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Algorithms of Scientific Computing

Exercise 1

According the Hint:

If $X_l = -X_{12-l}$, then $X_6 = -X_{12-6}$ holds. This is possible only if also $X_6 = 0$ holds. Analog we get $X_0 = -X_{12-0} = -X_{12}$. Here the value X_{12} is the declination for the ascension of 360°, which is the same as the declination value for 0° due to the periodicity of the data. Thus, it must also apply that $X_0 = X_{12}$. So we can conclude that $X_0 = 0$ must hold.

With these considerations we can compute the values a_k and b_k, for example with the Python-Worksheet `pallas1.py`.

According the coefficients:

We guess that the interpolation of the axis symmetrical data should only need the axis symmetrical basis functions (i.e. all cos functions), while the interpolation of the point symmetrical data will only depends on the point symmetric basis functions (i.e. all sin functions). Hence, in one case all coefficients $b_k = 0$, while in the other all $a_k = 0$.

To show this we can insert the symmetrical constraints into the equation for the interpolation

$$X_l = a_0 + \sum_{k=1}^{5} \left(a_k \cos\left(\frac{\pi k l}{6}\right) + b_k \sin\left(\frac{\pi k l}{6}\right) \right) + a_6 \cos(\pi l) \,. \tag{1}$$

For X_{12-l} it must hold:

$$\begin{aligned}
X_{12-l} &= a_0 + \sum_{k=1}^{5} \left(a_k \cos\left(\frac{\pi k(12-l)}{6}\right) + b_k \sin\left(\frac{\pi k(12-l)}{6}\right) \right) + a_6 \cos(\pi(12-l)) \\
&= a_0 + \sum_{k=1}^{5} \left(a_k \cos\left(2\pi k - \frac{\pi k l}{6}\right) + b_k \sin\left(2\pi k - \frac{\pi k l}{6}\right) \right) + a_6 \cos(12\pi - l\pi) \\
&= a_0 + \sum_{k=1}^{5} \left(a_k \cos\left(\frac{\pi k l}{6}\right) - b_k \sin\left(\frac{\pi k l}{6}\right) \right) + a_6 \cos(\pi l)
\end{aligned}$$

If $X_l = X_{12-l}$, then holds $X_l - X_{12-l} = 0$, i.e.:

$$
\begin{aligned}
& a_0 + \sum_{k=1}^{5} \left(a_k \cos\left(\frac{\pi k l}{6}\right) + b_k \sin\left(\frac{\pi k l}{6}\right)\right) + a_6 \cos(\pi l) \\
- & \left(a_0 + \sum_{k=1}^{5} \left(a_k \cos\left(\frac{\pi k l}{6}\right) - b_k \sin\left(\frac{\pi k l}{6}\right)\right) + a_6 \cos(\pi l) \right) = 0.
\end{aligned}
$$

Simplified this results in (for all l):

$$
\begin{aligned}
& 2\sum_{k=1}^{5} b_k \sin\left(\frac{\pi k l}{6}\right) = 0 \\
\Rightarrow \quad & b_k = 0 \quad \text{for all } k.
\end{aligned}
$$

Remark: To be precise we would need to show that the solution $b_k = 0$ for all k is the only solution (uniqueness). We will skip this step here and note further that we would generally need to show the uniqueness of the trigonometric interpolation, since otherwise the Exercise would not have been properly stated at all. The uniqueness follows from the fact that the matrix is invertible (See the matrix from the lecture, which is, however, for the complex DFT).

Analog we get, if $X_l = -X_{12-l}$ which means $X_l + X_{12-l} = 0$:

$$
\begin{aligned}
& 2a_0 + 2\sum_{k=1}^{5} a_k \cos\left(\frac{\pi k l}{6}\right) + 2a_6 \cos(\pi l) = 0 \\
\Rightarrow \quad & a_k = 0 \quad \text{for all } k.
\end{aligned}
$$

Exercise 2

In accordance with standard FFT-splitting, we form the sum formula for the c_k in:

$$
\begin{aligned}
c_k &= \frac{1}{12}\sum_{l=0}^{11} X_l e^{-i2\pi k l/12} \\
&= \frac{1}{12}\sum_{l=0}^{5} \left(X_{2l} e^{-i2\pi k(2l)/12} + X_{2l+1} e^{-i2\pi k(2l+1)/12} \right) \\
&= \frac{1}{12}\left(\sum_{l=0}^{5} X_{2l} e^{-i2\pi k l/6} + e^{-i2\pi k/12} \sum_{l=0}^{5} X_{2l+1} e^{-i2\pi k l/6} \right)
\end{aligned}
$$

We use this to compute the c_k for $k = 0, \ldots, 5$. To compute c_6 we reformulate as following:

$$
\begin{aligned}
c_6 = c_{0+6} &= \frac{1}{12}\left(\sum_{l=0}^{5} X_{2l} e^{-i2\pi(0+6)l/6} + e^{-i2\pi(0+6)/12} \sum_{l=0}^{5} X_{2l+1} e^{-i2\pi(0+6)l/6}\right) \\
&= \frac{1}{12}\left(\sum_{l=0}^{5} X_{2l} e^{-i2\pi 0l/6} + e^{-i2\pi 0/12} \cdot e^{-i2\pi 6/12} \sum_{l=0}^{5} X_{2l+1} e^{-i2\pi 0l/6}\right) \\
&= \frac{1}{12}\left(\sum_{l=0}^{5} X_{2l} e^{-i2\pi 0l/6} - \underbrace{e^{-i2\pi 0/12}}_{=1} \sum_{l=0}^{5} X_{2l+1} e^{-i2\pi 0l/6}\right).
\end{aligned}
$$

This is now the butterfly scheme for c_0 and c_6!

Now we define the coefficients for the required length 6 DFTs

$$
\begin{aligned}
\widetilde{c}_k &:= \sum_{l=0}^{5} X_{2l} e^{-i2\pi kl/6} \\
\widehat{c}_k &:= \sum_{l=0}^{5} X_{2l+1} e^{-i2\pi kl/6},
\end{aligned}
$$

for each $k = 0, \ldots, 5$, the coefficients c_k are calculated:

$$
\begin{aligned}
c_k &= \frac{1}{12}\left(\widetilde{c}_k + e^{-i2\pi k/12} \cdot \widehat{c}_k\right) \quad \text{for} \quad k = 0, \ldots, 5 \\
c_6 &= \frac{1}{12}\left(\widetilde{c}_0 - \widehat{c}_0\right).
\end{aligned}
$$

We calculate the Fourier transform of the 12 real data, dividing them into 2 real Fourier transforms of length 6.

Calculation of the length 6-DFTs using length 3 DFTs

In exactly the same was, the coefficients $\widetilde{c}_k$ and $\widehat{c}_k$ are calculated according to the FFT-Butterfly scheme:

$$
\begin{aligned}
\widetilde{c}_k &= \sum_{l=0}^{2} X_{4l} e^{-i2\pi kl/3} + e^{i2\pi k/6} \sum_{l=0}^{2} X_{4l+2} e^{-i2\pi kl/3} \\
\widetilde{c}_{k+3} &= \sum_{l=0}^{2} X_{4l} e^{-i2\pi kl/3} - e^{i2\pi k/6} \sum_{l=0}^{2} X_{4l+2} e^{-i2\pi kl/3}
\end{aligned}
$$

and

$$\begin{aligned}
\widehat{c}_k &= \sum_{l=0}^{2} X_{4l+1} e^{-i2\pi kl/3} + e^{i2\pi k/6} \sum_{l=0}^{2} X_{4l+3} e^{-i2\pi kl/3} \\
\widehat{c}_{k+3} &= \sum_{l=0}^{2} X_{4l+1} e^{-i2\pi kl/3} - e^{i2\pi k/6} \sum_{l=0}^{2} X_{4l+3} e^{-i2\pi kl/3},
\end{aligned}$$

for each $k = 0, 1, 2$.

since all X_l are real, we can use the symmetry and write

$$\widehat{c}_{6-k} = \widehat{c}_k^* \qquad \text{and} \qquad \widetilde{c}_{6-k} = \widetilde{c}_k^*.$$

Since $\widehat{c}$ and $\widetilde{c}$ are each 6-periodic, the following holds: $\widehat{c}_{-k} = \widehat{c}_k^*$ respectively, $\widetilde{c}_{6-k} = \widetilde{c}_k^*$ but the index k for this case is $k = 0, \ldots, 6$.

We define the above required four DFTs of length 3 as

$$\begin{aligned}
\mathcal{F}_k^{(0,4,8)} &:= \sum_{l=0}^{2} X_{4l} e^{-i2\pi kl/3} & \mathcal{F}_k^{(1,5,9)} &:= \sum_{l=0}^{2} X_{4l+1} e^{-i2\pi kl/3} \\
\mathcal{F}_k^{(2,6,10)} &:= \sum_{l=0}^{2} X_{4l+2} e^{-i2\pi kl/3} & \mathcal{F}_k^{(3,7,11)} &:= \sum_{l=0}^{2} X_{4l+3} e^{-i2\pi kl/3}.
\end{aligned}$$

Then the $\widetilde{c}_k$s are computed from the following Butterflies:

$$\begin{aligned}
\widetilde{c}_k &= \mathcal{F}_k^{(0,4,8)} + e^{i\pi k/3} \mathcal{F}_k^{(2,6,10)} \qquad \text{for} \quad k = 0, 1, 2 \\
\widetilde{c}_3 &= \mathcal{F}_0^{(0,4,8)} - \mathcal{F}_0^{(2,6,10)} \\
\widetilde{c}_k &= \widetilde{c}_{N-k}^* \qquad \text{for} \quad k = 4, 5
\end{aligned}$$

and the $\widehat{c}_k$ as well.

$$\begin{aligned}
\widehat{c}_k &= \mathcal{F}_k^{(1,5,9)} + e^{i\pi k/3} \mathcal{F}_k^{(3,7,11)} \qquad \text{for} \quad k = 0, 1, 2 \\
\widehat{c}_3 &= \mathcal{F}_0^{(1,5,9)} - \mathcal{F}_0^{(3,7,11)} \\
\widehat{c}_k &= \widehat{c}_{N-k}^* \qquad \text{for} \quad k = 4, 5
\end{aligned}$$

Computation of the 3-DFTs

We can easily compute the 3-DFTs relatively easy, e.g.:

$$
\begin{aligned}
\mathcal{F}_0^{(0,4,8)} &= \sum_{l=0}^{2} X_{4l} \\
\mathcal{F}_1^{(0,4,8)} &= \sum_{l=0}^{2} X_{4l} e^{-i2\pi l/3} \\
\mathcal{F}_2^{(0,4,8)} &= \left\{ \mathcal{F}_1^{(0,4,8)} \right\}^*
\end{aligned}
$$

Exercise 3: DFT of Mirrored data

We define $g_n := f_{N-n}$ for $n = 1, \ldots, N$ and compute for $k = 1, \ldots, N$ the corresponding Fourier coefficients G_k:

$$
\begin{aligned}
G_k &= \frac{1}{N} \sum_{n=1}^{N} g_n \omega_N^{-kn} = \frac{1}{N} \sum_{n=1}^{N} f_{N-n} \omega_N^{-kn} = \frac{1}{N} \sum_{n=N-1}^{0} f_n \omega_N^{-k(N-n)} \\
&= \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{kn} \omega_N^{-kN} = \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{kn} = \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-(-k)n} \\
&= F_{-k}
\end{aligned}
$$

Thus, the Fourier coefficients are also mirrored With respect to the 1 shifted index.

The coefficients F_{-k} belong to the Ansatzfunctions $e^{i2\pi(-k)x}$, which unlike the original Ansatzfunctions, $e^{i2\pi kx}$, move in the "mirrored" direction. Since the coefficients remain the same, the result is the "mirrored" signal.

Exercise 3: DFT and „Padding“

For the classic Fast Fourier Transform the number of discrete data must be a power of two. If this is not the case, one could try to fill up the dataset by "zero" entries like this:

$$
\hat{f}_n := \begin{cases} f_n & \text{if} \quad n \leq N-1 \\ 0 & \text{if} \quad N \leq n \leq M-1 \end{cases}
$$

The Fourier coefficients $\widehat{F}_k$ of the extended dataset then add up to

$$
\widehat{F}_k = \frac{1}{M} \sum_{n=0}^{M-1} \hat{f}_n \omega_M^{-kn} = \frac{1}{M} \sum_{n=0}^{N-1} f_n \omega_M^{-kn}.
$$

This looks like if the $\widehat{F}_k$ are just the $\frac{N}{M}$ multiple of the original coefficients from the transform of length N:

$$F_k = \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-kn}.$$

However, this is not the case, since

$$\omega_N^{-kn} \neq \omega_M^{-kn}.$$

So, the frequencies of the base functions do change.

If we take the Fourier transform as an interpolation problem, then the extension of the dataset is equal to an increment of the number of supporting points. Since the observed interval stays the same ($[0, 2\pi]$), the distance between the supporting points must decrease. By padding the dataset with "zeros" we actually compressed the signal and therefore the signal must be assembled from higher-frequency oscillations.

We go on with the equation from above. First we show that

$$\omega_M^{-kn} = e^{-i2\pi kn/M} = e^{-i2\pi kn(N/M)/N} = \left(\omega_N^{-kn}\right)^{N/M}$$

holds and therefore

$$\widehat{F}_k = \frac{1}{M} \sum_{n=0}^{N-1} f_n \left(\omega_N^{-kn}\right)^{N/M} = \frac{N}{M} \cdot \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-k(N/M)n}$$

In general we cannot express this by the F_k. But if kN/M is an integer number, we get

$$\widehat{F}_k = \frac{N}{M} \cdot \frac{1}{N} \sum_{n=0}^{N-1} f_n \omega_N^{-k(N/M)n} = \frac{N}{M} F_{kN/M}$$

Explanation: The Fourier components $\widehat{F}_k$ of the compressed signal belong to the wavenumber k. In the original signal the same component would belong to the oscillation with wavenumber kN/M. If kN/M is an integer number, this Fourier component is also computed in the "short" transformation and can be taken from the "long" transformation directly without being changed. If kN/M is not an integer number, then there is no according component in the "short" transformation.