Lesson 4

CSPP58001 Numerical Methods:
TA: Kyle Gerard Felker

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1 Stability

To this point we've studied both explicit and implicit discretizations of our model equation, the simple linear for of the heat equation with constant diffusivity. We observed that our choice of explicit discretization technique – the so-called Forward Time Center Space (FTCS) – was only stable for the choice of

$$C \equiv \frac{\alpha \Delta t}{\Delta x^2} \leq \frac{1}{2n}$$

where $n = 1, 2, 3$ is the dimensionality of the problem. We saw the effect of instability when the solution "blew up" for values just beyond this threshold. For our implicit methods – backward Euler and Crank Nicholson – there was apparently no limit on the size of C to yield a stable solution (accuracy is another issue, something which will be clarified shortly). Now we will study the theoretical basis for this phenomenon.

1.1 Ordinary Differential Equation

We begin by looking at a simple system – a simple linear first order ordinary differential equation (one independent variable) with constant coefficients:

$$\frac{du}{dt} = -\alpha u \tag{1}$$

where α is a positive constant (as with the heat equation – negative diffusivity is non-physical) and $u = u(t)$. If we denote the Initial condition is $u(0) = u_0$, then it should be clear that an analytical solution exists in this case, which is $\boxed{u(t) = u_0 e^{-\alpha t}.}$ Note that since α is positive the solution goes to zero as $t \to \infty$.

Now we will approximate the solution in the same manner as the full heat equation – by discretizing the system (here only in time since there is no spatial coordinate).

Forward Euler

$$\frac{u_{n+1} - u_n}{\Delta t} = -\alpha u_n$$
$$u_{n+1} = (1 - \alpha\Delta t)u_n \tag{2}$$

It is clear that at each time step we multiply the estimated solution at the previous time step by the quantity $1 - \alpha\Delta t$, so that at some arbitrary time step k in the future, the following recursion relation yields the solution:

$$u_k = (1 - \alpha\Delta t)^k u_0 \tag{3}$$

We are always interested in two things: consistency and stability of the approximation. In this case, the stability condition is clear: $|1 - \alpha\Delta t| < 1$. Otherwise evaluating the kith power would yield a solution that rapidly grew in time. we know from the analytical solution that the correct behavior is to tend to zero, and thus that a solution that blows up is a numerical artifact due to too large a choice of Δt.

Now we discretize using an implicit method – the simplest one (though not the most accurate) is Backward Euler, where the derivative is evaluated at the future time step:

Backward Euler

$$\frac{u_{n+1} - u_n}{\Delta t} = -\alpha u_{n+1}$$
$$u_{n+1} + \alpha\Delta t u_{n+1} = u_n$$
$$u_k = (1 + \alpha\Delta t)^{-k} u_0 \to 0 \;\forall\; \alpha\Delta t \tag{4}$$

It should be clear that this formulation is unconditionally stable. That is, no matter how large Δt, the solution is correctly driven to its true steady state value.

1.2 1-D Heat Equation Forward Euler

Our solution at each timestep n at position j is given by

$$u_{n+1,j} = u_{n,j} + \frac{\alpha\Delta t}{\Delta x^2}[u_{n,j+1} - 2u_{n,j} + u_{n,j-1}]$$

Let's rewrite this in matrix form: $u_{n+1} = Au_n$ where

$$A = \begin{bmatrix} 1-2c & c & 0 & \dots & & \\ c & 1-2c & c & 0 & \dots & \\ 0 & c & 1-2c & c & 0 & \dots \\ \vdots & \dots & \ddots & & & \end{bmatrix} \tag{5}$$

and c is $\alpha \Delta t \Delta x^{-2}$, a constant. Now, we can see that $\boxed{u_k = A^k u_0}$ as in the scalar ODE. Furthering this analogy, how can we determine what the stability condition is? What does it mean for a matrix to be "less than one" so that the solution stays bounded? In other words, what determines if the k applications of the matrix to the solution drives the solution to the correct steady state or forces it to diverge (go to infinity)[1]. To understand this requires a more general discussion of the concept of eigenvalues and eigenvectors of a matrix. After we understand eigenvalues and eigenvectors, in next week's lecture we will use them to analyze the stability of our heat equation example.

2 Eigenvalues and Eigenvectors

Consider a square matrix A and a vector $\vec{x}$. Think of A as an operator $A\colon \mathbb{R}^n \to \mathbb{R}^n$, where $\mathbb{R}^n$ is a Euclidean vector space. The matrix A is a discrete operator which changes vectors in the vector space. Suppose we find a very special vector such that for some value of $\lambda \neq 0$

$$A\vec{x} = \lambda \vec{x} \tag{6}$$

where $\lambda \in \mathbb{R}$ (i.e. is a scalar). The set of these such vectors are the eigenvectors of A. The scalars which are associated with them are their corresponding eigenvalues. Geometrically, the eigenvalues represent the amount which the vector is stretched or contracted by A (but $\vec{x}$ is not rotated, by definition!). For a square $n \times n$ matrix, there will be n eigenvalues and eigenvectors. The eigenvalues may be repeated. Note that eigenvalues can be real or imaginary, but this is a distinction we will not worry about until later.

[1] Note that we can derive an analytical solution in the 2d case as well and show that the solution in steady state should go to zero for homogeneous boundary conditions

2.1 Determining the eigenvalues

Analytically For small matrices it is possible to compute the eigenvalues/vectors analytically (for more realistic sized systems we will develop numerical techniques, but studying the analytical method gives insight into eigenvector properties). Note that Equation 6 can be rearranged to give

$$(A - I\lambda)\vec{x} = 0$$

This is equivalent to saying that the matrix $A - I\lambda$ is singular, or $\det(A - I\lambda) = 0$, since the transformation takes a nonzero vector into the null space, and information is "lost", i.e. there is no way to invert the transformation. (See chapter 4 in Strang). We can solve the nth order polynomial from the determinant relation to find the eigenvalues.

$\boxed{\text{Example: Find the eigenvalues and eigenvectors of A}}$

$$A = \begin{bmatrix} 4 & -5 \\ 2 & -3 \end{bmatrix}$$

Using the identity above,

$$A - I\lambda = \begin{bmatrix} 4 - \lambda & -5 \\ 2 & -3 - \lambda \end{bmatrix}$$

$\det(A - I\lambda) = \lambda^2 - \lambda - 2 = 0$ The roots of this equation are $\lambda = -1, 2$. We substitute the eigenvalues back into the equation separately to find their eigenvectors. We get the vectors $\vec{x} = (1, 1)$ and (5 ,2), respectively.

Properties of eigenvalues

- $\sum \lambda_i$ = trace(A), where the trace of A is the sum of the diagonal elements
- $\lambda_1 \times \ldots \lambda_i$ = det(A)
- The eigenvalues of a triangular matrix are the diagonal elements

2.2 Eigendecomposition

Let A be an $n \times n$ matrix. Define S as the special matrix whose columns are the n eigenvectors of A.

$$S = \begin{bmatrix} \vec{x_1} & \vec{x_2} & \ldots & \vec{x_n} \\ \vdots & \ddots & \ldots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \tag{7}$$

What is AS?

$$AS = \begin{bmatrix} A\vec{x_1} & A\vec{x_2} & \dots & A\vec{x_n} \\ \vdots & \ddots & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \tag{8}$$

Since $\vec{x_i}$ are eigenvectors with corresponding eigenvectors λ_i,

$$AS = \begin{bmatrix} \vec{x_1} & \vec{x_2} & \dots & \vec{x_n} \\ \vdots & \ddots & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \dots & \vdots \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & 0 & \dots \\ 0 & \lambda_2 & 0 & \dots \\ 0 & \vdots & \ddots & \dots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} = S\Lambda \tag{9}$$

Or alternatively, $A = S\Lambda S^{-1}$. This is incredibly useful for computing powers of A. For example, consider

$$A^2 = S\Lambda S^{-1} S\Lambda S^{-1}$$

Since matrix multiplication is associative and a matrix times its inverse is the identity matrix, we have

$$A^k = S\Lambda^k S^{-1} \tag{10}$$

Returning back to our original problem with the heat equation, we now know how to easily compute

$$u_k = S\Lambda^k S^{-1} u_0$$

The stability condition can be proved to be related to the spectral radius, defined as

$$\rho(A) = \max(|\lambda_i|) < 1 \tag{11}$$

3 Going Backwards: Connecting discrete to continuous

$\boxed{\text{Example: compound interest}}$ Let 6 % be the annual interest of a loan, P_0 the principal. How the interest accumulates depends on the period of compounding. Let the interest first compound once annually, for 5 years.

$$P_k = (1.06)^k P_0$$

$$P_5 = (1.06)^5(1000) = \$1338$$

Now let the interest compound monthly

$$P_{60} = (1.0 + \frac{.06}{12})^{60}1000 = \$1349$$

Finally, let the interest compound daily

$$P_{5\times 365} = (1.0 + \frac{.06}{365})^{5\times 365}1000 = \$1349.83$$

Observe the trend

$$\lim_{\Delta t \to 0} \frac{P_{k+1} - P_k}{\Delta t} = \frac{dP}{dt} = 0.06P \tag{12}$$

We already know how to solve this ODE; $P(t) = P_0 e^{0.06t}$. Now let's try this process with a matrix rather than a scalar.

$\boxed{\text{Example: Fibonacci Sequence (Strang example)}}$

$F = \{0, 1, 1, 2, 3, 5, 8 \ldots\}$ is the Fibonacci Sequence. What if we want to know F_{1000}? The general form of the sequence is $F_{k+2} = F_{k+1} + F_k$. In matrix form,

$$u_k = \begin{bmatrix} F_{k+l} \\ Fk \end{bmatrix} \tag{13}$$

$$u_{k+1} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} u_k \tag{14}$$

Now, try to use eigendecomposition to find large iterations.