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Simulating the nonlinear Schrödinger equation

David A. Meyer

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

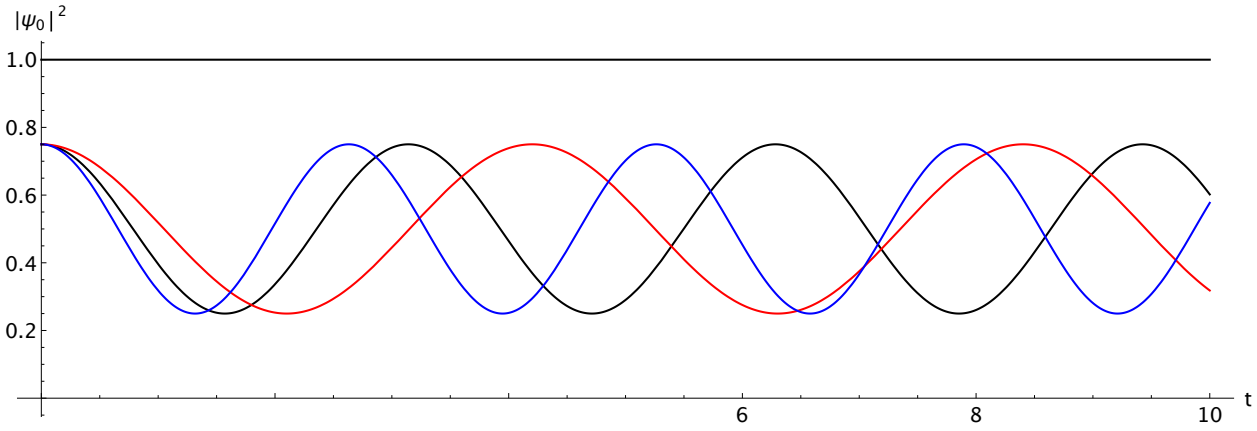
$$U = e^{i\gamma L\Delta t} \quad \text{and} \quad V_j = e^{-i(V-gK(j))\Delta t}.$$

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 $\psi(j+1) = V_jU\ldots V_0U\psi(j)$.
    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.

We can begin to assess the accuracy of our simulations by comparing them with numerical solutions of equation (1) for various choices of the parameters. The figure below shows these for $V = 0$, $\gamma = 1$, and $g \in \{-1, 0, 1\}$, with initial condition $\psi(0) = \cos(\pi/6)|0\rangle + \sin(\pi/6)|1\rangle$:



And the next figure shows the these for $V(0) = -1$, $V(1) = 0$, the same values of γ and g as above, with initial condition $\psi(0) = \cos(\pi/4)|0\rangle + \sin(\pi/4)|1\rangle$: