29 October 2022

Simulating the nonlinear Schrödinger equation

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Nonlinear Schrödinger equations describe the time evolution of various physical systems, *e.g.*, a Bose-Einstein condensate. In dimensionless form the $1+1$ dimensional equation with a potential and a cubic nonlinearity is

$$i\frac{\partial}{\partial t}\psi(t,x) = \Big(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) - g|\psi(t,x)|^2\Big)\psi(t,x). \tag{1}$$

If we discretize space by $\mathbb{Z}\Delta x \subset \mathbb{R}$, the second derivative with respect to x becomes

$$\frac{\partial^2}{\partial x^2}\psi(t,x) \approx \frac{\psi(t,x+\Delta x) - 2\psi(t,x) + \psi(t,x-\Delta x)}{\Delta x^2},$$

and we can rewrite the partial differential equation (1) as an ordinary differential equation for a vector $\psi(t)$ with components indexed by $\mathbb{Z}$,

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = \big(-\gamma L + V - gK(t)\big)\psi(t), \tag{2}$$

where

$$V = \begin{pmatrix} \ddots & & & & \\ & V_0 & & & \\ & & V_1 & & \\ & & & \ddots & \end{pmatrix} \quad \text{and} \quad K(t) = \begin{pmatrix} \ddots & & & & \\ & |\psi_0(t)|^2 & & & \\ & & |\psi_1(t)|^2 & & \\ & & & \ddots & \end{pmatrix}$$

are the potential and nonlinear operators, respectively, and

$$L = \begin{pmatrix} \ddots & & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & & \ddots & \end{pmatrix}$$

is the Laplacian, with $\gamma = 1/(2\Delta x^2)$.

If we think of the integer lattice in $\mathbb{R}$ as a graph with vertices the integers and edges connecting x and $x+1$ for all $x \in \mathbb{Z}$, notice the this Laplacian has the form $L = A - D$, where A is the *adjacency matrix* for the graph ($A_{xy} = 1$ when there is an edge connecting vertices x and y; $A_{xy} = 0$ otherwise) and D is the diagonal matrix with D_{xx} being the degree of vertex x (the number of vertices to which x is connected). This is the *graph Laplacian*.

Our goal is to evolve according to (2) for different choices of the underlying graph, G, and potential. For example, in a graph with two vertices connected by an edge,

$$L = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{3}$$

Notice that if $\psi(t)$ satisfies (2), then

$$i\frac{\mathrm{d}}{\mathrm{d}t}e^{-i\alpha t}\psi(t) = \alpha e^{-i\alpha t}\psi(t) + ie^{-i\alpha t}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = e^{-i\alpha t}\big(-\gamma L + V - gK(t) + \alpha I\big)\psi(t),$$

which tells us that if we add a constant times the identity to the evolution operator on the right hand side of (2), it has the effect only of multiplying the solution by $e^{-i\alpha t}$. Thus, if it is convenient, we can, for example, replace L in (3) by $L = X$. As long as L has off-diagonal terms, however, while V and $K(t)$ are diagonal, and so commute with each other, they do not commute with L unless they are proportional to the identity. Nevertheless, for $\Delta t \ll 1$, the time evolution can be approximated as

$$\psi(n\Delta t) \approx \Big(\prod_{j=1}^{n} e^{-i(V-gK(j\Delta t))\Delta t}e^{i\gamma L\Delta t}\Big)\psi(0);$$

this is the *first order Trotter product formula*. (We can eventually consider higher order Suzuki-Trotter formulas.) For notational convenience, we write $\psi(j) = \psi(j\Delta t)$ and $K(j) = K(j\Delta t)$, and define

$$U = e^{i\gamma L\Delta t} \quad \text{and} \quad V_j = e^{-i(V-gK(j))\Delta t}.$$

Since V_j depends on the state, $\psi(j)$, of the system, however, we need to estimate it. Our approach is:

0. Initialize the state $\psi(0)$.
1. Compute $\phi(0) = U\psi(0)$.
2. Measure $\phi(0)$.
3. Repeat steps 0-2 N times; use the results to estimate $|\phi_x(0)|^2$ and thus V_0.
4. Set $j = 0$.
5. While $j < n$,
    6. Re-initialize $\psi(0)$ and compute $\psi(j+1) = V_jU \dots V_0U\psi(j)$.
    7. Compute $\phi(j+1) = U\psi(j+1)$.
    8. Measure $\phi(j+1)$.
    9. Repeat steps 6-8 N times; use the results to estimate $|\phi_x(j+1)|^2$ and thus V_{j+1}.
    10. Set $j = j+1$.

We would like to understand how the accuracy of this simulation procedure depends upon Δx, n, N, the estimation method for $|\phi_x(j)|^2$, V, and G.