OPTIMIZATION OF BIOPROCESSES

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INTRODUCTION IN OPTIMIZATION

What is the optimization?

The optimization is the process of obtaining the best solution, provided that “good” or “bad” can be measured and modified.

In engineering the goal is to obtain a “maximum” (e.g., the best productivity, the highest yield) or a “minimum” (e.g., the lowest cost of production, the lowest energy consumption). In both cases the term “optimum” is used and involves quantitative measurements. Thus, **OPTIMIZATION is the process of reaching the optimum**.

Optimization theory is a branch of mathematics that involves the quantitative study of the optima of the optimization methods.

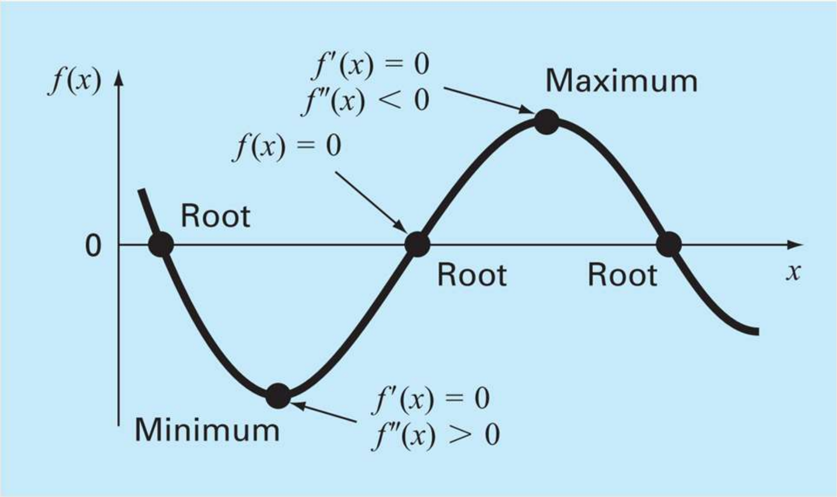
<u>Practical optimization</u> is the collection of method/algorithms that are used to find optima.

Optimization problems can be found in many finds, including engineering. Some examples of optimization problems are:

- modeling, characterization, and design of devices, circuits, and systems;
- design of tools, instruments, and equipment;
- design of structures and buildings;
- process control;
- approximation theory, curve fitting, solution of systems of equations;
- forecasting, production scheduling, quality control;
- maintenance and repair;
- inventory control, accounting, budgeting,

General approaches of optimization:

1. Analytical methods,
2. Graphical methods,
3. Experimental methods,
4. Numerical methods.



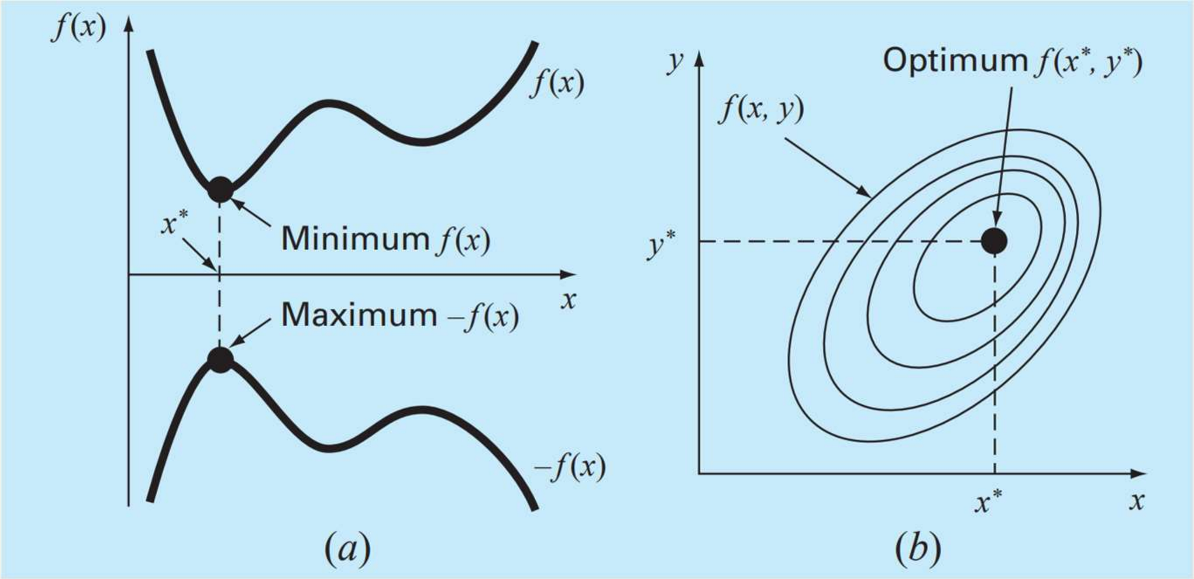
Classification of the optimization methods:

According to the presence/absence of constraints:

- optimization methods without constraints,
- optimization methods with constraints

According to the dimension of the function that must be optimized:

- One-dimensional optimization problems
- Multidimensional optimization problems



ONE-DIMENSIONAL UNCONSTRAINED OPTIMIZATION METHODS

Definitions:

Local optimum (minimum/maximum) is not as good as the global optimum that is expected. Possible solution: graphical representation, if available, or repeating the search several times and selecting the best optimum.

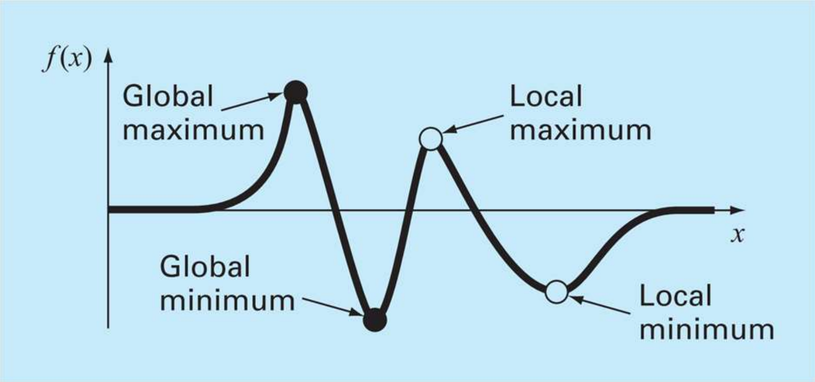
Multimodal functions have more that one optimum. They have both local and global optima. Optimization methods target unimodal functions or section of functions.

Lower/upper bounds are the ends of the interval which is known to have on optimum.

Range of uncertainty is the interval between the lower and upper bounds.

Objective function is the function that is optimized.

Stopping criterion is the function that can stop the search algorithm.



Classification of one-dimensional optimization methods

1. *Search methods* (e.g., bisection method, Fibonacci search method, golden ratio search method etc.). They are based on successively reducing the range of uncertainty down to a sufficiently short interval that contains the optimum and that falls into the tolerance of the stopping criterion.

2. *Approximation methods* (e.g., quadratic/parabolic interpolation method, cubic interpolation method etc.). They are based on the approximation of the objective function with a polynomial whose optimum can be determined analytically. The range of uncertainty is reduced also, but the stopping criterion consists in reaching two times the same optimum. These methods involves more calculation, but they are faster and more precise.

3. *Mixed methods* (e.g., the algorithm of Davies, Swann and Campey). It uses search for determine the range of uncertainty and approximation for finding the optimum.

PARABOLIC INTERPOLATION

Takes advantage of the fact that a second-order polynomial often provides a good approximation to the shape of *f(x)* near an optimum

If a second-order polynomial of the form

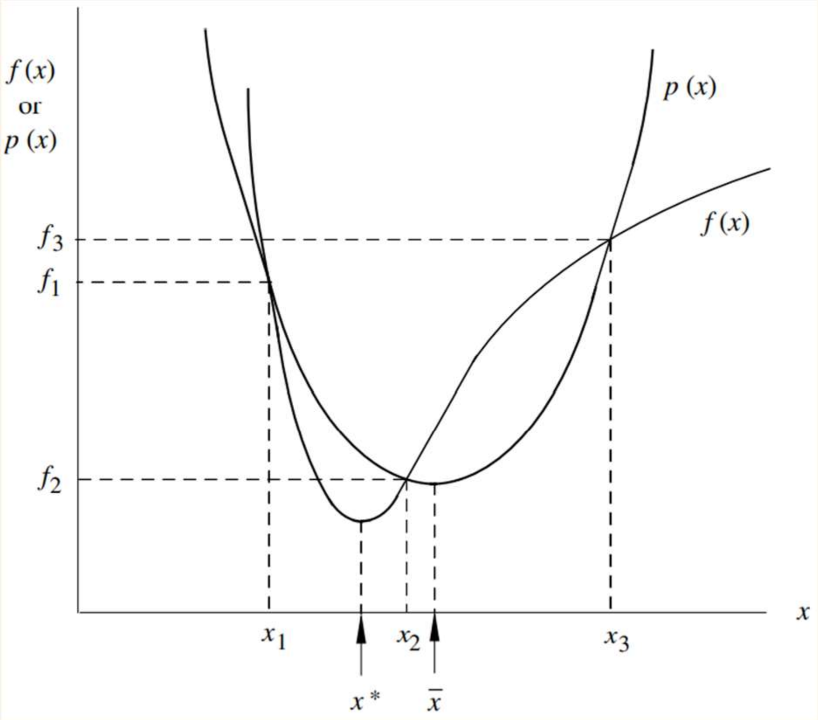
$$p(x) = a_0 + a_1 x + a_2 x^2$$

is assumed, where a_0, a_1, and a_2 are constants, a quadratic interpolation method is obtained.
Let,

$$p(x_i) = a_0 + a_1 x_i + a_2 {x_i}^2 = f(x_i) = f_i$$

for *i* = 1, 2, and 3 where $[x_1, x_3]$ is a bracket on the minimizer x* of *f(x)*.

If the values f_i are known, the three constants a_0, a_1, and a_2 can be deduced by solving the three simultaneous equations above.



The minimizer $\bar{x}$ of $p(x)$ is close to x^*, and if $f(x)$ can be accurately represented by a second-order polynomial, then $\bar{x} \approx x^*$. If $f(x)$ is a quadratic function, then $p(x)$ becomes an exact representation of $f(x)$ and $\bar{x} = x^*$.

The first derivative of $p(x)$ with respect to x is: $$p'(x) = a_1 + 2a_2 x$$

and if: $$p'(x) = 0 \quad \text{and} \quad a_2 \neq 0$$

$$\bar{x} = -\frac{a_1}{2a_2}$$

By solving the equations $p(x_i)$:

$$a_1 = -\frac{(x_2^2 - x_3^2)f_1 + (x_3^2 - x_1^2)f_2 + (x_1^2 - x_2^2)f_3}{(x_1 - x_2)(x_1 - x_3)(x_2 - x_3)}$$

$$a_2 = \frac{(x_2 - x_3)f_1 + (x_3 - x_1)f_2 + (x_1 - x_2)f_3}{(x_1 - x_2)(x_1 - x_3)(x_2 - x_3)}$$

By substituting a_1 and a_2 in $\bar{x}$ we obtain the **equation of interpolation**:

$$\bar{x} = \frac{(x_2^2 - x_3^2)f_1 + (x_3^2 - x_1^2)f_2 + (x_1^2 - x_2^2)f_3}{2[(x_2 - x_3)f_1 + (x_3 - x_1)f_2 + (x_1 - x_2)f_3]}$$

Parabolic interpolation algorithm (for maximum)

1. Define x_1 and x_3 (the bounds of the range of uncertainty)
2. Define x_2 (a guess between x_1 and x_3 or the middle of the interval)
3. Define ε (tolerance); set $\bar{x}_0$ to 10^6
4. Compute f_1, f_2 and f_3
5. Compute $\bar{x}$
6. If $x_2 < \bar{x}$

    if $f_2 > f(\bar{x})$

      $x_3 = \bar{x}$

    if $f_2 < f(\bar{x})$

      $x_1 = x_2$

      $x_2 = \bar{x}$

   if $x_2 > \bar{x}$

    if $f_2 < f(\bar{x})$

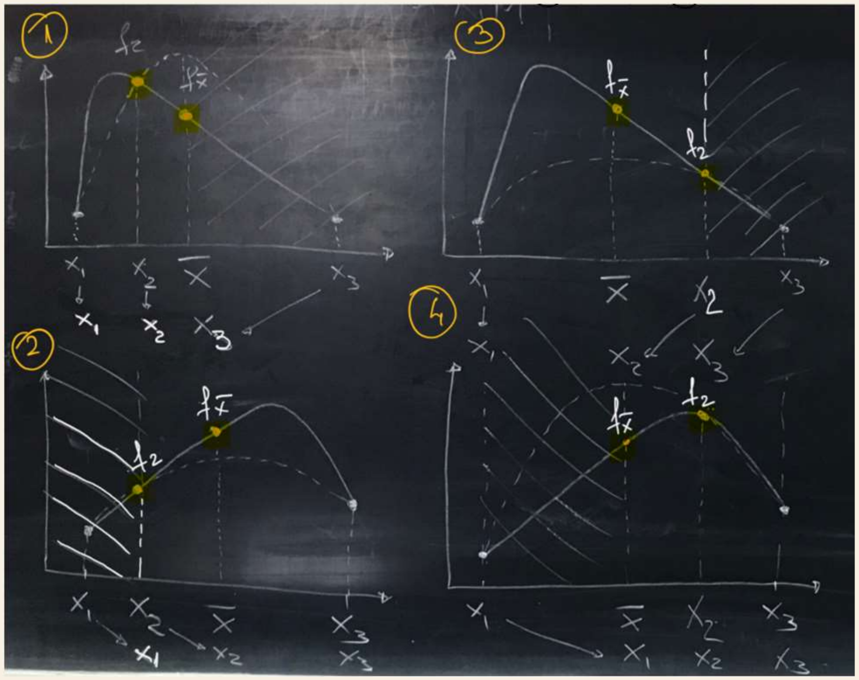
      $x_3 = x_2$

      $x_2 = \bar{x}$

    if $f_2 > f(\bar{x})$

      $x_1 = \bar{x}$

7. While $|\bar{x} - \bar{x}_0| > \varepsilon$, repeat from step 4



OPTIMIZATION TOOLBOX IN MATLAB

fminbnd Single-variable bounded nonlinear function minimization.

```
X = fminbnd(FUN,x1,x2)
```

fminsearch Multidimensional unconstrained nonlinear minimization

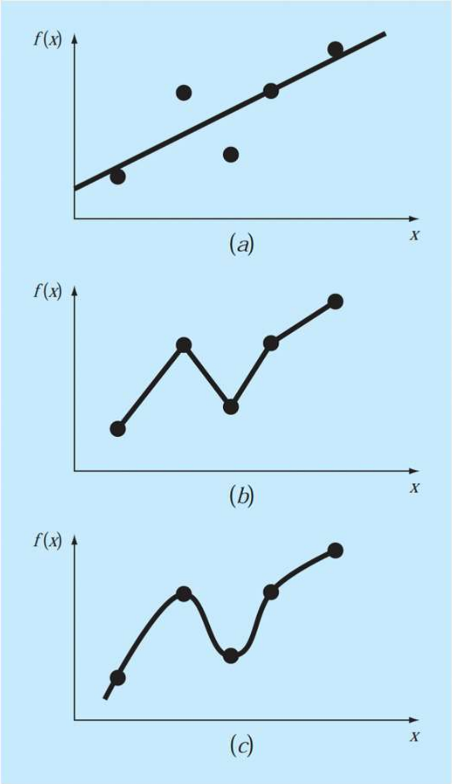
```
X = fminsearch(FUN,X0)
```

fmincon finds a constrained minimum of a function of several variables.

```
X = fmincon(FUN,X0,A,B,Aeq,Beq,LB,UB)
```

CURVE FITTING

Data is given for disctete values along a continuum. Estimates may be required at points between these discrete values



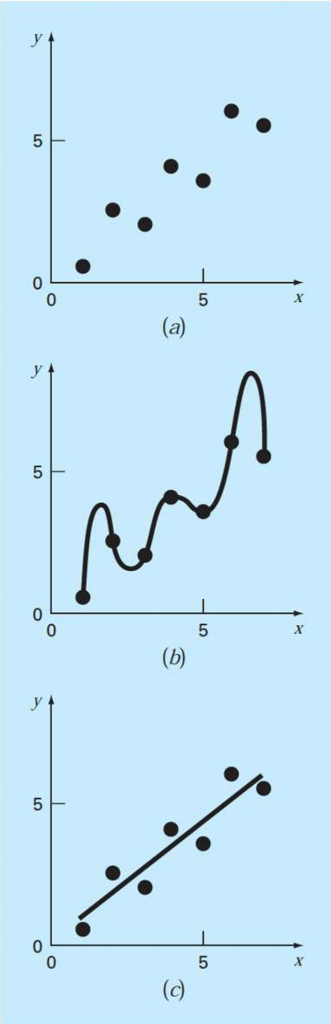
Three attempts to fit a "best" curve through five data points.

(a) Least-squares regression,

(b) linear interpolation,

(c) curvilinear interpolation.

Least-Squares Regression

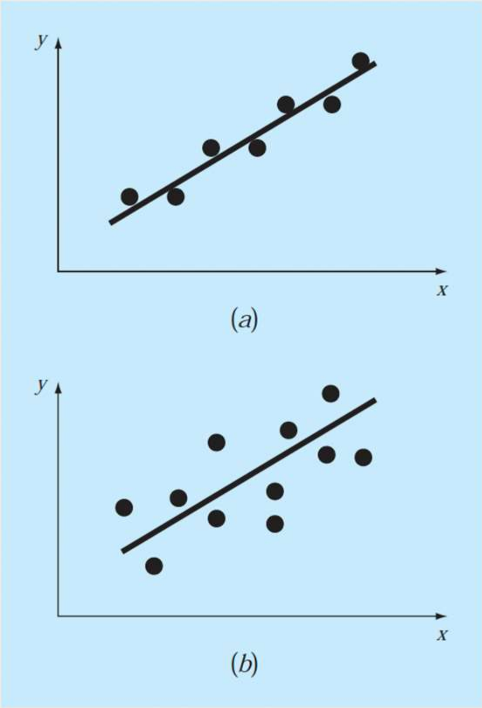


(a) Data exhibiting significant error.

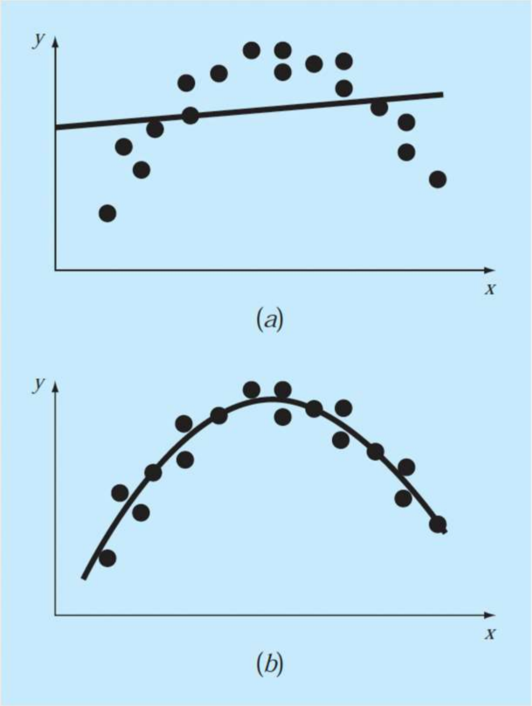
(b) Polynomial fit oscillating beyond the range of the data. Non-linear regression.

(c) More satisfactory result using the least-squares fit. Linear regression.

Criteria for the **best** fit

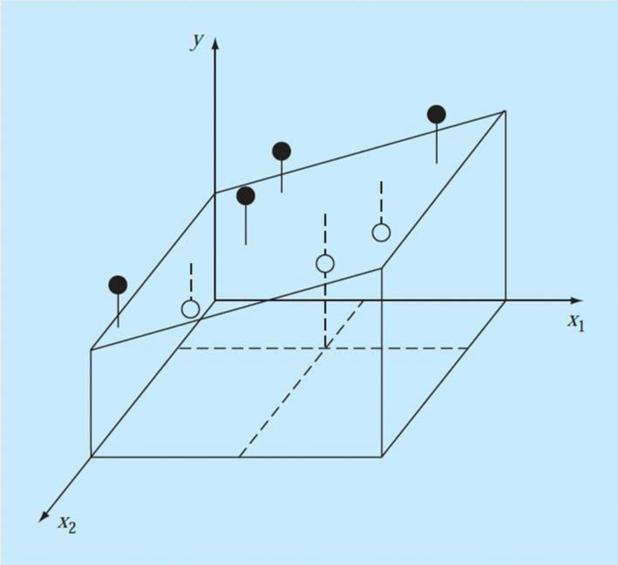


Linear regression with
(a) small and (b) large residual errors.



(a) Data that is ill-suited for linear least-squares regression.
(b) Indication that a parabola is preferable.

$$\sum_{i=1}^{n} Error_i^2 = \sum_{i=1}^{n} \left(y_{i,measured} - y_{i,model}\right)^2$$



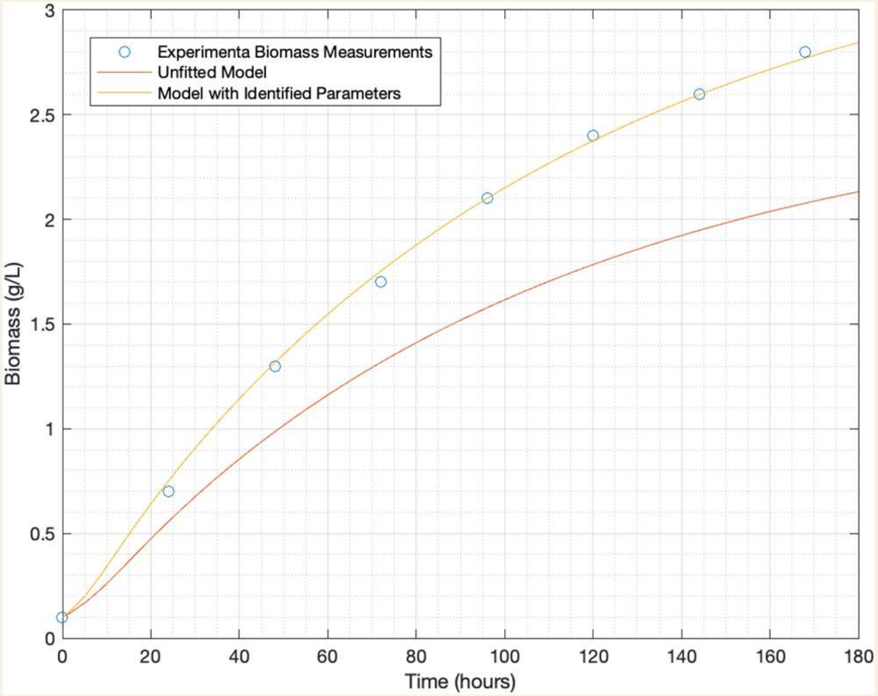
Graphical depiction of multiple linear regression where y is a linear function of x1 and x2.

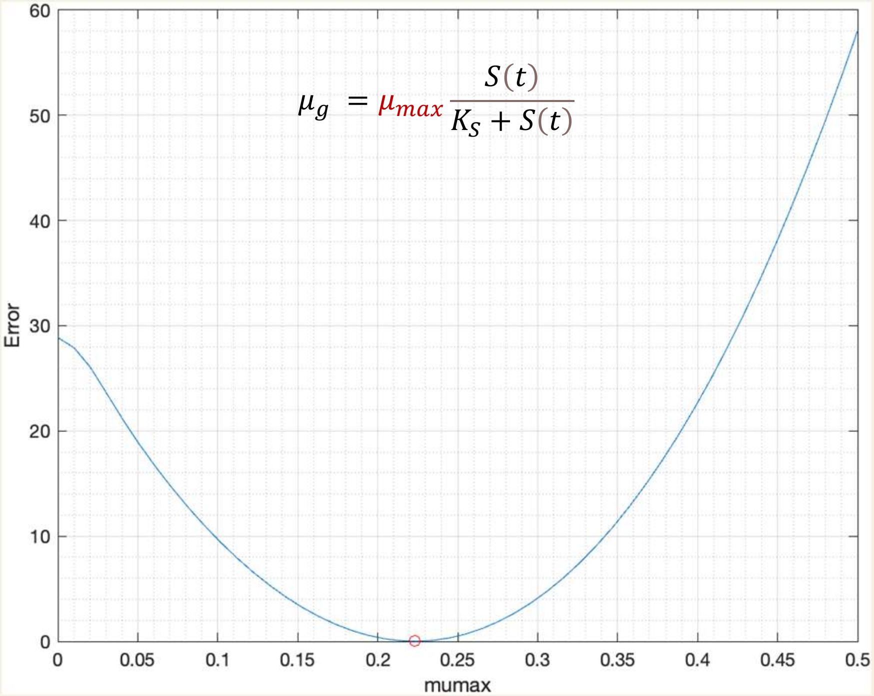
Parameter Identification in a Aerobic Wastewater Treatment Process

One-dimensional optimization to identify the specific growth rate, μ_{max}, that fit the measured data

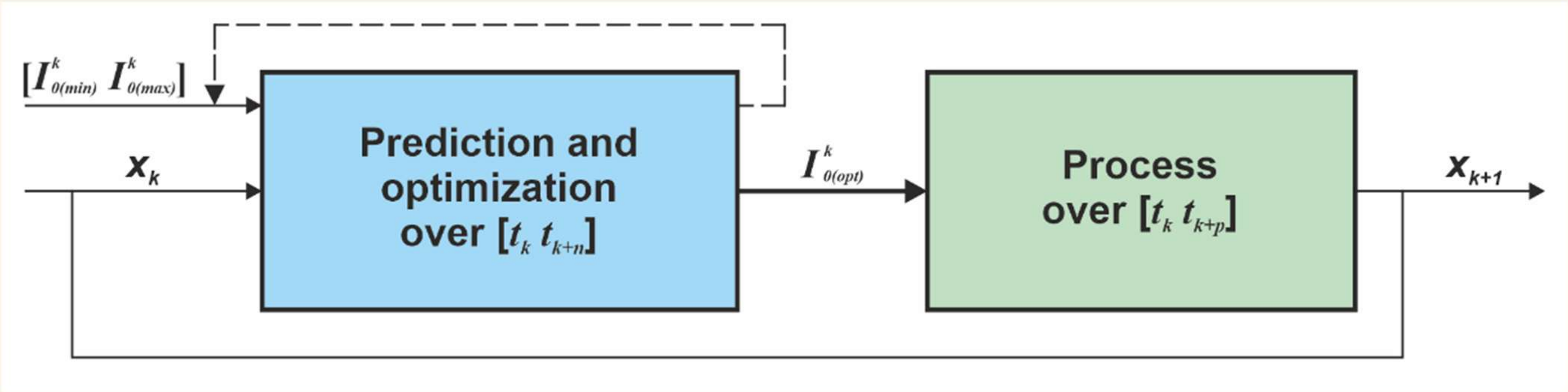
$$\frac{dX}{dt} = r_x$$

$$r_x = \mu X = \mu_g X - \mu_d X$$





THE CLOSED-LOOP CONTROL SYSTEM



THANK YOU

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