Computational Physics
Lecture 3

sieversj@ukzn.ac.za

git clone https://github.com/ukzncompphys/lecture3_2018.git

Variables

```
Jonathans-MacBook-Pro:lecture3 sievers$ cat simple_variables.py
x=5
y=3.0
z=x+y
print 'z is ' + repr(z)
print 'z is a ' + repr(type(z))
print 'x is a ' + repr(type(x))
print 'y is a ' + repr(type(y))

Jonathans-MacBook-Pro:lecture3 sievers$ python simple_variables.py
z is 8.0
z is a <type 'float'>
x is a <type 'int'>
y is a <type 'float'>
Jonathans-MacBook-Pro:lecture3 sievers$
```

- Python has several built-in variable types. These include strings, floats, ints, boolean.
- You can create variables by assigning to them.
- You can see what type variables are with the *type* command.
- You can print their values with the *print* command. *repr* will return value as a string
- strings can be combined with '+'. Types may be automatically converted.

```
>>> z=3
>>> print 'z is ',z
z is  3
```

Numpy

- Python has no built in arrays. Use NUMerical PYthon (numpy) for math functionality

- Many functions work on numpy arrays - usually much (much) faster than going through interpreter

- *numpy.arange* works like *range*, but returns numpy array instead of a list.

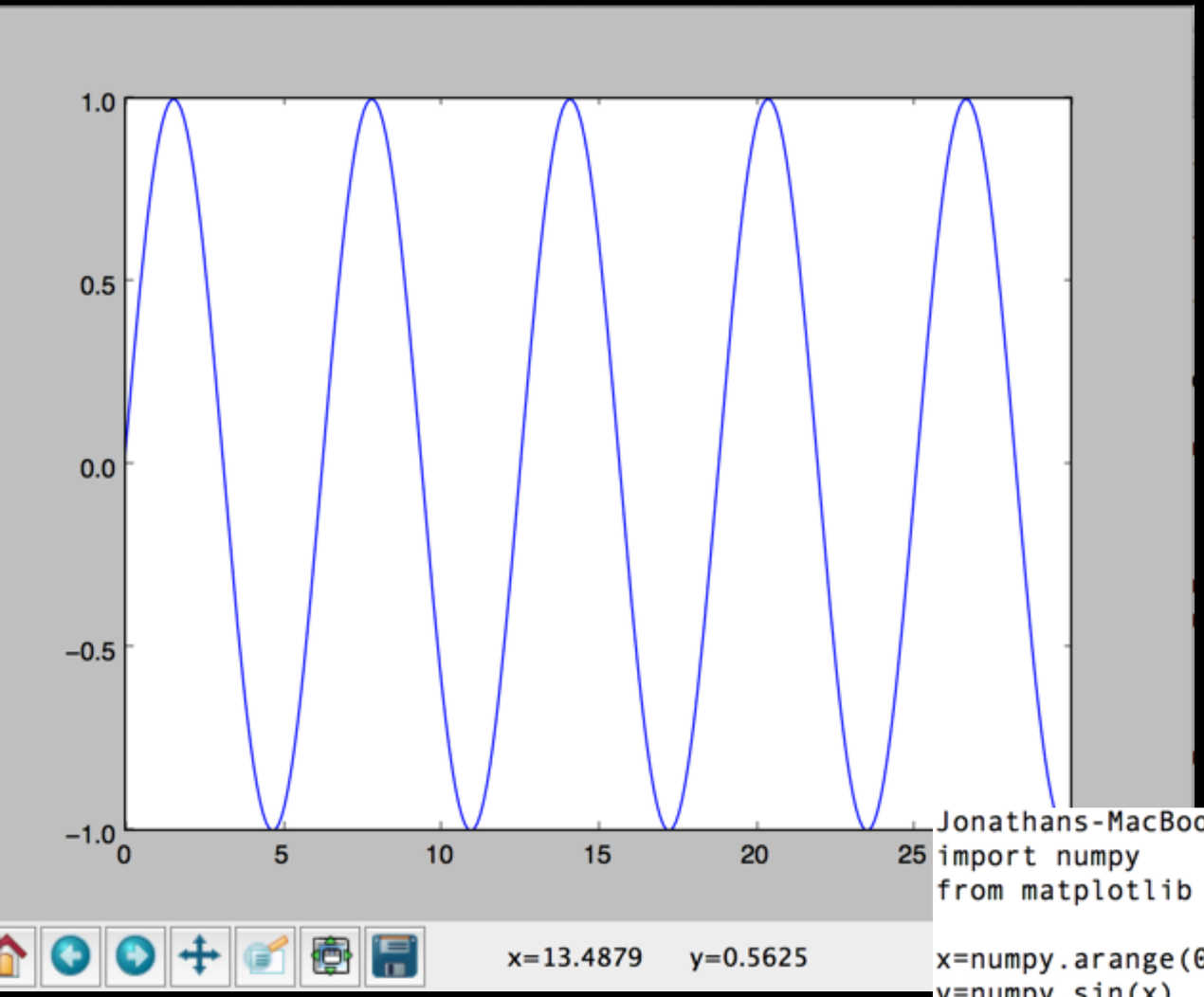
note - numpy.arange with three arguments will space values by 3rd argument.

```
Jonathans-MacBook-Pro:lecture3 sievers$ cat numpy_example.py
import numpy
x=numpy.arange(0,10)
print x**2
print 'type(x) is ' + repr(type(x))

x=range(0,10)
print 'type(x) is now ' + repr(type(x))
print x**2

Jonathans-MacBook-Pro:lecture3 sievers$ python numpy_example.py
[ 0  1  4  9 16 25 36 49 64 81]
type(x) is <type 'numpy.ndarray'>
type(x) is now <type 'list'>
Traceback (most recent call last):
  File "numpy_example.py", line 8, in <module>
    print x**2
TypeError: unsupported operand type(s) for ** or pow(): 'list' and 'int'
Jonathans-MacBook-Pro:lecture3 sievers$
```

Plotting

- Let's make a plot! Say, sin(x) from 0 to 30
- How would we do this? To the tubes!

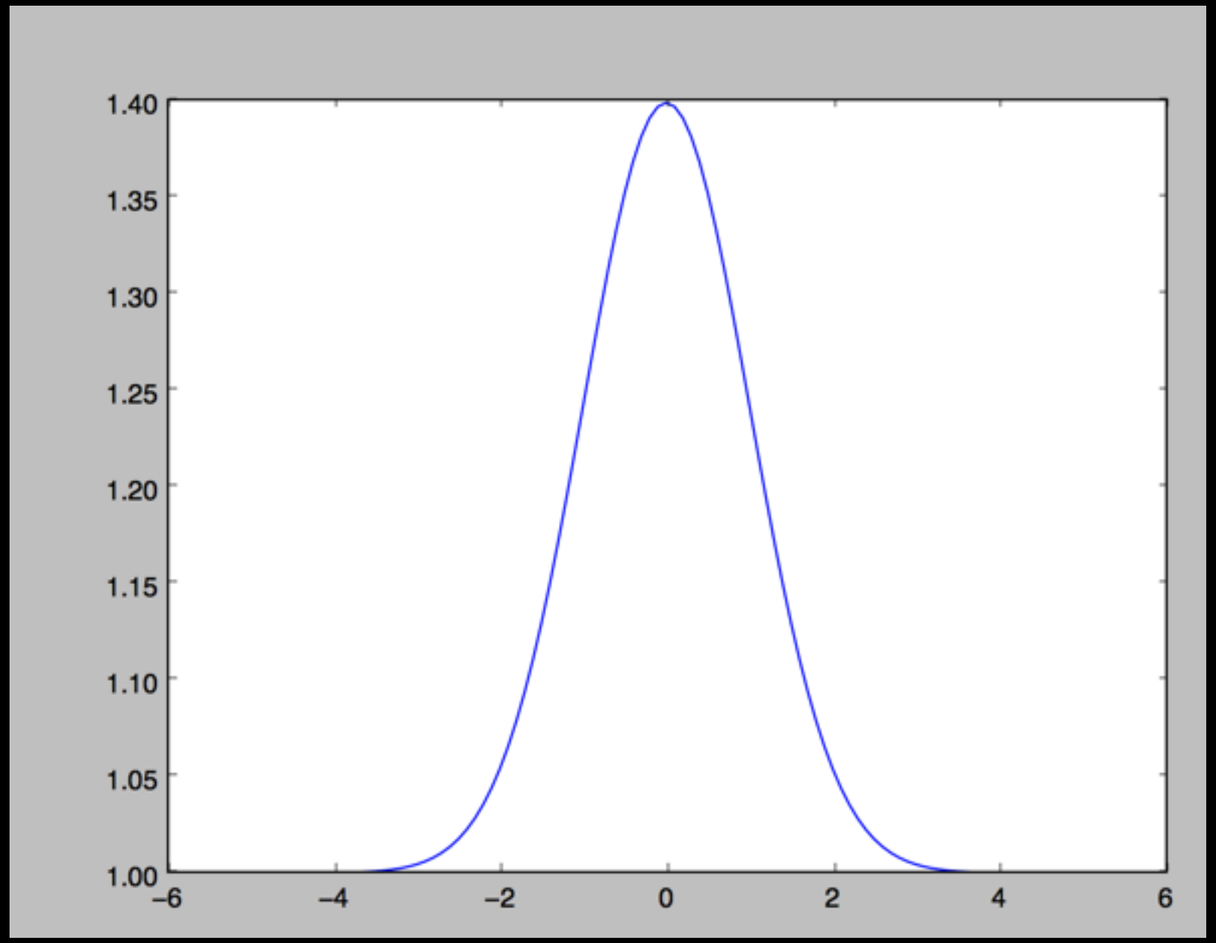
Example




```
Jonathans-MacBook-Pro:lecture3 sievers$ cat matplotlib_example.py
import numpy
from matplotlib import pyplot as plt

x=numpy.arange(0,30,0.1)
y=numpy.sin(x)

plt.plot(x,y)
plt.show()
Jonathans-MacBook-Pro:lecture3 sievers$ python matplotlib_example.py
```

Functions in Python

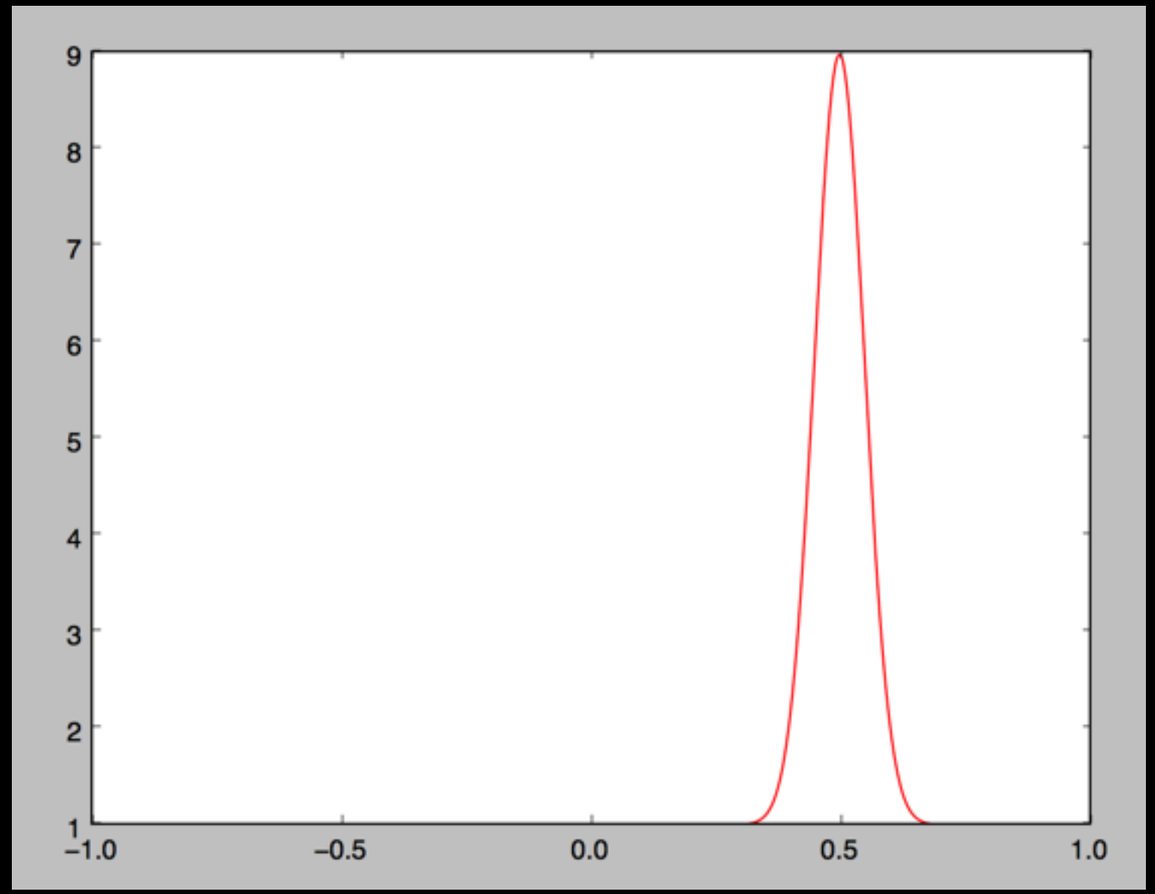
```
import numpy
from matplotlib import pyplot as plt
#functions defined with def
#arguments can be given default values
def mygauss(x,cent=0,sig=0.1):
    y=numpy.exp(-0.5*(x-cent)**2/sig**2)
    #pick this normalization so area under
    #gaussian is one.
    y=1+y/numpy.sqrt(2*numpy.pi*sig**2)
    return y

#only run this part if script is executed
if __name__ == "__main__":
    dx=0.1
    x=numpy.arange(-5,5,dx)
    y=mygauss(x,0,1)
    y2=mygauss(x,sig=1)
    print 'y total is ' +repr(y.sum()*dx)

    plt.plot(x,y)
    plt.show()
```



numpy arrays know how do to a lot of things. Can sum all elements with e.g. y.sum(). arrays also know their dimensions (shape), min,max, etc.

Functions Ctd.

```
import numpy
from matplotlib import pyplot as plt
#we can import functions we just wrote!
import func_example

x=numpy.arange(-1,1,0.002)
#functions are referenced by the file they're in
y=func_example.mygauss(x,cent=0.5,sig=0.05)
#we can assign the function to a variable
gg=func_example.mygauss
y2=gg(x,cent=0.5,sig=0.05)
delt=numpy.abs(y2-y)
print 'error is ' + repr(delt.sum())
#will output:
#error is 0.0
plt.plot(x,y,'r')
plt.show()
```



Integration

- We know have the tools to do some simple definite integrals
- Recall fundamental definition - sum ($f(x_i)*dx$) as dx-> 0
- How would we approximate integral of sin from 0 to pi?
- Before we do that, what *should* the answer be?

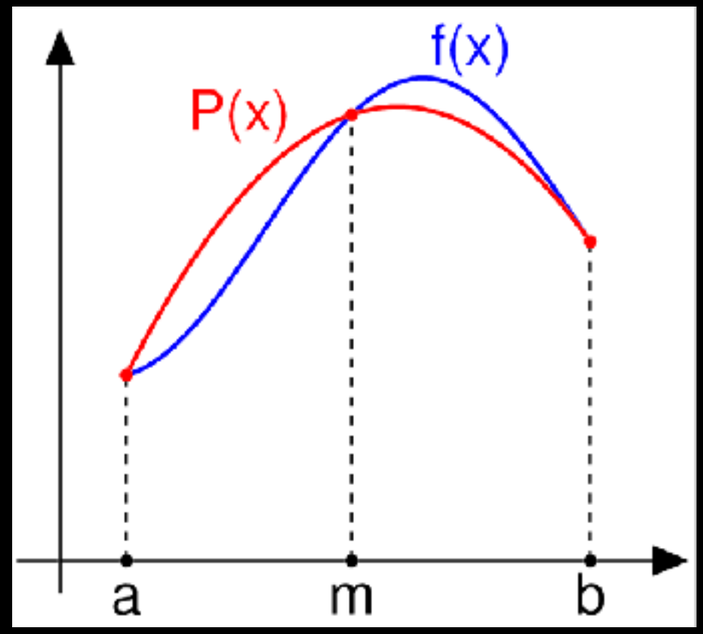
Example

- Here's some code that does the numerical integral of sin while varying the step size. How well does it work?
- you might also want to play with numpy.linspace…

```
import numpy

x0=0
x1=numpy.pi

mydelts=[0.5,0.1,0.03,0.01,0.003,0.001]
for dx in mydelts:
    x=numpy.arange(x0,x1,dx)
    y=numpy.sin(x)
    tot=y.sum()*dx
    print 'integral is ' + repr(tot) + ' with dx=' + repr(dx)
```

```
Jonathans-MacBook-Pro:lecture3 sievers$ python sin_integral.py
integral is 1.9836405445028298 with dx=0.5
integral is 1.9995479597125 98 with dx=0.1
integral is 1.9999407675824561 with dx=0.03
integral is 1.9999900283082466 with dx=0.01
integral is 1.9999992133611066 with dx=0.003
integral is 1.9999999540409921 with dx=0.001
Jonathans-MacBook-Pro:lecture3 sievers$
```

Simpson's Rule



- Let's integrate a quadratic over three points.
- Draw a straight line between the left and right points. The middle point is now off the straight line by $y_{mid}-0.5*(y_{left}+y_{right})$
- What is the average value of $(1-x^2)$ between -1 and 1?
- Area is now $1/2*(y_{left}+y_{right})+2/3*(y_{mid}-0.5*(y_{left}+y_{right}))$
- simplify: area=$1/6*y_{left}+2/3*y_{mid}+1/6*y_{right}$.
- for a bunch of points, string together segments, y_{right} become y_{left} of the next segment.
- Simpson's rule: integral=$dx*(1/6\ y_0 + 2/3y_{odd} + 1/3y_{even} + 1/6\ y_{last})$

4th Order Runge-Kutte

- Sometimes we want to integrate ODE's, dy/dx=f(x,y)
- Tricker than simple integration, because we can't evaluate at arbitrary points since y is changing.
- One standard technique is 4th-order Runge-Kutta, analagous to Simpson's rule. Make estimates of function using left edge, 2 in center, and one at right.
- RK4 reduces to Simpson's rule if dy/dx=f(x) only (not f(x,y)). For smooth functions, RK4 should be accurate to 4th order.

RK4 Recipe

- for step size h, let k_1=h*f(x,y) (left edge)
- k_2=h*f(x+h/2,y+k_1/2) (first mid-point estimate)
- k_3=h*f(x+h/2,y+k_2/2) (second mid-point estimate)
- k_4=h*f(x+h,y+k_3) (right edge)
- y(x+h)=y(x)+(k_1+2k_2+2k_3+k_4)/6

In Practice

```
import numpy
def myfun(x,y,a):
    #evaluate dydx=a*x*y
    return x*y*a
def rkstep(x,y,h,a,func):
    k1=h*func(x,y,a);
    k2=h*func(x+0.5*h,y+0.5*k1,a);
    k3=h*func(x+0.5*h,y+0.5*k2,a);
    k4=h*func(x+h,y+k3,a);
    dy=(k1+2*k2+2*k3+k4)/6
    return dy
y0=2.0
x0=4.0
x1=10
a=0.5
h=0.01
y=y0
for x in numpy.arange(x0,x1,h):
    #print "(x,y)="+repr(x)+' '+repr(y)
    y=y+rkstep(x,y,h,a,myfun)
print "at end (x,y)=" + repr(x+h) + ' ' + repr(y)
#can solve analytically:
#dy/y=axdx, log(y)=0.5*ax^2+c, y=c*exp(0.5*ax^2)
#at (x0,y0)=c=y0/exp(0.5*ax0**2)
c=y0/numpy.exp(0.5*a*x0**2)
print "predicted: " + repr(c*numpy.exp(0.5*a*(x+h)**2))
```

```
Jonathans-MacBook-Pro-3:lecture3_2015 sievers$ python rk4.py
at end (x,y)=9.999999999998721 2637630368.8623924
predicted: 2637631468.9647431
```

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

- $F(k)=\int f(x)*\exp(-2\pi ikx)dx$ (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)
- $F(k)=\sum f(x)\exp(-2\pi ikx/N)$ 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:
  $\sum\exp(-2\pi ikx)\exp(2\pi ik'x)=\sum\exp(2\pi i(k'-k)x)$. N if k'==k, otherwise 0.
- So, $A^{-1}=1/N*\text{conj}(A)$. $IFT=1/N\sum F(k)\exp(-2\pi ikx)$.
- 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)
```

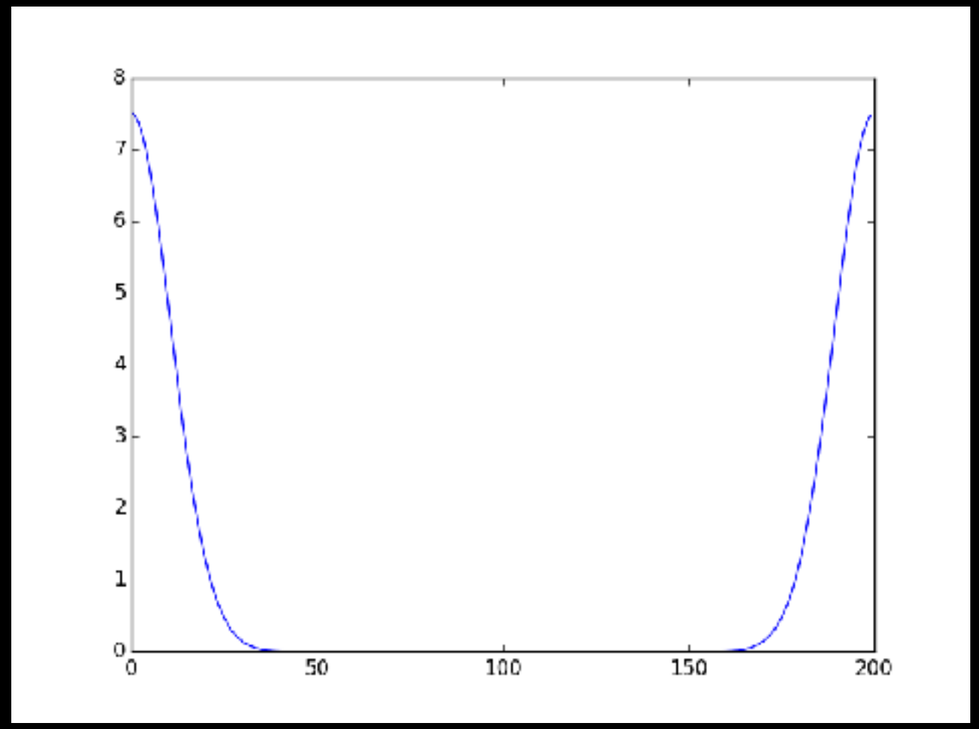
```
Jonathans-MacBook-Pro:lecture4 sievers$ python dft_columns.py
(8+0j)
(-4.28626379702e-16+4.4408920985e-16j)
(8+0j)
(3.44169137634e-15-1.11022302463e-15j)
Jonathans-MacBook-Pro:lecture4 sievers$
```

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

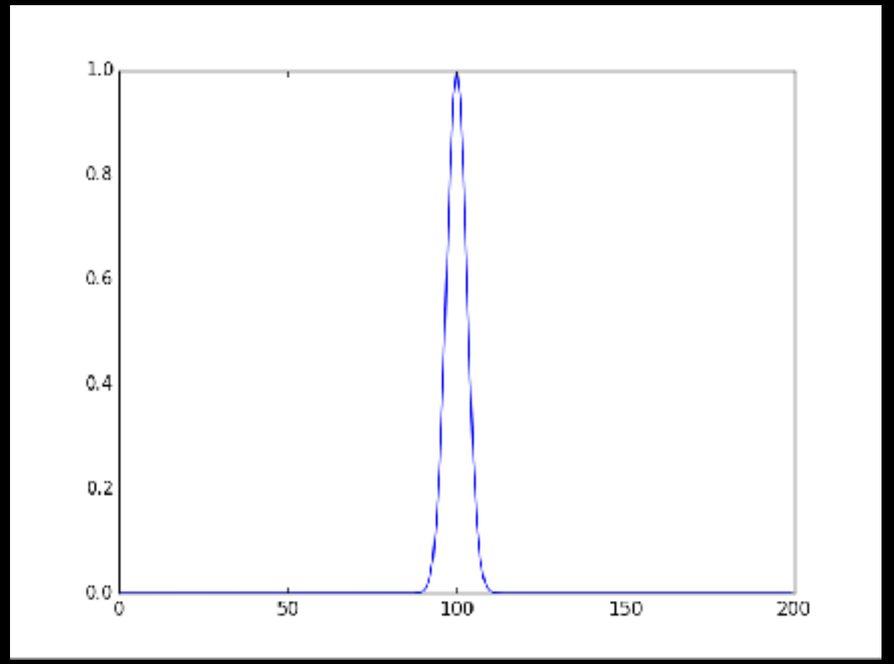
DFTs with Numpy

- 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==fft(ifft(f))==ifft(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()
```



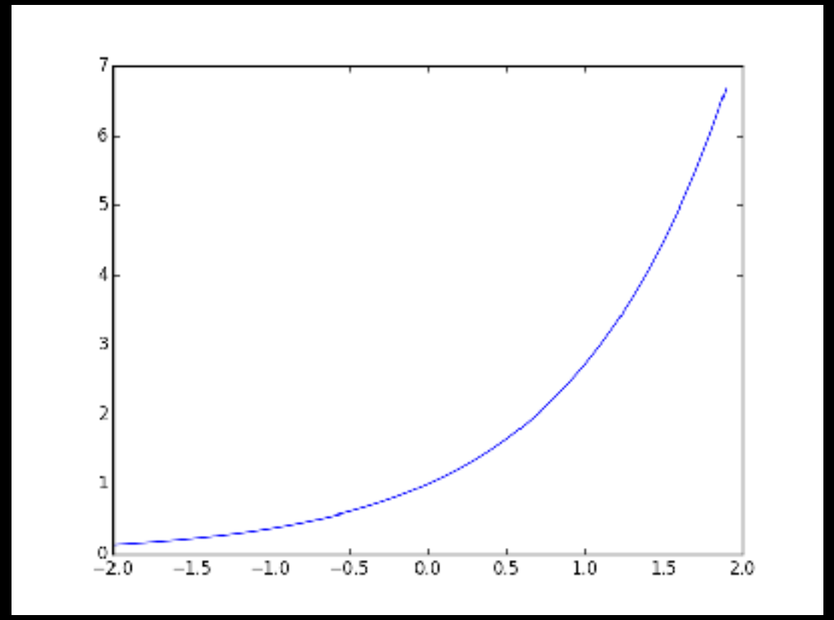
- Right: input Gaussian
- Top: DFT of the Gaussian

Periodicity

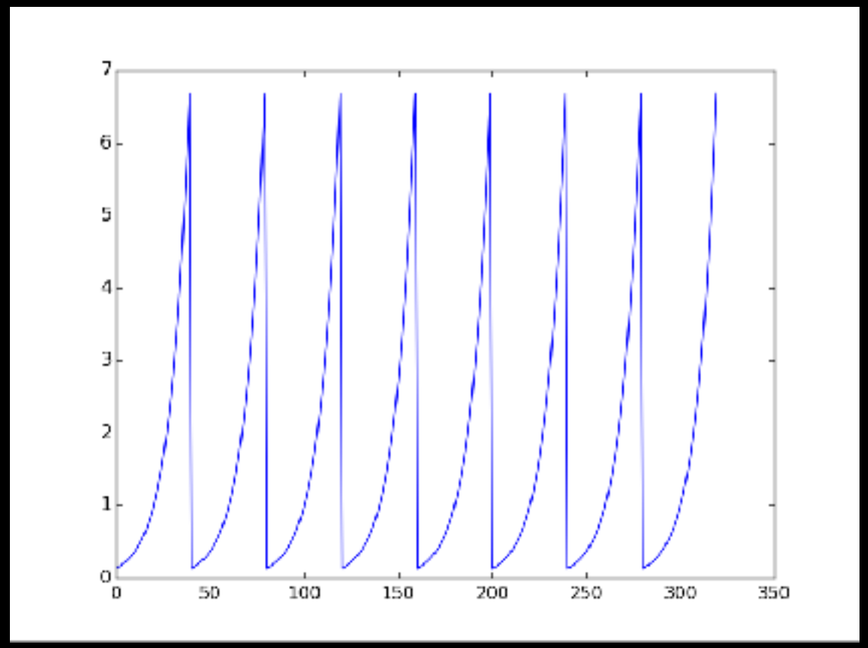
- $f(x)=\sum F(k) \exp(-2\pi ikx/N)$
- What is $f(x+N)$? $\sum F(k) \exp(-2\pi ik(x+N)/N)$
- $=\sum F(k) \exp(-2\pi ik)\exp(-2\pi ikx/N)$.
- $\exp(-2\pi ik)=1$ for integer k, so $f(x+N)==f(x)$
- DFT's are periodic - they just repeat themselves ad infinitum.

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



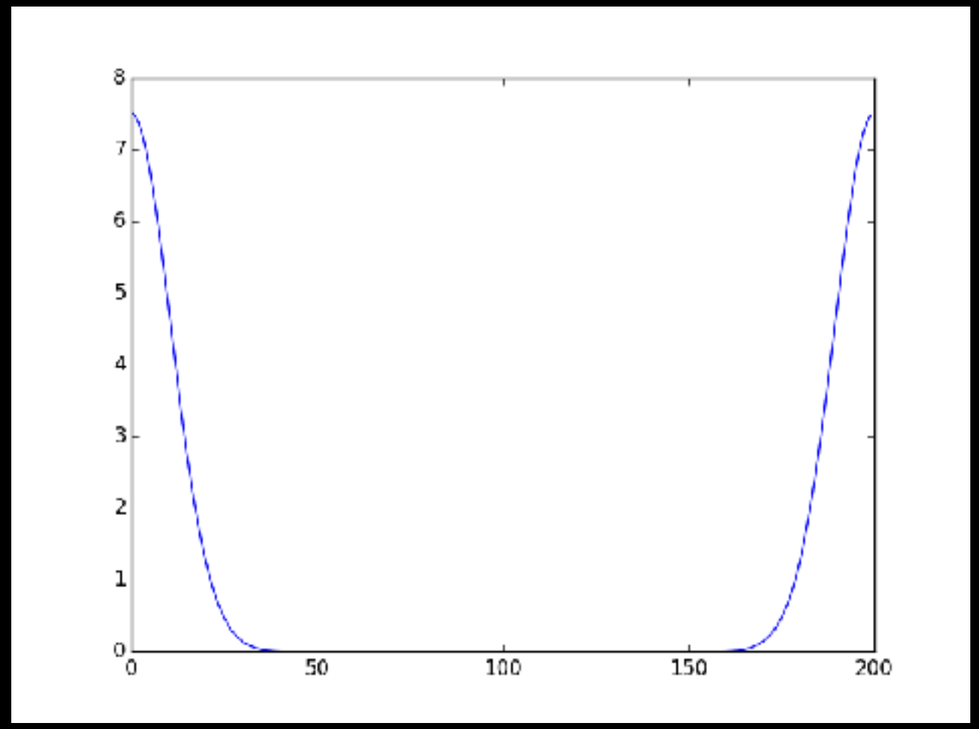
Aliasing

- $f(x)=\sum F(k)\ \exp(2\pi ikx/N)$
- What if I had higher frequency, $k>N$? let $k^*=k-N$ (i.e. k^* low freq.)
- $f(x)=\sum F(k)\ \exp(2\pi i(k^*+N)x/N=\sum F(k)\exp(2\pi ix)\exp(2\pi ik^*x/N)$
- for x integer, middle term goes away: $\sum F(k^*+N)\exp(2\pi ik^*x/N)$
- 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.

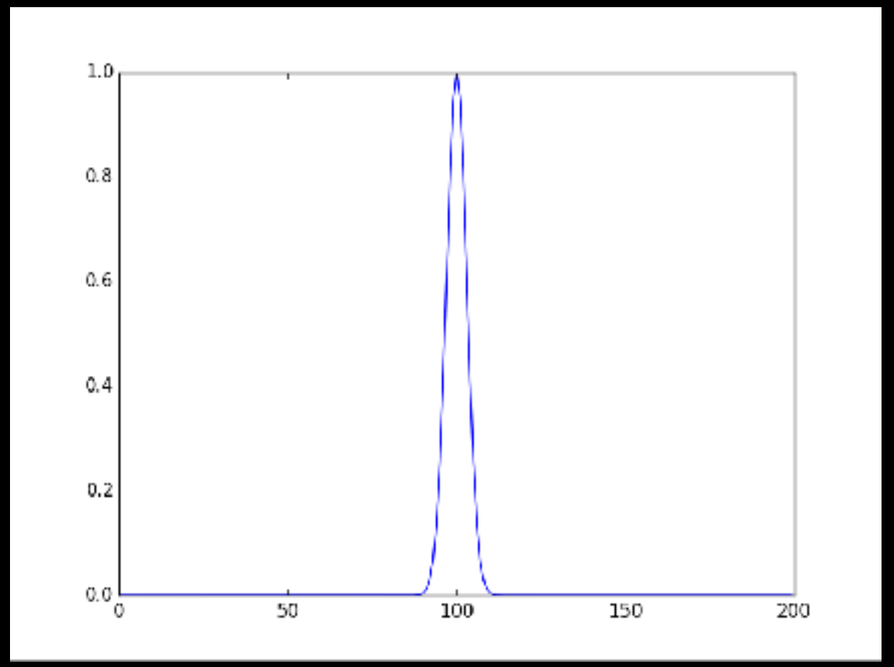
Negative Frequencies

- 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 ν - then I get full information if I sample *twice* per frequency, $dt=1/(2\nu)$. 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.

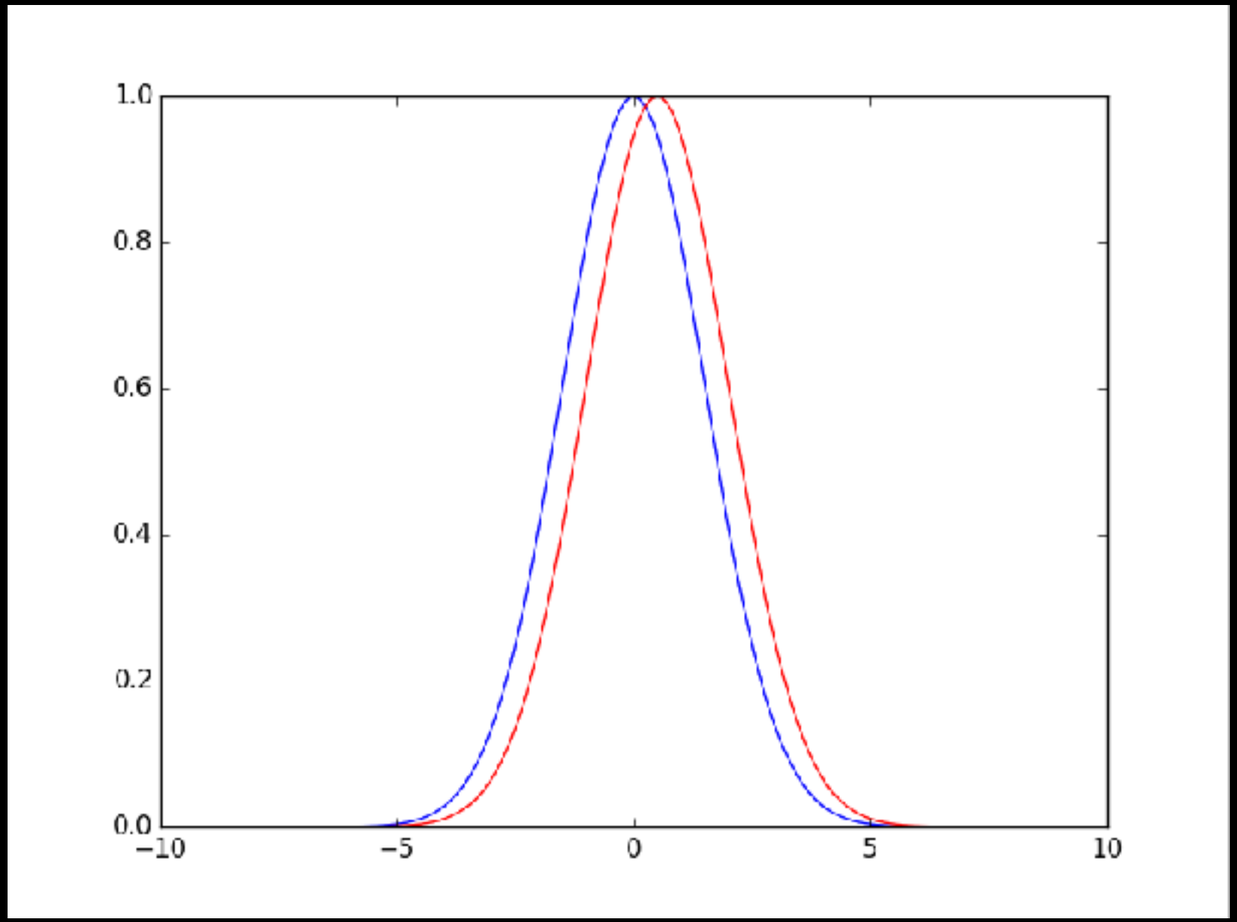
Flipping

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

Shifting

- What is FFT(x+dx)? $\sum f(x+dx)\exp(-2\pi ikx/N)$.
- $x^*=x+dx$: $F(k)=\sum f(x^*)\exp(-2\pi ik(x^*-dx)/N)$
- $F(k)=\exp(2\pi ikdx/N)\sum f(x^*)\exp(-2\pi ikx^*/N)$
- 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 $x^*=-x$
- $F(-k)=\sum f(-x^*)\exp(2\pi ikx^*/N)$ = conj(F(k)) by flipping
- So, if f(x) is real, F(k)=conj(F(N-k))
- If N even, F(N/2)=conj(F(N/2)), so F(N/2) must be real.

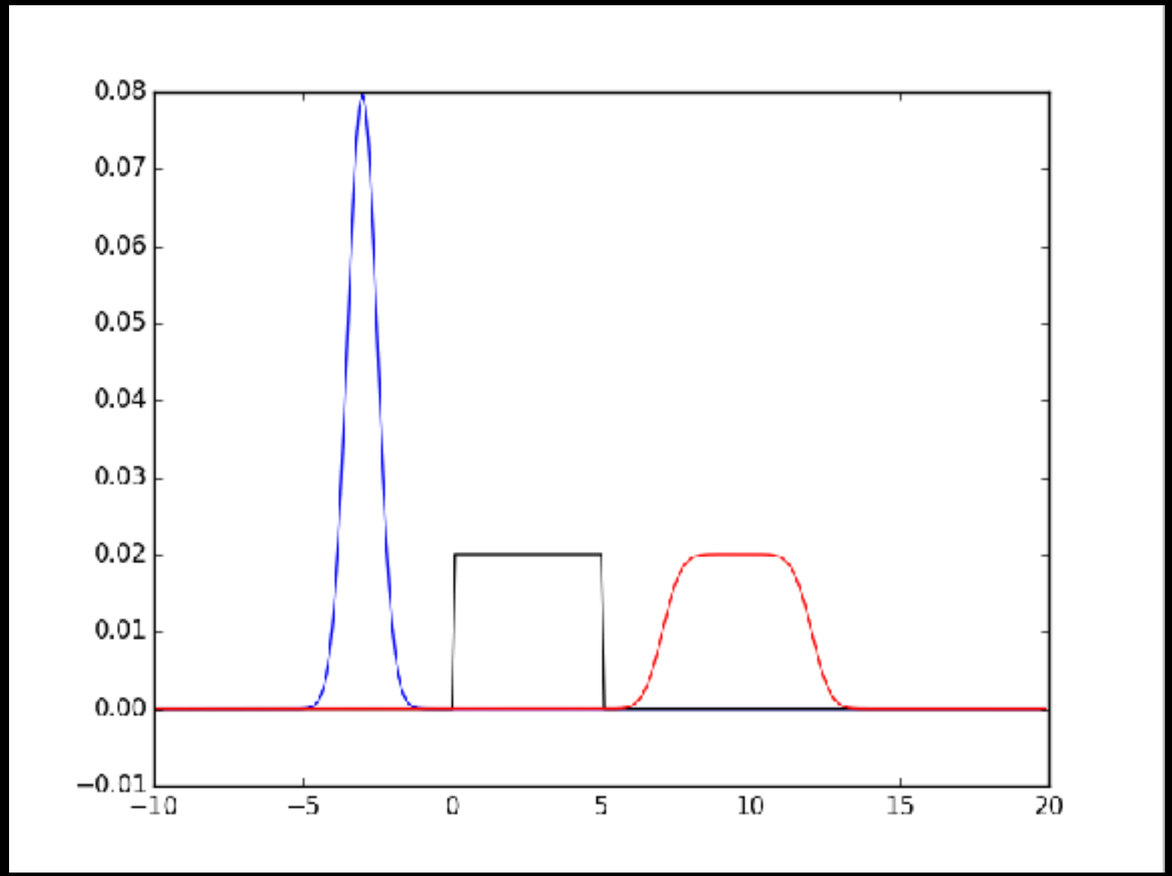
```
>>> x=numpy.random.randn(8)
>>> xft=numpy.fft.fft(x)
>>> for xx in xft:
...   print xx
...
(-4.53568815727+0j)
(-0.174046761579+2.08827239558j)
(2.15348308858+2.32162497273j)
(-0.423040513854-3.72126858798j)
(2.75685372591+0j)
(-0.423040513853+3.72126858798j)
(2.15348308858-2.32162497273j)
(-0.174046761579-2.08827239558j)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

Convolution Theorem

- Convolution defined to be $conv(y)=f \otimes g == \int f(x)g(y-x)dx$
- $\sum_x \sum F(k)exp(2\pi ikx) \sum conj(G(k'))exp(2\pi ik'x)exp(-2\pi ik'y/N)$
- Reorder sum: $\sum\sum F(k)conj(G(k'))exp(-2\pi ik'y/N)\sum_x exp(2\pi i(k+k')x)$
- equals zero unless $k'==-k$. Cancels one sum, conjugates G
- $f \otimes g=\sum F(k)G(k)exp(2\pi iky/N)=ift(dft(f)*dft(g))$
- 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 $DFT=\sum f(x)\exp(-2\pi ikx/N) = \sum f_{even}(x)\exp(-2\pi ik(2x)/N) + \sum f_{odd}(x)\exp(-2\pi ik(2x+1)/N)$
- $=F_{even}+\exp(-2\pi ik/N)F_{odd}$. Let $W_k=\exp(-2\pi ik/N)$
- if $k>N/2$, then $k^*=k-N/2$ and $DFT=F_{even}+\exp(-2\pi ik^*/N+i\pi)F_{odd}=F_{even}-W_kF_{odd}$.

FFT cont'd

- So $F(k)=F_{even}(k)+W_k F_{odd}(k)$ $(k<N/2)$ or $F_{even}(k)-W_k F_{odd}(k)$ $(k>=N/2)$
- 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

- Write a python script to make a vector of n evenly spaced numbers between 0 and pi/2. i.e. x[0]=0, x[-1]=pi/2 (5)

- Use this vector to integrate cos(x) from 0 to pi/2 for a range # of points using the simple method. include 10,30,100,300,1000 points between 0 and pi/2. How does error scale with # of points? (5)

- Python supports array slicing - x[5:10:2] will take points 5,7,9 from x. x[5::2] will take points 5,7,9… from x. How can I take all odd points from an array? How can I take all even points from an array, but skipping the first and last points? (5)

- Write a python function to integrate this vector using Simpson's rule. How does error scale with # of points? How many points did we need to use in part 2 to get same accuracy as 11 points with Simpson's rule? (10)

- Plot the errors as a function of # of points using Simpson's rule and standard sum. You will want to use a log scale here - look at logplot.py in the github distribution (5)

Bonus Points

- the scipy module has built in integration functions in scipy.integrate. The quad routine will do numerical integrals. quad will try to put its effort where the function changes quickly.

- Look at scipy_quad_example.py, which uses scipy to integrate our Gaussian function over two different ranges. The integrals should be (almost) identical - yet they are not. Can you figure out why? (5)

- Can you write another function that will always give the correct answer to this integral? (5) Hint - you may want to do two integrals instead of one.