Computational Physics
Lecture 6

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git clone https://github.com/ukzncompphys/lecture6_2016.git

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.

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))

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

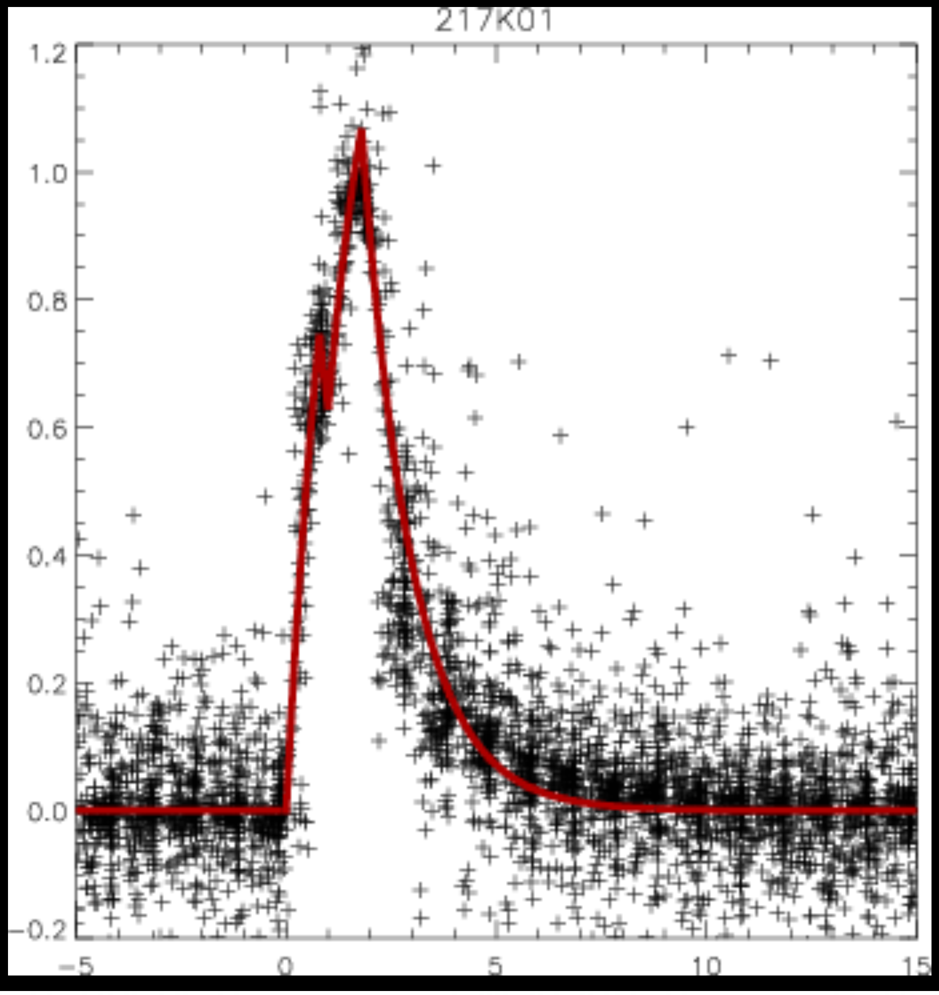
Real Data Symmetry

- If I know F(k), what is F(N-k) is f(x) is real?
- F(N-k)=F(-k) (from alias theorem)
- F(-k)=∑f(x)exp(2πi(-k)x/N. let x*=-x
- F(-k)=∑f(-x*)exp(2πikx*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.

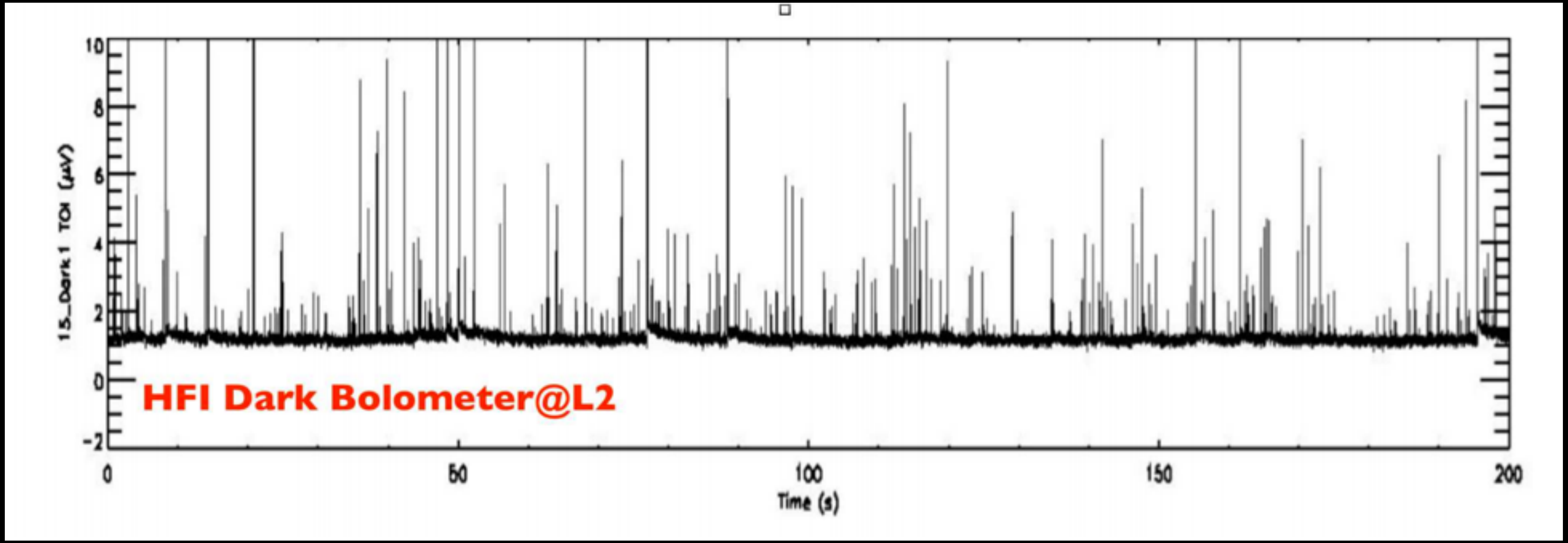
```
>>> x=numpy.random.randn(8)
>>> xft=numpy.fft.fft(x)
>>> for xx in xft:
...   print xx
...
(-4.53568815727+0j)
(-0.174046761579+2.08827239558j)
(2.15348308858+2.32162497273j)
(-0.423040513854-3.72126858798j)
(2.75685372591+0j)
(-0.423040513853+3.72126858798j)
(2.15348308858-2.32162497273j)
(-0.174046761579-2.08827239558j)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

Convolution

- Say we have instrument with some response.
  - cosmic ray hits detector, raises temperature. Temperature decays
  - out-of-focus camera smears image
- Observed signal at time *t* is true signal at time t' time response/smearing for $\delta t = t - t'$. But, must integrate over all times.
- So, $f_{obs}(t) = \int f(t')g(t-t')\, dt'$. This is a convolution.



Cosmic Rays from Planck Satellite

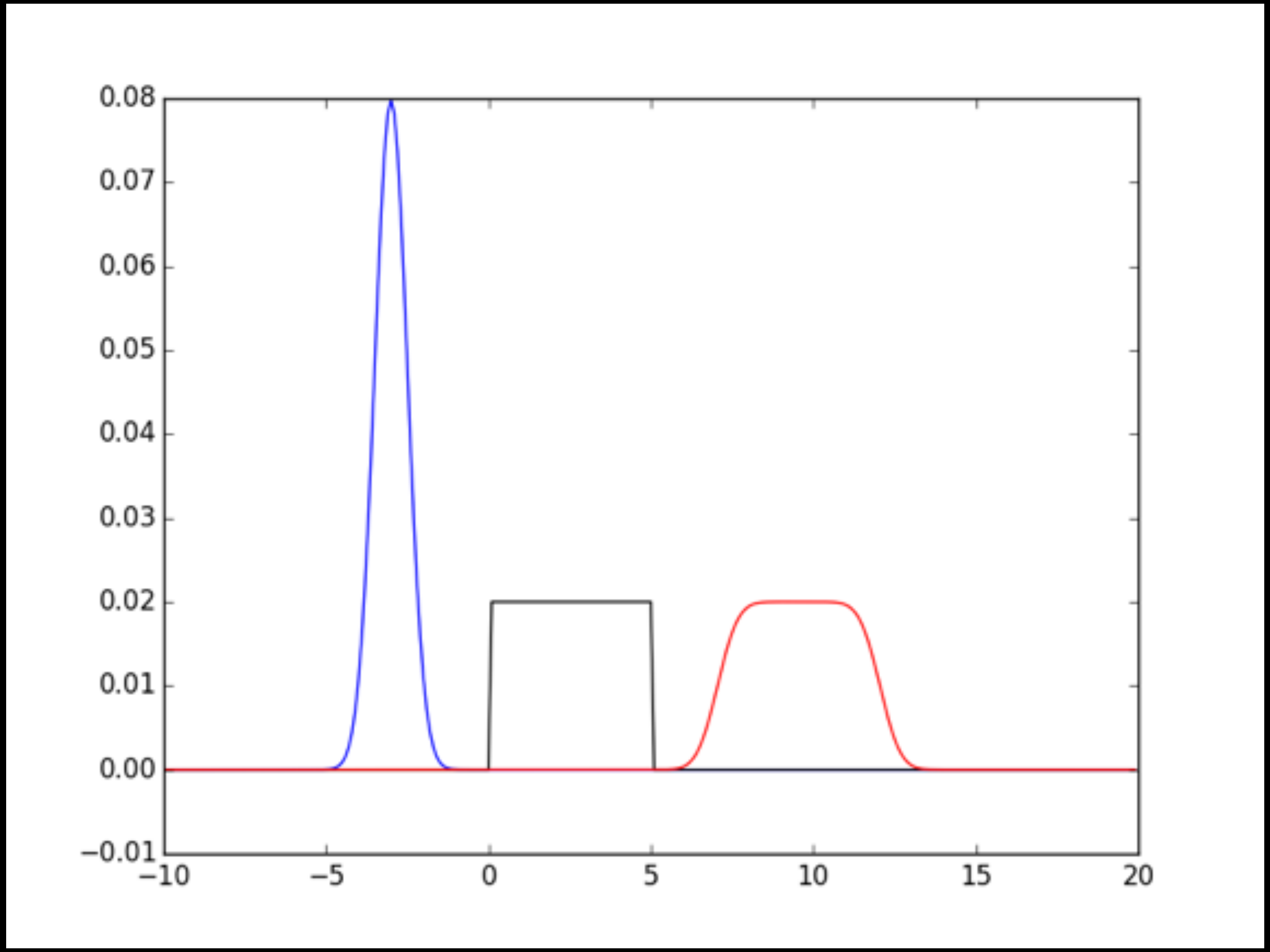


Convolution Theorem

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

Convolution Example

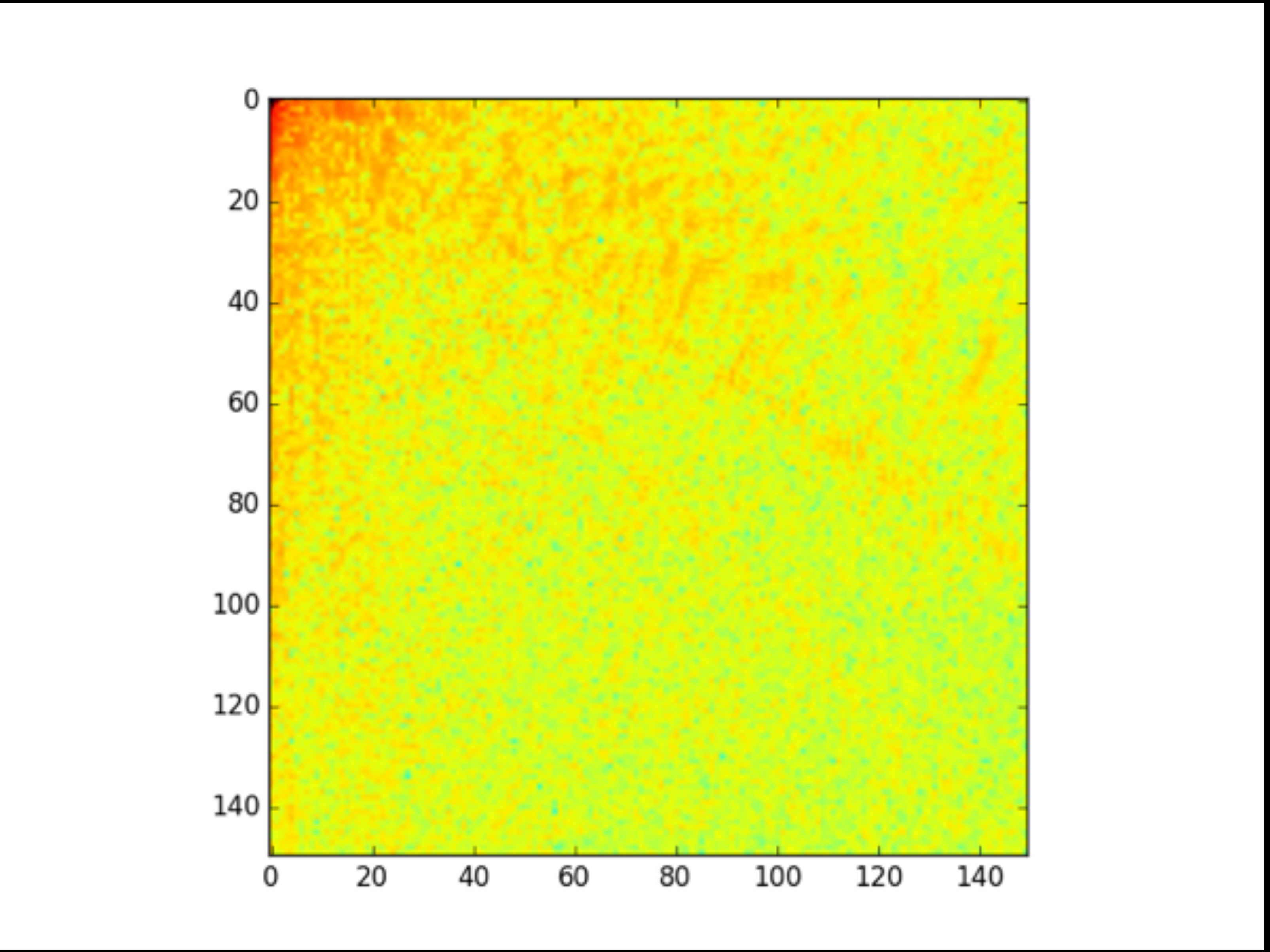
```
from numpy import arange,exp,real
from numpy.fft import fft,ifft
from matplotlib import pyplot as plt
def conv(f,g):
    ft1=fft(f)
    ft2=fft(g)
    return real(ifft(ft1*ft2))

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()
```



2D Fourier Transforms

- Fourier transform defined in 2 dimensions:
- $F(k,l)=\int\int f(x,y)\exp(-ikx)\exp(-ily)dxdy$
- 2D FT's extremely common in image processing.
- JPEGs in fact are based on picking out modes from image FT's.

numpy.fft.fft2



Smoothing Images

- Out-of-focus images are convolutions.
- Can defocus an image by convolving with a blurry kernel
- Let’s fuzz out map by a Gaussian.

```python
def get_fft_vec(n):
    vec=numpy.arange(n)
    vec[vec>n/2]=vec[vec>n/2]-n
    return vec
def smooth_map(map,npix,smooth=True):
    nx=map.shape[0]
    ny=map.shape[1]
    xind=get_fft_vec(nx)
    yind=get_fft_vec(ny)

    #make 2 1-d gaussians of the correct lengths
    sig=npix/numpy.sqrt(8*numpy.log(2))
    xvec=numpy.exp(-0.5*xind**2/sig**2)
    xvec=xvec/xvec.sum()
    yvec=numpy.exp(-0.5*yind**2/sig**2)
    yvec=yvec/yvec.sum()

    #make the 1-d gaussians into 2-d maps using numpy.repeat
    xmat=numpy.repeat([xvec],ny,axis=0).transpose()
    ymat=numpy.repeat([yvec],nx,axis=0)

    #if we didn't mess up, the kernel FT should be strictly real
    kernel=numpy.real(numpy.fft.fft2(xmat*ymat))

    #get the map Fourier transform
    mapft=numpy.fft.fft2(map)
    #multiply/divide by the kernel FT depending on whath we're after
    if smooth:
        mapft=mapft*kernel
    else:
        mapft=mapft/kernel
    #now get back to the convolved map with the inverse FFT
    map_smooth=numpy.fft.ifft2(mapft)

    #since numpy gets imaginary parts from roundoff, return the real part
    return numpy.real(map_smooth)
```

smooth_map.py

```
import numpy
from matplotlib import pyplot as plt
import smooth_map

meerkat=plt.imread('meerkat_small.jpg')

smoothed_map=numpy.zeros(meerkat.shape)
unsmoothed_map=numpy.zeros(meerkat.shape)
npix_smooth=3.5
npix_restore=4
for i in range(3):
    tmp=numpy.squeeze(meerkat[:,:,i])
    tmp_smooth=smooth_map.smooth_map(tmp,npix_smooth)
    smoothed_map[:,:,i]=tmp_smooth
    tmp2=smooth_map.smooth_map(tmp_smooth,npix_restore,False)
    unsmoothed_map[:,:,i]=tmp2
```

Deconvolution

- Well, if I smear out by multiplying FT's, I can unsmear by dividing, right?
- If yes, worth billions and billions of your favo(u)rite currency. Save those fuzzy pictures…
- Maybe. Let's try smoothing image by 3.5 pixels, then unsmoothing by 4.
- What happened?

Deconvolution

- smoothing lowers high-frequency signal
- unsmoothing *must* raise it back up.
- if there's any noise, it gets amplified by unsmoothing.
- If I smooth, then write to jpg, I round to nearest integer. Equivalent to adding noise.
- So, think those fuzzy license plates in google maps are safe?

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

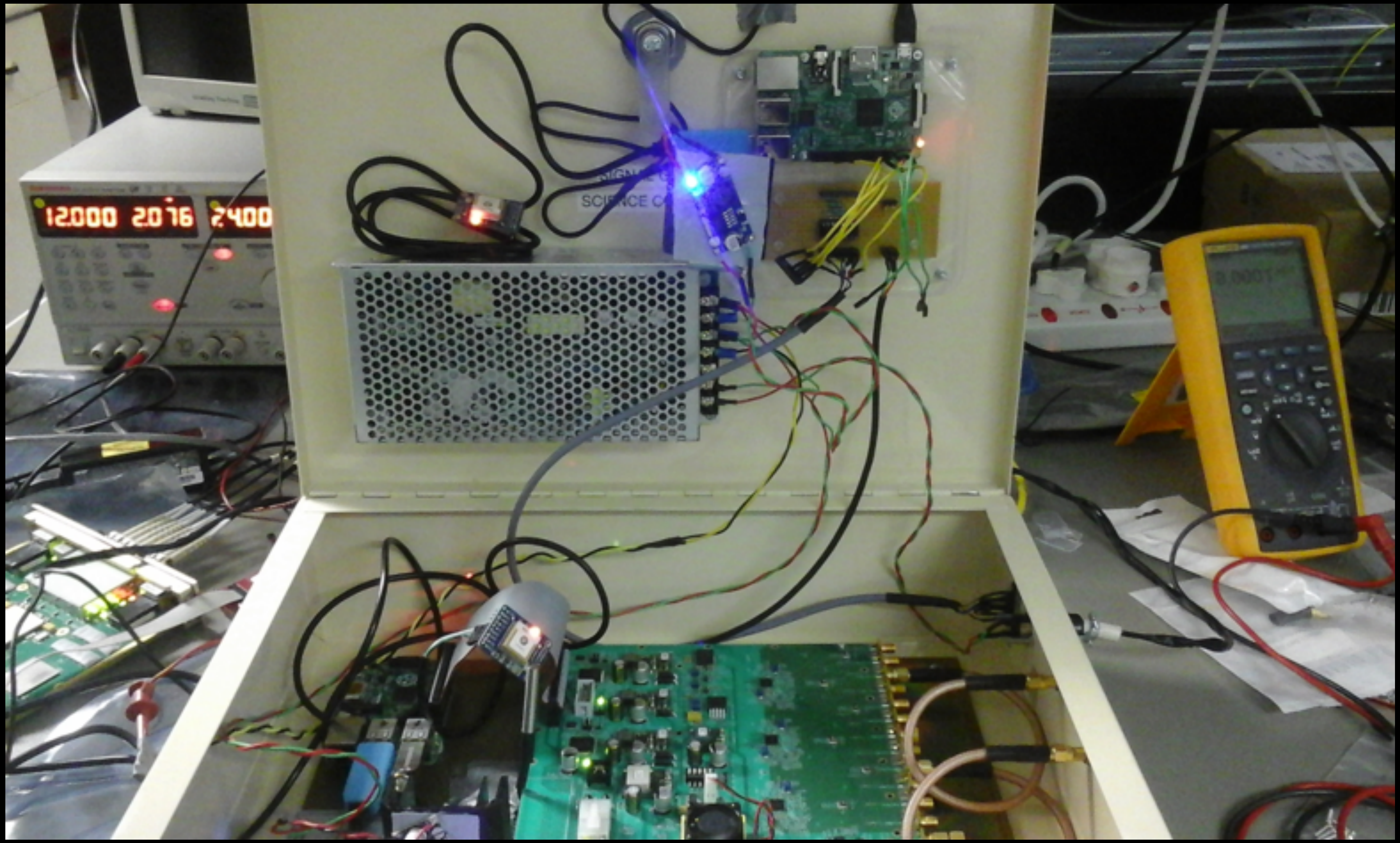
- So $F(k)=F_{even}(k)+W_kF_{odd}(k)$ $(k<N/2)$ or $F_{even}(k)-W_kF_{odd}(k)$ $(k>=N/2)$
- So, can get *all* the frequencies if I have 2 half-length FFTs.
- Well, just do the same thing again. FFT of a single element is itself.
- This algorithm works for arrays whose length is a power of 2
- Popularized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

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
>>>
```



Instrument deployed to Marion Island (2000 km south of SA) right now. Looking for signal from the first stars in the universe. Main job of back end is to FFT 4 billion numbers/second. Uses 30W total.

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★g is $\int f(x)g(x+y)$. Through a similar proof, one can show f★g=ift(dft(f)*conj(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)