Deterministic Fourier Features

Suppose we have time-series data, with a PSD stationary kernel k. Consider the following process:

(i) Evaluate the kernel from lags $-T$ to T, and construct vector

$$\xi \coloneqq (k(0), k(T), \ldots, k(1), k(1), \ldots, k(T))$$

For convenience, we define $\omega \coloneqq \frac{2\pi}{N}$ with $N \coloneqq 2T+1$.

(ii) Take the DFT of ξ:

$$S_j \coloneqq \sum_{t=0}^{N-1} \xi_t \exp(-i\omega j t)$$

for $j = 0, \ldots, N-1$. Since the true spectral density of k is nonnegative (and the DFT is an approximation), take T large enough so that all $S_j \geq 0$. If not possible, clip small negative values to zero.

(iii) Let $\mathcal{I}$ be the set of all indices $j \in \{0, \ldots, N-1\}$ such that S_j is among the $2r$ largest values (excluding S_0). This forms the sequence

$$\tilde{S}_j = \begin{cases} S_0, & j = 0 \\ S_j, & j \in \mathcal{I} \\ 0, & \text{o.w.} \end{cases}$$

Note that by symmetry, $S_j = S_{N-j}$, for $1 \leq j \leq N-1$, so that we always take pairs, ensuring the same symmetry in $\tilde{S}$.

(iv) Take the inverse DFT of $\tilde{S}$:

$$\begin{aligned} \tilde{\xi}_t &\coloneqq \frac{1}{N} \sum_{j=0}^{N-1} \tilde{S}_j \exp(i\omega j t) \\ &= \frac{1}{N}\left[S_0 + 2\sum_{j\in\mathcal{I}} S_j \cos(\omega j t)\right] \end{aligned}$$

for $t = 0, \ldots, N-1$. Some remarks:

- The sequence is of the form (Lemma 1)

$$\tilde{\xi} = \left(\tilde{k}(0), \tilde{k}(T), \ldots, \tilde{k}(1), \tilde{k}(1), \ldots, \tilde{k}(T)\right)$$

- The equality using cosines follows from Lemma 2.

(v) Define the low-rank kernel (as shown in $\tilde{\xi}$ above)

$$\tilde{k}(t) = \begin{cases} \tilde{\xi}_0, & t = 0 \\ \tilde{\xi}_{T+t}, & t \in \{1, \ldots, T\} \\ \tilde{k}(-t), & t \in \{-T, \ldots, -1\} \end{cases}$$

Note that this kernel satisfies (Lemma 3)

$$\tilde{k}\left(t-t'\right)=\left\langle \phi\left(t\right),\phi\left(t'\right)\right\rangle \tag{1}$$

for $t-t'\in\{-T,\ldots,T\}$, where

$$\phi\left(t\right)\coloneqq\frac{1}{\sqrt{N}}\begin{bmatrix}\sqrt{S_{0}}\\ \begin{bmatrix}\sqrt{2S_{j}}\cos\left(\omega jt\right)\\ \sqrt{2S_{j}}\sin\left(\omega jt\right)\end{bmatrix}_{j\in\mathcal{I}}\end{bmatrix}\in\mathbb{R}^{2r+1}$$

Note that we need $S\geq0$ to take the square roots.

We can then do GP inference on this approximated kernel, which reduces the computation to $O\left(r^{3}\right)$. Note that if we can compute the DTFT, we can directly pick the top r modes from it, instead of using the DFT.

1 Auxiliary results

Lemma 1

We have that $\tilde{\xi}_{t}=\tilde{\xi}_{N-t}$ for $t=1,\ldots,T-1$.

Proof. Ignoring the normalization,

$$\begin{aligned}\tilde{\xi}_{N-t} & \propto\sum_{j=0}^{N-1}\tilde{S}_{j}\exp\left(i\omega j\left(N-t\right)\right)\\
 & =\sum_{j=0}^{N-1}\tilde{S}_{j}\exp\left(-i\omega jt\right)\\
 & =\tilde{S}_{0}+\sum_{j=1}^{N-1}\tilde{S}_{N-j}\exp\left(i\omega\left(N-j\right)t\right)\\
 & =\sum_{j=0}^{N-1}\tilde{S}_{j}\exp\left(i\omega jt\right)\\
 & \propto\tilde{\xi}_{t}
\end{aligned}$$

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Lemma 2

We have that

$$\tilde{\xi}_{t}=\frac{1}{N}\left[S_{0}+2\sum_{j\in\mathcal{I}}S_{j}\cos\left(\omega jt\right)\right]$$

for $t=0,\ldots,N-1$.

Proof. Let us begin by noting that

$$\begin{aligned}
\sum_{j=T+1}^{N-1} \tilde{S}_j \exp\left(i\omega jt\right) &= \sum_{j=T+1}^{N-1} \tilde{S}_{N-j} \exp\left(-i\omega\left(N-j\right)t\right) \\
&= \sum_{j=1}^{T} \tilde{S}_j \exp\left(-i\omega jt\right)
\end{aligned}$$

Hence,

$$\begin{aligned}
\tilde{\xi}_t &= \frac{1}{N} \sum_{j=0}^{N-1} \tilde{S}_j \exp\left(i\omega jt\right) \\
&= \frac{1}{N} \left[\tilde{S}_0 + 2\sum_{j=1}^{T} \tilde{S}_j \cos\left(\omega jt\right)\right]
\end{aligned}$$

and the claim follows from the definitions of $\tilde{S}$ and $\mathcal{I}$. ∎

Lemma 3: Proof of Eq. (1)

For $0 \leq t - t' \leq N - 1$, recall that

$$\begin{aligned}
\tilde{\xi}_{t-t'} &= \frac{1}{N} \left[S_0 + 2\sum_{j\in\mathcal{I}} S_j \cos\left(\omega j\left(t-t'\right)\right)\right] \\
&= \frac{1}{N} \left[S_0 + 2\sum_{j\in\mathcal{I}} S_j \left[\cos\left(\omega jt\right)\cos\left(\omega jt'\right) + \sin\left(\omega jt\right)\sin\left(\omega jt'\right)\right]\right] \\
&= \left\langle \phi\left(t\right), \phi\left(t'\right)\right\rangle
\end{aligned}$$