Computational Physics (PHYS6350)

Lecture 22: Fourier transform

- Discrete Fourier transform (DFT)
- Fast Fourier Transform (FFT)

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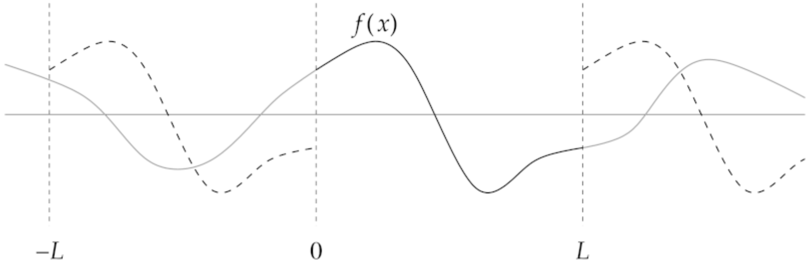
Course materials: https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Fourier transform

Periodic functions (e.g. over x ∈ [0,L]) permit Fourier decomposition

$$f(x) = \sum_{k=-\infty}^{\infty} \gamma_k \exp\left(i \frac{2\pi k x}{L} \right)$$

If a function is not periodic, it can always be forced to be periodic



Fourier coefficients read

$$\gamma_k = \frac{1}{L} \int_0^L f(x) \exp\left(-i \frac{2\pi k x}{L} \right) dx.$$

Applications:

- signal processing (e.g. frequencies)
- image compression
- solutions to partial differential equations
- convolutions of functions

Fourier transform: sines and cosines

If function is even (symmetric) around the midpoint $x = L/2$, it permits cosine series

$$f(x) = \sum_{k=0}^{\infty} \alpha_k \cos\left(\frac{2\pi kx}{L}\right) \qquad \alpha_k = \frac{2-\delta_{k0}}{L}\int_0^L f(x)\cos\left(\frac{2\pi kx}{L}\right)dx$$

If function is odd (antisymmetric) around the midpoint $x = L/2$, it permits sine series

$$f(x) = \sum_{k=1}^{\infty} \beta_k \sin\left(\frac{2\pi kx}{L}\right) \qquad \beta_k = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{2\pi kx}{L}\right)dx$$

The coefficients are related to the ones of the exponential series

$$\gamma_k = \frac{1+\delta_{k0}}{2}\left[\alpha_{|k|} - i\,\mathrm{sign}(k)\beta_{|k|}\right]$$

Evaluating Fourier coefficients

$$\gamma_k = \frac{1}{L}\int_0^L f(x)\,\exp\left(-i\frac{2\pi k x}{L}\right)dx.$$

Apply N-point trapezoidal rule

$$\gamma_k \simeq \frac{1}{L}\frac{L}{N}\left[\frac{f(0)}{2} + \frac{f(L)}{2} + \sum_{n=1}^{N-1} f(x_n)\exp\left(-i\frac{2\pi k x_n}{L}\right)\right] \qquad h = L/N \qquad x_n = hn$$

The function is periodic, f(0) = f(L), thus

$$\gamma_k = \frac{1}{N}\sum_{n=0}^{N-1} y_n \exp\left(-i\frac{2\pi k n}{N}\right) \qquad y_n \equiv f(x_n).$$

This is the **discrete Fourier transform (DFT)**.

Typically one uses the coefficients without the factor 1/N, i.e.

$$c_k = \sum_{n=0}^{N-1} y_n \exp\left(-i\frac{2\pi k n}{N}\right)$$

If y_n are all real,

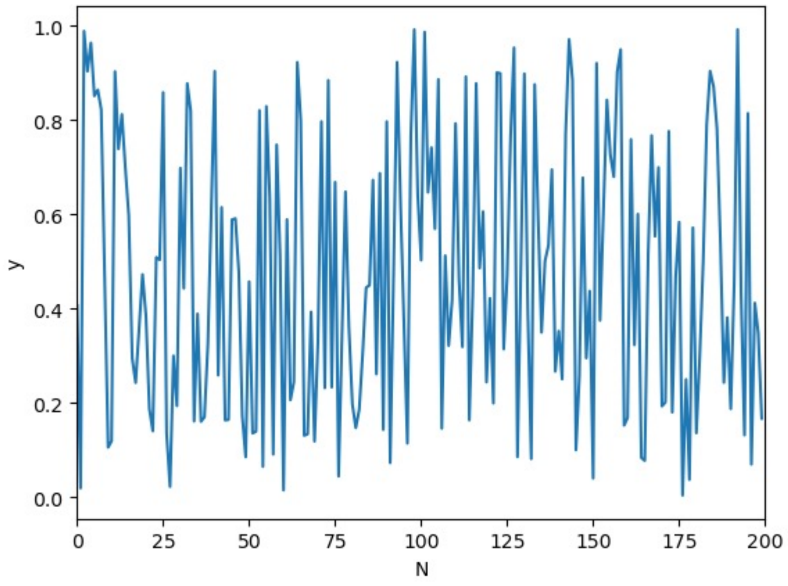
$$c_{N-k} = c_k^*$$

Evaluating Fourier coefficients

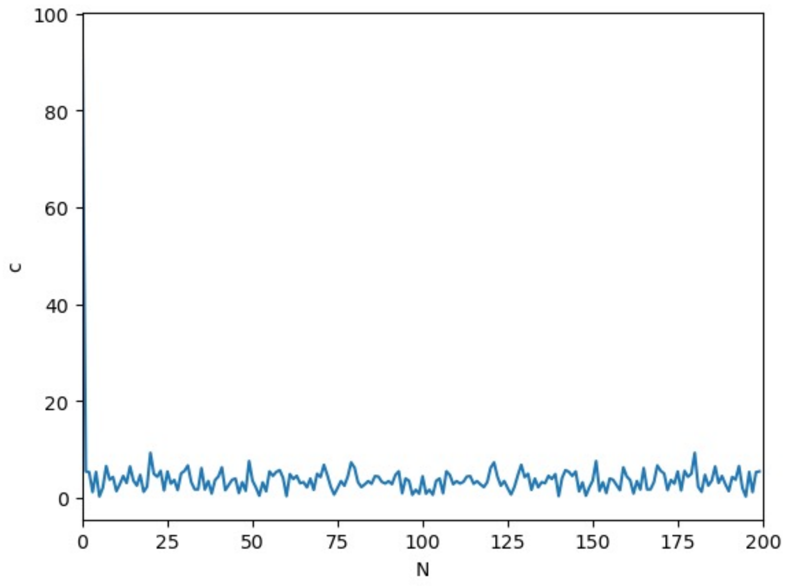
```python
def dft(y):
    N = len(y)
    c = np.zeros(N, complex)
    for k in range(N):
        for n in range(N):
            c[k] += y[n] * np.exp(-2j * np.pi * k * n / N)
    return c
```

```python
N = 200
y = np.random.rand(N)
#print("y = ", y)
plt.plot(y)
plt.xlim(0,N)
plt.show()

c = dft(y)
#print("c = ", c)
plt.plot(np.abs(c))
plt.xlim(0,N)
plt.show()
```

Function



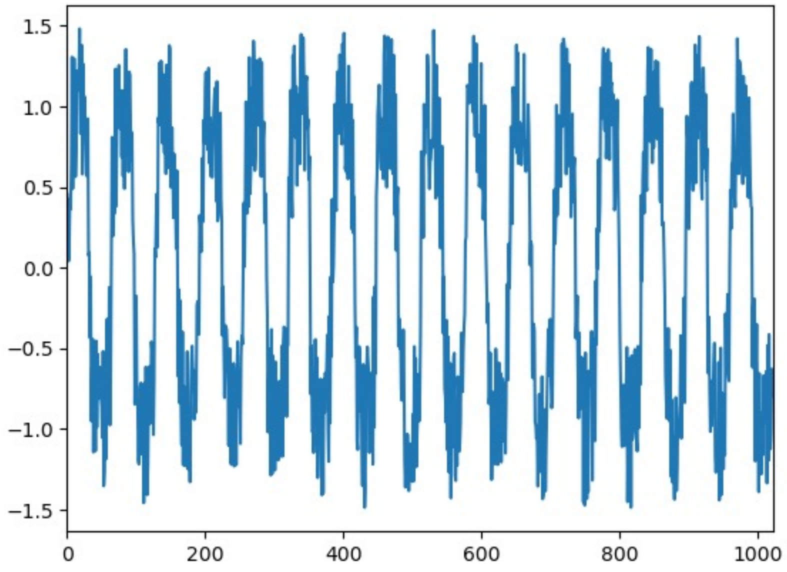
Fourier transform

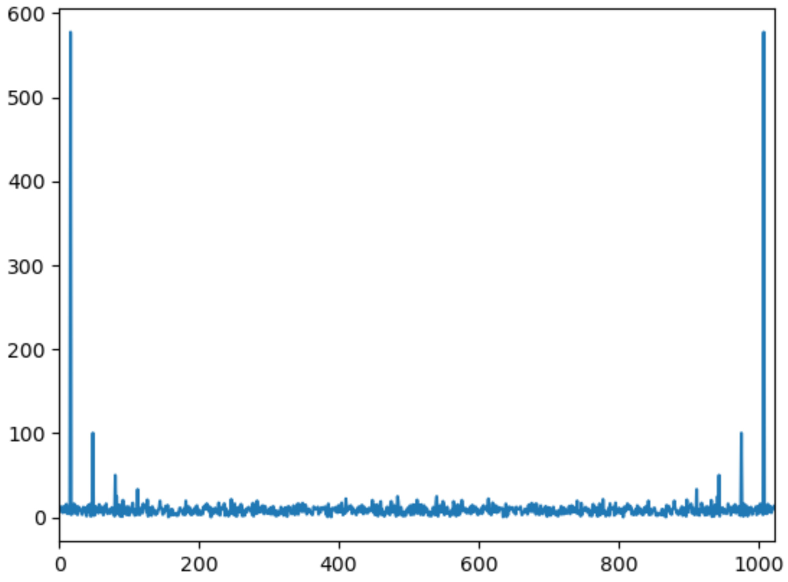


Evaluating Fourier coefficients

Consider a wavelike form with noise

```
## Data from http://www-personal.umich.edu/~mejn/cp/programs/dft.py
y = np.loadtxt("pitch.txt",float)
plt.plot(y)
plt.xlim(0,len(y))
plt.show()

c = dft(y)
plt.plot(np.abs(c))
plt.xlim(0,len(y))
plt.show()
```





Inverse Fourier transform

Consider the following geometric progression

$$\sum_{k=0}^{N-1} e^{i2\pi km/N} = \frac{1 - e^{i2\pi m}}{1 - e^{i2\pi m/N}} = \delta_{m0}.$$

We use this now to evaluate the following sum

$$\begin{aligned}
\sum_{k=0}^{N-1} c_k \exp\left(i\frac{2\pi kn}{N}\right) &= \sum_{k=0}^{N-1}\sum_{k'=0}^{N-1} y_{k'} \exp\left(-i\frac{2\pi k'k}{N}\right) \exp\left(i\frac{2\pi kn}{N}\right) \\
&= \sum_{k=0}^{N-1}\sum_{k'=0}^{N-1} y_{k'} \exp\left(i\frac{2\pi(n-k')k}{N}\right) \\
&= \sum_{k'=0}^{N-1} y_{k'}\,\delta_{n-k',0} \\
&= N y_n.
\end{aligned}$$

$$y_n = \frac{1}{N}\sum_{k=0}^{N-1} c_k \exp\left(i\frac{2\pi kn}{N}\right),$$

inverse discrete Fourier transform (inverse DFT)

Inverse DFT

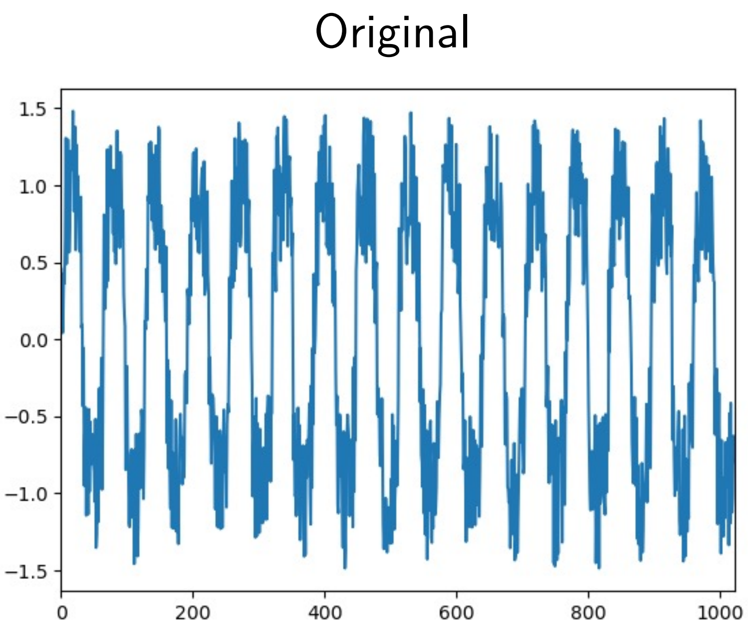
```python
def inverse_dft(c):
    N = len(c)
    y = np.zeros(N, complex)
    for k in range(N):
        for n in range(N):
            y[n] += c[k] * np.exp(2j * np.pi * k * n / N)
    return y / N
```

```python
N = 20
y = np.random.rand(N)
print("y = ", y)
c = dft(y)
print("c = ", c)
yinv = inverse_dft(c)
print("y = ", yinv)
```

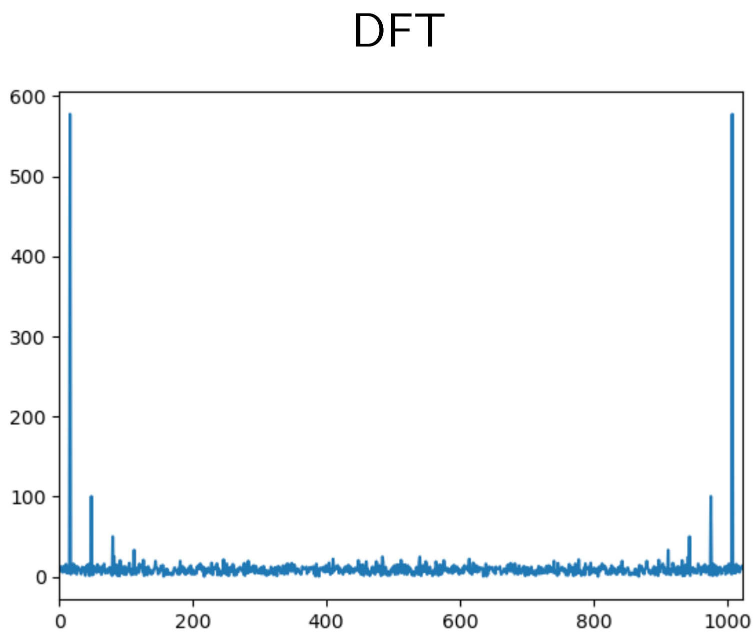
```
y =  [0.86046716 0.48175562 0.06576607 0.73962908 0.61970857 0.26800379
 0.82606492 0.47751752 0.56001126 0.25493145 0.01241648 0.6918537
 0.81113769 0.27735761 0.09617065 0.17598327 0.27550172 0.93691544
 0.50237258 0.1342621 ]
c =  [ 9.06782667+0.00000000e+00j  0.41721559-6.84001863e-01j
  0.0708089 +3.20029273e-01j  0.04707852+1.44889560e+00j
 -1.17455143-1.23742486e+00j  1.6240357 +2.81762241e-04j
  0.9057288 -7.21848714e-01j  2.18903831-1.12193177e+00j
 -0.06718515-4.86177561e-01j -0.03711474+5.50581297e-01j
  0.19140753+4.00264145e-15j -0.03711474-5.50581297e-01j
 -0.06718515+4.86177561e-01j  2.18903831+1.12193177e+00j
  0.9057288 +7.21848714e-01j  1.6240357 -2.81762241e-04j
 -1.17455143+1.23742486e+00j  0.04707852-1.44889560e+00j
  0.0708089 -3.20029273e-01j  0.41721559+6.84001863e-01j]
y =  [0.86046716-4.10782519e-16j 0.48175562+6.66133815e-16j
 0.06576607-1.69309011e-16j 0.73962908-2.47649123e-15j
 0.61970857-1.02834408e-15j 0.26800379-1.90680804e-15j
 0.82606492+3.33066907e-17j 0.47751752-2.77555756e-17j
 0.56001126+5.27355937e-16j 0.25493145-2.27595720e-16j
 0.01241648+1.91513472e-15j 0.6918537 -7.04991621e-16j
 0.81113769+8.63198402e-16j 0.27735761+1.77913240e-15j
 0.09617065+2.32869279e-15j 0.17598327+7.63278329e-16j
 0.27550172+2.06501483e-15j 0.93691544+1.67643677e-15j
 0.50237258-7.99360578e-16j 0.1342621 -1.44884105e-15j]
```

Recover the original function up to round-off error

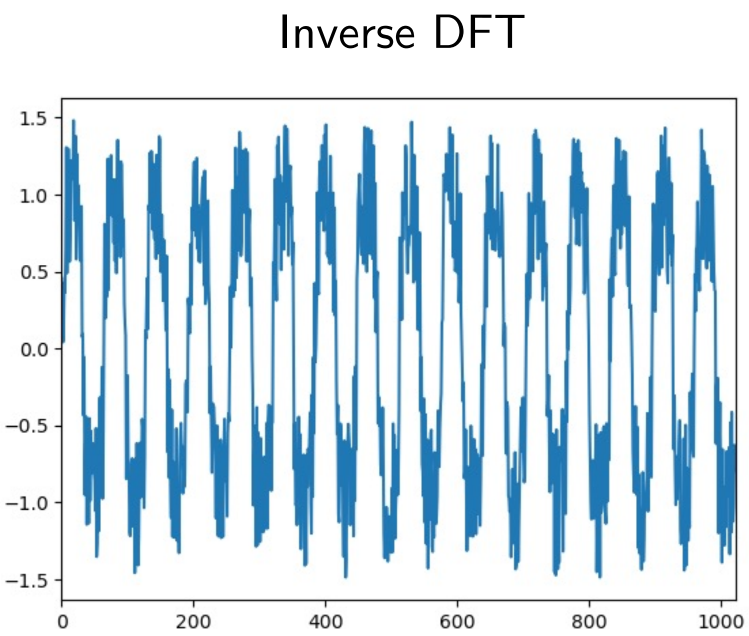
Inverse DFT



Original
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
200
400
600
800
1000



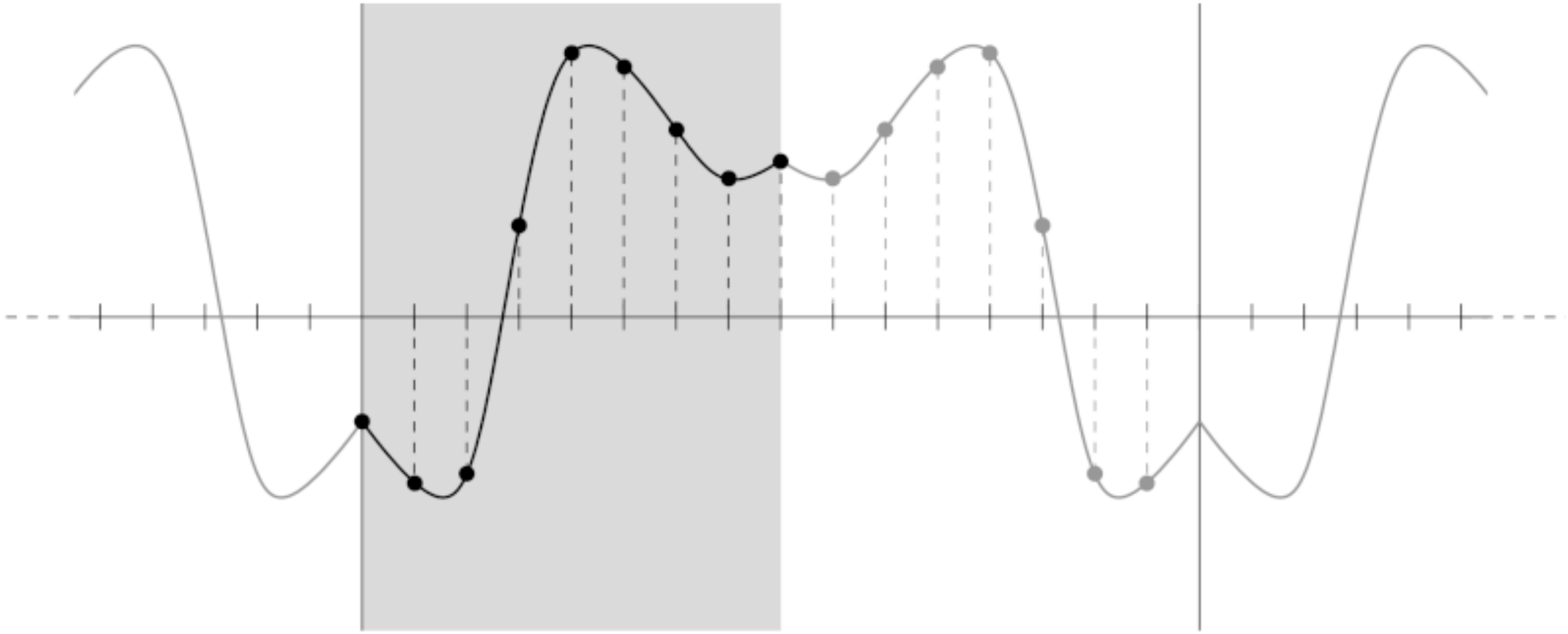
DFT
600
500
400
300
200
100
0
0
200
400
600
800
1000



Inverse DFT
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
200
400
600
800
1000

Discrete cosine and sine transforms

Mirror the function over $x \in [0, L/2]$ and make it (anti)symmetric around $x = L/2$. Then apply the standard Fourier transform



With some optimizations one can avoid using complex numbers

Fast Fourier Transform

DFT complexity: $O(N^2)$

```python
def dft(y):
    N = len(y)
    c = np.zeros(N, complex)
    for k in range(N):
        for n in range(N):
            c[k] += y[n] * np.exp(-2j * np.pi * k * n / N)
    return c
```

Impractical for large data sets

Can we do better?

Fast Fourier Transform (FFT) algorithms achieve $O(N \log N)$

Fast Fourier Transform: Cooley-Tukey algorithm (1965)

To see how it works, let us consider a case where N is a power of two $N = 2^M$ and we want to compute the Fourier transform of $(y_0, y_1, \ldots, y_N)$. By definition we have

$$c_k = \sum_{n=0}^{N-1} y_n \exp\left(-i\frac{2\pi kn}{N}\right).$$

We can split the sum into even and odd elements

$$\begin{aligned}
c_k &= \sum_{n=0}^{N/2-1} y_{2n} \exp\left(-i\frac{2\pi k(2n)}{N}\right) + \sum_{n=0}^{N/2-1} y_{2n+1} \exp\left(-i\frac{2\pi k(2n+1)}{N}\right) \\
&= \sum_{n=0}^{N/2-1} y_{2n} \exp\left(-i\frac{2\pi kn}{N/2}\right) + \exp\left(-i\frac{2\pi k}{N}\right) \sum_{n=0}^{N/2-1} y_{2n+1} \exp\left(-i\frac{2\pi kn}{N/2}\right) \\
&= E_k + \exp\left(-i\frac{2\pi k}{N}\right) O_k.
\end{aligned}$$

c_k can be expressed as a sum of two elements, one is kth element from a DFT of all even elements, $(y_0, y_2, \ldots, y_{N-2})$, and another is a kth element from a DFT of all odd elements, $(y_1, y_3, \ldots, y_{N-1})$.

Fast Fourier Transform: Cooley-Tukey algorithm (1965)

The interpretation makes sense if $k < N/2$.

Other Fourier components can be expressed as $k + N/2$ and read

$$c_{k+N/2} = \sum_{n=0}^{N/2-1} y_{2n} \exp\left(-i\frac{2\pi(k+N/2)n}{N/2}\right) + \exp\left(-i\frac{2\pi(k+N/2)}{N}\right) \sum_{n=0}^{N/2-1} y_{2n+1} \exp\left(-i\frac{2\pi(k+N/2)n}{N/2}\right)$$
$$= E_k - \exp\left(-i\frac{2\pi k}{N}\right) O_k .$$

Combine with

$$c_k = E_k + \exp\left(-i\frac{2\pi k}{N}\right) O_k .$$

To compute DFT of $(y_0,\ldots,y_N)$ we only need to compute *two N/2 DFTs* of even and odd components of y.

Divide and conquer: continue recursively until $N = 1$, where $c_k = y_k$

At each step N is halved

Complexity: O(N log N)

FFT implementation

```python
# Compute DFT of (y_st, y_st+s, y_st+2s, ..., y_st+(N-1)s)
def fft_recursive(y, st, N, s):
    if (N == 1):
        return np.array([y[st]])
    else:
        c = np.empty(N, complex)
        c1 = fft_recursive(y, st, N//2, 2*s)
        c2 = fft_recursive(y, st + s, N//2, 2*s)
        for k in range(N//2):
            p = c1[k]
            q = np.exp(-2j*np.pi*k/N) * c2[k]
            c[k] = p + q
            c[k + N//2] = p - q
        return c

# N = len(y) must be a power of 2
def fft(y):
    N = len(y)
    return FFT_recursive(y, 0, N, 1)
```

FFT vs simple DFT

```
%%time

# Try naive DFT
cdft = dft(y)
```

```
CPU times: user 2.02 s, sys: 26.3 ms, total: 2.05 s
Wall time: 1.61 s
```

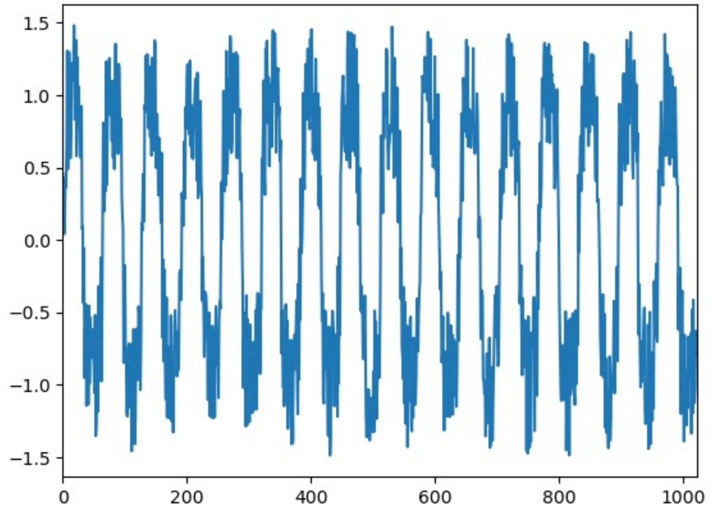
```
%%time

# Now compare to FFT
cfft = fft(y)

print(cdft - cfft)
```

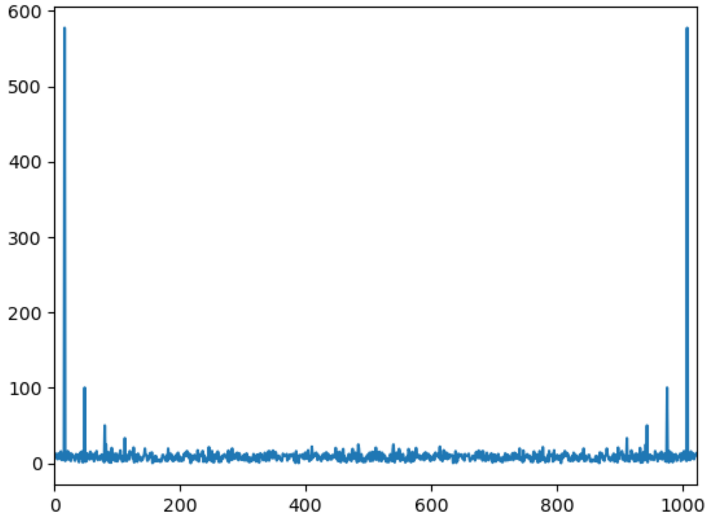
```
[-7.95807864e-13+0.00000000e+00j  4.66293670e-14+6.43929354e-14j
 -2.57571742e-14+4.08562073e-14j ...  1.42890144e-11-1.61026747e-12j
  2.72741829e-11+5.71453995e-12j  1.94777527e-12-1.27142741e-12j]
CPU times: user 5.85 ms, sys: 86 µs, total: 5.93 ms
Wall time: 5.88 ms
```

FFT for the signal

```
%%time

print("N = ",len(y))
y = np.loadtxt("pitch.txt",float)
plt.plot(y)
plt.xlim(0,len(y))
plt.show()

c = fft(y)
plt.plot(np.abs(c))
plt.xlim(0,len(y))
plt.show()
```

```
N =  1024

CPU times: user 307 ms, sys: 9.85 ms, total: 317 ms
Wall time: 121 ms
```

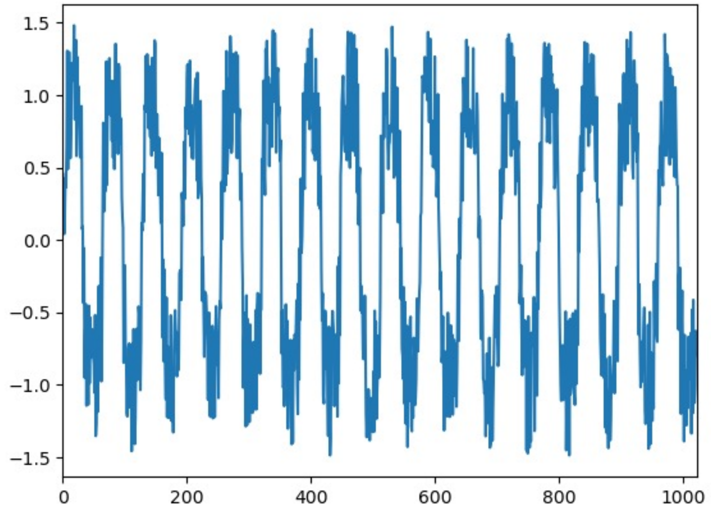


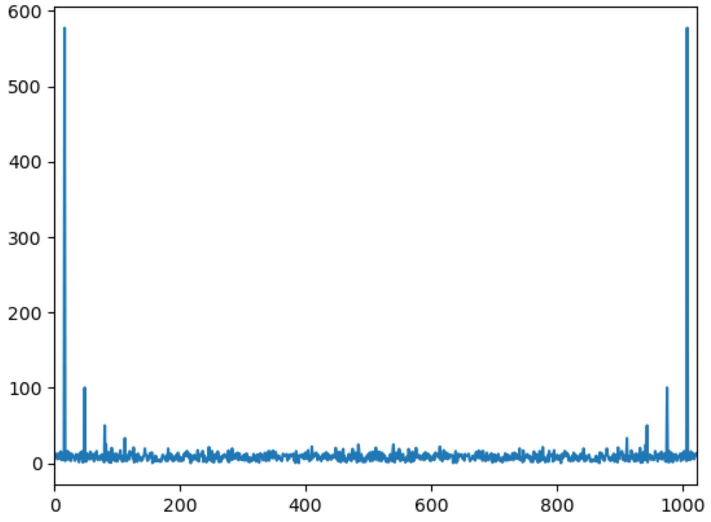


FFT for the signal

```
%%time

print("N = ",len(y))
y = np.loadtxt("pitch.txt",float)
plt.plot(y)
plt.xlim(0,len(y))
plt.show()

c = fft(y)
plt.plot(np.abs(c))
plt.xlim(0,len(y))
plt.show()
```

```
N =  1024

CPU times: user 307 ms, sys: 9.85 ms, total: 317 ms
Wall time: 121 ms
```





Numpy: `np.fft.fft(y)`

```
CPU times: user 299 ms, sys: 10.1 ms, total: 309 ms
Wall time: 118 ms
```