## CPS 5310: Introduction to Mechanistic Models

Natasha Sharma, Ph.D.

## Prerequisites

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I must stress on the review of the
1 Calculus III This means the knowledge of Calculus I and II is already assumed. Specifically, differentiation, integration.
2 Matrix Algebra This means, arithmetic operations involving matrices. Specifically, eigenvalues and eigenvectors.

## What you have learnt so far...

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- CPS 5401: Introduction to Computational Science learnt computational tools to prepare you to model problem arising in engineering and sciences.


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- Phenomenological models-Glimpse of modeling of the probabilistic nature


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■ Remainder of CPS 5310, focussed on deterministic models represented by

1 Linear Programming Problems (just this lecture)

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1 Linear Programming Problems (just this lecture)
2 Differential Equations (remainder of the course!)


## What you have learnt so far...

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- Phenomenological models-Glimpse of modeling of the probabilistic nature
- Remainder of CPS 5310, focussed on deterministic models represented by
1 Linear Programming Problems (just this lecture)
2 Differential Equations (remainder of the course!)
- Programming tools to solve these models.


## What we will cover...

After formally introducing the concept of mathematical models, we will focus on three main components-

- Ordinary Differential Equations (ODEs)


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After formally introducing the concept of mathematical models, we will focus on three main components-

- Ordinary Differential Equations (ODEs)
- Partial Differential Equations (PDEs)

■ Use of computational tools (such as Maxima and Matlab) to solve these equations.

## Mathematical Models: Defintion

A Mathematical Model is a triplet (S, Q,M) where

- $S$ denotes a system
- $Q$ is a question relating to $S$
- $M$ is a set of mathematical statements expressed as $M=\left\{\sum_{1}, \sum_{2}, \sum_{3}, \cdots\right\}$ which can be used to answer $Q$.


## How to set up a model?

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1 Determine the unknown quantities to be calculated in the problem.

2 Give precise definitions of the unknowns (including the units).

3 Translate the information in the problem description into mathematical statements.

## Classification of Mathematical Models

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The model is classified based on the mathematical question asked.

## Example

## Linear Programming Problem (LPP):

Trying to maximize profit or minimize cost under some constraints like limited resources and in the presence of alternate course of actions to choose from.
The objective and constraints in linear programming problems must be expressed in terms of linear equations or inequalities.

## Classification of Mathematical Models

## Example

Mixture Problems: Mixtures (and mixture problems) are made whenever different types of items are combined to create a third, mixed item.
Example: White gold is $75 \%$ pure gold. How many grams of pure gold and white gold should be mixed to obtain 100 grams of yellow gold given that yellow gold contains $92 \%$ pure gold?

## Model I: Linear Programming Problem

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## Example

Suppose a farmer has a piece of land of area A square kilometer. This land can be planted with either wheat or barley or some combination of the two. Suppose that the farmer has a permissible amount $F$ of fertilizer and $P$ of pesticide which can be used each of which is required in different amounts per unit area for wheat $\left(F_{1}, P_{1}\right)$ and for barley $\left(F_{2}, P_{2}\right)$. Let $S_{1}$ and $S_{2}$ be the selling prices of wheat and barley respectively. How many square kilometers should be planted with wheat versus barley to maximize the revenue ?

## Solution

- S: Farm Land

■ Q: How many square kilometers should be planted to maximize revenue?

- M: Mathematical Statements transforming the problem into a maximization problem constrained to some limited resources.


## Example continued

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1 Determine the unknown quantities to be calculated in the problem. $x_{w}$ and $x_{b}$
2 Give precise definitions of the unknowns (including the units). $x_{w}$ denotes the area with wheat planted while $x_{b}$ denotes the area with barley planted.
3 Translate the information in the problem description into mathematical statements.

$$
\begin{array}{r}
x_{w} \geq 0, x_{b} \geq 0 \\
x_{w}+x_{b} \leq A \\
F_{1} x_{w}+F_{2} x_{b} \leq F \\
P_{1} x_{w}+P_{2} x_{b} \leq P  \tag{4}\\
\text { maximize } S_{1} x_{w}+S_{2} x_{b}
\end{array}
$$

## Product Mix Problem

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## Example

The Pear Company produces two products: A and B. The production process for each product is similar in that both require a certain number of hours of electronic work and a certain number of labor hours in the assembly department. Each unit of A takes 4 hours of electronic work and 2 hours in the assembly shop. While each unit of B requires 3 hours in electronics and 1 hour in assembly. During the current production period, 240 hours of electronic time are available, and 100 hours of assembly department time are available. Each unit of $A$ sold yields a profit of $\$ 7$; each unit of product $B$ produced may be sold for a $\$ 5$ profit.
Determine the best possible combination of product $A$ and $B$ to be manufactured to reach the maximum profit.

## Mathematical Problem

| Department | Product A | Product B | Available hours this week |
| :---: | :---: | :---: | :---: |
| Electronic | 4 | 3 | 240 |
| Assembly | 2 | 1 | 100 |

## Mathematical Problem

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3 Translate the information in the problem description into mathematical statements.

$$
\begin{align*}
& x_{a} \geq 0, x_{b} \geq 0  \tag{6}\\
& 4 x_{a}+3 x_{b} \leq 240  \tag{7}\\
& 2 x_{a}+x_{b} \leq 100  \tag{8}\\
& \text { maximize } 7 x_{a}+5 x_{b} \tag{9}
\end{align*}
$$

## Mathematical Problem

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\end{align*}
$$

4 Interaction between constraints: Eliminate non-physical choices of $x_{a}$ and $x_{b} \cdot x_{a}=70$ is not possible choice!

## In-class Activity

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## Example

LP Electronics Corporation primarily manufactures four highly technical products, which it supplies to aerospace firms that hold NASA contracts. Each of the products must pass through the following departments before they are shipped: wiring, drilling, assembly, and inspection. The time requirements in each department (in hours) for each unit produced and its corresponding profit value are summarized in table 1.
The production time available in each department each month and the minimum monthly production requirement to fulfill contracts are given by table 2 .

1. Each month, the production manager has the responsibility of specifying production levels for each product in the coming month so as to maximize the profit. Please set up the mathematical model.

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## Example

| Product | Wiring | Drilling | Assembly | Inspection | Unit Profit <br> (in dollars) |
| :---: | :---: | :---: | :---: | :---: | :---: |
| XJ201 | 0.5 | 3 | 2 | 0.5 | 9 |
| XM897 | 1.5 | 1 | 4 | 1.0 | 12 |
| TR29 | 1.5 | 2 | 1 | 0.5 | 15 |
| BR788 | 1.0 | 3 | 2 | 0.5 | 11 |

Table: Time requirements

| Department | Capacity | Product | Minimum Production Level |
| :---: | :---: | :---: | :---: |
| Wiring | 1500 | XJ201 | 150 |
| Drilling | 2350 | XM897 | 100 |
| Assembly | 2600 | TR29 | 300 |
| Inspection | 1200 | BR788 | 400 |

Table : Production time available and minimum monthly production requirement

## Model II: Mixing Problem

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## Example

White gold is $75 \%$ pure gold. How many grams of pure gold and white gold should be mixed to obtain 100 grams of yellow gold given that yellow gold contains $92 \%$ pure gold?

## Mixing Problem

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1 Determine the unknown quantities to be calculated in the problem: $x_{w g}$ and $x_{p g}$,

## Mixing Problem

1 Determine the unknown quantities to be calculated in the problem: $x_{w g}$ and $x_{p g}$,
2 Give precise definitions of the unknowns. $x_{w g}$ and $x_{p g}$ denotes the gms of white and pure gold to be mixed respectively.

## Mixing Problem

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1 Determine the unknown quantities to be calculated in the problem: $x_{w g}$ and $x_{p g}$,
2 Give precise definitions of the unknowns. $x_{w g}$ and $x_{p g}$ denotes the gms of white and pure gold to be mixed respectively.
3 Translate the information in the problem description into mathematical statements: $\left\{\sum_{1}, \ldots, \sum_{5}\right\}$

$$
\begin{align*}
x_{w g}+x_{p g} & =100  \tag{10}\\
\frac{75}{100} x_{w g}+x_{p g} & =92 \tag{11}
\end{align*}
$$

## In-class Activity

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## Example

Which volumes of fluids $A$ and $B$ should be mixed to obtain 150 liter of a fluid $C$ that contains $70 \mathrm{gl}^{-1}$ of a substance if $A$ and $B$ contain $50 \mathrm{gl}^{-1}$ and $80 \mathrm{gl}^{-1}$, respectively?

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## Example

Suppose the fluids A, B, C, D contain the substances $S_{1}, S_{2}, S_{3}$ according to the table below (concentration in grams per liter):

|  | A | B | C | D |
| :---: | :---: | :---: | :---: | :---: |
| $S_{1}$ | 2.5 | 8.2 | 6.4 | 12.7 |
| $S_{2}$ | 3.2 | 15.1 | 13.2 | 0.4 |
| $S_{3}$ | 1.1 | 0.9 | 2.2 | 3.1 |

What is the concentration of $S_{3}$ in a mixture of these fluids that contains $75 \%$ (percentage by volume) of fluids $A$ and $B$ and which contain $4 \mathrm{gl}^{-1}$ and $5 \mathrm{gl}^{-1}$ of the substances $S_{1}$ and $S_{2}$, respectively?

## To Do List before the next class

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■ Set up a bitbucket account using your university email address. https://bitbucket.org.

- Look into the first software tool Maxima. http://maxima.sourceforge.net.
■ Using LaTeX for turning in homework. https://www.overleaf.com/gallery/tagged/homework

