a known volume of water. A known concentration of sodium hydroxide in water, stored in a graduated pipe ( buret), is released slowly into the beaker, the solution is stirred continuously, and the pH of the solution is measured at specified time intervals. We will model the pH in the beaker as a function of time.

What is pH? Recall that the pH of a solution is a measure of its acidity. In fact, it is defined to be the negative logarithm, base ten, of the concentration of protons $H^+$ (in units of mol / l) or

$$\text{pH} := -\log_{10}[H^+].$$

For sodium hydroxide in water, we have

$$NaOH \rightleftharpoons Na^+ + OH^-.$$  

The forward dissociation constant is very large compared with the association constant. Almost all of the sodium hydroxide dissociates to sodium and $OH^-$ ions. The sodium does not react with acetic acid. Thus, we are only interested in the $OH^-$ ions. A solution of $A$ mol / l of $NaOH$ has $A$ mol / l of $OH^-$ for “all practical purposes.” Let us assume that all of the $NaOH$ dissociates. The solution enters at a rate of $B$ ml / sec. We must not mix units. Thus, we should express this concentration as $B/1000$ l / sec. It follows that $OH^-$ ions enters the acetic acid solution at the rate of

$$AB \text{ mol / sec}.$$  

The concentration of this ion changes during the addition of $NaOH$ because the volume is changing from 100 ml via the function

$$\text{vol} = \frac{1}{10} + \frac{B}{1000} t.$$  

A model of the ion concentration entering the solution (measured in mol / l) as a function of time is

$$\frac{AB}{\left(\frac{1}{10} + \frac{B}{1000} t\right)}.$$  \hspace{1cm} (5.14)

Using the model (5.14) for addition of $OH^-$ (during the addition of the
Conservation of Mass

<table>
<thead>
<tr>
<th>sec</th>
<th>pH</th>
<th>sec</th>
<th>pH</th>
<th>sec</th>
<th>pH</th>
<th>sec</th>
<th>pH</th>
</tr>
</thead>
<tbody>
<tr>
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<td>2.567</td>
<td>16</td>
<td>3.590</td>
<td>32</td>
<td>4.196</td>
<td>48</td>
<td>4.490</td>
</tr>
<tr>
<td>2</td>
<td>2.563</td>
<td>18</td>
<td>3.738</td>
<td>34</td>
<td>4.240</td>
<td>50</td>
<td>4.514</td>
</tr>
<tr>
<td>4</td>
<td>2.563</td>
<td>20</td>
<td>3.852</td>
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<td>4.283</td>
<td>52</td>
<td>4.540</td>
</tr>
<tr>
<td>6</td>
<td>2.563</td>
<td>22</td>
<td>3.923</td>
<td>38</td>
<td>4.327</td>
<td>54</td>
<td>4.564</td>
</tr>
<tr>
<td>8</td>
<td>2.689</td>
<td>24</td>
<td>3.979</td>
<td>40</td>
<td>4.363</td>
<td>56</td>
<td>4.590</td>
</tr>
<tr>
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<td>26</td>
<td>4.042</td>
<td>42</td>
<td>4.396</td>
<td>58</td>
<td>4.607</td>
</tr>
<tr>
<td>12</td>
<td>3.279</td>
<td>28</td>
<td>4.094</td>
<td>44</td>
<td>4.436</td>
<td>60</td>
<td>4.632</td>
</tr>
<tr>
<td>14</td>
<td>3.418</td>
<td>30</td>
<td>4.148</td>
<td>46</td>
<td>4.462</td>
<td>62</td>
<td>4.656</td>
</tr>
</tbody>
</table>

Figure 5.3: The data in this table is produced by a pH meter while a one molar sodium hydroxide solution is added to a one molar solution of acetic acid and water.

NaOH solution, our basic model (5.4) is modified to

\[ w' = c - dwz + \frac{AB}{\left(\frac{1}{100} + \frac{B}{1000t}\right)}, \]

\[ x' = byz - ax, \]

\[ y' = ax - byz, \]

\[ z' = ax - byz + c - dwz. \]  \( (5.15) \)

The flow rate \( B \) does not remain constant. The flow is turned on after the acetic acid solution is in steady state and turned off when the measurement device is stopped or the reservoir of NaOH is empty. The model can be used to make predictions via numerical integration.

An experiment was performed where a solution of one mol/l of NaOH is added to a solution of one mol/l of acetic acid at the rate of 0.5 ml/sec. The beaker containing the solution was stirred continuously and a pH sensor recorded the pH of the solution every two seconds for 74 sec (see Table 5.3). The flow of NaOH was started at 5 sec. The results of this experiment and a simulation using the model (5.15) are depicted in Figure 5.4. The agreement is excellent (compare, Exercise 5.11).

We note that the solution pH does not rise significantly during the titration if not too much base is added. The presence acid buffers the solution to the addition of the strong base. Buffering is an essential process in the living organisms. The pH of essential fluids, for example blood, must remain within some narrow range for certain biochemical processes to work properly. While our model is viable for small concentrations of the base, sodium hydroxide, it does not seem to predict the correct titration curve (pH versus the amount
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Figure 5.4: Plots of pH versus time in seconds for the addition of NaOH in acetic acid. The continuous graph is from the mathematical model (5.15); the discrete graph is from the data in Table 5.3.

of added base) over a larger range of additional OH\(^-\). A better model is the subject of the next section.

**Exercise 5.11.** (a) The results of experiment and simulation using the mathematical model (5.15) depicted in Figure 5.4 show excellent agreement. On the other hand, transient in the solutions of the model are very short. Good results can also be obtained by a static model based on the assumption that the mixtures are instantaneously in steady state. Discuss this alternative. Hint: This approach is used in textbooks on basic chemistry. (b) The accuracy of predictions from the model should depend on the accuracy of its parameters. How sensitive is the result to the given parameters. (c) Which choice of parameters best fits the experimental data?

**Exercise 5.12.** Prove the generalization of Bendixson’s theorem due to Dulac:

If a vector field has a periodic integral curve in the plane and the vector field is defined on the entire planar region bounded by this curve, then every positive function multiple of the vector field must have its divergence change sign in the region bounded by the curve. *This result is useful when a given vector field X does not have fixed sign in a region to be tested for the existence of periodic orbits. If there is a positive function f defined on the region, and the new vector field fX has fixed sign, then there are no periodic orbits in the region.*
5.3 An Improved Titration Model

The titration of a weak acid by a strong base (for example, titration of acetic acid by sodium hydroxide) stays in the buffer region, where the change in pH is not too great for small additions of the base until some critical amount of base is added. At this point a sharp rise in pH occurs. The pH levels off as more base is added. This general behavior is typical and is easily observed in experiments. Appropriate mathematical models build from rate equations, which are discussed in this section, predict the observed behavior.

Recall that we have introduced the chemical reactions for the dissociation of water

\[ H_2O \rightleftharpoons H^+ + OH^- \]

and acetic acid

\[ CH_3COOH + H_2O \rightleftharpoons CH_3COO^- + H^+; \]

or, in shorthand,

\[ AcH + H_2O \rightleftharpoons Ac^- + H^+, \]

and sodium hydroxide

\[ NaOH \rightleftharpoons Na^+ + OH^- . \]

The water concentration is considered to be very large compared with the concentrations of the other species. To account for the additional OH\(^-\) ions from the dissociated sodium hydroxide, one additional reaction should be included:

\[ CH_3COOH + OH^- \rightleftharpoons CH_3COO^- + H_2O. \]  \(5.16\)

In the previous section, we ignored the rate constants in this equation and simply changed the OH\(^-\) concentration in the mixture.

Using the notation of system (5.4), incorporating the water concentration into the forward rate constant for the dissociation of water and the backward rate constant \(e\) for reaction (5.16), and using \(f\) for the forward rate constant in the reaction (5.16), we have the rate equations

\[ w' = c - dwz + ey - fxw, \]

\[ x' = byz - ax + ey - fxw, \]

\[ y' = ax - byz - ey + fxw, \]

\[ z' = ax - byz + c - dwz. \]  \(5.17\)
Figure 5.5: Simulated titration curve (that is, pH versus initial molarity) of sodium hydroxide added to an 0.1 molar acetic acid solution.

We do not know the exact values of the rate constants $e$ and $f$. To determine their ratio, let us recall that

$$K_w = \frac{W_f}{W_b} \approx 10^{-14}$$

(see, equation (5.5)). At steady state for the system (5.17),

$$W_f[H_2O] - W_b[H^+][OH^-] = C_f[OH^-][AcH] - C_b[H_2O][Ac^-].$$

A rearrangement of the formula is

$$C_f K_w - C_b K_a = \frac{[H^+]}{[AcH]} (W_f - w_b K_w) = 0.$$

Thus, we have

$$\frac{e}{f} = \frac{C_f}{C_b} = \frac{K_a}{K_w} \approx 10^9.$$

Using the rate constants

$$a = 10^5, \quad b = \frac{a}{10^{-4.75}}, \quad c = 10^{-14}, \quad d = 1, \quad e = 10^{-9}, \quad f = \frac{e}{10^{-9}},$$

the titration curve depicted in Figure 5.5 is computed by first integrating system (5.17) forward with initial acetic acid concentration 0.1 mol/l until an equilibrium pH is reached, which is approximately 2.88. The equilibrium values of the states are used as initial conditions for the states during the
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titration simulation (see Exercise 5.14). An initial $OH^-$ concentration is set and the states are evolved forward in time (by numerical integration) until (an approximation of) equilibrium is reached. The corresponding pH is then plotted as a function of the initial $OH^-$. The figure shows a buffering region with relatively unchanged pH for low concentrations of the base, a region of rapid pH increase, and a region of high pH for the addition of high concentrations of the base.

The steep change in pH in Figure 5.5 is not an obvious prediction from the model. Why does this happen? To explain this phenomenon without numerical approximations, let us consider the steady states in more detail.

The dynamical system (5.17) has two first-integrals:

$$x + y = 0, \quad z - y - w$$

(see the discussion on page 50.) Using the chemistry at the initial time—which is after the acid solution is in equilibrium and at the instant the base is added, we have that $y = x(0) - x$ and $w = z - y + w(0)$. We may reduce our model to the two-dimensional system

$$\dot{y} = a(x(0) - y) - byz - ey + f(x(0) - y)(z - y + w(0)), \quad (5.18)$$
$$\dot{z} = a(x(0) - y) - byz + c - dz(z - y + w(0)). \quad (5.19)$$

Using the parameter values

$$a = 10^5, \quad b = 10^{10}, \quad c = 10^{-14}, \quad d = 1, \quad e = 10^{-9}, \quad f = 1.$$  

The equations for the steady states—the right-hand sides of the differential equations set to zero—have some small and some large coefficients. Inspection of these coefficients suggests defining $\mu$, a new parameter that has value $10^{-5}$ in our model, so that the coefficients are expressed in the form

$$a = 1/\mu, \quad b = 1/\mu^2, \quad c = 10\mu^3, \quad d = 1, \quad e = 10\mu^2, \quad f = 1.$$  

We may treat $\mu$ as an order parameter (which orders the relative sizes of the coefficients) and reduces the number of parameters. The equations for the steady states are equivalent to

$$\begin{align*}
-10yz + (1 - 10y)\mu + (w(0) - y - 10w(0)y + 10y^2 + z - 10yz)\mu^2 - 100y\mu^4 &= 0, \\
-10yz + (1 - 10y)\mu - (10w(0)z - 10yz + 10z^2)\mu^2 + 100\mu^5 &= 0.
\end{align*} \quad (5.20)$$
We may solve for the state variable $y$ in the second equation, where it appears linearly, and substituting this solution into the first equation. A minor miracle occurs: the equation for $z$ factors and the desired steady state is the positive root of the cubic polynomial

$$p(z) := -10w(0)z^2 - 10z^3 + z\mu - 10w(0)z\mu - 10z^2\mu + 100z\mu^3 + 100\mu^4.$$  

The pH is $-\log_{10} z$. The derivative of this expression with respect to $w(0)$ is

$$\frac{-1}{z} \frac{dz}{dw(0)} = \frac{10(z + \mu)}{20w(0)z + 30z^2 + (10w(0) - 1)\mu + 20z\mu - 100\mu^3}.$$  

The rate of change of the pH with respect to $w(0)$ is large near values of $z$ that are nearly roots of both the cubic polynomial $p$ and its derivative with respect to $z$. If we ignore terms of order at least four in $\mu$, then $z = 0$ is such a point provided that $w(0) = 1/10$. Thus, for $z$ near zero (as it must be when the base and the acid are both close to being neutralized), we expect the pH to have a large derivative for $w(0)$ near $1/10$, which explains the numerical result depicted in Figure 5.5 (compare, Exercise 5.16).

The kinetic theory expressed in the models discussed here predicts phenomena that are in complete agreement with physical experiments. Thus, we may have a high level of confidence that the underlying theory is correct. To make such a statement about a class of mathematical models is satisfying; the validation (and invalidation) of models is of course a strong motivation for doing applied mathematics.

**Exercise 5.13.** Redraw Figure 5.4 using the improved titration model. Is there a difference?

**Exercise 5.14.** Redraw Figure 5.5 using an alternative method: do not integrate the differential equations; solve for the steady states. Which method is more efficient?

**Exercise 5.15.** Redraw Figure 5.5 using the cubic polynomial (5.21) to solve for $z$ as a function of $w(0)$.

**Exercise 5.16.** (a) The roots of the cubic polynomial $p$ in equation (5.21) may be determined explicitly using Cardano’s formula. Can it be used to explain the shape of titration curves? (b) It is possible to determine the discriminant of a cubic. It is zero exactly when the cubic has a multiple root. The discriminant is
also equal to the resultant of the cubic and its first derivative. Find the lowest order approximation in powers of $\mu$ for the discriminant of $p$ and show that it vanishes for $w(0) = 1/10$. Hint: Learn the meaning of the concepts mentioned in the problem: discriminant and resultant.

**Exercise 5.17.** A titration of 0.1 molar acetic acid with sodium hydroxide is discussed in the section. The point of mutual neutralization occurs for the addition of approximately 0.1 mole of the base. Repeat the analysis, using the same methods, for titration of 0.3 molar acetic acid with sodium hydroxide.

**Problem 5.18.** The titration curve depicted in Figure 5.5 is obtained by a static model; that is, we set the new $OH$ concentration, integrate to steady state, determine the pH and iterate this process. A dynamic model would predict results for a titration where the sodium hydroxide solution is poured continuously into the acetic acid solution. Model (5.15) is a first approximation of such a model. Create a model that can be used to predict titration curves consistent with Figure 5.5.

### 5.4 Reaction, Diffusion, and Convection

Conservation of mass is a fundamental physical law used to model many physical processes.

#### 5.4.1 Fundamental and Constitutive Model Equations

Let us suppose that some substance (considered to have mass) is distributed in $\mathbb{R}^n$ and let $\Omega$ denote a bounded region in $\mathbb{R}^n$ with boundary $\partial \Omega$ and outer normal $\eta$. The density of the substance is represented by a function $u: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$, where $u(x, t)$ is the numerical value of the density in some units of measurement at the site with coordinate $x \in \mathbb{R}^n$ at time $t$.

The time rate of change of the amount of the substance in $\Omega$ is given by the negative flux of the substance through the boundary of $\Omega$ plus the amount of the substance generated in $\Omega$; that is,

$$\frac{d}{dt} \int_{\Omega} u \, d\mathcal{V} = -\int_{\partial\Omega} X \cdot \eta \, d\mathcal{S} + \int_{\Omega} f \, d\mathcal{V},$$

where $X$ is the velocity vector field (sometimes called the diffusion flux) of the substance (with units of mass per area per time); $d\mathcal{V}$ is the volume element; $d\mathcal{S}$ is the surface element; the vector field $\eta$ is the outer unit normal
field on the boundary of $\Omega$; and $f$, a function of density, position and time, represents the amount of the substance generated in $\Omega$ per volume per time. The minus sign on the flux term is required because we are measuring the rate of change of the amount of substance in $\Omega$. If, for example, the flow is all out of $\Omega$, then $X \cdot \eta \geq 0$ and the minus sign is required because the rate of change of the amount of substance in $\Omega$ must be negative.

Using the divergence theorem (also called Gauss’s theorem) to rewrite the flux term and by interchanging the time derivative with the integral of the density, we have the relation

$$\int_{\Omega} u_t d\mathcal{V} = -\int_{\Omega} \text{div} X d\mathcal{V} + \int_{\Omega} f d\mathcal{V}.$$  

Moreover, because the region $\Omega$ is arbitrary in this integral identity, it follows that

$$u_t = -\text{div} X + f. \quad (5.22)$$

To obtain a useful dynamical equation for $u$ from equation (5.22), we need a constitutive relation between the density $u$ of the substance and the flow field $X$. It is not at all clear how to derive this relationship from the fundamental laws of physics. Thus, we have an excellent example of an important problem where physical intuition must be used to propose a constitutive law whose validity can only be tested by comparing the results of experiments with the predictions of the corresponding model. Problems of this type lie at the heart of applied mathematics and physics.

For equation (5.22), the classic constitutive relation—called Darcy’s, Fick’s, or Fourier’s law depending on the physical context—is

$$X = -K \text{grad} u + \mu V \quad (5.23)$$

where $K \geq 0$ and $\mu$ are functions of density, position, and time; and $V$ denotes the flow field for the medium in which our substance is moving. The minus sign on the gradient term represents the assumption that the substance diffuses from higher to lower concentrations.

By inserting the relation (5.23) into the balance law (5.22), we obtain the dynamical equation

$$u_t = \text{div}(K \text{grad} u) - \text{div}(\mu V) + f. \quad (5.24)$$

Also, if we assume that the diffusion coefficient $K$ is equal to $k^2$ for some constant $k$, the function $\mu$ is given by $\mu(u, x, t) = \gamma u$ where $\gamma$ is a constant,
and $V$ is an incompressible flow field ($\text{div} V = 0$); then we obtain the most often used reaction-diffusion-convection model equation

$$u_t + \gamma \text{grad } u \cdot V = k^2 \Delta u + f. \quad (5.25)$$

In this equation, the gradient term is called the convection term, the Laplacian term is called the diffusion term, and $f$ is the source term.

Let us also note that if the diffusion coefficient is zero, the convection coefficient is given by $\gamma = 1$, the source function vanishes, and $V$ is not necessarily incompressible, then the dynamical equation (5.24) reduces to the law of conservation of mass, also called the continuity equation, given by

$$u_t + \text{div}(uV) = 0. \quad (5.26)$$

Because equation (5.25) is derived from general physical principles, this PDE is used to model all physical processes where reaction, diffusion, or convection is involved.

In case the substrate medium is stationary (that is, $V = 0$), the model equation (5.25) is the diffusion (or heat) equation with a source

$$u_t = k^2 \Delta u + f. \quad (5.27)$$

Using Fourier’s law, this equation is the basic model equation for heat flow.

The derivation of the model equation (5.25) should help to explain the widespread appearance of the Laplacian in applied mathematics: It is the divergence of the gradient vector field that we suppose carries some substance from higher to lower concentrations.

**Exercise 5.19.** Show that the gradient of a function evaluated at a point $p$ points in the direction of maximum increase of the function at $p$. Also, the gradient is orthogonal to each level set of the function at each point on a level set.

**Exercise 5.20.** Discuss the meaning of the divergence of a vector field. In particular, discuss positive divergence, negative divergence, and zero divergence. Give examples. Hint: You may wish to consider the equation

$$\text{div } X(p) = \lim_{\Omega \to \{p\}} \frac{1}{\text{vol}(\Omega)} \int_{\partial \Omega} X \cdot \eta \, dS.$$
5.4.2 The Reaction-Diffusion Model in One Spatial Dimension

One-dimensional Diffusion

Let us consider the diffusion of heat in a bar with insulated ends (that is, zero heat flux through each end of the bar) under the assumptions that the temperature in every cross-section perpendicular to the bar’s axis has uniform temperature and there are no heat sources or sinks along the bar. We are given the initial temperature distribution along the bar. The problem is to determine the temperature as time increases.

Under our assumptions, we need only consider the spatial distribution of heat along the axis of the bar that we idealize as an interval of real numbers. For a bar of length $L$, we thus let $x$ in the open interval $(0, L)$ denote the spatial coordinate. The basic model equation (5.27) with no heat sources or sinks in this case is

$$u_t = \kappa u_{xx}, \quad (5.28)$$

where $u(x, t)$ is the temperature at position $x$ along the bar at time $t \geq 0$ and $\kappa > 0$ is a constant (called the diffusivity) that depends on the material used to construct the bar. The value of $\kappa$ must be determined by experiment.

A function $f : (0, L) \rightarrow \mathbb{R}$ representing the initial temperature along the bar gives the initial condition

$$u(x, 0) = f(x). \quad (5.29)$$

Zero flux conditions at each end of the bar provide the boundary conditions

$$u_x(0, t) = 0, \quad u_x(L, t) = 0. \quad (5.30)$$

These boundary conditions are also called the zero Neumann boundary conditions.

The problem is to find a function $u$ that satisfies the partial differential equation (5.28), the initial condition (5.29), and the boundary conditions (5.30). This is a classic problem first solved by Joseph Fourier in 1822. His basic ideas, which have far reaching consequences, are milestones in the history of science. Fourier’s law of heat conduction—heat flows from regions of high temperature to regions of lower temperature—In the derivation of the PDE (5.28). His mathematical solution of our heat problem uses another important innovation called Fourier series, which will be introduced here.
A fundamental idea that often works for linear PDEs whose spatial domains are rectangular is separation of variables. We simply look for solutions in the form \( u(x, t) = X(x)T(t) \), where \( X \) and \( T \) are unknown functions. Inserting this guess into our PDE yields the formula

\[
X(x)T'(t) = \kappa X''(x)T(t),
\]

which must hold if \( X(x)T(t) \) is a solution. Let us assume for the moment that \( X(x) \) and \( T(t) \) do not vanish and rearrange the last formula to the form

\[
\frac{T'(t)}{\kappa T(t)} = \frac{X''(x)}{X(x)}.
\]

If \( X(x)T(t) \) is a solution that does not vanish, the left-hand side of the equation a function of \( t \) alone and the right-hand side a function of \( x \) alone. This implies that the left-hand side and the right-hand side of the equation are equal to the same constant \( c \). In other words, there must be a constant \( c \) such that

\[
T'(t) = c\kappa T(t), \quad X''(x) = cX(x);
\]

that is, \( X \) and \( T \) must be solutions of the given ordinary differential equations.

The ODE \( X''(x) = cX(x) \) is easily solved for each of the usual cases: \( c > 0 \), \( c = 0 \), and \( c < 0 \). Indeed, for \( c = \lambda^2 > 0 \), the general solution is

\[
X(x) = ae^{\lambda x} + be^{-\lambda x},
\]

for \( c = 0 \),

\[
X(x) = ax + b;
\]

and, for \( c = -\lambda^2 < 0 \),

\[
X(x) = a \cos \lambda x + b \sin \lambda x.
\]

Our solution must satisfy the boundary conditions. This is possible only for \( c = 0 \) and \( X(x) = b \) or \( c < 0 \) and

\[
X(x) = a \cos \frac{n\pi}{L}x,
\]

where \( n \) is an integer. Since cosine is an even function, all of the solutions for \( c < 0 \) are obtained with \( n \) ranging over the non-negative integers.
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For \( c = -\lambda^2 = -\left(\frac{n\pi}{L}\right)^2 \), the corresponding solution of \( T'(t) = c\kappa T(t) \) is

\[
T(t) = e^{-(\kappa n^2 \pi^2 / L^2) t}.
\]

Thus we have constructed an infinite number of solutions:

\[
u_n(x, t) = X_n(x) T_n(t) = e^{-(\kappa n^2 \pi^2 / L^2) t} \cos \frac{n\pi}{L} x, \quad n = 0, 1, 2, \ldots, \infty.
\]

By a simple calculation, if \( u \) and \( v \) are solutions of our PDE and boundary conditions, then so is every linear combination (also called superposition) \( au + bv \), where \( a \) and \( b \) are scalars. It follows that every finite sum

\[
u(x, t) = b_0 + \sum_{n=1}^{N} b_n e^{-(\kappa n^2 \pi^2 / L^2) t} \cos \frac{n\pi}{L} x
\]

is a solution of the PDE and the boundary conditions.

What about the initial condition? One fact is clear: If

\[
f(x) = b_0 + \sum_{n=1}^{N} b_n \cos \frac{n\pi}{L} x
\]

for some choice of \( b_0, b_1, b_2, \ldots, b_N \), then the function \( u \) in display (5.31) is a solution of our PDE, boundary conditions, and initial conditions. This result suggests the question: Which functions \( f \) can be written as a sum of cosines? The surprising answer, first given by Fourier, is that most functions defined on the interval \([0, L]\) can be written as an infinite sum of cosines (or sines). We will discuss this result in more detail in subsequent sections. A more precise statement is that every function \( f \) defined on \([0, L]\) that is continuously differentiable, except possibly at a finite number of jump discontinuities, can be represented by a convergent Fourier cosine series; that is,

\[
f(x) = b_0 + \sum_{n=1}^{\infty} b_n \cos \frac{n\pi}{L} x.
\]

This is a very powerful result. With it, we know that our model equation has a solution for all initial conditions we are likely to encounter. In fact, once we have expressed the initial condition \( f \) as a Fourier series,

\[
u(x, t) := b_0 + \sum_{n=1}^{\infty} b_n e^{-(\kappa n^2 \pi^2 / L^2) t} \cos \frac{n\pi}{L} x
\]
is a solution of our PDE with its boundary and initial conditions.

It turns out that there is a simple method to determine the Fourier coefficients $b_n$ of a function $f$ defined on $[0, L]$. Fourier’s theorem tells us that our function $f$ may be expressed as in display (5.32) and that the sum on the right-hand side of the equation may be integrated term-by-term. Thus,

$$\int_0^L f(x) \, dx = \int_0^L b_0 \, dx + \sum_{n=1}^{\infty} \int_0^L b_n \cos \frac{n\pi}{L} x \, dx.$$

Every integral in the infinite summation vanishes. Hence,

$$b_0 = \frac{1}{L} \int_0^L f(x) \, dx.$$

For each positive integer $m$, we have that

$$\int_0^L f(x) \cos \frac{m\pi}{L} x \, dx = \int_0^L b_0 \cos \frac{m\pi}{L} x \, dx + \sum_{n=1}^{\infty} \int_0^L b_n \cos \frac{n\pi}{L} x \cos \frac{m\pi}{L} x \, dx.$$

As before, the first integral on the right-hand side of the equation vanishes. The integrals of products of cosines behave in the best possible way: they all vanish except for the product where $n = m$. (Check this statement carefully; it is a basic result that makes Fourier series useful.) Using this fact,

$$\int_0^L f(x) \cos \frac{m\pi}{L} x \, dx = \int_0^L b_m \cos^2 \frac{m\pi}{L} x \, dx = b_m \frac{L}{2},$$

and we have the general formula

$$b_m = \frac{2}{L} \int_0^L f(x) \cos \frac{m\pi}{L} x \, dx.$$

All the Fourier coefficients may be computed simply by integrating the product of the given function and an appropriate cosine. A similar result holds for Fourier sine series. Indeed, a function $f$ in the same class of functions may be represented as the Fourier sine series

$$f(x) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi}{L} x.$$
We have constructed a solution of our initial boundary value problem. But, it would be useless for applied mathematics if there were more than one solution. Which solution would we choose? Fortunately, it is easy to show that our solution is unique. Suppose on the contrary that there were two solutions \( u \) and \( v \). By superposition, \( w := u - v \) is also a solution of the same boundary value problem but with zero initial condition; that is,

\[
w_t = \kappa w_{xx}, \quad w(x, 0) = 0, \quad w_x(0, t) = 0, \quad w_x(L, t) = 0.
\]

Note that

\[
\int_0^L w_t w \, dx = \int_0^L \kappa w_{xx} w \, dx.
\]

By an application of integration by parts on the right-hand integral and taking the time-derivative outside the left-hand integral, we have the equality

\[
\frac{d}{dt} \int_0^L \frac{1}{2} w^2 \, dx = \kappa w_w \big|_0^L - \int_0^L w_x^2 \, dx.
\]

Using the boundary conditions,

\[
\frac{d}{dt} \int_0^L \frac{1}{2} w^2 \, dx = -\kappa \int_0^L w_x^2 \, dx.
\]

It follows that

\[
\int_0^L \frac{1}{2} w^2 \, dx
\]

is a non-negative function that does not increase as \( t \) increases. But, at \( t = 0 \), the initial condition is \( w = 0 \). Hence, \( w \) must be the zero function for all \( t > 0 \) for which the solution exists; and, \( u = v \), as desired.

The analytic solution of our diffusion model equation solves can be used to answer questions and make predictions from the model. When we add heat sources and sinks to our model or make other modifications, especially those that produce nonlinear terms, our analytic solution method will likely fail. In these cases we may use approximate solutions obtained with numerical computations. Our diffusion model serves as a simple example to illustrate a method for approximating the solutions of partial differential equations.

To make a numerical computation, we must be given the diffusivity \( k \), the length of the spatial domain \( L \) and the initial data \( f \). The first step is to discretize space and time. This may be done by choosing a positive integers.
\[ N \text{ with corresponding spatial increment } \Delta x := L/N, \text{ a temporal increment } \Delta t, \text{ and agreeing to consider the value of } u \text{ only at the interior spatial domain points with coordinates } x_i := i\Delta x = iL/N \text{ for } i = 1, 2 \ldots N - 1 \text{ and temporal coordinates } j\Delta t \text{ for } j = 0, 1, 2, \ldots, \text{ where we leave open the number of time-steps we plan to compute. In other words, we will approximate the values of } u \text{ at the interior grid-points } U_i^j = u(i\Delta x, j\Delta t). \]

Having discretized space and time, we will also discretize the PDE by approximating the time and space derivatives. For this, we use Taylor theorem. Recall that for a function \( f \) that is \((n + 1)\)-times continuously differentiable at a point \( a \), the value of \( f \) at a nearby point \( x \) is given by

\[
\begin{align*}
f(x) &= f(a) + f'(a)(x - a) + \frac{1}{2!} f''(a)(x - a)^2 + \frac{1}{3!} f'''(a)(x - a)^3 \\
&\quad + \cdots + \frac{1}{n!} f^n(a)(x - a)^n + \frac{1}{(n + 1)!} f^{n+1}(c)(x - a)^{n+1} \\
\end{align*}
\]  

for some number \( c \) that lies between \( a \) and \( x \). We often say that the right-hand side of the last formula is the taylor expansion of the function \( f \) at \( a \). Let us consider a point \( (x, t) \) and the nearby point \( (x, t + \Delta t) \). By an application of Taylor’s formula to the function \( \Delta t \mapsto u(x, t + \Delta t) \) at \( \Delta t = 0 \), we have the expansion

\[
u(x, t + \Delta t) = u(x, t) + u_t(x, t)\Delta t + \frac{1}{2!} u_{tt}(x, c)\Delta t^2.
\]

A rearrangement yields the equation

\[
u_t(x, t) = \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} - \frac{1}{2!} u_{tt}(x, c)\Delta t.
\]

and the approximation

\[
u_t(x, t) \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t}
\]

with an error of order \( \Delta t \). Using our discretization, we may approximate the left-hand side of our PDE by

\[
u_t(i\Delta x, j\Delta t) \approx \frac{U_{i+1}^j - U_i^j}{\Delta t}.
\]  

(5.35)
By a similar procedure, note that up to an error of fourth-order in $\Delta x$,

$$u(x - \Delta x, t) = u(x, t) - u_x(x, t)\Delta x + \frac{1}{2}u_{xx}(x, t)\Delta x^2 - \frac{1}{3!}u_{xxx}(x, t)\Delta x^3,$$

$$u(x + \Delta x, t) = u(x, t) + u_x(x, t)\Delta x + \frac{1}{2}u_{xx}(x, t)\Delta x^2 + \frac{1}{3!}u_{xxx}(x, t)\Delta x^3.$$

These equations may be added and rearranged to obtain the approximation

$$u_{xx}(x, t) \approx \frac{u(x - \Delta x, t) - 2u(x, t) + u(x + \Delta x, t)}{\Delta x^2}$$

with an error of order $\Delta x^2$, which is better than our approximation of the time derivative. Using our discretization, we may approximate the right-hand side of our PDE by

$$u_{xx}(i\Delta x, j\Delta t) \approx \frac{U_{j+1}^i - 2U_j^i + U_{j-1}^i}{\Delta x^2}.$$  (5.36)

By equating the approximations (5.35) and (5.36) and rearranging the result, we have the discrete approximation of our PDE

$$U_{j+1}^i = U_j^i + \frac{\kappa \Delta t}{\Delta x^2}(U_{j-1}^i - 2U_{j}^i + U_{j+1}^i).$$  (5.37)

The left-hand side of equation (5.37) is the value of $u$ at the $(j + 1)^{\text{st}}$ time step; all values of $u$ on the right-hand side are evaluated at the $j^{\text{th}}$ time step. Since we are given the values of $u$ at the zeroth time step via the initial condition, we may simply bootstrap up to any desired time by iteration. Well, almost... We have not yet taken into account the boundary conditions. For example, we are given the values of $U_0^i$ for $i = 1, 2, 3 \ldots N - 1$. To obtain the values at $U_1^i$ we need $U_0^0$ at the left end and $U_N^0$ at the right end of the bar. As a simple approximation of the Neumann boundary conditions (which require $u_x$ to vanish at each end), we may insist that for all time steps

$$U_0^j = U_1^j, \quad U_N^j = U_{N-1}^j.$$  (5.38)

If $u$ is constant over the intervals $[x_0, x_1]$ and $[x_{N-1}, x_N]$, then $u_x$ is zero at the ends of the bar, which have spatial coordinates $x_0$ and $x_N$. This is of course not the only possible method to insure the boundary conditions are met; but, at least, it is simple to implement in a computer code.
All the ingredients are now in place to approximate the PDE (5.28) with Neumann boundary conditions (5.30) and initial condition (5.29) on a computer. Simply impose the end conditions (5.38) at each step, set \( j = 1 \) and compute \( U_i^1 \) for \( i = 1, 2, 3, \ldots N - 1 \) using the equation (5.37), repeat the process to compute \( U_i^2 \) using the previously computed values \( U_i^1 \), and continue the same way in general to compute \( U_i^{j+1} \) over \( i = 1, 2, 3, \ldots N - 1 \) using the previously computed values \( U_i^j \). The process is stopped when the product of the number of steps and the increment \( \Delta t \) reaches the desired final time.

Our numerical scheme may also be viewed in vector form. Define the \( N - 1 \)-vector \( W^j \) to be the transpose of the row vector \((U_1^j, U_2^j, U_3^j, \ldots, U_{N-1}^j)\), let \( \alpha = \kappa \Delta t / \Delta x^2 \), and define the \((N - 1) \times (N - 1)\)-matrix \( A \) whose main diagonal is \( (1 - \alpha, 1 - 2\alpha, 1 - 2\alpha, 1 - 2\alpha, \ldots, 1 - 2\alpha, 1 - \alpha) \) (that is, the first and last components are \( 1 - \alpha \) and the other components are all \( 1 - 2\alpha \)), and whose first super-diagonal and first sub-diagonal elements are all \( \alpha \). In case \( N = 5 \), the matrix is

\[
A = \begin{pmatrix}
1 - \alpha & \alpha & 0 & 0 \\
\alpha & 1 - 2\alpha & \alpha & 0 \\
0 & \alpha & 1 - 2\alpha & \alpha \\
0 & 0 & \alpha & 1 - \alpha
\end{pmatrix}.
\]

The iteration scheme (5.37) may be written in the compact form

\[
W^{j+1} = AW^j.
\]

In other words, the iteration scheme is simply matrix multiplication by \( A \). The special first and last rows of \( A \) are due to the Neumann boundary conditions.

The initial vector \( W^0 \) is given by the initial condition for the PDE. The numerical scheme is implemented by iteration: \( W^1 = AW^0, W^2 = AW^1, \) and so on; or, in a more compact form

\[
W^{j+1} = A^j W^j
\]

where \( A^j \) means the \( j \)th power of the matrix \( A \) and \( W^j \) means the \( j \)th element in the sequence whose first three elements are \( W^1, W^2, \) and \( W^3 \).

Our numerical scheme has at least two potential difficulties: The approximation of the time derivative \( u_t \) by our discretization is less accurate than our approximation of the spatial derivative \( u_{xx} \), and numerical instabilities
will occur unless the temporal and spatial discretizations are chosen appropriately. Alternative numerical methods that overcome the first difficulty will be discussed in Section 5.4.4.

The condition for numerical stability is

$$\kappa \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}. \quad (5.39)$$

This requirement is explained in Section 5.4.4. Numerical instabilities that lead to meaningless numerical results are likely to occur if this condition, called the Courant-Friedricks-Lewy condition, is not met (see Exercise 5.25). In practice, the Courant-Friedricks-Lewy condition determines the maximum allowable time-step size for our numerical method after a spatial discretization is set.

To give some indication of how the Courant-Friedricks-Lewy condition arises, suppose that a roundoff error is introduced in the computer at the first computational step. Instead of computing $W^1$, the machine computes $W^1 + \epsilon$ (where $\epsilon$ is an $N-1$-vector representing the error). Of course, further errors might be introduced at subsequent steps. But, for simplicity, consider the propagation of the first error only and assume that after the first error occurs the arithmetic is exact. Under these conditions, we will compute

$$W^2 = AW^1 + A\epsilon, \quad W^3 = A^2W^1 + A^2\epsilon, \quad W^4 = A^3W^1 + A^3\epsilon, \ldots.$$ 

The error propagates as $A^j\epsilon$. Our method will produce useless results if the norm of this propagated error grows as $j$ increases.

What would happen if the matrix $A$ were the diagonal $2 \times 2$-matrix

$$A = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}?$$

Clearly

$$A^j = \begin{pmatrix} a^j & 0 \\ 0 & b^j \end{pmatrix}.$$ 

If either $|a| > 1$ or $|b| > 1$ and there is a corresponding nonzero element of the vector $\epsilon$, then the size of the propagated error will grow. For example, if $|b| > 1$ and $\epsilon$ is the transpose of the vector $(0.01, 0.035)$ the number $b^j0.035$ will grow to infinity as $j$ goes to infinity. In this case, roundoff errors will be amplified under iteration and our numerical approximation of the PDE will
become useless. On the other hand, if both \( |a| \) or \( |b| \) are less than or equal to one, then the propagated error will remain bounded as \( j \) goes to infinity. The same is true for general diagonal matrices.

The matrix \( A \) for our numerical scheme is not diagonal. But, it has a special form: \( A \) is symmetric; that is, \( A \) is equal to its transpose. Every symmetric matrix is diagonalizable; in other words, if \( A \) is symmetric, then there is an invertible matrix \( B \) such that \( B^{-1}AB \) is diagonal. Also, every eigenvalue of a symmetric matrix is real. Using these facts, let us suppose that every eigenvalue of our matrix \( A \) lies in the closed interval \([-1, 1]\). The matrix \( C := B^{-1}AB \) has the same eigenvalues as \( A \). (Why?). Iterations of a vector \( v \) by \( C \) remain bounded because \( C \) is diagonal and all its eigenvalues have absolute value less than or equal to one. In fact,

\[
|C^j v| \leq |v|
\]

for all vectors \( v \) and all positive nonzero integers \( j \). Iteration of \( v \) by the matrix \( A \) also remains bounded because

\[
|A^j v| = |(BCB^{-1})^j v| \leq |BC^j B^{-1} v| \leq \|B\| \|B^{-1} v\| \leq \|B\| \|B^{-1}\| |v|.
\]

In fact, if the Courant-Friedricks-Lewy condition (5.39) is satisfied, all eigenvalues of \( A \) are in the closed interval \([-1, 1]\) (see Section 5.4.4).

**Exercise 5.21.** (a) Solve the diffusion equation on the spatial domain \([0, L]\) with initial condition and zero Dirichlet boundary conditions:

\[
 u_t = \kappa u_{xx}, \quad u(x, 0) = f(x), \quad u(0, t) = 0, \quad u(L, t) = 0.
\]

(b) Show that your solution is unique.

**Exercise 5.22.** Solve the diffusion equation on the spatial domain \([0, L]\) with initial condition and non zero Neumann boundary conditions:

\[
 u_x(0, t) = a, \quad u_x(L, t) = b,
\]

where \( a \) and \( b \) are real numbers. Hint: Look for a solution \( u = v + w \), where \( v \) is a function that satisfies the boundary conditions and \( w \) satisfies the PDE with zero boundary conditions.

**Exercise 5.23.** Solve the diffusion equation on the spatial domain \([0, L]\) with initial condition and non zero Dirichlet boundary conditions:

\[
 u(0, t) = a, \quad u(L, t) = b,
\]

where \( a \) and \( b \) are real numbers.
Exercise 5.24. The zero flux boundary condition for the diffusion equation has the physical interpretation that no substance is lost as time increases. Prove this fact by showing that the time-derivative of the total amount of substance (its integral over the spatial domain) vanishes.

Exercise 5.25. (a) Write a computer code to implement the method described in this section to approximate the solution of the diffusion equation in one space-dimension on a finite interval with Neumann boundary conditions and given initial conditions. As a test case, consider the spatial domain to be one unit in length, the diffusivity $\kappa = 1$, and the initial data given by $f(x) = 1 + \cos \pi x$. Compare your numerical results with the analytic solution. (b) Test the Courant-Friedricks-Lewy number by choosing at least the discretizations $\Delta t/\Delta x^2 = 0.4$ and $\Delta t/\Delta x^2 = 0.6$. Discuss your results.

Exercise 5.26. The following is a constitutive model for the ink diffusion experiment in Section 3.3: Let $u(x, t)$ denote the concentration of ink at position $x$ at time $t$ and $L$ the trough length. Also let $a$ and $b$ be positive constants. The model equation of motion for $u$ is the initial boundary value problem

$$u_t = \kappa u_{xx}, \quad u_x(0, t) = u_x(L, t) = 0, \quad u(x, 0) = \begin{cases} a, & 0 \leq x \leq b, \\ 0, & x > b. \end{cases}$$

(a) What constitutive law is used to construct this model? (b) Show that the model predicts the presence of ink at every position along the trough for every positive time. Does this fact invalidate the model? (c) Show that the model predicts that the total amount of ink remains constant in time. (d) Define the diffusion front to be the largest distance from the origin where the ink concentration is 1% of $a$. Use the model to determine the diffusion front. If necessary, choose values for the parameters in the problem. (e) Is the distance of the diffusion front from the origin a linear function of time? If not, what type is this function? (f) Calibrate the model to the data given in Section 3.3 and discuss the model prediction in view of the experimental data. (g) Construct a model that takes into account two (or three) space dimensions. Compare the new front speed with the front speed obtained for the one-dimensional model. (h) Can you refine the model to give a more accurate representation of the diffusion experiment? You may wish to perform a similar diffusion experiment.

Propagation of a Mutant Gene

Consider a population with a mutant gene whose concentration is $u$. Its allele (the parent gene) has concentration $1 - u$. The individuals in the population
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diffuse along a one-dimensional spatial domain (for example a shoreline) and they interact with each other to produce offspring. A simple model (introduced in 1937 independently by R. A. Fisher [26] and A. N. Kolmogorov, I. Petrovskii and N. Piscounov [39]) is

$$u_t = \kappa u_{xx} + au(1 - u).$$

(5.40)

The choice of the model interaction term, given by $f(u) = au(1 - u)$, may be more fully justified using probability theory (see [39]). This term is perhaps the simplest model of interaction (a product) that agrees (qualitatively) with experiments. The constant $a$ is meant to model the utility of the gene for the organism to survive: $a > 0$ for an advantageous mutation; $a < 0$ for a disadvantageous mutation.

There is a natural scientific question: How will an advantageous mutation spread if it occurs in some individual or group of individuals at a specified spatial location?

The quantity $u(x, t)$ is the number of individuals at time $t$ at shoreline position $x$ with the mutant gene divided by the total number of individuals in the population at $x$. Of course this is an idealization. In reality, we would measure this ratio over some area (a fixed width times a length of shoreline). The concentration is more precisely defined to be the limit of this ratio as the area of the region shrinks to zero at $x$ for the fixed time $t$. Thus, $u$—the ratio of two tallies—is a dimensionless quantity. The time-derivative $u_t$ has the dimensions of inverse time. In symbols, we write $[u_t] = 1/T$, where in this formula the square brackets denote units of the enclosed expression and $T$ denotes the unit of time (perhaps $T$ is years). The diffusion term has units $[\kappa u_{xx}] = [\kappa]/L^2$. These must agree with the units of the time derivative. Thus, $[\kappa]/L^2 = 1/T$ and $[\kappa] = L^2/T$. Likewise, the units of the interaction term are carried by $a$ and $[a] = 1/T$; thus, $a$ has the appropriate units for a rate.

We are unlikely to know good values of the diffusivity $\kappa$ (a measure of how fast the organisms carrying the mutant gene spread along the shoreline) or $a$ (which is the growth rate of the population with the mutant gene). Thus, we should not expect to make reliable quantitative predictions; rather, we should use the model to predict the qualitative behavior of the spread of a mutant gene.

The qualitative behavior of the solutions of our model are independent of the (positive) parameters $\kappa$ and $a$. In fact, we can simply eliminate the
Figure 5.6: Graphs of the spatial distribution of the mutant gene modeled by PDE (5.42) at times $t = 5, 15, 30$ and $45$ are depicted for the condition (5.43) with $a = -2$, $b = 2$, and $\mu = 0.01$. The plotted curves are thicker as time increases. The numerical method is forward Euler on the spatial domain $[-100, 100]$ with Neumann boundary conditions, time step $0.25$, and a spatial grid of $200$ interior points.

By substitution into the model PDE (5.40), we have

$$
\frac{1}{\tau} u_s = \kappa \frac{1}{\ell^2} u_{\xi \xi} + au(1-u)
$$

and, by rearranging, the equation

$$
u_s = \kappa \frac{\tau}{\ell^2} u_{\xi \xi} + \tau au(1-u).
$$

We may choose

$$
\tau = \frac{1}{a}, \quad \ell = \sqrt{\frac{\kappa}{a}}.
$$

(5.41)
to obtain the desired dimensionless model equation

\[ u_s = u_{\xi\xi} + u(1 - u). \]

Reverting to the usual notation, we will discuss the PDE

\[ u_t = u_{xx} + u(1 - u). \quad (5.42) \]

For our biological problem, we may consider the PDE for \( x \) on the whole real line; or, we may impose the Dirichlet condition (\( u \) vanishes at the ends of the portion of the shoreline under consideration) or the Neumann condition (\( u_x \) vanishes at these points). Both make sense in this biological context.

The model (5.42) is a non-linear PDE; the superposition of solutions is generally not a solution. There is no known general explicit solution (cf. Exercise 5.27). But, it is possible to prove that unique solutions exist for appropriate initial conditions \( u(x, 0) = f(x) \) (see, for example, [59]). Let us assume these results.

We may gain some insight into the behavior predicted from this model by assuming there is no diffusion. In this case, we simply have the ODE \( \dot{u} = u(1 - u) \) (see Exercise 2.2). There are two steady states \( u = 0 \) and \( u = 1 \). Also, if \( 0 < u(0) < 1 \), then the corresponding solution \( u(t) \) grows monotonically to \( u = 1 \) as \( t \) goes to infinity. Thus, with the passage of time, the mutant gene eventually is established in the entire population at each location along the shoreline. Is this basic conclusion altered when the model takes diffusion (and thus spatial dependence) into account?

The next obvious step in our analysis is numerical experimentation. Let us suppose that the initial population with the mutant gene is localized to one place along the shoreline. This situation may be modeled by an initial \( u \) of the form

\[ u(x, 0) = f(x) = \begin{cases} 0; & x < a, \\ \mu; & a \leq x \leq b, \\ 0; & x > b, \end{cases} \quad (5.43) \]

where \( a < b \) and \( 0 < \mu \leq 1 \).

Some of the results of a typical numerical experiment are depicted in Figure 5.6. The spread of the mutant gene is a wave spreading in both directions from the spatial location of the initial population that carried the mutation. The wave speed for this simulation is approximately 10.

To help determine the wave speed in general, let us note that in our scaling (5.41), the characteristic velocity is length divided by time. Our
Figure 5.7: Graphs of the spatial distribution of the mutant gene modeled by PDE (5.42) at times $t = 20, 40, 60$ and $80$ are depicted for the condition (5.43) with $a = -100$, $b = -90$, and $\mu = 1$. The plotted curves are thicker as time increases. The numerical method is forward Euler on the spatial domain $[-100, 100]$ with Neumann boundary conditions, time step 0.1, and a spatial grid of 200 interior points.

The basic prediction obtained from our PDE model for the spread of a mutant gene from a location where the mutation arises is the spread of this gene as a wave moving in both directions away from the primary location with the concentration of the mutant gene approaching unity as the wave passes each remote location.

A related scenario is the spread of a mutant gene that is already dominant on one side of a location along our beach but not present on the other side. Some of the results of a numerical experiment are reported in Figure (5.7). These results suggest the local concentration of the mutant gene rises to dominate the population where the mutation is already present and it spreads
Figure 5.8: A portion of the phase portrait for the ODE system (5.49) with $c = 3$ is depicted. The flow crosses each thick line segment in the same direction. The thick curve is an approximate trajectory connecting the rest points at $(0, 0)$ and $(1, 0)$.

to the right at a constant speed with each location being fully saturated as the wave front passes. A mathematical idealization of this situation leads to the question: Is there a solution $u$ of the dimensionless model equation (5.42) such that

$$0 \leq u(x, t) \leq 1, \quad \lim_{t \to -\infty} u(x, t) = 0, \quad \lim_{t \to \infty} u(x, t) = 1? \quad (5.45)$$

The existence of a solution of this type would show that some solutions of the PDE have the same qualitative behavior as a solution of $\dot{u} = u(1 - u)$ (that is, the model differential equation without diffusion) with initial value $u(0)$ restricted to $0 < u(0) < 1$.

Inspection of the Figure (5.7) (or better yet an animation) suggests that the spatial concentration quickly approaches a wave that maintains its profile while moving to the right with constant velocity. Ideally, there is some function $\phi : \mathbb{R} \to \mathbb{R}$ such that

$$u(x, t) = \phi(x - ct), \quad (5.46)$$
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where \( c > 0 \) is the wave speed. A solution of this form is called a traveling wave with wave form \( \phi \).

By substitution of the formula (5.46) into the PDE (5.42), we obtain the differential equation

\[
-c\phi'(x - ct) = \phi''(x - ct) + \phi(x - ct)(1 - \phi(x - ct)),
\]

which we may view as an ordinary differential equation for the unknown wave profile \( \phi \) with auxiliary conditions

\[
0 \leq \phi \leq 1, \quad \lim_{s \to -\infty} \phi(s) = 1, \quad \lim_{s \to \infty} \phi(s) = 0.
\]

A basic fact is that if \( c \geq 2 \), then there is a solution of the ODE

\[
\dot{\phi} + c\dot{\phi} + \phi(1 - \phi) = 0 \quad (5.48)
\]

that satisfies the auxiliary conditions.

The second-order ODE (5.48) is equivalent to the system of ODEs

\[
\begin{align*}
\dot{\phi} &= v, \\
\dot{v} &= -cv - \phi(1 - \phi)
\end{align*} \quad (5.49)
\]

in the phase plane.

Our system (5.49) has two rest point in the phase plane \((0, 0)\) and \((1, 0)\). The rest point at the origin is asymptotically stable and the rest point at \((1, 0)\) is a saddle point. If \( c \geq 2 \), then the triangle depicted by thick line segments is positively invariant. The horizontal segment connects the rest points, the ray with negative slope is in the direction of the eigenspace corresponding to the negative eigenvalue of the linearized system matrix at \((0, 0)\) with the largest absolute value, and the ray with positive slope is in the direction of the eigenspace corresponding to the unstable manifold of the linearized system matrix at \((1, 0)\). For \( c < 2 \), the eigenvalues of the linearized system at the origin are complex. Thus, the incoming unstable trajectory from the saddle point winds around the origin and \( \phi \) has negative values, violating the condition that \( 0 \leq \phi \leq 1 \) (see [17] for a detailed proof and Exercise 5.34).

The connecting orbit in Figure (5.8) corresponds to the desired function \( \phi \) that defines a traveling wave solution. Of course, \( \phi \) is the first coordinate function of the corresponding solution of the ODE system (5.49). Its graph, which has the profile of the expected traveling wave, is depicted in
Figure 5.9: The figure depicts an approximation of the graph of the function \( \phi \) that is the first coordinate function of the solution of the ODE system (5.49) with \( c = 3 \) along the unstable manifold of the saddle point at \((1,0)\) that connects this point to the sink at the origin.

Figure 5.9. Kolmogorov, Petrovskii and Piscounov [39] proved that solutions of the PDE (5.42) with initial data such that \( 0 \leq u(x,0) \leq 1 \), \( u(x,0) = 1 \) for \( x \leq a \) and \( u(x,0) = 0 \) for \( x \geq b > a \) approach a traveling wave solution with wave speed \( c = 2 \) (see Exercise 5.33).

**Exercise 5.27.** Show that \( u(x,t) = \phi(x - ct) \) is a solution of the PDE (5.42) in case \( c = 5/\sqrt{6} \), \( K \) is a constant, and

\[
\phi(z) = (1 + Ke^{z/\sqrt{6}})^{-2}.
\]

**Exercise 5.28.** (a) Repeat the experiment reported in Figure 5.6. (b) Repeat the experiment with Dirichlet boundary conditions and compare the results.

**Exercise 5.29.** How does the speed of the wave front(s) of solutions of the PDE (5.42) depend on the amplitude of the initial population with the mutant gene?

**Exercise 5.30.** How does the speed of the wave front(s) of solutions of the PDE (5.42) depend on the length of the spatial interval occupied by the initial population with the mutant gene?

**Exercise 5.31.** Use numerical experiments to test the characteristic velocity approximation in display (5.44). Set an initial mutant gene concentration and vary the parameters \( \kappa \) and \( a \) in the PDE (5.40).
Exercise 5.32. Reproduce Figures 5.7–5.9.

Exercise 5.33. Use numerical experiments to verify the theorem of Kolmogorov, Petrovskii and Piscounov [39] that solutions of the PDE (5.42) with initial data such that \( 0 \leq u(x,0) \leq 1, u(x,0) = 1 \) for \( x \leq a \) and \( u(x,0) = 0 \) for \( x \geq b > a \) approach a traveling wave solution with wave speed \( c = 2 \).

Exercise 5.34. (a) Find the system matrix at each rest point of system 5.49, find the eigenvalues and eigenvectors, and determine the stability types of the rest points. Show the triangle as in Figure 5.8 is positively invariant by proving the vector field corresponding to the system of differential equations points into the region bounded by the triangle along the boundary of the region.

5.4.3 Reaction-Diffusion Systems: the Gray-Scott Model and Pattern Formation

Let us consider two concentrations \( u \) and \( v \) in some process involving diffusion of each concentration and some interaction between the two substances. We can imagine interacting populations (for example a predator and its prey) or a chemical reaction.

Absent diffusion, the interaction of two species is often modeled by a (nonlinear) system of ordinary differential equations

\[
\dot{u} = f(u, v), \quad \dot{v} = g(u, v). \tag{5.50}
\]

For example, the basic interaction between a predator concentration \( u \) and its prey concentration \( v \) might be modeled by

\[
\dot{u} = -au + buv, \quad \dot{v} = cv(1 - \frac{1}{k}v) - buv. \tag{5.51}
\]

Here \( a \) is the death rate of the predator, \( c \) is the growth rate of the prey, \( k \) is the carrying capacity of the prey’s environment, and \( b \) is the success rate of the predator. By taking into account the (spatial) diffusion of the two species, we obtain the reaction-diffusion model

\[
u_t = \lambda \Delta u - au + buv, \quad v_t = \mu \Delta v + cv(1 - \frac{1}{k}v) - buv, \tag{5.52}
\]

where now \( u \) and \( v \) are functions of space and time.