Numerical Methods II
Fourier Transforms and the FFT

Aleksandar Donev
Courant Institute, NYU[1]
donev@courant.nyu.edu

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Outline

Trigonometric Orthogonal Polynomials

Periodic Functions

- Consider now interpolating / approximating **periodic functions** defined on the interval $I = [0, 2\pi]$:

$$\forall x \quad f(x + 2\pi) = f(x),$$

as appear in practice when analyzing signals (e.g., sound/image processing).

- Also consider only the space of complex-valued **square-integrable functions** $L^2_{2\pi}$,

$$\forall f \in L^2_w : \quad (f, f) = \|f\|^2 = \int_0^{2\pi} |f(x)|^2 \, dx < \infty.$$

- Polynomial functions are not periodic and thus basis sets based on orthogonal polynomials are not appropriate.
- Instead, consider sines and cosines as a basis function, combined together into **complex exponential functions**

$$\phi_k(x) = e^{ikx} = \cos(kx) + i\sin(kx), \quad k = 0, \pm 1, \pm 2, \ldots$$

Fourier Basis Functions

$$\phi_k(x) = e^{ikx}, \quad k = 0, \pm 1, \pm 2, \ldots$$

- It is easy to see that these are **orhogonal** with respect to the continuous dot product

$$(\phi_j, \phi_k) = \int_{x=0}^{2\pi} \phi_j(x)\phi_k^{\star}(x)dx = \int_0^{2\pi} \exp\left[i(j-k)x\right] dx = 2\pi\delta_{ij}$$

- The complex exponentials can be shown to form a complete **trigonometric polynomial basis** for the space $L^2_{2\pi}$, i.e.,

$$\forall f \in L^2_{2\pi}: \quad f(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ikx},$$

where the **Fourier coefficients** can be computed for any **frequency or wavenumber** k using:

$$\hat{f}_k = \frac{(f, \phi_k)}{2\pi} = \frac{1}{2\pi} \cdot \int_0^{2\pi} f(x)e^{-ikx}dx.$$

Truncated Fourier Basis

- For a general interval $[0, X]$ the **discrete frequencies** are

$$k = \frac{2\pi}{X}\kappa \qquad \kappa = 0, \pm 1, \pm 2, \ldots$$

Length

- For non-periodic functions one can take the limit $X \to \infty$ in which case we get **continuous frequencies**.
- Now consider a **discrete Fourier basis** that only includes the first N basis functions, i.e.,

$$\begin{cases} k = -(N-1)/2, \ldots, 0, \ldots, (N-1)/2 & \text{if } N \text{ is odd} \\ k = -N/2, \ldots, 0, \ldots, N/2 - 1 & \text{if } N \text{ is even}, \end{cases}$$

and for simplicity we focus on N odd.

- The least-squares **spectral approximation** for this basis is:

$$f(x) \approx \phi(x) = \sum_{k=-(N-1)/2}^{(N-1)/2} \hat{f}_k e^{ikx}.$$

Discrete Dot Product

- Now also discretize a given function on a set of N **equi-spaced nodes**

$$x_j = jh \text{ where } h = \frac{2\pi}{N}$$

where $j = N$ is the same node as $j = 0$ due to periodicity so we only consider N instead of $N + 1$ nodes.

- We also have the **discrete dot product** between two discrete functions (vectors) $\mathbf{f}_j = f(x_j)$:

$$\mathbf{f} \cdot \mathbf{g} = h \sum_{j=0}^{N-1} f_i g_i^{\star}$$

- The discrete Fourier basis is **discretely orthogonal**

$$\phi_k \cdot \phi_{k'} = 2\pi \delta_{k,k'}$$

Proof of Discrete Orthogonality

The case $k = k'$ is trivial, so focus on

$$\phi_k \cdot \phi_{k'} = 0 \text{ for } k \neq k'$$

$$\sum_j \exp\left(ikx_j\right) \exp\left(-ik'x_j\right) = \sum_j \exp\left[i\left(\Delta k\right) x_j\right] = \sum_{j=0}^{N-1} \left[\exp\left(ih\left(\Delta k\right)\right)\right]^j$$

where $\Delta k = k - k'$. This is a geometric series sum:

$$\phi_k \cdot \phi_{k'} = \frac{1 - z^N}{1 - z} = 0 \text{ if } k \neq k'$$

since $z = \exp\left(ih\left(\Delta k\right)\right) \neq 1$ and
$z^N = \exp\left(ihN\left(\Delta k\right)\right) = \exp\left(2\pi i\left(\Delta k\right)\right) = 1$.

Discrete Fourier Transform

- The **Fourier interpolating polynomial** is thus easy to construct

$$\phi_N(x) = \sum_{k=-(N-1)/2}^{(N-1)/2} \hat{f}_k^{(N)} e^{ikx}$$

where the **discrete Fourier coefficients** are given by

$$\hat{f}_k^{(N)} = \frac{\mathbf{f} \cdot \phi_k}{2\pi} = \frac{1}{N} \sum_{j=0}^{N-1} f(x_j) \exp\left(-ikx_j\right)$$

- Simplifying the notation and recalling $x_j = jh$, we define the the **Discrete Fourier Transform** (DFT):

$$\hat{f}_k \neq \hat{f}_k^{N} = \frac{1}{N} \sum_{j=0}^{N-1} f_j \exp\left(-\frac{2\pi ijk}{N}\right)$$

Discrete spectrum

- The set of discrete Fourier coefficients $\hat{\mathbf{f}}$ is called the **discrete spectrum**, and in particular,

$$S_k = \left|\hat{f}_k\right|^2 = \hat{f}_k \hat{f}_k^\star,$$

  is the **power spectrum** which measures the frequency content of a signal.
- If f is real, then $\hat{f}$ satisfies the **conjugacy property**

$$\hat{f}_{-k} = \hat{f}_k^\star,$$

  so that half of the spectrum is redundant and $\hat{f}_0$ is real.
- For an even number of points N the largest frequency $k = -N/2$ does not have a conjugate partner. It is special and **must be treated with care**.

Fourier Spectral Approximation

- **Discrete Fourier Transform** (DFT): $\varphi(x) = \sum_k f_k e^{ikx}$

$$\text{Forward } \mathbf{f} \rightarrow \hat{\mathbf{f}} : \quad \hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j \exp\left(-\frac{2\pi ijk}{N}\right)$$

$$\text{Inverse } \hat{\mathbf{f}} \rightarrow f : \quad f(x_j) \approx \phi(x_j) = \sum_{k=-(N-1)/2}^{(N-1)/2} \hat{f}_k \exp\left(\frac{2\pi ijk}{N}\right)$$

- There is a very fast algorithm for performing the **forward and backward DFTs (FFT)**.
- There is **different conventions** for the DFT depending on the interval on which the function is defined and placement of factors of N and 2π.

  Read the documentation to be consistent!

$$\varphi(x) = \sum_{-(N-1)/2}^{(N-1)/2} \hat{f}_k e^{ikx}$$

If $\vec{x}$ is arbitrary, use

Non-Uniform FFT (NUFFT)

If $\vec{x}$ is on a regular grid

$M > N$

$$\sum_{-(M-1)/2}^{(M+1)/2} \hat{f}_k e^{ikx}$$

$$f_{|k| > (N-1)/2} = 0$$

<u>Interpft</u>:

- Padd $\hat{f}$ with zeros
- $\to$ Do iFFT

Spectral Convergence (or not)

- The Fourier interpolating polynomial $\phi(x)$ has **spectral accuracy**, i.e., exponential in the number of nodes N

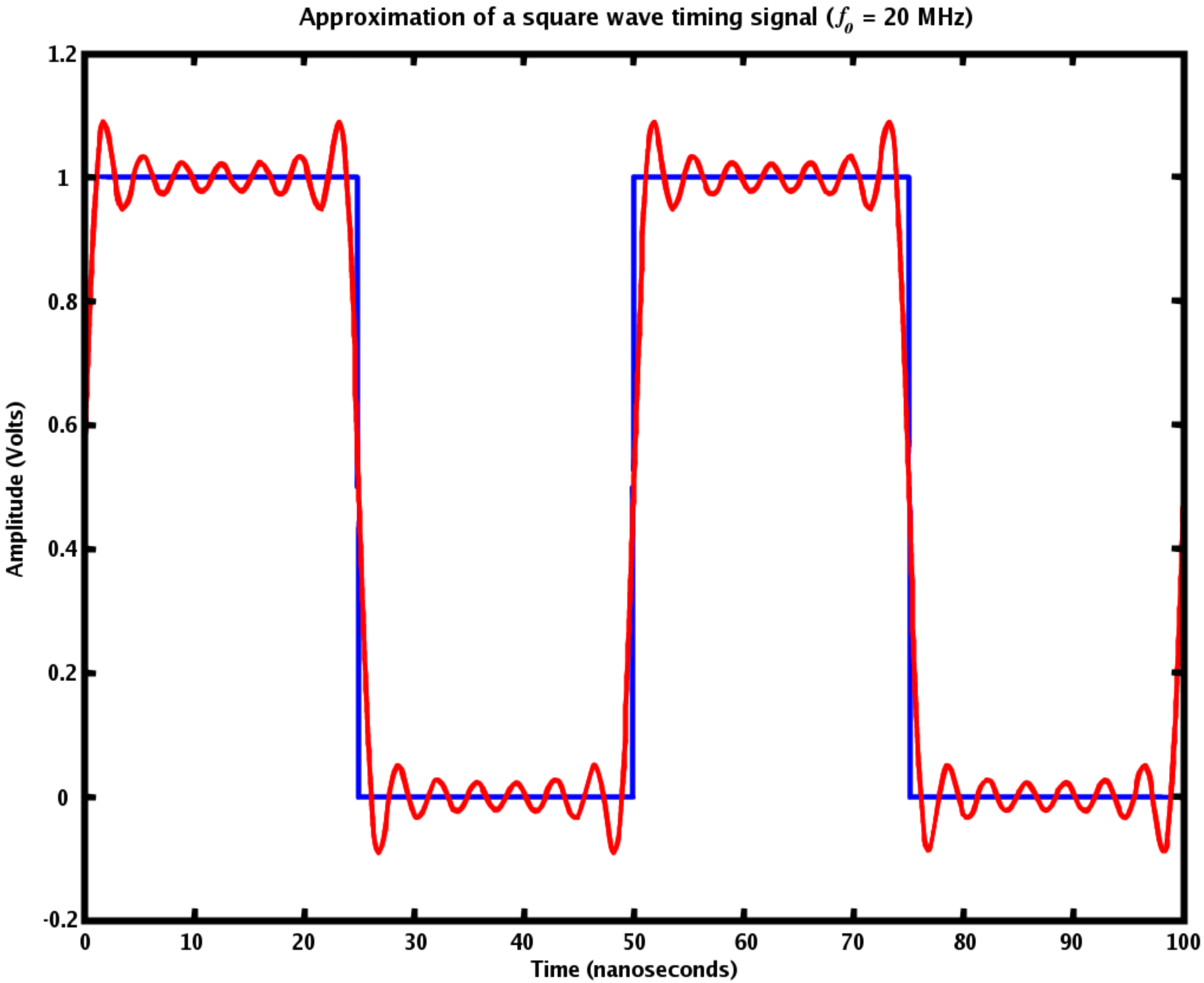
$$\|f(x) - \phi(x)\| \sim e^{-N}$$

for **analytic functions** (more details shortly).

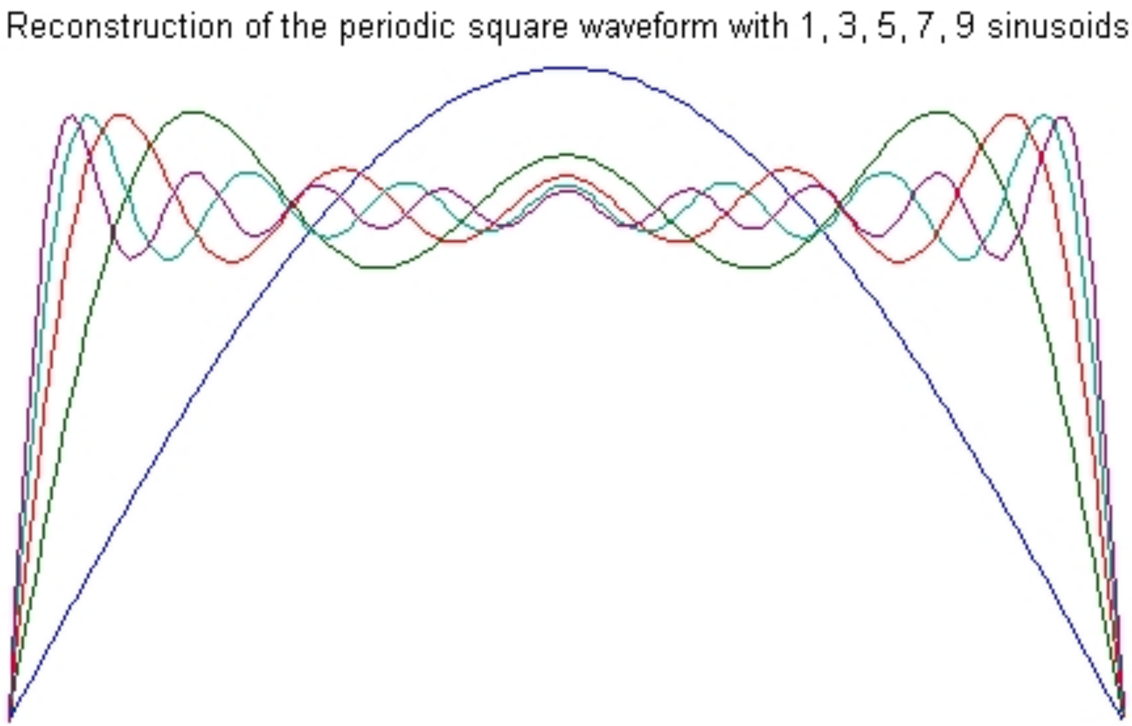
- Specifically, nice functions exhibit **rapid decay of the Fourier coefficients** with k, e.g., exponential decay $\left|\hat{f}_k\right| \sim e^{-|k|}$.
- Discontinuities cause slowly-decaying Fourier coefficients, e.g., power law decay $\left|\hat{f}_k\right| \sim k^{-1}$ for **jump discontinuities**.
- Jump discontinuities lead to slow convergence of the Fourier series for non-singular points (and no convergence at all near the singularity), so-called **Gibbs phenomenon** (ringing):

$$\|f(x) - \phi(x)\| \sim \begin{cases} N^{-1} & \text{at points away from jumps} \\ \text{const.} & \text{at the jumps themselves} \end{cases}$$

Gibbs Phenomenon

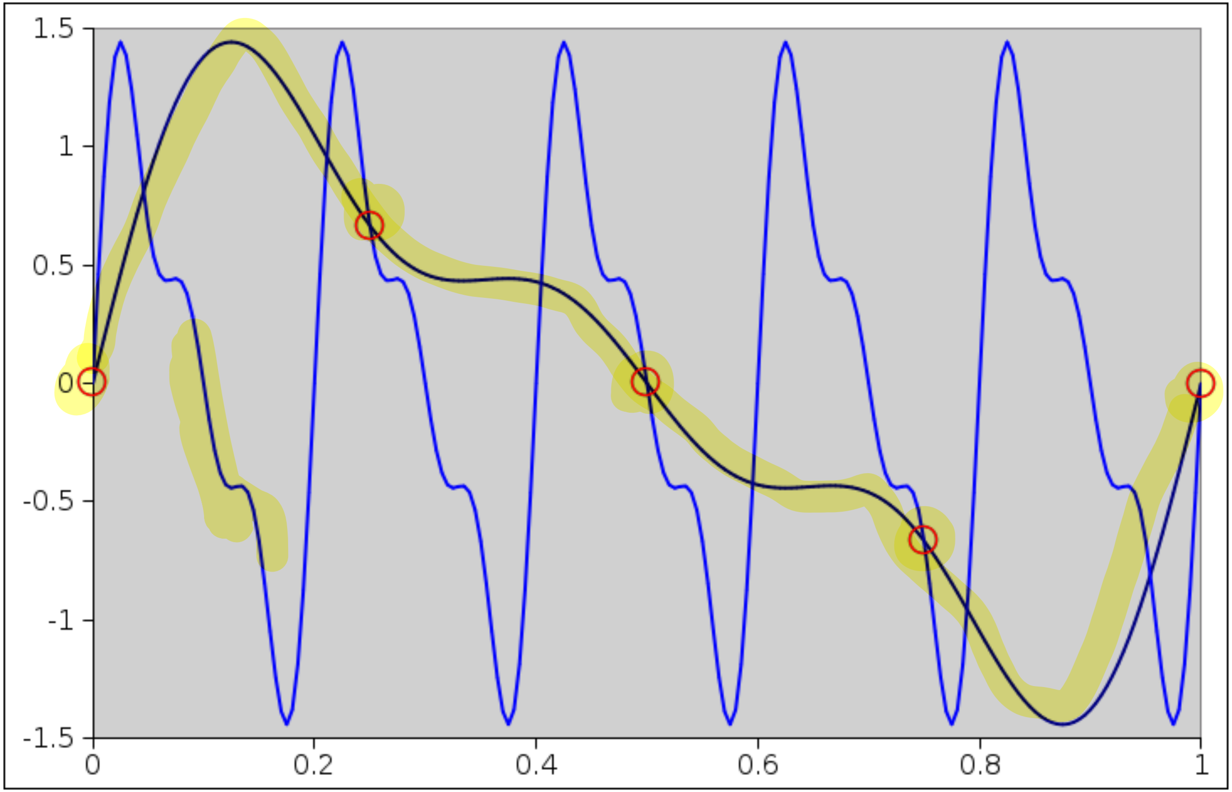


Gibbs Phenomenon



Aliasing

If we sample a signal at too few points the Fourier interpolant may be wildly wrong: **aliasing** of frequencies k and $2k, 3k, \ldots$



e^{ikx}

e^{2ikx}

Approximation Theory

Trigonometric projection vs. interpolation

- I will temporarily switch to notation in paper on periodic chebfun in paper of Trefethen *et al*, assuming *odd* number of points for simplicity:

$$f\left(t \in [0, 2\pi]\right) \text{ discretized with } N = 2n + 1 \text{ points } t_m = \frac{2\pi m}{N}$$

$$\text{Trigonometric projection: } f_n(t) = \sum_{k=-n}^{n} c_k e^{ikt}$$

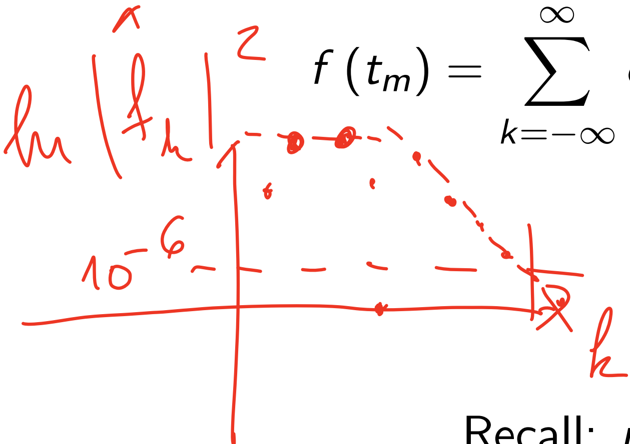
$$\text{Trigonometric interpolant: } p_n(t) = \sum_{k=-n}^{n} \tilde{c}_k e^{ikt}.$$

- **Aliasing** means that one cannot distinguish two different Fourier modes on a given grid:

$$\exp\left(ikt_m\right) = \exp\left(i\left(k + jN\right) t_m\right)$$

Poisson Summation Formula

- Observe that because of aliasing:



$$f(t_m) = \sum_{k=-\infty}^{\infty} c_k e^{ikt_m} = \sum_{k=-n}^{n} \sum_{j=-\infty}^{\infty} c_{k+jN} e^{i(k+jN)t_m}$$

$$= \sum_{k=-n}^{n} \left(\sum_{j=-\infty}^{\infty} c_{k+jN} \right) e^{ikt_m}$$

$$\text{Recall: } p_n(t_m) = \sum_{k=-n}^{n} \tilde{c}_k e^{ikt_m}$$

- Since the trigonometric interpolant is unique, we get Poisson's summation formula

CFT

DFT

$$\tilde{c}_k = \sum_{j=-\infty}^{\infty} c_{k+jN}$$

The importance of smoothness

- **Total variation** of differentiable function (can be generalized):

$$\mathrm{TV}[f] = \int_0^{2\pi} \left| f'(x) \right| dx, \quad \text{denote } V = \mathrm{TV}\left[f^{(\nu)} \right].$$

- We have two cases where we have nice error estimates:
  - If f is $\nu \geq 0$ times **differentiable**, then

$$|c_k| \leq \frac{V}{2\pi \left| k \right|^{\nu+1}}$$

    which can be proved by integrating $c_k = (2\pi)^{-1} \int_0^{2\pi} f(x) e^{-ikx} dx$ by parts $\nu + 1$ times.
  - If $f(t)$ is **analytic** in a half-strip around the real axis of half-width α and bounded by $|f(t)| < M$, then

$$|c_k| \leq M e^{-\alpha |k|}$$

    which can be proved by shifting the contour of integration above or below the real line by α.

Approximation error: Differentiable

- If f is $\nu \geq 1$ times **differentiable** then

$$\|f - f_n\|_\infty = \left\| \sum_{|k|>n} c_k e^{ikt} \right\|_\infty \leq \sum_{|k|>n} |c_k|$$

$$\leq 2 \sum_{k=n+1}^{\infty} \frac{V}{2\pi k^{\nu+1}} \approx 2 \int_n^\infty \frac{V}{2\pi k^{\nu+1}} dk$$

- Performing the integral we get that if f is $\nu \geq 1$ times **differentiable**, then

$$\|f - f_n\|_\infty \leq \frac{V}{\pi \nu n^\nu}$$

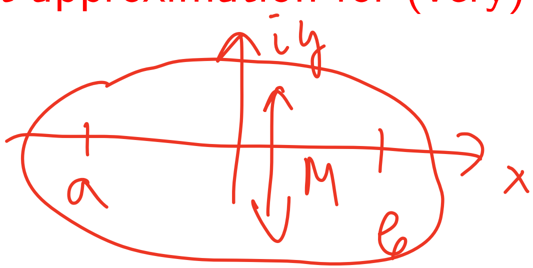
- You can replace f_n with p_n if you multiply the r.h.s. by 2 to account for the additional aliasing error.

Approximation error: Analytic

- If $f(t)$ is **analytic** in the half strip then

$$\|f - f_n\|_\infty \leq 2 \sum_{k=n+1}^{\infty} Me^{-\alpha k} = \frac{2Me^{-\alpha n}}{e^{\alpha} - 1} \text{ (geometric series sum)}$$

- You can replace f_n with p_n if you multiply the r.h.s. by 2 to account for the additional aliasing error.
- The Fourier interpolating trigonometric polynomial is spectrally accurate and a really great approximation for (very) smooth functions.



Trapezoidal Rule

- Consider using the trapezoidal rule to approximate a **periodic integral**:

$$I = \int_0^{2\pi} f(x)dx = c_0$$

$$I_N = \frac{2\pi}{N} \sum_{m=1}^{N} f(t_m) = \tilde{c}_0.$$

- If f is $\nu \geq 1$ times **differentiable** then

$$|I_N - I| \leq \frac{4V}{N^{\nu+1}}.$$

- If $f(t)$ is **analytic** in the half strip then trapezoidal rule is spectrally accurate:

$$|I_N - I| \leq \frac{4\pi M}{e^{\alpha N} - 1}.$$

Fast Fourier Transform

DFT

- Recall the transformation from real space to frequency space and back:

$$\mathbf{f} \rightarrow \hat{\mathbf{f}}: \quad \hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j \exp\left(-\frac{2\pi ijk}{N}\right), \quad k = -\frac{(N-1)}{2}, \ldots, \frac{(N-1)}{2}$$

MATLAB

$$\hat{\mathbf{f}} \rightarrow \mathbf{f}: \quad f_j = \sum_{k=-(N-1)/2}^{(N-1)/2} \hat{f}_k \exp\left(\frac{2\pi ijk}{N}\right), \quad j = 0, \ldots, N-1$$

- We can make the forward-reverse **Discrete Fourier Transform** (DFT) more symmetric if we shift the frequencies to $k = 0, \ldots, N$:

$$\text{Forward } \mathbf{f} \rightarrow \hat{\mathbf{f}}: \quad \hat{f}_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} f_j \exp\left(-\frac{2\pi ijk}{N}\right), \quad k = 0, \ldots, N-1$$

$$\text{Inverse } \hat{\mathbf{f}} \rightarrow \mathbf{f}: \quad f_j = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \hat{f}_k \exp\left(\frac{2\pi ijk}{N}\right), \quad j = 0, \ldots, N-1$$

FFT

- We can write the transforms in matrix notation:

$$\hat{\mathbf{f}} = \frac{1}{\sqrt{N}} \mathbf{U}_N \mathbf{f}$$

$$\mathbf{f} = \frac{1}{\sqrt{N}} \mathbf{U}_N^{\star} \hat{\mathbf{f}},$$

$O(N \log N)$

FFT

where the **unitary Fourier matrix** (*fft*(*eye*(*N*)) in MATLAB) is an $N \times N$ matrix with entries

$$u_{jk}^{(N)} = \omega_N^{jk}, \quad \omega_N = e^{-2\pi i/N}.$$

- A **direct** matrix-vector multiplication algorithm therefore takes $O(N^2)$ multiplications and additions.
- Is there a faster way to compute the **non-normalized**

$$\hat{f}_k = \sum_{j=0}^{N-1} f_j \omega_N^{jk} \quad ?$$

FFT

- For now assume that N is even and in fact a power of two, $N = 2^n$.
- The idea is to split the transform into two pieces, **even and odd** points:

$$\sum_{j=2j'} f_j \omega_N^{jk} + \sum_{j=2j'+1} f_j \omega_N^{jk} = \sum_{j'=0}^{N/2-1} f_{2j'} \left(\omega_N^2\right)^{j'k} + \omega_N^k \sum_{j'=0}^{N/2-1} f_{2j'+1} \left(\omega_N^2\right)^{j'k}$$

- Now notice that

$$\omega_N^2 = e^{-4\pi i/N} = e^{-2\pi i/(N/2)} = \omega_{N/2}$$

- This leads to a **divide-and-conquer algorithm**:

$$\hat{f}_k = \sum_{j'=0}^{N/2-1} f_{2j'} \omega_{N/2}^{j'k} + \omega_N^k \sum_{j'=0}^{N/2-1} f_{2j'+1} \omega_{N/2}^{j'k}$$

$$\hat{f}_k = \mathbf{U}_N \mathbf{f} = \left(\mathbf{U}_{N/2} \mathbf{f}_{even} + \omega_N^k \mathbf{U}_{N/2} \mathbf{f}_{odd}\right)$$

FFT Complexity

- The **Fast Fourier Transform** algorithm is **recursive**:

$$FFT_N(\mathbf{f}) = FFT_{\frac{N}{2}}(\mathbf{f}_{even}) + \mathbf{w} \boxdot FFT_{\frac{N}{2}}(\mathbf{f}_{odd}),$$

  where $w_k = \omega_N^k$ and $\boxdot$ denotes element-wise product. When $N = 1$ the FFT is trivial (identity).
- To compute the whole transform we need $\log_2(N)$ steps, and at each step we only need N multiplications and $N/2$ additions at each step.
- The total **cost of FFT** is thus much better than the direct method's $O(N^2)$: **Log-linear**

$$O(N \log N).$$

- Even when N is not a power of two there are ways to do a similar **splitting** transformation of the large FFT into many smaller FFTs.
- Note that there are different **normalization conventions** used in different software.

In MATLAB

- The forward transform is performed by the function $\hat{f} = \mathit{fft}(f)$ and the inverse by $f = \mathit{fft}(\hat{f})$. Note that $\mathit{ifft}(\mathit{fft}(f)) = f$ and f and $\hat{f}$ may be complex.
- In MATLAB, and other software, the frequencies are not ordered in the "normal" way $-(N-1)/2$ to $+(N-1)/2$, but rather, the nonnegative frequencies come first, then the positive ones, so the "funny" ordering is

$$0, 1, \ldots, (N-1)/2, \quad -\frac{N-1}{2}, -\frac{N-1}{2} + 1, \ldots, -1.$$

  This is because such ordering (shift) makes the forward and inverse transforms symmetric.
- The function *fftshift* can be used to order the frequencies in the "normal" way, and *ifftshift* does the reverse:

$$\hat{f} = \mathit{fftshift}(\mathit{fft}(f)) \text{ (normal ordering)}.$$

FFT-based noise filtering (1)

```
Fs = 1000;                          % Sampling frequency
dt = 1/Fs;                          % Sampling interval
L = 1000;                           % Length of signal
t = (0:L-1)*dt;                     % Time vector
T=L*dt;                             % Total time interval

% Sum of a 50 Hz sinusoid and a 120 Hz sinusoid
x = 0.7*sin(2*pi*50*t) + sin(2*pi*120*t);
y = x + 2*randn(size(t));           % Sinusoids plus noise

figure(1); clf;
plot(t(1:100),y(1:100),'b--'); hold on
title('Signal Corrupted with Zero-Mean Random Noise')
xlabel('time')
```

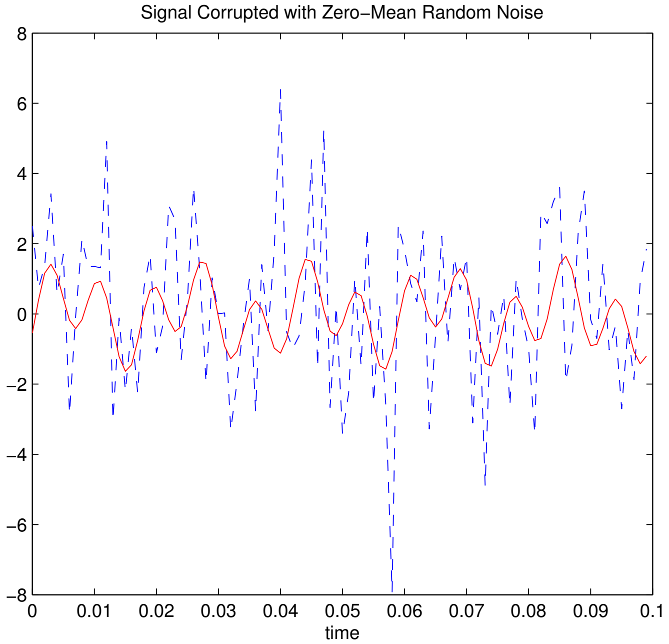
FFT-based noise filtering (2)

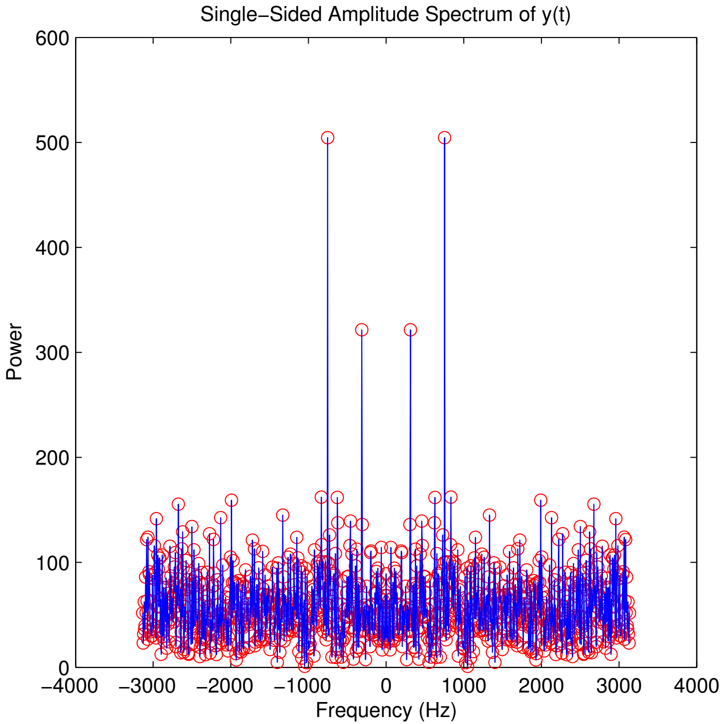
```
if(0)
   N=(L/2)*2; % Even N
   y_hat = fft(y(1:N));
   % Frequencies ordered in a funny way:
   f_funny = 2*pi/T* [0:N/2-1, -N/2:-1];
   % Normal ordering:
   f_normal = 2*pi/T* [-N/2 : N/2-1];
else
   N=(L/2)*2-1; % Odd N
   y_hat = fft(y(1:N));
   % Frequencies ordered in a funny way:
   f_funny = 2*pi/T* [0:(N-1)/2, -(N-1)/2:-1];
   % Normal ordering:
   f_normal = 2*pi/T* [-(N-1)/2 : (N-1)/2];
end
```

FFT-based noise filtering (3)

```
figure(2); clf; plot(f_funny, abs(y_hat), 'ro'); hold

y_hat=fftshift(y_hat);
figure(2); plot(f_normal, abs(y_hat), 'b-');

title('Single-Sided Amplitude Spectrum of y(t)')
xlabel('Frequency (Hz)')
ylabel('Power')

y_hat(abs(y_hat)<250)=0; % Filter out noise
y_filtered = ifft(ifftshift(y_hat));
figure(1); plot(t(1:100),y_filtered(1:100),'r-')
```

FFT results


Signal Corrupted with Zero−Mean Random Noise
8
6
4
2
0
−2
−4
−6
−8
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
time


Single−Sided Amplitude Spectrum of y(t)
600
500
400
300
200
100
0
Power
−4000
−3000
−2000
−1000
0
1000
2000
3000
4000
Frequency (Hz)

Multidimensional FFT

- DFTs and FFTs generalize straightforwardly to higher dimensions due to separability: **Transform each dimension independently**

$$\hat{f} = \frac{1}{N_x N_y} \sum_{j_y=0}^{N_y-1} \sum_{j_x=0}^{N_x-1} f_{j_x,j_y} \exp\left[-\frac{2\pi i \left(j_x k_x + j_y k_y\right)}{N}\right]$$

$$\hat{\mathbf{f}}_{k_x,k_y} = \frac{1}{N_x} \sum_{j_y=0}^{N_y-1} \exp\left(-\frac{2\pi i j_y k_x}{N}\right) \left[\frac{1}{N_y} \sum_{j_y=0}^{N_y-1} f_{j_x,j_y} \exp\left(-\frac{2\pi i j_y k_y}{N}\right)\right]$$

- For example, in two dimensions, **do FFTs of each column, then FFTs of each row of the result**:

$$\hat{\mathbf{f}} = \mathcal{F}_{row}\left(\mathcal{F}_{col}\left(\mathbf{f}\right)\right)$$

- The cost is N_y one-dimensional FFTs of length N_x and then N_x one-dimensional FFTs of length N_y:

$$N_x N_y \log N_x + N_x N_y \log N_y = N_x N_y \log\left(N_x N_y\right) = N \log N$$

Conclusions

Conclusions/Summary

- **Periodic functions** can be approximated using basis of **orthogonal trigonometric polynomials**.
- The Fourier basis is **discretely orthogonal** and gives **spectral accuracy** for smooth functions.
- Functions with discontinuities are not approximated well: **Gibbs phenomenon**.
- The **Discrete Fourier Transform** can be computed very efficiently using the **Fast Fourier Transform** algorithm: $O(N \log N)$.