MINLP applications, part II: Water Network Design and some applications of black-box optimization

Claudia D'Ambrosio

CNRS & LIX, École Polytechnique
dambrosio@lix.polytechnique.fr

5th Porto Meeting on MATHEMATICS for INDUSTRY, April 11, 2014

Water Distribution Network (WDN)

- **design**: choice of a diameter for each pipe, with other fixed design properties (e.g., the topology and pipe lengths). "Worse case" water demand.
- **operation**: decide how to distribute the water at each time period. For each time period, different water demand.

Introduction

Water Distribution Network (WDN) **optimal design**:
choice of a diameter for each pipe, with other fixed design properties (e.g., the topology and pipe lengths).

MINLP problem:

- discrete variables: set of commercially-available diameters;
- hydraulic constraints on water flows and pressures;
- minimize the cost (function of the selected diameters).

History of this Work

- 2002-2005: from Cristiana Bragalli's PhD thesis to my Master thesis, **linearization.**
- 2005-2012: **mixed integer nonlinear programming** techniques.
- 2013-????: understand why in this context MINLP approaches outperform the MILP ones while in the gas distribution context the linearization is an option.

Let's start with the detailed problem description...

Notation

Sets:

$\mathbf{E}$ = set of pipes;

$\mathbf{N}$ = set of junctions;

$\mathbf{S}$ = set of source junctions ($S \subset N$);

$\delta_+(\mathbf{i})$ = set of pipes with tail juction i ($i \in N$);

$\delta_-(\mathbf{i})$ = set of pipes with head juction i ($i \in N$).

Parameters for each pipe $e \in E$:

$\mathbf{len}(\mathbf{e})$ = length of pipe e;

$\mathbf{k}(\mathbf{e})$ = roughness coefficient of pipe e;

$\mathbf{d_{min}}(\mathbf{e}), \mathbf{d_{max}}(\mathbf{e})$ = min and max diam. of pipe e;

$\mathbf{v_{max}}(\mathbf{e})$ = max speed of water in pipe e;

$\mathfrak{D}(\mathbf{e}, \mathbf{r}), \mathfrak{C}(\mathbf{e}, \mathbf{r})$ = value and cost of the rth discrete diameter for pipe e ($r = 1, \ldots, r_e$).

Notation

Parameters for each junction $i \in N \setminus S$:

$\mathbf{dem(i)}$ = demand at junction i;

$\mathbf{elev(i)}$ = physical elevation of junction i;

$\mathbf{ph_{min}(i), ph_{max}(i)}$ = min and max pressure head at junction i.

Parameters for each source junction $i \in S$:

$\mathbf{h_s(i)}$ = fixed hydraulic head of source junction i;

Variables

$\mathbf{Q}(\mathbf{e})$ = flow in pipe e ($e \in E$);

$\mathbf{H}(\mathbf{i})$ = hydraulic head of junction i ($i \in N$);

$\mathbf{D}(\mathbf{e})$ = diameter of pipe e ($e \in E$).

$\mathbf{X}(\mathbf{e}, \mathbf{r})$ = 1 is r-th diameter is selected for pipe e,
0 otherwise ($e \in E$).

The simplified model

$$\min \sum_{e \in E} len(e) \sum_{r=1}^{r_e} \mathfrak{C}(e,r) \cdot X(e,r)$$

$$\sum_{e \in \delta_-(i)} Q(e) - \sum_{e \in \delta_+(i)} Q(e) = dem(i) \qquad (\forall\ i \in N \setminus S)$$

$$-v_{max}(e) \sum_{r=1}^{r_e} \frac{\pi}{4} \mathfrak{D}^2(e,r) X(e,r) \leq Q(e) \leq v_{max}(e) \sum_{r=1}^{r_e} \frac{\pi}{4} \mathfrak{D}^2(e,r) X(e,r) \qquad (\forall\ e \in E)$$

$$H(i) - H(j) = \frac{\mathrm{sgn}(Q(e))|Q(e)|^{1.852} \cdot 10.7 \cdot len(e)}{k(e)^{1.852} \cdot D(e)^{4.87}} \qquad (\forall\ e = (i,j) \in E)$$

$$D(e) = \sum_{r=1}^{r_e} \mathfrak{D}(e,r) X(e,r) \qquad (\forall e \in E)$$

$$\sum_{r=1}^{r_e} X(e,r) = 1 \qquad (\forall e \in E)$$

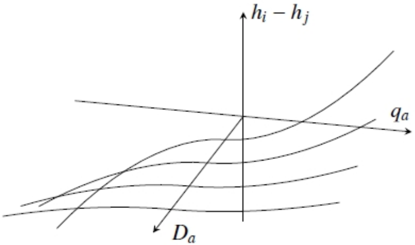
$$d_{min}(e) \leq D(e) \leq d_{max}(e) \qquad (\forall e \in E)$$

$$ph_{min}(i) + elev(i) \leq H(i) \leq ph_{max}(i) + elev(i) \qquad (\forall\ i \in N \setminus S)$$

$$H(i) = h_s(i) \qquad (\forall\ i \in S)$$

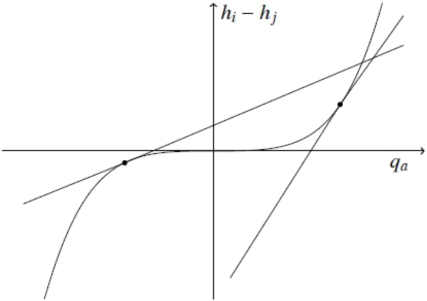
$$X(e,r) \in \{0,1\} \qquad (\forall e \in E, r \in \{1, \ldots, r_e\})$$

Hazen-Williams Equation



For each discrete diameter, a univariate nonlinear curve.

Hazen-Williams Equation

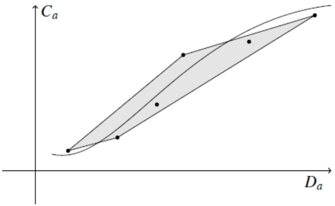


Outer approximation cannot work – feasible region cut!

Modeling Tricks

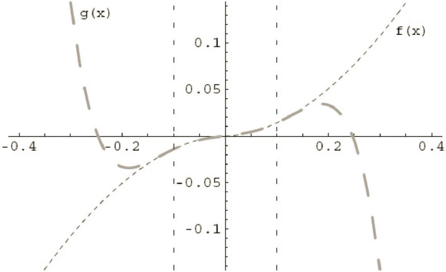
- Continuous objective function $C_e(D(e))$?
- Nondifferentiability! See $\text{sgn}(Q(e))|Q(e)|^{1.852}$
- Reformulate with $A(e)$ instead of $D(e)$!

Continuous objective function



Continuous fitted polynomial might give a better bound wrt the continuous relaxation of the discrete defined cost function.

Nondifferentiability



Algorithmic Tricks

Bonmin:

- Open-source code for solving general MINLP problems (`https://projects.coin-or.org/Bonmin`);
- Several algorithmic choices: a NLP-based Branch-and-Bound algorithm, an outer-approximation decomposition algorithm, a Quesada and Grossmann's Branch-and-Cut algorithm, and a hybrid outer-approximation based Branch-and-Cut algorithm;
- Exact for convex MINLPs;
- Heuristic for nonconvex MINLPs.

Algorithmic Tricks

Bonmin branch-and-bound algorithm: : solve NLP relaxation at each node of the search tree and branch on variables.
NLP solver used:
Ipopt (open-source `https://projects.coin-or.org/Ipopt`).
It founds a local optima: no valid bound for nonconvex MINLPs.

Different starting points for root/each node.
Still not a valid LB!

Fathom only if $z \leq \mathrm{LB} + \Delta z$ with $\Delta z < 0$, i.e., **continue branching** even if the solution value to the current node is worse than the best-known solution.
If $|\Delta z|$ is too big, few nodes are fathomed, extreme case: complete enumeration!

Algorithmic Tricks

Bonmin modifications:

I.1 Ad-hoc definition of the cutoff_decr option value (Δz).

I.2 Properly evaluating the objective value of integer feasible solutions through the definition of 2 objective functions: LB and UB objective function;

Computational results

Instances.

name	number of ...					unit
	junctions	reservoirs	pipes	duplicates	diameters	cost
shamir	7	1	8	–	14	$
hanoi	32	1	34	–	6	$
blacksburg	31	1	35	–	11	$
New York	20	1	21	21	12	$
foss_poly_0	37	1	58	–	7	lira
foss_iron	37	1	58	–	13	€
foss_poly_1	37	1	58	–	22	€
pescara	71	3	99	–	13	€
modena	272	4	317	–	13	€

Computational results

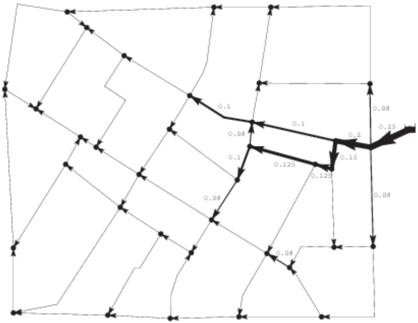
Characteristics of the 50 continuous solutions at the root node.

	mean	% dev. first	% dev. min	% dev. max	std dev	coeff var
shamir	401,889.00	-4.880	-4.880	59.707	37,854.70	0.0941920
hanoi	6,134,520.00	-0.335	-1.989	2.516	91,833.70	0.0149700
blacksburg	114,163.00	1.205	-0.653	2.377	861.92	0.0075499
New York	82,646,700.00	0.605	-47.928	31.301	16,682,600.00	0.2018540
foss_poly_0	68,601,200.00	-1.607	-1.748	15.794	2,973,570.00	0.0433457
foss_iron	182,695.00	-2.686	-2.686	61.359	16,933.80	0.0926891
foss_poly_1	32,195.40	26.186	-17.193	42.108	4,592.63	0.1426490
pescara	1,937,180.00	-6.311	-6.596	54.368	274,956.00	0.1419370
modena	2,559,350.00	-0.254	-0.396	9.191	38,505.80	0.0150452

Computational results for the MINLP model. Time limit 7200 seconds.

	$v_{disc}(\bar{x}^{best})$	time	% dev. $v_{disc}(\bar{x}^{first})$
shamir	419,000.00	1	0.000
hanoi	6,109,620.90	191	0.000
blacksburg	118,251.09	2,018	0.178
New York	39,307,799.72	5	0.000
foss_poly_0	70,680,507.90	41	0.000
foss_iron	178,494.14	464	0.000
foss_poly_1	29,117.04	2,589	0.119
pescara	1,820,263.72	2,084	0.724
modena	2,576,589.00	3,935	0.055

Practical use of MINLP solutions



Computing valid lower bounds with Baron

`Baron`: considered one of the best solver for global optimization.
It uses:

- under and over estimators to compute valid LB for nonconvex MINLPs;
- spatial Branch-and-Bound to improve estimation quality and enforce integrality.

It provides (possibly) the global solution of nonconvex MINLPs (a lower bound otherwise).
Used to measure the quality of the proposed solutions.

Computing valid lower bounds with Baron

Computational results for the MINLP model comparing `Baron` and `Bonmin`

	Baron				Bonmin
	UB (2h)	LB (2h)	UB (12h)	LB (12h)	% gap
shamir	419,000.00	419,000.00	419,000.00	419,000.00	0.00
hanoi	6,309,727.80	5,643,490.00	6,219,567.80	5,783,950.00	5.63
blacksburg	n.a.	55,791.90	n.a.	105,464.00	12.12
New York	43,821,000.00	29,174,000.00	43,821,000.00	29,174,000.00	34.74
foss_poly_0	n.a.	64,787,300.00	n.a.	64,787,300.00	9.10
foss_iron	n.a.	170,580.00	n.a.	170,580.00	4.64
foss_poly_1	n.a.	25,308.20	n.a.	25,308.20	15.05
pescara	n.a.	1,512,640.00	n.a.	1,512,640.00	20.34
modena	n.a.	2,073,050.00	n.a.	2,073,050.00	24.29

Literature comparison

- Dandy et al. (1996): genetic algorithm;
- Savic and Walters (1997): meta-heuristic approaches for the optimization, and they work with the constraints by numerical simulation;
- Cunha and Sousa (1999): similar to Savic and Walters.

	Savic and Walters (1997)		Savic and Walters (1997)		Cunha et Sousa (1999)	
	SW99 rel.	MINLP[a]	SW99 res.	MINLP[a]	CS99	MINLP[a]
hanoi	6.073 e+06	6.066 e+06	6.195 e+06	6.183 e+06	6.056 e+06	6.056 e+06

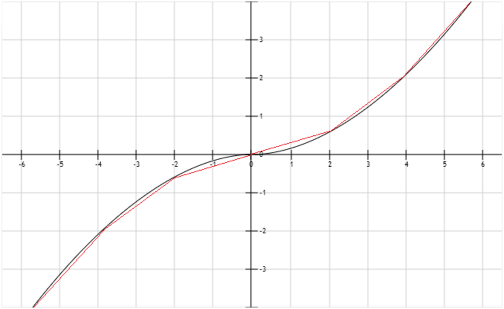
	Savic and Walters (1997)		Savic and Walters (1997)		Dandy et al. (1996)	
	SW99 rel.	MINLP[a]	SW99 res.	MINLP[a]	DSM96	MINLP[a]
New York	37.13 e+06	36.38 e+06	40.42 e+06	40.47 e+06	38.8 e+06	38.8 e+06

MILP approach

The nonlinear parts of the models: Hazen-Williams equations.

- Linearize the Hazen-Williams equations (for each Diameter $\rightarrow$ piecewise linear approximation of univariate functions).

Additional continuous and binary variables and additional constraints (proportional to the quality of the approximation).



MILP approach: results

`shamir`: the same solution found with the MINLP approach.
`hanoi`: a worse and slightly infeasible solution in 40 CPU minutes.
`blacksburg` and `New York`: a worse solution in 48 CPU hours!!!
Real-world instances: even worse results.

Feasibility test: on the rather small instance `hanoi` (32 junctions, 1 source, 34 pipes and 6 diameter types), the MILP solver fed with the optimal diameter choices needs 180 linearization points before certifying feasibility.

When all the diameters/areas have been selected, the objective function is a constant and we need **complete enumeration** to find the values of the other variables!

Collins et al. 1977; Raghunathan 2013 proved that original feasibility testing of a set of diameter sizes can be reformulated as a convex (continuous) optimization problem!

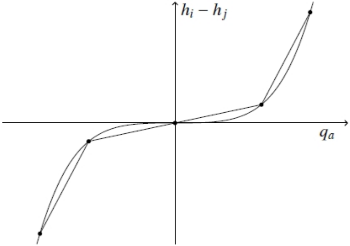
Gas Distribution Network and linearization

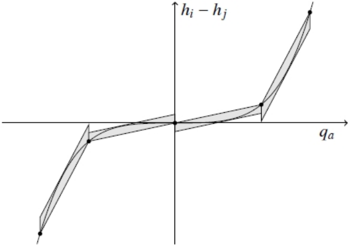
- Huge project on gas distribution network in Germany.
- Among all, the people from ZIB and the group of Alexander Martin (Erlangen) are involved.
- Different kind of piecewise linear approximation were employed successfully.

Actually Martin et al. also employed successfully piecewise linear approximation to water distribution network.

What's wrong with our piecewise linear approximation???

A possible improved piecewise linear approximation (relaxation)





Water Distribution Network: design vs. operation

WDN design:

$$H(i) - H(j) = \Psi(e,r)\frac{\mathrm{sgn}(Q(e))|Q(e)|^{1.852}}{D(e)^{4.87}}$$

WDN operation (with pumps):

$$H(i) - H(j) = \frac{\Psi(e,r)}{D(e)^{4.87}}\mathrm{sgn}(Q(e))|Q(e)|^{1.852} + \beta(e)y(e)$$

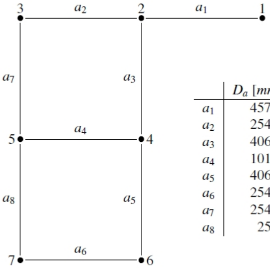
where $\beta(e)$ is the efficiency of a pump operating on pipe e and $y(e)$ is the variable associated with the decision of activating the pump or not.

$\beta(e)y(e)$ plays the role of “slack variable”.

- **Design**: if the diameters are fixed, a unique solution exists (if any).
- **Operation**: potentially multiple feasible solution (more expensive if the pump is used).

Water Distribution Network: design vs. operation

Shamir example:



	D_a [mm]
a_1	457.2
a_2	254.0
a_3	406.4
a_4	101.6
a_5	406.4
a_6	254.0
a_7	254.0
a_8	25.4

	$i = 1$	2	3	4	5	6	7
$\underline{h}_i$ [m]	210	180	190	185	180	195	190

Pumps are somehow able to compensate for the approximation error made by MILP approximations

$$H(i) - H(j) = \frac{\Psi(e,r)}{D(e)^{4.87}} \text{sgn}(Q(e))|Q(e)|^{1.852} + \beta(e)y(e)$$

Black-box Optimization

A.K.A.

What if we do not have an explicit form of
the involved functions, first, and second derivatives?

Smart buildings design

Decision variables

- Building orientation
- Material choice for different building layers
- Windows size

Objective

- minimize energy consumption to garantee a given temperature in each parts of the building within one year

Simulator: EnergyPlus

`http://apps1.eere.energy.gov/buildings/energyplus/`

Oil reservoir engineering

Decision variables

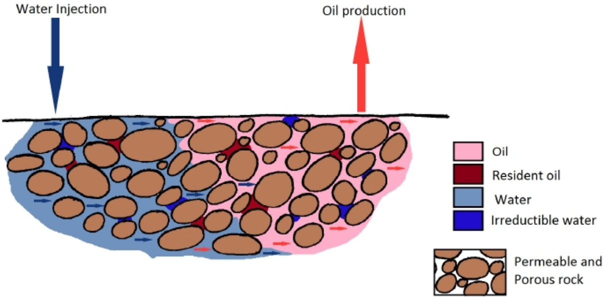
- Wells to construct
- Wells type (injector/producer)
- Wells coordinates

Objective

- maximize cumulative oil production or net present value

Open-source software: NOMAD
`http://www.gerad.ca/nomad/Project/Home.html`

Oil reservoir engineering



Black-box Optimization

- Direct/Pattern Search methods
- Trust Region methods
- Radial Basis Function methods
- Surrogate models

"Introduction to Derivative Free Optimization" by Andrew R. Conn, Katya Scheinberg, Luis N. Vicente