OPTIMIZING OVER NONLINEAR NETWORKS WITH DUALITY CUTS

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POTENTIAL-DRIVEN FLOW NETWORK

- transportation of a commodity on a digraph $G = (N, A)$
- flow q_a: measure of volume/rate on arcs (sign=direction)

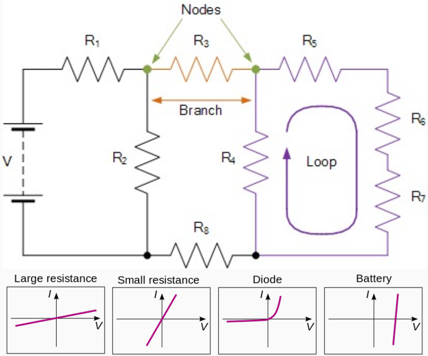
$$q_{n^+} = q_{n^-} \quad \text{(flow conservation at nodes)}$$

- potential h_n: measure of energy at nodes

$$\Delta h_a = \phi_a(q_a) \quad \text{(flow/potential equilibrium on arcs)}$$

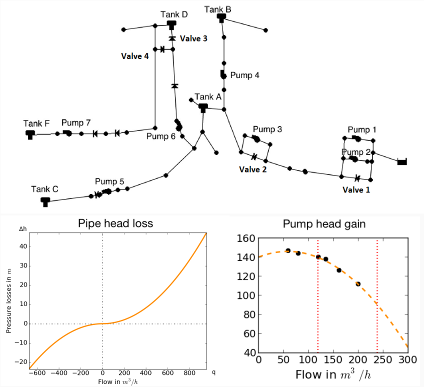
- model for many physical systems: electricity, water, gas, heat, telecommunications, transportation, vascular, elastic/spring

EX: ELECTRIC CIRCUIT



- connected conductors (resistors, batteries,...)
- current I: flow rate through conductors
- voltage V: potential difference at ends
- resistance V/I: constant (Ohm's law) or not
- Kirchhoff's current law (flow conservation)

EX: HYDRAULIC NETWORK



- pipes, pumps, valves
- water flow rate Q
- hydraulic head H: pressure + elevation
- resistance: friction (Darcy-Weisbach's law)
- demand satisfaction (flow conservation)

steady-state equilibrium

Given boundary conditions (some fixed flows or potentials), find all flows and potentials with:

- flow conservation at nodes
- flow/potential equilibrium on arcs

Different formulations for different boundary conditions.

EX: PIPE NETWORK ANALYSIS PROBLEM

- connected digraph $G = (N, A)$ with incidence matrix $I_{AN} \in \{0, 1, -1\}^{A \times N}$
- flow/potential drop relation ϕ_A on all arcs
- boundary conditions: nodes $N = J \cup R$ with either fixed demands d_J or fixed potentials h_R (reservoirs)

$$
\begin{aligned}
NAP(A, d_J, h_R) = \{(q_A, h_J) \in \mathbb{R}^A \times \mathbb{R}^J, & & & \text{(flows, potentials)} \\
q_j = d_j & \quad & \forall j \in J, & \quad \text{(flow conservation)} \\
h_a = \phi_a(q_a) & \quad & \forall a \in A\} & \quad \text{(resistance)}
\end{aligned}
$$

with $q_n = I_{An}^T q_A$ residual flow at node n and $h_a = -I_{aN} h_N$ potential drop along arc a.

THE LINEAR CASE

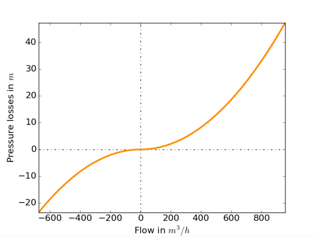
- $h_a = \phi_a(q_a) = r_a q_a$ for any arc a
- Ohm's law (electric), Fourier's law (thermal), Poiseulle's law (viscous fluids)
- well studied in the electric context (ohmic conductors): existence, unicity, reduction, optimal distribution/differential
- solution minimizes power dissipation:

$$D = \sum_A r_a q_a^2 = \sum_A h_a q_a.$$

THE NONLINEAR CASE: ASSUMPTIONS ON ϕ_A

resistance function ϕ_a *continuous* or smooth, *strictly increasing*, bijective on $\mathbb{R}$

- antiderivative $\Phi_a(q) = \int_0^q \phi_a(s)ds$
  $\Rightarrow$ smooth, strictly convex, coercive
- conductivity function ϕ_a^{-1}: $q_a = \phi_a^{-1}(h_a)$
  $\Rightarrow$ smooth, strictly increasing



Examples:

- friction in pipes $\phi_a(q) = sgn(q)\alpha_a|q|^d$ with $d = 2$ (water) or $d = 1.852$ (gas)
- discharge pressure in pumps $\phi_a(q) = \alpha_a q|q| + \beta_a q + \kappa_a$ with $\alpha_a > 0$

SMOOTH NONCONVEX EQUATION SYSTEM

- in many practical applications, the boundary conditions ensure the existence and unicity of the flow/potential equilibrium
  see e.g. [Rockafellar (1984) *Network Flows and Monotropic Optimization*]
- system $F(x) = 0$ can be solved with the Newton-Raphson algorithm.

ex: the pipe network analysis problem

if $G = (N, A)$ weakly connected, $R \neq \varnothing$, ϕ_a smooth strictly increasing then

$$NAP(A, d_J, h_R) = \{(q_A, h_J) \mid q_J = d_J, h_A = \phi_A(q_A)\}$$

with $\phi_A(q_A) = (\phi_a(q_a))_{a \in A}$ has a unique solution.

Application of the Newton-Raphson algorithm proposed in [Todini&Pilati 1988] implemented in the EPANET simulator

CONVEX OPTIMIZATION REFORMULATION

primal minimization problem:

$(q_A, h_J) \in NAP(A, d_J, h_R)$ for some h_J if and only if q_A solves

$$P(A, q_J, h_R) : \min_{q_A}\{f(q_A) = \Phi_A(q_A) + h_R q_R \mid q_J = d_J\}$$

with $\Phi_A(q_A) = \sum_{a \in A} \Phi_a(q_a)$.

- Lagrangian multiplier theorem holds on P by convexity of Φ_a:

$$L(q_A, h_J) = \Phi_A(q_A) + h_R q_R + h_J(q_J - d_J) \text{ given multipliers } h_J$$

$$\text{NAP is KKT:} \begin{cases} h_A = \phi_A(q_A) & (\frac{\partial L}{\partial q_A} = 0 \text{ 1st-order condition}) \\ q_J = d_J & (\frac{\partial L}{\partial h_J} = 0 \text{ primal feasibility}) \end{cases}$$

- solution is unique by strict convexity of Φ_a.

strong duality holds:

$(q_A, h_J) \in NAP(A, d_J, h_R)$

- if and only if q_A solves

$$P(A, q_J, h_R) : \min_{q_A}\{f(q_A) = \Phi_A(q_A) + h_R q_R \mid q_J = d_J\}$$

- if and only if

$$\begin{cases} f(q_A) \leq L(h_J) = \min\limits_{q_A} \{L(q_A, h_J) = f(q_A) + h_J(q_J - d_J)\} & \text{(strong duality)} \\ q_J = d_J & \text{(primal feasibility)} \end{cases}$$

as f convex and $q_J = d_J$ linear: (q_A, h_J) is a saddle point of L

$$\begin{aligned} L(q_A, h_J) &= \Phi_A(q_A) + h_R q_R + h_J(q_J - d_J) \\ &= \Phi_A(q_A) - h_A q_A - h_J d_J. \end{aligned}$$

$q_a \mapsto \Phi_a(q_a) - h_a q_a$ is convex and reaches its minimum at $q_a = \phi_a^{-1}(h_a)$, then:

analytical formulation and decomposition:

$$L(h_J) = \min_{q_A} L(q_A, h_J) = \sum_{a \in A} L_a(h_a) - h_J d_J$$

with $L_a(h_a) = \Phi_a(\phi_a^{-1}(h_a)) - h_a \phi_a^{-1}(h_a)$ concave.

CONVEX REFORMULATION

$NAP(A, d_J, h_R)$ is equivalent to:

$$
\begin{aligned}
CNAP(A, d_J, h_R) = \{(q_A, h_J) \in \mathbb{R}^A \times \mathbb{R}^J \\
&\sum_{a \in A} g_a(q_a, h_a) + h_N q_N \leq 0 \qquad \text{(strong duality } f(q_A) \leq L(h_J)\text{)} \\
&q_J = d_J\}.
\end{aligned}
$$

with $g_a(q_a, h_a) = \Phi_a(q_a) - L_a(h_a) = \Phi_a(q_a) - \Phi_a(\phi_a^{-1}(h_a)) + h_a \phi_a^{-1}(h_a)$ convex.

- aggregated form of $h_a = \phi_a(q_a)\ \forall\, a \in A$
- if ϕ_a is quadratic then g_a is cubic
- convex if (A, d_J, h_R) are fixed

- network design: select the arc characteristics to satisfy a fixed demand and minimize installation costs
- network operation: operate dynamically the controllable arcs to satisfy a varying demand and minimize operation costs

nonconvex (MI)NLPs with a bilevel structure:

1. select one (or a sequence) topology A and boundary conditions (d_J, h_R)
2. check existence of an equilibrium $(q_A, h_J) \in NAP(A, d_J, h_R)$

SOLUTION METHODS

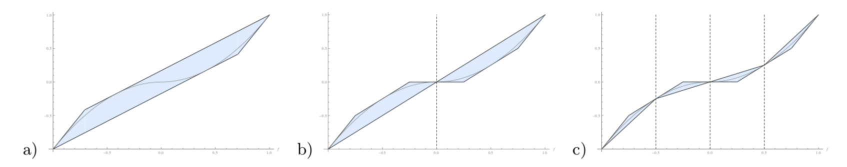
bilevel structure

1/ select (A, d_J, h_R) 2/ check $NAP(A, d_J, h_R)$

- one monolithic approximated model (e.g. piecewise-linear)
- two independent blocks: black-box optimization (e.g metaheuristics + simulation)
- in-between: the outer block includes a static or dynamic relaxation of the inner block (Bender's decomposition, bundle method, LP-NLP branch and bound,...)

tractable relaxations of $h_a = \phi_a(q_a)$:

- convex/polyhedral outer-approximation
- pwl under- and over-estimators



[Fügenschuh 2013]

computed statically in a preprocessing step
or refined dynamically at trial points (OA cuts, spatial b&b separation,...)

add a relaxation of $CNAP$ in the outer block:

aggregated valid inequality

$$\sum_{a \in A} g_a(q_a, h_a) + h_N q_N \leq 0$$

with $g_a(q_a, h_a) = \Phi_a(q_a) - \Phi_a(\phi_a^{-1}(h_a)) + h_a \phi_a^{-1}(h_a)$ convex when (A, h_R) given.

EX 1: PIPE SIZING

- every node has a fixed demand d_J or a fixed head h_R (sources)
- arcs are pipes to select in a discrete set K:

$$x_{ak} \in \{0,1\} \text{ select pipe of type } k \text{ on arc } a \in A?$$

- model on graph $G = (N, A^K)$ with replicated arcs:

$$\min \sum_a \sum_k c_k x_{ak}$$

$$s.t. (q_A, h_J) \in NAP(A^K x_K, d_J, h_R)$$

$$x_{ak} = 0 \implies q_{ak} = h_{ak} = 0 \qquad \forall a \in A, k \in K$$

$$\sum_{k \in K} x_{ak} = 1 \qquad \forall a \in A.$$

EX 1: PIPE SIZING (CONT.)

$$\min \sum_a \sum_k c_k x_{ak}$$

$$s.t. (q_A, h_J) \in NAP(A^K x_K, d_J, h_R)$$

$$x_{ak} = 0 \implies q_{ak} = h_{ak} = 0 \qquad \forall a \in A, k \in K$$

$$\sum_{k \in K} x_{ak} = 1 \qquad \forall a \in A.$$

strong duality constraint is convex [Tassef 2021]

$$\sum_{a \in A} \sum_{k \in K} g_{ak}(q_{ak}, h_{ak}) + h_N q_N \leq 0$$

EX 2: PUMP SCHEDULING

- controllable arcs (pumps, valves) are switch on/off on a discrete horizon T:

$$x_{at} \in \{0,1\} \text{ active arc } a \in A \text{ on time } t \in T?$$

- fixed demand d_{JT} known for all time steps
- fixed head h_{R0} (tank level) known only at time 0
- head h_{Rt} bounded and depends (linearly) on flow $q_{R(t-1)}$
- a sequence-dependent sequence of NAPs:

$$\min \sum_a \sum_t c^0_{at} x_{at} + c^1_{at} q_{at}$$

$$\begin{aligned}
s.t. (q_{At}, h_{Jt}) &\in NAP(Ax_t, d_{Jt}, h_{Rt}) && \forall t \in T \\
x_{at} = 0 &\implies q_{at} = 0 && \forall a \in A, t \in T \\
h_{R(t+1)} &= h_{Rt} + s_R q_{Rt} && \forall t \in T \\
\underline{H}_R \leq h_{Rt} &\leq \overline{H}_R && \forall t \in T.
\end{aligned}$$

$$\min \sum_a \sum_t c^0_{at} x_{at} + c^1_{at} q_{at}$$

$$s.t. (q_{At}, h_{Jt}) \in NAP(Ax_t, d_{Jt}, h_{Rt}) \qquad \forall t \in T$$

$$x_{at} = 0 \implies q_{at} = 0 \qquad \forall a \in A, t \in T$$

$$h_{R(t+1)} = h_{Rt} + s_R q_{Rt} \qquad \forall t \in T$$

$$\underline{H}_R \leq h_{Rt} \leq \overline{H}_R \qquad \forall t \in T.$$

strong duality constraints are not convex

$$\sum_{a \in A} g_a(q_{at}, h_{at}) x_{at} + h_{Jt} d_{Jt} + h_{Rt} q_{Rt} \leq 0, \quad \forall t \in T$$

EX 2: PUMP SCHEDULING (CONT.)

strong duality constraints are not convex

$$\sum_{a \in A} g_a(q_{at}, h_{at}) x_{at} + h_{Jt} d_{Jt} + h_{Rt} q_{Rt} \leq 0, \quad \forall t \in T$$

- bad news: a loose relaxation of the bilinear term may *absorb* the duality gap
- good news: tank capacities are exogenous bounds on h_{Rt} and q_{Rt} to tighten McCormick's relaxation

The strong duality constraint

$$\sum_{a \in A} g_a(q_{at}, h_{at})x_{at} + h_{Jt}d_{Jt} + h_{Rt}q_{Rt} \leq 0, \quad \forall t \in T$$

Linearize g_a at some feasible points $(q_a^*, \phi_a(q_a)^*)$ and take the McCormick's envelope for the bilinear terms $h_{rt}q_{rt}$, $r \in T$:

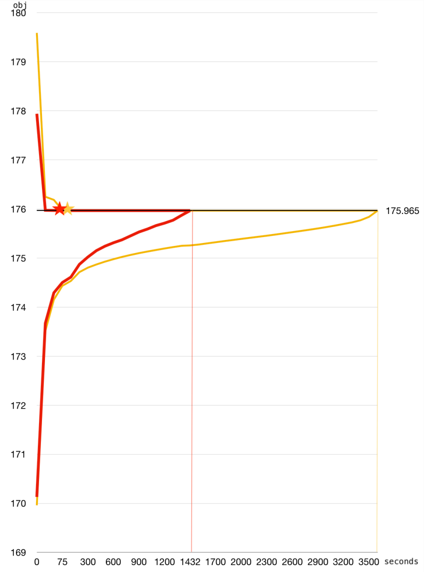
$$\begin{aligned}
&\sum_{a \in A} g_{at} + h'_{Rt} + h_{Jt}d_{Jt} \leq 0 && \forall t \in T \\
&x_{at} = 0 \implies q_{at} = h_{at} = 0 && \forall a \in A \\
&g_{at} \geq \phi_a(q_a^*)(q_{at} - q_a^* x_{at}) + q_a^* h_{at} && \forall t \in T, \forall a \in A, q_a^* \in \mathcal{Q}_a \\
&h'_{rt} \in MC_{[\underline{H}_r, \overline{H}_r]}(h_{rt}q_{rt}) && \forall t \in T, \forall r \in R.
\end{aligned}$$

COMPUTATION

with or without duality constraints

impact on the primal/dual bounds in a LP-NLP BB [Bonvin, Demassey, Lodi 2020]

generated at preprocessing:
5 linearization/pipes and 10/pumps



REFERENCES

- our papers on the pump scheduling problem are available on `https://sofdem.github.io/`
- code (partially) available on: `https://github.com/sofdem/gopslpnlpbb`