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SS 2017
Worksheet 4
24.5.2017

Algorithms of Scientific Computing

Exercise 1: Fourier Series

The Fourier coefficients are given as

$$c_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx} \, \mathrm{d}x.$$

We plug in our three functions and compute their Fourier coefficients.

a) Recall $\int f(x)\delta(x)\,\mathrm{d}x = f(0)$. The integral gives the amplitude of $f(x)$ at the delta spike. We can also shift the integral used to computed the Fourier coefficients by any given a, here chosen between $-\pi$ and 0 ($-\pi < a < 0$). We need to do this in this case because you cannot have a Dirac delta spiking at the border of an integral (it isn't defined in that case). Then the repeating Dirac delta $DD(x)$ yields:

$$\begin{aligned}
c_k &= \frac{1}{2\pi} \int_a^{a+2\pi} DD(x) e^{-ikx} \, \mathrm{d}x \\
&= \frac{1}{2\pi} \left(\int_a^{a+\pi} DD(x) e^{-ikx} \, \mathrm{d}x + \int_{a+\pi}^{a+2\pi} -DD(x) e^{-ikx} \, \mathrm{d}x \right) \\
&= \frac{1}{2\pi} \left(e^{-ik\cdot 0} - e^{-ik\cdot\pi} \right) \\
&= \frac{1}{2\pi} \left(1 - (-1)^k \right)
\end{aligned}$$

If k is even, then the coefficients are 0, otherwise the Fourier coefficients are constant with $\frac{1}{\pi}$. In other words, all odd frequencies are equally important and necessary to approximate a delta spike. The Fourier series then is

$$F(x) = \frac{1}{\pi} \sum_{\substack{k=-\infty \\ k \text{ odd}}}^{\infty} e^{ikx}.$$

b) We compute the Fourier coefficients of the square wave $SW(x)$:

$$
\begin{aligned}
c_k &= \frac{1}{2\pi}\int_0^{2\pi} SW(x)e^{-ikx}\,\mathrm{d}x \\
&= \frac{1}{2\pi}\left(\int_0^{\pi} SW(x)e^{-ikx}\,\mathrm{d}x + \int_{\pi}^{2\pi} SW(x)e^{-ikx}\,\mathrm{d}x\right) \\
&= \frac{1}{2\pi}\left(\int_0^{\pi} e^{-ikx}\,\mathrm{d}x + \int_{\pi}^{2\pi} -e^{-ikx}\,\mathrm{d}x\right) \\
&= \frac{1}{2\pi}\left(\left[\frac{1}{-ik}\,e^{-ikx}\right]_0^{\pi} + \left[\frac{1}{ik}\,e^{-ikx}\right]_{\pi}^{2\pi}\right) \\
&= \frac{1}{\pi}\left(\frac{-1}{ik}\,e^{-ik\pi} + \frac{1}{ik}\right) \\
&= \frac{-i}{k\pi}\left(1 - e^{-ik\pi}\right)
\end{aligned}
$$

We start with the complex Fourier series and apply a sequence of simplifications.

① For even k, the term $1 - e^{-ik\pi}$ vanishes. For odd k, $1 - e^{-ik\pi}$ simplifies to 2.

② Combine positive and negative terms.

③ $\sin(kx) = \frac{e^{ikx} - e^{-ikx}}{2i}$

$$
\begin{aligned}
F(x) &= \sum_{k=-\infty}^{\infty} \frac{-i}{k\pi}\left(1 - e^{-ik\pi}\right) e^{ikx} \\
&\overset{①}{=} \sum_{\substack{k=-\infty \\ k \text{ odd}}}^{\infty} \frac{-2i}{k\pi}\, e^{ikx} \\
&\overset{②}{=} \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \left(\frac{-2i}{k\pi}\, e^{ikx} + \frac{2i}{k\pi}\, e^{-ikx}\right) \\
&= \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{2i}{k\pi}\left(e^{-ikx} - e^{ikx}\right)\frac{2i}{2i} \\
&\overset{③}{=} \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{2i \cdot 2i}{k\pi}\sin(kx) \\
&= \frac{4}{\pi}\sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{\sin(kx)}{k}
\end{aligned}
$$

All imaginary parts vanish and we obtain the common form of the Fourier series of the square wave. As the square wave is an odd function, it is no surprise that we are left with only sines. Note the factor $1/k$. Although the series in infinite and we need all frequencies to represent the jumps, higher coefficients are less important than lower frequencies. This is the key difference to the delta spikes.

c) Fourier coefficients of the repeating ramp $RR(x)$:

$$\begin{aligned}
c_k &= \frac{1}{2\pi}\int_0^{2\pi} RR(x)e^{-ikx}\,\mathrm{d}x \\
&= \frac{1}{2\pi}\left(\int_0^{\pi} RR(x)e^{-ikx}\,\mathrm{d}x + \int_{\pi}^{2\pi} RR(x)e^{-ikx}\,\mathrm{d}x\right) \\
&= \frac{1}{2\pi}\left(\int_0^{\pi} xe^{-ikx}\,\mathrm{d}x + \int_{\pi}^{2\pi} -xe^{-ikx}\,\mathrm{d}x\right) \\
&= \frac{1}{2\pi}\left(\left[\frac{e^{-ikx}(1+ikx)}{k^2}\right]_0^{\pi} - \left[\frac{e^{-ikx}(1+ikx)}{k^2}\right]_{\pi}^{2\pi}\right) \\
&= \frac{1}{\pi k^2}\left(e^{-ik\pi}(1+ik\pi) - 1 - ik\pi\right)
\end{aligned}$$

Fourier series:

$$F(x) = \frac{1}{\pi}\sum_{k=-\infty}^{\infty}\frac{1}{k^2}\left(e^{-ik\pi}(1+ik\pi) - 1 - ik\pi\right)e^{ikx}$$

We could derive the real-valued Fourier series analogously to the square wave. There is, however, a much simpler way. The Dirac delta, the square wave and the repeating ramp can be obtained by integrating and differentiating, respectively. Integrating the Dirac delta gives the square wave divided by 2[1]; integrating the square wave gives the ramp. We can use this insight to easily derive the real-valued Fourier series of the Dirac delta by differentiating the square pulse (and adding the factor 2). We can further derive the real-valued series for the ramp function from the square pulse by integrating. The only piece missing is the integration constant.

$$\begin{aligned}
DD: &\quad \frac{4}{\pi}\sum_{\substack{k=1\\ k\text{ odd}}}^{\infty}\cos(kx) \\
SW: &\quad \frac{4}{\pi}\sum_{\substack{k=1\\ k\text{ odd}}}^{\infty}\frac{\sin(kx)}{k} \\
RR: &\quad c_0 - \frac{4}{\pi}\sum_{\substack{k=1\\ k\text{ odd}}}^{\infty}\frac{\cos(kx)}{k^2}
\end{aligned}$$

The meaning of the constant c_0 gives us its value: It is the average value of the function, so $c_0 = \pi/2$ for the ramp.

If we had to truncate a series, then an interesting question is how many terms we need to achieve a certain accuracy. We can answer this by looking at the decay rate of the coefficients. Integration makes functions smoother; higher frequencies become less important. This result translates to the discrete Fourier transform in a very similar manner.

[1] The dirac spike is in some sense a jump of size one at a discontinuitie, in our case we want to do a jump of size 2 at the discontinuities of the square wave so we need to add a factor 2

function	**decay rate**
delta	1
square wave	$1/k$
ramp	$1/k^2$

Exercise 2: DFT and Least Squares Approximation

Since the Euclidean norm is defined by a scalar product, the function giving the error $E(\alpha_0, \ldots, \alpha_{N-1}) = ||\mathbf{f} - \Phi_N(x)||_2^2$ is a quadratic function that attains its extremum where $\nabla E(\alpha_0, \ldots, \alpha_{N-1})$ vanishes.

Given that the k-th partial derivative is given by

$$\frac{\partial E}{\partial a_k} = \sum_{n=0}^{N-1} \left[e^{-i2\pi nk/N} \left(f_n - \sum_{p=0}^{N-1} \alpha_p e^{i2\pi np/N} \right) \right], \tag{1}$$

we set each partial derivative to zero and obtain

$$\sum_{n=0}^{N} \left[e^{-i2\pi nk/N} \left(f_n - \sum_{p=0}^{N-1} \alpha_p e^{i2\pi np/N} \right) \right] = 0. \tag{2}$$

Rearranging the terms gives us the set of N equations

$$\sum_{n=0}^{N-1} f_n \omega_N^{-nk} = \sum_{p=0}^{N-1} \alpha_p \underbrace{\sum_{n=0}^{N-1} \omega_N^{n(p-k)}}_{N\delta_N(p-k)}, \tag{3}$$

where $\omega_N = e^{i2\pi/N}$ and $\delta_N(k)$ is known as the modular Kronecker delta defined by

$$\delta_N(k) = \begin{cases} 1 & \text{if } k = 0 \text{ or a multiple of } N, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

.

Next, we will show that $\sum_{n=0}^{N-1} \omega_N^{n(p-k)} = N\delta_N(p-k)$. ω_N^k are complex exponentials that for $k = 0, \ldots, N-1$ are the Nth roots of unity.

$$(\underbrace{\omega_N^k}_{:=z})^N = \left(e^{i2\pi k/N} \right)^N = e^{i2\pi k} = 1 \tag{5}$$

We can rewrite $z^N - 1 = 0$ as

$$z^N - 1 = (z-1)\left(z^{N-1} + z^{N-2} + \ldots + z + 1 \right) = (z-1) \sum_{n=0}^{N-1} z^n = 0. \tag{6}$$

A product is zero, if one of the factors evaluates zero. We have a case distinction.

1. $z = \omega_N^{p-k}$ where $p-k$ is not a multiple of N. Then $z \neq 1$. The product can only evaluate zero if the second term evaluates zero. Hence

$$\sum_{n=0}^{N-1} z^n = \sum_{n=0}^{N-1} \left(\omega_N^{p-k}\right)^n = 0 \tag{7}$$

2. $z = \omega_N^{p-k}$ where $p-k$ is a multiple of N. Then $\omega_N^{p-k} = 1$ and

$$\sum_{n=0}^{N-1} z^n = \sum_{n=0}^{N-1} \left(\omega_N^{p-k}\right)^n = \sum_{n=0}^{N-1} 1 = N. \tag{8}$$

Using this result in equation (3) we obtain

$$\sum_{n=0}^{N-1} f_n \omega_N^{-nk} = N\alpha_k, \tag{9}$$

for $k = 0, \ldots, N-1$. We get that α_ks correspond exactly to the DFT coefficients

$$\alpha_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-nk}. \tag{10}$$

The least squares error is minimised when the coefficients of the trigonometric polynomial correspond to the DFT coefficients.

The FFT algorithm can be used to efficiently compute the α_k.

Exercise 3: Fast Discrete Sine Transform

The butterfly scheme is retrieved as usual:

$$\begin{aligned}
F_k &= \frac{1}{2N} \sum_{n=-N+1}^{N} f_n \omega_{2N}^{-kn} = \frac{1}{2}\left(\frac{1}{N} \sum_{n=-N/2+1}^{N/2} f_{2n}\omega_{2N}^{-2kn} + \frac{1}{N} \sum_{n=-N/2+1}^{N/2} f_{2n-1}\omega_{2N}^{-k(2n-1)}\right) \\
&= \frac{1}{2}\Bigg(\underbrace{\frac{1}{N} \sum_{n=-N/2+1}^{N/2} f_{2n}\omega_N^{-kn}}_{=:G_k} + \underbrace{\frac{1}{N} \sum_{n=-N/2+1}^{N/2} f_{2n-1}\omega_N^{-kn}}_{=:H_k} \omega_{2N}^{k}\Bigg) \\
&= \frac{1}{2}\left(G_k + \omega_{2N}^k H_k\right) \\
F_{k+N} &= \frac{1}{2}\left(G_{k+N} + \omega_{2N}^{k+N} H_{k+N}\right) = \frac{1}{2}\left(G_k - \omega_{2N}^k H_k\right)
\end{aligned}$$

For the datasets $g_n := f_{2n}$ and $h_n := f_{2n-1}$, respectively, we can try to find other symmetries:

$$g_{-n} = f_{2(-n)} = -f_{-2n} = -f_{2n} = -g_n$$

The "odd" data also shows an odd symmetry and therefore lead to another Sine Transform but with half length.

Analog for the data with odd indices:

$$h_{-n} = f_{2(-n)-1} = f_{-2n-1} = -f_{2n+1} = -f_{2(n+1)-1} = -h_{n+1}$$

Again we get an "odd" symmetry. However, this is the transform shown in the lecture, known as Quarter-Wave-DST, again with half length.

For a dataset with the symmetry constraint $f_{-n} = -f_{n+1}$ we get accordingly

$$g_{-n} = f_{2(-n)} = f_{-2n} = -f_{2n+1} = -h_{n+1}$$

and

$$h_{-n} = f_{-2n-1} = f_{-2n+1} = -f_{2n+2} = -f_{2n-1} = -g_{n+1}$$