Working Paper: Estimate density function through Fast Fourier Transformation

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Abstract. This is the specification for estimating a function and its derivatives/antiderivatives of any order through fast Fourier transformation(FFT).

1. cos expansion of even functions

For an even continuous periodic function h on $[-\pi, \pi]$, we have by the standard Fourier analysis

$$h(x) = \sum_{j \geq 0} A'_j \cos(jx)$$

where

$$A_j = \frac{2}{\pi} \int_0^{\pi} h(x) \cos(jx) dx. \tag{1}$$

and

$$A'_0 = A_0/2, \qquad A'_j = A_j, \quad j \geq 1. \tag{2}$$

REMARK 1. *We shall use similar notation* $\{c_j\}'_{j \geq 0}$ *for any sequence* $\{c_j\}_{j \geq 0}$, *i.e.*

$$c'_0 = c_0/2, \qquad c'_j = c_j, \quad j \geq 1. \tag{3}$$

Assume a function $f(x)$ is defined over the interval $[L, R]$. Extend it to an even periodic function over the real number space $\mathbb{R}$, and denote the extended function also by f. Transform the interval $[L, R]$ to $[0, \pi]$ by

$$y = \frac{\pi(x - L)}{l}, \quad x \in [L, R] \tag{4}$$

where $l = R - L$. We have

$$f(x) = \frac{A_0}{2} + \sum_{j=1}^{\infty} A_j \cos \frac{j\pi(x - L)}{l} = \sum_{j=0}^{\infty} A'_j \cos \frac{j\pi(x - L)}{l}, \quad x \in [L, R] \tag{5}$$

where

$$A_j = \frac{2}{l} \int_L^R f(x) \cos \frac{j\pi(x - L)}{l} dx. \tag{6}$$

Using first N terms in above series to Approximate f,

$$\tilde{f}_N(x) = \sum_{j=0}^{N-1} (-1)^j A'_j \cos(\pi j \frac{x-(2L-R)}{l}). \tag{7}$$

Let $F(x,0) = \tilde{f}_N(x)$ and

$$\begin{aligned} F(x,k) &:= F(x,k+1)', \quad k = -1,-2,-3,\dots \\ F(x,k) &:= \int_L^x F(u,k-1)du, \quad k = 1,2,3\dots, \end{aligned}$$

denote the derivatives and anti derivatives of order k of $\tilde{f}_N$ respectively. The explicit expression (7) of $\tilde{f}_N$ make it possible for us to compute effectively $F(x,k)$ at the points $\{x_k\}_{k=0}^N$:

$$x_k = (2L-R) + k \times \lambda, \quad \lambda = \frac{2(R-L)}{N}, 0 \le k \le N \tag{8}$$

Note that

$$x_0 = 2L - R, \quad x_{N/2} = L, \quad x_N = R.$$

By (7),

$$F(x_k, 0) = \sum_{j=0}^{N-1} A'_j (-1)^j \cos(2kj\pi/N) = \Re \sum_{j=0}^{N-1} A'_j (-1)^j \omega_N^{kj} \tag{9}$$

where $\omega_N = e^{2\pi i/N}$. For any complex number z, $\Re(z)$ and $\Im(z)$ denote the real part and imaginary part of z respectively. of the complex number z. The equation (9) can be obtained by inverse FFT ($ifft$):

$$\{F(x_k,0)\}_{0\le k\le N-1} = N \times \Re\left\{ifft(\{(-1)^j A'_j\}_{0\le j\le N-1})\right\}. \tag{10}$$

One can apply (7) to derive s-th order derivatives ($s = -1, -2, \cdots$)

$$\begin{aligned} F(x, -(2h-1)) &= (-1)^h \sum_{j=0}^{N-1} (-1)^j (j\pi/l)^{2h-1} A'_j \sin(\pi j \frac{x-(2L-R)}{l}) \\ F(x,-2h) &= (-1)^h \sum_{j=0}^{N-1} (-1)^j (j\pi/l)^{2h} A'_j \cos(\pi j \frac{x-(2L-R)}{l}). \end{aligned}$$

and apply inverse FFT to estimate the values at $\{x_k\}_{0\le k\le N-1}$

$$\{F(x_k, -(2h-1))\} = (-1)^h N \times \Im(ifft\{(-1)^j (j\pi/l)^{2h-1} A'_j\}) \tag{11}$$
$$\{F(x_k, -(2h))\} = (-1)^h N \times \Re(ifft\{(-1)^j (j\pi/l)^{2h} A'_j\}) \tag{12}$$

For anti derivatives $F(x,s)$ $(s = 1,2,\ldots)$, one can use induction to show for $h \geq 1$

$$\begin{aligned} F(x,2h-1) &= (-1)^{h-1}\sum_{j=0}^{N-1}(-1)^j\frac{\hat{A}_j l^{2h-1}}{(j\pi)^{2h-1}}\sin(j\pi\frac{x-(2L-R)}{l}) \\ &+ \sum_{m=1}^{h-1}\frac{(-1)^{h-m-1}}{(2m-1)!}(x-L)^{2m-1}\sum_{j=0}^{N-1}\frac{\hat{A}_j l^{2(h-m+1)}}{(\pi j)^{2(h-m+1)}} \\ &+ \frac{A'_0(x-L)^{2h-1}}{(2h-1)!} \qquad (13) \end{aligned}$$

and

$$\begin{aligned} F(x,2h) &= (-1)^{h}\sum_{j=0}^{N-1}(-1)^j\frac{\hat{A}_j l^{2h}}{(j\pi)^{2h}}\cos(j\pi\frac{x-(2L-R)}{l}) \\ &+ \sum_{m=1}^{h}\frac{(-1)^{h-m}}{(2m-2)!}(x-L)^{2m-2}\sum_{j=0}^{N-1}\frac{\hat{A}_j l^{2(h-m+1)}}{(\pi j)^{2(h-m+1)}} \\ &+ \frac{A'_0(x-L)^{2h}}{(2h)!} \qquad (14) \end{aligned}$$

where

$$\hat{A}_0 = 0, \quad \hat{A}_j = A'_j = A_j, \quad j \geq 1$$

For $h \geq 1$,

$$\begin{aligned} \{Z(h,k)\}_{0\leq k\leq N-1} &= \sum_{j=0}^{N-1}(-1)^j\frac{\hat{A}_j l^{2h-1}}{(j\pi)^{2h-1}}\sin(j\pi\frac{x_k-(2L-R)}{l}) \\ &= N\times\Im(ifft\{(-1)^j\frac{\hat{A}_j l^{2h-1}}{(j\pi)^{2h-1}}\}) \end{aligned}$$

and

$$\begin{aligned} \{Y(h,k)\}_{0\leq k\leq N-1} &= \sum_{j=0}^{N-1}(-1)^j\frac{\hat{A}_j l^{2h}}{(j\pi)^{2h}}\cos(j\pi\frac{x_k-(2L-R)}{l}) \\ &= N\times\Re(ifft\{(-1)^j\frac{\hat{A}_j l^{2h}}{(j\pi)^{2h}}\}) \end{aligned}$$

Notice that

$$Y(h,\frac{N}{2}) = \sum_{j=0}^{N-1}\frac{\hat{A}_j l^{2h}}{(j\pi)^{2h}}$$

One can rewrite (13) as

$$\begin{aligned}\{F(x_k, 2h-1)\}_k &= (-1)^{h-1}\{Z(j,k)\}_k + \{\frac{A_0'(x_k-L)^{2h-1}}{(2h-1)!}\}_k \\ &+ \{\sum_{m=1}^{h-1} \frac{(-1)^{h-m-1}Y(\frac{N}{2}, h-m+1)}{(2m-1)!}(x_k-L)^{2m-1}\}_k\end{aligned} \tag{15}$$

and rewrite (14) as

$$\begin{aligned}\{F(x_k, 2h)\}_k &= (-1)^{h}\{Y(j,k)\}_k + \{\frac{A_0'(x_k-L)^{2h}}{(2h)!}\}_k \\ &+ \{\sum_{m=1}^{h} \frac{(-1)^{h-m}Y(\frac{N}{2}, h-m+1)}{(2m-2)!}(x_k-L)^{2m-2}\}_k\end{aligned} \tag{16}$$

Since we assume that $f_X = 0$ outside $[L, R]$, one should only take the second parts of F:

$$F(i,h) = F(N/2 : (N-1), h), \quad h = 0, 1, \ldots \frac{N}{2} - 1$$

2. Estimate certain relevant integrations

2.1. Exp

FFT method can also be used to compute the following integration, which is required for our purpose.

$$E(x,t) = \int_L^x e^{tu}\tilde{f}_N(u)du, \quad t \geq 0, \quad x < R \tag{17}$$

In fact,

$$\begin{aligned}E(x,t) &= e^{tx}\sum_{j=0}^{N-1} \frac{\frac{1}{t}\cos(j\pi(x-L)/l) + \frac{j\pi}{lt^2}\sin(j\pi(x-L)/l)}{1+(\frac{j\pi}{tl})^2}A_j' \\ &- \sum_{j=0}^{N-1} \frac{e^{tL}/t}{1+(\frac{j\pi}{tl})^2}A_j' \\ &= e^{tx}\sum_{j=0}^{N-1} \frac{\frac{1}{t}(-1)^j\cos(j\pi(x-(2L-R))/l)}{1+(\frac{j\pi}{tl})^2}A_j' \\ &+ e^{tx}\sum_{j=0}^{N-1} \frac{\frac{j\pi}{lt^2}(-1)^j\sin(j\pi(x-(2L-R))/l)}{1+(\frac{j\pi}{tl})^2}A_j'\end{aligned} \tag{18}$$

$$- \sum_{j=0}^{N-1} \frac{e^{tL}/t}{1+(\frac{j\pi}{tl})^2} A'_j \tag{19}$$

We can use FFT inverse transformation to obtain $\{E(x_k,t)\}_{k=0}^{N-1}$.

2.2. POWER FUNCTION

using integration by parts, we can calculate the following integration for any nonnegative integer j

$$P(a,b,c,j) = \int_a^b (x-c)^j \tilde{f}_X(x)dx, \quad [a,b] \subseteq [L,R]$$

In fact,

$$P(a,b,c,j) = \sum_{k=0}^{j} \frac{(-1)^k j!}{(j-k)!} \{F(b,k)(b-y)^{j-k} - F(a,k)(a-y)^{j-k}\} \tag{20}$$

3. normalized density

We assume that density function $f(x)$ is effectively defined on the symmetric range $[L,R]$ with $L=-R$. Using the Fourier expansion (5),

$$f(x) \approx \frac{A_0}{2} + \sum_{j=1}^{\infty} A_j \cos\frac{j\pi(x+R)}{l}, \quad x \in [L,R] \tag{21}$$

where A_j is defined by 6.

Let $h(x)$ is the normralized function over the range $[-R,R]$ and is approximated by the Fourier expansion

$$h(x) = \sum_{0\le j<M} c_j cos\frac{j\pi x}{R}. \tag{22}$$

Rewrite $h(x)$ to align with the Fourier expansion (21) of $f(x)$,

$$\begin{aligned} h(x) &= \sum_{0\le j<M} c_j(-1)^j \cos\frac{j\pi}{R}(x+R) \\ &= \sum_{0\le k<2M} h_k \cos\frac{k\pi}{2R}(x+R) \end{aligned} \tag{23}$$

where

$$h_k = \begin{cases} (-1)^j c_j & k = 2j \\ 0 & otherwise \end{cases} \tag{24}$$

Let $g(x) = f(x)h(x)$, we need to find the cos expansion of $g(x)$ over the range $[-R, R]$.

$$g(x) = \sum_{j=0}^{\infty} B_j \cos \frac{j\pi(x+R)}{2R}, \quad x \in [L, R] \tag{25}$$

where

$$B_0 = \frac{1}{l} \int_L^R f(x)h(x)dx \tag{26}$$

and

$$B_j = \frac{2}{l} \int_L^R f(x)h(x) \cos \frac{j\pi(x+R)}{2R} dx, \qquad j \geq 1 \tag{27}$$

By (23) and (26)

$$B_0 = h_0 A_0 + \frac{1}{2} \sum_{1 \leq k < 2M} A_k h_k \tag{28}$$

and by (23) and (27), for $j > 0$,

$$\begin{aligned} B_j &= \frac{2}{l} \int_L^R f(x) \cos \frac{j\pi}{2R}(x+R) \sum_{0 \leq k < 2M} h_k \cos \frac{k\pi}{2R}(x+R)dx, \\ &= \sum_{0 \leq k < 2M} \frac{h_k}{l} \int_L^R f(x) \cos \frac{(j+k)\pi}{2R}(x+R)dx, \\ &+ \sum_{0 \leq k < 2M} \frac{h_k}{l} \int_L^R f(x) \cos \frac{(j-k)\pi}{2R}(x+R)dx, \\ &= I_j + II_j \end{aligned} \tag{29}$$

where

$$I_j = \sum_{0 \leq k < 2M} \frac{h_k}{l} \int_L^R f(x) \cos \frac{(j+k)\pi}{2R}(x+R)dx = \frac{1}{2} \sum_{0 \leq k < 2M} h_j A_{j+k}. \tag{30}$$

For $0 \leq j < 2M$,

$$II_j = \sum_{0 \leq k < 2M} \frac{h_k}{l} \int_L^R f(x) \cos \frac{(j-k)\pi}{2R}(x+R)dx,$$

$$
\begin{aligned}
&= \sum_{0\le k<2M, k\neq j} \frac{h_k}{l}\int_L^R f(x)\cos\frac{(j-k)\pi}{2R}(x+R)dx + \frac{h_j}{l}\int_L^R f(x)dx \\
&= \frac{1}{2}\sum_{0\le k<2M} h_k A_{j-k} + \frac{1}{2}h_j A_0 \qquad (31)
\end{aligned}
$$

where $A_{-k} = A_k$ for any positive integer k. For $j \geq 2M$,

$$
II_j = \frac{1}{2}\sum_{0\le k<2M} h_k A_{j-k} \qquad (32)
$$

If we like to approximate $g(x)$ using N terms, then we need $\{A_j\}_{0\le j<2M+N}$, and we have

$$
g(x) \approx \sum_{j=0}^{N-1} B_j \cos\frac{j\pi(x+R)}{2R}, \quad x \in [L, R] \qquad (33)
$$

where

$$
\begin{aligned}
B_0 &= h_0 A_0 + \frac{1}{2}\sum_{1\le k<2M} A_k h_k \\
B_j &= \frac{1}{2}h_j A_0 + \frac{1}{2}\sum_{0\le k<2M} h_j A_{j+k} + \frac{1}{2}\sum_{0\le k<2M} h_k A_{j-k}, \quad 0 < j < 2M \\
B_j &= \frac{1}{2}\sum_{0\le k<2M} h_j A_{j+k} + \frac{1}{2}\sum_{0\le k<2M} h_k A_{j-k} \quad j \geq 2M \qquad (34)
\end{aligned}
$$