MDCorr Notes

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1 Correlations

There are general relationships between correlations and Fourier transforms. Especially, there is the convolution theorem. Define the convolution as

$$g(t) * h(t) \equiv \int_{-\infty}^{\infty} g(\tau)\, h(t-\tau)\, \mathrm{d}\tau. \tag{1}$$

Define the Fourier transform as

$$H(f) \equiv \mathcal{F}\{h(t)\}(f) = \int_{-\infty}^{\infty} h(t)\, e^{2\pi i f t}\, \mathrm{d}t \tag{2}$$

and the inverse,

$$h(t) = \mathcal{F}^{-1}\{H(f)\} = \int_{-\infty}^{\infty} H(f)\, e^{-2\pi i f t}\, \mathrm{d}f \tag{3}$$

The convolution theorem states:

$$\mathcal{F}\{g * h\} = G(f)\, H(f) \tag{4}$$

The correlation of two functions may be written as,

$$\mathrm{Corr}(g, h) = g(t) * h(-t) \tag{5}$$

If both g and h are real, then

$$\begin{aligned} \mathrm{Corr}(g, h) &= G(f)\, H(f)^* \\ \mathrm{Corr}(g, h) &= \mathcal{F}^{-1}\{\mathcal{F}\{g\}\, \mathcal{F}\{h\}^*\} \end{aligned} \tag{6}$$

If the correlation is with the same real function [1], i.e., it is a real autocorrelation, then the solution takes a simple form

$$\mathrm{Corr}(g, g) = \mathcal{F}^{-1}\left\{|G|^2\right\}. \tag{7}$$

This is known as the "Wiener-Khinchin Theorem".

2 Discretization

The Discrete Fourier Transform (DFT) of a complex series x_n with size N is computed as

$$X_k = \sum_{n}^{N-1} x_n e^{2\pi i k n/N}, \tag{8}$$

and its inverse,

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} X_k e^{-2\pi i k n / N}. \tag{9}$$

There is a corresponding discrete theorem called the circular convolution theorem.

3 FFT

The DFT can be denoted,

$$\begin{aligned} \boldsymbol{X} &= \mathscr{F}_N \left\{ \boldsymbol{x} \right\} \\ \boldsymbol{x} &= \mathscr{F}_N^{-1} \left\{ \boldsymbol{X} \right\} \end{aligned} \tag{10}$$

where N is the size of the input and output vectors of the tranform operation. Now suppose N is divisible by some integer a. The sum can be decomposed into parts,

$$\begin{aligned} X_k &= \sum_{s=0}^{a-1} \sum_{m=0}^{N/a} x_{am+s} e^{2\pi i k (am+s)/N} \\ &= \sum_{s=0}^{a-1} e^{2\pi i k s/N} \sum_{m=0}^{N/a} x_{am+s} e^{2\pi i k (am)/N} \\ &= \sum_{s=0}^{a-1} e^{2\pi i k s/N} \sum_{m=0}^{N/a} x_{am+s} e^{2\pi i k m/(N/a)} \\ \mathscr{F}_N \left\{ \boldsymbol{x} \right\}_k &= \sum_{s=0}^{a-1} e^{2\pi i k s/N} \mathscr{F}_{N/a} \left\{ \boldsymbol{x} \right\}_k \end{aligned} \tag{11}$$

Thus the Fourier transform can be decomposed into the sum of smaller Fourier transforms. This results in a computational speedup because $\mathscr{F}_{N/a} \left\{ \boldsymbol{x} \right\}_k$ is periodic in k with periodicity N/a. Thus

$$\mathscr{F}_{N/a} \left\{ \boldsymbol{x} \right\}_k = \mathscr{F}_{N/a} \left\{ \boldsymbol{x} \right\}_{k \bmod N/a}. \tag{12}$$

Therefore

$$\mathscr{F}_N \left\{ \boldsymbol{x} \right\}_k = \sum_{s=0}^{a-1} e^{2\pi i k s/N} \mathscr{F}_{N/a} \left\{ \boldsymbol{x} \right\}_{k \bmod N/a}. \tag{13}$$

Similarly,

$$\mathscr{F}_N^{-1} \left\{ \boldsymbol{x} \right\}_n = \frac{1}{N} \sum_{s=0}^{a-1} e^{-2\pi i n s/N} \mathscr{F}_{N/a}^{-1} \left\{ \boldsymbol{X} \right\}_{n \bmod N/a}. \tag{14}$$

The single thread runtime of this substep l with size n_l is

$$\begin{aligned} R_l \left(n_l \right) &= a_l n_l + a_l R_{l-1} \left(n_l / a_l \right) \\ &= a_l \left(n_l + R_{l-1} \left(n_l / a_l \right) \right) \end{aligned} \tag{15}$$

This is because each $k \in 0, ..., n_s - 1$ must be evaluated. Assuming a_s R_{s+1} subproblems have already been performed, that leaves an $O\left(1\right)$ read operation from the child calculation and a butterfly operations for each k. If N has the prime factorization a_p of length P, then there will be P layers. Enumerate these layers starting from a base case $a_1, a_2, ..., a_P$.

$$\begin{aligned}
R_2 &= a_2\left(n_2 + R_1\right) \\
R_3 &= a_3\left(n_3 + a_2\left(n_2 + R_1\right)\right) \\
R_4 &= a_4\left(n_4 + a_3\left(n_3 + a_2\left(n_2 + R_1\right)\right)\right) \\
&= a_4 n_4 + a_4 a_3 n_3 + a_4 a_3 a_2 n_2 + a_4 a_3 a_2 R_1 \\
&\vdots \\
R_P = R\left(N\right) &= \sum_{l=2}^{P} n_l \prod_{p=2}^{P} a_p + R_1 \prod_{p=1}^{P} a_p \\
&= \sum_{l=2}^{P} n_l \prod_{p=l}^{P} a_p + R_1 N
\end{aligned} \tag{16}$$

The size of each layer is given by

$$n_l = \prod_{p=1}^{l-1} a_p \tag{17}$$

Thus

$$R = \sum_{l=1}^{P} a_l \prod_{p=1}^{P} a_p = N \sum_{l=1}^{P} a_l \tag{18}$$

The indices respect a similar recursive relationship

$$x_{n,l} = a_l x_{n,l} + s_l \tag{19}$$

In explicit form,

$$\begin{aligned}
x_{n,l-1} &= a_l x_{n,l} + s_l \\
x_{n+1,l} &= \frac{x_{n_l} - s_l}{a_l}
\end{aligned} \tag{20}$$

- explicit index mapping
- complex number respresentation.
- The RDF cutoff must coordinate with the ghost mapping when the realspace cutoff is small.
- This can be fixed with the command

```
comm_modify cutoff {RDF cutoff + skin}.
```

References

[1] William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. *Numerical recipes in C (2nd ed.): the art of scientific computing.* Cambridge University Press, USA, 1992.