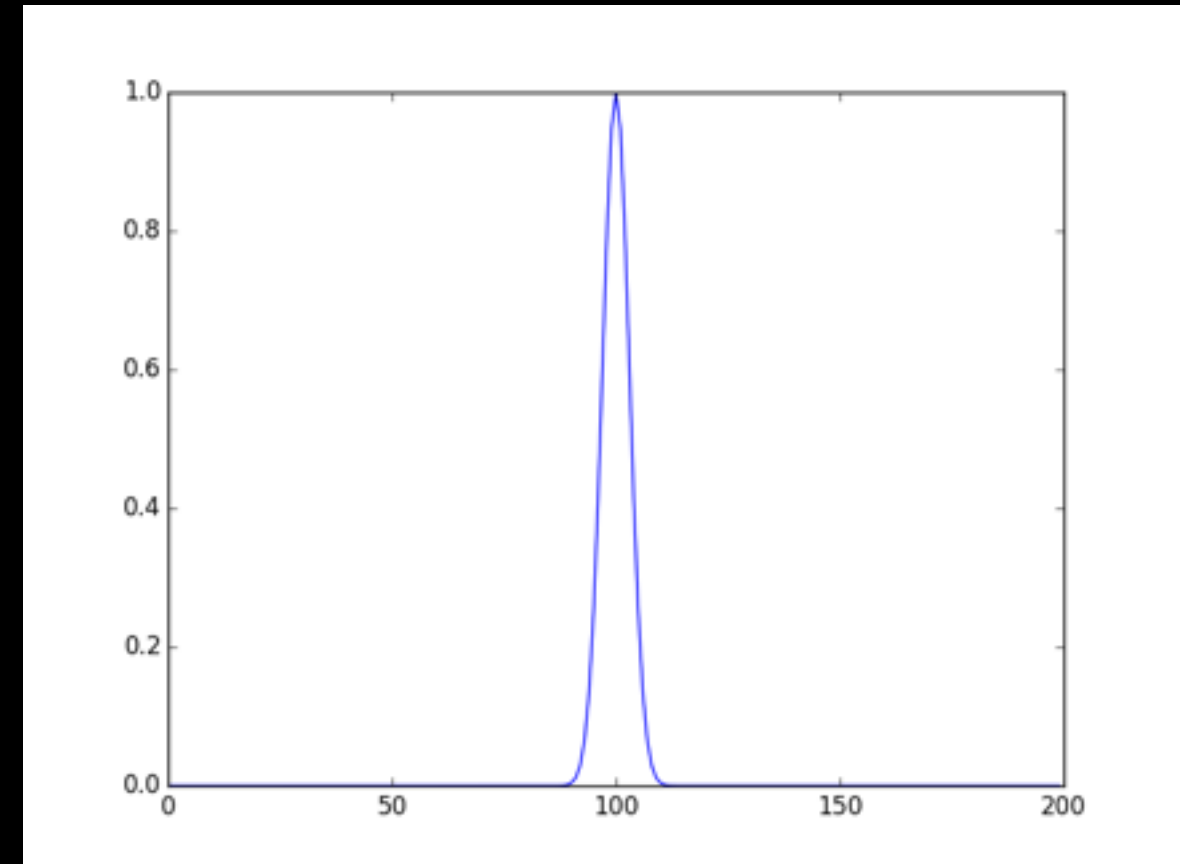
# DFT in Action, Redux



```
import numpy
from matplotlib import pyplot as plt

x=numpy.arange(-10,10,0.1)
y=numpy.exp(-0.5*x**2/(0.3**2))
yft=numpy.fft.fft(y)
plt.plot(numpy.abs(yft))
plt.savefig('gauss_dft')
plt.show()
```

- FFT makes more sense now - negative frequencies have been aliased to high frequency.



# Flipping

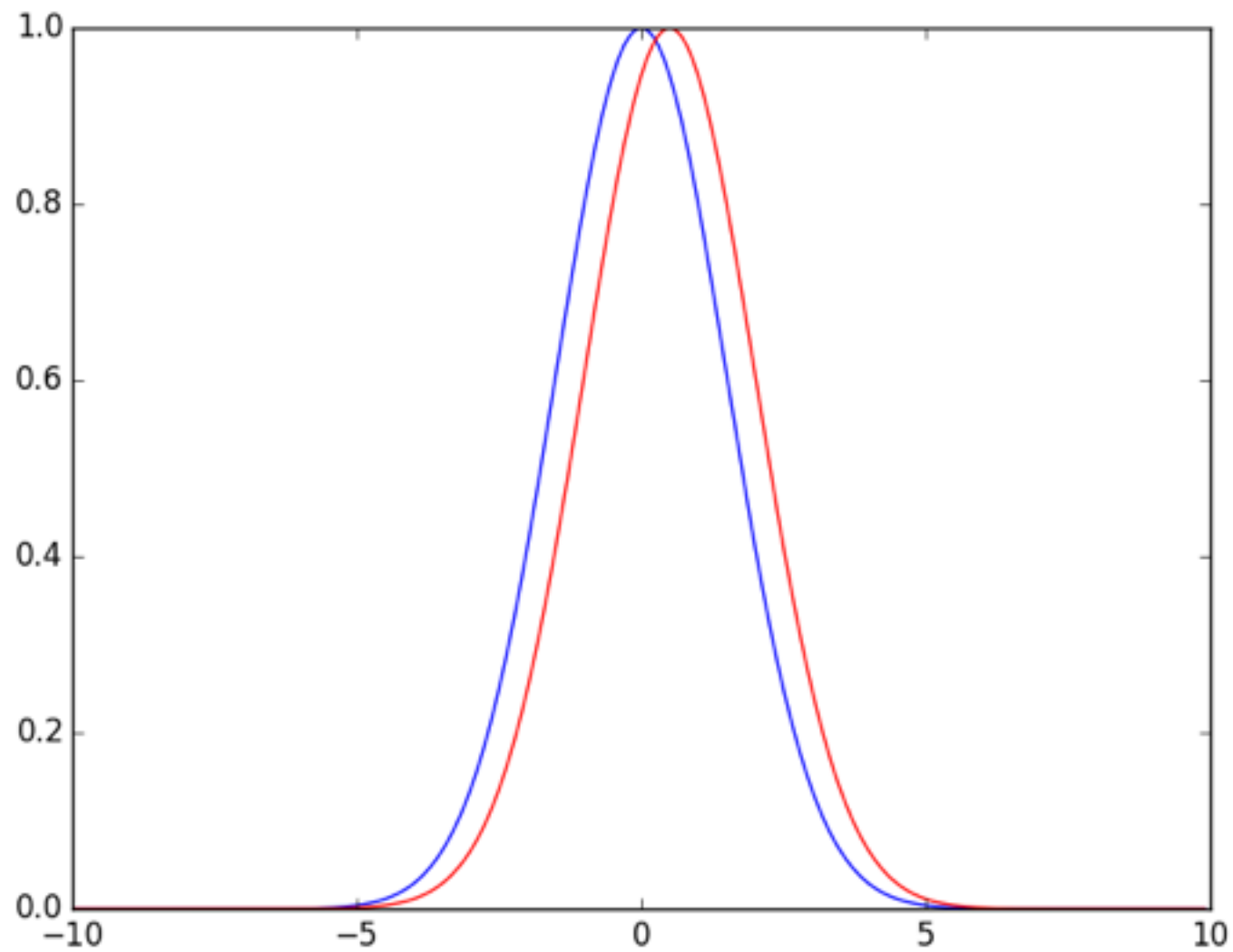
- What is DFT of  $f(-x)$ ?
- $\sum f(-x) \exp(2\pi i k x / N)$ ,  $x^* = -x$ ,  $\sum f(x^*) \exp(2\pi i k (-x) / N)$
- $\text{DFT}(f(-x)) = \sum f(x) \exp(-2\pi i k x / N) = \text{conj}(F(k))$

# Shifting

- What is  $\text{FFT}(x+dx)$ ?  $\sum f(x+dx)\exp(2\pi i k x/N)$ .
- $x^*=x+dx$ :  $F(k)=\sum f(x^*)\exp(2\pi i k (x^*-dx)/N)$
- $F(k)=\exp(-2\pi i k dx/N)\sum f(x^*)\exp(2\pi i k x^*/N)$
- So, just apply a phase gradient to the DFT to shift in  $x$



# Shifting Example



```
import numpy
from matplotlib import pyplot as plt

x=numpy.arange(-10,10,0.1)
y=numpy.exp(-0.5*x**2/(1.5**2))
N=x.size
kvec=numpy.arange(N)
yft=numpy.fft.fft(y)
J=numpy.complex(0,1)
dx=5.0;
yft_new=yft*numpy.exp(-2*numpy.pi*J*kvec*dx/N)
y_new=numpy.real(numpy.fft.ifft(yft_new))
plt.plot(x,y)
plt.plot(x,y_new,'r')
plt.savefig('shifted_gaussian')
plt.show()
```

# Real Data Symmetry

- If I know  $F(k)$ , what is  $F(N-k)$  if  $f(x)$  is real?
- $F(N-k)=F(-k)$  (from alias theorem)
- $F(-k)=\sum f(x)\exp(2\pi i(-k)x/N)$ . let  $x^*=-x$
- $F(-k)=\sum f(-x^*)\exp(2\pi i k x^*/N) = \text{conj}(F(k))$  by flipping
- So, if  $f(x)$  is real,  $F(k)=\text{conj}(F(N-k))$
- If  $N$  even,  $F(N/2)=\text{conj}(F(N/2))$ , so  $F(N/2)$  must be real.

```
>>> x=numpy.random.randn(8)
>>> xft=numpy.fft.fft(x)
>>> for xx in xft:
...     print xx
...
(-4.53568815727+0j)
(-0.174046761579+2.08827239558j)
(2.15348308858+2.32162497273j)
(-0.423040513854-3.72126858798j)
(2.75685372591+0j)
(-0.423040513853+3.72126858798j)
(2.15348308858-2.32162497273j)
(-0.174046761579-2.08827239558j)
>>>
```

# Convolution Theorem

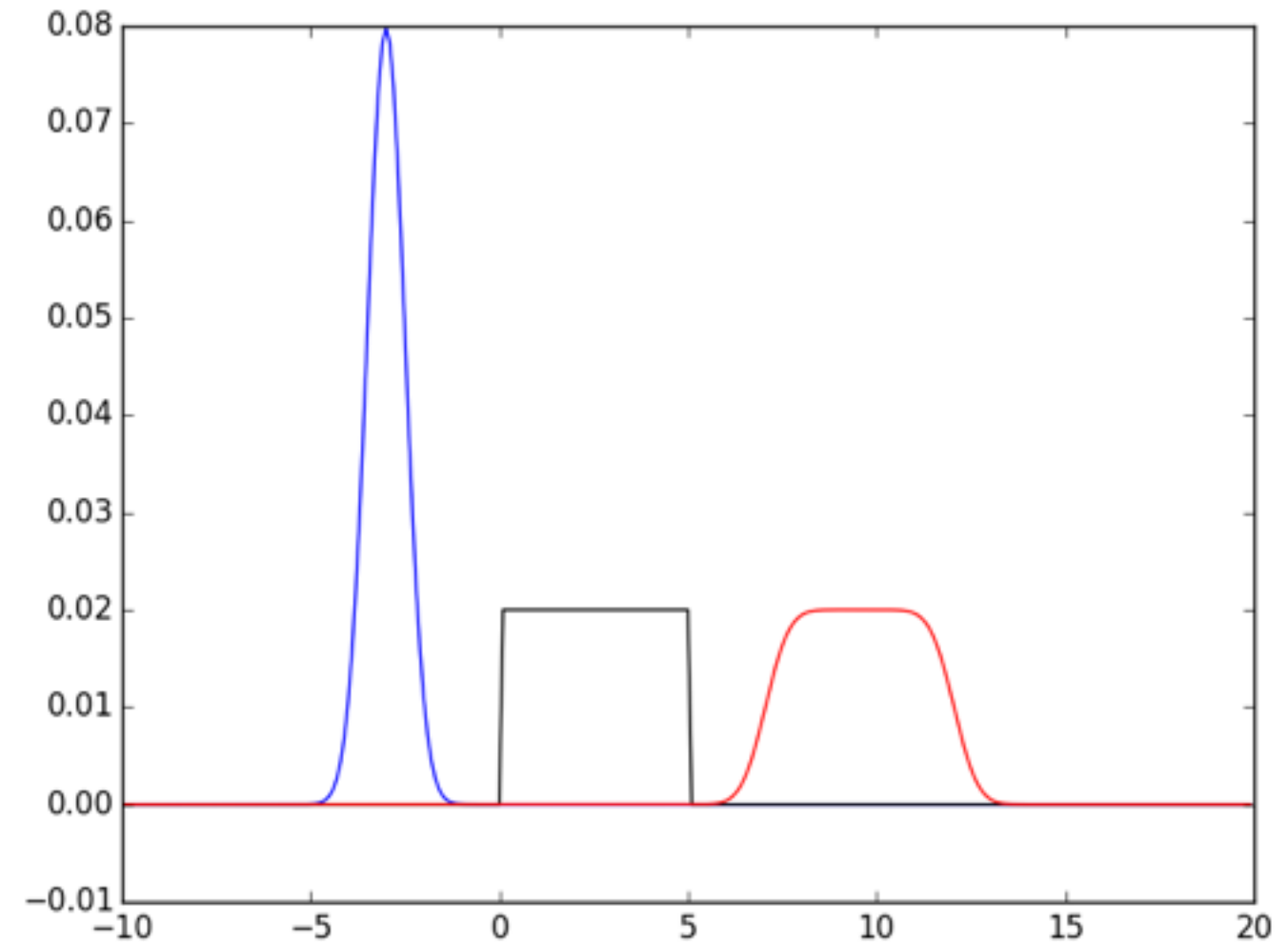
- Convolution defined to be  $\text{conv}(y) = f \otimes g = \int f(x)g(y-x)dx$
- $\sum_x \sum F(k) \exp(-2\pi i k x) \sum \text{conj}(G(k')) \exp(-2\pi i k' x) \exp(2\pi i k' y/N)$
- Reorder sum:  $\sum \sum F(k) \text{conj}(G(k')) \exp(2\pi i k' y/N) \sum_x \exp(-2\pi i (k+k')x)$
- equals zero unless  $k' = -k$ . Cancels one sum, conjugates  $G$
- $f \otimes g = \sum F(k)G(k) \exp(-2\pi i k y/N) = \text{ift}(\text{dft}(f) * \text{dft}(g))$
- So, to convolve two functions, multiply their DFTs and take the IFT

# Convolution Example

```
from numpy import arange,exp,real
from numpy.fft import fft,ifft
from matplotlib import pyplot as plt
def conv(f,g):
    ft1=fft(f)
    ft2=fft(g)
    return real(ifft(ft1*ft2))

x=arange(-10,20,0.1)
f=exp(-0.5*(x+3)**2/0.5**2)
g=0*x;g[(x>0)&(x<5)]=1
g=g/g.sum()
f=f/f.sum()
h=conv(f,g)

plt.plot(x,f,'b')
plt.plot(x,g,'k')
plt.plot(x,h,'r')
plt.savefig('convolved')
plt.show()
```



# Fast Fourier Transform

- How many operations does a DFT take?
- Have an  $N$  by  $N$  matrix operating on a vector of length  $N$  - clearly  $N^2$  operations, right?
- Nope! Otherwise we'd never use them. What's actually going on?
- Note  $\text{DFT} = \sum f(x) \exp(2\pi i k x / N) = \sum f_{\text{even}}(x) \exp(2\pi i k (2x) / N) + \sum f_{\text{odd}}(x) \exp(2\pi i k (2x + 1) / N)$
- $= F_{\text{even}} + \exp(2\pi i k / N) F_{\text{odd}}$ . Let  $W_k = \exp(2\pi i k / N)$
- if  $k > N/2$ , then  $k^* = k - N/2$  and  $\text{DFT} = F_{\text{even}} + \exp(2\pi i k^* / N + i\pi) F_{\text{odd}} = F_{\text{even}} - W_k F_{\text{odd}}$ .

# FFT cont'd

- So  $F(k) = F_{\text{even}}(k) + W_k F_{\text{odd}}(k)$  ( $k < N/2$ ) or  $F_{\text{even}}(k) - W_k F_{\text{odd}}(k)$  ( $k \geq N/2$ )
- So, can get *all* the frequencies if I have 2 half-length FFTs.
- Well, just do the same thing again. FFT of a single element is itself.
- This algorithm works for arrays whose length is a power of 2
- Popularized by Cooley/Tukey in early computer days. Later found to go back to Gauss in 1805. Changes computational work from  $n^2$  to  $n \log n$ .

# Sample FFT

- Routine uses *recursion* - function calls itself. Recursion can be very powerful, but also easy to goof.
- `numpy.concatenate` will combine arrays - note that they have to be passed in as a tuple, hence the extra set of parenthesis
- Modern FFT routines deal with arbitrary length arrays. Fastest Fourier Transform in the West (FFTW) standard packaged - usually used by numpy.

```
from numpy import concatenate,exp,pi,arange,complex
def myfft(vec):
    n=vec.size
    #FFT of length 1 is itself, so quit
    if n==1:
        return vec
    #pull out even and odd parts of the data
    myeven=vec[0::2]
    myodd=vec[1::2]

    nn=n/2;
    j=complex(0,1)
    #get the phase factors
    twid=exp(-2*pi*j*arange(0,nn)/n)

    #get the dfts of the even and odd parts
    eft=myfft(myeven)
    oft=myfft(myodd)

    #Now that we have the partial dfts, combine them with
    #the phase factors to get the full DFT
    myans=concatenate((eft+twid*oft,eft-twid*oft))
    return myans
```

```
>>> import myft
>>> x=numpy.random.randn(32)
>>> xft1=numpy.fft.fft(x)
>>> xft2=myft.myfft(x)
>>> print numpy.sum(numpy.abs(xft1-xft2))
2.33937690259e-13
>>>
```

# Tutorial Problems

- Write a function that will shift an array by an arbitrary amount using a convolution (yes, I know there are easier ways to do this). The function should take 2 arguments - an array, and an amount by which to shift the array. Plot a gaussian that started in the centre of the array shifted by half the array length. (10)
- The correlation function  $f \star g$  is  $\int f(x)g(x+y)$ . Through a similar proof, one can show  $f \star g = \text{ift}(\text{dft}(f) * \text{conj}(\text{dft}(g)))$ . Write a routine to take the correlation function of two arrays. Plot the correlation function of a Gaussian with itself. (10)
- Using the results of part 1 and part 2, write a routine to take the correlation function of a Gaussian (shifted by an arbitrary amount) with itself. How does the correlation function depend on the shift? Does this surprise you? (10)
- The circulant (wrap-around) nature of the dft can sometimes be problematic. Write a routine to take the convolution of two arrays \*without\* any danger of wrapping around. You may wish to add zeros to the end of the input arrays. (10)



# Tutorial Bonus Problem

- You have a sample code that calculates an FFT of an array whose length is a power of 2. Using that routine as a guideline, write an FFT routine that works on an array whose length is a power of 3 (e.g. 9, 27, 81). Verify that it gives the same answer as `numpy.fft.fft` (10)