STAT 153 & 248 - Time Series
Lecture Six

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1 Recap from last lecture

In the last lecture, we discussed fitting the sinusoidal model:

$$y_t = \beta_0 + \beta_1 \cos(2\pi f t) + \beta_2 \sin(2\pi f t) + \epsilon_t \qquad \text{with } \epsilon_t \overset{\text{i.i.d}}{\sim} N(0, \sigma^2) \tag{1}$$

to the observed time series $y_1, \dots, y_n$. We looked at both the MLE and Bayesian inference for estimating the unknown parameters $f, \beta_0, \beta_1, \beta_2, \sigma$. The main parameter is f which we reasoned can be taken to lie in the interval $[0, 1/2]$ (this is because the observed times are $1, \dots, n$).

In both the MLE and Bayesian approaches, a key role for inferring f is played by the following criterion function:

$$RSS(f) := \min_{\beta_0, \beta_1, \beta_2} \sum_{t=1}^{n} (y_t - \beta_0 - \beta_1 \cos(2\pi f t) - \beta_2 \sin(2\pi f t))^2 = \|y - X_f \hat{\beta}_f\|^2$$

where

$$y = \begin{pmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_n \end{pmatrix} \quad \text{and} \quad X_f = \begin{pmatrix} 1 & \cos(2\pi f(1)) & \sin(2\pi f(1)) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cos(2\pi f(n)) & \sin(2\pi f(n)) \end{pmatrix} \quad \text{and} \quad \hat{\beta}_f = (X_f^T X_f)^{-1} X_f^T y.$$

$RSS(f)$ is simply the residual sum of squares in the linear regression model obtained by fixing the frequency parameter f. The MLE for f is obtained by minimizing $RSS(f)$ over $f \in [0, 1/2]$ while the Bayesian posterior is given by:

$$I\{0 < f < 1/2\} |X_f^T X_f|^{-1/2} \left(\frac{1}{RSS(f)} \right)^{(n-3)/2}.$$

We discussed how the MLE can be calculated (approximately) and how the Bayesian posterior can be evaluated (approximately) by taking a fine grid of values of f inside the domain $[0, 1/2]$ (for the Bayesian posterior, it is important to not go too close to the boundary values 0 and 0.5 because the term $X_f^T X_f$ will be close to singular for such f).

2 Fourier Frequencies and Computation of $RSS(f)$

$RSS(f)$ describes how well the sinusoid with frequency f fits the observed data $y_1, \dots, y_n$. A plot of $RSS(f)$ over different frequencies f is frequently used as an exploratory data analysis tool for identifying "which periodicities are present in the data". This tool is often used even when one is not interested in eventually fitting the simple model (1) to the observed data.

For computing $RSS(f)$, as discussed in the previous lecture, we need a grid of values for f. The most commonly used grid is given by:

$$\mathcal{F} := \left\{0, \frac{1}{n}, \frac{2}{n}, \dots, \frac{[n/2]}{n}\right\} \tag{2}$$

where $[n/2]$ is the largest integer smaller than or equal to $n/2$.

A frequency of the form j/n where $j \in \{0, 1, 2, \dots, n-1\}$ and n is the observed data size is called a **Fourier Frequency**. So the grid (2) consists of all Fourier frequencies that are in the range $[0, 1/2]$.

The main reason for taking the grid to consist of Fourier Frequencies is that $RSS(f), f \in \mathcal{F}$ can be computed very efficiently (in time $O(n \log n)$) using a classical algorithm known as the Fast Fourier Transform (FFT). We explain the high level details behind this fact today (without going into the workings of the FFT algorithm).

3 Formula for $RSS(f)$ when f is a Fourier Frequency

When f is a Fourier Frequency, one can write down a more explicit formula for $RSS(f)$. For this, first note that for every f,

$$\begin{aligned} RSS(f) &= \|y - X_f\hat{\beta}_f\|^2 \\ &= (y - X_f\hat{\beta}_f)^T(y - X_f\hat{\beta}_f) = y^Ty - \hat{\beta}_f^T X_f^T y - y^T X_f \hat{\beta}_f + \hat{\beta}_f^T X_f^T X_f \hat{\beta}_f. \end{aligned}$$

Plugging in $\hat{\beta}_f = (X_f^T X_f)^{-1} X_f^T y$ above, we get

$$\begin{aligned} RSS(f) &= y^Ty - y^TX_f(X_f^TX_f)^{-1}X_f^Ty - y^TX_f(X_f^TX_f)^{-1}X_f^Ty \\ &\quad + y^TX_f(X_f^TX_f)^{-1}X_f^TX_f(X_f^TX_f)^{-1}X_f^Ty \\ &= y^Ty - y^TX_f(X_f^TX_f)^{-1}X_f^Ty - y^TX_f(X_f^TX_f)^{-1}X_f^Ty \\ &\quad + y^TX_f(X_f^TX_f)^{-1}X_f^Ty \\ &= y^Ty - y^TX_f(X_f^TX_f)^{-1}X_f^Ty \end{aligned}$$

Now

$$X_f^T X_f = \begin{pmatrix} n & \sum_{t=1}^n \cos(2\pi ft) & \sum_{t=1}^n \sin(2\pi ft) \\ \sum_{t=1}^n \cos(2\pi ft) & \sum_{t=1}^n \cos^2(2\pi ft) & \sum_{t=1}^n \cos(2\pi ft)\sin(2\pi ft) \\ \sum_{t=1}^n \sin(2\pi ft) & \sum_{t=1}^n \cos(2\pi ft)\sin(2\pi ft) & \sum_{t=1}^n \sin^2(2\pi ft). \end{pmatrix}$$

Now suppose that $f \in (0, 0.5)$ and suppose that f is a Fourier frequency i.e., it is of the form $f = j/n$ for some integer j. Then it turns out that

$$\begin{aligned}
&\sum_{t=1}^{n} \cos(2\pi f t) = 0 \qquad \sum_{t=1}^{n} \sin(2\pi f t) = 0 \\
&\sum_{t=1}^{n} \cos^2(2\pi f t) = \frac{n}{2} \qquad \sum_{t=1}^{n} \sin^2(2\pi f t) = \frac{n}{2} \\
&\sum_{t=1}^{n} \cos(2\pi f t) \sin(2\pi f t) = 0
\end{aligned} \tag{3}$$

As a result, for such f,

$$X_f^T X_f = \begin{pmatrix} n & 0 & 0 \\ 0 & n/2 & 0 \\ 0 & 0 & n/2 \end{pmatrix} \quad \text{so that} \quad (X_f^T X_f)^{-1} = \begin{pmatrix} 1/n & 0 & 0 \\ 0 & 2/n & 0 \\ 0 & 0 & 2/n \end{pmatrix}$$

This gives

$$\begin{aligned}
&y^T X_f (X_f^T X_f)^{-1} X_f^T y \\
&= y^T \begin{pmatrix} 1 & \cos(2\pi f(1)) & \sin(2\pi f(1)) \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & \cos(2\pi f(n)) & \sin(2\pi f(n)) \end{pmatrix} \begin{pmatrix} 1/n & 0 & 0 \\ 0 & 2/n & 0 \\ 0 & 0 & 2/n \end{pmatrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot & 1 \\ \cos(2\pi f(1)) & \cdot & \cdot & \cdot & \cos(2\pi f(n)) \\ \sin(2\pi f(1)) & \cdot & \cdot & \cdot & \sin(2\pi f(n)) \end{pmatrix} y \\
&= \begin{pmatrix} \sum_t y_t & \sum_t y_t \cos(2\pi f t) & \sum_t y_t \sin(2\pi f t) \end{pmatrix} \begin{pmatrix} 1/n & 0 & 0 \\ 0 & 2/n & 0 \\ 0 & 0 & 2/n \end{pmatrix} \begin{pmatrix} \sum_t y_t \\ \sum_t y_t \cos(2\pi f t) \\ \sum_t y_t \sin(2\pi f t) \end{pmatrix} \\
&= \frac{1}{n} \left(\sum_t y_t \right)^2 + \frac{2}{n} \left(\sum_t y_t \cos(2\pi f t) \right)^2 + \frac{2}{n} \left(\sum_t y_t \sin(2\pi f t) \right)^2 \\
&= n\bar{y}^2 + \frac{2}{n} \left(\sum_t y_t \cos(2\pi f t) \right)^2 + \frac{2}{n} \left(\sum_t y_t \sin(2\pi f t) \right)^2 .
\end{aligned}$$

Therefore for Fourier frequencies in the range $(0, 0.5)$, we get

$$RSS(f) = y^T y - n\bar{y}^2 - \frac{2}{n} \left(\sum_t y_t \cos(2\pi f t) \right)^2 - \frac{2}{n} \left(\sum_t y_t \sin(2\pi f t) \right)^2$$

or equivalently

$$RSS(f) = \sum_t (y_t - \bar{y})^2 - \frac{2}{n} \left(\sum_t y_t \cos(2\pi f t) \right)^2 - \frac{2}{n} \left(\sum_t y_t \sin(2\pi f t) \right)^2 \tag{4}$$

When $f = 0$ and $f = 1/2$, the above formula needs to be slightly modified. When $f = 0$, the sinusoidal model (1) simply becomes:

$$y_t = \beta_0 + \beta_1 + \epsilon_t \qquad \text{with } \epsilon_t \overset{\text{i.i.d}}{\sim} N(0, \sigma^2).$$

There is only one effective parameter coefficient parameter $(\beta_0 + \beta_1)$ here which will be estimated by $\bar{y}$ so that RSS becomes

$$RSS(0) = \sum_t (y_t - \bar{y})^2. \tag{5}$$

When $f = 1/2$ and n is even (when n is odd, $1/2$ cannot be a Fourier frequency so it will not be considered), the model (1) becomes

$$y_t = \beta_0 + \beta_1 \cos(\pi t) + \epsilon_t = \beta_0 + \beta_1 (-1)^t + \epsilon_t.$$

For this model, it is easy to check that

$$X^T X = \begin{pmatrix} n & 0 \\ 0 & n \end{pmatrix}$$

so that

$$RSS(1/2) = \sum_t (y_t - \bar{y})^2 - \frac{1}{n} \left(\sum_t y_t (-1)^t \right)^2 \tag{6}$$

Let us not worry too much about the edge cases $f = 0$ and $f = 1/2$, and focus on the formula (4). Note again that this formula holds whenever $f \in (0, 0.5)$ and f is a Fourier frequency (i.e., nf is an integer).

4 Proof of the identities in (3)

Note that $0 < f < 1/2$ and that nf is an integer.

$$\begin{aligned}
&\sum_{t=1}^{n} \cos(2\pi f t) \\
&= \frac{1}{2} \sum_{t=1}^{n} e^{2\pi i f t} + \frac{1}{2} \sum_{t=1}^{n} e^{-2\pi i f t} \\
&= \frac{1}{2} \frac{e^{2\pi i f}}{e^{2\pi i f} - 1} \left(e^{2\pi i n f} - 1 \right) + \frac{1}{2} \frac{e^{-2\pi i f}}{e^{-2\pi i f} - 1} \left(e^{-2\pi i n f} - 1 \right) \\
&= \frac{1}{2} \frac{e^{2\pi i f}}{e^{2\pi i f} - 1} \left(\cos(2\pi n f) - 1 + i \sin(2\pi n f) \right) + \frac{1}{2} \frac{e^{-2\pi i f}}{e^{-2\pi i f} - 1} \left(\cos(2\pi n f) - 1 - i \sin(2\pi n f) \right) \\
&= 0
\end{aligned}$$

because $\cos(2\pi n f) = \cos(2\pi(\text{integer})) = 1$ and $\sin(2\pi n f) = \sin(2\pi(\text{integer})) = 0$.

Similarly

$$\begin{aligned}
&\sum_{t=1}^{n} \sin(2\pi f t) \\
&= \frac{1}{2i} \sum_{t=1}^{n} e^{2\pi i f t} - \frac{1}{2i} \sum_{t=1}^{n} e^{-2\pi i f t} \\
&= \frac{1}{2i} \frac{e^{2\pi i f}}{e^{2\pi i f} - 1} \left(e^{2\pi i n f} - 1 \right) - \frac{1}{2i} \frac{e^{-2\pi i f}}{e^{-2\pi i f} - 1} \left(e^{-2\pi i n f} - 1 \right) \\
&= \frac{1}{2i} \frac{e^{2\pi i f}}{e^{2\pi i f} - 1} \left(\cos(2\pi n f) - 1 + i \sin(2\pi n f) \right) - \frac{1}{2i} \frac{e^{-2\pi i f}}{e^{-2\pi i f} - 1} \left(\cos(2\pi n f) - 1 - i \sin(2\pi n f) \right) \\
&= 0
\end{aligned}$$

Next note

$$\sum_{t=1}^{n} \cos^2(2\pi f t) = \sum_{t=1}^{n} \frac{1 + \cos(4\pi f t)}{2} = \frac{n}{2} + \frac{1}{2} \sum_{t=1}^{n} \cos(4\pi f t)$$

and

$$\sum_{t=1}^{n} \sin^2(2\pi ft) = \sum_{t=1}^{n} \frac{1-\cos(4\pi ft)}{2} = \frac{n}{2} - \frac{1}{2}\sum_{t=1}^{n} \cos(4\pi ft).$$

The quantity $\sum_t \cos(4\pi ft)$ which appears in both the above terms turns out to be zero because

$$\begin{aligned}
&\sum_{t=1}^{n} \cos(4\pi ft) \\
&= \frac{1}{2}\sum_{t=1}^{n} e^{4\pi ift} + \frac{1}{2}\sum_{t=1}^{n} e^{-4\pi ift} \\
&= \frac{1}{2}\frac{e^{4\pi if}}{e^{4\pi if}-1}\left(e^{r\pi inf}-1\right) + \frac{1}{2}\frac{e^{-4\pi if}}{e^{-4\pi if}-1}\left(e^{-4\pi inf}-1\right) \\
&= \frac{1}{2}\frac{e^{4\pi if}}{e^{4\pi if}-1}\left(\cos(4\pi nf)-1+i\sin(4\pi nf)\right) + \frac{1}{2}\frac{e^{-4\pi if}}{e^{-4\pi if}-1}\left(\cos(4\pi nf)-1-i\sin(4\pi nf)\right) \\
&= 0
\end{aligned}$$

because $\cos(4\pi nf) = \cos(4\pi(\text{integer})) = 1$ and $\sin(4\pi nf) = \sin(4\pi(\text{integer})) = 0$.

Finally

$$\begin{aligned}
&\sum_{t=1}^{n} \cos(2\pi ft)\sin(2\pi ft) \\
&= \sum_{t=1}^{n} \sin(4\pi ft) \\
&= \frac{1}{2i}\sum_{t=1}^{n} e^{4\pi ift} - \frac{1}{2i}\sum_{t=1}^{n} e^{-4\pi ift} \\
&= \frac{1}{2i}\frac{e^{4\pi if}}{e^{4\pi if}-1}\left(e^{r\pi inf}-1\right) - \frac{1}{2i}\frac{e^{-4\pi if}}{e^{-4\pi if}-1}\left(e^{-4\pi inf}-1\right) \\
&= \frac{1}{2i}\frac{e^{4\pi if}}{e^{4\pi if}-1}\left(\cos(4\pi nf)-1+i\sin(4\pi nf)\right) - \frac{1}{2i}\frac{e^{-4\pi if}}{e^{-4\pi if}-1}\left(\cos(4\pi nf)-1-i\sin(4\pi nf)\right) \\
&= 0
\end{aligned}$$

The intermediate calculations above include the terms $e^{2\pi if}-1$ and $e^{4\pi if}-1$ in the denominators. We need to make sure that these terms are not zero (otherwise the above proofs would not be valid).

$$e^{2\pi if} - 1 = \cos(2\pi f) - 1 + i\sin(2\pi f)$$

which cannot be zero because $\cos(2\pi f) < 1$ for $f \in (0, 0.5)$, and

$$e^{4\pi if} - 1 = \cos(4\pi f) - 1 + i\sin(4\pi f)$$

which also cannot be zero because $\cos(4\pi f) < 1$ for $f \in (0, 0.5)$.

5 The Periodogram

Given a time series dataset $y_1, \dots, y_n$, its periodogram is the function $I(f), 0 < f < 1/2$, defined as follows:

$$I(f) := \frac{1}{n}\left(\sum_{t=1}^{n} y_t \cos(2\pi ft)\right)^2 + \frac{1}{n}\left(\sum_{t=1}^{n} y_t \sin(2\pi ft)\right)^2 \qquad \text{for } f \in (0, 0.5)$$

From the formula (4), we have

$$RSS(f) = \sum_t (y_t - \bar{y})^2 - 2I(f) \qquad \text{when } f \in (0, 0.5) \text{ is a Fourier Frequency.}$$

The periodogram $I(f)$ can be written in the following alternative way:

$$I(f) = \frac{1}{n} \left| \sum_{t=1}^{n} y_t e^{-2\pi i f t} \right|^2$$

where $|\cdot|$ denotes complex modulus. As we shall discuss in detail next lecture,

$$\sum_{t=1}^{n} y_t \exp(-2\pi i f t)$$

(when f is a Fourier frequency) is closely related to the Discrete Fourier Transform (DFT) of $y_1, \ldots, y_n$. The DFT can be efficiently computed using the Fast Fourier Transform (FFT) algorithm. This gives a way of computing $I(f)$ and $RSS(f)$ at Fourier frequencies efficiently.