

# Simulation and optimization in transportation: an overview

Michel Bierlaire

Transport and Mobility Laboratory  
School of Architecture, Civil and Environmental Engineering  
Ecole Polytechnique Fédérale de Lausanne

November 6, 2014



# Outline

- 1 Simulation
- 2 Simulation-based optimization
- 3 Black box algorithms
- 4 Noise reduction
- 5 Open box algorithms
- 6 Conclusions



# Transport policies



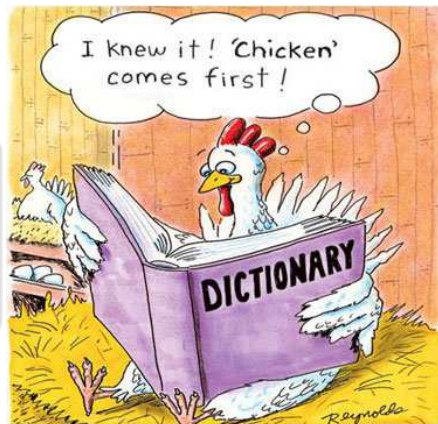
## Complexity

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

# Transport policies

## Causal effects

- Very important to identify the causal effects
- Failure to do so may generate wrong 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
- Before and after analysis



Example: improving safety

## Accidents in Kid City



# Example: improving safety

Accidents in Kid City: 



# Example: improving safety

## Accidents in Kid City





## Example: improving safety

## Accidents in Kid City



# Example: improving safety

Accidents in Kid City: 



# Example: improving safety

## Conclusions

- The “Drive safely” signs have a significant impact on safety
- The number of accidents has been reduced by 57%, from 21 down to 9.



# Example: improving safety

## 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

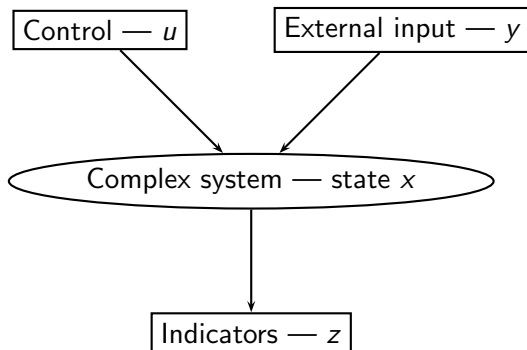


# Simulation: what it is not in engineering

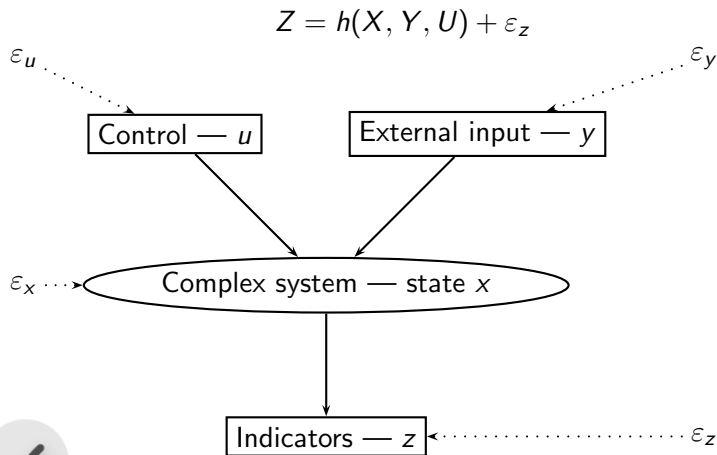


# Simulation

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



# Simulation





# 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

# Simulation

## Sampling

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

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

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



# Simulation

## Empirical distribution function

$$F_e(x) = \frac{1}{R} \#\{z^r \leq x\},$$

For any  $x \in \mathbb{R}$ ,

$$E[F_e(x)] = F(x)$$

and

$$\text{var}(F_e(x)) = \frac{1}{R} F(x)(1 - F(x)).$$



# Statistics

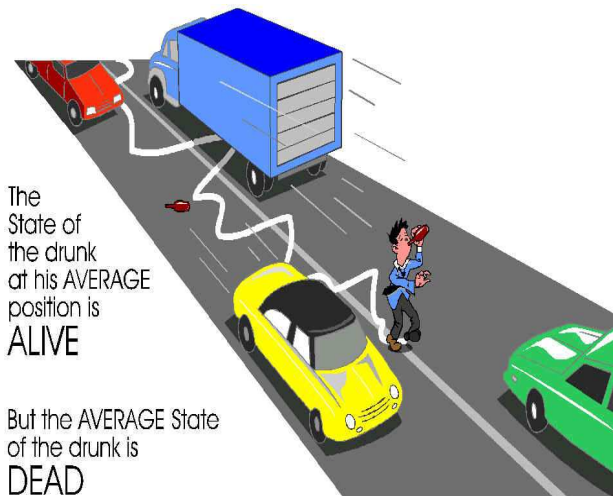


## Indicators

- Mean:  $E[Z] \approx \bar{Z}_R = \frac{1}{R} \sum_{r=1}^R z^r$
- Variance:  $\text{Var}(Z) \approx \frac{1}{R} \sum_{r=1}^R (z^r - \bar{Z}_R)^2$
- 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)

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

... except if  $h$  is linear.



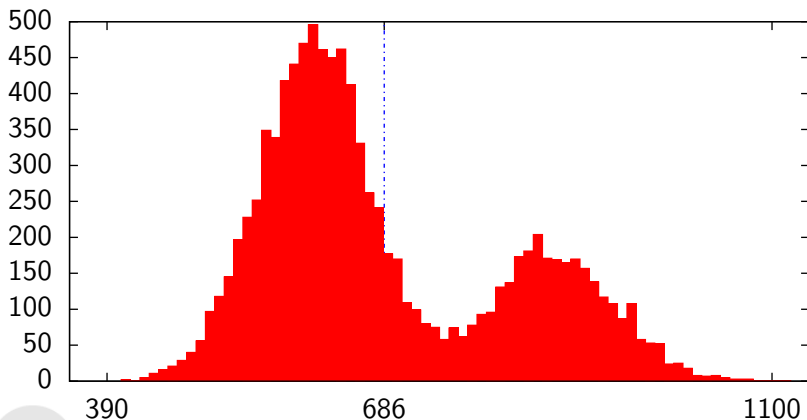
# There is more than the mean



## 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 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

- 1 Simulation
- 2 **Simulation-based optimization**
- 3 Black box algorithms
- 4 Noise reduction
- 5 Open box algorithms
- 6 Conclusions



# 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

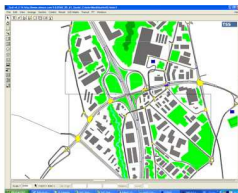
$$g(u) = 0.$$

## 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)

# Outline

- 1 Simulation
- 2 Simulation-based optimization
- 3 Black box algorithms**
- 4 Noise reduction
- 5 Open box algorithms
- 6 Conclusions



# Scenario based optimization

## Method

- Identify a list of scenarios  $u_1, \dots, u_N$
- 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

© MARK ANDERSON

WWW.ANDERTOONS.COM



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



# Nonlinear programming

## General approach

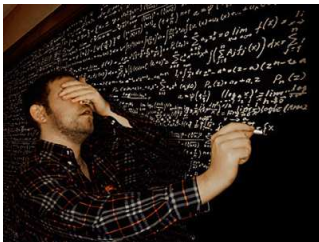
- $f(u) = S^R(h(X, Y, u) + \varepsilon_z)$  is a nonlinear function of  $u$
- In general, it is continuous and differentiable
- As  $h$  is a computer program, the derivatives are not available

## Methods

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



# Automatic differentiation



## Method

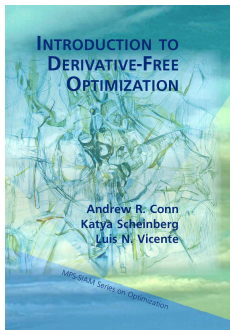
Griewank (2000), Naumann (2012)

- 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

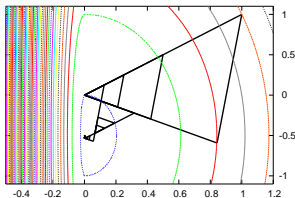


## Comments

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



# Direct search



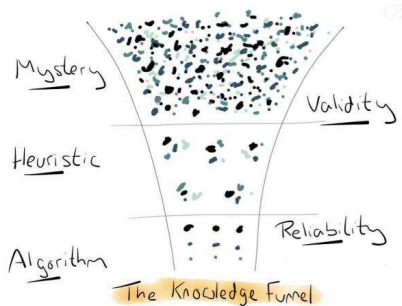
## Method

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

## Comments

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

# 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...

# Outline

- 1 Simulation
- 2 Simulation-based optimization
- 3 Black box algorithms
- 4 Noise reduction**
- 5 Open box algorithms
- 6 Conclusions



# Example of simulation

## Machine with 4 states wrt wear

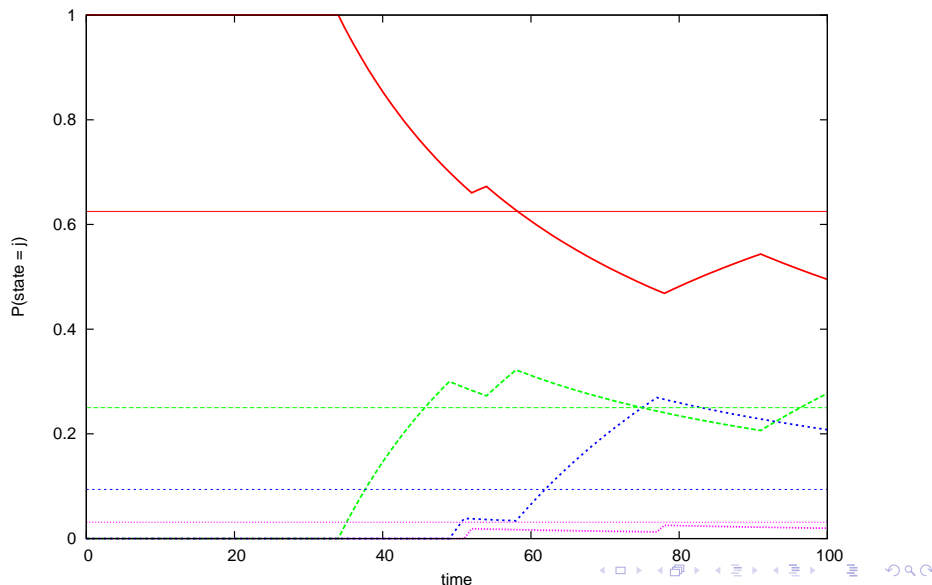
- perfect condition,
- partially damaged,
- seriously damaged,
- completely useless.

## Transition

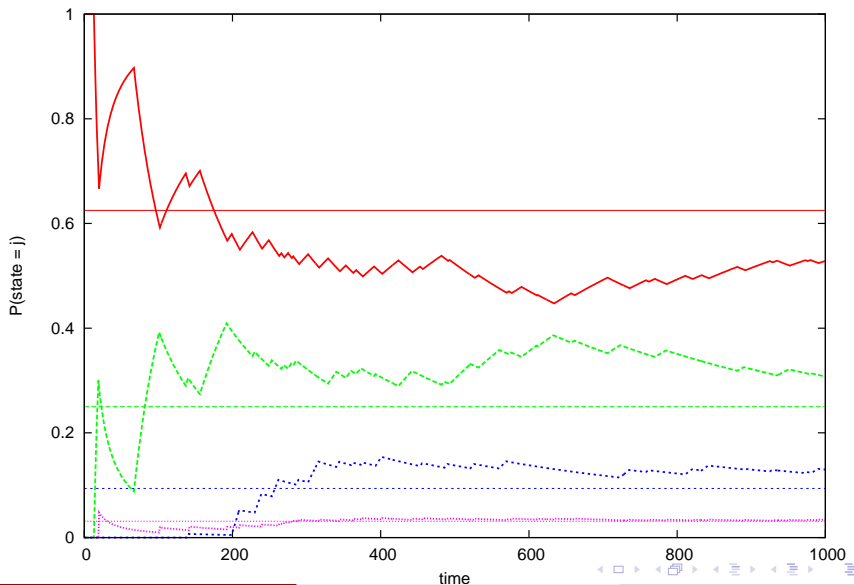
$$\begin{pmatrix} 0.95 & 0.04 & 0.01 & 0.0 \\ 0.0 & 0.90 & 0.05 & 0.05 \\ 0.0 & 0.0 & 0.80 & 0.20 \\ 1.0 & 0.0 & 0.0 & 0.0 \end{pmatrix}$$



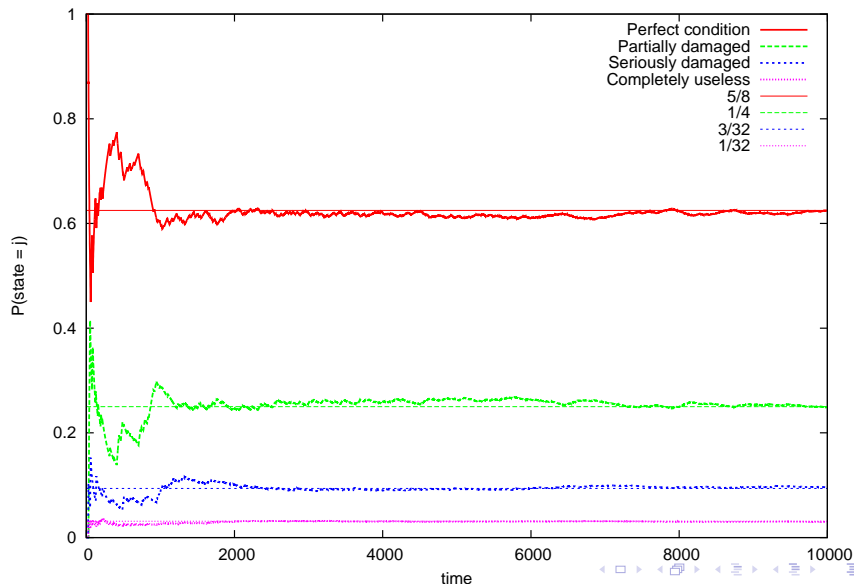
# Noise reduction: $R = 100$





Noise reduction:  $R = 1000$ 

# Noise reduction: $R = 10000$

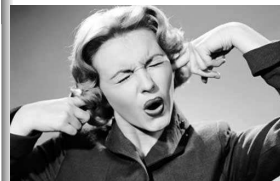


# Noise reduction methods

## Adaptive Monte-Carlo

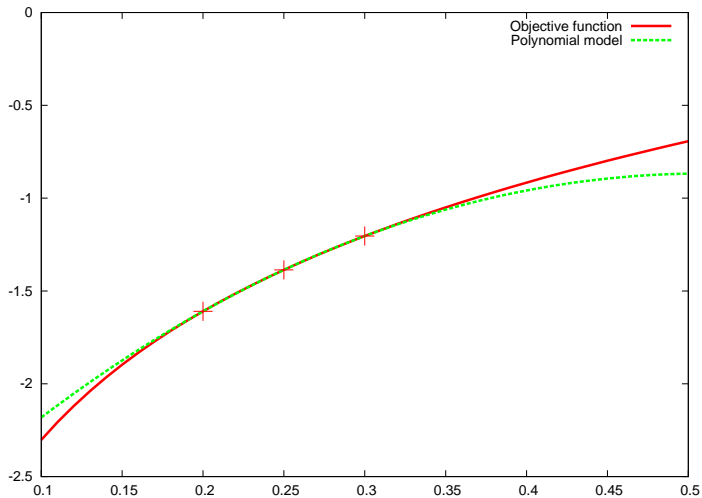
Bastin et al. (2006)

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



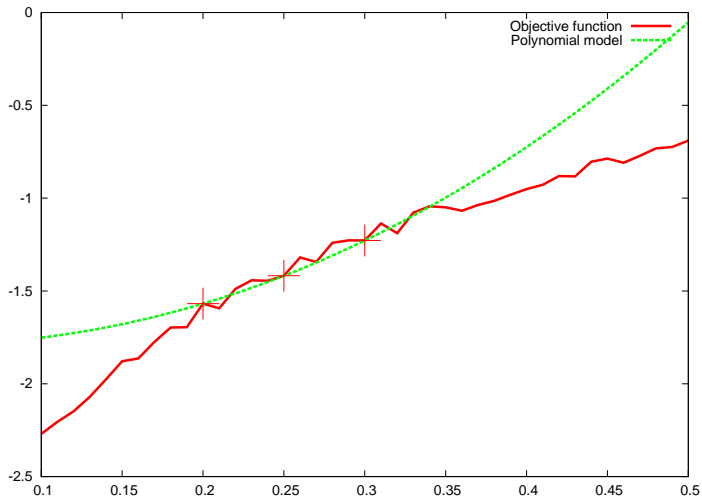
# Noise reduction methods

## Interpolation: true function



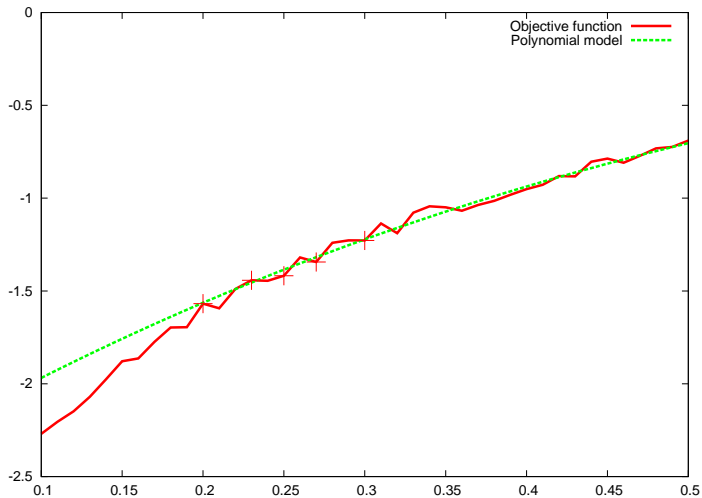
# Noise reduction methods

## Interpolation: simulated function



# Noise reduction methods

## Least-square fitting: simulated function



# 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)



# Outline

- 1 Simulation
- 2 Simulation-based optimization
- 3 Black box algorithms
- 4 Noise reduction
- 5 Open box algorithms**
- 6 Conclusions





# Open box algorithms

## What are we simulating?

- $h(\cdot)$  is a detailed description of our system
- We need simulation because it is complicated
- We open the box, and 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

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
- engineering
  - mathematics



# Metamodel approach

## Ongoing research

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



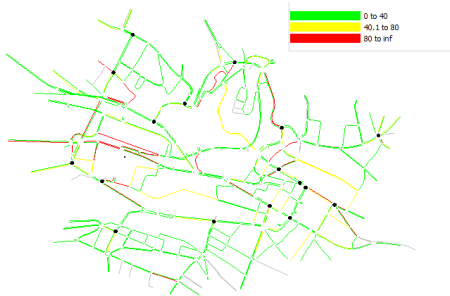
# Large scale problems

Simulated travel time (with 50 draws) Osorio and Chong (ta)

Initial signal plan



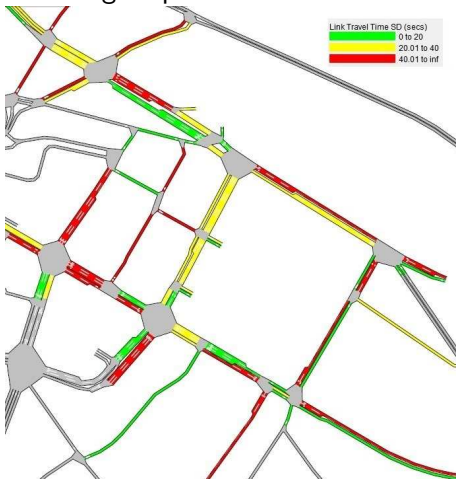
Optimized signal plan



# Reliability

Simulated standard deviation (with 50 draws) Chen et al. (2013)

Initial signal plan



Optimized signal plan



# Outline

- 1 Simulation
- 2 Simulation-based optimization
- 3 Black box algorithms
- 4 Noise reduction
- 5 Open box algorithms
- 6 Conclusions**



# Summary

## Simulation

- Number of draws
- Beyond the mean

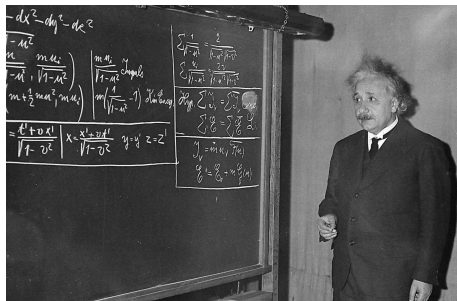
## Black box algorithms

- 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*.

## 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.

## 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.