Lecture 4

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1 Stiff ODEs

1.1 Motivation

Consider the linear ode system:

$$\begin{cases} \boldsymbol{y}' = \boldsymbol{\Lambda}\boldsymbol{y}, \quad t \geq 0 \\ \boldsymbol{y}(0) = \boldsymbol{y}_0 \neq 0 \end{cases} \quad \text{where } \boldsymbol{\Lambda} = \begin{pmatrix} -100 & 1 \\ 0 & -\frac{1}{10} \end{pmatrix} \tag{1}$$

$\boldsymbol{\Lambda}$ is a diagonizable matrix, which we can write as $\boldsymbol{\Lambda} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^{-1}$, and

$$\boldsymbol{V} = \begin{pmatrix} 1 & 1 \\ 0 & \frac{999}{10} \end{pmatrix}, \quad \boldsymbol{D} = \begin{pmatrix} -100 & 0 \\ 0 & -\frac{1}{10} \end{pmatrix}$$

By theory, the entries of diagonal matrix $\boldsymbol{D}$ are the eigenvalues of $\boldsymbol{\Lambda}$. We can derive the exact solution of the system: $\boldsymbol{y} = e^{\boldsymbol{\Lambda}t}\boldsymbol{y}_0 = \boldsymbol{V}e^{\boldsymbol{D}t}\boldsymbol{V}^{-1}\boldsymbol{y}_0$. Where $e^{\boldsymbol{D}t}$, the exponential of a matrix is defined as a matrix of same dimension in taylor expansion of $e^{(\cdot)}$. In this case $\boldsymbol{e^{Dt}}$ is a diagonal matrix with entries e^{-100t} and $e^{-\frac{1}{10}t}$. So there exists constant $\boldsymbol{x}_1, \boldsymbol{x}_2$, such that $\boldsymbol{y}(t) = \boldsymbol{x}_1 e^{-100t} + \boldsymbol{x}_2 e^{-\frac{1}{10}t}$. Compared with the second term, e^{-100t} is small (for $t \geq 0$), so this is approximately $\boldsymbol{y} \sim \boldsymbol{1}e^{-\frac{1}{10}t}$.

On the other hand we try solve the system with euler's method: $\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\boldsymbol{\Lambda}\boldsymbol{y}_n = (\boldsymbol{I} + h\boldsymbol{\Lambda})\boldsymbol{y}_n$. So we have

$$\begin{aligned} \boldsymbol{y}_n &= (\boldsymbol{I} + h\boldsymbol{\Lambda})^n \boldsymbol{y}_0 = \boldsymbol{V}(\boldsymbol{I} + h\boldsymbol{D})^n \boldsymbol{V}^{-1}\boldsymbol{y}_0 = \boldsymbol{V}\begin{pmatrix} 1 - 100h & 0 \\ 0 & 1 - \frac{1}{10}h \end{pmatrix}^n \boldsymbol{V}^{-1}\boldsymbol{y}_0 \\ &= \boldsymbol{c}_1(1 - 100h)^n + \boldsymbol{c}_2(1 - \tfrac{1}{10}h)^n \end{aligned} \tag{2}$$

The exact solution decays with t, we want the numerical solution to possess this property, i.e. to decay with n. This requires $|1 - 100h| < 1$ and $|1 - \frac{1}{10}h| < 1$, *depending on our choice of* h. We *should* choose $0 < h < \frac{1}{50}$ and $0 < h < 20$ to make the numerical solution decay with n. The problem is that we can not foresee this problem all the time, so we are possible to select an improper h, like $h = \frac{1}{10}$. Which will make the first term blow up with n, and clearly in this case the numerical solution does not match the decaying property of the exact solution.

1.2 Stiffness

Def. **Stiffness**: An ODE system is said to be *stiff* if the numerical solution requires a very *small* h, i.e. a significant depression of step size, to avoid blow up. We also define the *stiffness ratio* for the linear system $\boldsymbol{y}' = \boldsymbol{A}\boldsymbol{y}$ as the largest eigenvalue of $\boldsymbol{A}$ / the smallest eigenvalue of $\boldsymbol{A}$. We look at the (eigenvalues of) Jacobian $\nabla_{\boldsymbol{y}}\boldsymbol{f}$ as an approximation for nonlinear systems $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$.

Ex. A Chemical Reaction ODE System:

$$\begin{cases} y_1' = -0.04y_1 + 10^4 y_2 y_3 \\ y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2 \\ y_3' = 3 \cdot 10^7 y_2^2 \end{cases} \tag{3}$$

An observation is the conservation of mass: $(y_1 + y_2 + y_3)' = 0$, and we may want to preserve this property in numerical computing. In this system, y_3 is a *fast* variable, since it has the largest change rate; y_2 is *intermediate* and y_1 is *slow*. In general, fast variable requires a small h, and determines the appropriate step size.

2 Absolute Stability

Def. **Absolute Stability**: Apply a numerical method for $y' = f(t, y)$ to a linear ODE:

$$\begin{cases} y' = \lambda y, \quad t \geq 0 \\ y(0) = y_0 \neq 0 \end{cases} \tag{4}$$

for certain fixed $\bar{h} = \lambda h, \lambda \in \mathbb{C}$ (complex plane). $\{y_n\}$ is the path of numerical solution, if $\{y_n\}$ strictly decays to 0 as $n \to \infty$, i.e. $\lim_{n\to\infty} y_n = 0$, we call the method as absolute stable (A-stable). Moreover, the region $\{\bar{h} : \bar{h} \text{ is A-stable}\} \subseteq \mathbb{C}$ is called the region of absolute stability of the method.