An Introduction to Simulation Optimization

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Introductory Tutorials
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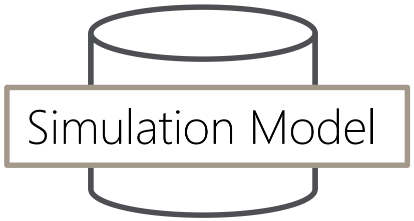
Contents

What is Simulation Optimization?

Simulation



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Choosing the decision variables to optimize some (expected) performance measure.

Optimization

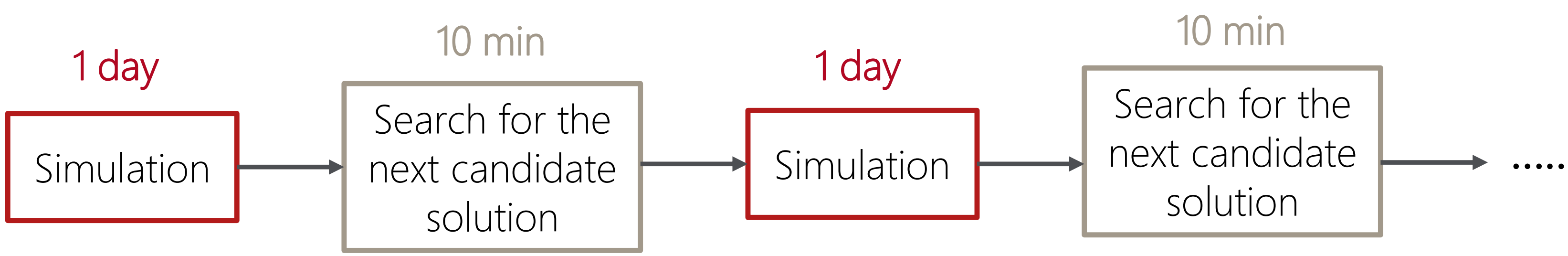
+

Having uncertainty in the objective and/or constraints.

Other names: "Simulation-based Optimization" or "Optimization via Simulation".

Simulation Optimization is Hard

- Mathematical: Cannot evaluate the objective and/or constraints exactly.
  - The noisy evaluation of a function is small. Is the function really small?
- Computational: Simulation/optimization alone is computationally expensive.



- More in the coming section…

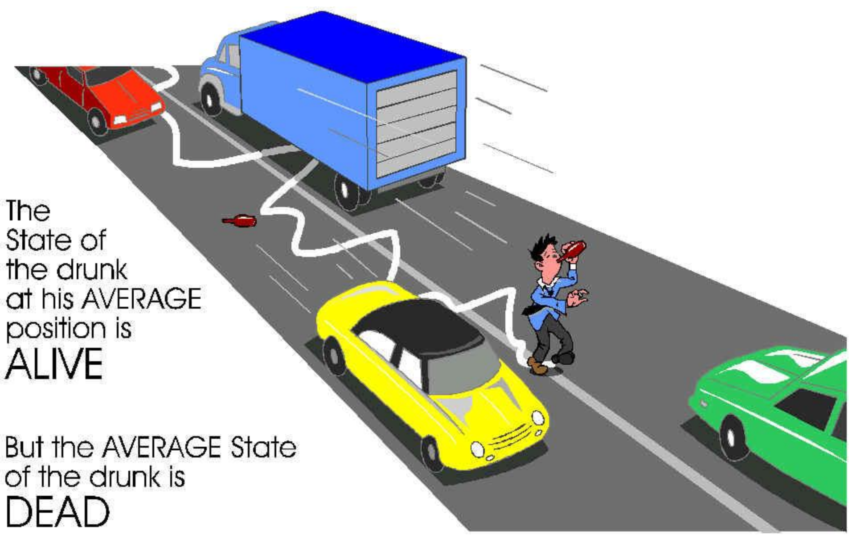
So why not replacing all random variables with estimates of their means?

The Flaw of Averages: Deadly Highway

Consider a drunk person wandering on a divided highway:

Random Position: $\xi \sim \text{Uniform}[0, 1]$

Vital Status: $$f(y) = \begin{cases} \text{dead} & \text{if } y \neq \frac{1}{2}, \\ \text{alive} & \text{if } y = \frac{1}{2}. \end{cases}$$



$$f(E\xi) \neq Ef(\xi)!!!$$

"Alive" "Dead"

(Savage, 2015)

The Flaw of Averages: Newsvendor

Donald, the newsboy, is deciding how many newspaper x to stock at the beginning of the day so he can maximize the expected profit $\pi(x) = E\pi(x,\xi) = pE(\min(x,\xi)) - cx$ wrt/ a random demand ξ.

Consider the normally distributed demand ξ .

The mean μ = 1000, and stdev σ = 300, p=$5, c=$3.

$\max \pi(x) =$ $1420 when $x = \mu + \Phi^{-1}(\frac{p-c}{p})\sigma =$ 924

$\max \pi(x, E\xi) =$ $2000 when $x = E\xi =$ 1000

The difference seems small – but it is 40% of the profit!

(the actual avg. profit with x = 1000 is ~$1220.)

It can be shown with Jensen's Inequality that replacing the demand by its mean would always overestimate the expected profit.

What We Talk About When We Talk About Simulation Optimization

ξ : the randomness in the system (e.g. demand)
x : the set of decision variables (e.g. stock)
$f(x,\xi)$: the output for the objective for one replication of the simulation logic (e.g. profit for a day)
Θ : the search space (e.g. stock>0)

$$\min_{x \in \Theta} f(x)$$

Expected Values:

$$f(x) = Ef(x,\xi)$$

e.g. Maximize the expected return of a portfolio

Quantiles:

$$f(x) = \inf\{y : P(f(x,\xi) \leq y) \geq \alpha\}$$

e.g. Minimize the value-at-risk of a portfolio

Applications of Simulation Optimization

Problem	ξ	x	$f(x, \xi)$
Newsvendor	Demand	Starting inventory	(-) Daily profit
Financial Optimization	Stock Price	Portfolio	(-) Return
Supply Chain Inventory (s-S)	Demand	Base stock level (Order-up-to level)	Inventory holding cost
Queuing System, e.g. Call centers	Arrivals	Number of Servers	Waiting time
Healthcare, e.g. Ambulance	Call Arrivals	Base locations	Response time

Scope and Other References

- In this tutorial:
  - What is simulation optimization?
  - Some common issues one encounters when solving such problems
  - Tools and principles
  - Using simulation optimization: a bike-sharing example

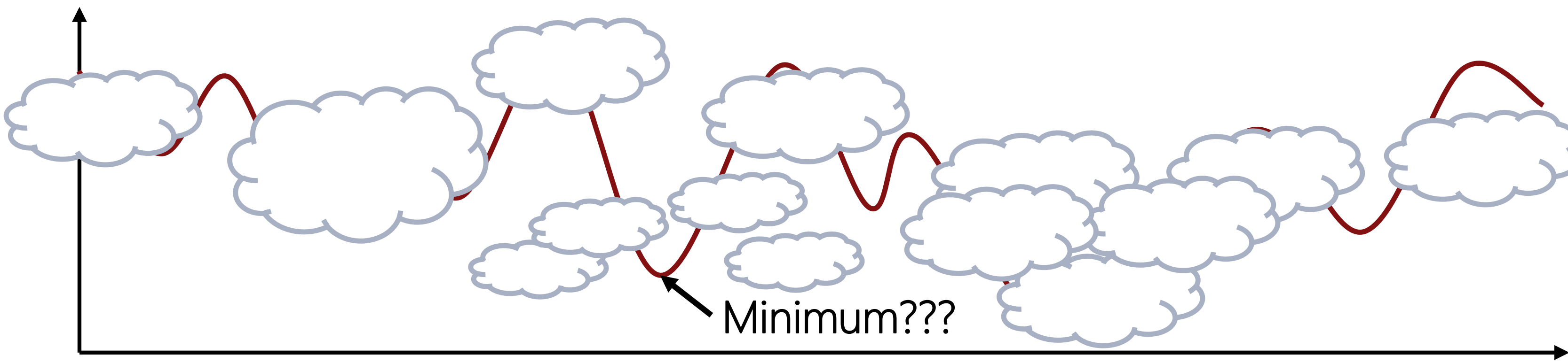
- Not in this tutorial: Detailed methodology, and advanced stuff… please come to the talks in the Simulation Optimization or Analysis Methodology tracks!

- Other references for further interest:
  - Previous WSC tutorials: Fu 2001, Fu, Glover, and April 2005, Fu, Chen, and Shi 2008, Chau, Fu, Qu, and Ryzhov 2014
  - Book chapters (Intro): Chapter 12 of Banks, Carson, Nelson, and Nicol 2010
  - Book (Advanced): Fu 2015
  - See our paper for more!

Contents

Local vs. Global Solutions

- Searching on a function:
  - Global optimum: the true minimum/maximum on the entire domain.
  - Local optimum: the point where no nearby improvement can be found.

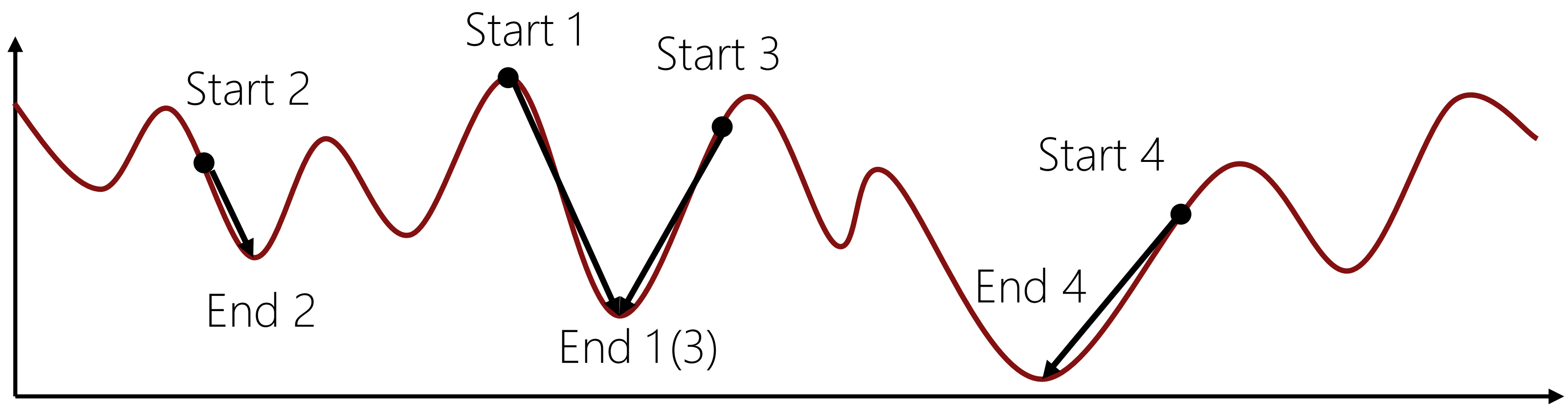


- Similar to finding the lowest point in the US, but:
  - in heavy fog: only local information available
  - with a broken altimeter: can only measure altitude with noise
  - and a teleporter machine: can sample anywhere

  How to differentiate The Grand Canyon from Death Valley?

Local vs. Global Solutions

- Unless the function is convex, the best an algorithm can promise is to locate a local minimum.
- Solution: Can use random restart:



  - Not-too-rolling landscape: may be effective
  - Very-rolling landscape: will visit the global minimum eventually… after lots of restarts!

Many Decision Variables = Huge Search Space

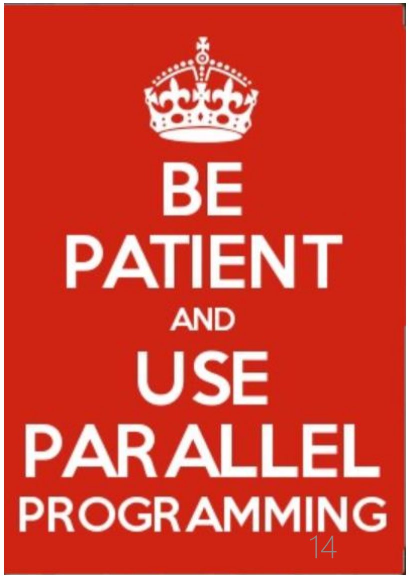
- Consider a call center:
  - ξ = call arrivals
  - d = number of shifts
  - x_i = number of agents at shift i, $x_i \leq n$
  - c = cost per agent
  - $f(x)$ = average speed of answer minus the cost of labor

- $(n+1)^d$ possible values of x:
  - If d = 24 and n = 10, 11^24 = 984973267580761109471841!!

Huge Search Space: What can we do?

- Exploit domain knowledge
  - Start searching from the current shift schedule
- Use an algorithm that is aware of the function structure
  - The average speed of answer is decreasing in x.
  - There is diminishing returns wrt increasing x.

- Be patient
- Parallel programming can greatly reduce the computational time!
  - But can you defeat the curse of dimensionality?
  - Having two shift alternatives: 11^48 values!



Continuous vs. Discrete Decision Variables

- Continuous decision variables:
  - There are efficient local search algorithms that can exploit continuity and differentiability.
  - "Close" points are expected to have "close" function values.
- Discrete decision variables:
  - "Continuity" doesn't come naturally.

Optimizing in the Presence of Noise

- Suppose in replication i, we obtain output $f(x, \xi_i)$. Let the objective be denoted as $f(x) = E(f(x, \xi))$.

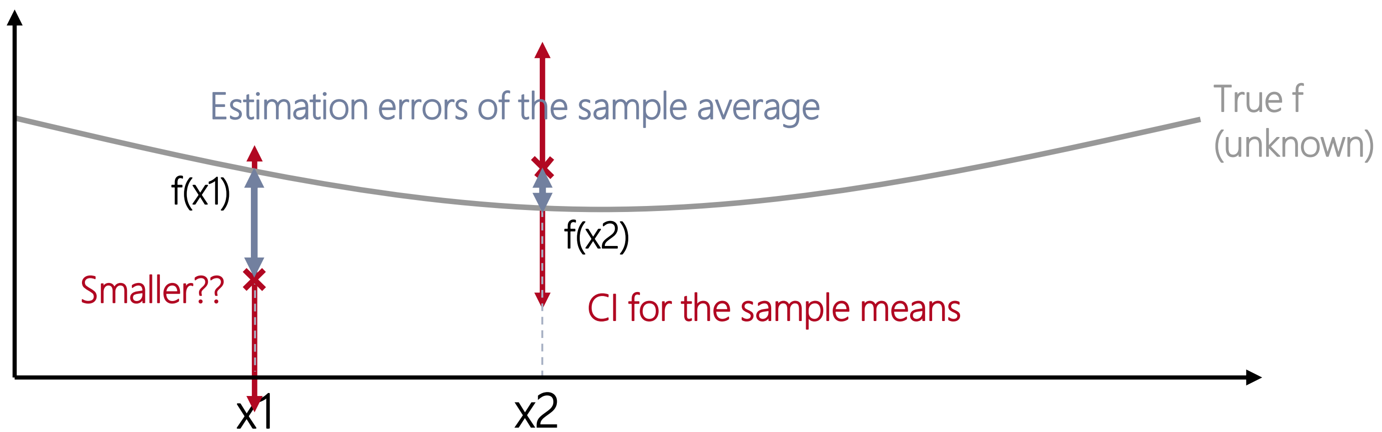
- How far is $f_n(x) = \frac{1}{n}\sum_{i=1}^{n} f(x, \xi_i)$ from $f(x)$?

- If $f_n(x_1) < f_n(x_2)$, does it imply $f(x_1) < f(x_2)$?

- Solution: We can increase the runlength at x_1 and x_2 to be more sure.
  - But how about other x values?

Simulation Noise can Swamp the Signal

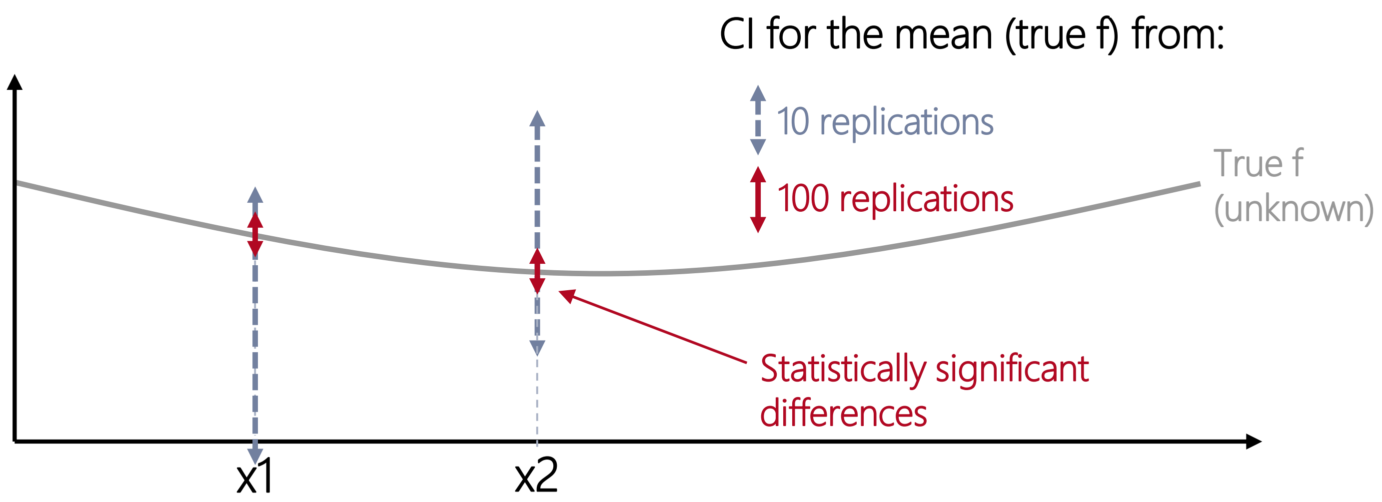
- When the difference in the simulation noise is bigger than the difference in the function values:



- Solutions:
  - Carefully choose the runlength to ensure statistically significant differences
  - Use Common Random Numbers

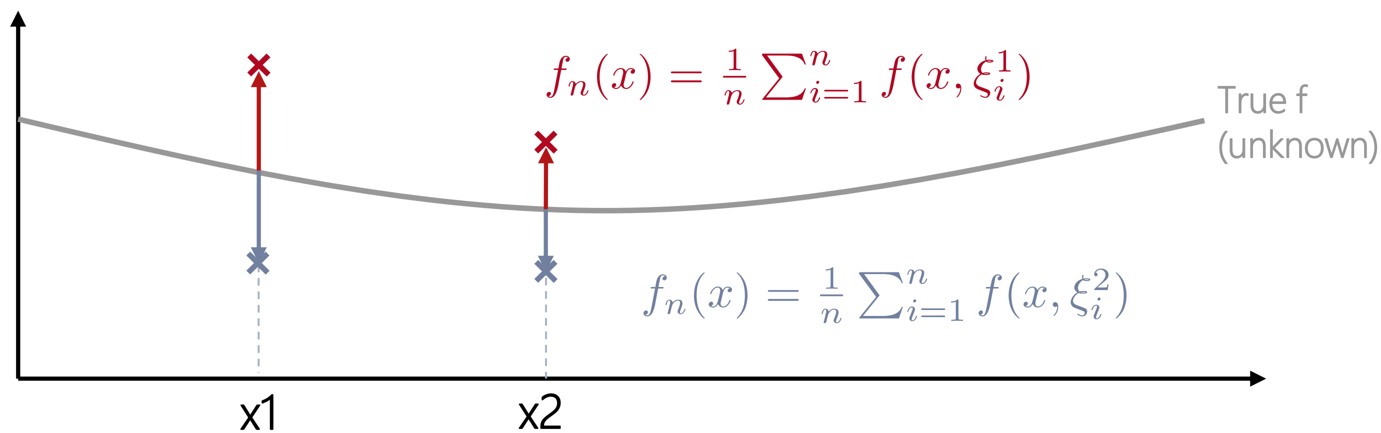
Simulation Noise can Swamp the Signal

- Carefully choose the runlength to ensure statistically significant differences:



Common Random Numbers (CRN)

- Idea: Use the same set of ξ to evaluate $f_n(x_1)$ and $f_n(x_2)$.



- E.g. Consider the newsvendor problem:
  - Comparing starting stocks x_1 and x_2 .
  - CRN means comparing the two with exact the same demands.
- To use: Many software has random number stream implemented. Use the same stream to simulate the systems being compared.

Failing to Recognize an Optimal Solution

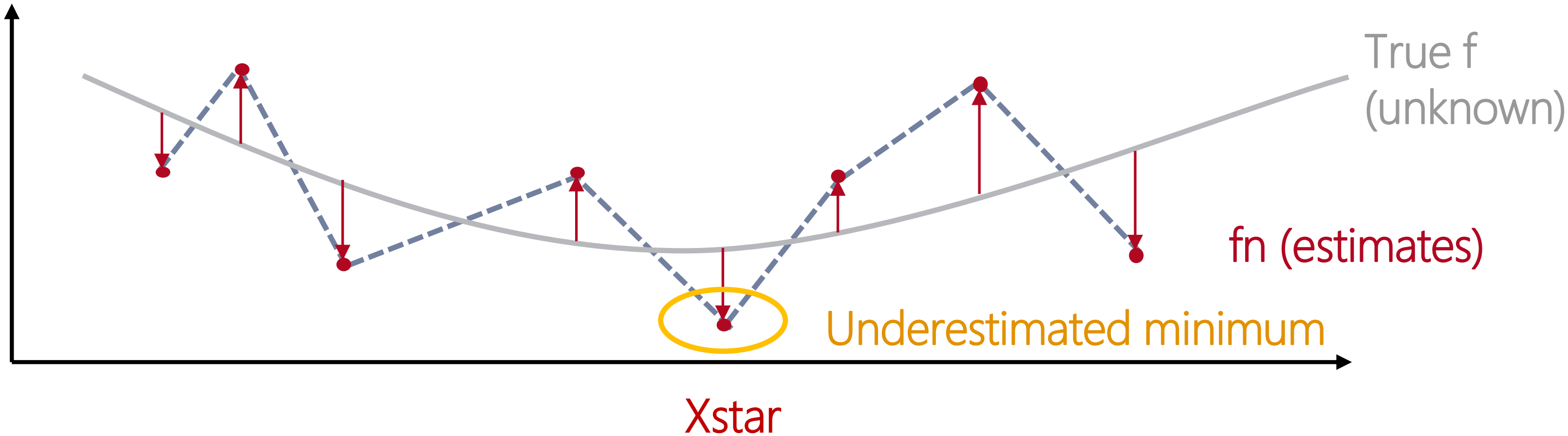
Even if we visited every point in the solution space, how do we know which one is optimal, given we can only obtain noisy evaluations of the objective?

- Again, carefully choose runlength.
- Use ranking & selection to "clean up" the solutions! † (later)

† : Hong, Nelson, and Xu 2015

Poor Estimates of the Optimal Value

- For the optimal solution x^* of a minimizing problem, the min of the estimates underestimates the true min:



- Solution: take x^* and run a longer simulation using independent sample (new random stream).

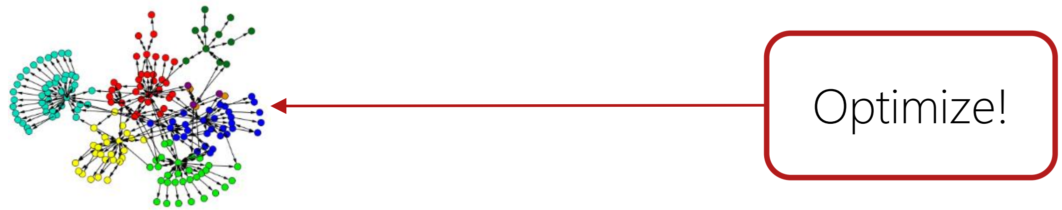
When to stop?

- Since objective is noisy, it is hard to differentiate noise from the actual progress. Usually most algorithms are stopped when a computational budget is reached.

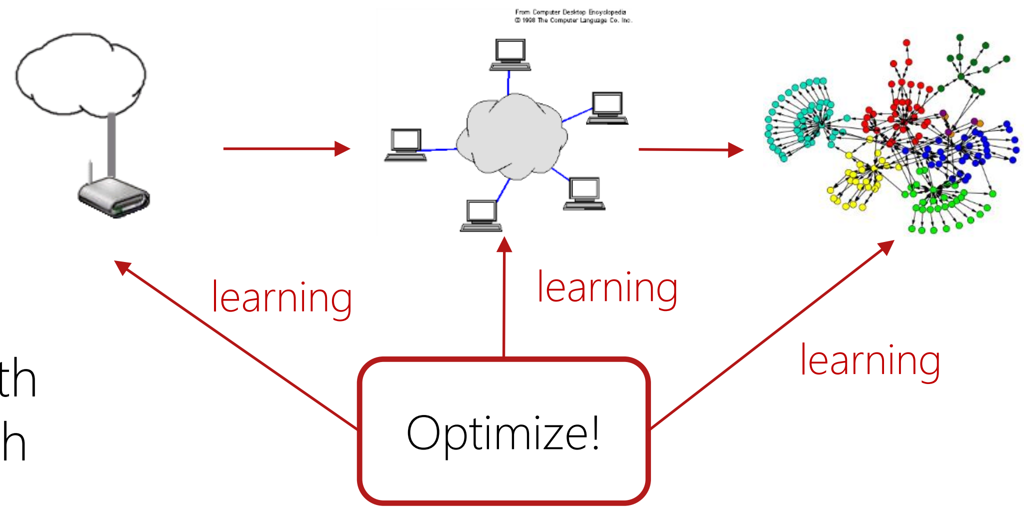
- “Smarter” ways to stop:
  - Start the optimization algorithm with a small number of replications.
  - Then sequentially increase the sample size to “refine” the solution until “steady”.

Model Madness

"Textbook":



A Succession of Models:



- Build a sequence of models with increasing complexity, and each one answers the question to some degree.

Summary

We talked about issues arising from:

- Nonlinear Optimization:
  - Local vs. Global solutions
  - Huge search space
  - Discrete vs. Continuous variables
- Simulation Noise:
  - Optimizing in the presence of noise
  - Simulation noise can swamp the signal
  - Failing to recognize an optimal solution
  - Getting poor estimates of the objective of the estimated optimal solution
  - When to stop
- Modeling:
  - Model Madness

Contents

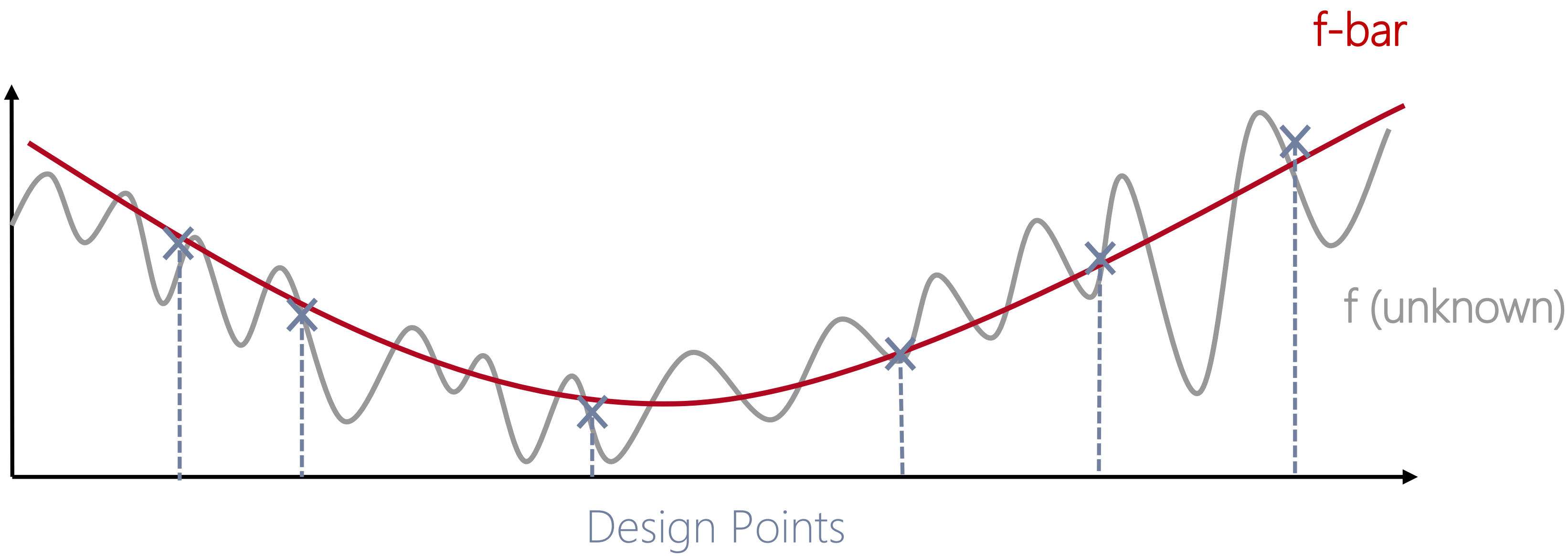
Sample Average Approximation

- Idea: Use sample average ($f_n(x) = \frac{1}{n}\sum_{i=1}^{n} f(x,\xi_i)$) to estimate the expectation ($f(x) = Ef(x,\xi)$).
  - If the inputs $\xi_1,\ldots,\xi_n$ are fixed, optimizing f_n is a deterministic program.
- To use: Assign a stream of random numbers ξ_i to rep i.
- Pros: Very flexible, works on constrained problems, and reliable when n is large
- Cons: User needs to choose the deterministic optimization algorithm.
- Example: Call center:
  - Wish to optimize the expected customer waiting time
  - Use the average customer waiting time over 1000 simulated days as an estimate
  - Optimize this average with different staffing schedules over the same 1000 days (using CRN)

More: Kim, Pasupathy, and Henderson 2015.

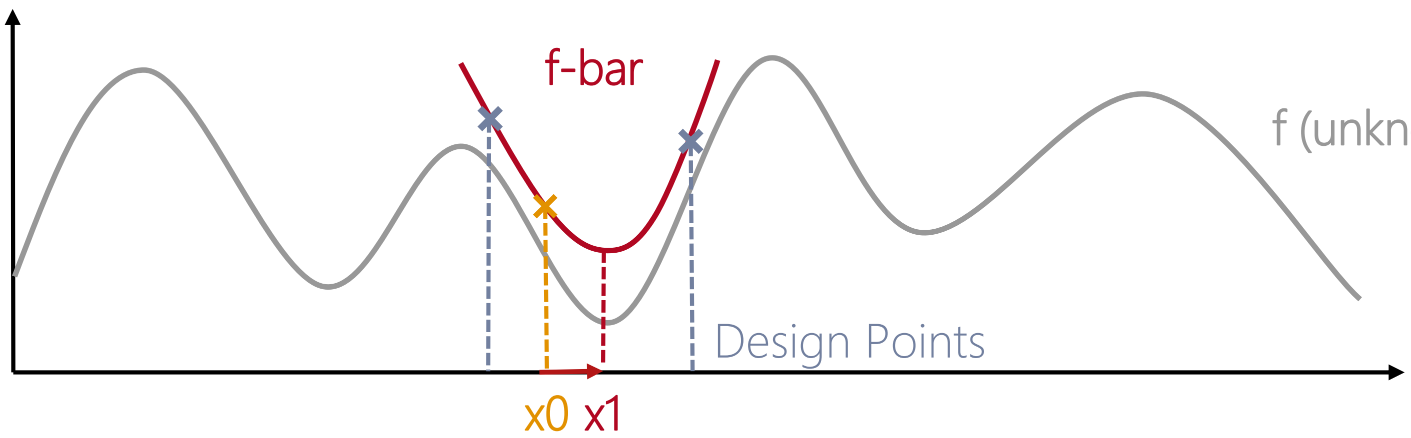
Metamodeling

- Also called Response Surface Methodology.
- Idea: Based on some design points, approximate the true function f by some simple-to compute function $\bar{f}$ (e.g. polynomial), and optimize $\bar{f}$ instead.



Metamodeling

- Global metamodel: Used when the search space is small.
- Local metamodel: Used to move to the next candidate solution.



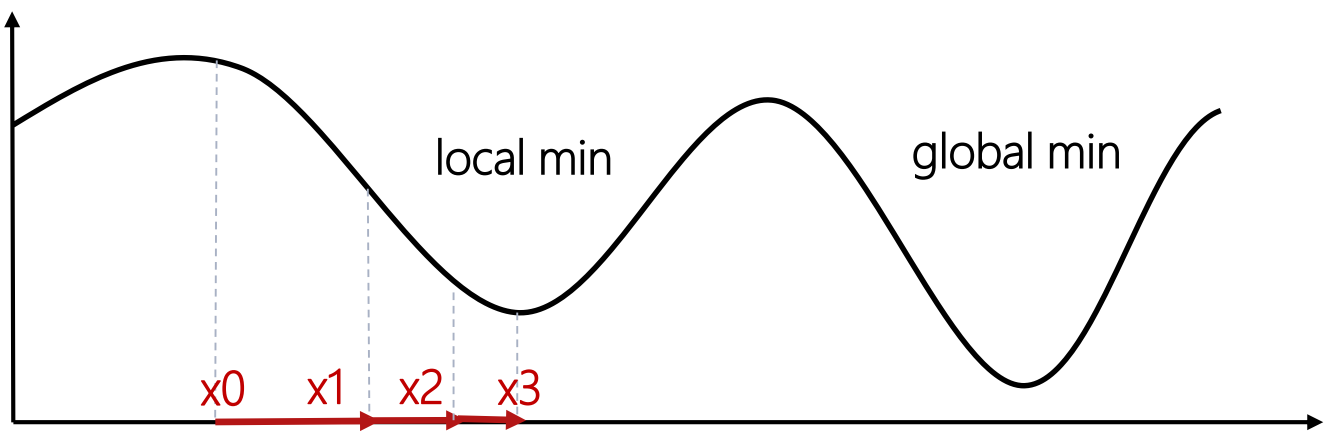
- Pros: The metamodel is structured and thus easy to optimize.
- Cons: Relies on the experiment design, needs smoothness to work well

More: Barton 2009, Kleijnen 2015.

Stochastic Approximation (SA) and Gradient Estimation

- Idea: Similar to the Steepest Descent Algorithm, SA iteratively step into the (estimated) negative gradient direction.

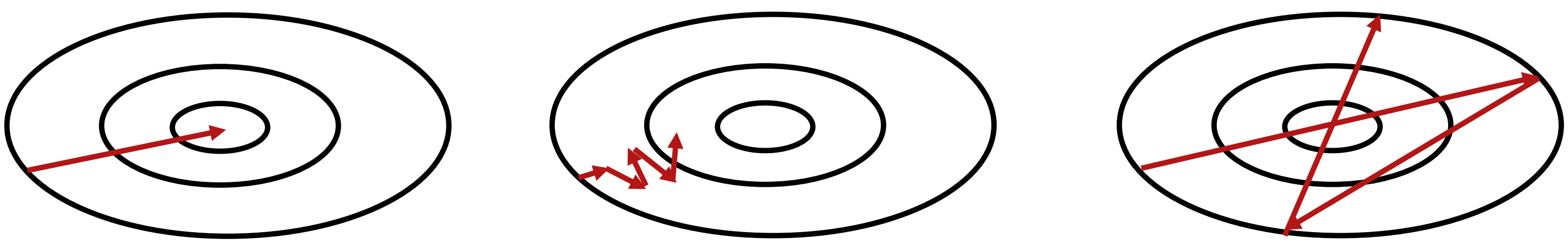
$$x_{n+1} = x_n - \alpha_n g(x_n, \xi_n)$$



- Applies to: finding the local optimum of a smooth function over a continuous space

Stochastic Approximation (SA) and Gradient Estimation

- Gradient Estimation $g(x_n, \xi_n)$:
  - e.g. Finite differences (easiest, but biased): make a small perturbation in each dimension
  - Others yield unbiased estimates in special cases.
- Pros: Fast, works on (simple) constrained problems
- Cons: Performance greatly depends on the choice of the step size
- To use: Need to code it directly



More: Chau and Fu 2015.

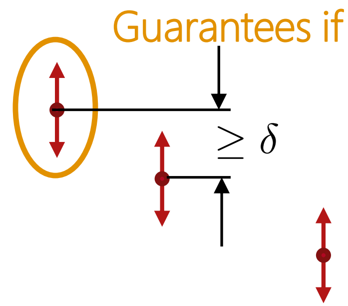
Ranking and Selection

- Idea: Exhaustively test all solutions and rank them. The goal is to return the system with the lowest mean.
- A common frequentist procedure:
  1. Start by obtaining a small sample (say, 10) on each system.
  2. Use the initial sample to decide how much to further simulate each system.
- The procedures differs by the allocation of samples and the statistical guarantee provided.
- The total sample sizes can be different for each system!
  - The choice of sample sizes can be quite complicated.
  - Usually it is larger for the system with higher variance and/or closer to the optimum.

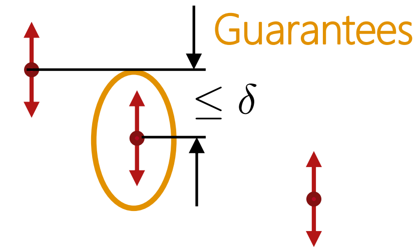
Ranking and Selection: Statistical Guarantee

User input: δ

- Probability of correct selection (PCS):
  - Guarantees (say, w.p. 95%) to choose the best system only if it is better than the second best by at least δ
  - δ is called the "indifference zone" parameter.



- Probability of good selection (PGS):
  - Guarantees (say, w.p. 95%) the selected system is worse than the best system by at most δ



- Algorithms providing PCS/PGS guarantees are usually very conservative.
- Other methods that are more efficient but without guarantee:
  - "Optimal Computing Budget Allocation" for maximizing PCS/PGS †.
  - "Expected Value of Perfect Information" for the most "economic" choice ‡.

†‡: see Chen, Chick, and Lee 2015; More: Kim and Nelson 2006.

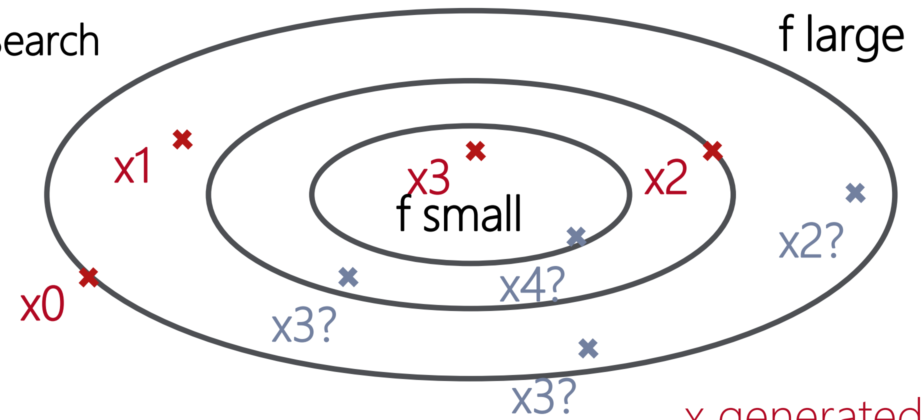
Ranking and Selection

- Applies to: A finite and “small” (say, <500) search space, so each solution can be estimated by at least a few simulation runs.
- The recent development of using parallel computing in R&S can handle larger search space (e.g. 10^6 systems) †.
- Example: Clean up step after an initial search
- To use: Implemented in some commercial software packages

†: see Luo and Hong 2011, Luo et al. 2015, Ni et al. 2015

Random Search Methods

- Idea: Iteratively choose the next sample point based some sampling strategy, and move to that point if it shows evidence of improvement.



- Applies to: any problem

Random Search Methods

- The sampling strategy:
  - deterministic or randomized
  - depends on the information of all the previous points, only a few previous points, or only the most recent point
  - trades off exploration vs. exploitation

- Pros: Easy to implement, no requirement for problem structure
- Cons: Few or no statistical guarantee, not using any model information
- Widely used in most commercial packages.

More: Andradottir 2015, Hong, Nelson, and Xu 2015, Fu, Glover, and April 2005, Olafsson 2006.

Contents

Problem Statement

- Citibike in NYC has approximately 330 stations and 6000 bikes.
- Users check out bikes at a station and return bikes to another station.
- Unhappy bikers are those who don't find a bike when they want one, or don't find a rack when they want one.
- In the event of a full rack, users go to a nearby bike station. A bike may be abandoned after a few attempts.

†

†: www.siegelgale.com, www.voltaicsystems.com, socialmediaweek.org

A Simulation Optimization Problem

x = #bikes to allocate to each station overnight

$$\underset{x}{\text{minimize}} \quad f(x)$$

(the expected number of unhappy bikers during morning rush)

$$\text{subject to} \quad \sum_i x_i = b$$

(total budget of bikes)

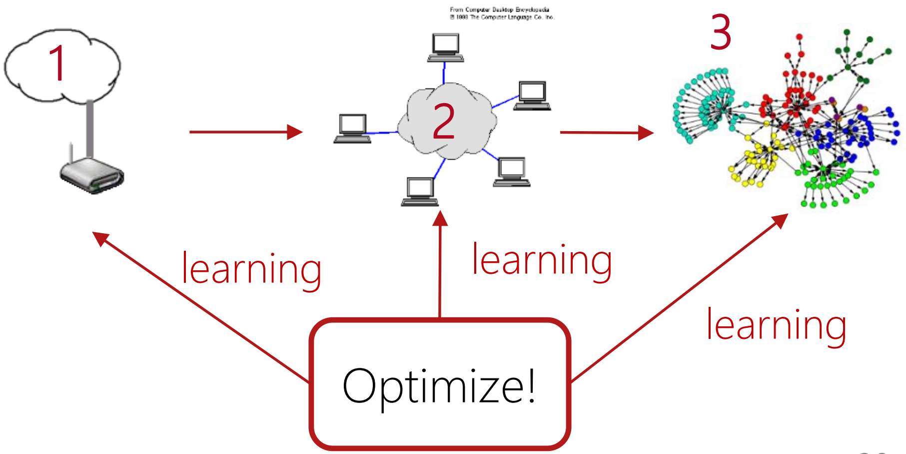
(Station capacities)

$$0 \leq x_i \leq r_i, x_i \text{ integer } \forall i,$$

Stages of Modeling

We built a sequence of more and more complex models to obtain intuition on how the system behaves and the form of a good allocation:

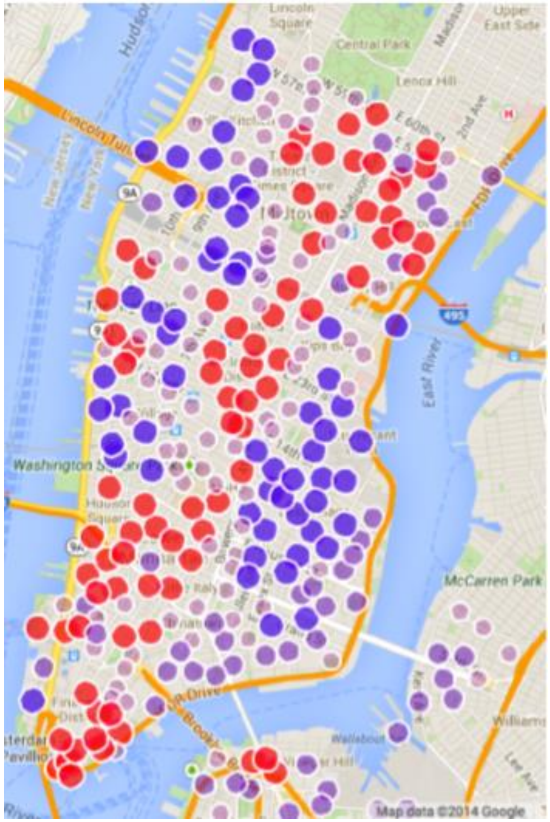
0. Half-full Stations
1. Fluid Model
2. Continuous-Time Markov Chain Model
3. Discrete Event Simulation



Let’s make every station half full

In fact, this was the original plan of Citibike.

What can go wrong?



†

Morning Rush Hour Demand:

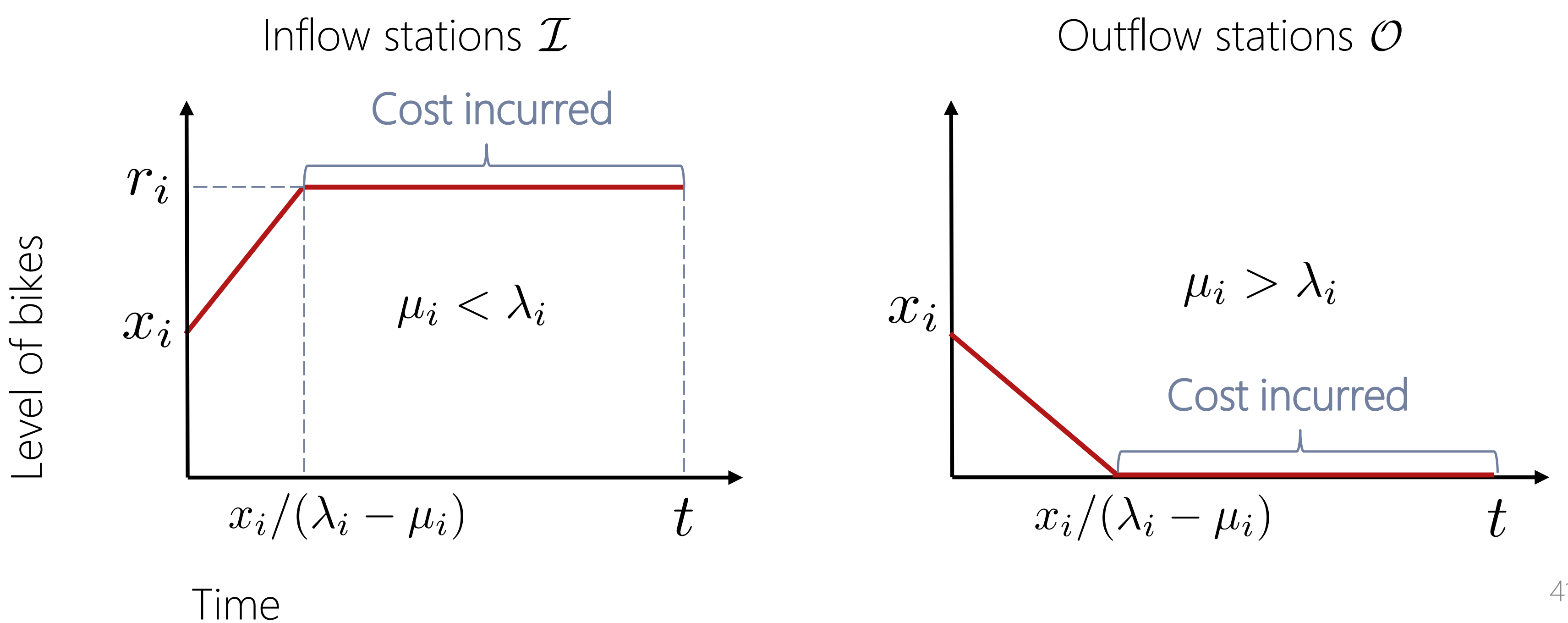
Blue stations: bike consumers (more empty)

Red stations: bike producers (more full)

†: O’Mahony and Shmoys 2015

A Fluid Model: Idea

- Ignore the randomness in the arrival and departure processes for now and assume that users pick up and drop off bikes at constant rates μ_i and λ_i.
- The level of bikes at a station is linear wrt/ time:

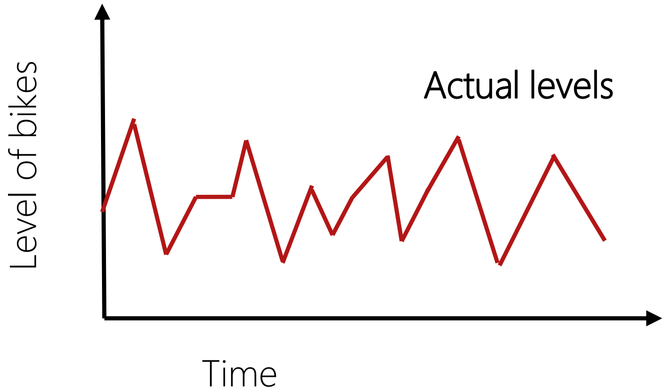


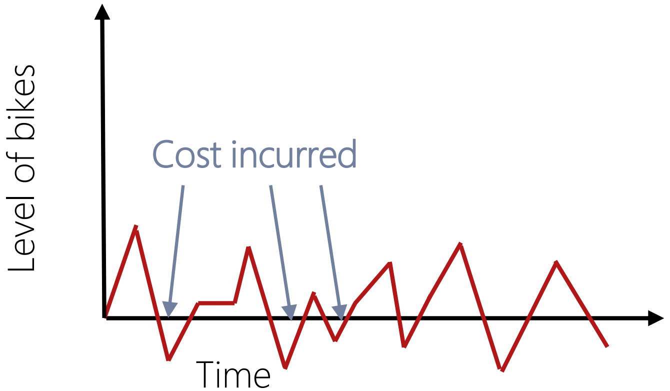
A Fluid Model: Insights

1. For the outflow stations, the min number of bikes x_i needed to ensure happy customers is $(\mu_i - \lambda_i)t$, which is the flow imbalance over the rush hour period.
2. There might be no way to avoid unhappy customers, unless we increase the capacity.
3. Adding a bike to any outflow station gives the same improvement - all unhappy customers are equal.

A Fluid Model: Problems

- As we expected, the solution would allocate no bikes to the inflow stations, and the minimum number of bikes to the outflow stations so they never run out of bikes, if the budget allows.
- This model is especially problematic for the near-balanced stations:
  - If $\lambda_i = \mu_i$, then it doesn't matter how many bikes we put at the station! So why not put 0?





A Continuous-Time Markov Chain Model

- Model the flows of customer arrivals at different stations as independent time-homogeneous Poisson processes.
- Assume that the stations never run out of bikes, then each station can be modeled as a $M/M/1/r_i$ queue independent of all other stations.
- This is a strong assumption to make!

- This model captures the stochastic nature of bike flows.
  - Once a station is full, it will not stay full for the rest of the period.

A Continuous-Time Markov Chain Model

- When $\lambda_i = \mu_i$, the solution $x_i = r_i/2$.
- $f(x)$ can be computed very efficiently without simulation.
- Also one can show f(x) is "convex"!
- This CTMC solution can be used as a starting solution for the simulation optimization.

A Discrete Event Simulation Model

- Each station generates trips according to a Poisson process. A trip is assigned a destination with probability $P_{ij}(s)$ and its duration is Poisson-distributed.
- A trip can have a few states:
  - "trip-start": there is bike available at the origin
  - "failed-start": otherwise, in which case the trip is cancelled
  - "trip-end": there is dock available at the destination
  - "failed-end": otherwise, in which case a trip to the nearest station is generated
  - "bad-end": the user abandons the bike after 3 failed attempts
- The objective is

$$f(x) = E_x[\#\text{failed-starts}] + E_x[\#\text{failed-ends}] + c_b E_x[\#\text{bad-ends}]$$

A Discrete Event Simulation Model

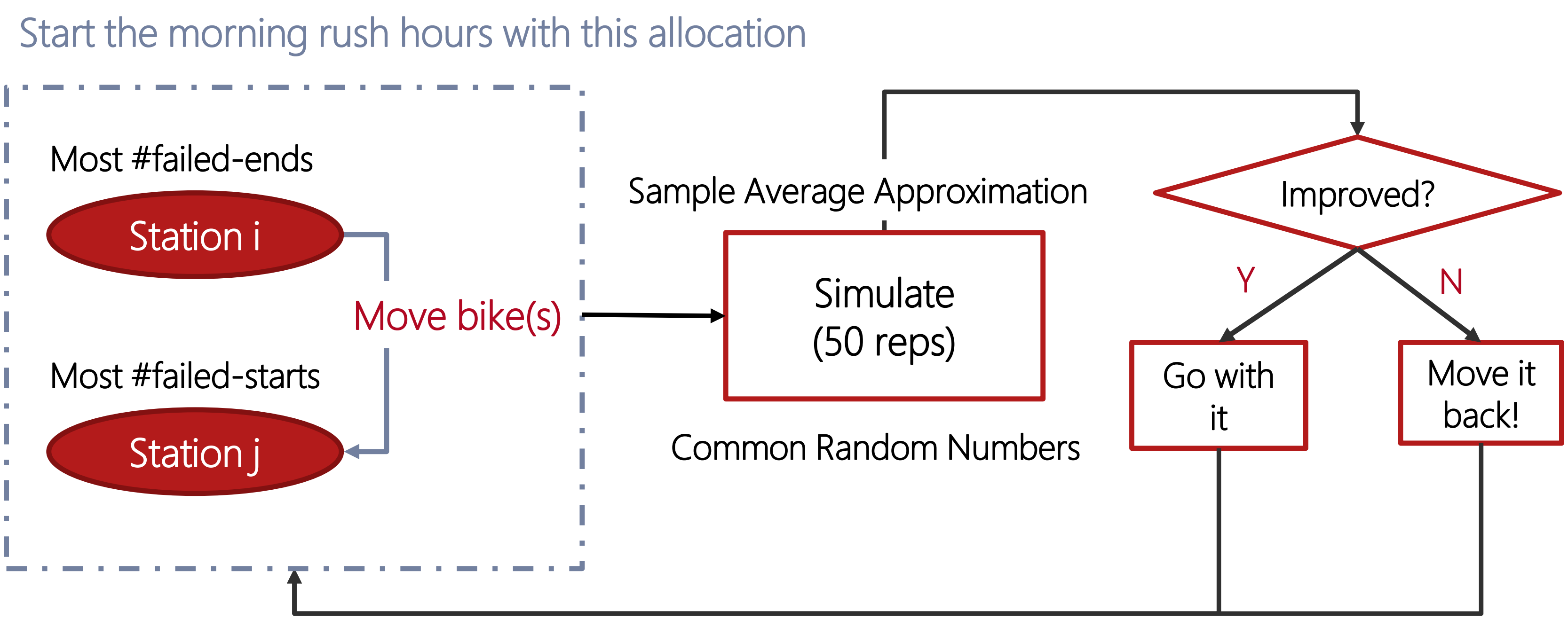
- The simulation is run for the morning rush hour period (7-9am).
- 1 rep = 0.2s. 50 reps gives 10s per fn evaluation.
- ~350 stations:
  - Random search (select two stations i and j to move a bike) hopeless:

    #ways to select I * #ways to select j = 350*349 = 122,150 possible pairs of stations!
  - "Gradient" search hopeless:

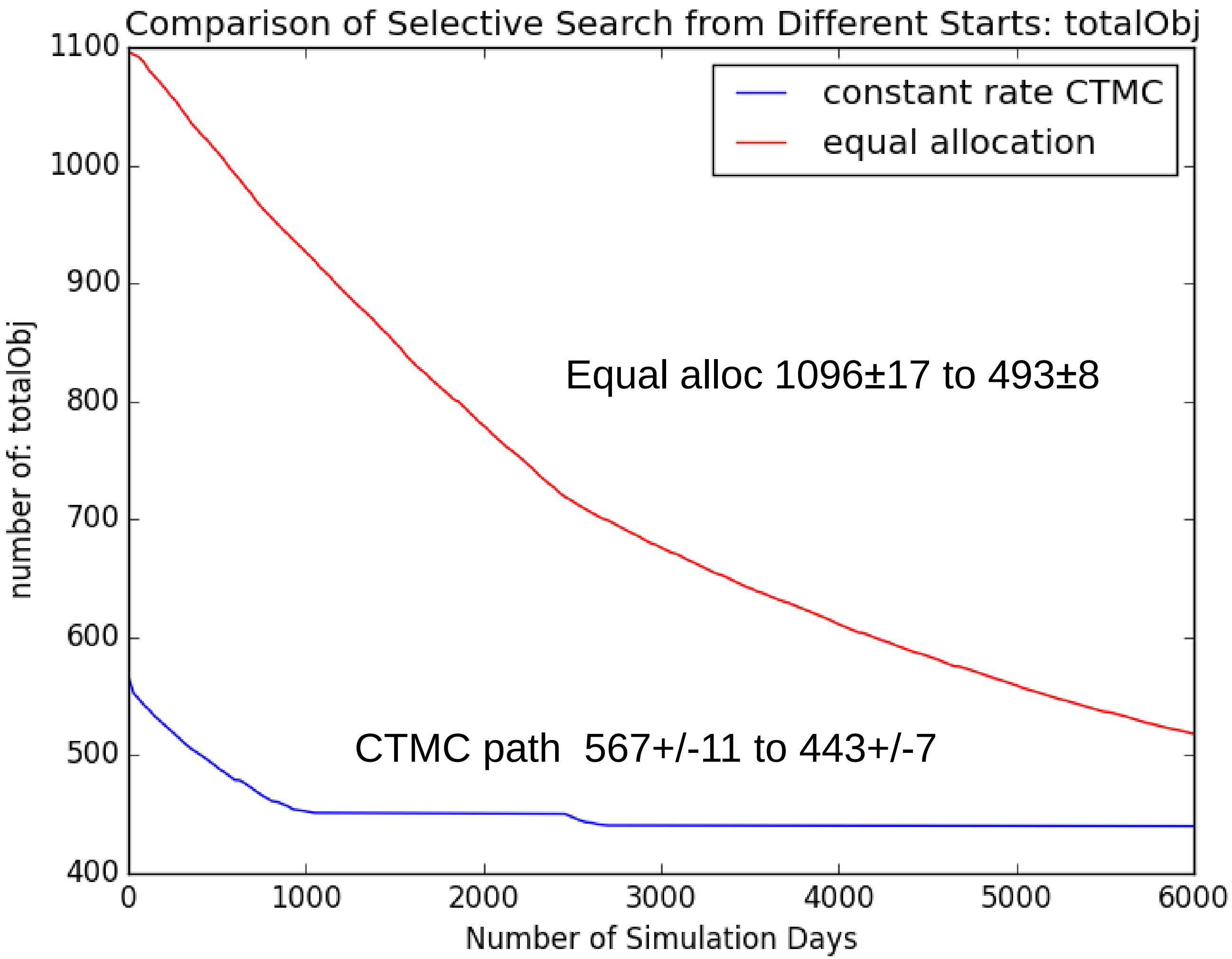
    350 dimensions to perturb

A Discrete Event Simulation Model

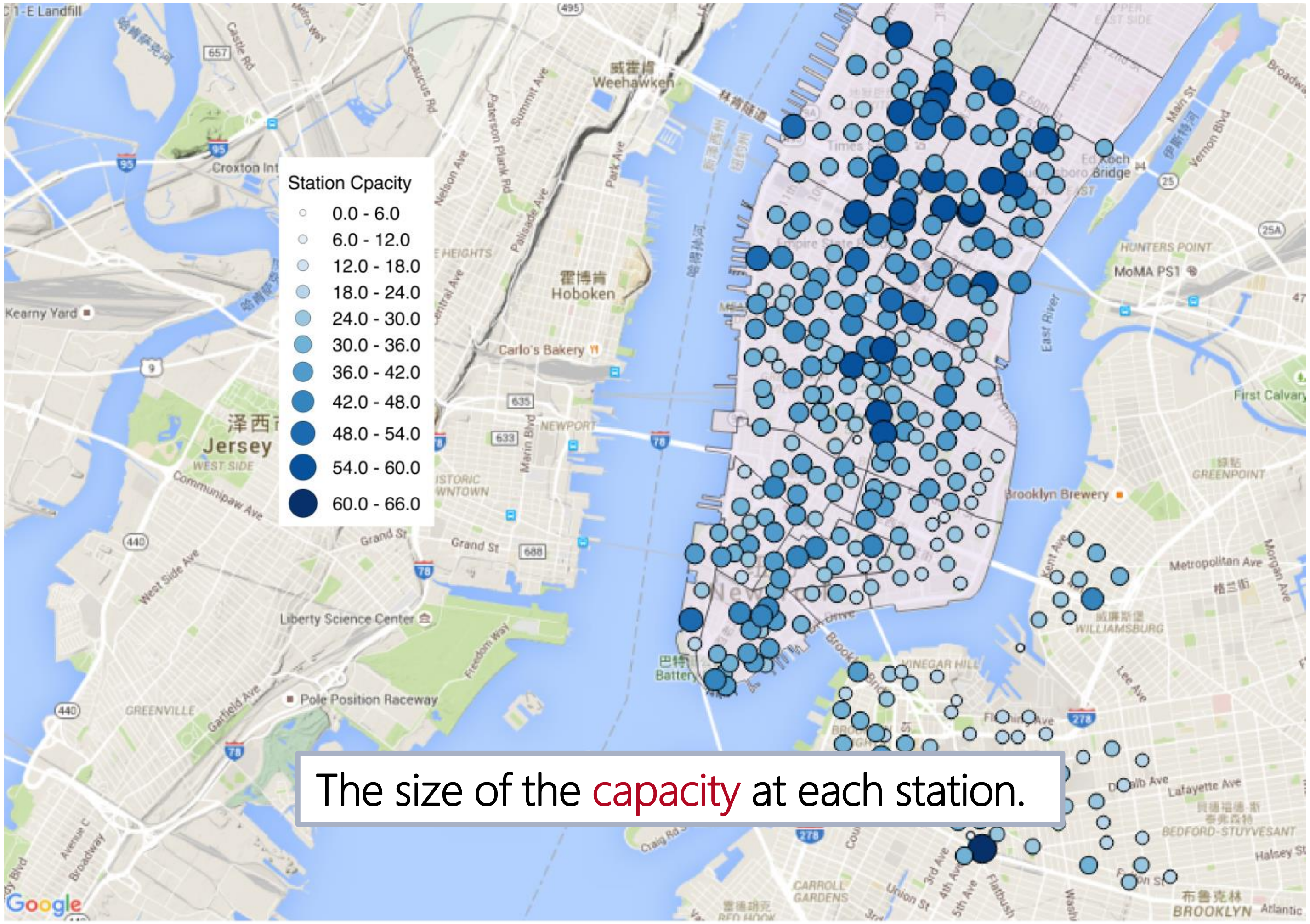
- Instead, swap bikes between the stations who have the most contributions to the objective:



Search from Different Starts

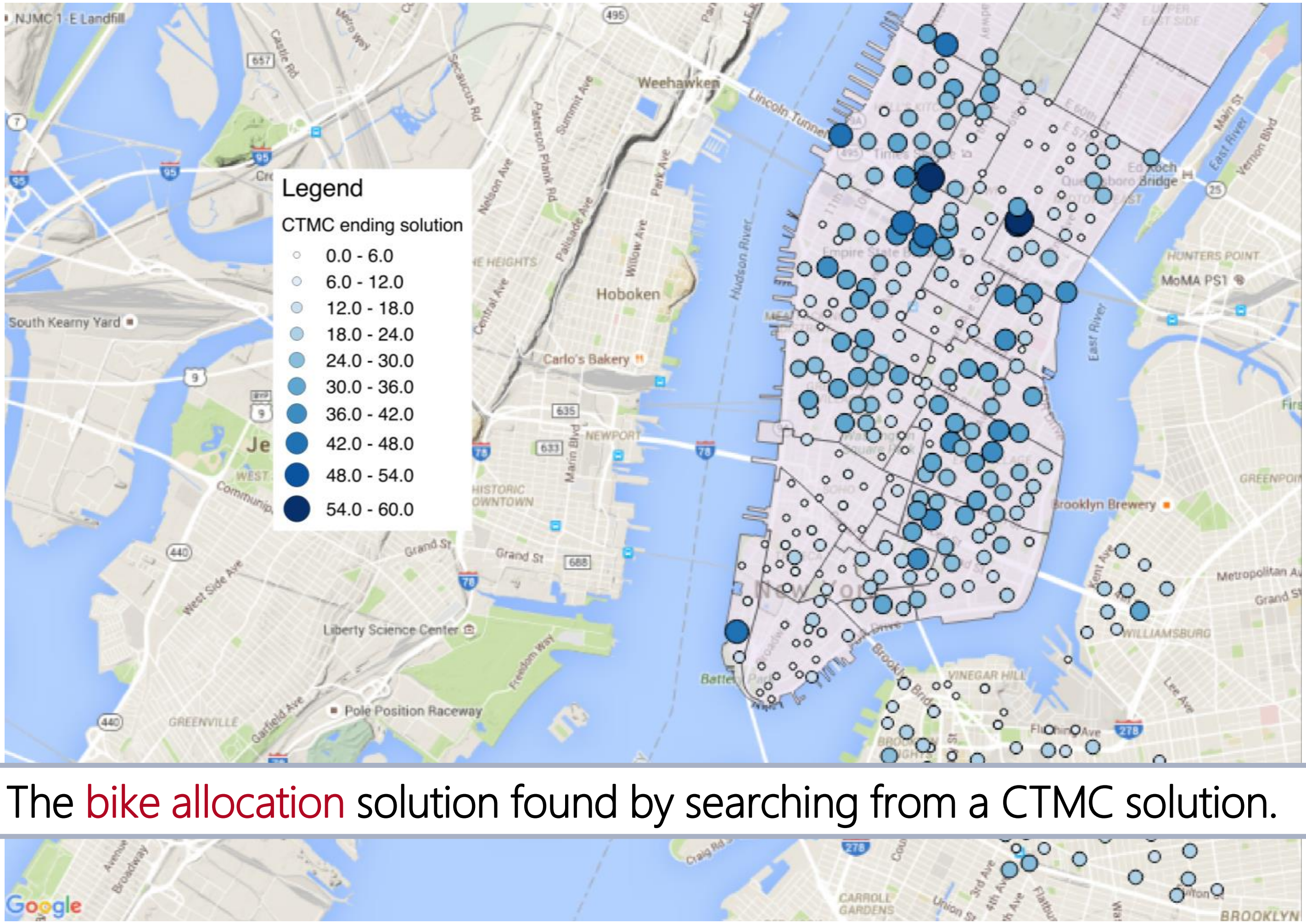


Station Capacities



The size of the capacity at each station.

The Ending Solution (Bike Allocation)



The bike allocation solution found by searching from a CTMC solution.

What have we learned?

- A succession of models can greatly assist in making simulation optimization possible!
- With huge search space, we need to take advantage of the problem structure.
- Common Random Numbers help when comparing different solutions.

- Next step: How to optimize dock allocation too?

Contents

1. Introduction
2. Common Issues and Remedies
3. Tools
4. Case Study: Bike Sharing

Takeaway

1. Simulation optimization is not easy.
2. Don't try to build one huge model and then optimize it.
3. If using standard tools, stick with low dimensional problems (not many variables).
4. Use Common Random Numbers with streams to compare systems.

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Thank you!

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