Bilevel Optimization in Infrastructure Planning (energy, water, environment, transportation)

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Outline

- Overivew
 - The Role of Optimization and Data Analytics for Improving Social Welfare
 - Bilevel Optimization/Mathematical Programs with Equilibrium Constraints (MPECS) for Improved Infrastructure Management (focus on energy, transport, water, the environment)
 - Optimization and Equilibrium Problem (complementarity problems short review)
- **③** "Bottom Level" Infrastructure Market Examples (deterministic/stochastic)
 - \bullet #1, Water markets for Water Quantity, Water Quality Improvement
 - #2, Nutrient Credit Exchange
 - 3 #3, Carbon Allowance Markets
 - #4, Flow-Based Transportation Pricing
- Bilevel Optimization-Focus on Energy
 - Selected Examples of Bilevel Optimization in Energy
 - ★ Energy Conservation
 - Wastewater-to-Energy
 - ★ Optimal Grid Tariffs



Detailed Power Generation/Transmission Infrastructure Investment Example

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- Overview of Optimization and Equilibrium Problems
- Complementarity Problems Short Review, Relation to Game Theory & Optimization Problems
- "Bottom Level" Examples
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Optimization and Data Analytics for Improving Social Welfare

- Use technology, management and economics to improve social welfare and achieve societal sustainability goals
- One key area to concentrate on is infrastructure, e.g., energy, transportation, water, the environment
- By improving these key areas, society as a whole, as well as individuals will see an improved quality of life
- If we consider just energy as an example (but also true of other areas of infrastructure), no "silver bullet" here, society will need a portfolio of options for
 - supply/demand (e.g., renewable but intermittent supply, demand response)
 - transmission/distribution
 - regulatory/policy incentives

to achieve the above goals

• Will need a combination of new technologies as well as market

equilibrium-based and optimization-based models to maximize benefits given limited resources and competing goals (i.e., multiobjectve, user vs. system equilibria)

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$"\,30,000\mbox{-foot"}\,/$ $"\,10,000\mbox{-meter"}$ Perspective: Modeling and Analysis of Data-Driven Systems with Autonomous Agents





Referenc

Bilevel Optimization Problem (or Mathematical Program with Equilibrium Constraints) [Gabriel et al., 2013]



 Ω set of constraints for (x, y)

 $x \in \mathbb{R}^{n_x}$ upper-level variables

 $y \in R^{n_y}$ lower-level variables

f(x,y) upper-level objective function

S(x) solution set of lower-level problem (opt. or game)





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Bilevel Optimization/MPEC Structure Example: River Systems





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Overview of Optimization Problems

The Big Picture



KEY LP=linear program ILP=integer linear program QP=quadratic program



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Reference:

Complementarity Problems, Mixed Complementarity Problems (MCP) [Gabriel et al., 2013]

(Mixed) Nonlinear Complementarity Problem MNCP Having a function $F: \mathbb{R}^n \to \mathbb{R}^n$, find an $x \in \mathbb{R}^{n_1}$, $y \in \mathbb{R}^{n_2}$ such that $F_i(x, y) \ge 0, x_i \ge 0, F_i(x, y) * x_i = 0$ for $i = 1, ..., n_1$ $F_i(x, y) = 0, y_i$ free, for $i = n_1 + 1, ..., n_i$ Example $F(x_1, x_2, y_1) = \begin{pmatrix} F_1(x_1, x_2, y_1) \\ F_2(x_1, x_2, y_1) \\ F_3(x_1, x_2, y_1) \end{pmatrix} = \begin{pmatrix} x_1 + x_2 \\ x_1 - y_1 \\ x_1 + x_2 + y_1 - 2 \end{pmatrix}$ so we want to find x_1, x_2, y_1 s.t. $x_1 + x_2 \ge 0$ $x_1 \ge 0$ $(x_1 + x_2)^* x_1 = 0$ $x_1 - y_1 \ge 0$ $x_2 \ge 0$ $(x_1 - y_1)^* x_2 = 0$ $x_1 + x_2 + y_1 - 2 = 0$ y_1 free



If all functions (linear) affine, we get the linear complementarity problem (LCP)

One solution: $(x_1, x_2, y_1) = (0, 2, 0)$, why? Any others?

Sources for Complementarity Problems: Linear Programming

Consider a (primal) linear program in the variables $x \in \mathbb{R}^n$:

$$\begin{array}{ll} \min_{x} & c^{T}x & (1a) \\ s.t. & Ax \ge b & (y) & (1b) \\ & x \ge 0 & (1c) \end{array}$$

and corresponding dual linear program in the variables $y \in {\mathbb R}^m$

$$\begin{array}{ll} max_y & b^T y & (2a) \\ s.t. & A^T y \leq c & (x) & (2b) \\ & y \geq 0 & (2c) \end{array}$$

and complementary slackness for both primal and dual problems:



$$(Ax - b)^T y = 0, (c - A^T y)^T x = 0$$

Reference

Sources for Complementarity Problems: LP Primal and Dual Feasibility, Complementary Slackness

We can rewrite things a bit to get the following equivalent form. Find $x \in R^n, y \in R^m$ such that:

$$0 \le c - A^T y \perp x \ge 0$$

$$0 \le Ax - b \perp y \ge 0$$
(4a)
(4b)

This is exactly the (monotone) linear complementarity problem (LCP) in nonnegative variables (x, y) and is exactly the KKT optimality conditions as applied to the primal LP. Here

$$F(x,y) = \begin{pmatrix} F_x(x,y) \\ F_y(x,y) \end{pmatrix} = \begin{pmatrix} c - A^T y \\ Ax - b \end{pmatrix} \text{ or }$$
(5)

 $F(x,y) = \begin{pmatrix} c \\ -b \end{pmatrix} + \begin{pmatrix} 0 & -A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$

(6)

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Reference

Sources for Complementarity Problems: KKT Optimality Conditions for Nonlinear Programs

Consider a nonlinear program of the following form where $f: R^n \to R, g_i: R^n \to R, i = 1, ..., m, h_j: R^n \to R, j = 1, ..., p$:

$$min_x \quad f(x)$$
 (7a)

s.t.
$$g_i(x) \le 0$$
 $i = 1, ..., m$ (λ_i) (7b)

$$h_j(x) = 0$$
 $j = 1, ..., p$ (γ_j) (7c)

The KKT conditions are to find primal variables $x \in R^n$ and Lagrange multipliers $\lambda \in R^m_+$, $\gamma \in R^p$ such that:

$$0 = \nabla f(x) + \sum_{i} \nabla g_{i}(x)\lambda_{i} + \sum_{j} \nabla h_{j}(x)\gamma_{j}, x \text{ free}$$

$$0 \leq -g(x) \perp \lambda \geq 0$$

$$0 = h(x), \quad \gamma \text{ free}$$
(8c)
(8c)
(8c)



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References

Selected Sources for Complementarity Problems: KKT Optimality Conditions for Nonlinear Programs

Putting all these conditions together, we get a mixed complementarity problem of the following form. Find vectors $\lambda \in R^m_+$, $x \in R^n$, $\gamma \in R^p$ such that:

$$F(x,\lambda,\gamma) = \begin{pmatrix} \nabla f(x) + \sum_{i} \nabla g_{i}(x)\lambda_{i} + \sum_{j} \nabla h_{j}(x)\gamma_{j} \\ -g(x) \\ h(x) \end{pmatrix}$$

with

$$\begin{array}{lll} 0 = F_x(x,\lambda,\gamma) & x \mbox{ free } & (9a) \\ 0 \leq F_\lambda(x,\lambda,\gamma) & \perp \lambda \geq 0 & (9b) \\ 0 = F_\gamma(x,\lambda,\gamma) & \gamma \mbox{ free } & (9c) \end{array}$$



 \Rightarrow Connection to game theory problems

Reference

Overview of Equilibrium Problems: Generalizing Certain Optimization and Game Theory Problems [Gabriel et al., 2013]





KKT=Karush-Kuhn-Tucker optimality conditions.

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Classical Examples of the "Bottom Level" of the Bilevel/MPEC Approach

- Wardrop Traffic Equilibrium Problem
 - originally from [Wardrop, 1952]
 - additive path costs
 - nonadditive path costs
- Spatial Price Equilibrium Problem
 - classical approach using linear programming from [Samuelson, 1952] then [Takayama and Judge, 1964]
 - discretely constrained equilibrium extension



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Wardrop Traffic Equilibrium [Wardrop, 1952]



A->B, 38.5 miles 62 kilometers About 53 minutes travel time Which route

to take for commuting?

Black, red, blue?

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Wardrop Traffic Equilibrium Principle

- Original formulation [Wardrop Equilibrium,1952] and then [Aashtiani and Magnanti, 1981]
- "At equilibrium, for each origin-destination pair the travel times on all routes serving the same OD pair, actually used are equal, and less than then travel times on all nonused routes."
- Wardrop user equilibrium principle: users will choose the minimum cost path between each OD pair resulting in paths with positive flow all having equal costs, paths with costs higher than the minimum will have no flow.
- Can express this traffic equilibrium problem in some cases in terms of arc flows f as opposed to path flows F.

$$\begin{split} (C_p(F)-u_i)F_p &= 0, \forall p \in P_i, i \in I\\ C_p(F)-u_i \geq 0, \forall p \in P_i, i \in I\\ \sum_{p \in P_i}F_p - D_i(u) &= 0, \forall i \in I\\ F_p \geq 0, \forall p \in P \end{split}$$



 $u_i \geq 0, \forall i \in I$

Reference O

Nonadditive Traffic Equilibrium Problem [Gabriel & Bernstein, 1997]

- Can extend the basic Wardrop traffic equilibrium problem to include non-additive path costs.
- In this case, the path flows are needed but you can avoid enumerating all the paths via an algorithm.
- The algorithm brings in paths only when an improvement towards finding an equilibrium can be detected by solving a related shortest-path problem.
- Some examples of nonadditive path costs:
 - Nonlinear value of time
 - Nonadditive tolls and fares
 - Pricing emissions fees
 - Congestion pricing



Reference O

Nonadditive Traffic Equilibrium Problem [Gabriel & Bernstein, 1997]

- An example of a nonadditive path costs function
- Indices: *a*-arc, *p*-path
- Flows: F-path flow, f-arc flow
- : Costs/time:
 - $t_a(f)$: time to traverse arc a
 - η_1 : time-based operating costs (e.g., gasoline consumption)
 - λ_a: arc-specific cost
 - $g_p(\cdot)$: function converting time to money

$$C_p(F) = \sum_{a \in A} \delta_{ap}(\lambda_a + \eta_1 t_a(f)) + g_p(\sum_{a \in A} \delta_{ap} t_a(f))$$



Spatial Price Equilibrium Problem in Power Markets

- Consider the problem of an independent system operator (ISO) that is trying to efficiently run a power network composed of of power generation nodes (S_1, S_2) and demand nodes (D_1, D_2, D_3)
- Cost minimization ("Transportation Problem") with the ISO's decisions x_{ij} the (primal) flow variables, ψ_i , θ_j the dual variables (Lagrange multipliers) at respectively, supply node i and demand node j, not so realistic since ψ_i and θ_j should be elastic not fixed





Spatial Price Equilibrium Model: Transportation Problem

$$\min_{x_{ij}} \sum_{i} \sum_{j} c_{ij} x_{ij}$$
(10a)
s.t. $\sum x_{ij} \le supply_i$ $(\psi_i), \forall i$ (10b)

$$\sum_{i}^{j} x_{ij} \ge demand_{j} \qquad \qquad (\theta_{j}), \quad \forall j \qquad (10c)$$

$$x_{ij} \ge 0 \qquad \qquad \forall i,j \qquad (10d)$$





Transportation Problem Formulation, Karush-Kuhn-Tucker Optimality Conditions

$$egin{aligned} 0 &\leq \psi_i + c_{ij} & - heta_j ot x_{ij} \geq 0, orall i, j \ 0 &\leq supply_i - \sum_j x_{ij} ot \psi_i \geq 0, orall i \ 0 &\leq \sum_i x_{ij} - demand_j ot heta_j \geq 0, orall j \ w_i & ot heta_j \geq 0, orall j \ \psi_i & ot heta_j \ \psi_i & ot heta_j \ \psi_j \end{aligned}$$



Spatial Price Equilibrium Problem in Power Markets

- x_{ij} := flow from supply i to demand j, $S_i := \sum_j x_{ij}, D_j := \sum_i x_{ij}$
- $\psi_i(S_i) :=$ inverse supply function
- $\theta_j(D_j)$:= inverse demand function
- c_{ij} := marginal transport cost

Overall MCP in terms of (nonnegative) flows x_{ij} is thus:

$$0 \le \psi_i \left(\sum_j x_{ij}\right) + c_{ij} - \theta_j \left(\sum_i x_{ij}\right) \perp x_{ij} \ge 0$$
(11)

• $x_{ij} > 0 \Rightarrow \psi_i \left(\sum_j x_{ij} \right) + c_{ij} = \theta_j \left(\sum_i x_{ij} \right)$ or marginal cost = marginal benefit

 $\psi_i\left(\sum_j x_{ij}\right) + c_{ij} - \theta_j\left(\sum_i x_{ij}\right) > 0 \Rightarrow x_{ij} = 0 \text{ or no flow when marginal or solution of the second s$

SPE Example with If-Then Logic, 4 Supply Nodes, 5 Demand Nodes [Gabriel, 2017]

- Consider a solution of the SPE with numbers on arcs referring to an equilibrium flow (color-coded by supply node).
- **Problem: Supply node 4 is inactive!** This might be costly to keep running.
- Want to keep the equilibrium notion but reroute flows somehow? How to do this?



SPE Example with 4 Supply Nodes, 5 Demand Nodes, Equity-Enforcing Constraints [Gabriel, 2017]

- If $\sum_{j} x_{ij} < \delta_i$ then $\sum_{j} x_{ij} \ge 0.25 \sum_{i} \sum_{j} x_{ij}$, re-routing equilibrium flows.
- With δ_i a minimum flow threshold (contractual?) and 0.25 the minimum guaranteed flow % (of total flows) for supply node *i*.
- See the new solution below with $\delta_i = 3, \forall i$. Want to generalize this MCP example, this leads to the DC-MCP which can be formulated as a mixed-integer, nonlinear program (MINLP).





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References

Some Motivation for Studying the Class of Discretely Constrained Equilibrium Problems

- These problems can apply integer/binary restrictions to equilibrium problems for more realism, richer applications (e.g., game theory plus go-no go decisions, if-then thresholds)
 - Allowing for autonomy in infrastructure networks/supply chains (e.g., energy) that need some additional logic constraints and/or distributional or other equity enforcement (e.g., discrete design variables), or multi-sector coupling (combined with logic variables)
 - Allowing for mixed equilibrium systems that involve volumes as well as discrete units (e.g., road traffic volume but accounting for a discrete number of emergency vehicles)
 - Equilibrium problems combined with combinatorial optimization
 - Relaxation of multi-agent, non-cooperative markets with discrete restrictions (e.g., unit commitment in power), for example [Weinhold & Gabriel, 2020]



Several Ways to Get DC-MCP

• Case 1:

- Having a mixed complementarity problem, there are additional discrete (usually binary) constraints imposed.
- See the first example for the spatial price equilibrium problem.
- Case 2:
 - There are multiple discretely constrained/binary-constrained problems which are relaxed, then KKT conditions used for these problems forming an MCP and the discrete/binary conditions imposed after this.
 - This does not always give an equilibrium that is discretely constrained, may need some sort of "extra payment" to the players to induce them towards an equilibrium [Weinhold & Gabriel, 2020]
 - See the second example for relaxed unit commitment.



Case 2 Example: Relaxed Unit-Commitment Problem [Weinhold & Gabriel, 2020]

- Try to select for each player p and their generating unit u, the best quantity of power generation $Q_{p,u}$ to maximize their profit
- Problem is that the variable $ON_{p,u}$ is binary so that this is a binary-constrained optimization problem, KKT conditions are not valid.
- Can relax $ON_{p,u} \in [0,1]$, gather all players' KKT conditions plus any market-clearing, then impose the binary conditions "after the fact".
- Will this work? Not always. See [Weinhold & Gabriel, 2020] for a two-level approach to make this work. Need extra payments to induce the players to a market equilibrium.



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2 "Bottom Level" Examples

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What is Being Modeled: Balancing Water Markets, Spatial and/or Temporal Positional Advantages

- Consider a river network with n users (nodes), $I = \{1, \ldots, n\}$
- Let D_i represent the nodes downstream of node i, U_i represent the nodes upstream of node *i*
- For all nodes in D_i , would they be willing to pay upstream nodes $i, i - 1, \ldots, 1$ something to:
 - Increase volume of water? Demand and supply for water can be stochastic.
 - Decrease volume of pollutants? Fate and transport of pollutants can be seemingly stochastic in nature.

so, how to compute payments? ill everyone do better with these water markets? Gabriel (UMD/NTNU)



Water Flow in a River-Water Quantity Example [Boyd et al., 2022]

- Generically, each node (player) withdraws/discharges water from the river
- Each player can also add their own supply
- There is an opportunity though to be more efficient by reducing consumptive losses
- Overall, each node solves an optimization problem related to maximizing benefits less costs with possible participation in consumptive loss-reduction markets





Land Use Heterogeneity-Water Quality Example [Boyd et al., 2023]

- Loading heterogeneity in the watershed
- Water runoff and pollutants could vary according to: land use, soil properties, vegegation
- Comparative advantages amount the various players in different regions of the watershed





Shultz et al. (2007)

Infrastructure Markets: Incentivizing Water Market Participation

- What we propose for water markets is voluntary participation in the consumptive-loss reduction markets- water quantity (see Boyd et al., 2022)) or pollution-reduction credits (see Boyd et al., 2023))
- This means, "downstream" river users pay "upstream" ones to improves the efficiency of water lost so more water makes it downstream (water quanity) or a similar sort of payment but to reduce pollutants upstream (e.g., sediment deposition, probabilistic processes) for overall river benefit (e.g., better flood control), TMDL chance constraints (reliability)
- Each river node will be modeled as solving a particular optimization problem, the concatenation of the resulting Karush-Kuhn-Tucker (KKT) optimality conditions plus system or market-clearing conditions gives rise to a mixed complementarity problem (MCP)
- A solution is flows and prices in the various river nodal markets (and other items)



This problem then is the "bottom level" of the two-level perspective presented earlier

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Virginia Nutrient Credit Exchange Association

- There are other markets similar to water with success stories
- Consider the Virginia Nutrient Credit Exchange Association
 - Established in 2005 to reduce nitrogen and phosphorus discharges to the Chesapeake Bay
 - Voluntary collective of owners of 105 wastewater treatment plants (WWTPs)
 - Pollution reduction goals exceeded by over 2,000% for nitrogen and 450% for phosphorus in 2011
 - Smaller WWTPs compensated larger facilities to upgrade on their behalf
 - Pollution levels can be stochastic based on many factors





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Carbon Allowance Markets: Regional Greenhouse Gas Initiative, https://www.rggi.org/

- Regional Greenhouse Gas Initiative (RGGI)
- RGGI is a cooperative, market-based effort among 11 U.S.
 states with a population of about 60 million to cap and reduce CO2 emissions from the power sector
- As of June 2022, RGGI states raised over \$5 billion in carbon allowance auctions for supporting communities for local energy, health and environmental goals

Carbon prices depending on tochastic supply/demand of memitted carbon are uncertain



https://www.nrdc.org/resources/regional-greenhouse-gas-initiative-model-nation



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Transportation: Flow-Based Pricing Outside Washington, DC

- Intercounty Connector (ICC), a way to avoid the Washington Beltway, save time
- To use the ICC, you need a transponder in your car, from which flow-based prices are charged
- The payment puts a value on free flow of travel
- There is no obligation to use the ICC, drivers can just use regular (non-tolled) roads and avoid fees Stochastic demand for the ICC?





- Clearly these infrastructure markets can work, the problem is how to incentivize everyone to participate
- Should there be some minimum participation required?
- Should there be legal mandates?
- How to handle the **uncertainty** in the markets/lower-level equilibrium problem?
- Should participation be voluntary based on some social improvement?
- In the a river system context
 - The work by Allen et al. (2022), determines appropriate taxes to "nudge" the user equilibrium (i.e., MCP) towards a social best using inverse optimization and LCP theory
 - The work by Boyd et al. (2023) analyzes water quality issues for the Anacostia River (Washington, DC) using a stochastic LCP formulation involving TMDLs (total maximum daily loadings) for pollutants





Bilevel Optimization in Energy: Cutting Across Sustainable Energy Technologies, Markets, and Policy

| Top Level | Design decisions (e.g., what materials, size of CCS plants) Dominant firm generation decisions Government policy decisions Investment decisions for technologies | | |
|-----------------|--|--|--|
| Bottom Level | Operational decisions (e.g., how to operate the technologies, the CCS plants) Rest of the market (competitive fringe, ISO) generation and endogenous market prices Market responses to policy Market responses to investments | | |



 $\label{eq:CCS} CCS{=} Carbon, \ capture, \ and \ sequestration.$

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Bilevel Optimization: Energy Conservation Example [B. R. Champion and S.A. Gabriel, 2015]



- Energy Conservation Programs
- Two-level optimization model to better manage energy conservation programs for agencies, schools
- More efficient decision-making for internal/outsourced energy project retrofits



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Bilevel Optimization: Stochastic Wastewater-to-Energy Example [U-tapao et al., 2016]

Top and Bottom Levels









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Summary

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Stochastic Bilevel Optimization: Optimal Grid Tariffs [Askeland et al., 2020]





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References

Overview: Power Generation/Transmission Infrastructure Investment Example [Bylling et al., 2019, 2020]



Linear Bilevel Programming Problem

$$\begin{array}{l} \min_{x,y,\lambda} c^T x + d^T y^* + k^T \lambda^* + g(y^*,\lambda^*) \quad (1a) \\ \text{s.t.} \quad Ax = b \quad (1b) \\ x \ge 0 \quad (1c) \\ y^* \in \operatorname{argmin}\{p^T y \quad (1d) \\ \text{s.t.} \quad Cy = Dx + e \quad (1e) \\ y \ge 0\} \quad (1f) \\ \lambda^* \in \operatorname{argmax}\{\lambda^T (Dx + e) \quad (1g) \\ \text{s.t.} \quad C^T \lambda \le p\} \quad (1h) \end{array}$$



Linear Bilevel Programming Problem

| $\min_{x,y,\lambda} c^T x + d^T y^* + k^T \lambda^* + {\pmb\lambda^{*T}} M y^*$ | (1a) | |
|--|------|--------------------------------------|
| s.t. $Ax = b$ | (1b) | |
| $x \ge 0$ | (1c) | Replace with $\lambda^T M y$ in most |
| $y^* \in \operatorname{argmin}\{p^T y$ | (1d) | |
| s.t. $Cy = Dx + e$ | (1e) | cases |
| $y\geq 0\}$ | (1f) | |
| $\boldsymbol{\lambda^*} \in \operatorname{argmax}\{\boldsymbol{\lambda}^T(Dx+e)\}$ | (1g) | |
| s.t. $C^T\lambda \leq p\}$ | (1h) | |



Reformulate the problem as

$\min_{x} c^T x + F(x) \tag{2a}$

s.t.
$$Ax = b$$
 (2b)

$$x \ge 0$$
 (2c)

with

$$F(x) = d^T y(x) + k^T \lambda(x) + \lambda(x)^T M y(x),$$
(3)





Proposition

- F is a piece-wise linear function (on *critical regions*).
 - F is possibly discontinuous (because of the dual variables).

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Bilevel Optimization in Infrastructure

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Mathematical Details-5

Data and approach

- Danish price regions DK1 and DK2 [7].
- Regions connected with 600 MW DC cable.
- Potiential generation investment in DK1 and DK2.
- Full year of demand data.



Figure: Source: nordpoolspot.com



Solution time



(a) No of LL problems from 10 to 100. (b) No of LL problems from 200 to 5000.

Figure: Solution times for increasing number of LL problems.



Summary

- Infrastructure management can be improved through the use of analysis using bilevel optimization/MPEC models directly taking into account stochastic elements (e.g., at the lower level)
- Users are autonomous agents with a top-level decision-maker testing out various policy regimes to seek overall best policies for social welfare
- Computational issues related to the bilevel structure- these can be overcome through the use of optimization/operations research techniques for small- or medium-scale problems
- For larger problems, there are opportunities for research to improve the related modeling and algorithmic approaches



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