Stochastic optimization of simulation models: management of water resources under uncertainty

Alexei A. Gaivoronski

Department of Industrial Economics and Technology Management
Norwegian University of Science and Technology

with contribution by Denis Becker, Paolo Pisciella, Zhonghua Su, Sondre Flinstad Harbo (NTNU)

Paola Zuddas, Giovanni Sechi, Jacopo Napolitano (University of Cagliari, Italy)

NTNU – Trondheim
Norwegian University of Science and Technology

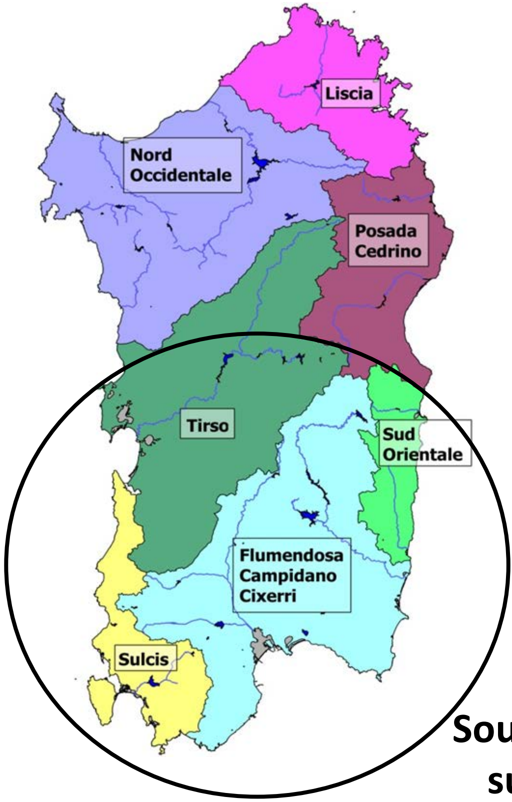
Alexei.Gaivoronski@iot.ntnu.no

IIASA, Laxenburg, October 31, 2017

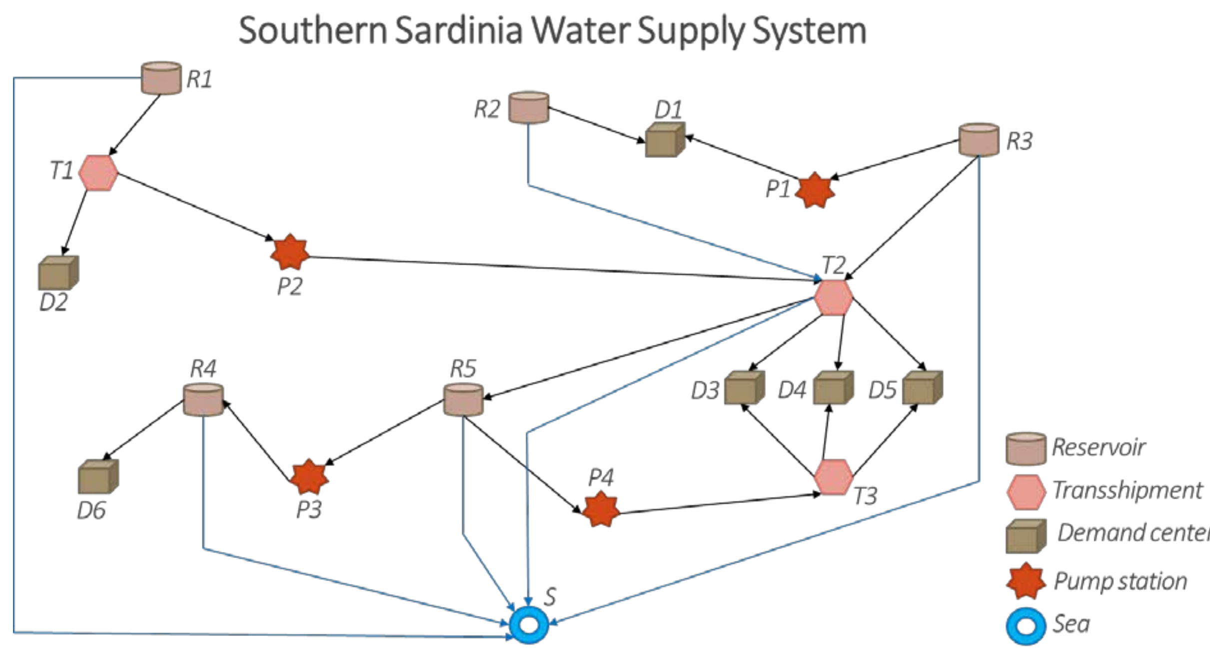
Contents

- Motivation
  - Water resources network in South Sardinia
- Methodology: Stochastic optimization of simulation models under uncertainty
  - Concurrent simulation and optimization with stochastic gradient methods
- Water resources management
  - Management of reconfigurable water network
  - Cost/risk tradeoff in management of scarce water resources

Motivation: complex water resource networks (and other networks too)



Southern-Sardinia supply system



- Uncertainty: water inflows, demand, prices for energy and agricultural production
- Many connected reservours
- Different demand classes: population, industry, agriculture, environment, energy
- Dynamics: at most monthly time step and at least yearly planning horizon
- Water deficit, Floods control, Climate change …. **VERY complex system**

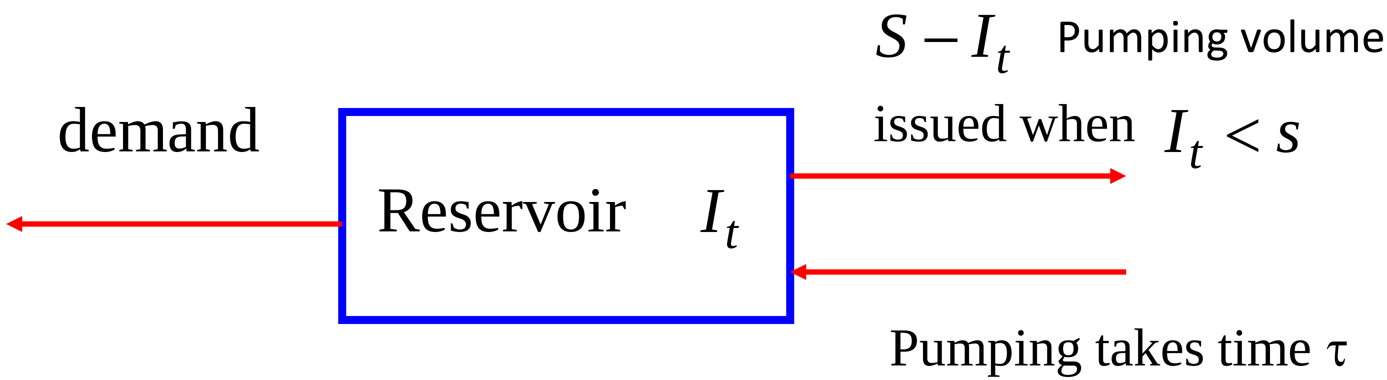
Possible methodology

- Stochastic programming with representation of uncertainty by scenario trees
  - **practical with only few periods and relatively simple uncertainty: exponential growth of complexity with the number of periods**
- Stochastic dynamic programming
  - **Practical with only very few states (reservours but not only): exponential growth of complexity with the number of states**
- Optimization of simulation models

Parametrized simulation model

- Time t=1,…T or infinite horizon
- System: state s_t, random parameters ω_t
- One or more decision making actors with decisions z_{ti} and **current objectives** $F_{ti}(z_{ti}, s_t, \omega_t)$ and **expected total objectives** $F_i = \Sigma_t F_{ti}(z_{ti}, s_t, \omega_t)$
- Decision hierarchy $z_{ti} = (z'_{ti}, z^*_{ti})$
  - **Tactical decisions** z'_{ti} : optimization or equilibrium problem for time t with **current objectives**
  - **Strategic decisions**: decision rule $z^*_{ti}(\mathbf{x_i}, s_t, \omega_t)$ where $\mathbf{x_i}$ are rule parameters
- State dynamics $s_t \longrightarrow s_{t+1}$
- The expected total objectives $F_i(\mathbf{x_i})$ depend on rule parameters and one simulation run k yields an observation of total objective $F_i(\mathbf{x_i}, \omega^k)$
- Rule parameters are obtained by solving stochastic optimization or equilibrium model with **expected total objectives** observed by running simulation model outlined above
- **We have developed solver SQG for solution of such problems implementing stochastic gradient methods**

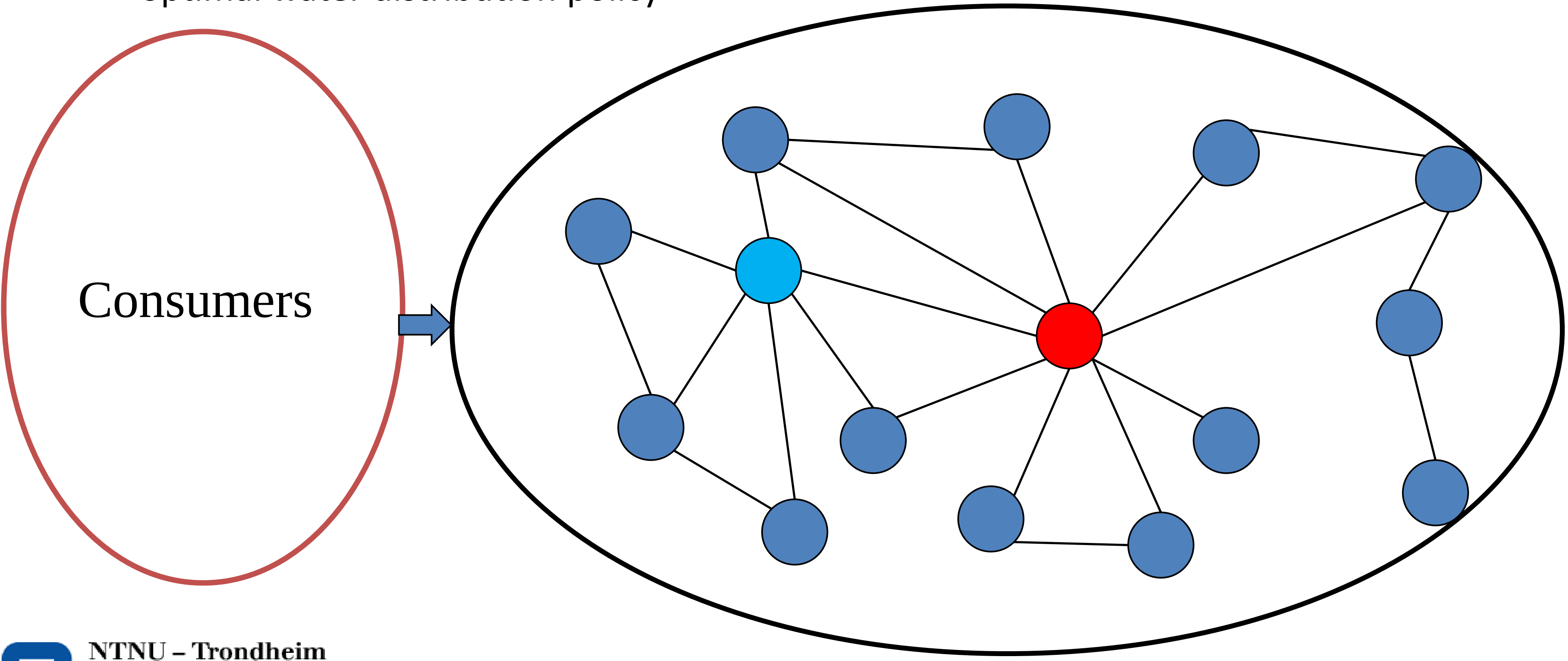
Stripped to the bones: single reservoir management with pumping



- (s,S) pumping policy
- Finding optimal (s,S) policy combining simulation and optimization

Opposite range: water dependent production and consumption ecosystem

- Consumers: water and water dependent production: hydro, agriculture, other
- Actors:
  - Producers: hydro energy, agriculture
  - Water storage for hydro production, interaction with other renewables
  - Regulation: water distribution authority
- Objective: find optimal investment strategies of actors and optimal water distribution policy



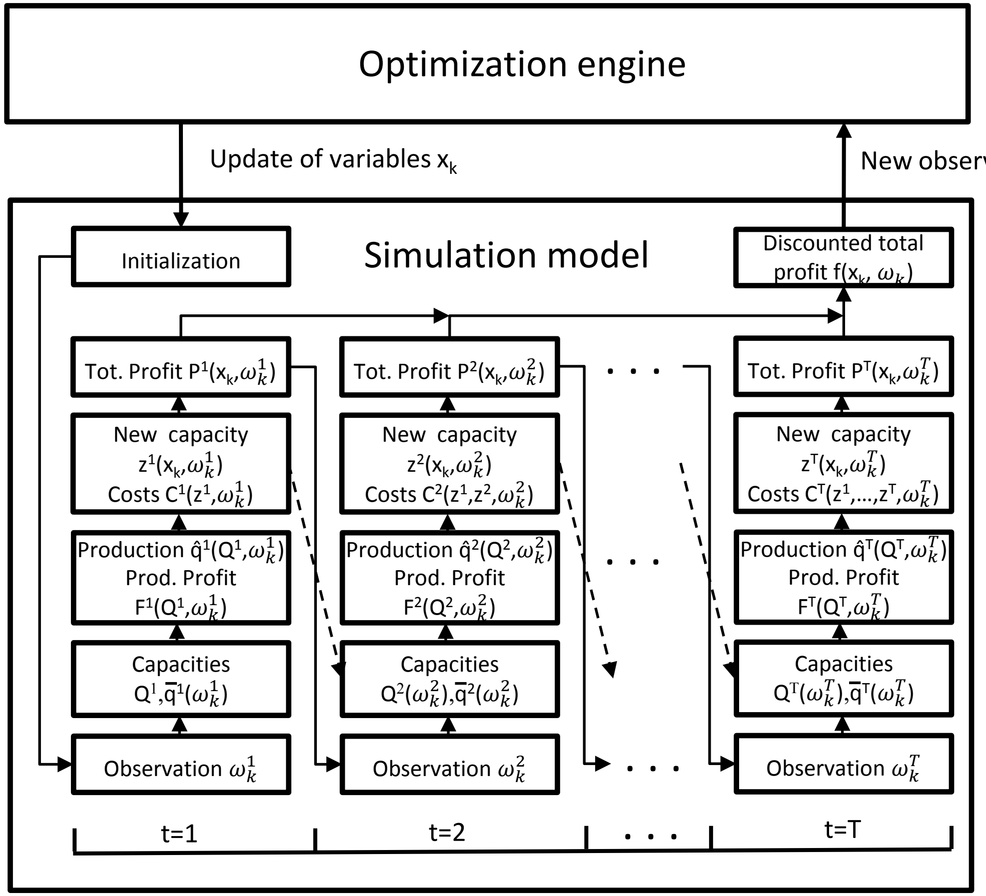
Alexei.Gaivoronski@iot.ntnu.no

Single simulation step

- Observe system parameters (costs, parameters of inverse demand function, production parameters, ecc.)
- Water authority distributes water
- Compute equilibrium production of all actors (prices depend on production of all actors) and observe profits
- Forecast optimal production expansion by every actor for observed system parameters and compute ROI for each actor (return on investment)
- Each actor decides whether to expand by checking if his ROI exceeds his acceptance threshold
- Acceptance threshold is the policy parameter for each actor, which is obtained by solving equilibrium problem on the upper level

Alexei.Gaivoronski@iot.ntnu.no

Simulation of producers and consumers in water ecosystem with investment decisions

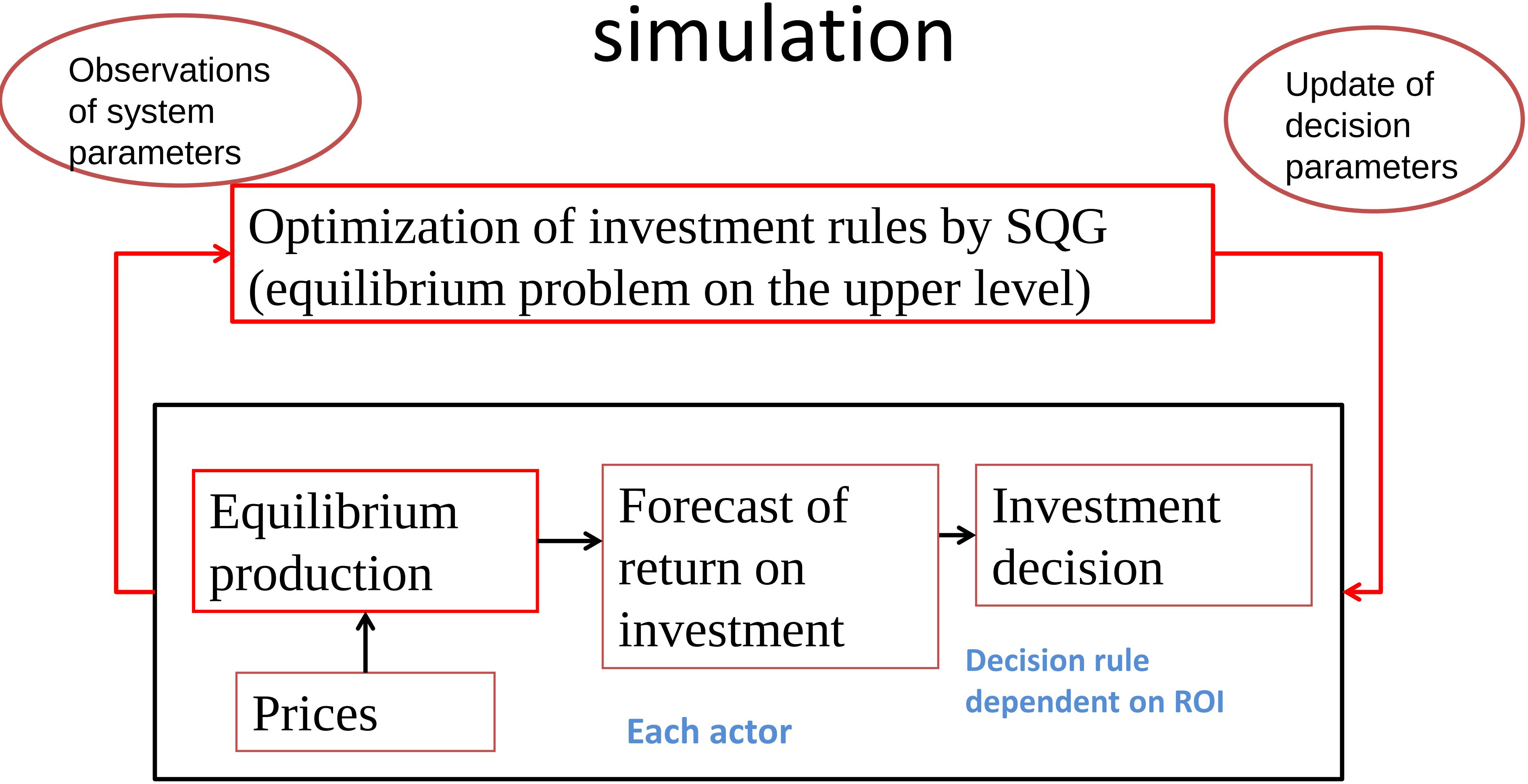


Policy parameters:
Upper level equilibrium or optimization

Capacity expansion:
Medium level equilibrium or optimization

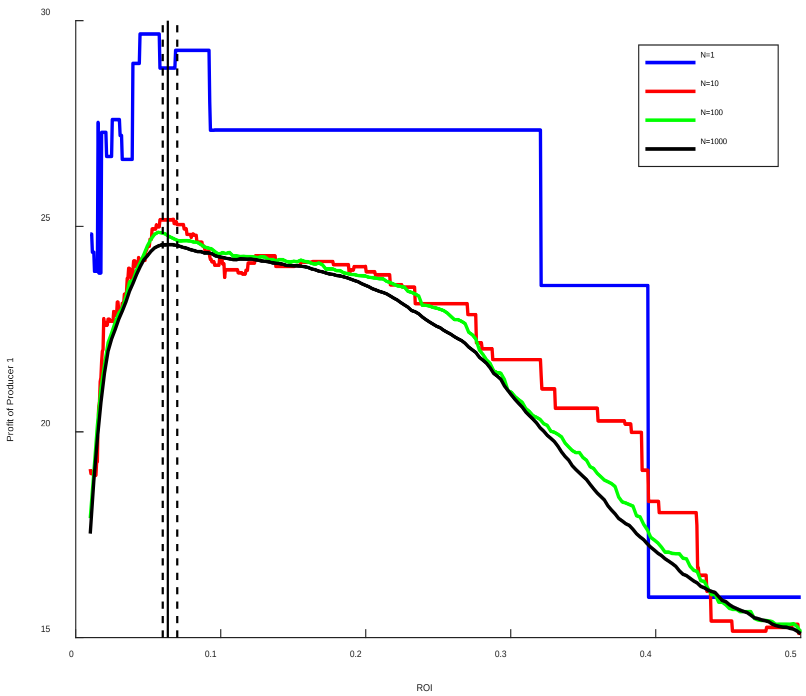
Production level:
Lower level equilibrium or optimization

Combination of optimization and simulation

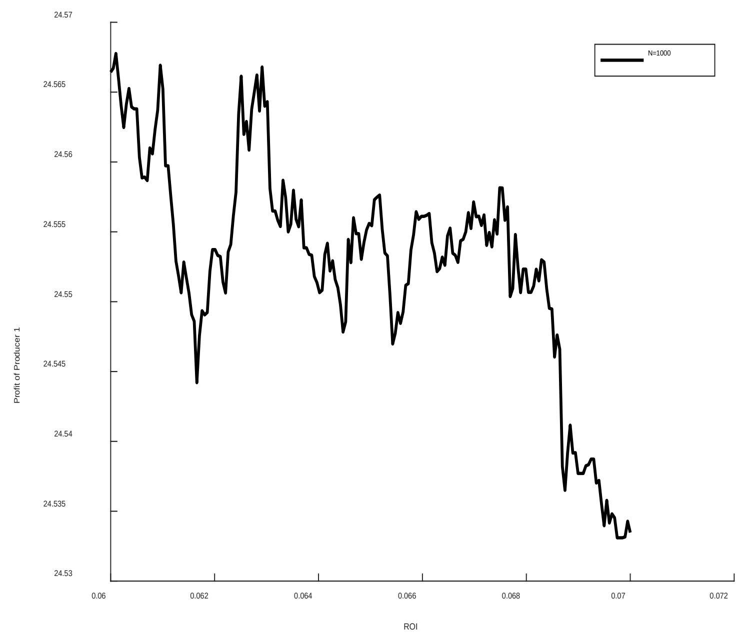


Strategic decision rule: threshold on return on investment (ROI)
Water distribution by water authority

Sample averages approximation



Magnified behavior in vicinity of maximum

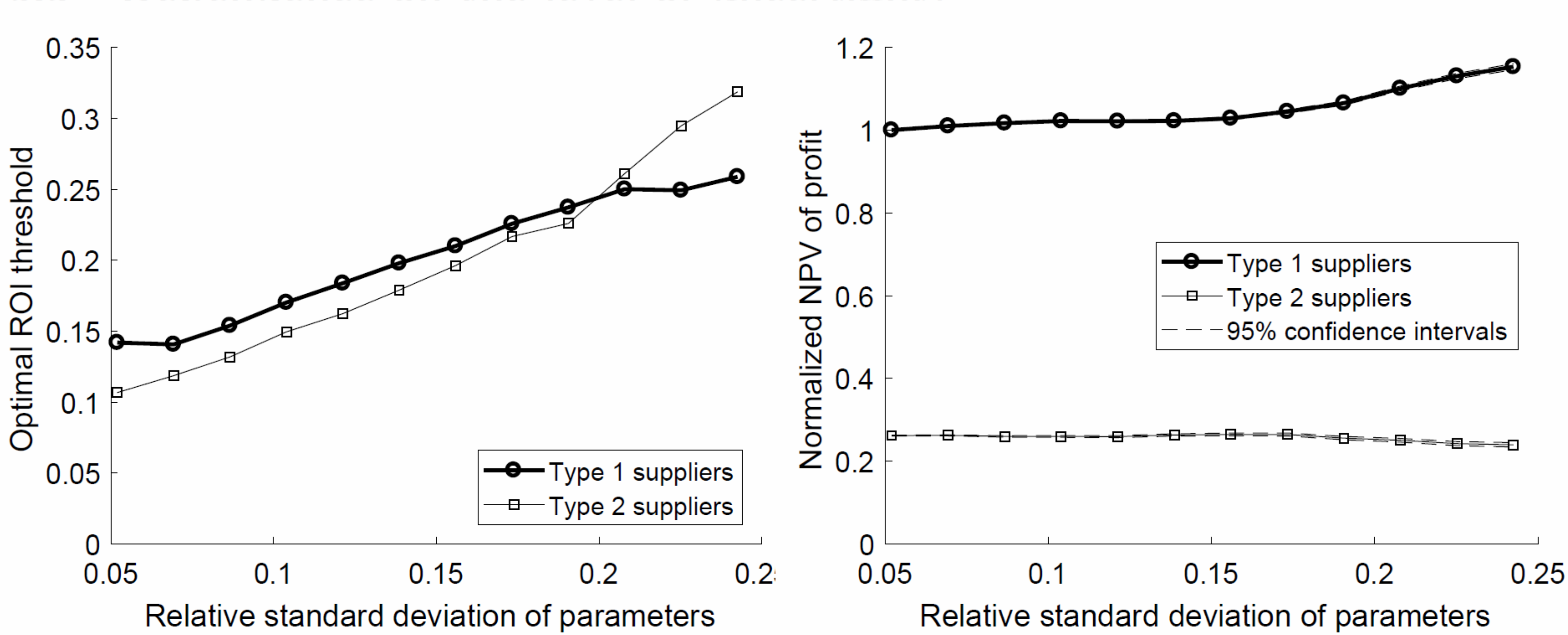


- Sample average approximation: simulate N sample paths and average the objective
- Apply NLP code to optimize this sample average
- **It will not work here due to discontinuous sample average irrespective of N**

  Very typical of simulation models
- Answer: **Stochastic gradient methods**

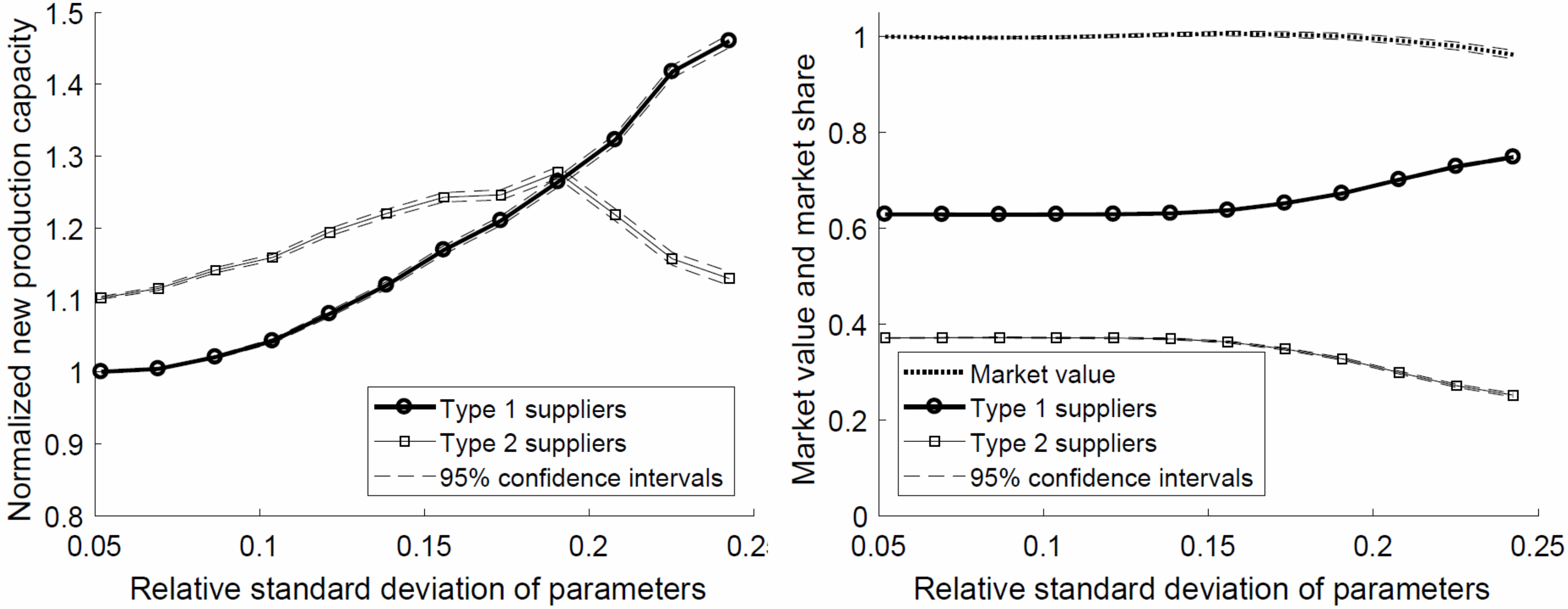
Some results: comparison with corporate finance theory

5.3 Dependence on the level of uncertainty



Alexei.Gaivoronski@iot.ntnu.no

Comparison with corporate finance theory



Big picture

- We develop combined simulation and optimization model which allow forecast of development of this ecosystem on the time scale of several decades
- Emphasis on uncertainty: consumption, prices, costs, production parameters …
- Complementary approach to scenario trees: reduced decision space, but more possibilities to model uncertainty with finer time grid and modeling of behavior of real actors
- Simulation model provides observations of performance, which depend on decision parameters.
- The values of decision parameters are optimized in parallel with simulation

Alexei.Gaivoronski@iot.ntnu.no

Answer: stochastic (quasi)gradient methods (SQG), Ermoliev

- Method for solution of stochastic optimization problems of the type

$$\max_{x \in X} \mathbb{E} f(x, \omega)$$

- Iterative process $x^{s+1} = \pi_X \left(x^s + \rho_s \xi_s \right)$
- Projection operator

$$\pi_X(y) \in X, \ \ \|\pi_X(y) - y\| = \min_{z \in X} \|z - y\|$$

- ξ_s is an estimate of the gradient of the objective function:

$$\mathbb{E}\left(\xi_s \mid x^1, \ldots, x^s \right) = F_x\left(x^s \right) + a_s$$

- ρ_s is a stepsize:

$$\sum_{s=0}^{\infty} \rho_s = \infty, \ \sum_{s=0}^{\infty} \rho_s^2 < \infty, \ \sum_{s=0}^{\infty} \rho_s \|a_s\| < \infty \ \ a.s.$$

Stochastic approximation: Kiefer & Wolfowitz, Kushner,
Optimization: Gaivoronski, Pflug, Shapiro …

SQG, continued

- Important difference: transient behavior, we can observe only estimate with the property

$$\mathbb{E}\left(\xi_s \mid x^1, \ldots, x^s\right) = F_x^s\left(x^s\right) + a_s$$

- **Convergence theorem**:
  - Functions $F^s(x)$ are convex and bounded on open set
  - Set X is convex and compact
  - ρ_s is nonnegative and

$$\sum_{s=0}^{\infty} \rho_s = \infty, \ \sum_{s=0}^{\infty} \rho_s^2 < \infty, \ \sum_{s=0}^{\infty} \rho_s \left\| a_s \right\| < \infty \ a.s., \ \mathbb{E}\left(\left\| F_x^s\left(x^s\right) - \xi_s - a_s \right\|^2 \mid \mathbb{B}_s \right) < \infty$$

  - Nonstationarity condition:

$$\frac{\sup_{x \in X} \left\| F^{s+1}(x) - F^s(x) \right\|}{\rho_s} \rightarrow 0 \ as \ s \rightarrow \infty$$

Then $\max_{x \in X} F^s(x) - F^s\left(x^s\right) \rightarrow 0$ with probability 1

Lot of work is needed to adapt this method to optimization of simulation models

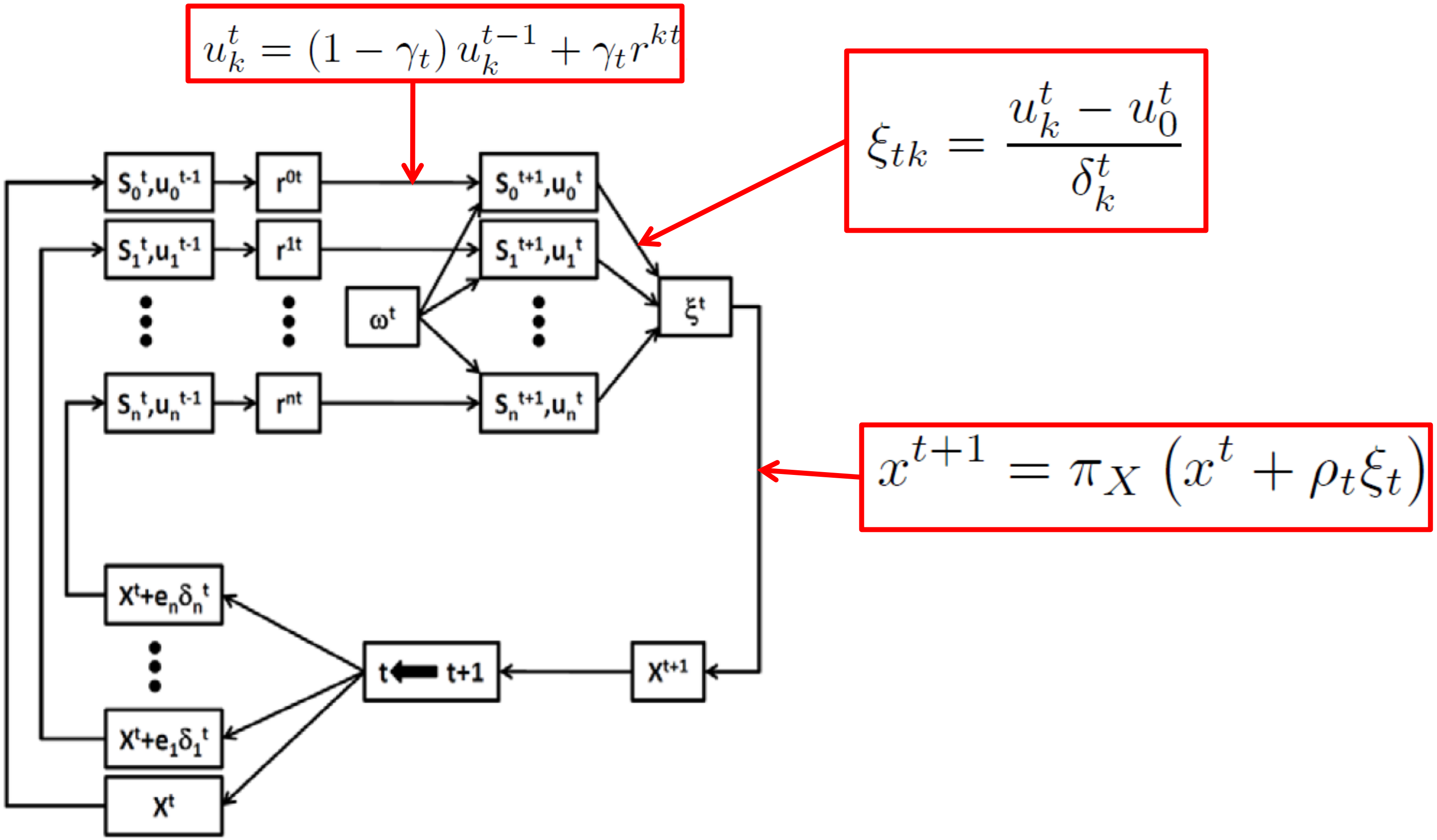
- Transient behavior
- Integration issues between simulation and optimization
- Obvious strategies do not work, for example brute force finite differences
  - At each step:
  - 1. Simulate the system from some initial state for current values of service parameters x^s during time horizon T, obtain the observation of objective $u_{0s}=R^T(x^s,w^s)$.
  - 2. Do the same for the values of x_i^s that differ from x^s in that the i-th variable is incremented by the value δ_s of finite differences, obtain the estimate u_{is}. Do it for all the service parameters.
  - 3. Compute the i-th component of the estimate of the gradient $\xi_i^s=(u_{is}-u_{0s})/\delta_s$
  - 4. Perform one step of the SQG method, obtain x^{s+1}
  - 5. Go to step 1.

This takes forever because T should be sufficiently large to get rid of the transient effects.

Integrated simulation and optimization

- Intertwine tightly simulation and optimization: change service parameters according to SQG method *every* simulation step
- Perform *n+1* parallel simulations for the current point and *n* shifts with the finite difference step for each of the *n* parameters using common random numbers
- Utilize previous information in the estimation of function values necessary for the finite differences
- This has an effect of filtering out both noise and transient effects
- Since optimization steps are so lightweight they can be performed by millions in a few minutes on laptop

Integrated simulation and optimization, continued



Optimal values of service parameters are obtained after the end of single simulation run consisting of n+1 simulation threads

Full description of the algorithm

1. Initialization. Select the following parameters of the algorithm:

T - *the number of time periods to perform simulation and optimization;*

$\rho_t \geq 0$ - *the sequence of step sizes for updating of the decision variables* x^t .

γ_t - *the sequence of multipliers for estimation of the objective function* $F(x)$ *from (5).*

θ_t - *the sequence of moving average multipliers for estimation of the solution of problem (5) from the iteration points*

δ_k^t - *the sequence of finite difference steps for approximating of the gradient of objective function,* $k = 1 : n$.

x^1 - *the starting point for the optimization algorithm.*

$S_k^1 = S^1$ - *the initial state for the simulation of the social network,* $k = 0 : n$.

Select the initial approximation $\tilde{x}^1 = x^1$ *to the solution of the problem (5), the initial estimates* $u_k^0 = u^0$ *of the value of* $F(x^1)$ *and the initial estimate* $\tilde{F}^1$ *to the optimal value of the problem.*

2. Generic step. Suppose that by the start of iteration $t = 1, ..., T$ *the* $k+1$ *simulation processes have arrived at the states* $S_k^t, k = 0 : n$, *the optimization algorithm has generated the value* x^t *of decision variables and* $k+1$ *estimation processes obtained the estimates* u_k^{t-1} *for the values of the objective function* $F(x)$ *at point* x^t *for* $k = 0$ *and points* $x^t + e_k\delta_k^t$ *for* $k = 1 : n$. *On iteration* t *the states* S_k^t, *the estimates* u_k^{t-1} *and point* x^s *are updated as follows.*

2a. The observations $r^{kt}, k = 0 : n$ *of the one period performance measure are obtained (for example, one period revenue from (4)). The observation* r^{kt} *is made from the state* S_k^t *using the values* x^t *of decision variables for* $k = 0$ *and* $x^t + e_k\delta_k^t$ *for* $k = 1 : n$.

2b. The observations ω^t *of random variables* ω *are generated.*

2c. The next states $S_k^{t+1}, k = 0 : n$ *of the social network are obtained using the observations* ω^t. *The state* S_0^{t+1} *is generated starting from the state* S_0^t *according to the network description (1)-(3) and using the value* x^t *of decision variables and the states* $S_k^{t+1}, k = 1 : n$ *are generated starting from the states* S_k^t *and using the values* $x^t + e_k\delta_k^t$ *of decision variables.*

Full description of the algorithm, continued

2d. The estimates u_k^t *of the objective function* $F(x)$ *at points* x^t *for* $k = 0$ *and* $x^t + e_k\delta_k^t$ *for* $k = 1 : n$ *are computed using the observations* r^{kt}*:*

$$u_k^t = (1 - \gamma_t)\, u_k^{t-1} + \gamma_t r^{kt}, \;\; k = 0 : n$$

2e. The finite difference approximation ξ^t *to the gradient of function* $F(x^t)$ *is computed as follows:*

$$\xi_t = (\xi_{t1}, ..., \xi_{tn})\,, \;\; \xi_{tk} = \frac{u_k^t - u_0^t}{\delta_k^t}$$

2f. The new value x^{t+1} *of the decision variables is computed as follows:*

$$x^{t+1} = \pi_X \left(x^t + \rho_t \xi_t\right)$$

2g. The current approximations to the optimal values of decision variables x *and the current approximation* $\tilde{F}^{t+1}$ *to the optimal value of the problem are computed as the moving average of the iteration points as follows:*

$$\tilde{x}^{t+1} = (1 - \theta_t)\, \tilde{x}^t + \theta_t x^{t+1}$$
$$\tilde{F}^{t+1} = (1 - \theta_t)\, \tilde{F}^t + \theta_t x^{t+1}$$

2h. Stop if $t = T$ *and take the average of the last* T_1 *values of* $\tilde{x}^t$ *and* $\tilde{F}^t$ *as the final approximations* $\tilde{x}$ *and* $\tilde{F}$ *to the optimal solution of the problem(5) and its optimal value.*$\square$

Implementation

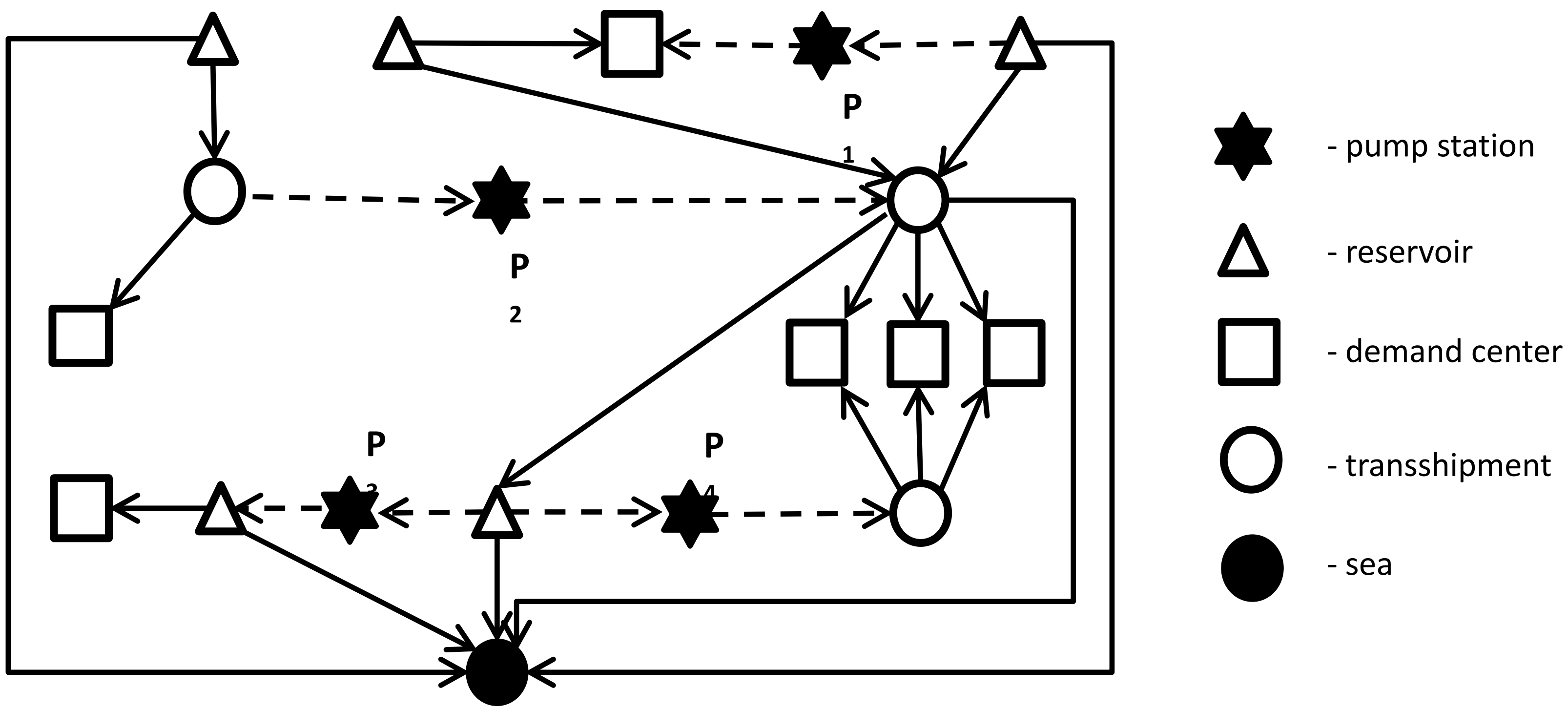
- We developed a framework for solving such problems: universal optimization engine, which takes as an input simulation models with appropriate interface
- Optimization engine is written in Matlab, it is developed together with former PhDs (Denis Becker and others). Gradually it is being enriched by new capabilities (like parallel execution, etc)
- Simulation is written in Matlab and is connected to optimization engine by specified rules

Contents

- Motivation
  - Water resources network in South Sardinia
- Methodology: Stochastic optimization of simulation models under uncertainty
  - Concurrent simulation and optimization with stochastic gradient methods
- **Water resources management**
  - **Management of reconfigurable water network**
  - **Cost/risk tradeoff in management of scarce water resources**

Management of reconfigurable water system network

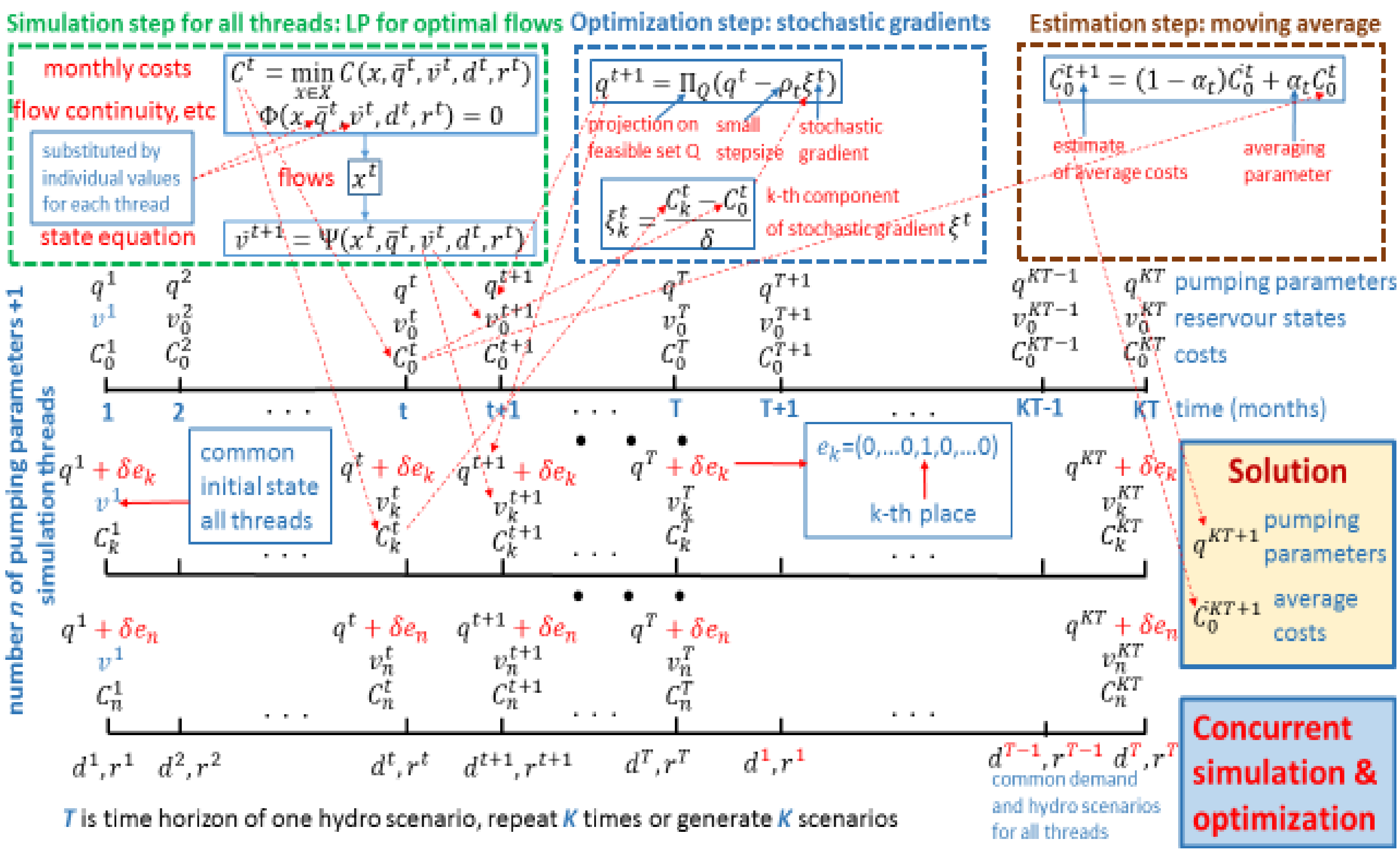
Simplified model of South Sardinia water management system



Graph where some links are temporary

- Simulation: Each time period: decide the network configuration according to parametrized rule
- Compute optimal flows by solving LP
- Get optimal rule parameter values by optimization of simulation model

Concurrent simulation and optimization



Network configuration rule

- Activate link when the weighted sum of volumes in critical reservoirs drops below the threshold level
- Volume weights and threshold levels are the rule parameters

$$\sum_{i \in V} h_{ik} v_i^t \leq q_k \sum_{i \in V} h_{ik} V_i^{\max}$$

Rule parameters

Network flow problem: objective

Minimize total costs during one period

$$\min_{\substack{v_i^{t+1}, v_{i-}^{t+1}, v_{i+}^{t+1} \geq 0, \\ x_{ik}^t, u_{pi}^t, u_{ni}^t \geq 0}} \left[\sum_{(i,k)\in\bar{P}} \left(c_p^{ik} - c_y^{ik}\right) x_{ik}^t + \sum_{i\in D} c_p^i u_{pi}^t + \sum_{i\in D} c_n^i u_{ni}^t + \sum_{k\in K_{i_0}^-} c_w^k x_{ki_0} + \sum_{i\in V} c_v^i v_{i-}^{t+1} \right]$$

c_p^{ik} - cost of pumping on link $(i,k) \in P$;

c_p^i - cost of nonsatisfaction of unit demand at demand node $i \in D$ within programmed deficit;

c_n^i - cost of nonsatisfaction of unit demand at demand node $i \in D$ beyond programmed deficit, it is assumed that $c_{ud}^i > c_{pd}^i$;

c_w^i - opportunity cost of spilled water to sea from node $i \in V \cup U$;

c_v^i - penalty for violating lower bound constraint on the volume of reservoir $i \in V$;

c_y^{ik} - penalty for pumping on link (i,k) less than g^{ki}, $c_y^{ik} > c_p^{ik}$. This penalty is introduced due to technological considerations: if pump is operating, it should operate with full capacity if there is enough water. It could happen that during some time period there is not enough water for pumping during the whole period. In this case the corresponding pump will operate only during some part of this period.

Network flow problem: constraints

Water conservation

$$v_i^{t+1} = \left(1 - \alpha_t^i\right) v_i^t + r_i^t + \sum_{k \in K_i^-} x_{ki}^t - \sum_{k \in K_i^+} x_{ik}^t, \; i \in V$$

$$\sum_{k \in K_i^-} x_{ki}^t - \sum_{k \in K_i^+} x_{ik}^t = 0, \;\; i \in U$$

Capacity constraints

$$v_i^{t+1} \le V_i^{\max}$$

$$0 \le x_{ij}^t \le g_{ij}, \;\; i,j \in V \cup U, \;\; (i,j) \in L \setminus P$$

$$0 \le x_{ij}^t \le \chi_{ij}\left(\bar{P}\right) g_{ij}, \;\; (i,j) \in P$$

Environmental constraint

$$v_i^{t+1} = V_i^{\min} + v_{i+}^{t+1} - v_{i-}^{t+1}$$

Demand satisfaction

$$\sum_{k \in K_i^-} x_{ki}^t + u_{pi}^t + u_{ni}^t = d_i^t, \;\; i \in D,$$

$$0 \le u_{pi}^t \le \beta_i d_i^t, \;\; u_{ni}^t \ge 0, \;\; i \in D$$

Programmed and onprogrammed deficit

Dependence of costs on rule parameters

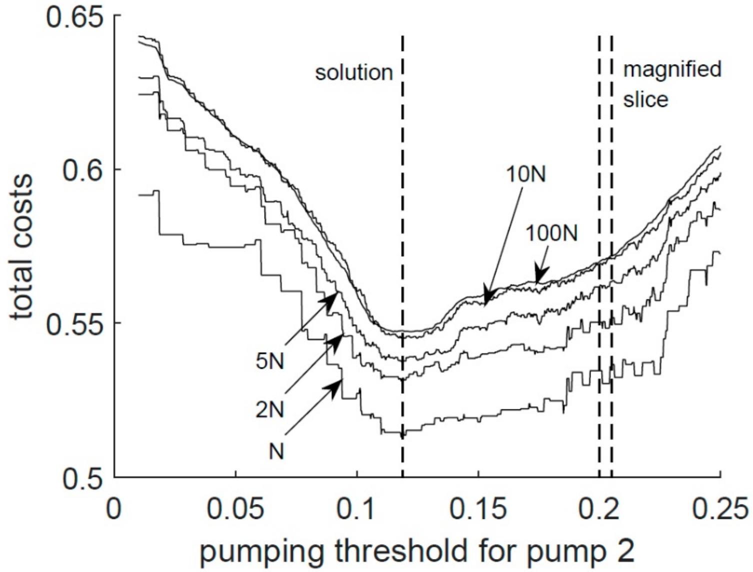


Figure 5. Dependence of costs on the value of pumping threshold for pump P2 for different simulation horizons

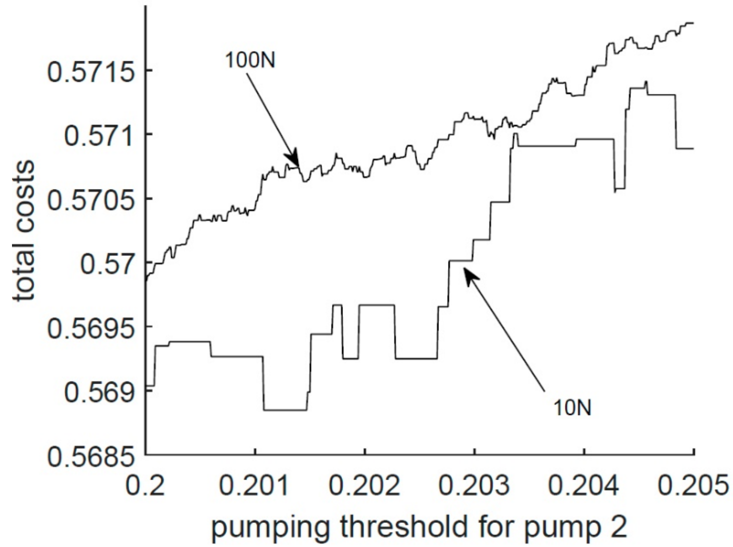


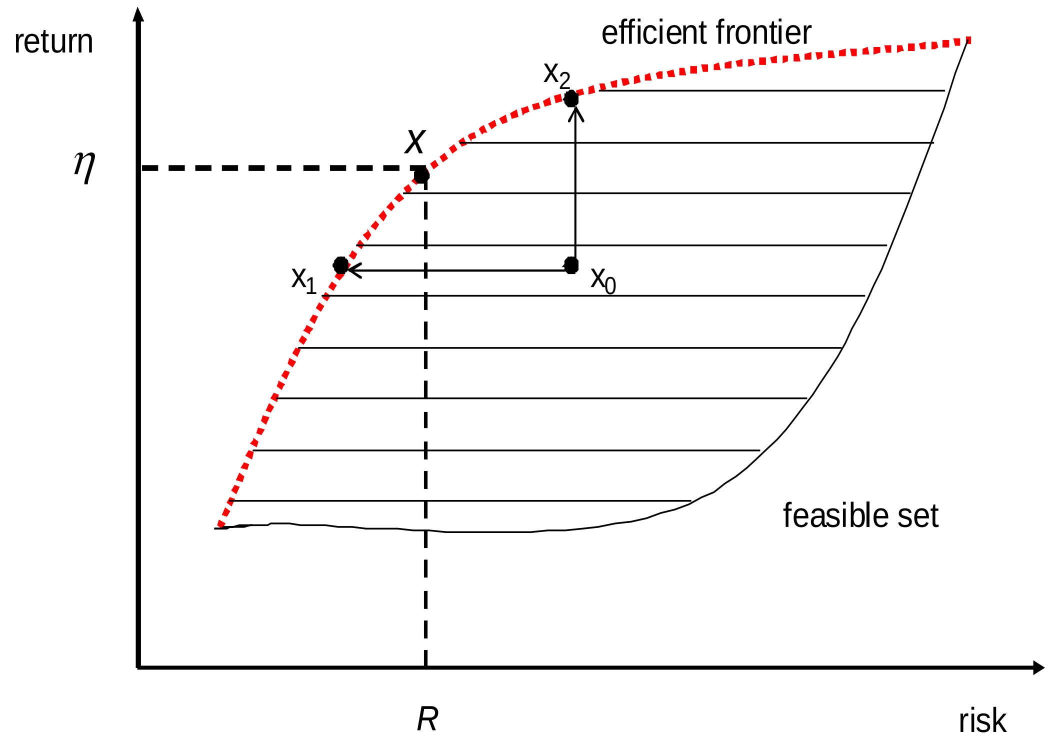
Figure 6. Dependence of costs on the value of pumping threshold for pump P2 for different simulation horizons, magnified portion

N=636 (the number of moinths in 53 years for which exists hydrological data

Cost/risk tradeoff in management of scarce water resources

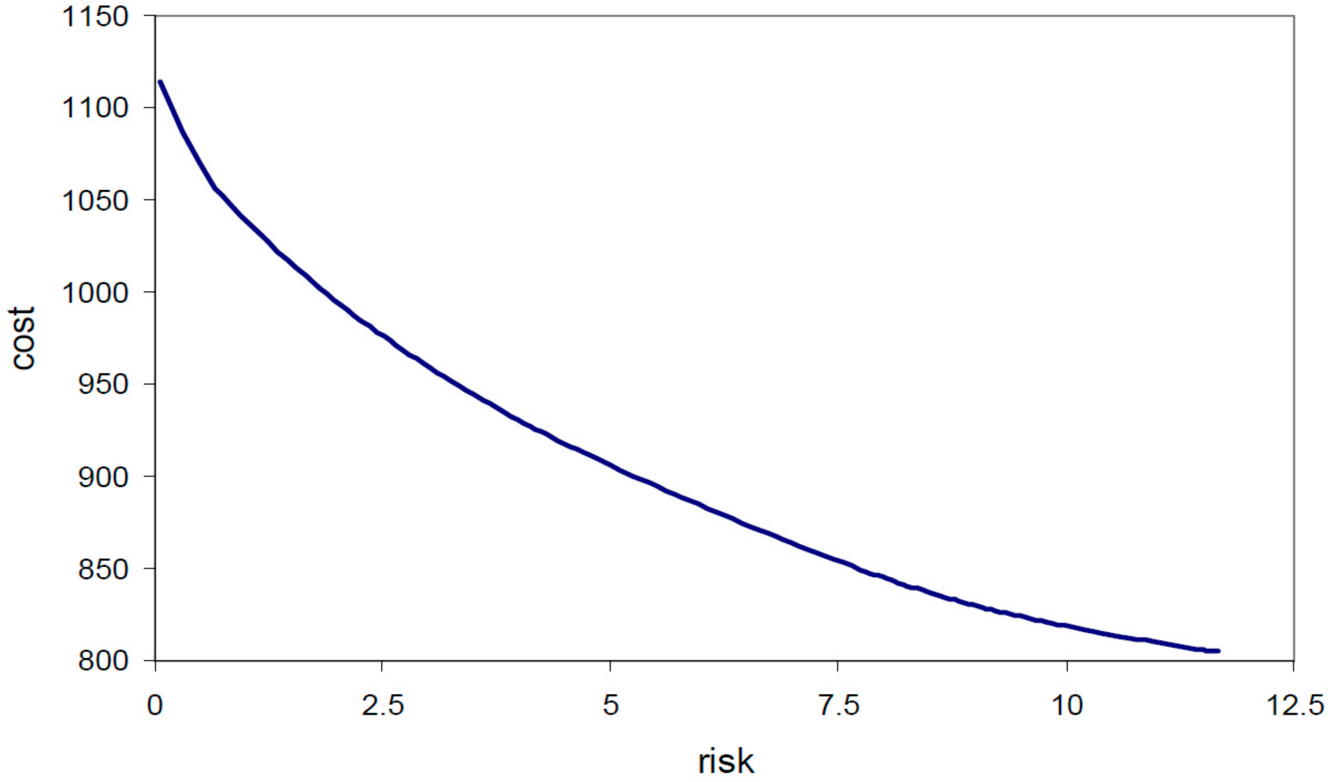
- View of portfolio theory of investment science:
  - Define benefit (costs/profits/public good)
  - Define risk (flood damages/extent of nonprogrammed deficits, measure of variation)
  - View water distribution between different uses as **water portfolio**, each portfolio brings benefit and risk
  - Construct efficient frontier by finding portfolios, which minimize risk for given benefit
  - Decision maker selects water portfolio from efficient frontier according to his risk preferences

Risk/return tradeoff



Harry Markowitz, Nobel prize in economics 1990, (for work done in 1952)

Water resources management in South Sardinia



Risk – extent of nonprogrammed deficit

Summary

- Combination of simulation and optimization is feasible and efficient in context of models of water resorces management ecosystems
- Integrated simulation and optimization approach powered by stochastic gradient methods is appropriate tool for solving complex nonlinear dynamic problems arising in water resources management
- Portfolio view brings a new perspective on the management of water systems