10.007: Modeling the Systems World

Week 01 - Cohort 2

Fundamentals of Mathematical Modelling

Term 3, 2017

Singapore University of
Technology & Design

Learning outcomes

- Modeling a real-world optimization problem using mathematical notation.
- Introduction to unconstrained optimization.
- Some tools to analyze a function in 2D.

Activity 1 (25 minutes): Steel production

We need 1000 kgs of stainless steel. Steel must have at least 1.5% manganese (Mn) and between 11% and 15% chromium (Cr). We obtain steel by mixing pig iron, possibly adding pure Mn.

Composition of pig iron:

Type of pig iron

	A	B	C
Cr	12%	3%	1.8%
Mn	1.3%	1.5%	1.2%

Cost (per kg):

Pig A	\$0.021
Pig B	\$0.025
Pig C	\$0.015
Mn	\$8.

It costs 0.5 cents to melt down a kg of pig iron.

Formulate a problem to decide which inputs we should mix to produce the steel while keeping the cost as small as possible.

Activity 1 (solution)

Decision variables: kgs of pig A (x_1), pig B (x_2), pig C (x_3), Mn (x_4).

Remember to factor in cost for melting pig iron!
E.g.: pig iron A costs $0.021 + 0.005 = 0.026$ per kg.

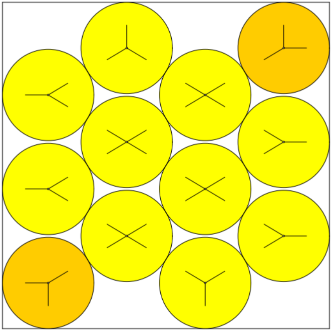
$$\left.\begin{array}{rrrrrcl}
\min & 0.026x_1+ & 0.03x_2+ & 0.02x_3+ & 8x_4 & & \\
\text{subject to:} & & & & & & \\
\text{(Tot. prod.)} & x_1+ & x_2+ & x_3+ & x_4 & = & 1000 \\
\text{(Mn min)} & 0.013x_1+ & 0.015x_2+ & 0.012x_3+ & x_4 & \geqslant & 15 \\
\text{(Cr min)} & 0.12x_1+ & 0.03x_2+ & 0.018x_3 & & \geqslant & 110 \\
\text{(Cr max)} & 0.12x_1+ & 0.03x_2+ & 0.018x_3 & & \leqslant & 150 \\
 & x_1 \geqslant 0, & x_2 \geqslant 0, & x_3 \geqslant 0, & x_4 \geqslant 0. & &
\end{array}\right\}$$

Activity 2 (20 minutes)

We want to decide the can size for a new energy drink. Shipping crates measure 1m × 1m × 0.2m. Can height is 0.2m (fixed), radius and number of cans per crate must be decided.

Write down an optimization problem to determine the maximum allowed radius if we want to fit 100 cans in a crate. All cans should have the same radius.

An example of how we could pack 12 cans inside the crate:



Activity 2 (solutions)

To understand the model, we start with an example with only three cans.

Decision variables: $(x_1, y_1), (x_2, y_2), (x_3, y_3)$ to represent the position of the center of the cans, r to represent the radius.

Constraints: cans do not overlap, and they are inside the crate.

$$
\left.
\begin{array}{rrcl}
\max & r & & \\
\text{(Overlap 1-2)} & \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} & \geqslant & 2r \\
\text{(Overlap 1-3)} & \sqrt{(x_1 - x_3)^2 + (y_1 - y_3)^2} & \geqslant & 2r \\
\text{(Overlap 2-3)} & \sqrt{(x_2 - x_3)^2 + (y_2 - y_3)^2} & \geqslant & 2r \\
\text{(InsideCrate)} \quad i = 1,2,3 & r \leqslant x_i & \leqslant & 1 - r \\
\text{(InsideCrate)} \quad i = 1,2,3 & r \leqslant y_i & \leqslant & 1 - r \\
 & r & \geqslant & 0.
\end{array}
\right\}
$$

Activity 2 (solutions cont'd)

Decision variables: (x_i, y_i), $\forall i \in \{1, \ldots, 100\}$ to represent the position of the center of the i-th can, and r to represent the radius.

Constraints: cans do not overlap, and they are inside the crate.

$$\left.\begin{array}{rrcccc}
 & \max & & & r & \\
(\text{Overlap}) & \forall i < j \leqslant 100 & & \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} & \geqslant & 2r \\
(\text{InsideCrate}) & \forall i \leqslant 100 & r \leqslant & x_i & \leqslant & 1 - r \\
(\text{InsideCrate}) & \forall i \leqslant 100 & r \leqslant & y_i & \leqslant & 1 - r \\
 & & & r & \geqslant & 0.
\end{array}\right\}$$

Unconstained Optimization

In general, we can write an optimization problem formally as

$$\min\{f(x) : x \in X\}.$$

We will learn a lot about how to solve optimization problems in this form in the next few weeks.

First, let us remember what we already know and focus on the simple case where $X = \mathbb{R}^n$.

In this case, the feasible region is the whole space and the problem is called unconstrained.

Global vs. local

Suppose we have the unconstrained optimization problem:

$$\min\{f(x) : x \in \mathbb{R}^n\} \qquad \text{(P)}.$$

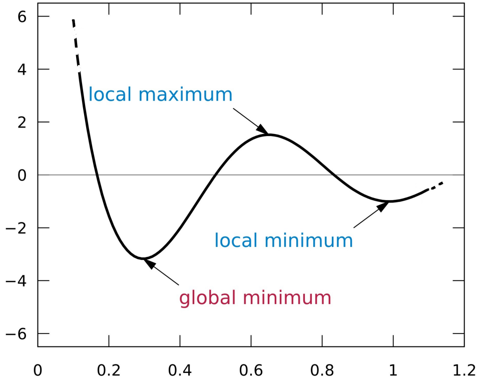
Definition

The point x^* is a global minimum of (P) if $f(x^*) \leqslant f(x)\ \forall x \in \mathbb{R}^n$.

The point x^* is a local minimum of (P) if there exists $\varepsilon > 0$ (possibly very small) such that $f(x^*) \leqslant f(x)$ for all points $x \in \mathbb{R}^n$ such that $\|x^* - x\| \leqslant \varepsilon$.

Global vs. local

Which of these points are global/local minima/maxima?



When is a local minimum automatically a global one?
Can you give a simple example?

Activity 3 (10 mins)

Consider the following univariate functions:

- $y = e^x$
- $y = sinx$
- $y = x$
- $y = x^2$
- $y = (x^2 - 1)(x + 1)$

Using the corresponding graphs discuss whether local/global minima/maxima exist or not.

A blast from the past

It is not easy to identify the global minima for many problems.

We first recall (from Math I and II) how to find the local minima of a problem given as:

$$\min\{f(x) : x \in \mathbb{R}^n\}.$$

Single-variable function $f(x)$:

- Find points with $f'(x) = 0$.

  For all such points:
- If $f''(x) > 0$, x is local min.
- If $f''(x) = 0$, check further.
- If $f''(x) < 0$, x is local max.

Two-variable function $f(x, y)$:

- Find points with $\nabla f(x, y) = (0, 0)$.

  For all such points:
- If $\det H_f(x, y) > 0$ and $f_{xx}(x, y) > 0$, (x, y) is local min. ($f_{xx}(x, y) < 0$, (x, y) is local max.)
- If $\det H_f(x, y) = 0$, check further.
- If $\det H_f(x, y) < 0$, saddle point.

Activity 4 (20 mins)

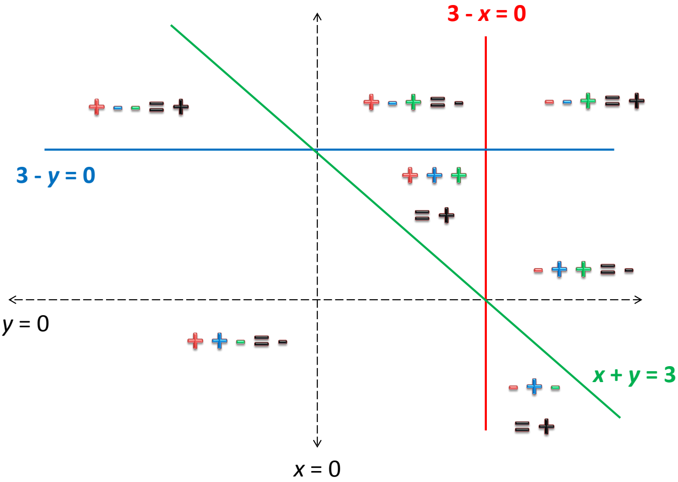
Let $f(x, y) = (3 - x)(3 - y)(x + y - 3)$.

1. Draw a sketch on the plane of the set of points (x, y) at which $f(x, y) = 0$.
2. Use the sketch to identify the regions of the plane at which $f(x, y) \geqslant 0$.
3. Find all points in the plane at which $\nabla f(x, y) = (0, 0)$.
4. Find which of these points are neither local maxima nor minima.
5. Show that there is a local maximum among these points.
6. Prove that $f(x, y)$ does not have a global minimum or maximum.

There are many ways to approach these questions!

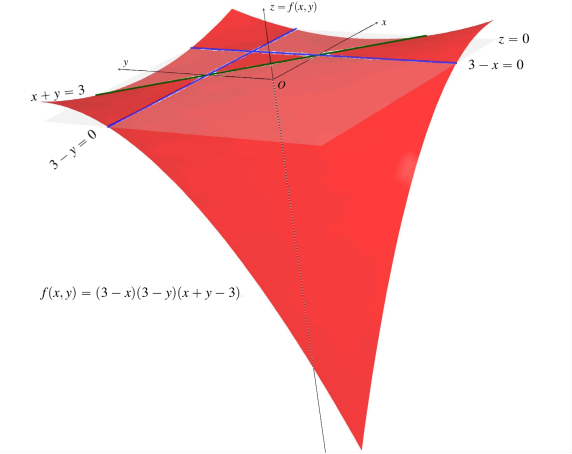
Activity 4 (solutions)

1 and 2. $f(x, y) = (3 - x)(3 - y)(x + y - 3)$.



Activity 4 (solutions)

A sketch of the function in 3D (not required):



Activity 4 (solutions)

$$f(x,y) = (3-x)(3-y)(x+y-3)$$

$$\nabla f(x,y) = \begin{pmatrix} (3-y)(6-2x-y) \\ (3-x)(6-x-2y) \end{pmatrix}.$$

3. $\nabla f(x,y) = (0,0)$ at four points: (3,3), (3,0), (0,3), (2,2).

4. We can see from the sketch that $(3,3), (3,0), (0,3)$ cannot be local optima because the function is equal to zero at these points while it can be both positive and negative values around them.

An alternative way to see this: the plane tangent to $f(x,y)$ at these three points is $z=0$ (it contains two of the lines $x=3, y=3, x+y=3$), but the surface is on both sides of it; so they are not local optima.

Activity 4 (solutions)

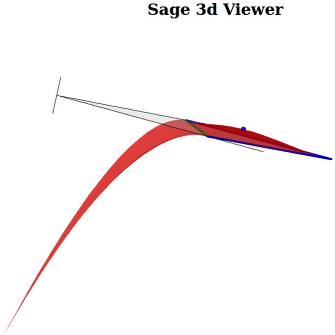
5. From the answer to question 3, the only local optimum can be at (2,2).

$$H_f(x,y) = \begin{pmatrix} 2y-6 & -9+2x+2y \\ -9+2x+2y & 2x-6 \end{pmatrix}, H_f(2,2) = \begin{pmatrix} -2 & -1 \\ -1 & -2 \end{pmatrix}.$$

Since $\det(H_f(2,2)) > 0$ and $f_{xx}(2,2) < 0$, we can conclude that $(2,2)$ is a local maximum.

Note that you can also answer this question quickly with a very useful theorem called the Extreme Value Theorem. We will learn this in Week 4.

Activity 4 (solutions)



$$f(x,y) = (3-x)(3-y)(x+y-3)$$

6. There is no global optimum for this function, since f can be arbitrarily large or small:

$$\lim_{N\to+\infty} f(3+N, 3+N) = \lim_{N\to+\infty} N^2(3+2N) = +\infty.$$

$$\lim_{N\to-\infty} f(3+N, 3+N) = \lim_{N\to-\infty} N^2(3+2N) = -\infty.$$

Summary

- Modeling, modeling and more modeling!
- Algebraic formulations to get used to "abstract" modeling.
- Introduction to unconstrained optimization.
- Local versus global minima.