As a model problem of general parabolic equations, we shall mainly consider the following heat equation and study corresponding finite difference methods and finite element methods:

\[
\begin{cases}
    u_t - \Delta u = f & \text{in } \Omega \times (0, T), \\
    u = 0 & \text{on } \partial \Omega \times (0, T), \\
    u(\cdot, 0) = u_0 & \text{in } \Omega.
\end{cases}
\]

Here \( u = u(x, t) \) is a function of spatial variable \( x \in \Omega \subset \mathbb{R}^n \) and time variable \( t \in (0, T) \). The ending time \( T \) could be +\( \infty \). The Laplace operator \( \Delta \) is taking with respect to the spatial variable. For the simplicity of exposition, we consider only homogenous Dirichlet boundary condition and comment on the adaptation to Neumann and other type of boundary conditions. Besides the boundary condition on \( \partial \Omega \), we also need to assign the function value at time \( t = 0 \) which is called initial condition. For parabolic equations, the boundary \( \partial \Omega \times (0, T) \cup \Omega \times \{ t = 0 \} \) is called the parabolic boundary. Therefore the initial condition can be also thought as a boundary condition.

1. Background on heat equation

For the homogenous Dirichlet boundary condition without source terms, in the steady state, i.e., \( u_t = 0 \), we obtain the Laplace equation:

\[
\Delta u = 0 \quad \text{in } \Omega \quad \text{and} \quad u|_{\partial \Omega} = 0.
\]

So \( u = 0 \) no matter what the initial condition is. Indeed the solution will decay to zero exponentially as \( t \to +\infty \). Let us consider the simplest 1-D problem

\[
u_{xx} = u_{xx} \quad \text{in } \mathbb{R}^1 \times (0, T), \quad u(\cdot, 0) = u_0.
\]

Apply Fourier transfer in space

\[
\hat{u}(k, t) = \int_{\mathbb{R}} u(x, t)e^{-ikx} \, dx.
\]

Then \( \hat{u_x} = (-ik)\hat{u}, \hat{u_{xx}} = -k^2\hat{u}, \) and \( \hat{u}_t = \hat{u}_t \). So we get the following ODE for each Fourier coefficient \( \hat{u}(k, t) \)

\[
\hat{u}_t = -k^2\hat{u}, \quad \hat{u}(\cdot, 0) = \hat{u}_0
\]

The solution in the frequency domain is \( \hat{u}(k, t) = \hat{u}_0 e^{-k^2 t} \). We apply the inverse Fourier transform back to \((x, t)\) coordinate and get

\[
u(x, t) = \frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R}} e^{-\frac{(x-y)^2}{4t}} u_0(y) \, dy.
\]

For a general bounded domain \( \Omega \), we cannot apply Fourier transform. Instead we can use the eigenfunctions of \( A = -\Delta_0 \) (Laplace operator with zero Dirichlet boundary condition). Since \( A \) is SPD, we know that there exists an orthonormal basis formed by eigenfunctions of \( A \), i.e., \( L^2 = \text{span}\{\phi_1, \phi_2, \ldots\} \) and \( A\phi_k = \lambda_k \phi_k \) for \( k = 1, 2, \ldots \).
We expand the function in such bases $u(x, t) = \sum_k u^k(t) \phi_k(x)$. The heat equation then becomes

$$u^k_t(t) = \lambda_k u^k, \quad u^k(0) = u_0^k$$

and the solution is

$$u^k = u_0^k e^{-\lambda_k t}, \quad \text{for} \quad k = 1, 2, \ldots$$

Each component will exponentially decay to zero since the eigenvalue $\lambda_k$ of $A$ is positive. And the larger the eigenvalue, the faster the decay rate. This spectral analysis is mainly for theoretical purpose and the numerical application is restricted to special domains for which the eigenfunctions can be found. In practice, for domains of complex geometry, it is much harder to finding out all eigenvalue and eigenfunctions than solving the heat equation numerically. In the following sections we will talk about finite difference and finite element methods.

2. Finite difference methods for 1-D heat equation

In this section, we consider a simple 1-D heat equation

$$(2) \quad u_t = u_{xx} + f \quad \text{in} \quad (0, 1) \times (0, T),$$

$$(3) \quad u(0) = u(1) = 0, \quad u(x, 0) = u_0(x).$$

to illustrate the main issues in the numerical methods for solving parabolic equations.

Let $\Omega = (0, 1)$ be decomposed into a uniform grid $\{0 = x_0 < x_1 < \ldots < x_{N+1} = 1\}$ with $x_i = ih, h = 1/N$, and time interval $(0, T)$ be decomposed into $\{0 = t_0 < t_1 < \ldots < t_M = T \}$ with $t_n = n\delta t, \delta t = T/M$. The tensor product of these two grids give a two dimensional rectangular grid for the domain $\Omega \times (0, T)$. We now introduce three finite difference methods by discretizing the equation (2) on grid points.

2.1. Forward Euler method. We shall approximate the function value $u(x_i, t_n)$ by $U^n_i$ and $u_{xx}$ by second order central difference

$$u_{xx}(x_i, t_n) \approx \frac{U^n_{i-1} + U^n_{i+1} - 2U^n_i}{h^2}.$$  

For the time derivative, we use the forward Euler scheme

$$(4) \quad u_t(x_i, t_n) \approx \frac{U^{n+1}_i - U^n_i}{\delta t}.$$  

Together with the initial condition and source $F^n_i = f(x_i, t^n)$, we end with the system

$$(5) \quad \frac{U^{n+1}_i - U^n_i}{\delta t} = \frac{U^n_{i-1} + U^n_{i+1} - 2U^n_i}{h^2} + F^n_i, \quad 1 \leq i \leq N, 1 \leq n \leq M$$

$$(6) \quad U^n_0 = u_0(x_0), \quad 1 \leq i \leq N, n = 0.$$  

To write (5) in a compact form, we introduce the parameter $\lambda = \delta t/h^2$ and the vector $U^n = (U^n_1, U^n_2, \ldots, U^n_N)^T$. Then (5) can be written as, for $n = 0, \ldots, M$

$$U^{n+1} = AU^n + \delta t F^n,$$

where

$$A = I + \lambda \Delta_h = \begin{pmatrix}
1 - 2\lambda & \lambda & 0 & 0 \\
\lambda & 1 - 2\lambda & \lambda & 0 \\
\vdots & \vdots & \vdots & \vdots \\
0 & \lambda & 1 - 2\lambda & \lambda \\
0 & 0 & \lambda & 1 - 2\lambda
\end{pmatrix}.$$
Starting from $t = 0$, we can evaluate point values at grid points from the initial condition and thus obtain $U^0$. After that, the unknown at next time step is computed by one matrix-vector multiplication and vector addition which can be done very efficiently without storing the matrix. Therefore it is also called time marching.

Remark 2.1. Because of the homogenous Dirichlet boundary condition, the boundary index $i = 0, N + 1$ is not included. For Neumann boundary condition, we do need to impose equations on these two boundary nodes and introduce ghost points for accurately discretize the Neumann boundary condition; See Finite difference methods for elliptic equations.

The first issue is the stability in time. When $f = 0$, i.e., the heat equation without the source, in the continuous level, the solution should be exponential decay. In the discrete level, we have $U^{n+1} = AU^n$ and want to control the magnitude of $U$ in certain norms.

Theorem 2.2. When the time step $\delta t \leq h^2/2$, the forward Euler method is stable in the maximum norm in the sense that if $U^{n+1} = AU^n$ then

$$\|U^n\|_\infty \leq \|U^0\|_\infty \leq \|u_0\|_\infty.$$ 

Proof. By the definition of the norm of a matrix

$$\|A\|_\infty = \max_{i=1,\ldots,N} \sum_{j=1}^N |a_{ij}| = 2\lambda + |1 - 2\lambda|.$$ 

If $\delta t \leq h^2/2$, then $\|A\|_\infty = 1$ and consequently

$$\|U^n\|_\infty \leq \|A\|_\infty \|U^{n-1}\|_\infty \leq \|U^{n-1}\|_\infty.$$ 

Theorem 2.2 and Exercise 4.1 imply that to ensure the stability of the forward Euler method in the maximum error, we have to choose the time step $\delta t$ in the size of $h^2$ which is very restrictive, say, $h = 10^{-3}$ then $t = 10^{-6}/2$. Although in one step, it is efficient, it will be very expensive to reach the solution at the ending time $T$ by moving forward with such tiny time step. For time dependent equations, we shall consider not only the computational cost for one single time step but also the total time to arrive a certain stopping time.

The second issue is the accuracy. We first consider the consistency error. Define $u^n_I = (u(x_1, t_n), u(x_2, t_n), \cdots, u(x_N, t_n))^T$. We denote a general differential operator as $L$ and its discritization as $L_h^n$. Note that the action $Lu$ is the operator $L$ acting on a continuous function $u$ while $L_h^n$ is applied to vectors such as $U^n$ or $u^n_I$. The called the truncation error is to pretend we know the exact function values and see what the error from the approximation of the differential operator. More precisely, for the heat equation we define $Lu = u_t - \Delta u$ and $L_h^n V = (V^{n+1} - V^n) / \delta t - \Delta u / h^2 V^n$ and the truncation error

$$\tau^n = L_h^n u^n_I - (Lu)^n_I.$$ 

The error is denoted by

$$E^n = U^n - u^n_I.$$ 

Estimate of the truncation error is straightforward using the Taylor expansion.

Lemma 2.3. Suppose $u$ is smooth enough. For the forward Euler method, we have

$$\|\tau^n\|_\infty \leq C_1 \delta t + C_2 h^2.$$
The convergence or the estimate of the error $E^n$ is a consequence of the stability and consistency. The method can be written as

$$L^n h U^n = F^n = (Lu)^n.$$

We then obtain the error equation

$$L^n h (U^n - u^n) = (Lu)^n - L^n h u^n, \tag{7}$$

which can be simply written as $L^n h E^n = -\tau^n$.

**Theorem 2.4.** For the forward Euler method, when $\delta t \leq h^2/2$ and the solution $u$ is smooth enough, we have

$$\|U^n - u^n\|_\infty \leq C t_n (\delta t + h^2).$$

**Proof.** We write out the specific error equation for the forward Euler method

$$E^{n+1} = A E^n - \delta t \tau^n.$$

Consequently

$$E^n = A^n E^0 - \delta t \sum_{l=1}^{n-1} A^{n-l-1} \tau^l.$$

Since $E^0 = 0$, by the stability and consistency, we obtain

$$\|E^n\|_\infty \leq \delta t \sum_{l=1}^{n-1} \|\tau^l\|_\infty \leq C n \delta t (\delta t + h^2) = C t_n (\delta t + h^2).$$

\[\square\]

### 2.2. Backward Euler method.

Next we introduce the backward Euler method to remove the strong constraint of the time step-size for the stability. The method is simply using the backward difference to approximate the time derivative. We list the resulting linear systems below:

$$\frac{U^n - U^n_{i-1}}{\delta t} = \frac{U^n_{i+1} + U^n_{i-1} - 2 U^n_i}{h^2} + F^n_i, \quad 1 \leq i \leq N, 1 \leq n \leq M \tag{8}$$

$$U^0_i = u_0(x_i), \quad 1 \leq i \leq N, n = 0. \tag{9}$$

In the matrix form (8) reads as

$$(I - \lambda \Delta h) U^n = U^{n-1} + \delta t F^n.$$

Starting from $U^0$, to compute the value at the next time step, we need to solve an algebraic equation to obtain

$$U^n = (I - \lambda \Delta h)^{-1} (U^{n-1} + \delta t F^n).$$

The inverse of the matrix, which involves the stiffness matrix of Laplacian operator, is not easy in high dimensions. For 1-D problem, the matrix is tri-diagonal and can be solved very efficiently by the Thomas algorithm.

The gain is the unconditional stability.

**Theorem 2.5.** For the backward Euler method without source term, i.e., $(I - \lambda \Delta h) U^n = U^{n-1}$, we always have the stability

$$\|U^n\|_\infty \leq \|U^{n-1}\|_\infty \leq \|u_0\|_\infty.$$
Proof. We shall rewrite the backward Euler scheme as
\[ (1 + 2\lambda)U_i^n = U_i^{n-1} + \lambda U_{i-1}^n + \lambda U_{i+1}^n. \]
Therefore for any \(1 \leq i \leq N\),
\[ (1 + 2\lambda)|U_i^n| \leq \|U_i^{n-1}\|_\infty + 2\lambda\|U_i^n\|_\infty, \]
which implies
\[ (1 + 2\lambda)\|U_i^n\|_\infty \leq \|U_i^{n-1}\|_\infty + 2\lambda\|U_i^n\|_\infty, \]
and the desired result then follows.  \(\square\)

The truncation error of the backward Euler method can be obtained similarly.

**Lemma 2.6.** Suppose \(u\) is smooth enough. For the backward Euler method, we have
\[ \|\tau^n\|_\infty \leq C_1\delta t + C_2h^2. \]

We then use stability and consistency to give error analysis of the backward Euler method.

**Theorem 2.7.** For the backward Euler method, when the solution \(u\) is smooth enough, we have
\[ \|U^n - u^n_I\|_\infty \leq Ct_n(\delta t + h^2). \]

**Proof.** We write the error equation for the backward Euler method as
\[ (1 + 2\lambda)E_i^n = E_i^{n-1} + \lambda E_{i-1}^n + \lambda E_{i+1}^n - \delta t\tau_i^n. \]
Similar to the proof of the stability, we obtain
\[ \|E^n\|_\infty \leq \|E^{n-1}\|_\infty + \delta t\|\tau^n\|_\infty \]
Consequently, we obtain
\[ \|E^n\|_\infty \leq \delta t \sum_{l=1}^{n-1} \|\tau^l\|_\infty \leq Ct_n(\delta t + h^2). \]

From the error analysis, to have optimal convergent order, we also need \(\delta t \approx h^2\) which is still restrictive. Next we shall give a unconditional stable scheme with second order truncation error \(O(\delta t^2 + h^2)\).

### 2.3. Crank-Nicolson method.

To improve the truncation error, we need to use central difference for time discretization. We keep the forward discretization as \((U_i^{n+1} - U_i^n)/\delta t\) but now treat it as an approximation of \(u_t(x_i, t_{n+1/2})\). That is we discretize the equation at \((x_i, t_{n+1/2})\). The value \(U_i^{n+1/2}\) is taken as average of \(U_i^n\) and \(U_i^{n+1}\). We then end with the scheme: for \(1 \leq i \leq N, 1 \leq n \leq M\)
\[ (11) \quad \frac{U_i^{n+1} - U_i^n}{\delta t} = \frac{1}{2} \frac{U_{i-1}^n + U_{i+1}^n - 2U_i^n}{h^2} + \frac{1}{2} \frac{U_{i-1}^{n+1} + U_{i+1}^{n+1} - 2U_i^{n+1}}{h^2} + F_i^{n+1/2}, \]
and for \(1 \leq i \leq N, n = 0\)
\[ U_i^0 = u_0(x_i). \]

In matrix form, (11) can be written as
\[ (I - \frac{1}{2}\lambda\Delta h)U_i^{n+1} = (I + \frac{1}{2}\lambda\Delta h)U_i^n + F_i^{n+1/2}. \]

It can be easily verify that the truncation error is improved to second order in time.
Lemma 2.8. Suppose $u$ is smooth enough. For Crank-Nicolson method, we have
\[ \| \tau^n \|_\infty \leq C_1 \delta t^2 + C_2 h^2. \]

In the next section, we shall prove Crank-Nicolson method is unconditionally stable in the $l^2$ norm and thus obtain the following second order convergence; See Exercise 13.

Theorem 2.9. For Crank-Nicolson method, we have
\[ \| E^n \| \leq C \tau_n (C_1 \delta t^2 + C_2 h^2). \]

3. VON NEUMANN ANALYSIS

A popular way to study the $L^2$ stability of the heat equation is through Fourier analysis and its discrete version. When $\Omega = \mathbb{R}$, we can use Fourier analysis. For $\Omega = (0, 1)$, we can use eigenfunctions of Laplacian operator. To study the matrix equation, we establish the discrete counterpart.

Lemma 3.1. Let $A = \text{diag}(b, a, b)$ be a $N \times N$ tri-diagonal matrix. The eigenvalues of $A$ are
\[ \lambda_k = a + 2b \cos \theta_k, \quad k = 1, \cdots, N \]
and the corresponding eigenvectors are
\[ \phi_k = \sqrt{2} \left( \sin \theta_k, \sin 2\theta_k, \cdots, \sin N \theta_k \right), \]
where
\[ \theta_k = k\theta = \frac{k\pi}{N + 1}. \]

Proof. It is can be easily verified by the direct calculation. \qed

Remark 3.2. The eigenvectors do not depend on the values $a$ and $b$!

We then define a scaling of $l^2$ inner product of two vectors as
\[ (U, V)_h = h U^T V = h \sum_{i=1}^N U_i V_i, \]
which is a mimic of $L^2$ inner product of two functions if we thought $U_i$ and $V_i$ represent the values of corresponding functions at grid points $x_i$.

It is straightforward to verify that the eigenvectors $\{ \phi_k \}_{k=1}^N$ forms an orthonormal basis of $\mathbb{R}^N$ with respect to $(\cdot, \cdot)_h$. Indeed the scaling $\sqrt{2}$ is introduced for the normalization. For any vector $V \in \mathbb{R}^N$, we expand it in this new basis
\[ V = \sum_{k=1}^N \hat{v}_k \phi_k, \quad \text{with} \quad \hat{v}_k = (V, \phi_k)_h. \]

The discrete Parseval identity is
\[ \| V \|_h = \| \hat{v} \|, \]
where $\hat{v} = (\hat{v}_1, \cdots, \hat{v}_N)^T$ is the vector formed by the coefficients. The $\hat{\cdot}$ in the coefficient indicates this is a mimic of Fourier transform in the discrete level.

Suppose
\[ U^{n+1} = AU^n, \]
with $A = \text{diag}(b, a, b)$. Then the stability in $\| \cdot \|_h$ is related to the spectrum radius of $A$. That is
\[ \| U^{n+1} \|_h \leq \| A \|_h \| U^n \|_h. \]
and since $A$ is symmetric with respect to $(\cdot, \cdot)_h$,
\[
\|A\|_h = \rho(A) = \max_{1 \leq k \leq N} |\lambda_k(A)|.
\]
Note that $\|\cdot\|_h = h^{1/2} \|\cdot\|$. The stability in the scaled $l_2$ norm is equivalent to that in $\|\cdot\|$ norm. Here the scaling $h$ is chosen to be consistent with the scaling of discrete Laplace operator.

Now we analyze the $l_2$-stability of the three numerical methods we have discussed. Recall that $\lambda = \delta/h^2$ and a circle on the plane can be described by the equation $|z - a| = r$ for a complex variable $z$. Then its real part is $\text{Re}(z) = a + r \cos \theta$. In the sequel, the inequality can be easily obtained by drawing circles.

**Forward Euler Method.**

\[
U^{n+1} = AU^n, \quad A = \text{diag}(\lambda, 1 - 2\lambda, \lambda).
\]

Thus
\[
\rho(A) = \max_{1 \leq k \leq N} |1 - 2\lambda + 2\lambda \cos \theta_k|.
\]

It is easy to verify that
\[
\lambda \leq 1/2 \implies \rho(A) \leq 1.
\]

Let us write $A = A_N$, the uniform stability (with respect to $N$) implies $\lambda \leq 1/2$, i.e.,
\[
\sup_N \rho(A_N) \leq 1 \implies \lambda \leq 1/2.
\]

Therefore we obtain the same condition as that for the maximum norm stability.

**Backward Euler Method.**

\[
U^{n+1} = A^{-1}U^n, \quad A = \text{diag}(-\lambda, 1 + 2\lambda, -\lambda).
\]

Thus
\[
\rho(A^{-1}) = \max_{1 \leq k \leq N} \frac{1}{|1 + 2\lambda - 2\lambda \cos \theta_k|},
\]

and
\[
\rho(A^{-1}) \leq 1 \quad \text{for any } \lambda > 0.
\]

Therefore the backward Euler is also unconditionally stable in $l_2$ norm.

**Crank-Nicolson Method.**

\[
U^{n+1} = A^{-1}BU^n, \quad A = \text{diag}(-\lambda, 2 + 2\lambda, -\lambda),
\]

\[
B = \frac{1}{2} \text{diag}(\lambda, 2 - 2\lambda, \lambda)
\]

Since $A$ and $B$ have the same eigenvectors, we have
\[
\rho(A^{-1}B) = \max_{1 \leq k \leq N} \frac{\lambda_k(B)}{\lambda_k(A)} = \max_{1 \leq k \leq N} \frac{|1 - \lambda + \lambda \cos \theta_k|}{|1 + \lambda - \lambda \cos \theta_k|},
\]

and
\[
\rho(A^{-1}B) \leq 1 \quad \text{for any } \lambda > 0.
\]

Therefore we proved Crank-Nicolson method is unconditionally stable in $l_2$ norm.
For general schemes, one can write out the matrix form and plug in the coefficients to do the stability analysis. This methodology is known as von Neumann analysis. Symbolically we replace

\[ U^n_j \leftarrow \rho^n e^{i\theta j} \]

in the scheme and obtain a formula of the amplification factor \( \rho = \rho(\theta) \). The uniform stability is obtained by considering inequality

\[ \max_{0 \leq \theta \leq \pi} \rho(\theta). \]

To fascinate the calculation, one can factor out \( \rho^n e^{i\theta j} \) and consider only the difference of indices.

The eigen-function is changed to \( e^{i\theta} = \cos \theta + i \sin \theta \) to account for possible different boundary conditions. The frequency of discrete eigenvectors \( \phi_k = e^{i\theta_k (1:N)^T} \) is changed to a continuous variable \( \theta \) in (12). We skip the index \( k \) and take the maximum of \( \theta \) over \([0, \pi]\) while the range of the discrete angle \( \theta_k \) satisfying \( h \pi \leq \theta_k \leq (1-h) \pi \).

4. Exercises

**Exercise 4.1.** Construct an example to show, numerically or theoretically, that if \( \delta t > h^2/2 \), then the forward Euler is not stable in the maximum norm, i.e.,

\[ \|U^n\|_\infty > \|U^0\|_\infty. \]

Apply the backward Euler method to the example you constructed to show that numerically the scheme becomes stable.

**Exercise 4.2.** Prove the maximum norm stability of Crank-Nicolson method with assumptions on \( \lambda \). What is the weakest assumption on \( \lambda \) you can impose? Is Crank-Nicolson method unconditionally stable in the maximum norm? You can google “Crank Nicolson method maxnorm stability” to read more.

**Exercise 4.3 (The \( \theta \) method).** For \( \theta \in [0, 1] \), we use the scheme: for \( 1 \leq i \leq N, 1 \leq n \leq M \)

\[ \frac{U^{n+1}_i - U^n_i}{\delta t} = (1 - \theta) \frac{U^n_{i-1} + U^n_{i+1} - 2U^n_i}{h^2} + \theta \frac{U^{n+1}_{i-1} + U^{n+1}_{i+1} - 2U^{n+1}_i}{h^2}, \]

and for \( 1 \leq i \leq N, n = 0 \)

\[ U^0_i = u_0(x_i). \]

Give a complete error analysis (stability, consistency, and convergence) of the \( \theta \) method. Note that \( \theta = 0 \) is forward Euler, \( \theta = 1 \) is backward Euler, and \( \theta = 1/2 \) is Crank-Nicolson method.

**Exercise 4.4 (Leap-frog method).** The scheme is an explicit version of Crank-Nicolson. For \( 1 \leq i \leq N, 1 \leq n \leq M \)

\[ \frac{U^{n+1}_i - U^{n-1}_i}{2\delta t} = \frac{U^n_{i-1} + U^n_{i+1} - 2U^n_i}{h^2}. \]

The computation of \( U^{n+1} \) can be formulated as linear combination of \( U^n \) and \( U^{n-1} \). Namely it is an explicit scheme. To start the computation, we need two ‘initial’ values. One is the real initial condition

\[ U^0_i = u_0(x_i), \quad 1 \leq i \leq N. \]
The other $U^1$, so-called computational initial condition, can be computed using one step forward or backward Euler method.

Give a complete error analysis (stability, consistency, and convergence) of the leap-frog method.