Mathematical Modelling

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What is modelling?

- A precise description of a system
- A formal summary of knowledge
- A tool that enables prediction
- An abstraction suitable for a particular purpose or question
- Modelling is a scientific method with "hypothesis" in a mathematical form

based on the premise

(TL) Torricelli's Law: The area of the region occupied by the crowd decreases proportionally to the width of the exit times the square root of its radius.

2.1 How is the premise expressed in the differential equation?

2.2 Sketch a slope field for this model

https://www.desmos.com/calculator/lxb4g6cuiz

and use it to study how the time it would take to evacuate that section depends on the parameters.

2.3 Using Euler's method, estimate how long it would take to evacuate a stadium with $\alpha = k = 1$, $\theta = \frac{\pi}{5}$ and $r(0) = 2$.

The following ordinary differential equation models a crowd leaving a stadium through an exit

$$2\theta r \frac{dr}{dt} = -k\alpha\sqrt{r}$$
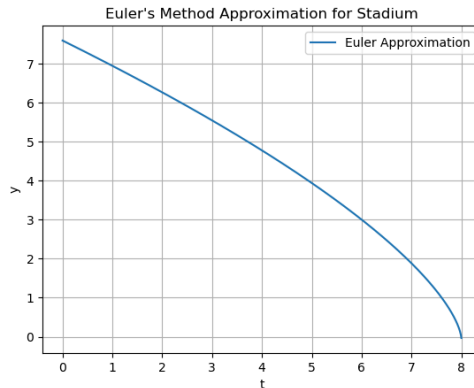
Ladd Peebles Stadium

According to the paper ''`A study of stadium exit design on evacuation performance`'' studying the Ladd Peebles stadium:

- The average person occupies 0.15m^2.

- The stadium fits 1200 people in one section.

3.1 According to an experiment in the paper, it took 8 minutes to evacuate the stadium. Use this to estimate k for Ladd Peebles.

3.2 In the same paper, "for safety, the maximum flow through an exit is 109 people per meter-width per minute." Does Ladd Peebles satisfy this safety concern?

Solution:

- $\theta r^2(0) = 1200 \cdot (0.15) \quad \Rightarrow \quad r(0) \approx 7.6m$

- $\theta = \pi$

- $\alpha = 1.5$

- To get everyone out in 8 minutes $\Rightarrow k = 7.33$ (time units are minutes)

- $p(t) = A(r(t))/(0.15 \cdot 1.5) =$ people per meter-width

- $p(t) = 2\theta \frac{1}{2} r^2(t)/(0.15 \cdot 1.5) = \frac{\theta}{0.225} r^2(t)$

- $p'(t) = \frac{1}{0.225} \underbrace{2\theta r \frac{dr}{dt}}_{-k\alpha\sqrt{r}} = -\frac{k\alpha}{0.225}\sqrt{r(t)} =$

  $-\frac{152}{3}\sqrt{r(t)}$

- Max at $t = 0$ when $|p'(t)| \approx 139.678$

Euler's Method Approximation for Stadium
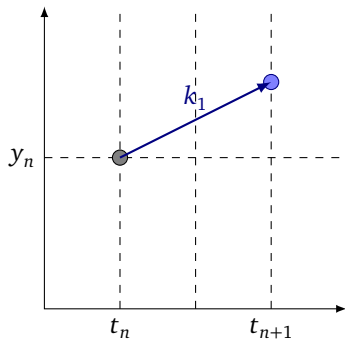
Max sqrt(y) is 2.756809750418044

Numerical Methods for:

$$y' = f(t, y)$$

4.1 Euler Method:
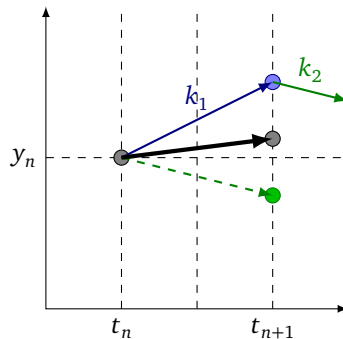
$$y_{n+1} = y_n + hk_1$$
$$k_1 = f(t_n, y_n)$$

4.2 Heun Method (Improved Euler):

$$y_{n+1} = y_n + h\frac{k_1 + k_2}{2}$$
$$k_1 = f(t_n, y_n)$$
$$k_2 = f(t_n + h, y_n + hk_1)$$

4.3 Runge-Kutta Method:

$$y_{n+1} = y_n + h \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}$$

$$k_1 = f(t_n, y_n)$$

$$k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1)$$

$$k_3 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2)$$

$$k_4 = f(t_n + h, y_n + hk_3)$$
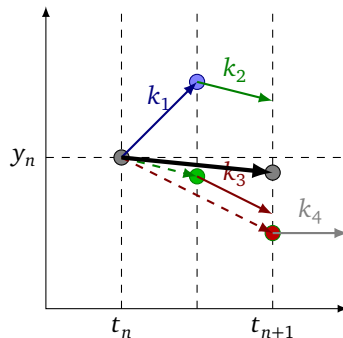
Desmos with all these three methods:
https://www.desmos.com/calculator/haolaltd9s

4.4 Consider the ODE $\frac{dy}{dx} = 2x \sin(x^2)$ and $y(0) = 0$. With a step $h = 0.1$, find the largest interval that the approximations stay within 0.1 distance of the exact solution.

Dimensional Analysis

Seven Fundamental Dimensions.
There are seven fundamental dimensions:

Dimension	Symbol	SI Unit	
length	L	metre	m
mass	M	kilogram	kg
time	T	second	s
electric current	I	ampere	A
temperature	Θ	kelvin	K
amount	N	mole	mol
light intensity	J	candela	cd

Note: Sometimes, we use charge Q (SI Unit coulomb C) as a fundamental dimension instead of current.

5.1 When can we add/subtract quantities? With different dimensions? With the same dimensions?

5.2 When can we equate quantities? With different dimensions? With the same dimensions?

5.3 When can we multiply/divide quantities? With different dimensions? With the same dimensions?

5.4 It is convenient to define some functions as a power series (e.g. $e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \cdots$). What condition on the dimension of x is required to be able to do this?

5.5 What are the dimensions of a derivative $\frac{dy}{dx}$? What are the dimensions of an integral $\int y\, dx$?

Modelling: Relationship between the variables in a model must be dimensionally consistent.

Consider the model for a mass undergoing radioactive decay:

$$\frac{dm}{dt} = -km$$

with $m(0) = m_0$.

6.1 What are the units of k? What are the units of $t_c = \frac{1}{k}$?

6.2 Introduce new variables: $\tau = \frac{t}{t_c}$ and $\overline{m}(\tau) = \frac{m(t)}{m_0}$. What is the ODE satisfied by $\overline{m}(\tau)$? What are its units? What are the parameters for this equation?

Consider the model for spruce budworm outbreak in Eastern Canada.[a]

$$\frac{dN}{dt} = RN\left(1 - \frac{N}{K}\right) - \frac{BN^2}{A^2 + N^2}.$$

The first term accounts for resource-limited population growth within a tree and the second term accounts for the predation of the budworms by birds.

7.1 What are the units of N, A, B, K?

7.2 Consider the new variables[b]:

- $x = N/A$ the non-dimensional budworm population
- $\tau = \frac{Bt}{A}$ the non-dimensional time
- $r = \frac{RA}{B}$ the non-dimensional growth rate
- $k = \frac{K}{A}$ the non-dimensional carrying capacity

What is the ODE satisfied by $x(\tau)$?

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[a]See "Nonlinear Dynamics and Chaos" by Strogatz.

[b]This is not the only way to do this.

Dimensional Matrix. The dimensional matrix $\mathcal{D}$ is a matrix where its (i, j) entry gives the power of the ith dimension of the jth variable.

Buckingham Pi Theorem. Any physical relation involving N dimensional variables can be written in terms of a complete set of $N - r$ independent dimensionless variables, where r is the rank of the dimensional matrix $\mathcal{D}$.

The notational convention for the Buckingham Pi Theorem is that the "pi's", $\Pi_1, \ldots, \Pi_{N-r}$ represent dimensionless variables and a relation between them is given by $F(\Pi_1, \ldots, \Pi_{N-r}) = 0$.

Consider a pendulum. We make assumptions:

- The pivot is frictionless

- The rod is massless

- Air resistance is neglected

- The ceiling is infinitely rigid

- $\cdots$

8.1 What are the units of the following variables of interest?

 (a) Period of the swing $[P] =$

 (b) Pendulum mass $[m] =$

 (c) Pendulum rod length $[l] =$

 (d) Gravitational acceleration $[g] =$

 (e) Amplitude of the swing $[\Theta] =$

8.2 Let us create the dimensional matrix:

- One column for each variable of interest
- One row for each dimension
- Each term contains the power of the corresponding dimension for the corresponding variable

$$
\mathcal{D} = \begin{array}{ccccc} [P] & [m] & [l] & [g] & [\Theta] \\ \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \end{array} \left[\qquad\qquad\qquad \right] \begin{array}{l} \leftarrow M \\ \leftarrow L \\ \leftarrow T \end{array}
$$

8.3 What is the rank of this matrix?

8.4 What is the dimension of the null space?

8.5 Find a basis for the null space.

For each vector of the null space basis,

$$\begin{bmatrix} 2 \\ 0 \\ -1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Buckingham Pi Theorem states that these correspond to non-dimensional variables Π_1 and Π_2:

$$\Pi_1 = \frac{P^2 g}{l} \quad \text{and} \quad \Pi_2 = \Theta$$

and that there is a relation between them:
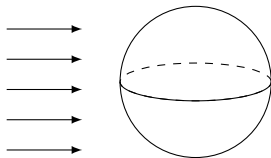
$$F(\Pi_1, \Pi_2) = 0 \quad \text{or} \quad \Pi_1 = f(\Pi_2) \quad \Leftrightarrow \quad \frac{P^2 g}{l} = f(\Theta)$$

which implies that

$$P = \sqrt{\frac{l}{g}} \cdot \overline{f}(\Theta),$$

or in other words, the fact that the *period of the pendulum is proportional to the square root of its length* is a consequence of a pure dimensional analysis of the variables in the problem.

Consider the flow past a sphere.

You don't need to know much about fluid dynamics to be able to deduce some properties of the flow.

The sphere is in a fluid (water) and we measure the force necessary to keep the sphere from moving downstream.

We want to understand how the drag force depends on the stream velocity.

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[a]This choice is part of the modelling process.

9.1 What are the units of the variables of interest[a]?

   (a) drag force $[F] =$

   (b) upstream velocity $[v] =$

   (c) fluid density $[\rho] =$

   (d) sphere diameter $[D] =$

   (e) fluid viscosity (its resistance to deformation by shear stress) $[\mu] =$

9.2 Create a dimension matrix $\mathcal{D}$.

9.3 What is its rank? What is the dimension of its null space? Find a basis for its null space.

9.4 What are the non-dimensional variables Π's from Buckingham Pi Theorem?

9.5 What relations do you obtain?

Solution:

$$\mathcal{D} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & -3 & 1 & -1 \\ -2 & -1 & 0 & 0 & -1 \end{bmatrix}$$

for rows M, L, T.

Its rank is 3, so there are 2 independent null vectors:

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 \\ -2 \\ -1 \\ -2 \\ 0 \end{bmatrix}$$

corresponding to

$$\Pi_1 = \frac{\rho v D}{\mu} \quad \text{and} \quad \Pi_2 = \frac{F}{\frac{1}{2}\rho v^2 D^2}$$

- $\Pi_1 =$ Reynolds number (Re) which determines

the relation between inertia and viscous forces in a fluid flow.

- $\Pi_2 =$ is the drag coefficient (C_d)

So dimensional analysis reveals:

$$\Pi_2 = f(\Pi_1)$$

which means that the drag coefficient depends on the fluid's Reynolds number.

Could have also obtained

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ -2 \end{bmatrix}$$

which gives a different Π_2 and a different relation.

Using python to find the null space gives yet another set of different Π_1 and Π_2.

```python
import numpy as np
from numpy.linalg import matrix_rank
from sympy import Matrix, nsimplify

D = np.array([[1,0,1,0,1],[1,1,-3,1,-1],[-2,-1,0,0,-1]])
Ds = Matrix([[1,0,1,0,1],[1,1,-3,1,-1],[-2,-1,0,0,-1]])

print(D)

print("\nRank(D)=",matrix_rank(D))

print("\nNull Space Basis for D is \n",-2*nsimplify(Ds, rational=True).nullspace(
```

```
[[ 1  0  1  0  1]
 [ 1  1 -3  1 -1]
 [-2 -1  0  0 -1]]

Rank(D)= 3

Null Space Basis for D is
 Matrix([[1], [-2], [-1], [-2], [0]])
 Matrix([[1], [0], [1], [0], [-2]])
```

10.1 Use Buckingham Pi Theorem on Exercise 6 about radioactive decay.

10.2 Use Buckingham Pi Theorem on Exercise 7 about the budworm population.

SYSTEMS OF ODEs

Optimization Problem[a]. A pig weighting 90 kg gains 3 kg per day and cost 45 cents a day to keep. The market price for pigs is 65 cents/kg, but is falling at 1 cent per day. When should the pig be sold?

[a]Adapted from "Mathematical Modelling" by Meerschaert.

Introduce variables:

- t = time at which the pig is sold (in days)

- w = weight of the pig (in kg)

- p = price of a pig (in \$/kg)

- C = cost of keeping the pig (in \$)

- R = revenue from selling the pig (in \$)

- P = profit from the sale of the pig (in \$)

11.1 Which of these variables depend on t? Based on the statement, what do we know about their values?

11.2 What is our goal?

11.3 Solve the problem.

11.4 Answer the question: when should the pig be sold and what is the profit?

Parameter Sensitivity.
Parameter sensitivity is a measure of how a model's response is affected by its parameters.
We quantify the **sensitivity** for the model output x and model parameter p by

$$S(x,p) = \frac{\partial x}{\partial p} \cdot \frac{p}{x},$$

which is dimensionless.

Example: If the time to sell or the profit depends strongly on a parameter, then the model is not very useful. If the model said to sell at $t = 1$ if the daily maintenance cost changed to 46 cents, then the recommendation would be very suspect!

11.5 Let $(t^\star, P^\star)$ be the optimal values found before.

What is the sensitivity of P over the parameter $c = $ the daily maintenance cost of keeping a pig?

11.6 Is $S(P^\star, c)$ positive/negative? What does that mean? Does that make sense?

11.7 What is the sensitivity of P over the parameter $p_0 = $ the initial price of a pig (in \$/kg)?

11.8 Is $S(P^\star, p_0)$ positive/negative? What does that mean? Does that make sense?

Solutions:

11.1
- $w(t) = 90 + 3t$
- $p(t) = 65 - t$
- $C(t) = 45t$
- $R(t) = p(t) \cdot w(t)$
- $P(t) = R(t) - C(t)$

11.2 The goal is to maximize $P(t)$ over $t \geq 0$.

11.3 $P(t) = (90 + 3t)(0.65 - 0.01t) - 0.45t$

$\dfrac{dP}{dt} = 3(0.65 - 0.01t) - 0.01(90 + 3t) - 0.45 = 0$

$t^\star = 10$

$P^\star(10) = 61.50$

11.4 The pig should be sold on day 10, which will give a profit of \$61.50.

11.5 We have $P = (90 + 3t)(0.65 - 0.01t) - ct$ and $t^\star = \frac{35}{2} - \frac{50}{3}c$.

We get $P^\star = \frac{25}{3}c^2 - \frac{35}{2}c + \frac{1083}{16}$ so that

$$S(P^\star, c) = \frac{\partial P^\star}{c} \frac{c}{P^\star}\big|_{c=0.45}$$

$$= \frac{\frac{50}{3}c^2 - \frac{35}{2}c}{\frac{25}{3}c^2 - \frac{35}{2}c + \frac{1083}{16}}\big|_{c=0.45} = -0.0731707$$

This model is insensitive with respect to the maintenance cost! =)

11.6 It is negative, which means that increasing the daily maintenance cost will decrease the profit, which makes sense.

11.7 We get $S(P^\star, p_0) = 1.26829$, so this model is moderately sensitive to the initial price for a pig. =|

11.8 The sensitivity is positive since increasing the initial price of a pig increases the profit also.

Robustness. How do the results depend on the assumptions?

We assumed:
- a linear increase in weight of the pig

- a linear decrease in the price of the pig

What happens if these were nonlinear? The prediction of prices is notoriously uncertain.

Prices are often modelled as stochastic processes (like Brownian motion). This would necessitate a different modelling approach.

In particular, we might then want to maximize the expected (average) profit. But if the variance is very large, then the farmer might prefer a lower expected profit if that means lowering the risk (variance). The farmer might consider maximizing the expected profit with a constraint on the variance of the profit.

Constrained Optimization. How do we solve optimization problems with constraints?

Lagrange Multipliers.

We want to minimize (or maximize) a function $f(x)$ with several constraints:

$$g_1(x) = c_1$$
$$\vdots$$
$$g_k(x) = c_k$$

If $x^\star \in \mathbb{R}^N$ is a local optimal of $f(x)$ which satisfies the above constraints, and $\nabla g_1(x^\star), \ldots, \nabla g_k(x^\star)$ are linearly independent, **then**

$$\nabla f(x^\star) = \lambda_1 \nabla g_1(x^\star) + \cdots + \lambda_k \nabla g_k(x^\star), \quad \text{(LM)}$$

for some scalars $\lambda_1, \ldots, \lambda_k$.

Notes:.

1. This is a necessary, but not sufficient condition.

2. To solve the optimization problem, find candidates x that satisfy it, and then pick the best one.

3. Points for which $\nabla g_1(x), \ldots, \nabla g_k(x)$ are linearly dependent should also be candidates.

4. (LM) $\Longleftrightarrow \nabla f(x^\star) \in \text{span}\{\nabla g_1(x), \ldots, \nabla g_k(x)\}$.

5. The "optimal" values for $\lambda_1, \ldots, \lambda_k$ give important insights on the problem – don't ignore them!

Consider the problem:

■ Maximize $x + y$ such that $x^2 + y^2 = 1$.
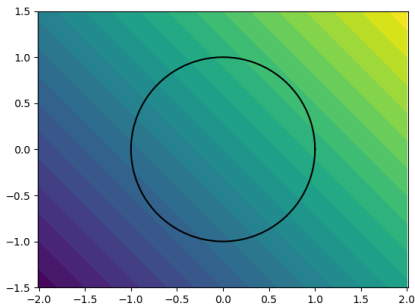
12.1 Use Lagrange Multipliers to find the maximum (and the minimum).

12.2 If the constraint was $x^2 + y^2 = c$, then what is:

(a) the maximizer point $(x^\star, y^\star)$?

(b) the Lagrange multiplier $\lambda^\star$?

(c) the maximum $f(x^\star, y^\star)$?

$$x^\star = y^\star = \frac{\sqrt{c}}{\sqrt{2}} \quad \text{and} \quad \lambda^\star = \frac{1}{\sqrt{2c}}$$
$$\max = x^\star + y^\star = \sqrt{2c}$$

12.3 Compare $\lambda^\star$ with $\dfrac{\partial f(x^\star, y^\star)}{\partial c}$.

$$\frac{\partial f(x^\star, y^\star)}{\partial c} = \frac{\sqrt{2}}{2\sqrt{c}} = \lambda^\star$$

12.4 Based on this relation, give an interpretation for the Lagrange Multiplier.

This means that if the constraint increased from 1 to $1 + \Delta = 1.1$, then we would expect the maximum to increase by approximately $\Delta \lambda^\star = \frac{\Delta}{\sqrt{2}} \approx 0.07$.

A manufacturer of lawn furniture makes two types of chairs, one with a wood frame and the other with an aluminum frame. The wood frame chair costs \$18 per unit to manufacture and aluminum frame chair costs \$10 per unit to manufacture. The company operates in a market where the number of units that can be sold depends on price. It is estimated that in order to sell x units per day of the wood chair and y units per day of the aluminum chair, the selling price cannot exceed $10 + 31x^{-0.5} + 1.3y^{-0.2}$ dollars per unit for the wood chair and $5 + 15y^{-0.4} + 0.8x^{-0.08}$ dollars per unit for the aluminum chair.

Let us first investigate the selling price model for **one type of** chair.

13.1 As more chairs of both types are sold in the market: $x \to \infty$, what do you expect will happen to their selling price?

13.2 As chairs become scarce: $x \to 0^+$, what happens to the price?

13.3 What family of functions satisfies both these conditions?
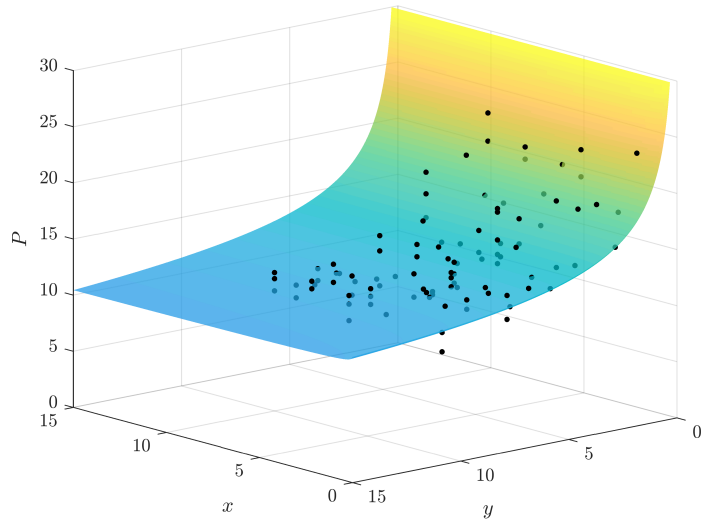
Historical prices and fitting surface $p = f(x, y)$.

A manufacturer of lawn furniture makes two types of chairs, one with a wood frame and the other with an aluminum frame. The wood frame chair costs \$18 per unit to manufacture and aluminum frame chair costs \$10 per unit to manufacture. The company operates in a market where the number of units that can be sold depends on price. It is estimated that in order to sell x units per day of the wood chair and y units per day of the aluminum chair, the selling price cannot exceed $10 + 31x^{-0.5} + 1.3y^{-0.2}$ dollars per unit for the wood chair and $5 + 15y^{-0.4} + 0.8x^{-0.08}$ dollars per unit for the aluminum chair.

14.1 We want to maximize the manufacturer's profit. What is the function to maximize?

14.2 This is a two-dimensional function, so we need to solve the system

$$\frac{\partial f}{\partial x} = 0$$

$$\frac{\partial f}{\partial y} = 0$$

Write down this system.

14.3 How can we find the solution?

Newton's Method.
This is a method to approximate the solution of the equation

$$f(x) = 0.$$

This is an iterative method, so we start with an initial approximation x_0.
For each successive approximation, take the linear approximation of f at x_i and take x_{i+1} to be the point where the linear approximation is 0.

14.4 From the description above, what is the formula for x_1 when using Newton's method?

14.5 Leveraging python.

(a) Go to `https://utoronto.syzygy.ca/jupyter`

(b) Download the file `https://github.com/bigfatbernie/IBLMathModeling/blob/main/python/chairs_newton.ipynb` and import it into the Jupyter Notebook

(c) In the file, introduce the partial derivative functions and an initial guess.

(d) Run the script

```
Minimum for  4.689577973016851  wooden chairs and  5.852031046491972  aluminum chairs
Profit =  52.072691798595706
```
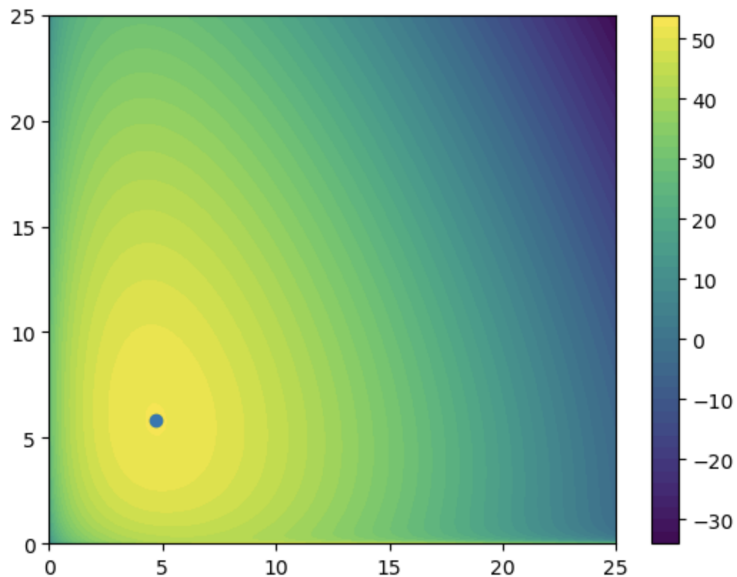
14.6 Leveraging python's minimization tools.

    (a) Go to https://utoronto.syzygy.ca/jupyter

    (b) Download the file https://github.com/bigfatbernie/IBLMathModeling/blob/main/python/chairs_fmin.ipynb and import it into Jupyter Notebook

    (c) In the file, introduce the profit function and an initial guess.

    (d) Run the script

A manufacturer of lawn furniture makes two types of chairs, one with a wood frame and the other with an aluminum frame. The wood frame chair costs $18 per unit to manufacture and aluminum frame chair costs $10 per unit to manufacture. The company operates in a market where the number of units that can be sold depends on price. It is estimated that in order to sell x units per day of the wood chair and y units per day of the aluminum chair, the selling price cannot exceed $10 + 31x^{-0.5} + 1.3y^{-0.2}$ dollars per unit for the wood chair and $5 + 15y^{-0.4} + 0.8x^{-0.08}$ dollars per unit for the aluminum chair.

Sensitivity. To compute $p^\star$, you can use https://github.com/bigfatbernie/IBLMathModeling/blob/main/python/chairs_sensitivity.ipynb

15.1 How sensitive is the profit to the parameter $c = 10$ (the production cost of the aluminum chair)

$$S(p^\star, c) \approx \frac{p^\star(c+h) - p^\star(c)}{h} \frac{c}{p^\star(c)}?$$

15.2 How sensitive is the profit to the parameter $b = 0.4$ (the exponent of y in the selling price of the aluminum chair)

$$S(p^\star, b) \approx \frac{p^\star(b+h) - p^\star(b)}{h} \frac{b}{p^\star(b)}?$$