Optimization and Simulation

Introduction

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Outline

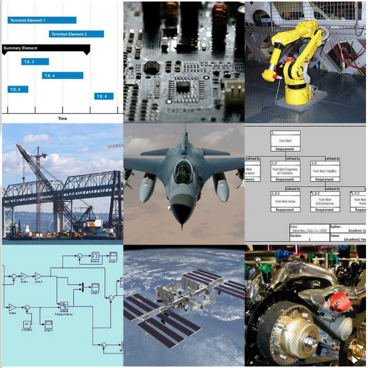
Engineering systems

Definition (Wikipedia)

Combination of components that work in synergy to collectively perform a useful function.

Properties

- Complex
- Large
- Designed
- Configurable
- Interactions with external world



Source: Wikipedia

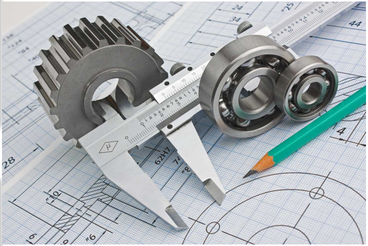
Engineering systems

Objectives

- Design
- Maintain
- Operate

Time horizon

- Long-term
- Medium-term
- Short-term

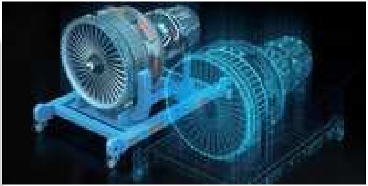


Source: Swiss Learning Exchange

Engineering systems

Mathematical and digital twins

- Modeling
- Simulation
- Optimization



Source: Konica Minolta

Engineering systems

	Modeling	Simulation	Optimization
Roles	Represent	Predict	Improve
How?	Capture causal effects	Capture the propagation of uncertainty	Investigate better configurations

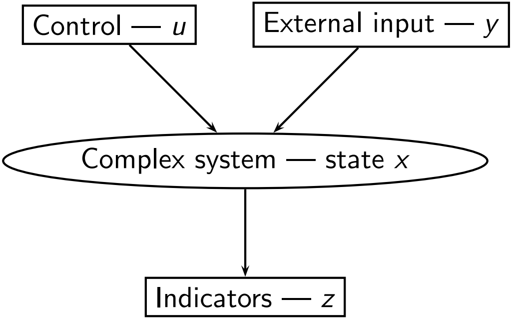
Outline

Modeling

System

A system can be seen as a black box, modeled by

$$z = h(x, y, u; \theta)$$



Modeling

$$z = h(x, y, u; \theta)$$

Example

A car:

- x captures the state of the system (e.g. speed, position of other vehicles)
- y captures external influences (e.g. wind)
- u captures possible human controls on the system (e.g. acceleration/deceleration)
- z represents indicators of performance (e.g. oil consumption).

Modeling

Decompose the complexity

- The model h is usually decomposed to reflect the interactions of the subsystems
- For example,
  - a car-following model captures the target speed of the driver,
  - an engine model derives the actual consumption as a function of the acceleration.

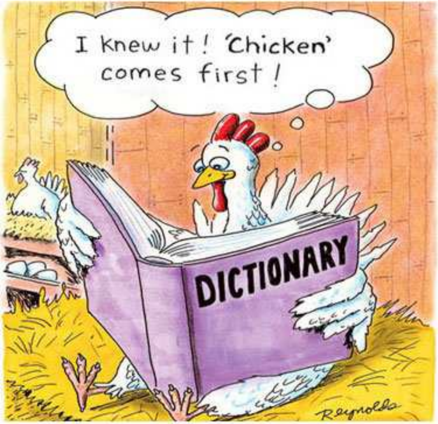
Modeling

Causal effects

- Very important to identify the causal effects
- Failure to do so may generate wrong conclusions

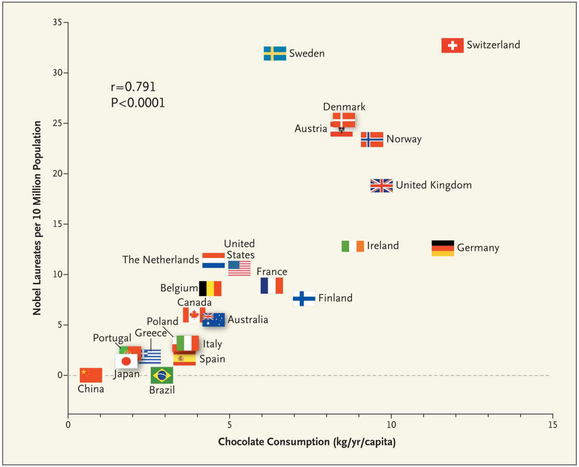
Forecasting

Assumption: causal effects are stable over time and configurations of the system.



Data can be misleading

Chocolate Consumption, Cognitive Function, and Nobel Laureates



Source: [Messerli, 2012]

Inference

Data collection

On an existing system, collect N observations of x_n, y_n, u_n, z_n, $n = 1, \ldots, N$.

Goodness of fit

For a given value of θ, "distance" $d_n(\theta)$ between

- the predicted value $h(x_n, y_n, u_n; \theta)$, and
- the observed value z_n.

Inference

Find $\widehat{\theta}$ that minimizes the total distance:

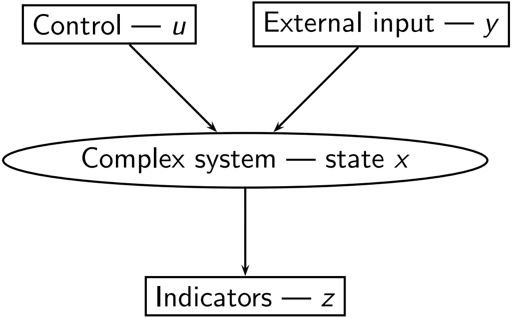
$$\widehat{\theta} = \text{argmin}_\theta \sum_{n=1}^{N} d_n(\theta).$$

Outline

Simulation

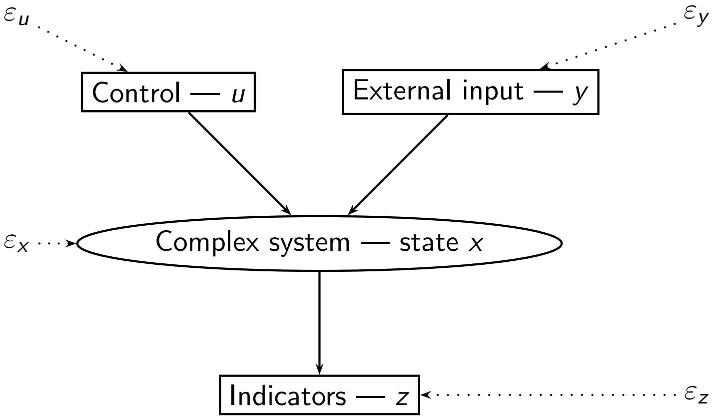
Simulation is more than simply applying the model.

$$z = h(x, y, u; \widehat{\theta})$$



Simulation

$$Z = h(X, Y, U; \widehat{\theta}) + \varepsilon_z$$



Simulation

Propagation of uncertainty

$$Z = h(X, Y, U; \widehat{\theta}) + \varepsilon_z$$

- Given the distribution of X, Y, U and ε_z
- what is the distribution of Z?

Simulation

Sampling

- Draw realizations of X, Y, U, ε_z
- Call them $x^r, y^r, u^r, \varepsilon_z^r$
- For each r, compute

$$z^r = h(x^r, y^r, u^r; \widehat{\theta}) + \varepsilon_z^r$$

- z^r are draws from the random variable Z

Analysis

- Generate many draws from Z.
- Analyze their empirical distribution.

Importance of number of draws

Theory vs. practice

- Theory: true distribution of Z when $r \to \infty$.
- Practice: finite number R of draws.
- If R is too small, simulator output is just noise.

Analogy with real world

- Nature also generates instances of a complex random variable.
- Experiments must be repeated in order to reach conclusions.

Example: policy analysis

- The real impact of a policy is difficult to analyze.
- Incomplete results that are consistent with expectations may lead to erroneous conclusions.

Example: improving safety

Accidents in Kid City

- The mayor of Kid City has commissioned a consulting company
- Objective: assess the effectiveness of safety campaigns
- They propose to use simulation

Example: improving safety

Accidents in Kid City

Example: improving safety

Accidents in Kid City: 

Example: improving safety

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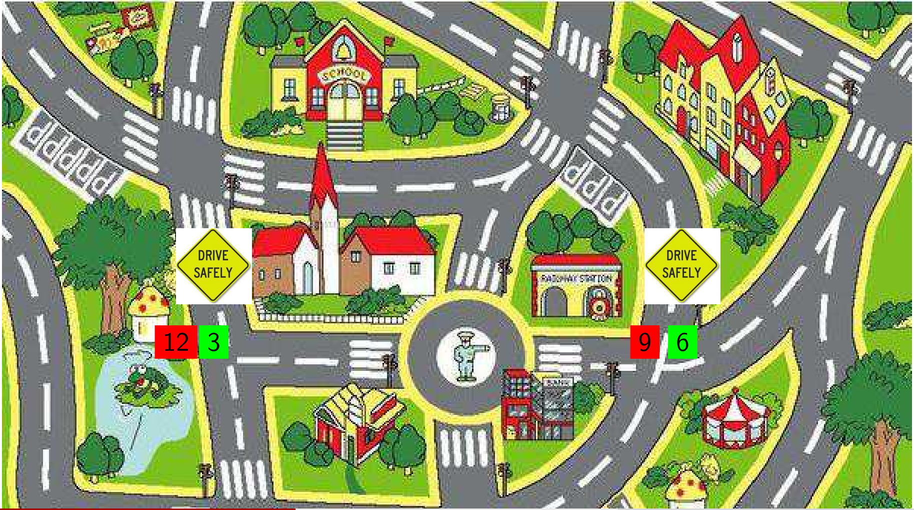
Accidents in Kid City:



Example: improving safety

Two major flaws

- Causal effects are not modeled
- Simulation performed with only one draw

What should have been done

- Simulate the number of accidents many times.
- If so, the average number of accidents is around 7, everywhere, with or without the sticker.
- A formal statistical test would not reject the null hypothesis that the sticker has no effect.

Outline

Simulation

Derivation of indicators from the distribution

- Mean
- Variance
- Modes
- Quantiles

Statistics

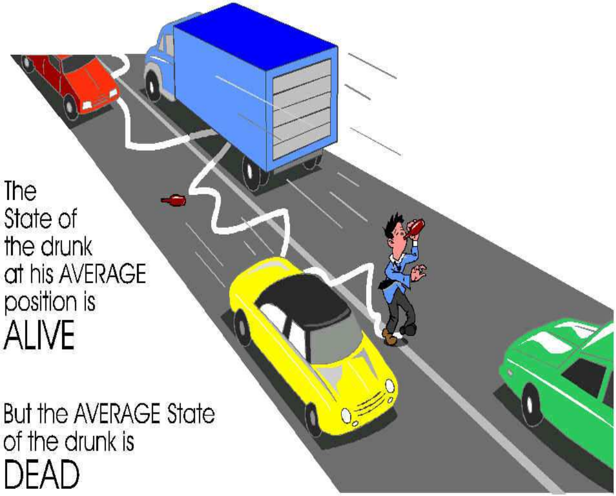
"Numbers don't lie. That's where we come in."

Indicators

- Mean: $\mathrm{E}[Z] \approx \bar{Z}_R = \frac{1}{R}\sum_{r=1}^{R} z^r$
- Variance: $\mathrm{Var}(Z) \approx \frac{1}{R}\sum_{r=1}^{R}\left(z^r - \bar{Z}_R\right)^2$.
- Modes: based on the histogram
- Quantiles: sort and select

Important: there is more than the mean

The mean



[Savage et al., 2012]

The mean

The flaw of averages

[Savage et al., 2012]

$$\mathrm{E}[Z] = \mathrm{E}[h(X, Y, U; \widehat{\theta}) + \varepsilon_z] \neq h(\mathrm{E}[X], \mathrm{E}[Y], \mathrm{E}[U]; \widehat{\theta}) + \mathrm{E}[\varepsilon_z]$$

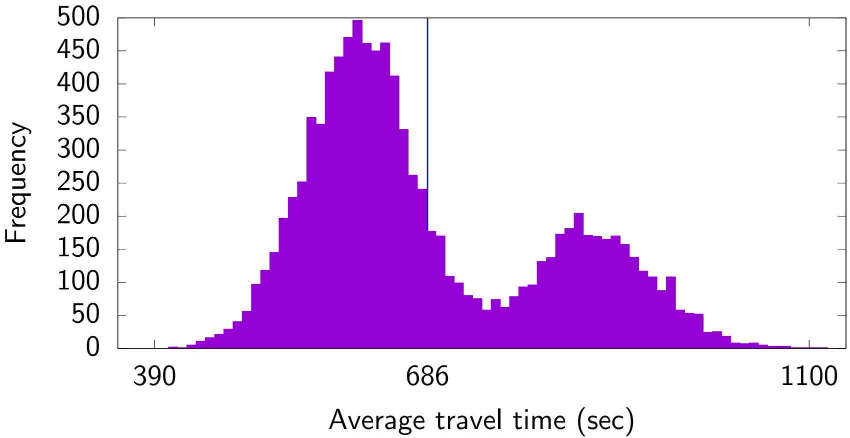
... except if h is linear.

There is more than the mean

Example

- Intersection with capacity 2000 veh/hour
- Traffic light: 30 sec green / 30 sec red
- Constant arrival rate: 2000 veh/hour during 30 minutes
- With 30% probability, capacity at 80%.
- Indicator: Average time spent by travelers

There is more than the mean



Pitfalls of simulation

Few number of runs

- Run time is prohibitive
- Tempting to generate partial results rather than no result

Focus solely on the mean

- The mean is useful, but not sufficient.
- For complex distributions, it may be misleading.
- Intuition from normal distribution (mode = mean, symmetry) do not hold in general.
- Important to investigate the whole distribution.
- Simulation allows to do it easily.

Challenges

- How to generate draws from Z?
- How to represent complex systems? (specification of h)
- How large R should be?
- How good is the approximation?

Pseudo-random numbers

Definition

- Deterministic sequence of numbers
- which have the appearance of draws from a $U(0,1)$ distribution

Typical sequence

$$x_n = a x_{n-1} \text{ modulo } m$$

- This has a period of the order of m
- So, m should be a large prime number
- For instance: $m = 2^{31} - 1$ and $a = 7^5$
- x_n/m lies in the $[0, 1[$ interval

Outline of the lectures

- Drawing from distributions
- Discrete event simulation
- Data analysis
- Variance reduction
- Markov Chain Monte Carlo

Reference

[Ross, 2012]

Outline

Optimization

Assumptions

- Control U is deterministic.

$$Z(u) = h(X, Y, u) + \varepsilon_z$$

- Various features of Z are considered: mean, variance, quantile, etc.

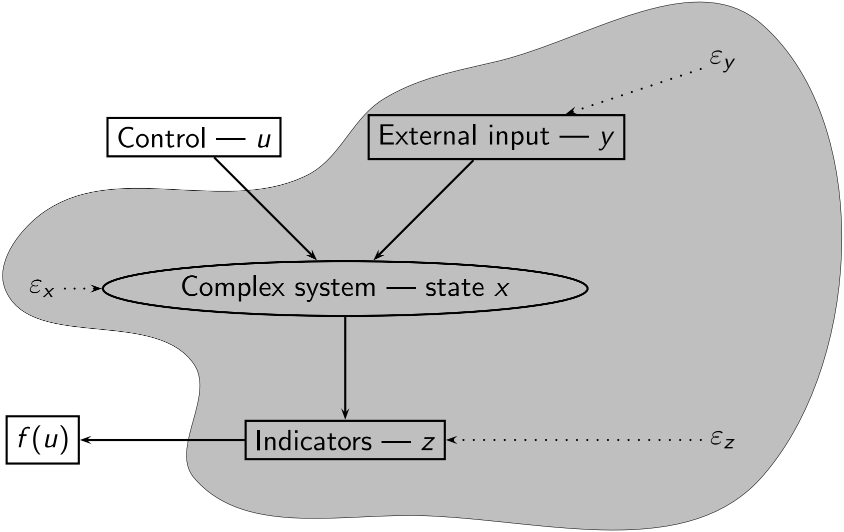
$$(z_1(u), \ldots, z_m(u))$$

- They are combined in a single indicator:

$$f(u) = g(z_1(u), \ldots, z_m(u))$$

- If not, it is called *multi-objective* optimization.

General framework: the black box



Optimization problem

$$\min_{u \in \mathbb{R}^n} f(u)$$

subject to

$$u \in \mathcal{U} \subseteq \mathbb{R}^n$$

- u: decision variables
- $f(u)$: objective function
- $u \in \mathcal{U}$: constraints
- $\mathcal{U}$: feasible set

In this course. . .

- Classical optimization problems
- Heuristics
- Multi-objective optimization

Summary

Modeling

- Decomposition of the complexity.
- Causal effects.

Simulation

- Propagation of uncertainty.
- Requires many draws.
- Analysis of the entire empirical distribution.
- There is more than the mean.

Optimization

- Identify the control that improves a function of the indicators.
- Optional: multi-objective optimization.

Bibliography

Messerli, F. (2012).
Chocolate consumption, cognitive function, and nobel laureates.
The New England Journal of Medicine, 367:1562–1564.

Ross, S. M. (2012).
Simulation.
Elsevier, fifth edition.

Savage, S., Danziger, J., and Markowitz, H. (2012).
The Flaw of Averages: Why We Underestimate Risk in the Face of Uncertainty.
Wiley.