### Simulation and optimization in transportation

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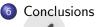
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### Outline



- 2 Simulation-based optimization
- 3 Black box algorithms
  - Noise reduction
- 💿 Open box algorithms





### Transport policies



#### Complexity

- Transport systems are complex
- Many elements interact
- Presence of uncertainty



3 / 55

June 4, 2014

### Transport policies

#### Causal effects

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







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June 4, 2014 4 / 55

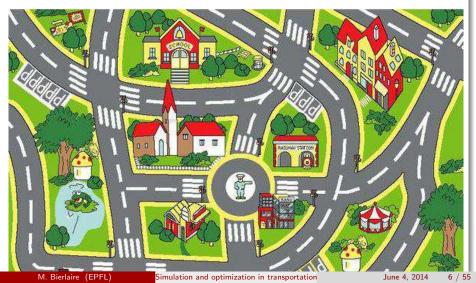
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#### Accidents in Kid City

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



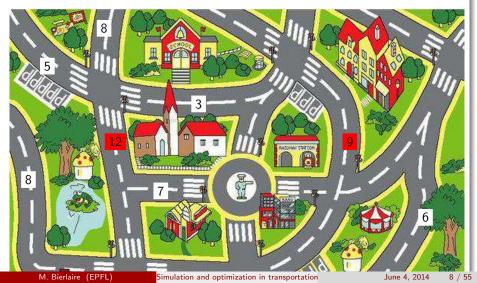
#### Accidents in Kid City



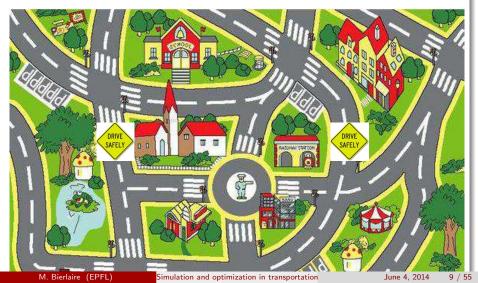
# Accidents in Kid City:



#### Accidents in Kid City



#### Accidents in Kid City



# Accidents in Kid City:



#### Two major flaws

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



### Capturing the complexity

#### Simulation

the act of imitating the behavior of some situation or some process by means of something suitably analogous

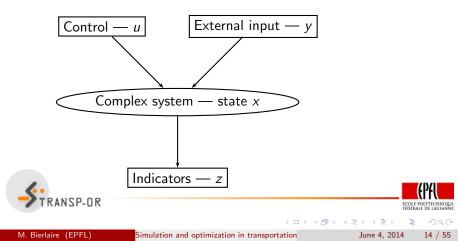


### Simulation: what it is not in engineering

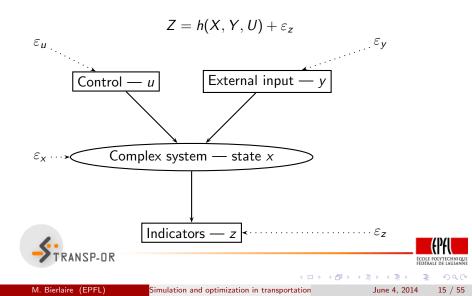


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$$z=h(x,y,u)$$



### Simulation



Propagation of uncertainty

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

• Given the distribution of X, Y, U and  $\varepsilon_z$ 

• what is the distribution of Z?

#### Derivation of indicators

- Mean
- Variance
- Modes
- Quantiles

M. Bierlaire (EPFL)

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#### Sampling

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

$$z^r = h(x^r, y^r, u^r) + \varepsilon_z^r$$

•  $z^r$  are draws from the random variable Z



### **Statistics**

@ MARK ANDERSON



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

#### Indicators

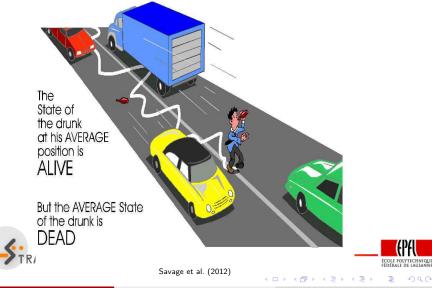
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- Mean:  $E[Z] \approx \overline{Z}_R = \frac{1}{R} \sum_{r=1}^R z^r$
- Variance:  $\operatorname{Var}(Z) \approx \frac{1}{R} \sum_{r=1}^{R} (z^r \overline{Z}_R)^2$ .
- Modes: based on the histogram
- Quantiles: sort and select

Important: there is more than the mean



### The mean



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June 4, 2014 19 / 55

#### The mean

#### The flaw of averages

Savage et al. (2012)

### $\mathsf{E}[Z] = \mathsf{E}[h(X, Y, U) + \varepsilon_z] \neq h(\mathsf{E}[X], \mathsf{E}[Y], \mathsf{E}[U]) + \mathsf{E}[\varepsilon_z]$

 $\dots$  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

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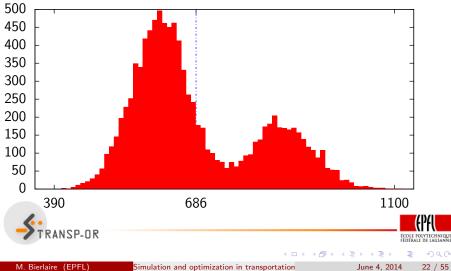
21 / 55

June 4, 2014

- 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 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.

### Outline

- Simulation-based optimization 2
- Black box algorithms



### Optimization

#### Assumptions

- U is deterministic.
- $S^{R}(Z)$  is the statistic of Z under interest (mean, quantile, etc.)
- R is the number of draws generated to obtain the statistics
- Distributions of X, Y and  $\varepsilon_z$  are known.

#### Optimization problem

$$\min_{u} f(u) = S^{R}(Z) = S^{R}(h(X, Y, u) + \varepsilon_{z})$$

subject to

$$g(u)=0.$$

## Optimization problem

#### Optimization problem

$$\min_{u} f(u) = S^{R}(Z) = S^{R}(h(X, Y, u) + \varepsilon_{z})$$

subject to

$$g(u)=0.$$

#### Difficulties

- R must be large, so calculating f is computationally intensive
- The derivatives of f are unavailable or very difficult to obtain



### Traffic simulation



#### Parameters calibration

- X: state of traffic
- Y: observed link flows
- u: parameters of the simulator
- h: traffic simulator
- Z: total squared difference between modeled and observed flows
- $S^{R}(Z)$ : mean squared error

### Traffic simulation



#### Traffic light optimization

- X: state of traffic
- Y: OD matrices
- u: traffic light configuration
- h: traffic simulator
- Z: total travel time
- $S^R(Z)$ : mean of total travel time Osorio and Bierlaire (2013)
- $S^R(Z)$ : std. dev. of total travel time Chen et al. (2013)



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June 4, 2014 29 / 55

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### Scenario based optimization



"Of course, this is a worst case scenario."

#### Method

- Identify a list of scenarios  $u_1, \ldots, u_N$
- Compute  $f(u_i)$  for each i

#### Comments

- Solution is feasible and realistic
- Limited computational effort
- No systematic investigation
- Relies only on the creativity of the analyst



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### Nonlinear programming

#### General approach

- $f(u) = S^{R}(h(X, Y, u) + \varepsilon_{z})$  is a nonlinear function of u
- In general, it is continuous and differentiable
- As h is a computer program, the derivatives are not available

#### Methods

- Automatic differentiation Griewank (2000)
- Derivative-free optimization Conn et al. (2009)
- Direct search Lewis et al. (2000)



### Automatic differentiation



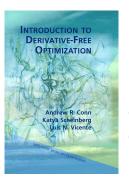
#### Method

Griewank (2000), Naumann (2012)

- A software is a sequence of a finite set of elementary operations
- Each of them is easy to differentiate
- Use chain rule to propagate



### Derivative-free optimization



#### Method

- Build a model of the function using interpolation
  - Lagrange polynomials
  - Splines
  - Kriging
- Use a trust region framework to guarantee global convergence

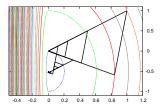
#### Comments

- Convergence theory
- Numerical issues with interpolation
- Need for a large number of interpolation points

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### Direct search



#### Method

- Generate a sequence of simplices
- using geometrical transformations maintaining the simplex structure

#### Comments

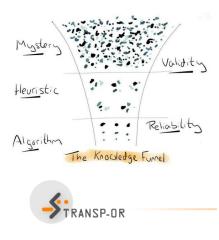
- Some do not always converge (Nelder-Nead)
- Convergence may be slow





June 4, 2014 34 / 55

### Heuristics



#### Neighborhood

- Simple modifications of u
- Feasible or infeasible

#### Local search

- Select a better neighbor
- Stop at a local optimum

#### Meta heuristics

- Escape from local optima
- Simulated annealing
- Variable neighborhood search
- and many others...

### Example of simulation

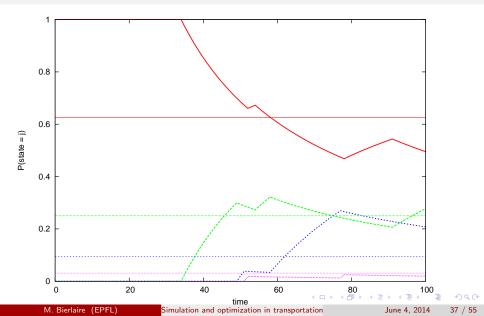
#### Machine with 4 states wrt wear

- perfect condition,
- partially damaged,
- seriously damaged,
- completely useless.

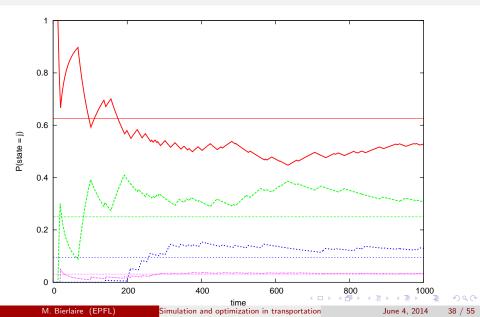
#### Transition 0.95 0.04 0.01 0.00.0 0.90 0.05 0.05 0.0 0.0 0.80 0.20 0.0 1.00.0 0.0



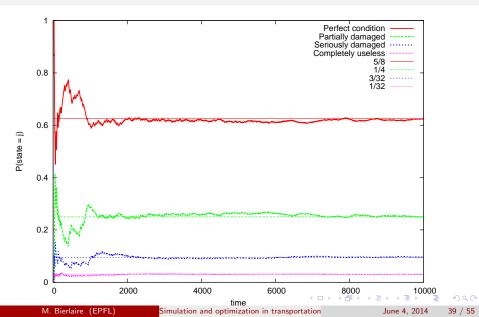
# Noise reduction: R = 100



# Noise reduction: R = 1000



## Noise reduction: R = 10000



# Noise reduction methods

#### Adaptive Monte-Carlo

Bastin et al. (2006)

- R varies across iterations
- Small R in early iterations
- R increases as the algorithm converges







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# Noise reduction methods

#### Least square fitting

Bierlaire et al. (2007), Bierlaire and Crittin (2006)





- Interpolation model + adaptive Monte-Carlo
- Each iterate considered as a sample
- Regression is used instead of interpolation

#### Comments

- Originally for systems of nonlinear equations
- An update formula à la Broyden can be derived
- Appropriate for large-scale applications (2 millions variables)

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### Open box algorithms



# Open box algorithms

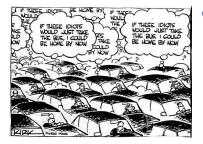
#### What are we simulating?

- h(·) is a detailed description of our system
- We need simulation because it is complicated
- We open the box, an build a simpler representation of the system





### Deterministic model



#### Congestion

Osorio and Bierlaire (2009)

- Queuing theory
- Closed form analytical equations
- Simplifying assumptions (e.g. stationarity)



### Metamodel

Osorio and Bierlaire (2013)

$$m(u, x; \alpha, \beta, q) = \alpha T(u, x, q) + \phi(u, \beta)$$

- $T(\cdot)$  analytical model
- $\phi(\cdot)$  interpolation model
- *u* control (traffic lights)
- x state variables



### Metamodel

• x state variables

Osorio and Bierlaire (2013)

$$m(u, x; \alpha, \beta, q) = \alpha T(u, x, q) + \phi(u, \beta)$$
  
•  $T(\cdot)$  analytical model  
•  $\phi(\cdot)$  interpolation model  
•  $u$  control (traffic lights)  
• mathematics



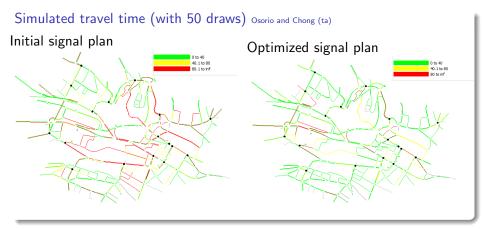
## Metamodel approach

#### Ongoing research

- Large scale problems Osorio and Chong (ta)
- Fuel consumption Osorio and Nanduri (ta)
- Emissions Osorio and Nanduri (2013)

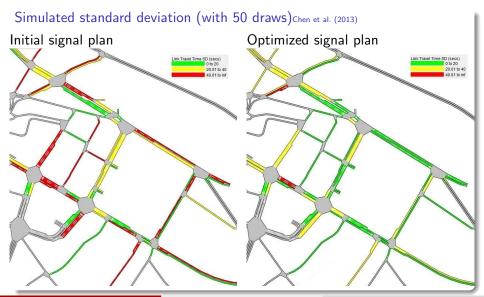


## Large scale problems



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# Reliability



### Outline

### Simulation

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# Summary

#### Simulation

- Number of draws
- Beyond the mean

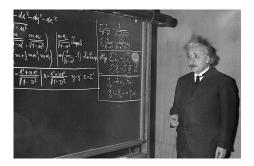
#### Black box algorithms

- Scenarios
- Automatic differentiation
- Derivative-free
- Direct search
- Heuristics
- Noise reduction

#### Open box algorithms

- Deterministic engineering model
- Metamodel

### Conclusion



Everything should be made as simple as possible, but no simpler

Albert Einstein

# Bibliography I

- Bastin, F., Cirillo, C., and Toint, P. L. (2006). Application of an adaptive monte carlo algorithm to mixed logit estimation. *Transportation Research Part B: Methodological*, 40(7):577–593.
- Bierlaire, M. and Crittin, F. (2006). Solving noisy large scale fixed point problems and systems of nonlinear equations. *Transportation Science*, 40(1):44–63.
- Bierlaire, M., Crittin, F., and Thémans, M. (2007). A multi-iterate method to solve systems of nonlinear equations. *European Journal of Operational Research*, 183(1):20–41.
- Chen, X., Osorio, C., and Santos, B. (2013). Travel time reliability in signal control problem: Simulation-based optimization approach. In *Proceedings of the Transportation Research Board (TRB) Annual Meeting January 13-17, 2013.*

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# Bibliography II

- Conn, A. R., Scheinberg, K., and Vicente, L. N. (2009). *Introduction to derivative-free optimization*, volume 8 of *MPS-SIAM series on optimization*. Siam.
- Griewank, A. (2000). *Evaluating derivatives. Principles and Techniques of Algorithmic differentiation.* Frontiers in Applied Mathematics. SIAM.
- Lewis, R. M., Torczon, V., and Trosset, M. W. (2000). Direct search methods: Then and now. *Journal of Computational and Applied Mathematics*, 124:191–207.
- Naumann, U. (2012). The Art of Differentiating Computer Programs: An Introduction to Algorithmic Differentiation. Number 24 in Software, Environments, and Tools. SIAM, Philadelphia, PA.
- Osorio, C. and Bierlaire, M. (2009). An analytic finite capacity queueing network model capturing the propagation of congestion and blocking. *European Journal of Operational Research*, 196(3):996–1007.

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# **Bibliography III**

- Osorio, C. and Bierlaire, M. (2013). A simulation-based optimization framework for urban traffic control. *Operations Research*, 61(6):1333–1345.
- Osorio, C. and Chong, L. (ta). A computationally efficient simulation-based optimization algorithm for large-scale urban transportation problems. *Transportation Science*.
- Osorio, C. and Nanduri, K. (2013). Emissions mitigation: coupling microscopic emissions and urban traffic models for signal control. MIT.
- Osorio, C. and Nanduri, K. (ta). Energy-efficient urban traffic management: a microscopic simulation-based approach. *Transportation Science*.
- Savage, S., Danziger, J., and Markowitz, H. (2012). *The Flaw of Averages:* Why We Underestimate Risk in the Face of Uncertainty. Wiley.

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