Estimate density function through fast Fourier transformation

Xiaorong Zou (xiaorzou@gmail.com)

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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

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

where

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

and

$$A'_0 = A_0/2, \qquad A'_j = A_j, \quad j \ge 1.$$
 (2)

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

$$c'_0 = c_0/2, c'_j = c_j, j \ge 1.$$
 (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

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

where l = R - L. We have

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

where

$$A_j = \frac{2}{l} \int_L^R f(x) \cos \frac{j\pi(x-L)}{l} dx.$$
 (5)

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Using first N terms in above series to Approximate f,

$$\tilde{f}_N(x) = \sum_{j=0}^{N-1} (-1)^j A_j' \cos(\pi j \frac{x - (2L - R)}{l}).$$
 (6)

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

$$F(x,k) := F(x,k+1)', \quad k = -1, -2, -3, \dots$$
$$F(x,k) := \int_{L}^{x} F(u,k-1)du, \quad k = 1, 2, 3 \dots,$$

denote the derivatives and anti derivatives of order k of \tilde{f}_N respectively. The explicit expression (6) of \tilde{f}_N make it possible for us to compute effectively F(x,k) at the points $\{x_k\}_{k=0}^N$:

$$x_k = (2L - R) + k \times \lambda, \quad \lambda = \frac{2(R - L)}{N}, 0 \le k \le N$$
 (7)

Note that

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

By (6),

$$F(x_k, 0) = \sum_{j=0}^{N-1} A'_j(-1)^j \cos(2kj\pi/N) = \Re \sum_{j=0}^{N-1} A'_j(-1)^j \omega_N^{kj}$$
 (8)

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 (8) can be obtained by inverse FFT (ifft):

$$\{F(x_k,0)\}_{0 \le k \le N-1} = N \times \Re \left\{ ifft(\{(-1)^j A_j'\}_{0 \le j \le N-1}) \right\}.$$
 (9)

One can apply (6) to derive s-th order derivatives $(s = -1, -2, \cdots)$

$$F(x, -(2h-1)) = (-1)^h \sum_{j=0}^{N-1} (-1)^j (j\pi/l)^{2h-1} A_j' \sin(\pi j \frac{x - (2L - R)}{l})$$

$$F(x, -2h) = (-1)^h \sum_{j=0}^{N-1} (-1)^j (j\pi/l)^{2h} A_j' \cos(\pi j \frac{x - (2L - R)}{l}).$$

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

$$\{F(x_k, -(2h-1))\} = (-1)^h N \times \Im(ifft\{(-1)^j (j\pi/l)^{2h-1} A_j'\}) (10)$$
$$\{F(x_k, -(2h))\} = (-1)^h N \times \Re(ifft\{(-1)^j (j\pi/l)^{2h} A_j'\}) \quad (11)$$

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

$$F(x,2h-1) = (-1)^{h-1} \sum_{j=0}^{N-1} (-1)^{j} \frac{\hat{A}_{j} l^{2h-1}}{(j\pi)^{2h-1}} \sin(j\pi \frac{x - (2L - R)}{l})$$

$$+ \sum_{m=1}^{h-1} \frac{(-1)^{h-m-1}}{(2m-1)!} (x - L)^{2m-1} \sum_{j=0}^{N-1} \frac{\hat{A}_{j} l^{2(h-m+1)}}{(\pi j)^{2(h-m+1)}}$$

$$+ \frac{A'_{0}(x - L)^{2h-1}}{(2h-1)!}$$
(12)

and

$$F(x,2h) = (-1)^{h} \sum_{j=0}^{N-1} (-1)^{j} \frac{\hat{A}_{j} l^{2h}}{(j\pi)^{2h}} \cos(j\pi \frac{x - (2L - R)}{l})$$

$$+ \sum_{m=1}^{h} \frac{(-1)^{h-m}}{(2m-2)!} (x - L)^{2m-2} \sum_{j=0}^{N-1} \frac{\hat{A}_{j} l^{2(h-m+1)}}{(\pi j)^{2(h-m+1)}}$$

$$+ \frac{A'_{0}(x - L)^{2h}}{(2h)!}$$

$$(13)$$

where

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

For $h \geq 1$,

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

and

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

Notice that

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

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One can rewrite (12) as

$$\{F(x_k, 2h-1)\}_k = (-1)^{h-1} \{Z(j,k)\}_k + \{\frac{A'_0(x_k-L)^{2h-1}}{(2h-1)!}\}_k$$

$$+ \{\sum_{m=1}^{h-1} \frac{(-1)^{h-m-1}Y(\frac{N}{2}, h-m+1)}{(2m-1)!} (x_k-L)^{2m-1}\}_k$$

and rewrite (13) as

$$\{F(x_k, 2h)\}_k = (-1)^h \{Y(j, k)\}_k + \{\frac{A'_0(x_k - L)^{2h}}{(2h)!}\}_k$$

$$+ \{\sum_{m=1}^h \frac{(-1)^{h-m}Y(\frac{N}{2}, h - m + 1)}{(2m-2)!} (x_k - L)^{2m-2}\}_k$$
(15)

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

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

2. Estimate certain relevant integrations

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

$$E(x,t) = \int_{L}^{x} e^{tu} \tilde{f}_{N}(u) du, \quad t \ge 0, \quad x < R$$
 (16)

In fact,

$$E(x,t) = e^{tx} \sum_{j=0}^{N-1} \frac{\frac{1}{t} \cos(j\pi(x-L)/l) + \frac{j\pi}{lt^2} \sin(j\pi(x-L)/l)}{1 + (\frac{j\pi}{tl})^2} A'_j$$

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

$$= e^{tx} \sum_{j=0}^{N-1} \frac{\frac{1}{t} (-1)^j \cos(j\pi(x - (2L - R))/l)}{1 + (\frac{j\pi}{tl})^2} A'_j$$

$$+ e^{tx} \sum_{j=0}^{N-1} \frac{\frac{j\pi}{lt^2} (-1)^j \sin(j\pi(x - (2L - R))/l)}{1 + (\frac{j\pi}{tl})^2} A'_j \qquad (17)$$

$$- \sum_{j=0}^{N-1} \frac{e^{tL}/t}{1 + (\frac{j\pi}{tl})^2} A'_j \qquad (18)$$

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

$$P(a,b,c,j) = \sum_{k=0}^{j} \frac{(-1)^k j!}{(j-k)!} \{ F(b,k)(b-y)^{j-k} - F(a,k)(a-y)^{j-k} \}$$
 (19)