Optimization and Machine Learning with Applications

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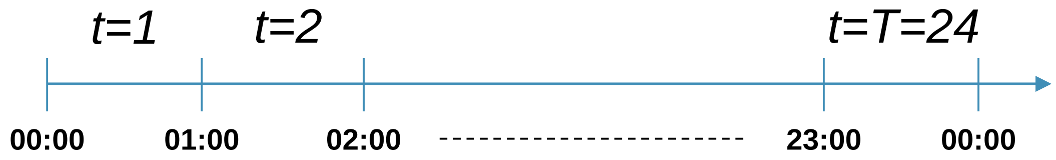
OAKS srl – Optimization Analytics Knowledge and Optimization

Pump Scheduling Optimization in Water Distribution Networks

- A problem usually addressed as **Global Optimization (GO)**
- The goal of **PSO** is to **minimize the energy cost**, while **satisfying hydraulic/operational constraints**
- A simplified formulation of the problem is the following:

$$\min \sum_{t=1}^{T} c_t E(x_t) \Delta t$$
$$s.t. \quad x_t \in U_t$$



- Where:
  - T is the time horizon (typically 24 hours)
  - Δt is the time step (typically 1 hour)
  - $x_t \in \mathbb{R}^p$ with *p* is the number of pumps (decision vector at *t*)
  - U_t is the feasibility set at *t*
  - c_t is the energy price per the unit of time [€/kWh]

$x_t^i \in \{0,1\}$ if pump *i* is an ON/OFF pump
$x_t^i \in [0,1]$ if pump *i* is a Variable Speed Pump

Pump Scheduling Optimization

- **PSO** is a typical problem in Operation Research community (Mala-Jetmarova et al., 2017)
- Many mathematical programming approaches (LP, IP, MILP) → they works with approximations
- Other approaches use simulation (i.e. EPANET 2.0)

Complex nonlinear objective function

$$\min \sum_{t=1}^{T} c_t E(x_t) \Delta t$$
$$s.t. \quad x_t \in U_t$$

Hydraulic feasibility

Mala-Jetmarova, H., Sultanova, N., Savic D. (2017). Lost in Optimization of Water Distri-bution Systems? A literature review of system operations, Environmental Modelling and Software, 93, 209-254.

Approaches based on water demand estimation/forecast

- **Simulation-Optimization:** minimizing the number of simulations required to find an optimal schedule, given a reliable forecast of the water demand

M. Castro-Gama, Q. Pan, E. A. Lanfranchi, A. Jomoski, D. P. Solomatine, "Pump Scheduling for a Large Water Distribution Network. Milan, Italy", Procedia Engineering, vol. 186, pp: 436-443, 2017.

M. Castro Gama, Q. Pan, M. A. Salman, and A. Jonoski, "Multivariate optimization to decrease total energy consuption in the water supply system of Abbiategrasso (Milan, Italy)," Environ. Eng. Manag. J., vol. 14, no. 9, pp. 2019–2029, 2015

F. De Paola, N. Fontana, M. Giugni, G. Marini, and F. Pugliese, "An Application of the Harmony-Search Multi-Objective (HSMO) Optimization Algorithm for the Solution of Pump Scheduling Problem," Procedia Eng., vol. 162, pp. 494–502, 2016.

***Candelieri, A., Perego, R., & Archetti, F. (2018). Bayesian optimization of pump operations in water distribution systems. Journal of Global Optimization, 71(1), 213-235**.*

Constrained GO with unknown constraints

- Although our proposed Bayesian Optimization approach is more efficient than other state-of-the-art methods, we concluded that the real problem is not modelling the objective function but **<u>estimating the feasible region within the search space</u>**

- In the **Constrained Global Optimization (CGO) with unknown constraints:**
  - **The set of constraints is "black-box"**, they can only be evaluated along with the function
  - Furthermore, $f(x)$ is typically **black-box** (itself), **multi-extremal** and **expensive**, and – more important – **<u>partially defined</u>**

BO with unknown constraints – state of the art

J. Bernardo, M. J. Bayarri, J. O. Berger, A. P. Dawid, D. Heckerman, A. F. M Smith and M. West, "Optimization under unknown constraints", Bayesian Statistics, 9(9), 229 (2011).

J. M. Hernández-Lobato, M. A. Gelbart, M. W. Hoffman, R. P. Adams and Z. Ghahramani, "Predictive entropy search for Bayesian Optimization with unknown constraints", in Proceedings of the 32nd International Conference on Machine Learning, 37 (2015).

Hernández-Lobato, J. M., Gelbart, M. A., Adams, R. P., Hoffman, M. W., & Ghahramani, Z. "A general framework for constrained Bayesian optimization using information-based search". The Journal of Machine Learning Research, 17(1), 5549-5601, (2016).

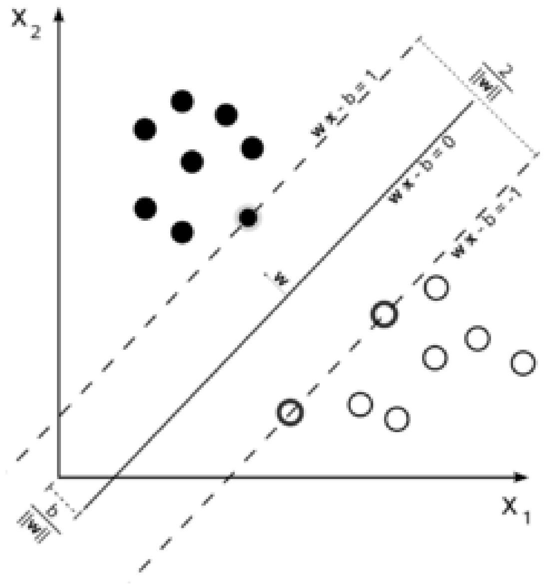
M. A. Gelbart, J. Snoek and R. P. Adams, "Bayesian Optimization with unknown constraints", arXiv preprint arXiv:1403.5607 (2014).

- We propose an approach where **no assumptions on constraints are needed**, the overall feasible region is modelled through a **Support Vector Machine** (SVM) classifier

A. Basudhar, C. Dribusch, S. Lacaze and S. Missoum, "Constrained efficient global optimization with support vector machines", Struct Multidiscip O, 46(2), 201-221 (2012).

A remind on SVM classification

- **Hard-margin classification**



Let $D = \left\{(x^i, y^i)\right\}_{i=1,\dots,n}$ denotes a dataset of pairs, where:

- x^i is a point in $\mathbb{R}^d$ and
- y^i is the associated «class label»: $y^i = \{+1, -1\}$

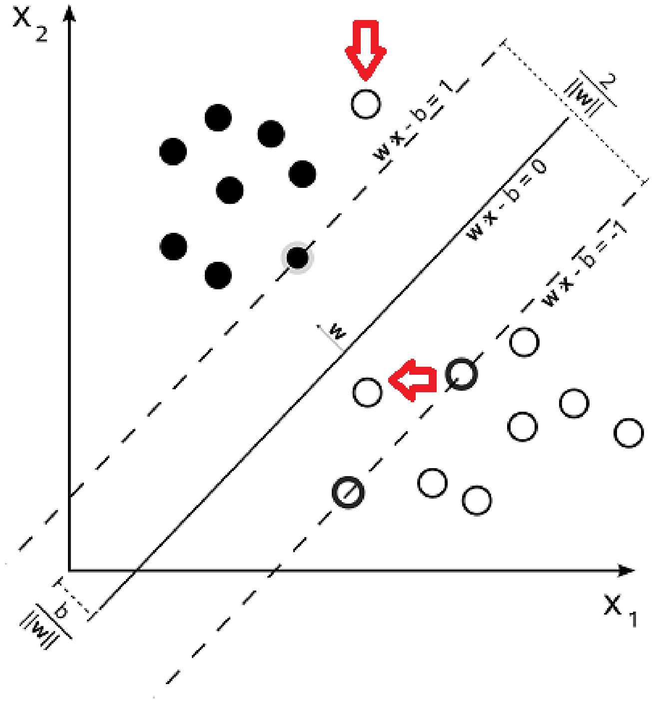
The goal is to find the **separating hyperplane** with **maximum margin**:

$$\min \frac{1}{2}\|w\|^2 \text{ s.t. } y^i\left(\langle w, x^i\rangle - b\right) \geq 1, \forall\, i = 1, \dots, n$$

Given a generic point $\bar{x} \in \mathbb{R}^d$, the label assigned to it by the SVM classifier (depending on the «learned» w and b) is given by $\operatorname{sign}(\langle w, x^i\rangle - b)$

A remind on SVM classification (cont'd)

- Hard-margin classification works only for **linearly separable data**
- **Soft-margin** classification was (initially) proposed to extend SVM to the case of **non-linearly separable data**



$$\min \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi^i$$

$$\text{s.t. } y^i\left(\langle w, x^i\rangle - b\right) \geq 1 + \xi^i,\ \ \forall\, i = 1, \dots, n$$

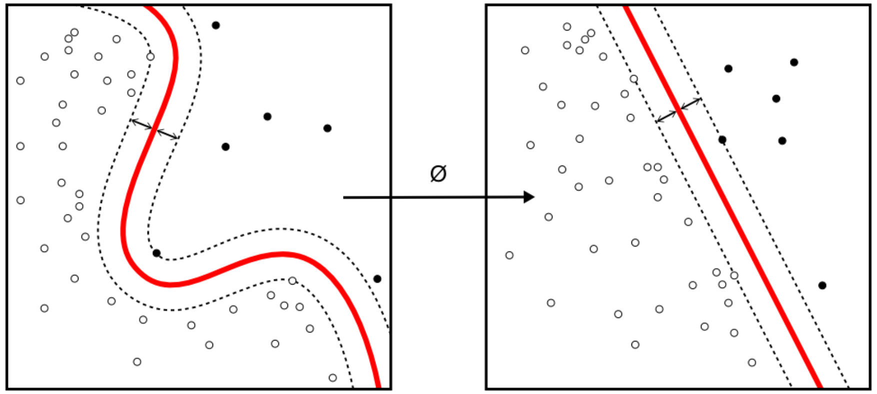
A remind on SVM classification (cont'd)

- Both Hard and Soft margin classification uses a **linear separation hyperplane** to classify data → to overcome limitations of linear classifier the ***"kernel trick"*** has been proposed

- For data not linearly separable in the **Input Space**, there is a function ϕ which "maps" them in a **Feature Space** where linear separation is possible

- Identifying ϕ is NP-hard!

- **Kernels** allow for computing distances in the Feature Space without the need to explicitly perfom the "mapping"



Scholkopf, B., & Smola, A. J. (2001). *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press.
Steinwart, I., & Christmann, A. (2008). *Support vector machines*. Springer Science & Business Media.

A two stages approach for CGO with unknown constraints

- The proposed formulation for **CGO with unknown constraints:**

$$\min_{x \in \Omega \subset X \subset \mathbb{R}^d} f(x)$$

Where $f(x)$ is a **black-box**, **multi-extremal**, **expensive** and **partially defined** objective function and Ω is the **unknown feasible region** within the box-bounded search space X

- Some notations:

  - $D_\Omega^n = \{(x^i, y^i)\}_{i=1,..,n}$ **feasibility determination** dataset;
  - $D_f^l = \{(x^i, f(x^i))\}_{i=1,..,l}$ **function evaluations** dataset,

with $l \leq n$ and where l is the number of feasible points out of the n evaluated so far;
where x^i is the i-th evaluated point and $y^i = \{+1, -1\}$ defines if x^i is feasible or infeasible, respectively.

First Stage: Feasibility Determination

- Aimed at finding an estimate $\tilde{\Omega}$ of the actual feasible region Ω in M function evaluations
- $\tilde{\Omega}^n$ is given by the (non-linear) separation hyperplane of the SVM classifier trained on D^n_Ω
- The next point x^{n+1} to evaluate (to improve the quality of the estimate $\tilde{\Omega}$) is chosen by considering:
  - Distance from the (current) non-linear separation hyperplane
  - Coverage of the search space

$$x^{n+1} = \underset{x \in X}{\operatorname{argmin}} \{d^n(h^n(x), x) + c^n(x)\}$$

$$d^n(h^n(x), x) = |h^n(x)| = \left| \sum_{i=1}^{n_{SV}} \alpha_i y_i k(x_i, x) + b \right|$$

Where $h(x) = 0$ is the (non linear) separation hyperplane

min coverage = max uncertainty

$$c^n(x) = \sum_{i=1}^{n} e^{-\frac{\|x^i - x\|^2}{2\sigma^2}}$$

First Stage: Feasibility Determination

- Function evaluation at x^{n+1} and datasets update:

$$y^{n+1} = \begin{cases} +1 \; if \; x^{n+1} \in \Omega \, ; \; with \; f(x^{n+1}) \\ -1 \; if \; x^{n+1} \notin \Omega \end{cases} \Rightarrow \begin{array}{c} D_{\Omega}^{n+1} = D_{\Omega}^{n} \cup \{(x^{n+1}, y^{n+1})\} \\ h^{n+1}(x) \, | D_{\Omega}^{n+1} \end{array}$$

And if $x^{n+1} \in \Omega \; (i.e. \, y^{n+1} = +1)$ $\Rightarrow$ $\begin{array}{c} D_f^{l+1} = D_f^l \cup \{(x^{n+1}, f(x^{n+1}))\} \\ l \leftarrow l + 1 \end{array}$

- The first stage ends after M function evaluations

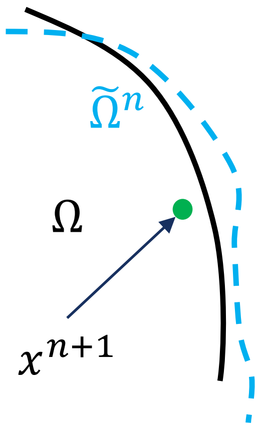
Second Stage: constrained BO

- "standard" BO but:
  - using, as a probabilistic surrogate model for $f(x)$, a GP fitted **only** on D_f^l
  - having an acquisition function (i.e. LCB) defined **only** on $\widetilde{\Omega}^n$

$$x^{n+1} = \underset{x \in \widetilde{\Omega}^n}{\operatorname{argmin}} \{LCB^n(x) = \mu^n(x) - \gamma^n \, \sigma^n(x)\}$$

- Function evaluation at x^{n+1} and datasets update:

$$D_\Omega^{n+1} = D_\Omega^n \cup \{(x^{n+1}, y^{n+1})\}$$ **Must be updated**



- **Case A:** $x^{n+1} \in \Omega \ (i.e.\, y^{n+1} = +1)$

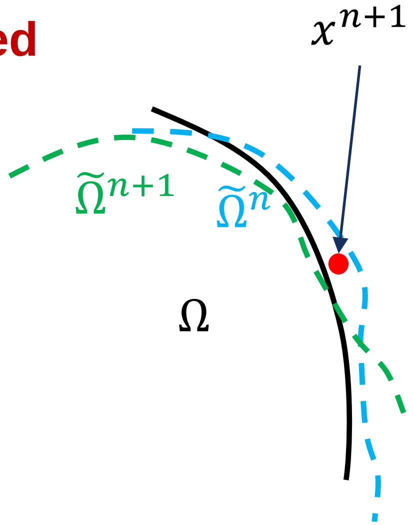
$$D_f^{l+1} = D_f^l \cup \{(x^{n+1}, f(x^{n+1}))\}$$
$$l \leftarrow l+1$$

No need to retrain SVM

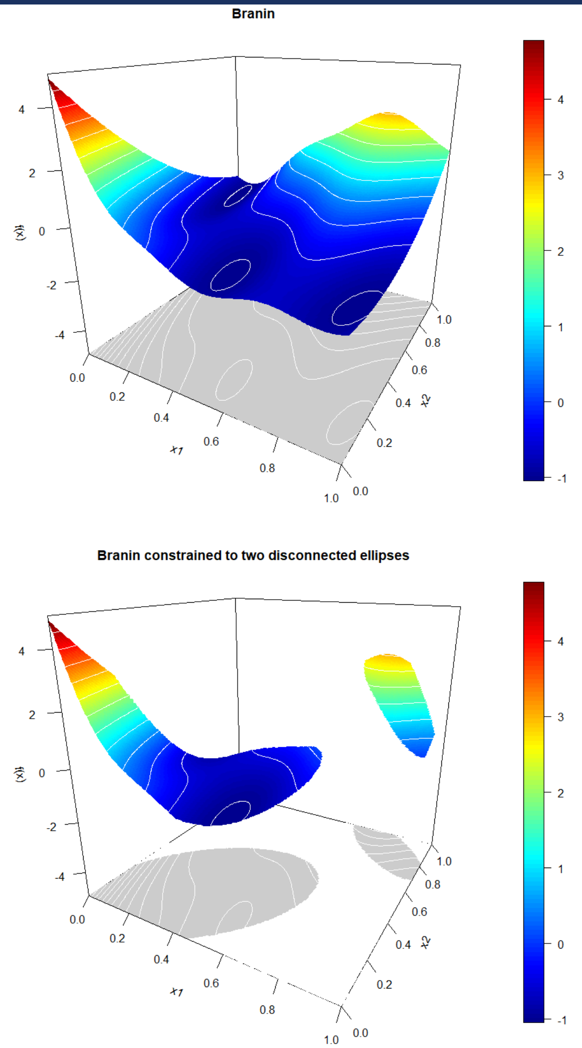
- **Case B:** $x^{n+1} \notin \Omega \ (i.e.\, y^{n+1} = -1)$

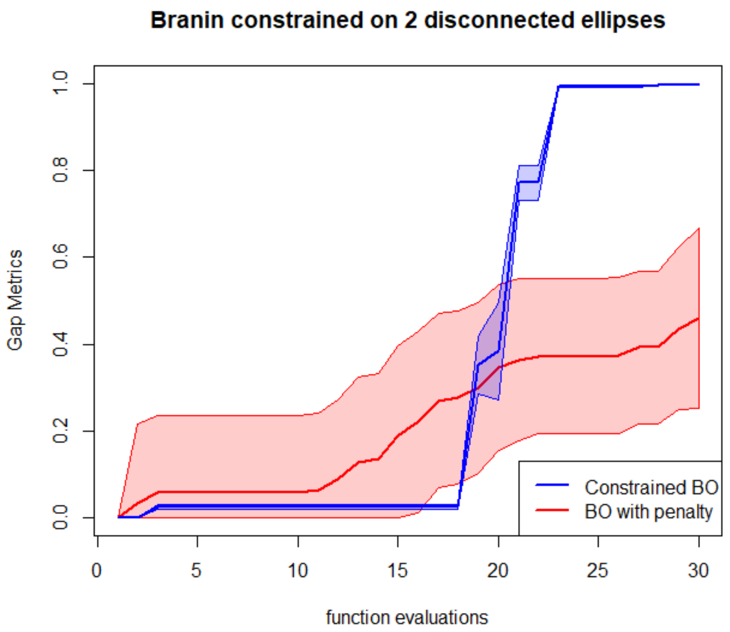
$$h^{n+1}(x) \mid D_\Omega^{n+1} \implies \widetilde{\Omega}^{n+1}$$

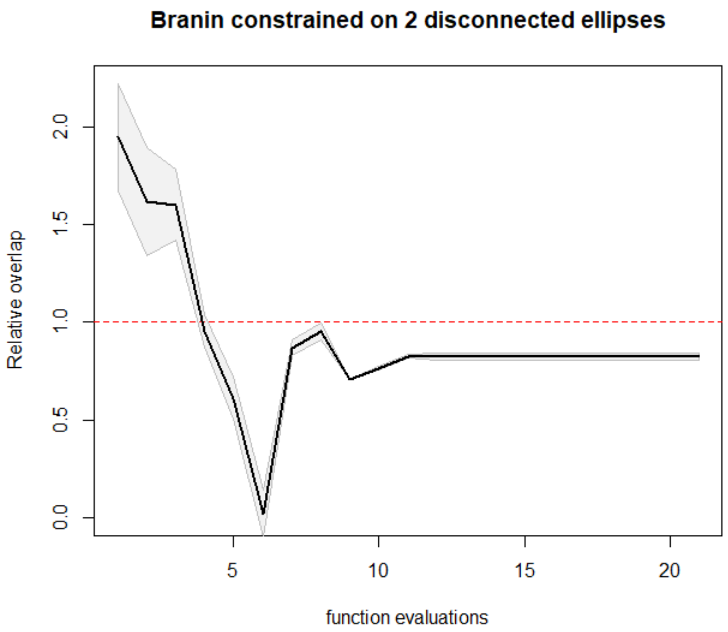
SVM must be retrained



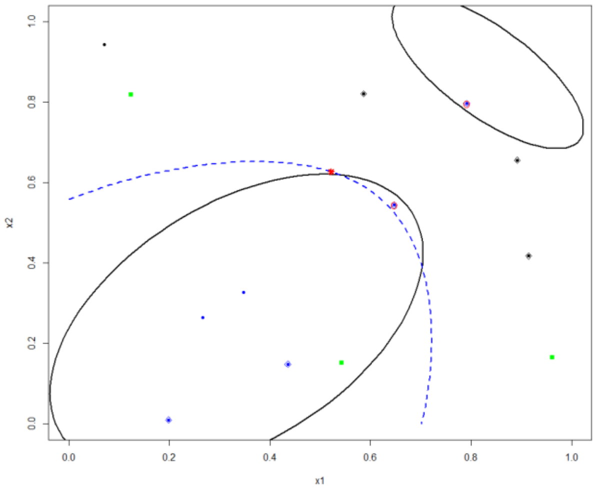
A simple test function: Branin 2D (rescaled) constrained to two elipses



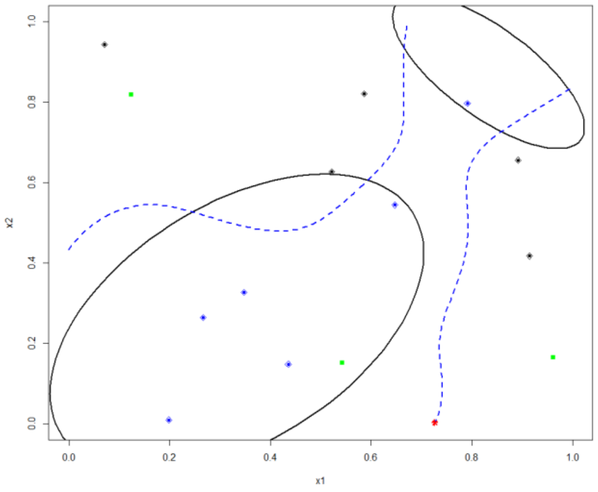




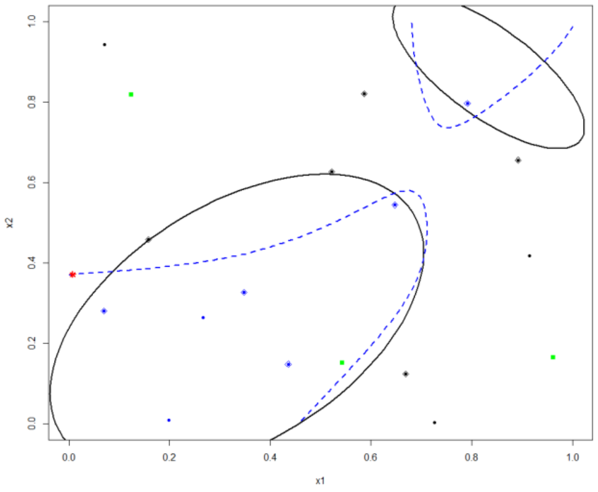
Initialization



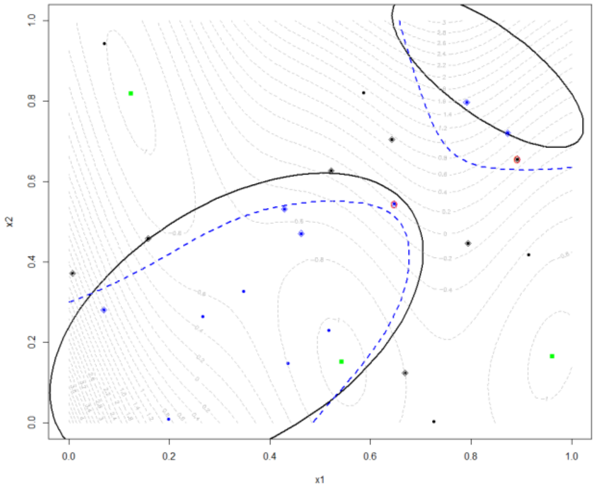
First Stage – 5 evaluations



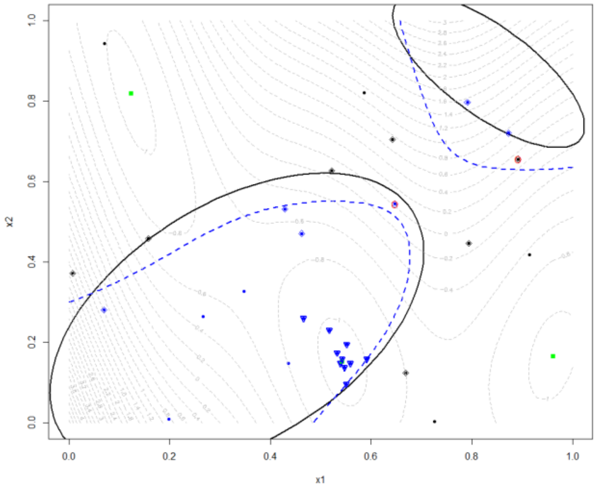
First Stage – 10 evaluations



Second Stage – starting



Second Stage – end



▪ Global optima (only 1 is feasible)
--- Boundaries of $\widetilde{\Omega}^n$
● Infeasible evaluation (1st stage)
● Feasible evaluation (1st stage)
* Next point to evaluate x^{n+1}
▼ Feasible evaluation (2nd stage)
▼ Infeasible evaluation (2nd stage)

Red-circled points are classification erros
Points into diamonds are Support Vectors

Summarizing…

- The **SVM+constrained BO framework** resulted more effective and efficient than BO with penalty
- It provides both a (better) optimal solution and a good approximation of the unknown feasible region
- A single SVM is sufficient for approximating the feasible region, instead of one GP per constraint (computational costs for training an SVM or a GP is $\mathcal{O}(n^3)$, with n the number of function evaluations)
- The approach is particularly well suited for **Simulation-Optimization** problems – or any other setting where infeasible evaluations are not *"disruptive"*
- **Sensitivity analysis is not possible** since the single constraints are not modelled

PSO via Approximate Dynamic Programming

Neither Supervised nor Unsupervised: Learning by doing!

Learning and Optimizing online – Goals:

- Identifying a **policy**, instead of a solution
- … thus, providing **a robust mechanism to generate solutions online**, in order to deal with uncertainty (i.e. on water demand)

- Online optimization means «decide (and act) at each decision step»
  - From $p \times T$ decision variables, in typical PSO approaches, to only p decision variables at each decision step
- … but balancing decisions (actions) for optimizing while learning something more about the system

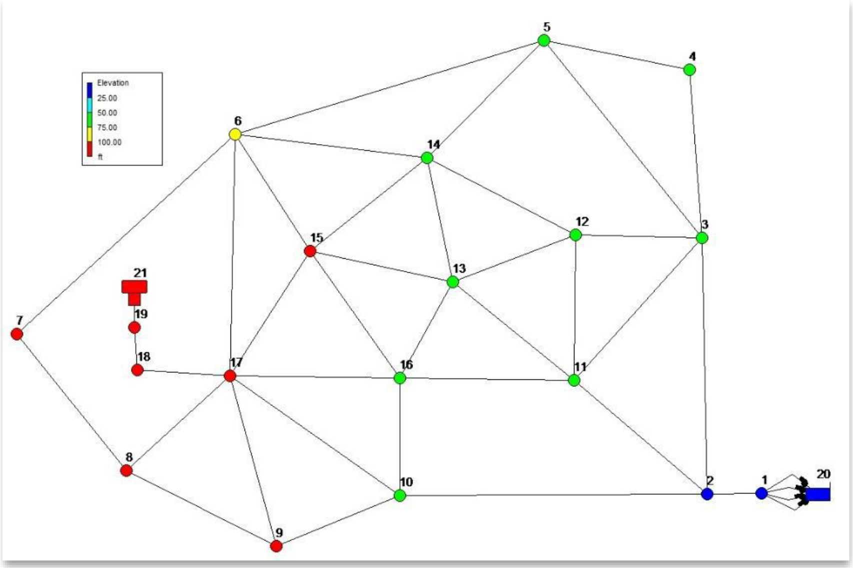
- **Information-acquisition** setting: a-priori knowledge is not available → Approximate Dynamic Programming (aka Reinforcement Learning)

Q-Learning

- A typical ADP algorithm, well known in the Reinforcement Learning community
- State-Action Value Function:
  - $Q^*(s,x) = \mathcal{R}(s,x) + \gamma \max_{x'} Q(s',x')$ for all s, all x and all policies
- Model-free
- ε-greedy policy to balance exploration-exploitation:
  - with probability ε → Make a random action x
  - with probability $1-\varepsilon$ → Select the best action known so far: $\operatorname{argmax}_x Q(s,x)$
- Updating rule:
  - $Q(s,x) \leftarrow Q(s,x) + \alpha\left[\mathcal{R}(s,x) + \gamma \max_{x'} Q(s',x') - Q\,(s,x)\right]$

PSO formulation as ADP problem

- **Use Case**: Anytown



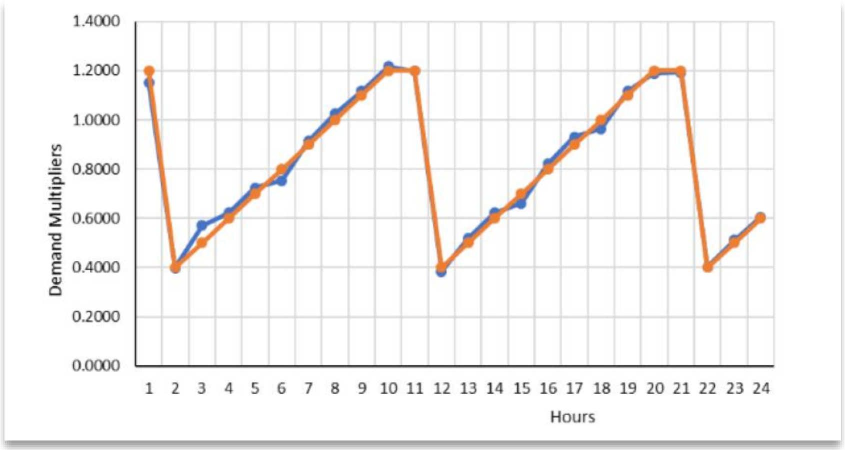
- **State Space**:
  - $s_t = (tank\ level, average\ pressure)$
  - Both tank level and average pressure discretized on 5 intervals
  - 5x5 = 25 possible states

- **Action Space**:
  - $x_t \in \mathbb{R}^p$, with $x_t^i = \{0,1\}\ \forall\ i = 1, \dots, p$
  - In this case study *p=4* → $2^4 = 16$ actions

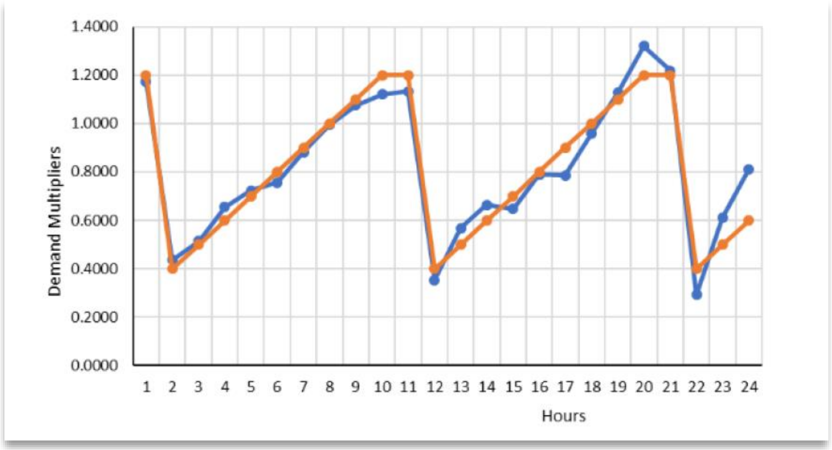
- **Reward**:
  - $\bar{C}_{t-1} - \bar{C}_t$ where $\bar{C}_t$ is the cumulated cost up to *t*
  - higher the increase in cumulated cost, lower is the reward → negative reward is a *«punishment»* (very large in case of infeasibility)

The impact of uncertainty

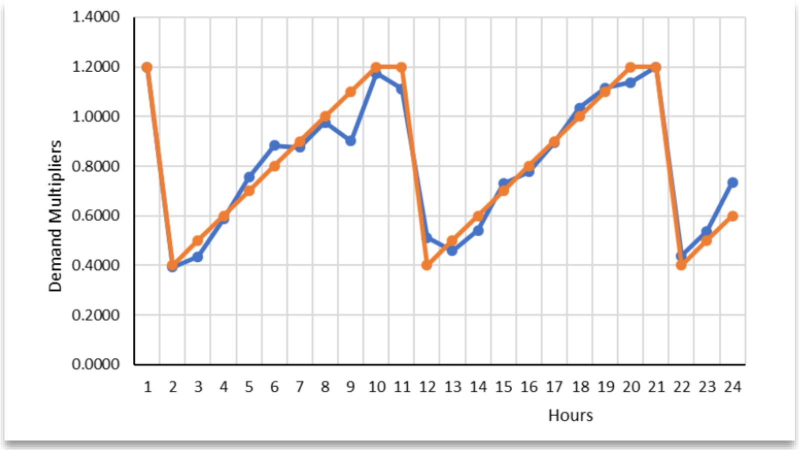
- Applying learned policy to three scenarios related to different modifications of the water demand



Scenario 1 – Actual vs forecasted demand (small variation)



Scenario 2 – Actual vs forecasted demand (larger variation)



Scenario 3 – Actual vs forecasted demand (entity of variationchanging from time step to time step)

The impact of uncertainty - Results

- Global optimum schedule remains feasible <u>only for the Scenario#1!!!</u>
- The learned policy was able to provide <u>a feasible schedule for each scenario</u> (even if sub-optimal)
- For the solutions obtained through ADP, the cost reduction with respect to the «naive» schedule (i.e. pumps always on) is reported

Demand variation	Cost Energy [$/day]	Max cost [$/day]	Cost reduction [$/day]
Scenario #1	1416.13	3925.52	2509.39 (63.92%)
Scenario #2	1414.75	3889.70	2474.95 (63.63%)
Scenario #3	1421.87	3959.58	2537.71 (64.09%)

Summarizing…

- Results proved that ADP/Reinforcement Learning (*Q*-learning):
  - can be used for **online-PSO**
  - is able to **learn** an optimal policy **by interacting** with the (pumping) system
  - is **«prediction free»**
  - is **robust** with respect to uncertainty (at least in terms of feasibility)

Water Management related projects and activities

ICeWater

SEVENTH FRAMEWORK PROGRAMME

ICT Solutions for Efficient Water Resources Management

Data4Water

Horizon 2020
European Union Funding
for Research & Innovation

CSA on smart, data driven e-services in water management

Seguici

RegioneLombardia

Smart tEcnologie per la Gestione delle risorse idriche ad Uso Irriguo e CIvile

PILGRIM

RegioneLombardia

Piattaforma ICT per la gestione della rete idrica Milanese

PerFORM WATER 2030

RegioneLombardia

An innovative project pathway for water utilities towards an integrated approach for water cycle management and its circular valorization

Thanks

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Extras: considerations on computational costs