

11.3: The Split-Step Fourier Method

As an example of the usefulness of the DFT, let us discuss a DFT-based method for performing numerical integration of a *partial* differential equation, known as the **split-step Fourier method**. Here, the method will be presented in the context of the time-dependent Schrödinger equation in 1D space:

$$i \frac{d\psi(x, t)}{dt} = \left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x, t) \right] \psi(x, t) \quad (11.3.1)$$

We have taken $\hbar = m = 1$ for simplicity. At each time, the wavefunction is a continuous function of x . Let us truncate and discretize this spatial coordinate, by defining a computational domain of length L containing N discretization points:

$$\psi_n(t) = \psi(x_n, t), \quad \text{where } x_n = -\frac{L}{2} + n\Delta x, \quad \Delta x = \frac{L}{N}. \quad (11.3.2)$$

Thus, the wavefunction at each time is represented by a complex vector, which we call a "state vector":

$$\vec{\psi}(t) = \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \\ \vdots \\ \psi_{N-1}(t) \end{pmatrix}. \quad (11.3.3)$$

Given an initial state vector $\vec{\psi}(t_a)$, the problem is to compute $\vec{\psi}(t_b)$ at a later time t_b . Note that this differs from previously-studied numerical ODE problems in one important respect: evolving in time involves taking second-order *spatial* derivatives. We won't go into the details, but it turns out that standard methods for time-stepping and discretizing space don't work very well here, because the errors from time-stepping and spatial discretization interact badly with one another. The split-step Fourier method provides a better way to solve the problem.

11.3.1 Factorizing the Time-Evolution Operator

The split-step Fourier method is based on the concept of the *time-evolution operator*. Given a wavefunction $\psi(x, t_j)$, the wavefunction after a small time step τ is

$$\psi(x, t_j + \tau) = U(t_j + \tau | t_j) \psi(x, t_j), \quad \text{where } U(t_j + \tau | t_j) \approx \exp \left\{ -i\tau \left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x, t_j + \tau/2) \right] \right\}. \quad (11.3.4)$$

Here, the $\exp(\dots)$ refers to the exponential of an operator (one involving spatial derivatives). We call $U(t_b | t_a)$ the time-evolution operator, which evolves the system from time t_a to t_b . The exponential of any operator \mathcal{A} is defined as the infinite series

$$\exp(\mathcal{A}) = I + \mathcal{A} + \frac{1}{2}\mathcal{A}^2 + \frac{1}{6}\mathcal{A}^3 + \dots \quad (11.3.5)$$

In this case, the exponential contains the Hamiltonian, which consists of a kinetic energy term and a potential energy term that do not generally commute. Due to this non-commutivity, the exponential cannot be simplified by factorization:

$$\exp \left\{ -i\tau \left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x, t_j + \tau/2) \right] \right\} \neq \exp \left\{ \frac{i\tau}{2} \left[\frac{\partial^2}{\partial x^2} \right] \right\} \exp \left\{ -i\tau V(x, t_j + \tau/2) \right\}. \quad (11.3.6)$$

However, we can obtain an approximate factorization by making use of the series definition of the exponential of an operator. One can show that

$$\exp(\mathcal{A} + \mathcal{B}) = \exp(\mathcal{A}/2) \exp(\mathcal{B}) \exp(\mathcal{A}/2) + O((\mathcal{A}, \mathcal{B})^3), \quad (11.3.7)$$

which is a variant of an important formula known as the **Baker–Campbell–Hausdorff formula**. On the right-hand side, note that $\exp(\mathcal{B})$ is sandwiched "symmetrically" between two copies of $\exp(\mathcal{A}/2)$. This symmetric arrangement reduces the approximation error to third order, by the cancellation of lower-order errors (in a manner similar to the mid-point formula for the discretized derivative). Applying this factorization to the time-evolution operator gives

$$U(t_j + \tau | t_j) \approx U_K \cdot U_V(t_j + \tau/2) \cdot U_K, \quad \text{where} \quad \begin{cases} U_K &= \exp\left[\frac{i\tau}{4} \frac{d^2}{dx^2}\right] \\ U_V(t) &= \exp[-i\tau V(x, t)] \end{cases} \quad (11.3.8)$$

In other words, the time-evolution operator decomposes into three pieces. That's why we call this a "split-step" algorithm: each time step from t_j to $t_j + \tau$ consists of applying a kinetic step, then applying a potential step, then applying another kinetic step, in sequence. As previously noted, we'll be working with state vectors (complex N -component vectors), defined through spatial discretization of the wavefunction. So we need to figure out how the above stepping operators act on these state vectors:

$$U_K \vec{\psi} = ??, \quad U_V \vec{\psi} = ?? \quad (11.3.9)$$

The potential stepping operator is simple to deal with. Since the state vector represents the wavefunction at different points in space, the potential operator is represented by a diagonal matrix, and its exponential is also diagonal:

$$U_V \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_{N-1} \end{pmatrix} = \begin{pmatrix} \exp[-i\tau V(x_0, t + \frac{\tau}{2})] & & \\ & \ddots & \\ & & \exp[-i\tau V(x_{N-1}, t + \frac{\tau}{2})] \end{pmatrix} \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_{N-1} \end{pmatrix} \quad (11.3.10)$$

11.3.2 Kinetic Step

The kinetic stepping operator, U_K , is less obvious. It contains spatial derivatives and is thus *not* diagonal in the current basis. The key thing to realize, however, is that this operator is diagonal in *wavenumber space*. Let us return to the continuous wavefunction, and write its Fourier representation:

$$\psi(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \Psi_k. \quad (11.3.11)$$

Then

$$U_K \psi(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left(-\frac{i\tau}{4} k^2\right) e^{ikx} \Psi_k. \quad (11.3.12)$$

Let us discretize space in steps of Δx , as discussed earlier, and also discretize the Fourier integrals by steps of Δk :

$$x_n = -\frac{L}{2} + n\Delta x, \quad (11.3.13)$$

$$k_n = -\frac{K}{2} + n\Delta k \quad (11.3.14)$$

The values of K and Δk will be chosen shortly. The discretized integrals become

$$\psi_m \approx \sum_{n=0}^{N-1} \frac{\Delta k}{2\pi} e^{ik_n x_m} \Psi_{k_n}, \quad (11.3.15)$$

$$(U_K \psi)_m \approx \sum_{n=0}^{N-1} \frac{\Delta k}{2\pi} e^{-\frac{i\tau}{4} k_n^2} e^{ik_n x_m} \Psi_{k_n}. \quad (11.3.16)$$

Let us now choose the k -space discretization parameters to be

$$\Delta k = \frac{2\pi}{N\Delta x} = \frac{2\pi}{L}, \quad K = N\Delta k = \frac{2\pi}{\Delta x} \Rightarrow k_n = -\frac{\pi}{\Delta x} + \frac{2\pi n}{N\Delta x}. \quad (11.3.17)$$

With this choice, we can show with a bit of algebra that the integral for ψ_m reduces to an IDFT:

$$\psi_m = (-1)^m \frac{1}{N} \sum_{n=0}^{N-1} \left(\frac{1}{\Delta x} e^{iN\pi/2} e^{-in\pi} \Psi_{k_n} \right) e^{\frac{2\pi i m n}{N}} \quad (11.3.18)$$

$$= (-1)^m \text{IDFT} \left\{ \frac{1}{\Delta x} e^{iN\pi/2} (-1)^n \Psi_{k_n} \right\}_m \quad (11.3.19)$$

$$\Rightarrow \Psi_{k_n} = \Delta x e^{-iN\pi/2} (-1)^n \text{DFT} \left\{ (-1)^m \psi_m \right\}_n \quad (11.3.20)$$

Likewise,

$$(U_{\mathcal{K}} \psi)_m = (-1)^m \text{IDFT} \left\{ \frac{1}{\Delta x} e^{iN\pi/2} (-1)^n e^{-\frac{i\tau}{4} k_n^2} \Psi_{k_n} \right\}_m \quad (11.3.21)$$

Putting these results together, we get

$$(U_{\mathcal{K}} \psi)_m = (-1)^m \text{IDFT} \left\{ e^{-\frac{i\tau}{4} k_n^2} \text{DFT} \left\{ (-1)^p \psi_p \right\}_n \right\}_m \quad (11.3.22)$$

$$\text{where } k_n = -\frac{\pi N}{L} + \frac{2\pi n}{L} \quad (11.3.23)$$

Hence, the $U_{\mathcal{K}}$ kinetic stepping operator can be implemented by taking a DFT, multiplying the resulting vector elements by $\exp(-i\tau k_n^2/4)$ phase factors, and taking an IDFT. The runtime of the stepping process is $O(N \log(N))$. The m , n , and p indices all run over the range $[0, 1, \dots, N-1]$, consistent with the standard definition of the DFT and IDFT.

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