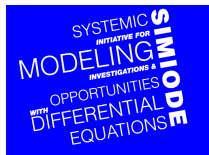


Introduction to Modeling

SIMIODE Remote Teaching Modules



Award #1940532



Modeling Project Preview

Simulating the spread of the common cold throughout a residence hall using markings on a floorplan, while investigating the effectiveness of social/hygienic behaviors in slowing the spread



- ▶ R.C. Harwood (2016), “1-037-S-CommonColdSpread,” <http://www.simiode.org/resources/3171>. (Student Version)
- ▶ RMT IntroModeling SimulationGuide.pdf (Handout of instructions for remote simulation)

Modeling Project Preview

“Although to penetrate into the intimate mysteries of nature and thence to learn the true causes of phenomena is not allowed to us, nevertheless it can happen that a certain fictive hypothesis [model equation] may suffice for explaining many phenomena.”—L. Euler

Questions we seek to answer with a fitting model equation:

- ▶ How does the number of residents infected, $x(t)$, vary with time?
- ▶ How effective are social/hygienic responses?
- ▶ How does our analysis for the common cold inform our preparation for more serious diseases?

Modeling Project Preview

Demonstration of Some Social/Hygienic Responses



Simulation Scenarios:

- ▶ Normal Behavior (Control)
- ▶ A: Surface Sterilization Response
- ▶ B: Reduced Exposure Response
- ▶ Both A & B

Modeling Project Preview

Project Template Spreadsheet

| Example Simulation Data and Model Fit for Introduction to Modeling Project | | | | | | | | | | |
|--|-------------|----------|-------------------------------|----------|--------------|-------------|--|----------|---------|----------|
| Differential Equation Model | Parameters | | a = | -0.35 | Total, N = | 26 | | | | |
| $x' = a(t-b), x(0)=1$ | | | b = | | 12 | Time step = | 1 | | | |
| Model Solution | | | | | | | | | | |
| $x(t) = a/2*(t-b)^2 + (1-a*b^2/2)$ | | | | | | | | | | |
| Time (rounds) | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | |
| Data: Susceptible | 25 | 24 | 22 | 17 | 12 | 7 | 4 | 2 | 1 | |
| Data: Infected | 1 | 2 | 4 | 9 | 14 | 19 | 22 | 24 | 25 | |
| Data: Change in Infected | 1 | 2 | 5 | 5 | 5 | 3 | 2 | 1 | 1 | |
| Data: (Infected) Derivative | 1.0000 | 1.5000 | 3.5000 | 5.0000 | 5.0000 | 4.0000 | 2.5000 | 1.5000 | 1.0000 | 0.5000 |
| Model: (Infected) Slope | 4.2000 | 3.8500 | 3.5000 | 3.1500 | 2.8000 | 2.4500 | 2.1000 | 1.7500 | 1.4000 | 1.0500 |
| Model: Infected | 1.0000 | 5.0250 | 8.7000 | 12.0250 | 15.0000 | 17.6250 | 19.9000 | 21.8250 | 23.4000 | 24.6250 |
| Model: Susceptible | 25.0000 | 20.9750 | 17.3000 | 13.9750 | 11.0000 | 8.3750 | 6.1000 | 4.1750 | 2.6000 | 1.3750 |
| Metrics for fitting model by hand | | | | | | | | | | |
| Square Errors | 0 | 9.150625 | 22.09 | 9.150625 | 1 | 1.890625 | 4.41 | 4.730625 | 2.56 | 1.890625 |
| | 2.278830442 | | Root Mean Square Error (RMSE) | | 0.9483042986 | | R ² Coefficient of Determination (Solution) | | | |

Questions to guide our modeling of the data:

- ▶ What pattern does this model equation describe?
- ▶ What is important about this model?
- ▶ What does the data look like?
- ▶ How well does this model fit the data?

Outline

Interpretation

Characterization

Visualization

Evaluation

What is a Differential Equation Model?

The embodiment of a dynamic pattern which allow us to predict the future

Knowing multiple ways to interpret a differential equation can help you solve/analyze it effectively and skillfully apply it as a model.

Equation: An equation involving one or more derivatives of an unknown variable

Description: A described pattern of how a quantity relates to its rates of change

Family: A relation between a family of solutions (*general solution*) and their derivatives

Fit: A derivative relation for a function (*specific solution*) which fits an additional condition(s)

Example

Equation:

$$x' + 4x = 0 \iff \frac{dx}{dt} = -4x$$

Description: Rate of change is negatively proportional to the amount

- ▶ *How does the amount $x(t)$ change over time?*
- ▶ *Can you think of a function whose 1st derivative is the same function multiplied by -4?*
- ▶ *Can you think of any others? If so, how are they related?*

Example

Family:

$$x = Ce^{-4t}$$

$$x' = -4Ce^{-4t}$$

$$x' + 4x = (-4C + 4C)e^{-4t} = 0$$

Fit:

$$x' + 4x = 0, x(0) = 2$$

$$x(0) = C = 2$$

$$\implies x(t) = 2e^{-4t}$$

Exponential Growth/Decay Model

Equation:

$$P' - rP = 0 \iff \frac{dP}{dt} = rP$$

with growth/decay rate r and population $P(t)$

Description: Rate of change is proportional (by r) to the population

Family:

$$P = Ce^{rt}$$

Fit:

$$P' = rP, P(0) = P_0$$

$$\implies P(t) = P_0 e^{rt}$$

Characterization of Differential Equations

Key characteristics determine the validity of solution methods and analytical techniques

Order Integer of the highest derivative in the equation

Linear? If all unknown terms are raised to the 1st power, scaled, and added together

Homogeneous? If all added terms in the equation are unknown

Autonomous? If the equation is not explicitly defined by the independent variable (t)

Characterize the following model equations

1. $\frac{dP}{dt} = rP \left(1 - \frac{P}{N}\right) - h$
2. $mx'' + k(x')^p = \frac{mMG}{(R+h-x)^2}$
3. $\frac{dA}{dt} = ac - b \left(\frac{A}{V+(a-b)t}\right)$

1. Logistic Growth with Harvesting Model

$$\frac{dP}{dt} = \left(r \left(1 - \frac{P}{N} \right) \right) P - h \iff \text{Rate of Change} = \text{Input} - \text{Output}$$

with exponential growth rate r , carrying capacity N , harvesting rate h , and population $P(t)$.

- ▶ *1st order, nonlinear, nonhomogeneous, and autonomous (assuming constant parameters)*
- ▶ *Description: A population's rate of change is equal to the balance between logistic growth input, proportional to population but constricted by a carrying capacity, and a constant harvesting rate output.*

2. Gravitational Motion Model (Falling)

$$mx'' = \frac{mMG}{(R+h-x)^2} - k(x')^p \iff ma = \sum F = F_g + F_d$$

with object's mass m , mass of the Earth M , universal gravitational constant G , radius of the Earth R , initial altitude h , drag coefficient k , power p , and altitude traveled $x(t)$.

- ▶ *This model is 2nd order, nonlinear, homogeneous, and autonomous (assuming constant parameters)*
- ▶ *Description: A falling object's acceleration is proportional to the sum of the forces of:
gravitational attraction (inversely proportional to the square of the distance between centers of mass) and
drag (negatively proportional to the powered velocity).*

2. Simplified Gravitational Motion Model (Falling)

$$m \frac{d^2x}{dt^2} = mg - k \left(\frac{dx}{dt} \right)^p \iff m \frac{dv}{dt} = mg - kv^p$$

with mass m , gravitational acceleration constant g , drag coefficient k , power p , altitude traveled $x(t)$, and velocity of descent $v(t)$.

- ▶ *This model is 1st order for v (but 2nd order for x), (non)linear (depends on p), nonhomogeneous, and autonomous (assuming constant parameters)*
- ▶ *Description: A falling object's acceleration is proportional to the sum of the forces of:
gravitational attraction (approximately constant) and
drag (negatively proportional to the powered velocity).*

3. Single Compartment Mixing Model

$$\frac{dA}{dt} = ac - \left(\frac{b}{V + (a-b)t} \right) A \iff \text{Rate of Change} = \text{Input} - \text{Output}$$

with flow rate in a , flow rate out b , material concentration flowing in c , initial volume V of tank, and amount of material $A(t)$ in the mixed tank

- ▶ *This model is 1st order, linear, nonhomogeneous, and not autonomous (unless $a = b$ and parameters are constant)*
- ▶ *Description: The amount of pollutant material in a mixture changes based upon the balance of constant input flow and output flow proportional to the current amount.*

Graphing a First Order Differential Equation

Crucial understanding of a differential equation model can be found more readily in visualizations of the shape and behavior than the algebraic form of the solution.

- ▶ Phase line by hand
- ▶ Slope field using DFIELD

What is a Phase Line?

If the equation is autonomous, $x' = f(x)$, then the vertical sign chart of the slope (phase line) guides us in sketching the shape of the family of solutions.

1. Find all equilibrium points $x = E$ where $x' = f(E) = 0$
2. Create a vertical sign chart for $f(x)$ about these E points
3. Draw the time axis and sketch the family of solutions by following the signs

Example Phase Line

Single Compartment Mixing Model (Steady Volume): $a = b, c, V > 0$

$$x' = ac - a\frac{x}{V}$$

1. Eq. pt. $x =$
2. Create a vertical sign chart:
3. Sketch family of solutions:

Now, use your sketch and what you know about the exponential growth/decay model to write down the family of solutions and then fit it to $x(0) = x_0$.

What is a Slope Field?

For differential equation, $x' = f(t, x)$, the slopes of the family of solutions can be scaled and plotted at discrete points to show the direction of any solution (slope field or direction field).

1. Use software to plot direction vectors $\langle 1, f(t, x) \rangle$ at various points (t, x) , scaling the vectors to fit
2. Plot initial condition point (t_0, x_0) and sketch the solution through it which follows the arrows

DFIELD Software

dfield is an example free software for plotting the slope/direction field

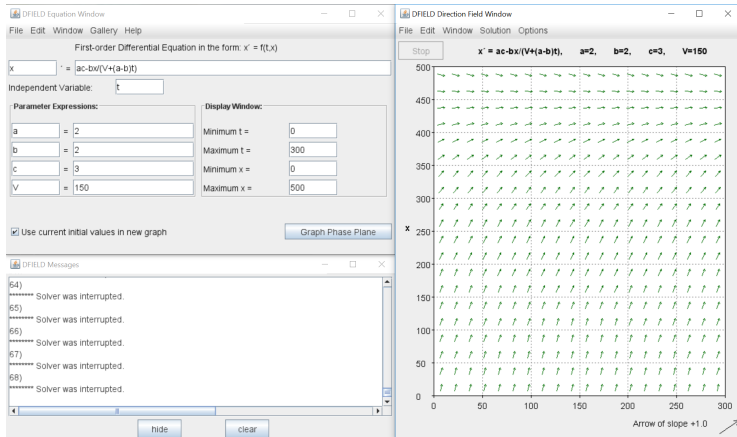


Figure: <http://www.cs.unm.edu/joel/dfield/>

Example Slope Field

Single Compartment Mixing Model (Steady Volume): $a = b = 2$ l/min, $c = 3$ g/l, and $V = 150$ l

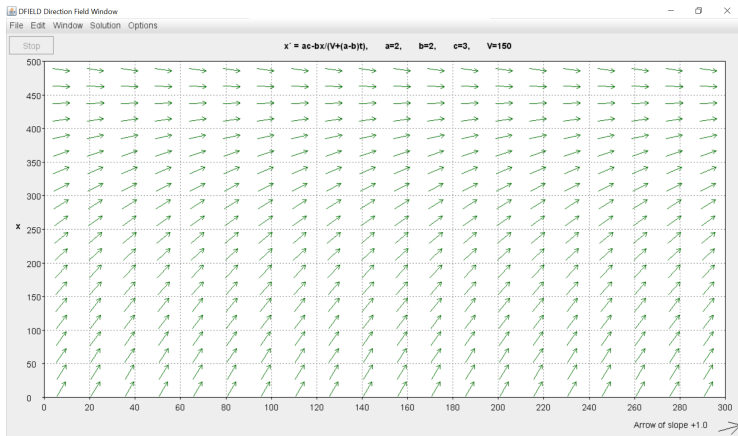


Figure: Sketch the solution

Example Slope Field

Single Compartment Mixing Model: $a = 1.5$ l/min, $b = 2$ l/min, $c = 3$ g/l, and $V = 150$ l

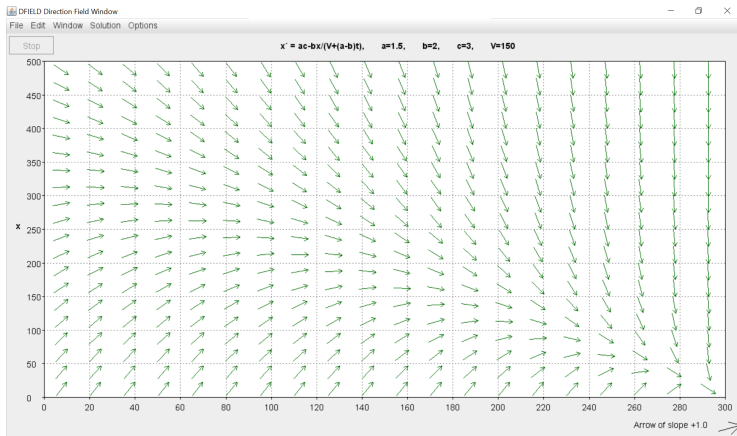


Figure: Sketch the solution

Evaluation of Numerical Solution and Model Fit to Data

Knowing how computed error of a numerical solution accumulates can help us fit our model to the noise inherent in data.

- ▶ Evaluating a Numerical Solution
- ▶ Fitting a Model to Data

What is a Numerical Solution?

Arithmetic computations that approximate the calculus of a differential equation

Caution: key characteristics may be preserved, but the accumulated errors can blur them.

Euler's Method

Given t_0, x_0 to solve $x' = f(t, x), x(t_0) = x_0$, choose $\Delta t, n$.

for $k = 0$ to $n-1$

- ▶ $x_{k+1} = x_k + \Delta t f(t_k, x_k) \leftarrow$ "Next = Current + Portion of Slope"
- ▶ $t_{k+1} = t_k + \Delta t$

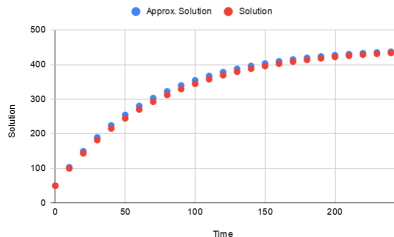
end

Example Numerical Solution

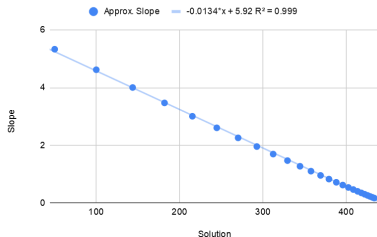
| Euler's Method Implementation | | | | | | | | | |
|--|-------------|-------------------------------|-------------|-------------|-------------|---|-------------|-------------|------------|
| | | | | a (l/min) = | 2 | Final index n= | 24 | | |
| Differential Equation: Mixing | | Parameters | | b (l/min)= | 2 | x_0 (g)= | 50 | | |
| $x' = a*c - b*x/(V+(a-b)*t)$ | | | | c (g/l) = | 3 | dt (min)= | 10 | | |
| Solution (when a=b) | | | | V (l) = | 150 | t_final (min) = | 240 | | |
| $x(t) = (x_0 - c*V)*exp(-a*t/V) + c*V$ | | | | | | | | | |
| Index | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Time | 0 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 |
| Approx. Solution | 50 | 103.3333333 | 149.5555556 | 189.6148148 | 224.3328395 | 254.4217942 | 280.4988883 | 303.0990366 | 322.685831 |
| Approx. Slope | 5.333333333 | 4.622222222 | 4.005925926 | 3.471802469 | 3.008895473 | 2.60770941 | 2.260014822 | 1.958679513 | 1.69752224 |
| Solution | 50 | 99.93067238 | 143.6286647 | 181.8719816 | 215.3415122 | 244.6331524 | 270.2684144 | 292.7037117 | 312.338485 |
| Metrics for Fit | | | | | | | | | |
| Squared Errors | 0.0000 | 11.5781 | 35.1280 | 59.9515 | 80.8440 | 95.8175 | 104.6626 | 108.0628 | 107.067 |
| | 7.626580113 | Root Mean Square Error (RMSE) | | | 0.99538061 | R^2 Coefficient of Determination (fitting solution by | | | |
| | | | | | | | | | 99.54% |

Example Numerical Solution

Approx. Solution and Solution vs. Time



Approx. Slope vs Solution



Model Fit to Data

Investigating a model's qualitative and quantitative fit begins with visualization.

- ▶ Graph various model equations to match shape of x data
- ▶ Plot x' data vs x data to visualize autonomous model $x' = f(x)$
- ▶ Plot x' data vs model slope $f(t, x)$ of data for 1:1 linear regression
- ▶ Plot model solution $x(t)$ and data x vs. time t and minimize error

Example Fitting of Model to Data

| Model-Data Regression: Automatic and by hand | | | | | | | | | |
|--|--------------|-------------------------------|--------------|-------------|--------------|--|--------------|--------------|------------|
| | | | | a (l/min) = | 1.675 | Final index n= | 24 | | |
| Differential Equation: Mixing | Parameters | | | b (l/min)= | 1.675 | x_0 (g)= | 50 | | |
| $x' = a*c - b*x/(V+(a-b)*t)$, $x(0)=x_0$ | | | | c (g/l) = | 2 | dt (min)= | 10 | | |
| Solution (when a=b) | | | | V (l) = | 100 | t_final (min) = | 240 | | |
| $x(t) = (x_0 - c*V)*exp(-a*t/V) + c*V$ | | | | | | | | | |
| Index | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
| Time | 0 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | |
| data | 50 | 70.85307013 | 118.0176364 | 96.67510369 | 139.4492384 | 123.6032882 | 147.9495719 | 140.2908872 | 150.693838 |
| change in data | 20.85307013 | 47.16456628 | -21.34253272 | 42.77413473 | -15.84595021 | 24.3462837 | -7.658684682 | 10.40294812 | 17.3512074 |
| data derivative (avg) | 2.085307013 | 3.40088182 | 1.291101678 | 1.0715801 | 1.346409226 | 0.4250166745 | 0.8343799509 | 0.1372131719 | 1.38770777 |
| fitted model solution | 50 | 73.13350741 | 92.69928705 | 109.247566 | 123.2437133 | 135.0813275 | 145.0933048 | 153.561201 | 160.723148 |
| model slope | 2.5125 | 2.1250 | 1.7973 | 1.5201 | 1.2857 | 1.0874 | 0.9197 | 0.7778 | 0.65 |
| Metrics for fitting model by hand | | | | | | | | | |
| Squared Errors | 0.1825 | 1.6278 | 0.2562 | 0.2012 | 0.0037 | 0.4387 | 0.0073 | 0.4104 | 0.53 |
| | 0.4217692924 | Root Mean Square Error (RMSE) | | | 0.7220692113 | R ² Coefficient of Determination (fitting solution by | | | |

Fit Model Shape

Match the shape of the model slope function to the derivative pattern in the data

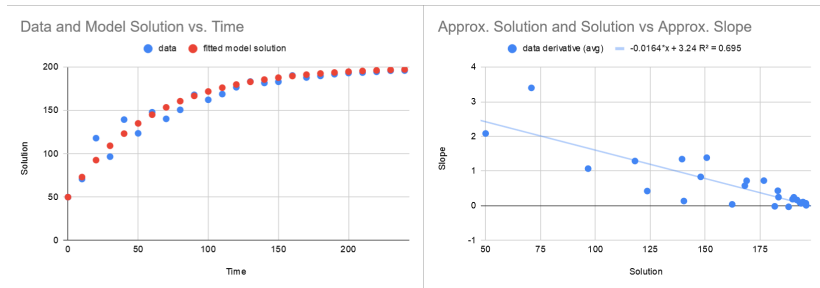


Figure: Qualitatively fit shape and quantitatively fit data's change to value. Equilibrium point: $cV \approx 200$. Slope function: $ac - \frac{a}{V}x = 3.12 - 0.0161x$. Given $V = 100$, compute $c \approx 2$ and estimate $a \approx 1.56$ or 1.61 .

Fit Model Parameters

Weave the chosen model shape through the data values

| Model-Data Regression: Automatic and by hand | | | | | | | | | |
|--|----|--------------|-------------------------------|--------------|-------------|-----------------|--|--------------|--------------|
| | | | | a (l/min) = | 1.675 | Final index n= | 24 | | |
| Differential Equation: Mixing | | Parameters | | b (l/min)= | 1.675 | x_0 (g)= | 50 | | |
| $x' = a*c - b*x/(V+(a-b)*t)$, $x(0)=x_0$ | | | | c (g/l) = | 2 | dt (min)= | 10 | | |
| Solution (when a=b) | | | | V (l) = | 100 | t_final (min) = | 240 | | |
| $x(t) = (x_0 - c*V)*exp(-a*t/V) + c*V$ | | | | | | | | | |
| Index | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Time | 0 | 10 | 20 | 30 | 40 | 50 | 60 | 70 | 80 |
| data | 50 | 70.85307013 | 118.0176364 | 96.67510369 | 139.4492384 | 123.6032882 | 147.9495719 | 140.2908872 | 150.693836 |
| change in data | | 20.85307013 | 47.16456628 | -21.34253272 | 42.77413473 | -15.84595021 | 24.3462837 | -7.658684682 | 10.40294812 |
| data derivative (avg) | | 2.085307013 | 3.40088182 | 1.291101678 | 1.0715801 | 1.346409226 | 0.4250166745 | 0.8343799509 | 0.1372131719 |
| fitted model solution | | 50 | 73.13350741 | 92.69928705 | 109.247566 | 123.2437133 | 135.0813275 | 145.0933048 | 153.561201 |
| model slope | | 2.5125 | 2.1250 | 1.7973 | 1.5201 | 1.2857 | 1.0874 | 0.9197 | 0.7778 |
| Metrics for fitting model by hand | | | | | | | | | |
| Squared Errors | | 0.1825 | 1.6278 | 0.2562 | 0.2012 | 0.0037 | 0.4387 | 0.0073 | 0.4104 |
| | | 0.4217692924 | Root Mean Square Error (RMSE) | | | 0.7220692113 | R ² Coefficient of Determination (fitting solution by | | |

Figure: Given $V = 100$, equilibrium of data ($c = 2$), and slope function. Update the value of a near 1.56 and 1.61 to minimize RMSE (maximize R^2).

Modeling Project Review

Simulating the spread of the common cold throughout a residence hall using markings on a floorplan, while investigating the effectiveness of social/hygienic behaviors in slowing the spread



- ▶ How does the number of residents infected, $x(t)$, vary with time?
- ▶ How effective are social/hygienic behaviors?
- ▶ How does our analysis for the common cold inform our preparation for more serious diseases?

Misleading Fit

Caution! Due to low number of data points, a bad model can still fit data surprisingly well.

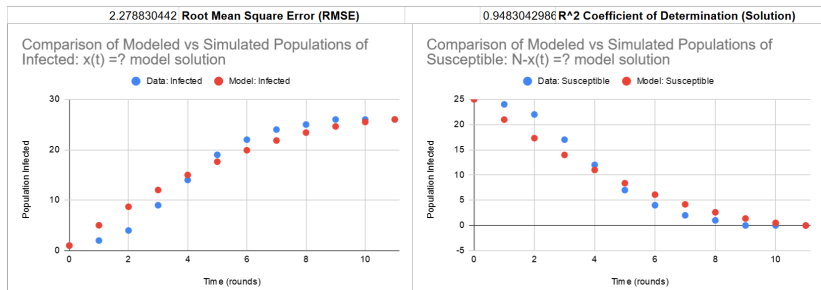


Figure: Model fit of data with low RMSE and very high R^2 , but where shape fit is poor.

Misleading Fit

Patterns in the data's derivative shows how bad our model was in form.

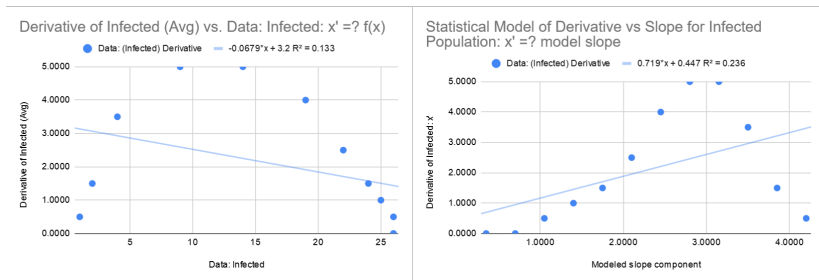


Figure: Linear pattern in slope function is an incorrect shape and makes a poor fit of the data's derivative.

Supplemental Resources for **Introduction to Modeling**

- ▶ Project: R. Corban Harwood (2016),
1-037-S-CommonColdSpread, www.simiode.org/resources/3171
1-037-T-CommonColdSpread, www.simiode.org/resources/3172
- ▶ Instructional Videos: SIMIODE Channel on YouTube
- ▶ All Module Materials for Teachers: www.simiode.org/modules
 - ▶ Guide for implementing instructional videos and activities
 - ▶ Adaptable source material for slides and handouts
 - ▶ Assessment guide with learning goals, examples, and rubrics

Send questions about **Introduction to Modeling** to
Corban Harwood, Prof. of Mathematics at George Fox U.
rharwood@georgefox.edu

More Teaching Resources Available at SIMIODE

The Systemic Initiative for Modeling Investigations and Opportunities with Differential Equations (SIMIODE) is a community of educators and students with a common interest in model-driven activity-based learning of differential equations.

- ▶ **FREE registration is available for all educators**
 - ▶ **FREE access to adaptable Open Education Resources (OER)**
 - ▶ **www.simiode.org/register**
- ▶ **Student Challenge in Undergraduate Differential Equations Modeling (SCUDEM)**
 - ▶ **Hosted by regional host sites (online for November 2020!)**
 - ▶ **www.simiode.org/scudem**

Example 2

Equation:

$$x'' + 4x = 0 \iff \frac{d^2x}{dt^2} = -4x$$

Description: Acceleration is negatively proportional to the position. Also, concavity is negatively proportional to function value.

- ▶ *How does the position $x(t)$ change over time?*
- ▶ *Can you think of a function whose 2nd derivative is the same function multiplied by -4?*
- ▶ *Can you think of any others? If so, how are they related?*

Example 2

Family:

$$x(t) = C_1 \cos(2t) + C_2 \sin(2t)$$

$$x''(t) = -4C_1 \cos(2t) - 4C_2 \sin(2t)$$

$$x'' + 4x = (-4C_1 + 4C_1) \cos(2t) + (-4C_2 + 4C_2) \sin(2t) = 0$$

Fit:

$$x'' + 4x = 0, \quad x(0) = 2, \quad x'(0) = -2$$

$$x(0) = C_1 + 0 = 2$$

$$x'(0) = 0 + 2C_2 = -2$$

$$\implies x(t) = 2 \cos(2t) - \sin(2t)$$

Model 2: Simple Harmonic Oscillator

Equation:

$$mx'' + kx = 0 \iff mx'' = -kx$$

with mass m , spring constant k , and displacement $x(t)$

Description:

Force is negatively proportional to displacement

Family:

$$x(t) = C_1 \cos(\omega t) + C_2 \sin(\omega t), \quad \omega = \sqrt{\frac{k}{m}}$$

Fit:

$$mx'' + kx = 0, \quad x(0) = x_0, \quad x'(0) = v_0$$

$$\implies x(t) = x_0 \cos(\omega t) + \frac{v_0}{\omega} \sin(\omega t)$$