Mathematical Modeling I, Fall 2018: Assignment 5
Due Friday Nov 30.
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This homework covers heat equation, parameter estimation, finite element method, hyperbolic PDEs, and epidemiology models. You can work in teams of up to three people. Submit one report per team.

1. [15 points] Consider the 1D heat equation,

$$\frac{\partial u}{\partial t} = q_1 \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, \pi), \quad t \in (0, 1)$$

with initial and boundary conditions

$$u(0, x) = q_2 \sin x,$$
$$u(t, 0) = u(t, \pi) = 0.$$

The solution of this problem can be found analytically, as discussed in class, and is $u(t, x) = u(t, x; \boldsymbol{q}) = q_2 \exp(-q_1 t) \sin x$. A sensor is placed at the point $x = \pi/4$ and collects measurements. We collect the (noisy) measurements in Table 1. Use OLS to estimate $\boldsymbol{q} = (q_1, q_2)^T$, and

observation times t_i	measurements y_i
0.05	0.4241
0.15	0.3380
0.25	0.2894
0.35	0.2229
0.45	0.1661
0.55	0.1111
0.65	0.1224
0.75	0.0920
0.85	0.0804
0.95	0.0604

Table 1: Measurement data.

report the following:

- the estimator $\hat{\boldsymbol{q}}_{\mathsf{OLS}}$ of the true parameter vector $\boldsymbol{q}_0$;
- the estimator $\hat{\sigma}^2_{\mathsf{OLS}}$ of the noise variance σ_0^2;
- a plot of your model fit to the given data; i.e., plot $u(t, \pi/4; \hat{\boldsymbol{q}}_{\mathsf{OLS}})$ versus the given data points (make sure to evaluate u on a finer grid than the observational grid);
- the covariance matrix estimator $\hat{\boldsymbol{\Sigma}}$, the standard errors, and 95% confidence intervals.

Also, do you observe any correlations? Discuss briefly.

Let $f(t, q) = u(t, \pi/4) = q_2 \exp(-q_1 t) \sin(\pi/4)$.

$$\hat{q}_{\mathsf{OLS}} = \arg\min_{q \in Q} \sum_{j=1}^{10} \left[Y_j - f(t_j, q) \right]^2 = (2.2310, 0.6744)^T$$

The function was minimized using Matlab's `fminunc` function. Multiple initial iterates yielded the above result.

$$\hat{\sigma}^2_{\text{OLS}} = \frac{1}{10-2}\sum_{j=1}^{10}\left[Y_j - f(t_j,\hat{q}_{\text{OLS}})\right]^2 = 1.7610\times 10^{-4}$$

The model fit to the data is shown is Figure 1.

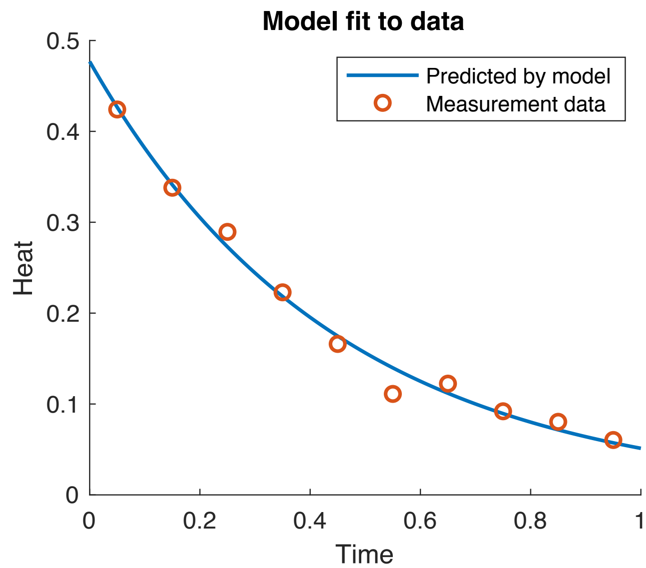


Figure 1: Model fit to data using $\hat{q}_{\text{OLS}} = (2.2310, 0.6744)^T$.

The covariance matrix $\hat{\Sigma} = \sigma^2[\chi^T\chi]^{-1}$ where $\chi_{jk} = \frac{\partial}{\partial q_k} f(t_j,\hat{q}_{\text{OLS}})$. Thus,

$$\hat{\Sigma} = \begin{bmatrix} 9.3759\times 10^{-03} & 1.3667\times 10^{-03} \\ 1.3667\times 10^{-03} & 3.5954\times 10^{-04}\end{bmatrix}.$$

Note that the standard error is $SE_k = \sqrt{\hat{\Sigma}_{kk}}$. Thus $SE_1 = 0.0968$, and $SE_2 = 0.0190$. To calculate the 95% confidence intervals, we use

$$P\{\hat{\boldsymbol{q}}_K - t_{1-0.05/2}SE_k(\hat{\boldsymbol{q}}) < \boldsymbol{q}_{0k} < \hat{\boldsymbol{q}}_k + t_{1-0.05/2}SE_k(\hat{\boldsymbol{q}})\} = 0.95$$

From Matlab,

$$t_{1-0.05/2} = \texttt{tinv(.95,8)} = 1.8595.$$

Thus

$$\begin{aligned} P\{2.2310 - 1.8595(0.0968) < \boldsymbol{q}_{01} < 2.2310 + 1.8595(0.0968)\} \\ = P\{2.0509 < \boldsymbol{q}_{01} < 2.4110\} = 0.95 \end{aligned}$$

and

$$\begin{aligned} P\{0.6744 - 1.8595(0.0190) < \boldsymbol{q}_{02} < 0.6744 + 1.8595(0.0190)\} \\ P\{0.6391 < \boldsymbol{q}_{02} < 0.7097\} = 0.95. \end{aligned}$$

To test for correlations between q_1 and q_2, I generated a sample of size 1000 of the parameters using Matlab's `mvnrnd` function.

Figure 2 shows a strong positive correlation between parameters q_1 and q_2. This correlation makes sense, since as q_1 increases, u decreases, and as q_2 increases, u increases.

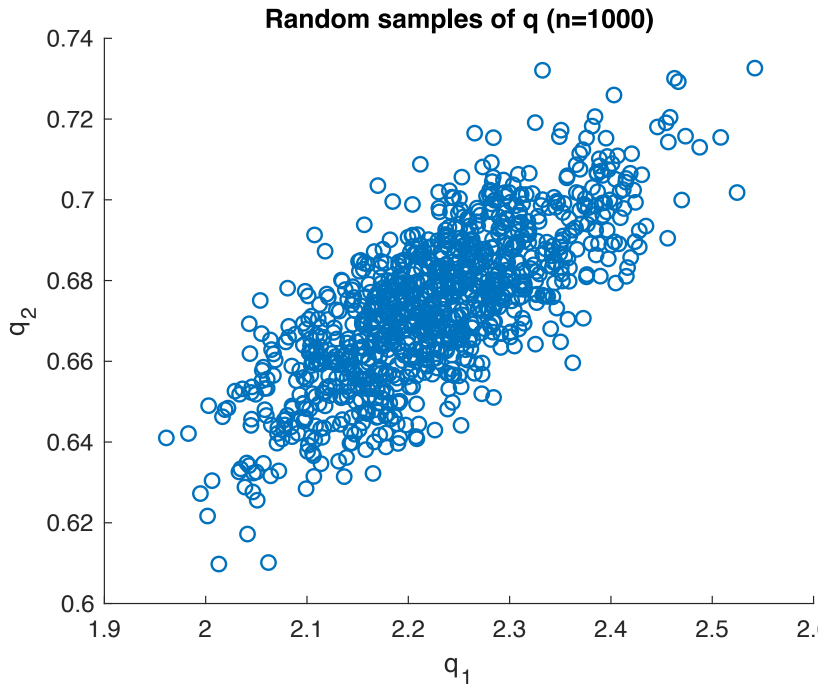


Figure 2: Scatter plot of parameters q_1 and q_2 generated according to the distribution $N(\hat{q}_{\mathsf{OLS}}, \hat{\Sigma})$.

2. [20 points] Consider the 1D steady advection-diffusion equation,

$$\begin{cases} -\kappa u'' + \nu u' = f, & \text{in } \Omega = (0,1), \\ u(0) = u(1) = 0, \end{cases} \tag{1}$$

where $\kappa > 0$ is the diffusion coefficient, $\nu > 0$ is the velocity, and f is a source term.

(a) The weak formulation of the problem is of the following form: find $u \in H_0^1(\Omega)$, such that

$$a(u,v) = \ell(v), \quad \forall v \in H_0^1(\Omega).$$

Derive the expression for the bilinear form $a(u,v)$ and the linear functional $\ell(v)$.

$$\int_0^1 (-\kappa u'' + \nu u')v \; dx = \int_0^1 fv \; dx.$$

Using integration by parts, we get

$$\int_0^1 (-\kappa u'' + \nu u')v \; dx = -ku'v\Big|_0^1 + \int_0^1 ku'v' \; dx + \int_0^1 \nu u'v \; dx = \int_0^1 (kv' + \nu v)u' \; dx,$$

therefore

$$\int_0^1 (kv' + \nu v)u' \; dx = \int_0^1 fv \; dx.$$

Now we have

$$a(u,v) = \int_0^1 (kv' + \nu v)u' \; dx$$

and

$$\ell(v) = \int_0^1 fv \; dx.$$

(b) Using a uniform mesh on $\Omega = (0,1)$ specified by a step-size $h = 1/(n+1)$ where $n \geq 1$ is an integer, and the classical hat functions, given by

$$\phi_i(x) = \begin{cases} \dfrac{x - x_{i-1}}{h} & \text{if } x \in [x_{i-1}, x_i), \\ \dfrac{x_{i+1} - x}{h} & \text{if } x \in [x_i, x_{i+1}), \\ 0 \quad \text{otherwise,} \end{cases}$$

as a basis of the finite element space V_h, derive a linear system resulting from the Galerkin finite element discretization of the problem.

In V_h, the weak form of the problem becomes: Find $u_h \in V_h = \text{span}\{\phi_j\}_{j=1}^n$ such that $a(u_h, v) = \ell(v)$ for all $v \in V_h$. This is equivalent to finding $u_h \in V_h$ such that $a(u_h, \phi_j) = \ell(\phi_j)$ for all $j = 1, \dots, n$.
Since $u_h \in V_h$, it can be written in the form $u_h = \sum_{i=1}^n u_i \phi_i$.
Note that

$$a\left(\sum_{i=1}^n u_i \phi_i, \phi_j\right) = \sum_{i=1}^n a(u_i \phi_i, \phi_j) = \sum_{i=1}^n u_i \ a(\phi_i, \phi_j).$$

Now the problem is: Find u_i $(i = 1, \dots, n)$, such that

$$\sum_{i=1}^n u_i \ a(\phi_i, \phi_j) = \ell(\phi_i),$$

which, in matrix-vector form, becomes: Find $\boldsymbol{U} \in \mathbb{R}^n$ such that $\mathbf{A}\boldsymbol{U} = \boldsymbol{F}$ where

$$A_{ij} = a(\phi_i, \phi_j) = \int_0^1 (k\phi_j' + \nu\phi_j)\phi_i' \ dx = k \int_0^1 \phi_j'\phi_i' \ dx + \nu \int_0^1 \phi_j \phi_i' \ dx$$

and

$$F_i = \ell(\phi_i) = \int_0^1 f\phi_j \ dx.$$

We will now find $\mathbf{A}$. First we will consider

$$\int_0^1 \phi_j'\phi_i' \ dx. \tag{2}$$

Note that unless $j = i$, $j = i+1$, or $j = i-1$, equation 2 is zero. Also, the cases where $j = i+1$ and $j = i-1$ are equivalent.
We will first consider the case where $j = i$:

$$\int_0^1 (\phi_i')^2 \ dx = \int_{x_{i-1}}^{x_i} (\phi_i')^2 \ dx + \int_{x_i}^{x_{i+1}} (\phi_i')^2 \ dx = \int_{x_{i-1}}^{x_i} \left(\frac{1}{h}\right)^2 dx + \int_{x_i}^{x_{i+1}} \left(-\frac{1}{h}\right)^2 dx = \frac{2}{h}$$

We will now consider the case where $j = i+1$ (same as $j = i-1$):

$$\int_0^1 \phi_i'\phi_{i+1}' \ dx = \int_{x_i}^{x_{i+1}} \phi_i'\phi_{i+1}' \ dx = \int_{x_i}^{x_{i+1}} \left(-\frac{1}{h}\right)\left(\frac{1}{h}\right) dx = -\frac{1}{h}$$

Next we will evaluate

$$\int_0^1 \phi_j \phi_i' \, dx. \tag{3}$$

Note that unless $j = i$, $j = i+1$, or $j = i-1$, equation 3 is zero.
We will first consider the case where $j = i$:

$$\int_0^1 \phi_i \phi_i' \, dx = \int_{x_{i-1}}^{x_i} \phi_i \phi_i' \, dx + \int_{x_i}^{x_{i+1}} \phi_i \phi_i' \, dx = \frac{1}{h} \int_{x_{i-1}}^{x_i} \phi_i \, dx - \frac{1}{h} \int_{x_i}^{x_{i+1}} \phi_i \, dx = 0$$

since

$$\int_{x_{i-1}}^{x_i} \phi_i \, dx = \int_{x_i}^{x_{i+1}} \phi_i \, dx.$$

We will now consider the case where $j = i+1$:

$$\int_0^1 \phi_{i+1} \phi_i' \, dx = \int_{x_i}^{x_{i+1}} \phi_{i+1} \phi_i' \, dx = -\frac{1}{h} \int_{x_i}^{x_{i+1}} \phi_{i+1} \, dx = -\frac{1}{h} \left(\frac{h}{2} \right) = -\frac{1}{2}$$

Now, if $j = i-1$:

$$\int_0^1 \phi_{i-1} \phi_i' \, dx = \int_{x_{i-1}}^{x_i} \phi_{i-1} \phi_i' \, dx = \frac{1}{h} \int_{x_{i-1}}^{x_i} \phi_{i-1} \, dx = \frac{1}{h} \left(\frac{h}{2} \right) = \frac{1}{2}$$

Therefore,

$$\mathbf{A} = \frac{k}{h} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} + \frac{\nu}{2} \begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{bmatrix}$$

Now we will find $\boldsymbol{F}$.

$$F_i = \int_0^1 f \phi_i \, dx = \int_{x_{i-1}}^{x_{i+1}} f \phi_i \, dx$$

We can use finite differences to approximate F_i:

$$F_i = \int_{x_{i-1}}^{x_{i+1}} f \phi_i \, dx \approx \frac{h}{2} [f(x_{i-1})\phi_i(x_{i-1}) + 2f(x_i)\phi_i(x_i) + f(x_{i+1})\phi_i(x_{i+1})] = \frac{h}{2} \big(2f(x_i) \big) = hf(x_i)$$

(c) Consider the problem (1), with the right hand side function $f \equiv 1$. In this case, the analytical solution to the problem is given by,

$$u(x) = \frac{1}{\nu} \Big[x - \frac{1 - e^{\frac{\nu}{\kappa} x}}{1 - e^{\frac{\nu}{\kappa}}} \Big].$$

Solve the problem with your finite-element code, with $\kappa = 0.1$ and $\nu = 1$ on a sufficiently fine mesh. Plot your finite-element solution and the analytic solution in the same plot to validate your code.

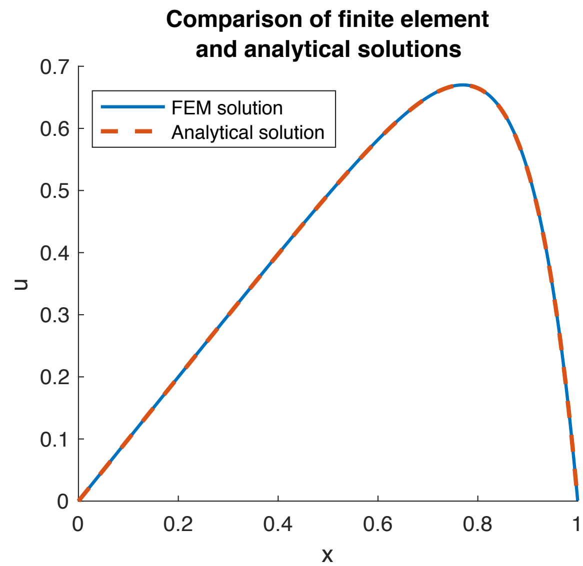
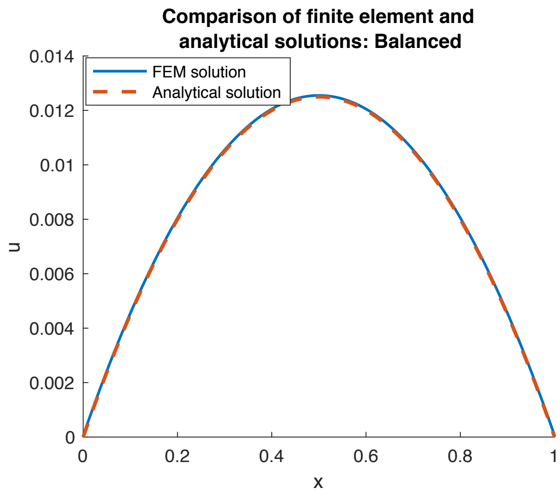


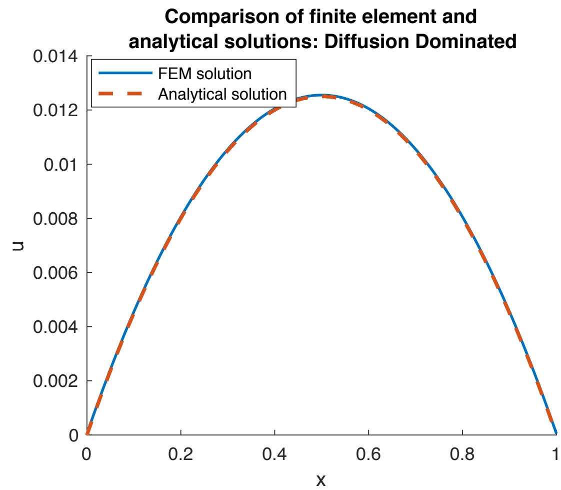
Figure 3: Comparison of analytic solution to FEM solution, generated with step-size $h = 10^{-4}$.

(d) Fix a sufficiently fine computational mesh for numerical tests (say with $n \geq 100$), and then run your code for the following regimes: diffusion dominated (small ν), balanced (ν and κ/h are comparable), advection dominated (ν as large as a reasonable resolution allows). Present the results in a way that allows comparison, and briefly comment on your results.

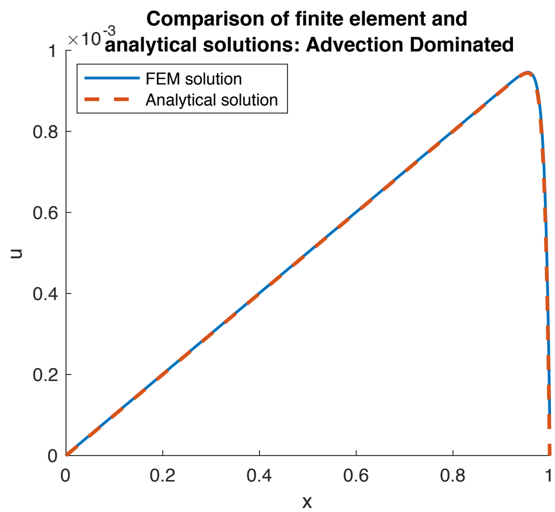
The following plots were all generated from codes using $h = 10^{-3}$ $(n = 1001)$ and $k = 10$. The balanced and diffusion dominated plots are fairly similar. Both are fairly symmetric, parabola-shaped curves, though the diffusion-dominated curve seems slightly skewed to the left end of the x-axis. They also have similar magnitude (u). The advection domitated plot differs dramatically from its balanced and diffusion dominated counterparts. The curve is very much skewed to the right end of the x-axis, behaving close to lineraly for nearly all x-values before sharply dropping off at x-values near one. Additionally, the maximum u-value reached by the advection dominated plot is about a tenth of that reached by the balanced and diffusion dominated plots.



(a) Balanced: $\nu = 0.01$, $k/h = 0.01$



(b) Diffusion dominated: $\nu = 10^{-4}$, $k/h = 0.01$



(c) Advection dominated: $\nu = 100$, $k/h = 0.01$

3. [10 points] Use the method of characteristics to solve the following problem

$$\frac{\partial u}{\partial t} + x\frac{\partial u}{\partial x} = -tu, \quad u(0,x) = \Phi(x),$$

Also, provide a plot of the solution in the x-t plane, with

$$\Phi(x) = \begin{cases} \sin^2 \pi x & x \in [0,1], \\ 0 & \text{otherwise}, \end{cases}$$

and for $(t,x) \in [0,5] \times [-1,10]$. (You can use Matlab's `surf` command.)

The total derivative of u is

$$\frac{du}{dt} = u_t + \frac{dx}{dt} u_x.$$

When $\frac{dx}{dt} = x$ (this is the characteristic curve),

$$\frac{du}{dt} = u_t + xu_x = -tu.$$

This ODE can easily be solved analytically:

$$u = Ce^{-\frac{1}{2}t^2} \qquad \text{where } C \text{ is a constant.}$$

Let $x(0)$ be denoted by x_0. Note that $\Phi(x_0) = u(0, x_0) = Ce^0 = C$.
Since $\frac{dx}{dt} = x$, $x(t) = x_0 e^t$, and consequently, $C = \Phi(xe^{-t})$. Thus,

$$u(t, x) = \Phi(xe^{-t})e^{-\frac{1}{2}t^2}.$$

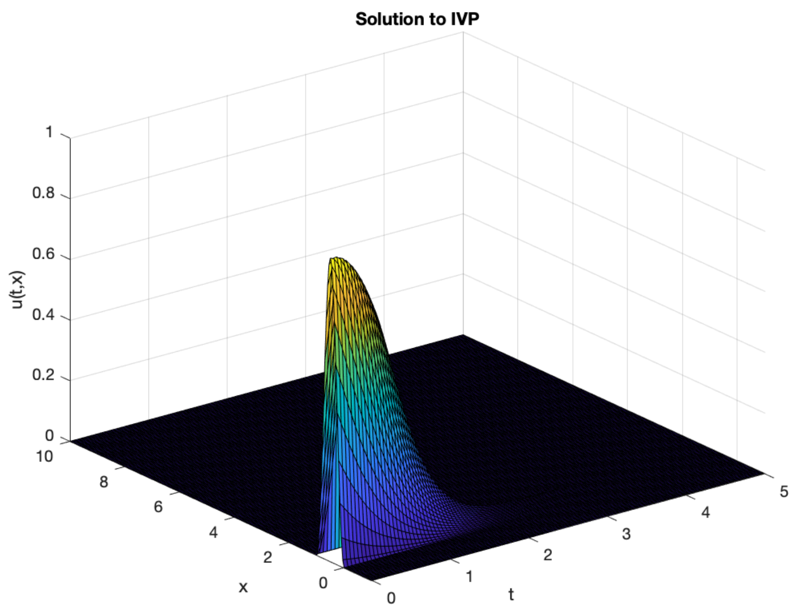


Figure 5: Plot of $u(t, x) = \Phi(xe^{-t})e^{-\frac{1}{2}t^2}$.

Extra credit.

Instructions: Solve only **one** of the following problems, which are weighted equally and are each worth **15** points.

1. Consider the following model of a spread of a disease

$$\frac{dS}{dt} = -\beta SI/N + \delta R$$
$$\frac{dI}{dt} = \beta SI/N - \gamma I$$
$$\frac{dR}{dt} = \gamma I - \delta R$$

with $\beta, \delta, \gamma > 0$, and where as usual S, I, and R denote the the susceptible, infected (and infectious), and recovered populations, respectively, and N is the total population $N = S + I + R$.

(a) Briefly explain the interpretaion of this mathematical model with regards to the dynamics of the spread of the disease.

Individuals move from S to I at a rate of $\frac{\beta}{N}SI$, which models the spread of disease via interaction of susceptible and infected people. Individuals move from I to R at a rate of γI, which represents the recovery of infected indivuals. Individuals move from R to I at a rate of δR, which represents immunity loss. This addition to the standard SIR model allows for individuals becoming sick multiple times.

(b) Derive the expression for the basic reproductive number R_0.

We consider the change in the number of infected people, $\frac{dI}{dt} = \beta SI/N - \gamma I$.
We assume that at the initial time, $S \approx N$. Thus

$$\frac{dI}{dt} = I\beta - \gamma I = I\beta\left(1 - \frac{\gamma}{\beta}\right).$$

We can see that $R_0 = \frac{\beta}{\gamma}$. Note that when $R_0 > 1$, $\frac{dI}{dt} > 0$. This means that the size of the infected population is increasing, and the epidemic will take off. Similarly, when $R_0 < 1$, $\frac{dI}{dt} < 0$, and the size of the infected population decreases. An epidemic will not take off in this scenario.

(c) Find the equilibrium points and analyze their stability in the cases of $R_0 < 1$ and $R_0 > 1$. [Hint: when doing the stability analysis, it is easier to consider the equations for $\frac{dS}{dt}$ and $\frac{dI}{dt}$ only, and note that $R = N - S - I$ can be substituted in the first equation.]

We first substitute $R = N - S - I$ into the equations for $\frac{dS}{dt}$ and $\frac{dI}{dt}$ and set them equal to zero. We get

$$\frac{dS}{dt} = -\frac{\beta}{N}SI + \delta(N - S - I) = 0$$

and

$$\frac{dI}{dt} = \frac{\beta}{N}SI - \gamma I = 0.$$

We can factor $\frac{dI}{dt}$ into

$$\frac{dI}{dt} = I\left(\frac{\beta}{N}S - \gamma\right) = 0.$$

We consider the first equilibrium point, where $I = 0$. Substituting into the equation for $\frac{dS}{dt}$, we get $\gamma(N - S) = 0$. That is, $S = N$. Thus the first equilbrium point is

$$(S^*, I^*) = (N, 0).$$

We now consider the second equilbrium point, where $\frac{\beta}{N}S - \gamma = 0$. Rearranging this, we have $S = \frac{N}{R_0}$. We substitute S into the equation for $\frac{dS}{dt}$ to get $I = \frac{\delta N(1-R_0^{-1})}{\gamma+\delta}$. Thus the second equilibrium point is

$$(S^*, I^*) = \left(\frac{N}{R_0}, \frac{\delta N(1 - R_0^{-1})}{\gamma + \delta}\right).$$

To analyze the stability of the equilibria, we conider the Jacobian of the system of equations involving just S and I, described above. We have

$$J = \begin{bmatrix} -\frac{\beta}{N}I - \delta & -\frac{\beta}{N}S - \delta \\ \frac{\beta}{N}I & \frac{\beta}{N}S - \gamma \end{bmatrix}.$$

To analyze the stability of the first equilbrium point, we consider

$$J(N, 0) = \begin{bmatrix} -\delta & -\beta - \delta \\ 0 & \beta - \gamma \end{bmatrix}.$$

Since this is an upper triangular matrix, its eigenvalues are

$$\lambda_1 = -\delta < 0$$

and

$$\lambda_2 = \beta - \gamma.$$

Note that when $\beta - \gamma > 0$ (i.e., $R_0 > 1$), $\lambda_2 > 0$ and the equilibrium point is a saddle point. In this case the equilibrium is unstable. When $\beta - \gamma < 0$, (i.e., $R_0 < 1$), $\lambda_2 < 0$ and the equilibrium is stable.

To analyze the stability of the second equilbrium point, we consider

$$J\left(\frac{N}{R_0}, \frac{\delta N(1 - R_0^{-1})}{\gamma + \delta}\right) = \begin{bmatrix} \frac{\delta(\gamma-\beta)}{\gamma-\delta} - \delta & -\gamma - \delta \\ \frac{\delta(\beta-\gamma)}{\gamma+\delta} & 0 \end{bmatrix}.$$

$$\det(J(S^*, I^*)) = (\gamma + \delta)\frac{\delta(\beta - \gamma)}{\gamma + \delta} = \delta(\beta - \gamma).$$

$$\text{trace}(J(S^*, I^*)) = \frac{\delta(\gamma - \beta)}{\gamma - \delta} - \delta$$

Note that $R_0 < 1$ implies $S < 0$, since $S = \frac{N}{R_0}$ and $N > 0$. It makes no sense to have a negative number of susceptible people, so it cannot be the case that $R - 0 < 1$. Thus we only consider the case where $R_0 > 1$.

If $R_0 > 1$, then $\beta > \gamma$ and $\det(J(S^*, I^*)) > 0$. This implies that $\lambda_1\lambda_2 > 0$, and consequently, that λ_1 and λ_2 have the same sign. The equilibrium is stable only when $\lambda_1, \lambda_2 < 0$.

This happens when trace$(J(S^*, I^*))\lambda_1 + \lambda_2 < 0$:

$$\begin{aligned} \frac{\delta(\gamma - \beta)}{\gamma - \delta} - \delta &< 0 \\ \delta\left(\frac{\gamma - \beta}{\gamma - \delta} - 1\right) &< 0 \\ \gamma - \beta &< \gamma - \delta \\ \beta &> \delta. \end{aligned}$$

Thus, this equilibrum point is stable when $\beta > \delta$.

(d) Numerically solve the system (you can use Matlab's ODE solvers) for choices of parameter values that result in $R_0 > 1$ and provide plots of S and I over time. Also, provide a plot of S versus I (the phase plane plot).

Figure 6 shows the time evolution of an epidemic modeled by SIR. Initially, there is one infected individual, 999 susceptible individuals, and no recovered individuals. However, an epidemic quickly occurs. This is to be expected, as $R_0 = 5$ in this simulation.

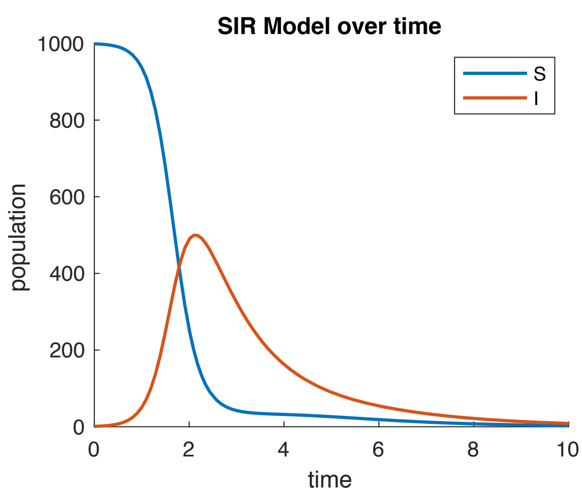


Figure 6: SIR model with $R_0 = 5$. $(\beta = 5, \gamma = 1, \delta = 0.2)$

Figure 7 shows the phase plane plot (S vs I).

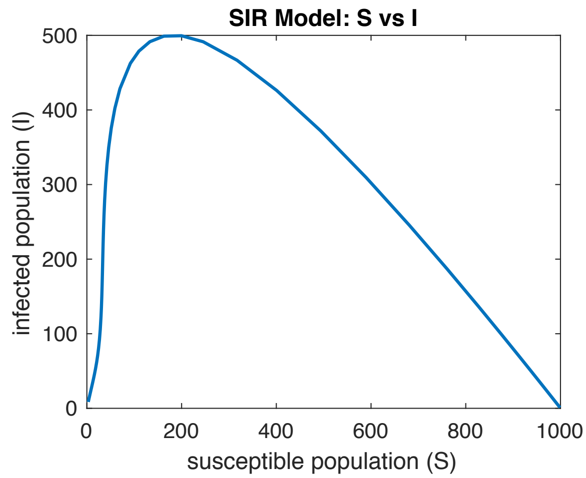


Figure 7: Phase plane plot.

References

[1] Michael Shearer and Rachel Levy. Partial differential equations: an introduction to Theory and Applications. Princeton University Press. 2015.