Stability and Leapfrog Scheme
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Context: consider the initial value problem for linear time-dependent PDEs. Denote the fully discretized scheme as $\mathbf{U}^{n+1} = S\mathbf{U}^n$. Here $\mathbf{U}$ is a column vector $[u_1, u_2, \cdots]^T$ where the subscript is spatial grid index. Assume we use linear discretizations, namely, S is a matrix.

Matrix Notations:

1. A^T is the transpose of A. A^* is the complex conjugate transpose.
2. Eigenvalues: $\mathrm{eig}_i(S)$ denotes the eigenvalue of S with i-th largest magnitude.
3. Jordan Normal Form: any matrix S can be decomposed as $S = P\Lambda P^{-1}$ where Λ is upper-triangular and the diagonal entries are eigenvalues of S.
4. Singular Value: the i-th largest one is denoted as $\sigma_i(S) = \sqrt{\mathrm{eig}_i(SS^*)} = \sqrt{\mathrm{eig}_i(S^*S)}$.
5. Normal Matrix: a matrix A is called normal if $AA^* = A^*A$.
6. The following are equivalent:
   (a) A is normal.
   (b) A is diagonalizable by a unitary matrix, i.e., $A = P\Lambda P^*$, Λ is a diagonal matrix and $PP^* = I$.
   (c) $\sigma_i(A) = |\,\mathrm{eig}_i(A)|$.

Stability Notations:

- Stability: $\|S^N U\| \le C\|U\|$ where C is a constant independent of Δt. Here $N = \frac{T}{\Delta t}$ is the total time steps. In other words, stability means $\|S^N\| \le C$.
- von Neumann Stability: $|\,\mathrm{eig}(S)| \le 1 + \mathcal{O}(\Delta t)$.

Neccesary and Sufficient Conditions for Stability:

1. To have stability $\|S^N\| \le C$, $\|S\| \le 1 + \mathcal{O}(\Delta t)$ is sufficient (due to $\|S^N\| \le \|S\|^N$ and $\lim\limits_{N\to+\infty}(1+\frac{1}{N})^N = e$) but not neccesary (see Example 1 below).
2. To have stability $\|S^N\| \le C$, vN-stability $|\,\mathrm{eig}(S)| \le 1 + \mathcal{O}(\Delta t)$ is neccesary ($S = P\Lambda P^{-1}$, then $S^N = P\Lambda^N P^{-1}$ implies $|\,\mathrm{eig}_i(S^N)| = |\,\mathrm{eig}_i(S)|^N$) but not sufficient (see Example 2 below).
3. If S is diagonalizable (for instance, S is normal or has distinct eigenvalues), i.e., $S = P\Lambda P^{-1}$ where Λ is a diagonal matrix and diagonal entries are eigenvalues. Then $S^N = P\Lambda^N P^{-1}$ implies $\|S^N\| \le \|P\|\|P^{-1}\|\|\Lambda\|^N$. In this case, $|\,\mathrm{eig}(S)| \le 1 + \mathcal{O}(\Delta t)$ is sufficient for stability $\|S^N\| \le C$.

Example 1: Consider the wave equation $u_{tt} = c^2 u_{xx}$ on a finite interval with periodic boundary conditions and the leapfrog scheme

$$\frac{U_j^{n+1} - 2U_j^n + U_j^{n-1}}{\Delta t^2} = c^2 \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2}. \tag{0.1}$$

Suppose $x_j = j\Delta x$ $(j = 0, 1, \cdots, m)$ denotes the spatial grid point. Let $\widetilde{U}^n$ be the Discrete Fourier Transform of U^n for any n, then we have

$$U_j^n = \sum_{k=-m/2}^{m/2} e^{\mathrm{i}kx_j} \widetilde{U}_j^n(k). \tag{0.2}$$

After plugging (0.2) into (0.1), we have

$$\sum_{k=-m/2}^{m/2} e^{\mathrm{i}kx_j} \left[\widetilde{U}_j^{n+1}(k) - (c\Delta t/\Delta x)^2(-2 + \cos k\Delta x)\widetilde{U}_j^n(k) - 2\widetilde{U}_j^n(k) + \widetilde{U}_j^{n-1}(k) \right] = 0.$$

Since $\{e^{\mathrm{i}kx_j} : k = -\frac{m}{2}, \cdots, \frac{m}{2}\}$ is a basis of $\mathbb{R}^m$, we get

$$\widetilde{U}_j^{n+1}(k) = (c\Delta t/\Delta x)^2(-2 + \cos k\Delta x)\widetilde{U}_j^n(k) + 2\widetilde{U}_j^n(k) - \widetilde{U}_j^{n-1}(k).$$

For convenience, we omit the subscript j and frequency variable k in $\widetilde{U}_j^n(k)$. For each fixed k, we have

$$\begin{pmatrix} \widetilde{U}^{n+1} \\ \widetilde{U}^n \end{pmatrix} = \begin{pmatrix} r^2(-2 + \cos k\Delta x) + 2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \widetilde{U}^n \\ \widetilde{U}^{n-1} \end{pmatrix} = G \begin{pmatrix} \widetilde{U}^n \\ \widetilde{U}^{n-1} \end{pmatrix}, \quad r = c\Delta t/\Delta x.$$

The eigenvalues of G are $\lambda_i = a \pm \sqrt{a^2 - 1}$ with $a = 1 + r^2(\cos k\Delta x - 1)$. To have $|\operatorname{eig}(G)| \le 1$, we need $r \le 1$. On the other hand, G is not a normal matrix and $\|G\| > 1$. But G is diagonalizable $G = P \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} P^{-1}$. Thus $\|G^N\| \le C$ if $r \le 1$.

Example 2: vN-stability is not sufficient. Consider a trivial "PDE" system

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \mathbf{0}$$

and a consistent scheme

$$\begin{pmatrix} u_j^{n+1} \\ v_j^{n+1} \end{pmatrix} = \begin{pmatrix} u_j^n - \frac{\Delta t^2}{2\Delta x^2}(v_{j+1}^n - v_{j-1}^n) \\ v_j^n \end{pmatrix}, \quad \Delta t = \Delta x.$$

After DFT, we get

$$\begin{pmatrix} \tilde{u}_j^{n+1} \\ \tilde{v}_j^{n+1} \end{pmatrix} = G \begin{pmatrix} \tilde{u}_j^n \\ \tilde{v}_j^n \end{pmatrix},$$

where the amplification matrix $G = \begin{pmatrix} 1 & \sin^2 k\Delta x \\ 0 & 1 \end{pmatrix}$. Obviously G satisfies vN-stability but $G^N = \begin{pmatrix} 1 & N\sin^2 k\Delta x \\ 0 & 1 \end{pmatrix}$. The scheme is not stable because $\|G^N\|$ depends on N thus is unbounded.