Skill Pill: Fourier Transforms

Lecture 3: Code 'n stuff

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Overview

1. What makes an FFT fast?
2. Spectral methods
3. Quantum mechanics

What makes an FFT fast?

- FT:

$$F(\xi) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i x \xi} \mathrm{dx}$$

$$f(x) = \frac{1}{N} \int_{-\infty}^{\infty} F(\xi) e^{2\pi i x \xi} \mathrm{d}\xi$$

- DFT:

$$F(k) = \sum_{n=0}^{N-1} f(n) e^{-2i\pi nk/N}$$

$$f(n) = \sum_{n=0}^{N-1} F(k) e^{2i\pi nk/N}$$

So, let's take the DFT and modify it a bit

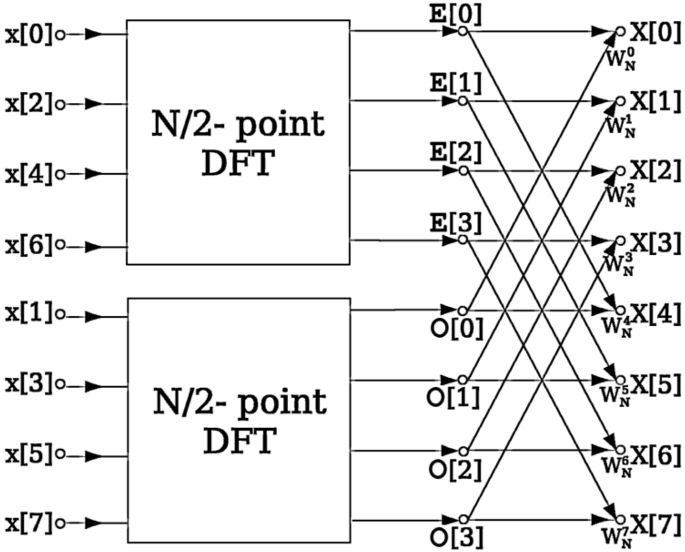
$$F(k) = \sum_{n=0}^{N-1} f(n) e^{-2\pi nk/N}$$

$$F(k) = \sum_{M=0}^{N/2-1} f(2m) e^{-i2\pi k(2m)/N} + \sum_{M=0}^{N/2-1} f(2m+1) e^{-i2\pi k(2m+1)/N}$$

$$F(k) = \sum_{M=0}^{N/2-1} f(2m) e^{-i2\pi k(2m)/N} + e^{-2i\pi k/N} \sum_{M=0}^{N/2-1} f(2m+1) e^{-i2\pi k(2m)/N}$$

We can continually subdivide out problem again and again to do this faster!

Butterfly diagram



- Any function can be represented as a sum of other functions, for example:

$$F \sim \sum_{n=0}^{N} a_n \sin(2\pi nx) + b_n \cos(2\pi nx)$$

- The new function can be called $\hat{I}(x)$, or the *interpolant*.
- So we have 2 spaces: *Configuration Space* and *Coefficient Space*
  - *Configuration Space*: $\hat{I}(x)$
  - *Coefficient Space*: $\sum_{n=0}^{N} a_n$
- Every Fourier transform brings us back and forth between these two spaces

- The difference between $\hat{I}(x)$ and $F(x)$ is known as aliasing error
- If we want to calculate the derivative of $F(x)$, it is simply

$$f'(x) = \hat{I}(x)' = \sum_{n=0}^{N} a_n'$$

where a_n are all functions used by $\hat{I}$

- This makes certain operations easy, but there is yet another method to calculate derivatives: *Pseudo-Spectral Methods*, like the *Split-Operator Method*
- With pseudo-spectral methods, we do not work fully in one space, but instead pop between both spaces to do our work

Application to Quantum Mechanics

- In quantum mechanics, there is the **Heisenberg uncertainty principle**:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

- This is quite similar to what you have been seeing, an expansion in real space, leads to a contraction in momentum space
- Incredibly, we can use the Split-Operator method for solving the Schrödinger equation (even if it's nonlinear!)

Application to Quantum Mechanics

- The Schrödinger equation looks like:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi = \left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\right)\Psi$$

  - Ψ is the wavefunction that we are solving for
  - V_0 is the potential, all in **real space**
  - $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = \frac{p^2}{2m}$ is the kinetic energy component in **momentum space**
- To solve this equation, we can naïvely say:

$$\Psi(t) = \Psi_0 e^H = \Psi_0 e^{V_0/2} e^{\frac{p^2}{2m}} e^{V_0/2}$$

- So we solve this equation by doing the following:

$$\cdots \Psi e^{\frac{V_0}{2}} \to FFT \to \Psi e^{\frac{p^2}{2m}} \to iFFT \to \Psi e^{\frac{V_0}{2}} \cdots$$

Conclusions

- FFT's are fast because of recursion (Cooley-Tukey algorithm!)
- FFT's are used all the time to simulate matter (Spectral methods)
- Psuedo-spectral methods are used in quantum mechanics to solve the Schrödinger equation
- Thanks for coming!