Optimization: a Ride on the Carousel (with an Eye to Energy)

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FLUID MACHINES AND ENERGY SYSTEMS

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Beware Mathematicians When They Seem to Speak Simple

Black-box Optimization

PDE-Constrained Optimization

NonLinear Nonconvex Problems

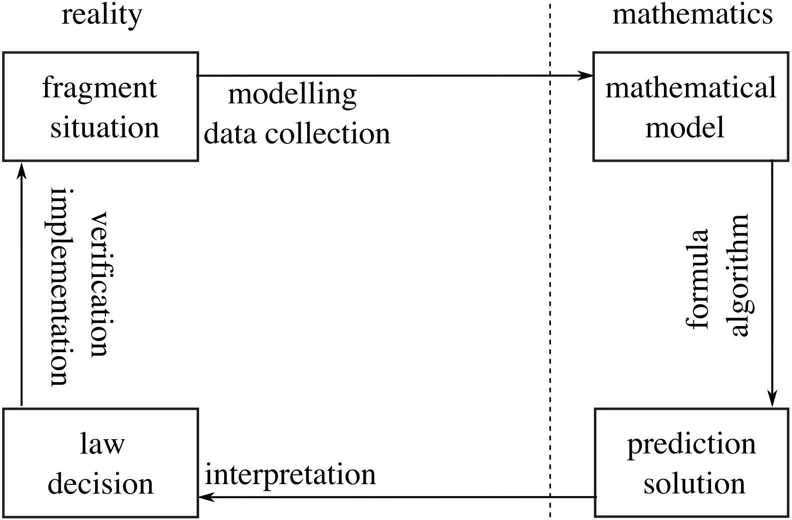
Mixed-Integer Convex (Linear) Problems

An Aside: Multiple Objectives

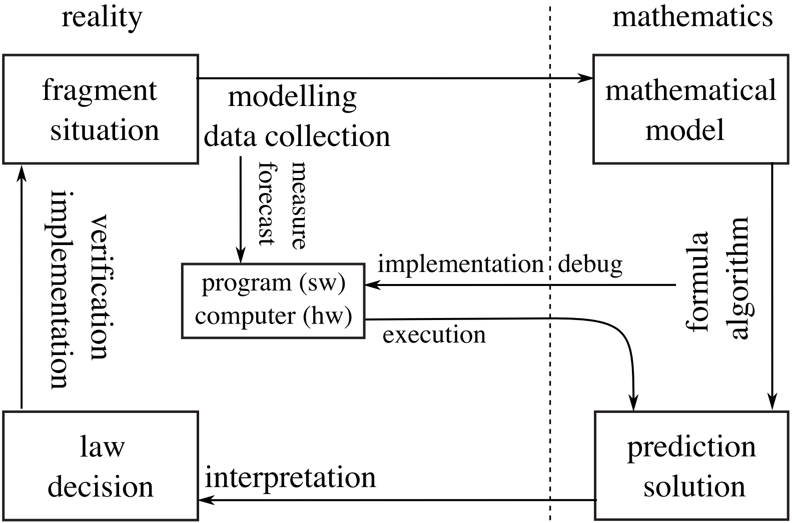
Do Not Underestimate Mixed-Integer Linear (Convex) Problems

Conclusions: Don't Be Afraid Of Optimization

- Everything you do, there always is at least one scarce resource (time, material, energy, money, manpower, data, knowledge, . . .)
- If you want to do more, there are basically two ways:
  - get more resources (slaughter some more of your neighbours, pollute some more the environment, . . .)
  - make better use of the resources you have
- Technology = learning to better exploit available resources
- This requires understanding of how the world works
- Understanding is almost invariably best expressed via mathematics (although not completely clear as to why this is the case)



- The fundamental cycle



- The fundamental cycle and its implementation

- Descriptive model: tells how the world (supposedly) is
- Prescriptive model: tells how the world (supposedly) should be
  a.k.a. optimization problem:

$$(P) \qquad f_* = \min \left\{ f(x) \; : \; x \in X \right\}$$

  - arbitrary set X = feasible region of possible choices x
  - typically X specified by $G \supset X$ (ground set) + constraints dictating required properties of feasible solutions $x \in X$
    [$\Longrightarrow x \in G \setminus X$ = unfeasible solution (??)]
  - $f : X \to Y$ objective function mapping preferences (cost)
  - optimal value $f_* \leq f(x) \forall x \in X$, $\forall v > f_* \, \exists x \in X$ s.t. $f(x) < v$
  - we want optimal solution: $x_* \in X$ s.t. $f(x_*) = f_*$
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- Everything looks pretty straightforward ... or is it?

- “Bad case” I: $X = \emptyset$ (“empty”)

  $$\min\{\, x \;:\; x \in \mathbb{R} \wedge x \leq -1 \wedge x \geq 1 \,\}$$

  there just is no solution (which may be important to know)

- “Bad case” II: $\forall M \, \exists x_M \in X$ s.t. $f(x_M) \leq M$ (“unbounded [below]”)

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  there are solutions as good as you like (which may be important to know)

- Not really bad cases, just things that can happen

- Solving an optimization problem actually three different things:
  - Finding x_* and proving it is optimal (how??)
  - Proving $X = \emptyset$ (how??)
  - Constructively prove $\forall M \, \exists x_M \in X$ s.t. $f(x_M) \leq M$ (how??)

- Often OK to find approximately optimal $\bar{x}$ and prove it (how??)

  $$f(\bar{x}) - f_* \leq \varepsilon \text{ (absolute)} \quad \text{or} \quad (\, f(\bar{x}) - f_* \,)/|\, f_* \,| \leq \varepsilon \text{ (relative)}$$

- Let's just stick to nonempty and bounded $X \implies \exists x_*$

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- Let's just stick to nonempty and bounded $X \Longrightarrow \exists x_*$ ... or does it?

- Things can be worse: not empty, not unbounded, but no x_* either:
  - $\min\{\, x \;:\; x \in \mathbb{R} \wedge x > 0 \,\}$ (“bad” X)
  - $\min\{\, 1 / x \;:\; x \in \mathbb{R} \wedge x > 0 \,\}$ (“bad” f and X)
  - $\min \left\{ f(x) = \left\{ \begin{array}{ll} x & \text{if } x > 0 \\ 1 & \text{if } x = 0 \end{array} \right. \;:\; x \in [\, 0 \,,\, 1 \,] \right\}$ (“bad” f)
- Still $\exists$ approximately optimal solutions $\forall\, \varepsilon > 0$, good enough for us
- Has to ensure somehow things don’t go awry
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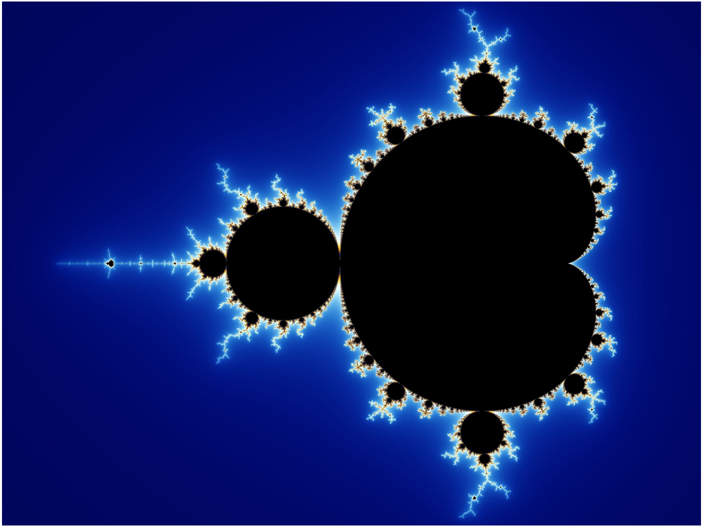

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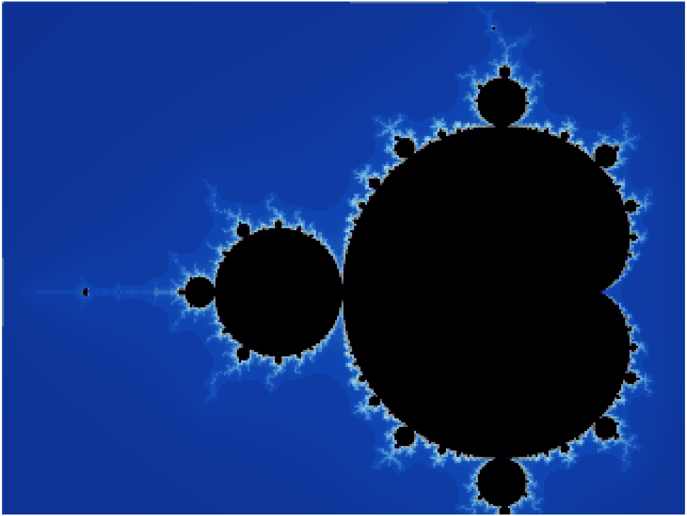

- $X \subset G \equiv$ (indicator) function $\imath_X : G \to \{ 0 , \infty \}$
- $x \in X \equiv \imath_X(x) \leq 0$ (constraint)
- All the difficulty lies in computing function values:

$$(P) \equiv \min \{ f(x) + \imath_X(x) \}$$

  the objective can take up all the complication of constraints

- Vice-versa also true: objective can always be linear

$$(P) \equiv \min \{ v \ : \ x \in X \ , \ v \geq f(x) \}$$

- And at least I can compute $f(x) / \imath_X(x)$, right? How hard can that be?
- Functions can be demonstrably impossible to compute $\Longrightarrow$ (P) demonstrably impossible to solve
- Even if not impossible, computing a function can be very hard

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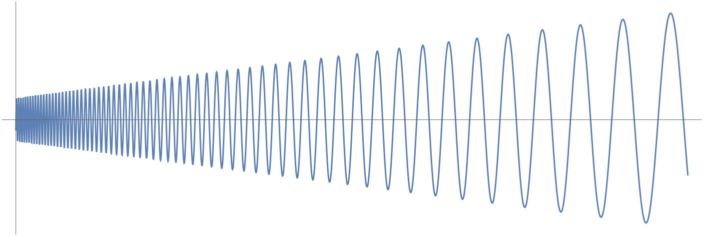
- (P) where $f(\cdot)$ / $\imath_X(\cdot)$ are "just any function" $\equiv$ complex mathematical model with no closed formulæ (most of them):
  - numerical integration
  - systems of PDEs
  - electromagnetic propagation models (ray-tracing, ...)
  - heat propagation models (heating/cooling of buildings, ...)
  - systems with complex management procedures (storage/plant design with route/machine optimization ...)
  - systems with stochastic components (+ possibly complex management) (queues in ERs, users of cellular networks, ...)
- A.k.a. simulation-based optimization: the system can only be numerically simulated as opposed to algebraically described
- Computation of $f(x)$ / $\imath_X(x)$ costly (can do few 100s/1000s of them)
- No information about the behaviour of $f(\cdot)$ "close" to x

- Typically require bound constraints: w.l.o.g. $X \subseteq [0, 1]^n$ (hence $X = [0, 1]^n$, other constraints "hidden" in $f(\cdot)$)
- Basically only (clever) "shotgun approach": fire enough rounds and eventually a good solution happens
- Good playground for population-based approaches (genetic algorithms, particle swarm, ...)
- Any other standard search (simulated annealing, taboo search, GRASP, variable-neighbourhood search, ...)
- Better idea: construct a model of $f(\cdot)$ out of past iterates to drive the search (regression, kriging, radial-basis functions, SVR, ML, ...)
- Bad news: none of these can possibly work efficiently (in theory)

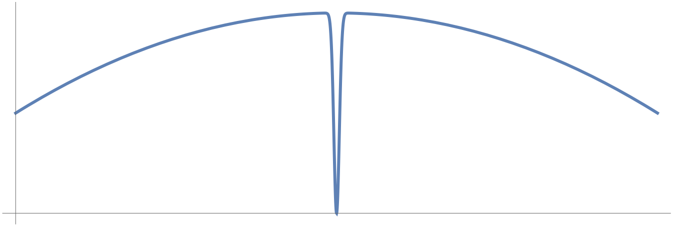
- If $f(\cdot)$ "swings wildly", things can be arbitrarily bad



- $f : \mathbb{R}^n \to \mathbb{R}$ (globally) Lipschitz continuous with constant L ($|f(x) - f(y)| \leq L||x - y|| \implies$ not too wild swings $\implies$ continuous)
- For each algorithm $\exists\, f(\cdot)$ s.t. finding ε-optimal solution requires $\geq O(L/\varepsilon)^n$ evaluations — that's very bad
- No free lunch theorem says "all algorithms equally bad"
- In practice is not as bad, but cost indeed grows very rapidly with n
- $n \approx 10 - 100$ if $f(\cdot)$ very costly, perhaps $n \approx 1000$ if not too costly

- $f(x)$ may be a random process:
  average performance computed via Montecarlo out of simulations
- Many examples:
  - behaviour of users
  - impact of weather on energy production/consumption
  - errors in measurement/impurity of materials ...
- Interesting tidbit: almost all approaches are inherently randomized
  (if you don't know anything, you may as well throw dices)
- Good part: can be trivially parallelized (as all Montecarlo do)
- Bad part: many runs = costly to compute average with high accuracy
- Intuitively, high accuracy only needed close to x_*
- But how do I tell if I'm close x_*? And which x_*?

- In a nutshell: if everything goes very, very well
  - you don't have many parameters (n in the few tens, ...)
  - you don't really need the best solution, a good one is OK
  - you have a lot of time and/or a supercomputer at hand
  - f is "nice enough": Lipschitz continuous, no isolated local minima, ...



- Good news: plenty of general-purpose black-box solvers, simple to use
- Bad news: difficult to choose/tune, none will ever scale to large-size
- In many cases, it is just what is needed
- Can we do better? Yes, we can if we have more structure

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- Fundamental concept: if you know the structure of $f(\cdot)/X$, exploit it
- Very important structure: Partial Differential Equations
- Model disparate phenomena as such as:
  - sound, heat, diffusion
  - electromagnetism (Maxwell's equations)
  - fluid dynamics (Navier–Stokes equations)
  - elasticity, ...
- Countless many applications:
  - weather forecast, ocean currents, pollution diffusion, ...
  - flows in pipes (water, gas, blood, ...)
  - air flow (airplane wing, car, wind turbine, ...)
  - behaviour of complex materials/objects (buildings, seismic models, ...)
- Optimal design/operation of many systems has PDE-defined $f(\cdot)/X$: PDE-Constrained Optimization (PDE-CO) problem

- General form of the problem:

$$\text{(PDE-CO)} \qquad \min \left\{ \, \ell(c,s) \; : \; \mathcal{H}(c,s) = 0 \;\; , \;\; \mathcal{G}(c,s) \geq 0 \, \right\}$$

  $x = [\, c \, , \, s \,]$, explicit description of X:
  - $s =$ state (pressure/velocity of air, force in material, . . .)
  - $c =$ controls (shape of wing/blade, position of actuators, . . .)
  - $\ell(c,s) =$ measure of function $\Longrightarrow$ typically involves integrals
  - $\mathcal{H}(c,s) =$ PDE constraints (Navier–Stokes equations, . . .)
  - $\mathcal{G}(c,s) =$ "other" algebraic constraints (min/max size/position, . . .)
- each $s_i : \mathbb{R}^k \to \mathbb{R}$ a function: $X \subset \mathbb{F}^n$
- often k small-ish: 2D/3D coordinates, fields, time (optimal control)
- controls may be functions or "simple" reals ($\equiv$ linear functions)
- $\mathbb{F}^n$ is a whole lot bigger than even $\mathbb{R}^n$ (all functions vs. linear ones): Banach space, infinite-dimensional while $\mathbb{R}^n$ has finite dimension n
- What did I gain from knowing ℓ, $\mathcal{H}$, $\mathcal{G}$?

- (the) "Space ($\mathbb{F}^n$) is big. Really big. You just won't believe how vastly, hugely, mind-bogglingly big it is."

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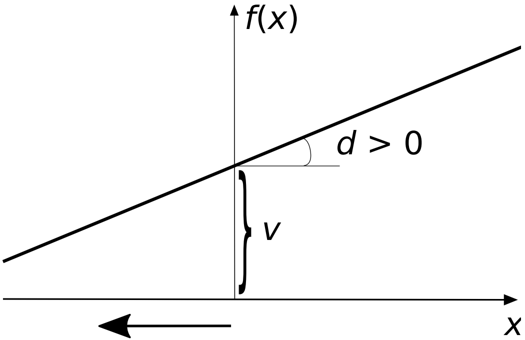

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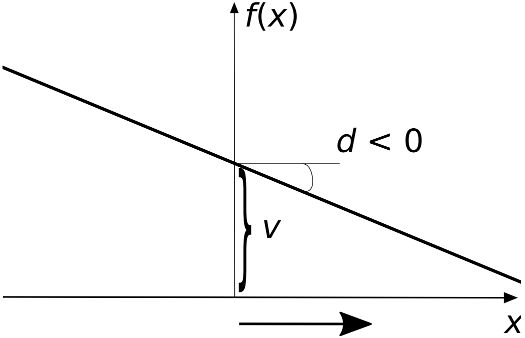

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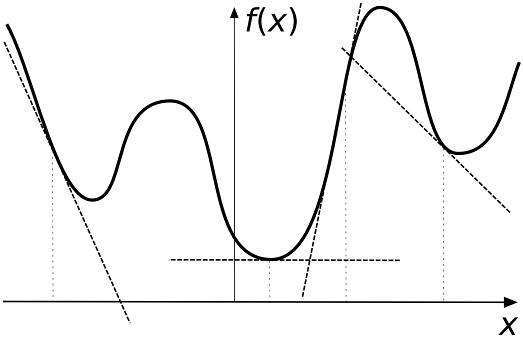

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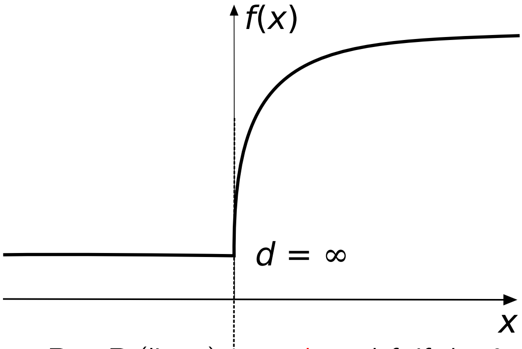

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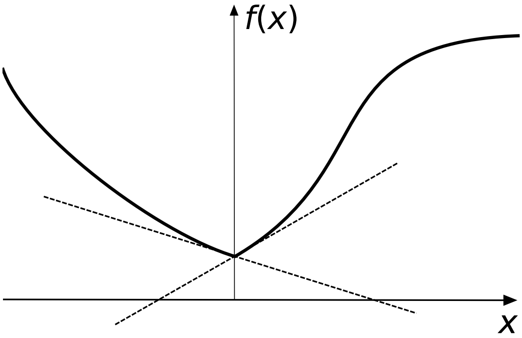

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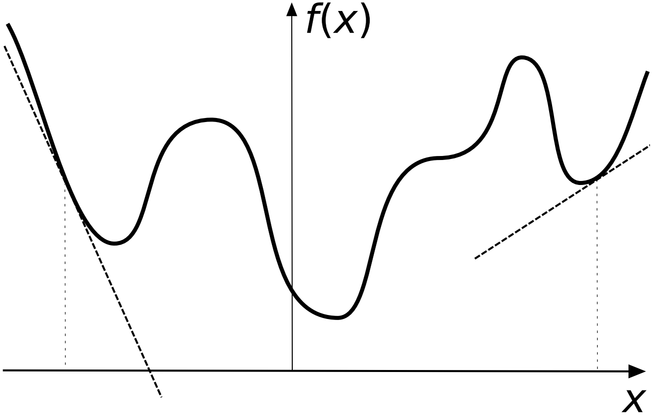
- Provided it exists ... and it is unique



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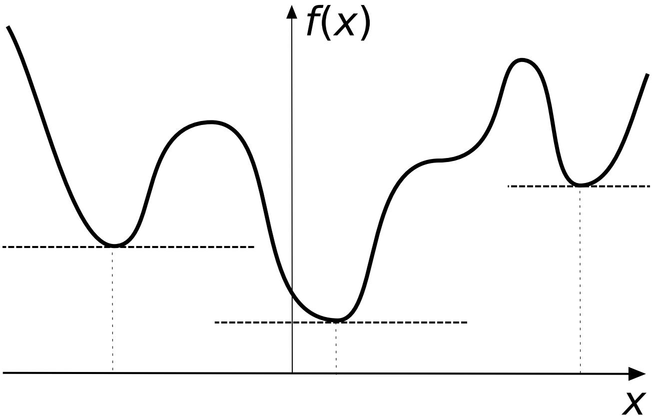

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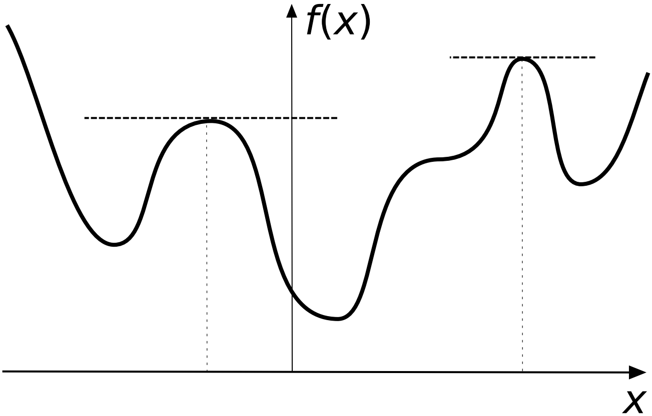

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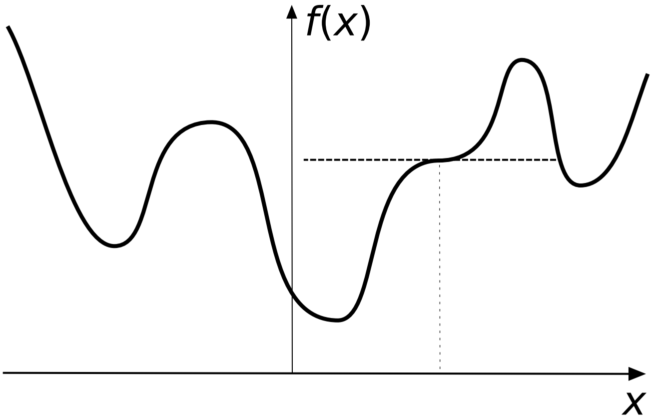
- However, $f'(x) = 0$ also in local (global) maxima



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- To find x_*, try finding stationary point x s.t. $f'(x) = 0$
- $f'(x) = 0$ (necessary, not sufficient) optimality condition: optimization is a system of (nonlinear) equations
- Still a lot hidden under the carpet:
  - what exactly is f' when $X \neq \mathbb{R}$?
  - $\imath_X$ has no derivative on "border" of $X \Longrightarrow$ has to "explicitly write" X as opposed to "hide" it in $\imath_X$ ($\mathcal{H}$, $\mathcal{G}$)
  - lots of "ifs" and "buts" (f' has to exist, X has to be "nice", ...)
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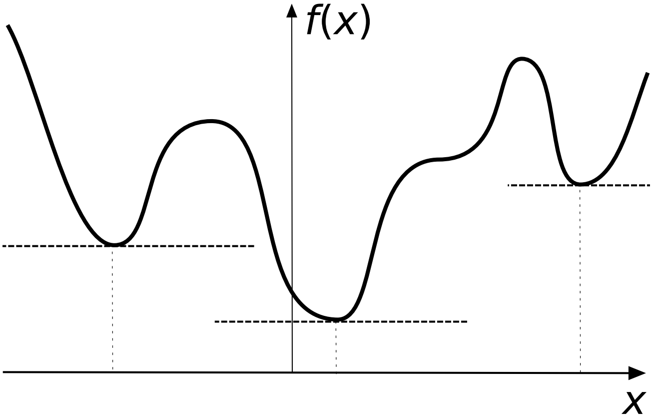
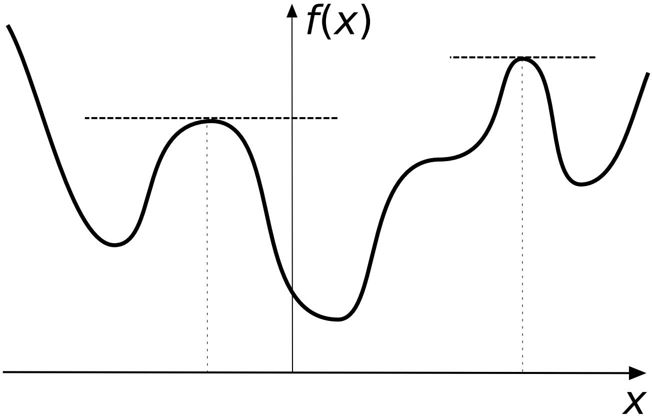
  - PDE systems have no closed-form solution anyway
    $\Longrightarrow$ have to discretize the PDE and solve approximately

- Still back to "have to compute $f(\cdot)$ numerically"
- However, can now prove that x $(= [\, c\,,\, u\,])$ is a (local) minimum
- Also, algorithms that use derivatives are vastly more efficient
  (we'll see more details later in a simpler setting)
- Can quickly reach a (local) minimum and stop there:
  no more random moves for fear of having missed a better point nearby
- $|f'(x)| \approx$ "distance" from x_*, useful to choose accuracy of simulation
- Explicit optimality conditions leads to multiple strategies:
  - first discretize, then write optimality conditions
  - first write optimality conditions, then discretize

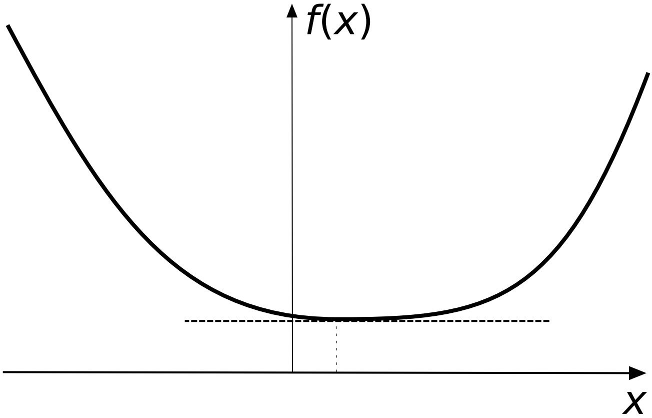
  (neither uniformly better, depends on the application)
- However, $f'(x) = 0$ only tells x may be a minimum,
  all is in vain if it rather is a maximum/saddle point
- There are ways to check it and ensure it'll never happen



- If f has local minima



- If f has local minima and maxima, f' must first $\nearrow$ and then $\searrow$
- What if f' monotone?



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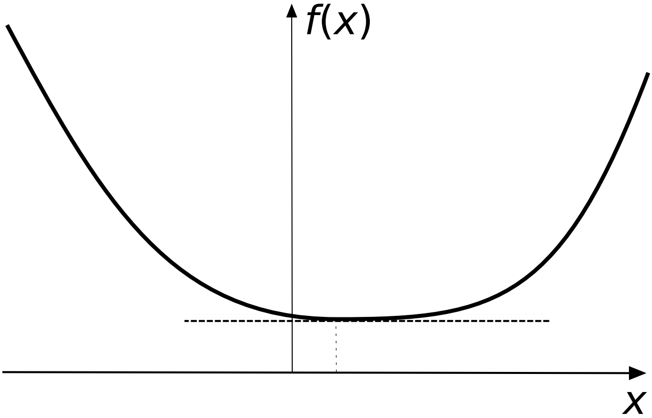

- If f has local minima and maxima, f' must first $\nearrow$ and then $\searrow$
- What if f' monotone? f convex function $\Longrightarrow$
  stationary point $\Longrightarrow$ local minimum $\Longrightarrow$ global minimum
- $f(\cdot)$ / X convex $\Longrightarrow$ x_* can be found "easily"
- (Restrictive) sufficient conditions to ensure $f(\cdot)$ / X convex

- In a nutshell: if everything goes very well
  - ℓ, $\mathcal{H}$ and $\mathcal{G}$ must have the right properties
  - details have to be worked out, options be wisely chosen
  - local optimality must be OK (or the problem convex to start with)
- There is no general-purpose PDE-OC solver,
  each case has to be dealt with individually
- However, tools are there, knowledge is there
- Problems of scale required by practical applications can be solved
  - with a little help from my (PDE-CO-savvy) friends
  - and possibly a supercomputer at hand
- As always, structure is your friend
  (e.g., optimal control has many specialized approaches exploiting time)
- Is it worth? In quite many cases, it is

Beware Mathematicians When They Seem to Speak Simple

Black-box Optimization

PDE-Constrained Optimization

NonLinear Nonconvex Problems

Mixed-Integer Convex (Linear) Problems

An Aside: Multiple Objectives

Do Not Underestimate Mixed-Integer Linear (Convex) Problems

Conclusions: Don't Be Afraid Of Optimization

- "Easier" problem: no PDE constraints, "only" algebraic ones

$$X = \{ x \in \mathbb{R}^n \,:\, g_i(x) \leq 0 \;\; i \in \mathcal{I} \,,\; h_j(x) = 0 \;\; j \in \mathcal{J} \}$$

  $\mathcal{I}$ = set of inequality constraints, $\mathcal{J}$ = set of equality constraints

- $G(x) = [\, g_i(x) \,]_{i \in \mathcal{I}} : \mathbb{R}^n \to \mathbb{R}^{|\mathcal{I}|}$, $H(x) = [\, h_i(x) \,]_{i \in \mathcal{J}} : \mathbb{R}^n \to \mathbb{R}^{|\mathcal{J}|}$

$$X = \{ x \in \mathbb{R}^n \,:\, G(x) \leq 0 \,,\; H(x) = 0 \}$$

  $G(\cdot)$, $H(\cdot)$ algebraic (vector-valued, multivariate) real functions

- Could always assume $|\mathcal{I}| = 1$ and $|\mathcal{J}| = 0$:
  - $h_j(x) = 0 \equiv h_j(x) \leq 0 \,\wedge\, -h_j(x) \leq 0$
  - $G(x) \leq 0 \equiv \max\{\, g_i(x) \,:\, i \in \mathcal{I} \,\} = g(x) \leq 0$

  but good reasons not to (exploit structure when is there)

- What does this gives to me? You know the drill: derivatives

- $f : \mathbb{R}^n \to \mathbb{R}$, partial derivative of f w.r.t. x_i at $x \in \mathbb{R}^n$:

  $$\frac{\partial f}{\partial x_i}(x) = \lim_{t \to 0} \frac{f(x_1, \ldots, x_{i-1}, x_i + t, x_{i+1}, \ldots, x_n) - f(x)}{t}$$

  just $f'(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_n)$ treating x_j for $j \neq i$ as constants

- Good news: computing derivatives mechanic, Automatic Differentiation software will do it for you, not only from formulæ but from code

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- Good news: computing derivatives mechanic, Automatic Differentiation software will do it for you, not only from formulæ but from code
  … provided they exist ($f(x) = |x|$, $f'(x) = ???$)
- Gradient = vector of all partial derivatives all important in optimization

$$\nabla f(x) := \left[\ \frac{\partial f}{\partial x_1}(x)\,,\ \ldots\ ,\ \frac{\partial f}{\partial x_n}(x)\ \right]$$

- $\nabla f(x) \approx [\, f(x + e_i \varepsilon) - f(x)] \,/\, \varepsilon$, $i = 1, \ldots, n$ (which ε?)
- f differentiable at $x \approx \forall i \ \frac{\partial f}{\partial x_i}(\cdot)$ continuous ($\Longleftarrow \exists$)
- $f \in C^1$: $\nabla f(x)$ continuous $\equiv f$ differentiable ($\Longrightarrow f$ continuous) $\forall\, x$
- $f \in C^1 \Longrightarrow$ finding local minimum (actually, stationary point) "easy": just go in the other direction ($-\nabla f(x)$ = steepest descent direction)

- Vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^m$, $f(x) = [\, f_1(x)\,,\, f_2(x)\,,\, \dots\,,\, f_m(x)\,]$
- Partial derivative: usual stuff, except with extra index

$$\frac{\partial f_j}{\partial x_i}(x) = \lim_{t\to 0} \frac{f_j(\, x_1\,, \dots, x_{i-1}\,, x_i + t\,, x_{i+1}\,, \dots, x_n\,) - f_j(\, x\,)}{t}$$

- $\nabla f(x) : \mathbb{R}^n \to \mathbb{R}^n$ itself has a gradient: Hessian of f

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_1}(x) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_1}(x) \\ \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) & \frac{\partial^2 f}{\partial x_2^2}(x) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_2}(x) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_n}(x) & \dots & \frac{\partial^2 f}{\partial x_n^2}(x) \end{bmatrix}$$

second-order partial derivative (just do it twice) $\quad \dfrac{\partial^2 f}{\partial x_j \partial x_i} \qquad \dfrac{\partial^2 f}{\partial x_i \partial x_i} = \dfrac{\partial^2 f}{\partial x_i^2}$

- $\nabla^2 f(x) \approx n$ times $\nabla f(x) \approx n^2$ times $f(x)$: packs a lot of information
- $f \in C^2$: $\nabla^2 f(x)$ continuous ($\Longrightarrow$ symmetric) $\equiv \nabla f$ differentiable $\forall\, x$
- $f \in C^2 \Longrightarrow$ finding local minimum (stationary point) “super-easy”

- $X = \mathbb{R}^n \Longrightarrow$ all depends on quality of derivatives of f:
  - $f \notin C^1 \Longrightarrow$ subgradient methods $\Longrightarrow$ sublinear convergence (error at step $k \approx 1/\sqrt{k}$, $O(1/\varepsilon^2)$ iterations)
  - $f \in C^1 \Longrightarrow$ gradient methods $\Longrightarrow$ linear convergence (error at step $k \approx \gamma^k$ with $\gamma < 1$, $O(1/\log(\varepsilon))$ iterations)
  - $f \in C^2 \Longrightarrow$ Newton-type methods $\Longrightarrow$ superlinear/quadratic convergence (error at step $k \approx \gamma^{k^2}/\gamma^{2^k}$ with $\gamma < 1$, $\approx O(1)$ iterations)
- All bounds $\approx$ independent from n (can be "hidden in the constants") $\Longrightarrow$ good for large-scale problems (n very large)
- Not all trivial, line search/trust region, globalization, ...
- Gradient methods can be rather slow in practice ($\gamma \approx 1$), need to cure zig-zagging (heavy ball, fast gradients, ...)
- Hessian a big guy, inverting it $O(n^3)$ a serious issue for large-scale: quasi-Newton/conjugate gradient only $O(n^2)$ / $O(kn)$ (but trade-offs)
- All in all, local (unconstrained) convergence very well dealt with

- Local optimality still "easy" to characterize via derivatives
- Karush-Kuhn-Tucker conditions: $\exists\, \lambda \in \mathbb{R}^{|\mathcal{I}|}_{+}$ and $\mu \in \mathbb{R}^{|\mathcal{J}|}$ s.t.

$$g_i(x) \leq 0 \;\; i \in \mathcal{I} \quad , \quad h_j(x) = 0 \;\; j \in \mathcal{J} \tag{KKT-F}$$

$$\nabla f(x) + \textstyle\sum_{i \in \mathcal{I}} \lambda_i \nabla g_i(x) + \sum_{j \in \mathcal{J}} \mu_j \nabla h_j(x) = 0 \tag{KKT-G}$$

$$\textstyle\sum_{i \in \mathcal{I}} \lambda_i g_i(x) = 0 \tag{KKT-CS}$$

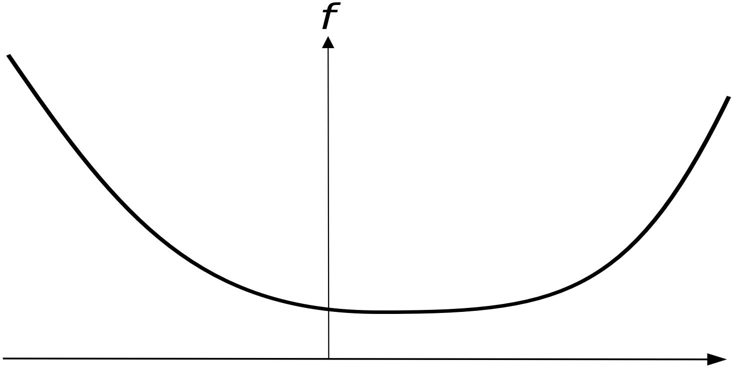
  $\equiv$ x stationary point of Lagrangian function (in x, λ / μ parameters)

  $L(\, x \,;\, \lambda \,,\, \mu \,) = f(x) + \sum_{i \in \mathcal{I}} \lambda_i g_i(x) + \sum_{j \in \mathcal{I}} \mu_j h_j(x)$ ($\rightsquigarrow$ duality ...)

- KKT Theorem: x local optimum + constraint qualifications $\Longrightarrow$ (KKT)
  a) Affine constraints: g_i and h_j affine $\forall\, i \in \mathcal{I}$ and $j \in \mathcal{J}$
  b) Slater's condition: g_i convex, h_j affine, $\exists\, \bar{x} \in X$ s.t. $g_i(\bar{x}) < 0 \; \forall\, i$
  c) Linear independence of $\nabla g_i(x)$ (i active) and $\nabla h_j(x)$ (all)
- (P) convex problem: (KKT) $\Longrightarrow$ x global optimum
- Otherwise, quite involved second-order optimality conditions ...

- In a nutshell, that $\exists$ efficient local algorithms
- At the very least, (KKT) $\approx$ tell x local minimum, stop the search
- Checking if (KKT) holds "easy" (Farkas' Lemma ...)
- Optimization $\equiv$ solving systems of nonlinear equations and inequalities
- Does not mean that algorithms are obvious:
  - several different forms (primal, dual, ...)
  - several different ideas (active set, projection, barrier, penalty, ...)
  - combinatorial aspects (active set choice) may make them inefficient
- Yet, provably and practically efficient algorithms are there if data of the problem nice (f, $G \in C^1/C^2$, H affine ...)
- Particularly relevant/elegant class: primal-dual interior point methods
- (Reasonably) robust and efficient implementations available, although numerical issues (linear algebra accuracy/cost) still nontrivial

- Unfortunately an entirely different game: sifting through all X required
- Derivatives a local object, can't give global information
  except in the convex case, where they actually do



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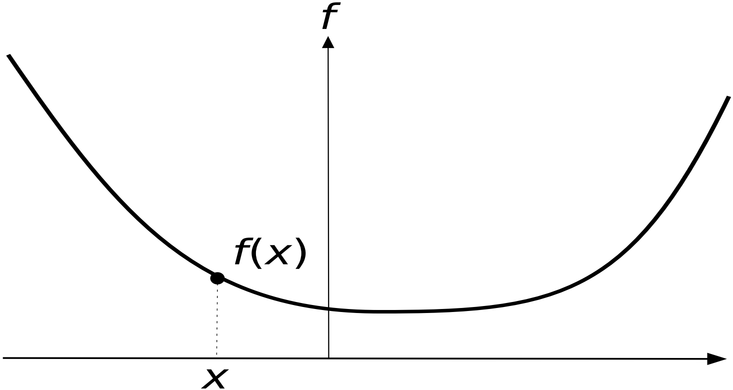

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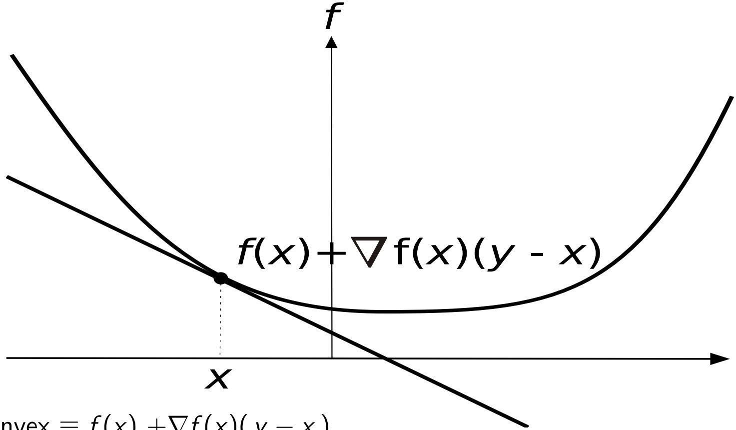

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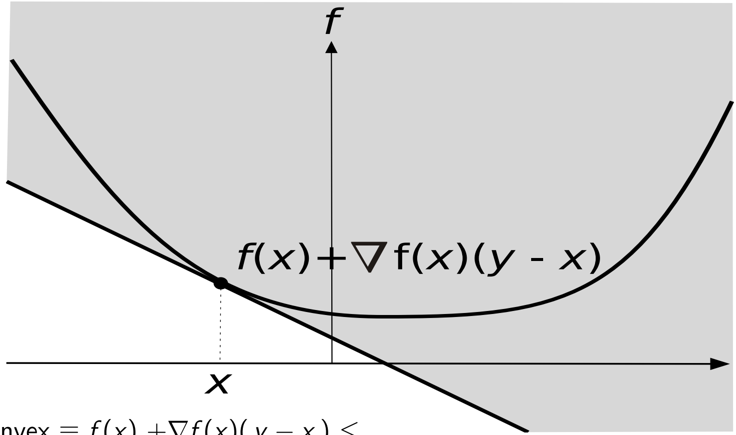

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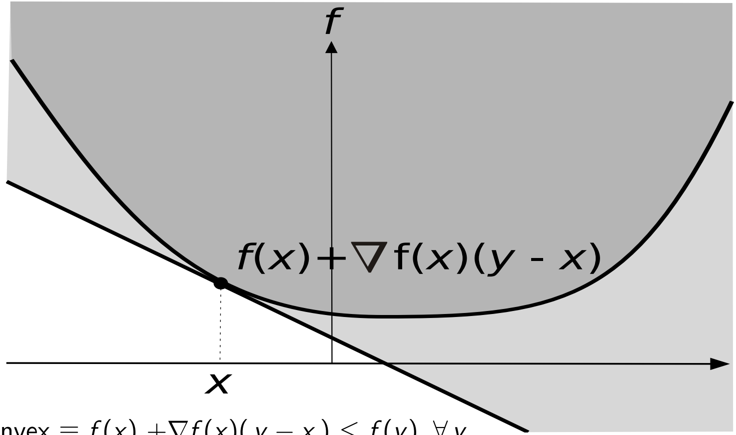

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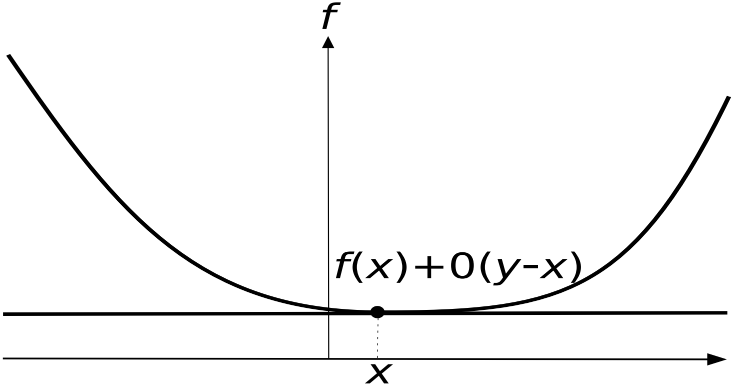

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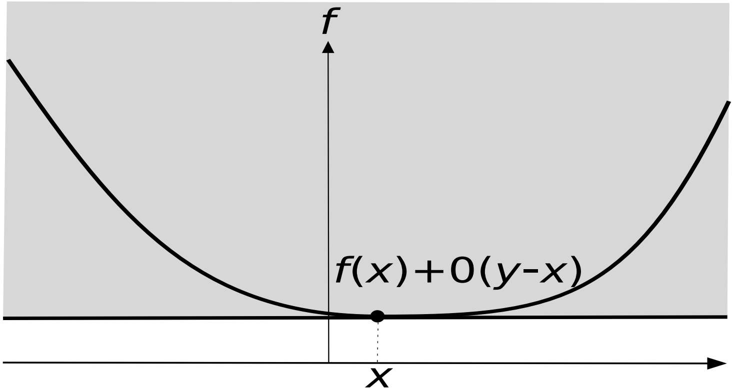

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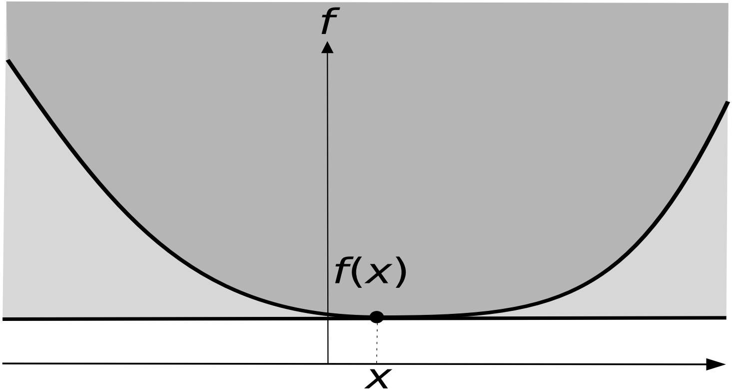

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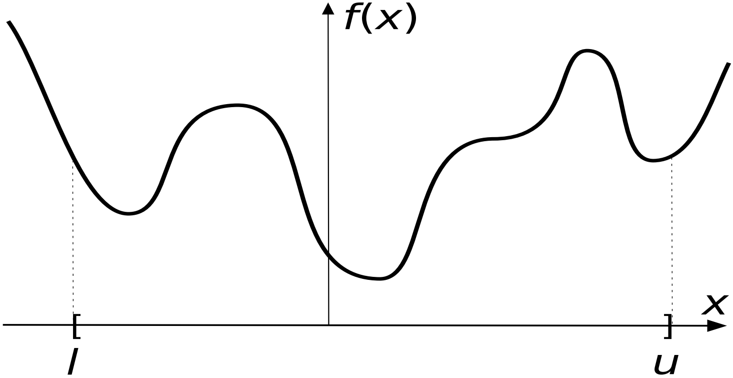
- Sift through all X $(= [\, l\, ,\ u\,])$ but using a clever guide



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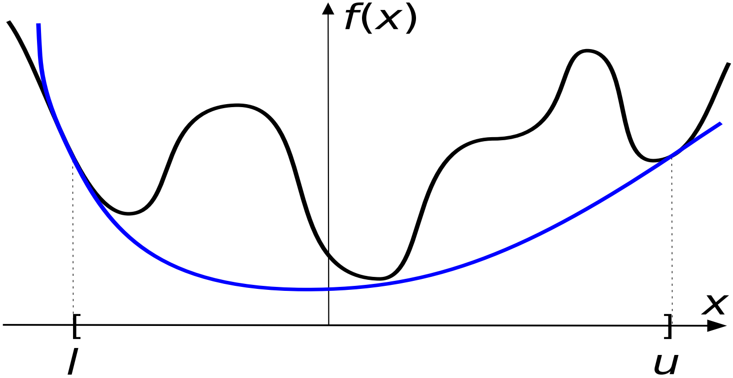

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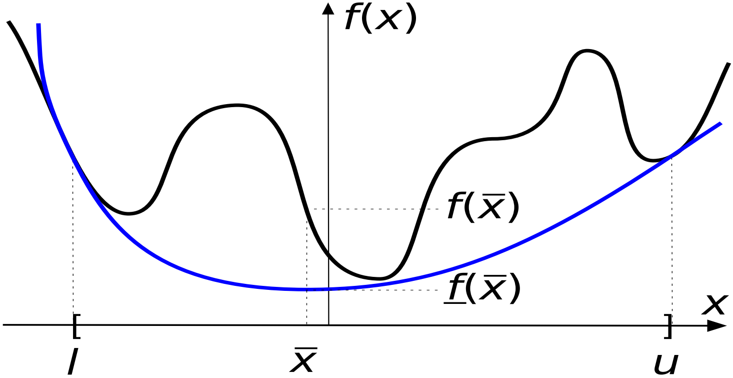

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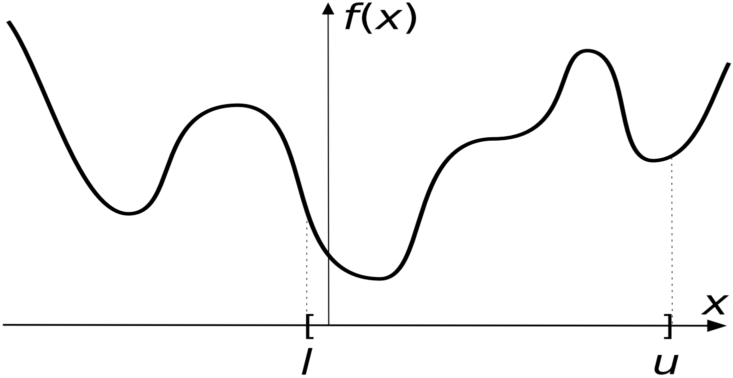

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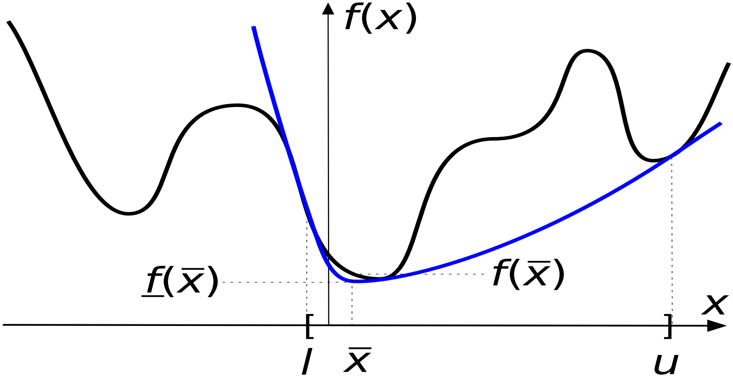

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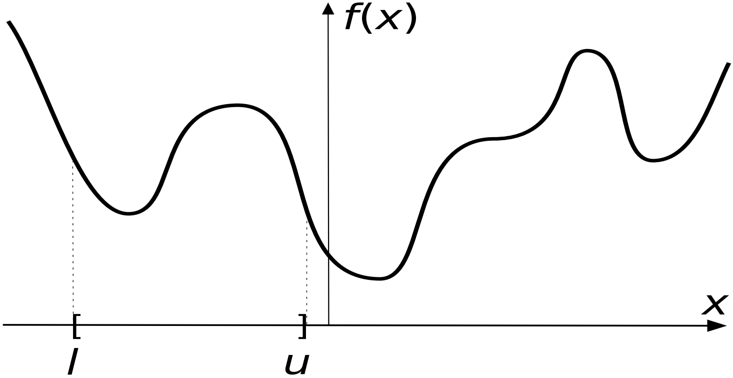

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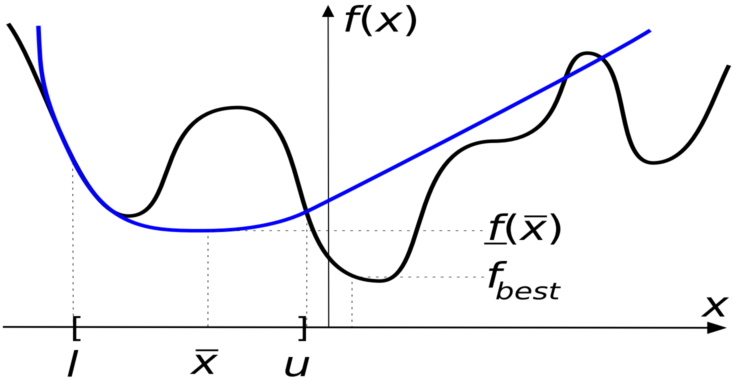

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- $\underline{f}$ depends on partition, smaller partition $\Longrightarrow$ better gap (hopefully)
- If on some partition $\underline{f}(\bar{x}) \geq$ best f-value so far, partition killed for good

- In a word? No
- Worst-case: keep dicing and slicing X until pieces "very small"
- However, in practice it depends on:
  - "how much nonconvex" f really is
  - how good $\underline{f}$ is as a lower approximation of f
- Best possible lower approximation: convex envelope
- Bad news: computing convex envelopes is hard
- Typical approach:
  - rewrite the expression of f in terms of unary/binary functions
  - apply specific convexification formulæ for each function
- Tedious job, bounds often rather weak
- Good news: implemented in available, well-engineered solvers
- Good news: immensely less inefficient in practice than blind search
  (at least, bounds allow to cut away whole regions for good)

- In a nutshell: if everything goes well
  - f, G and H must have the right properties
  - the less nonconvex they are, the better
  - the less "complicated" they are, the better
- Yet, there are general-purpose nonconvex MINLP solvers which can solve the problem to proven optimality
- Using them nontrivial, formulating the problem well crucial ($\equiv$ so that a "good $\underline{f}$ is available")
- Not really "large-scale", but 100s/1000s of variables often doable quickly enough with off-the-shelf tools
- Much larger problems also possible with special tools/effort
- As always, structure is your friend
- Is it worth? In quite many cases, it is (ask chemical Engineers)

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Conclusions: Don't Be Afraid Of Optimization

- Computing "good" convex approximation both complex and difficult
- One very relevant case in which at least "easy": integrality constraints
- $x_i \in \mathbb{Z}$, most often $x_i \in \{\, 0 \,,\, 1 \,\}$ very convenient for discrete choices (start machine/don't, make trip/don't, ...)
- Clearly nonconvex, $\exists$ nonlinear versions ($x_i(1 - x_i) \leq 0, \ldots$)
- Actually quite powerful: many different nonlinear nonconvex structures can be expressed via that + "simple" (linear) constraints
- Yet, this requires some rather weird formulation tricks
  $z = xy \equiv [\, (z \leq x) \wedge (z \leq y) \wedge (z \geq x + y - 1) \,]$ if all $x, y, z \in \{\, 0 \,,\, 1 \,\}$
- If all the rest in the problem convex, then a convex relaxation very easy: continuous relaxation ($x_i \in \mathbb{Z} \longrightarrow x_i \in \mathbb{R}$)
- This does not mean convex relaxation is good, but it may be
- At least makes life a lot easier to solution algorithms

- Finding good relaxations crucial for practical efficiency
- Solvers helped a lot by having few, well-controlled nonconvexities
- Mixed-Integer Convex Problems the easiest class of hard problems
- Especially famous special case: Mixed-Integer Linear Program

  $$(MILP) \quad \min \{\, cx \,:\, Ax \geq b \;,\; x_i \in \mathbb{Z} \;\; i \in I \,\}$$

  $\Longrightarrow$ continuous relaxation $\equiv$ Linear Program
- Very stable and efficient algorithms, some $\approx$ unique (simplex methods)
- Very powerful methods to improve relaxation quality (valid inequalities)
- Countless many results about special combinatorial structures (paths, trees, cuts, matchings, cliques, covers, knapsacks, ...)
- Clever approaches to exploit structure, though some work for MINLP too (Column/Row Generation, Dantzig-Wolfe/Benders' Decomposition, ...)

- Fundamental point: formulating the problem well is crucial
- Almost anything can be written as a MILP, albeit to some $\approx$ (not always a good idea: some nonlinearities "nice")
- Many different ways to write the same problem: apparently minor changes can make orders-of-magnitude difference
- Several of the best formulation weird and/or very large (appropriate tricks to only generate the strictly required part)
- Doing it "by hand" should not be required: solvers should be able to automatically find the best formulation (reformulate)
- Good news: the "perfect" formulation provably exists
- Bad news: it is provably ($\mathcal{NP}$-)hard to construct
- Doing it automatically is clearly difficult (but we should try harder)
- Meanwhile, a well-trained eye can make a lot of difference

- Good news: can "hide" many nonlinearities in a Linear Program
- Conic Program: $(P) \;\; \min\{\, cx \,:\, Ax \geq_K b \,\}$
  where $x \geq_K y \equiv x - y \in K$, K pointed convex cone, e.g.
  - $K = \mathbb{R}^n_+ \equiv$ sign constraints $\equiv$ Linear Program
  - $K = \mathbb{L} = \{\, x \in \mathbb{R}^n \,:\, x_n \geq \sqrt{\sum_{i=1}^{n-1} x_i^2} \,\} \equiv$ Second-Order Cone Program
  - $K = \mathbb{S}_+ = \{\, A \succeq 0 \,\} \equiv$ "$\succeq$" constraints $\equiv$ SemiDefinite Program
- Exceedingly smart idea: everything is linear, but the cone is not
  $\equiv$ a nonlinear program disguised as a linear one
- Contains as special case convex quadratic functions
- Many interesting (convex) nonlinear functions have a conic representation (but have to learn some even weirder formulation trick)
- Continuous relaxation almost as efficient as Linear Program
- Many combinatorial MILP tricks extend di MI-SOCP (valid surfaces, ...)
- Support in general-purpose software growing, already quite advanced

So, Can I Solve Mixed-Integer Linear (Convex) Problems?

- In a nutshell: unless something goes very bad
  - data of the problem by definition is nice
  - a feasible relaxation always there, bounds can be quite good
  - lots of good ideas (cutting planes, general-purpose heuristics, . . .)
- Plenty of general-purpose, well-engineered MILP/MI-SOCP solvers which can solve the problem to proven optimality
- Lots of useful supporting software: algebraic modelling languages, (there for MINLP too), IDEs, interfaces with database/spreadsheet, . . .
- 10000/100000 variables often doable in minutes/hours on stock hw/sw if you write the right model
- Much larger problems (10^6 / 10^9) also possible with special tools/effort
- As always, structure is your friend, and many known forms of structures
- Is it worth? In very many cases, it is

Beware Mathematicians When They Seem to Speak Simple

Black-box Optimization

PDE-Constrained Optimization

NonLinear Nonconvex Problems

Mixed-Integer Convex (Linear) Problems

An Aside: Multiple Objectives

Do Not Underestimate Mixed-Integer Linear (Convex) Problems

Conclusions: Don't Be Afraid Of Optimization

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  more than one objective, with incomparable units (apples & oranges)

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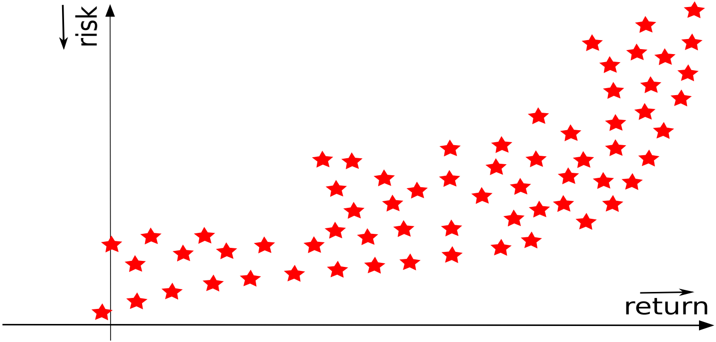
- Textbook example: portfolio selection problem



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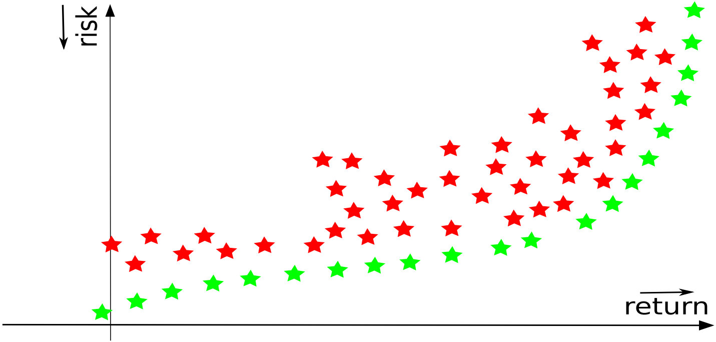

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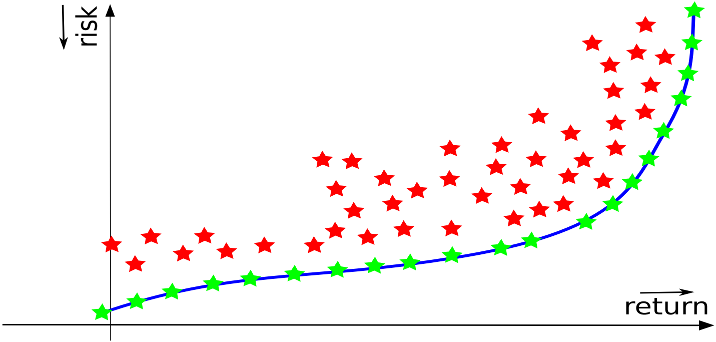

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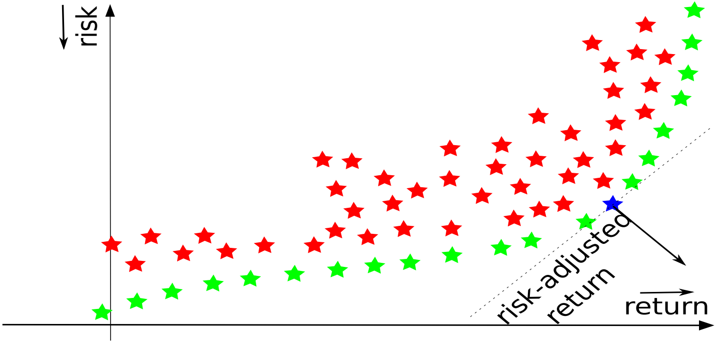

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- Two practical solutions: maximize risk-adjusted return,
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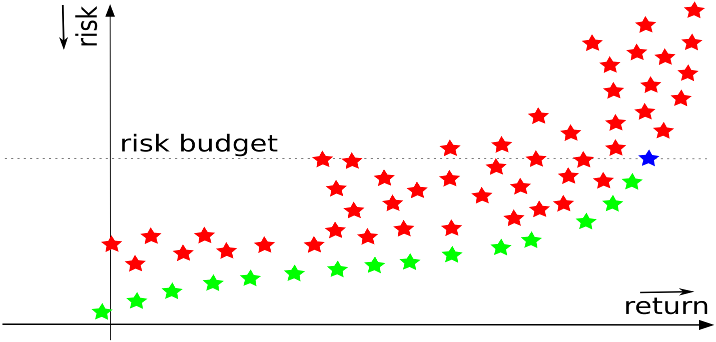

- No "best" solution, only non-dominated ones on the Pareto frontier
- Two practical solutions: maximize return with budget on maximum risk,
  a.k.a. budgeting $\min \{ f_1(x) : f_2(x) \leq \beta_2 , x \in X \}$ (which β_2??)

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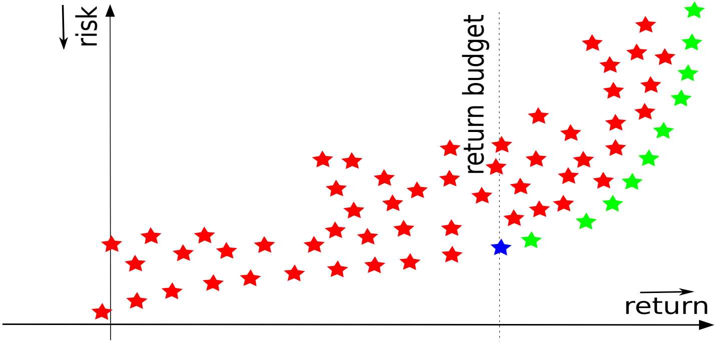

- No "best" solution, only non-dominated ones on the Pareto frontier
- Two practical solutions: minimize risk with budget on minimum return,
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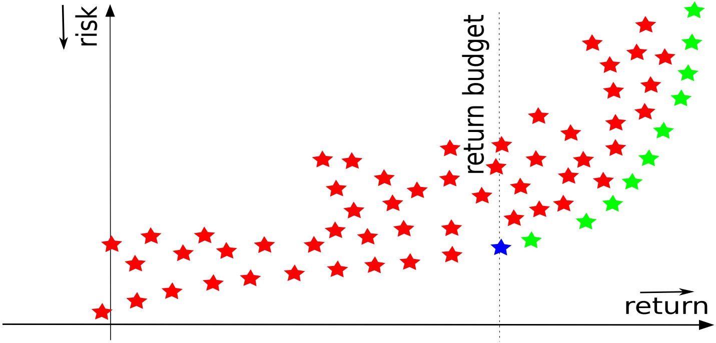

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  a.k.a. budgeting $\min \{ f_2(x) \; : \; f_1(x) \leq \beta_1 \, , \; x \in X \}$ (which β_1??)
- All a bit fuzzy, but it's the nature of the beast

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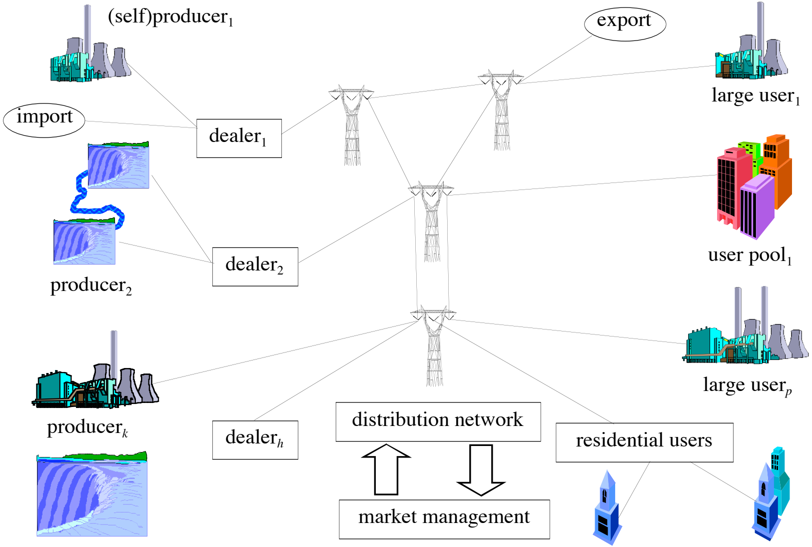
- Schedule a set of generating units over a set of time instants to satisfy the (forecasted) energy demand at each



- Gazzillions €€€ / $$$, enormous amount of research[1]
- Different types of production units, different constraints:
  - Thermal (comprised nuclear): min/max production, min up/down time, ramp rates on production increase/decrease, start-up cost depending on previous downtime, others (modulation, ...)
  - Hydro (valleys): min/max production, min/max reservoir volume, time delay to get to the downstream reservoir, others (pumping, ...)
  - Non programmable (ROR hydro) intermittent units (solar/wind, ...)
  - Fancy things (small-scale storage, demand response, smart grids, ...)
- The electrical network (AC/DC, transmission/distribution, OTS, ...)
- The right formulation of the individual units may make a lot of difference for thermals[2,3], hydros[4], ...

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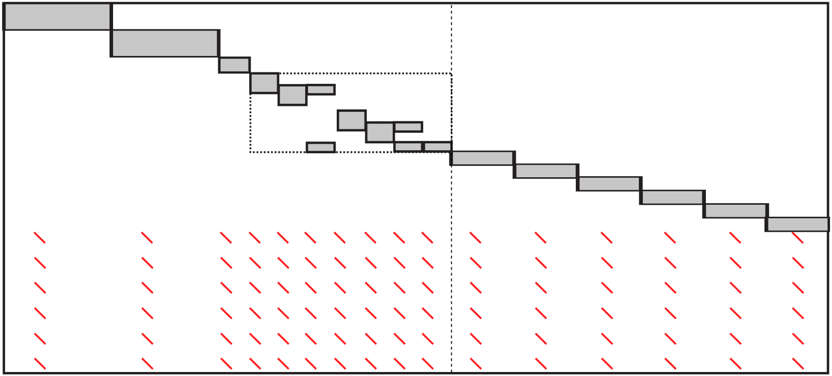
[1] van Ackooij, Danti Lopez, F., Lacalandra, Tahanan "Large-scale Unit Commitment Under Uncertainty [...]" *AOR*, 2018

[2] F., Gentile, Lacalandra "Tighter Approximated MILP Formulations for Unit Commitment Problems" IEEE TPWRS, 2009

[3] F., Gentile "New MIP Formulations for the Single-Unit Commitment Problems with Ramping Constraints" *TR*, 2015

[4] d'Ambrosio, Lodi, S. Martello. "Piecewise linear approxmation of functions of two variables in MILP models" *ORL*, 2010



- Many blocks of rather different shape and size + linking constraints
- A very-large-scale MIQP to be solved in <15' operationally
- Can be done via Lagrangian decomposition[5] and specialized solution methods for thermal[6]/hydro[7] units

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[5] F., Gentile, Lacalandra "Solving Unit Commitment Problems with General Ramp Contraints" *IJEPES*, 2008

[6] F., Gentile "Solving non-linear single-unit commitment problems with ramping constraints"' *OR*, 2006

[7] Taktak, D'Ambrosio "An overview on [...] unit commitment problem in hydro valleys" *Energy Systems*, 2017

- Maybe if this were the end, but it is just the beginning
- Data is uncertain: demand, wind/solar production, units/network state …which cannot be ignored (increased RES penetration …)
- Need methods to represent uncertainty[1]:
  - Robust Optimization: uncertain data lives anywhere in a (convex) uncertainty set (how chosen? too conservative, price-of-robustness, …)
  - Chance-Constrained Optimization: constraints hold with high probability (estimate distributions, nasty numerical integrals galore, …)
  - Stochastic Optimization[8]: here-and-now decisions in advance, recourse decisions when the uncertainty reveals itself
  - Hybrids[9], …
- UC typically stochastic: day-ahead commitment, to-the-minute dispatch
- Simplest approach scenario-based: each scenario ≈ a full UC $\Longrightarrow$ size increases by a factor # scenarios, which should be large

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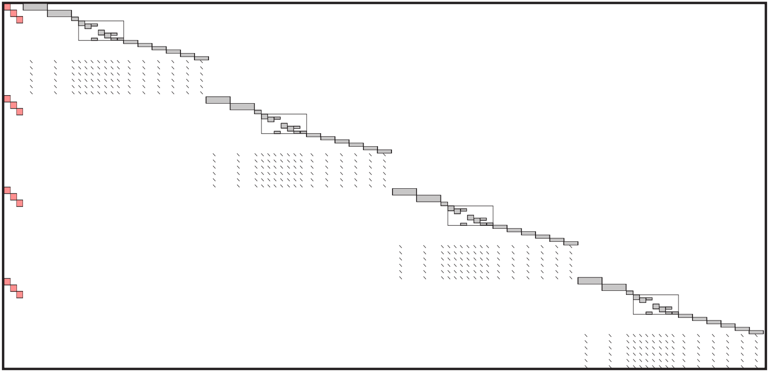
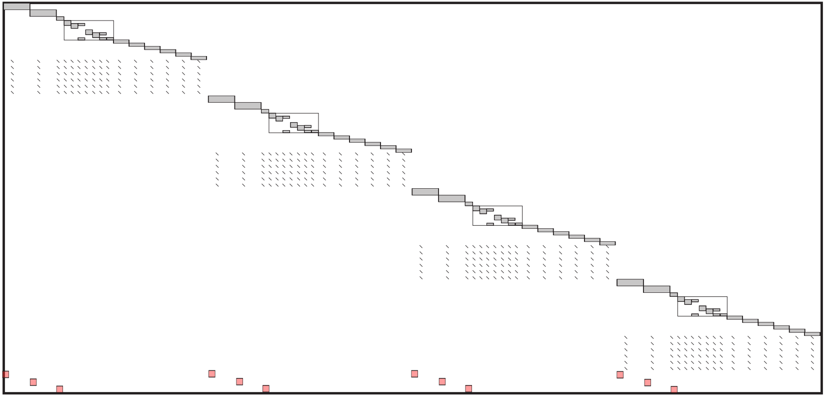
[8] Scuzziato, Finardi, F. "Comparing Spatial and Scenario Decomposition for Stochastic […]" *IEEE Trans. Sust. En.*, 2018
[9] van Ackooij, F., de Oliveira "Inexact Stabilized Benders' Decomposition Approaches, with Application […]" *CO&A*, 2016



- Perfect structure for Benders' decomposition: iteratively compute value function depending on linking variables
- Benders' decomposition with Lagrangian decomposition inside[10] (curiously, both happen to be the cutting-plane algorithm)
- . . . with (different) other subproblems inside

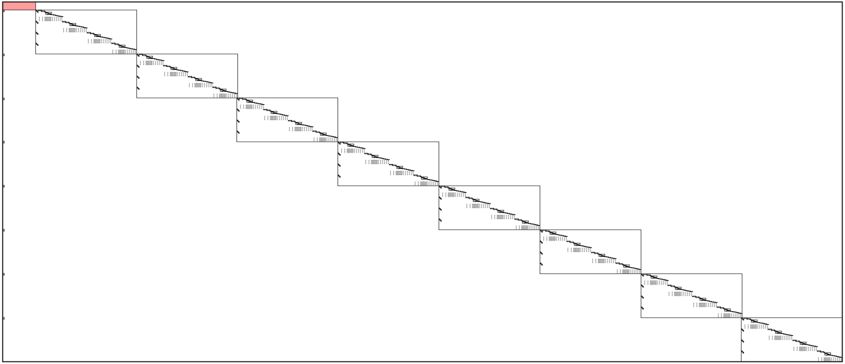
[10] van Ackooij, Malick "Decomposition algorithm for large-scale two-stage unit-commitment" *Ann. OR*, 2016



- Reformulation trick: split here-and-now variables, add copy constraints
  $\Longrightarrow$ perfect structure for Lagrangian decomposition again
- Lagrangian decomposition with Lagrangian decomposition inside ...
- Which is better? Very hard to say beforehand[8]

- Unit-Commitment is a short-term problem, lacks long-term strategies
- Issue: cost of water (none) / minimum reservoir volume (very low) $\Longrightarrow$ lot of water used $\Longrightarrow$ no water most of the year
- Hydro production most useful for peak shaving every day
- Computing value of water left in the reservoirs at T for each (significant) day of the year
- stochastic dual dynamic programming[11]:
  - proceed forward to construct solution
  - proceed backward to compute/refine lower bounds
  - sample the uncertain parameters, solve a parametric (uncertain) UC problem for each sample
  - construct stochastic cuts out of sampled dual information

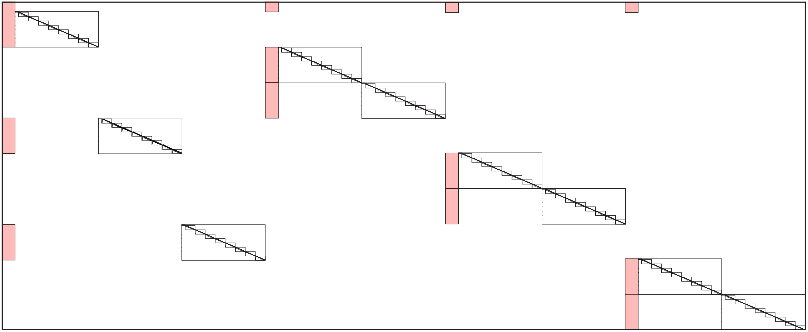
[11] Pereira, Pinto "Multi-stage stochastic optimization applied to energy planning" *Math. Prog.*, 1991



- Each block is scenario-uncertain on some data (RES production) and continuous-uncertain on other data (water inflows/outflows)

- SDDP + Benders + Lagrange + subproblems or
SDDP + Lagrange + Lagrange + subproblems or ...

- The energy system changes all the time, but modifications slow, extremely costly, with huge inertia
- Demand and production subject to very significant uncertainties: climate = RES production + demand, shifts in consumption patterns (EV, cryptocurrencies, ...), new technologies (shale, LED, ...), geo-political factors (energy security), economical factors (boost or boom), regulatory factors (EU energy market, ...), political factors (CO_2 emission treaties, nuclear power, ...), ...
- Planning long-term evolution very hard, yet necessary
- 20/30 years, 2/5 years steps (multi-level recourse), many scenarios



- Huge size, multiple nested structure
- Still OK for either Benders or Lagrange
- Benders + SDDP + Benders + Lagrange + subproblems or
  Lagrange + SDDP + Benders + Lagrange + subproblems ...

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- Is it "easy"? By no means
- Tools for doing this actually don't exist, writing them as I speak
- Large project, 4M€ (so not that large w.r.t. many others), but if we can shave 0.01% of total EU energy cost we re-pay them 1000-fold
- Is it the "typical" use of optimization? By no means, but:
  - hints at some useful techniques, in particular for uncertainty
  - nice idea: it helps if you know how to solve a subproblem
  - two inner levels actually useful in operations
  - if we can solve this, we can almost surely solve yours
- Usual project much more limited $\Longrightarrow$ doable with standard tools

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Conclusions: Don't Be Afraid Of Optimization

- Optimization problems are difficult

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- Many problems have structure that can be exploited
- First crucial choice: which class of optimization problems
- Trade-off model accuracy vs. model complexity not trivial
- However, apparently very complex problems may not be that difficult if one knows the right set of modelling tricks
- Lots of stable, well-developed software (even open-source), especially for the most "tractable" problems
- Optimal solutions not always needed, "just good" ones may be easy
- Some mad people having fun just with solving optimization problems
- Can be worth a lot of €€€/performance
- If it really helps, it probably can be done

- Learn a bit about it:
  - mathematics seems imposing but not really though (unless you want to)
  - lots of software whose inner workings you only need to partly understand (oftentimes we don't know all the details ourselves)
- Often off-the-shelf tools enough, but have to be used well
- Consider inviting an optimization-savvy friend:
  - (most of us) will typically bend backwards to make it work
  - seeing our toys actually useful to someone a great joy
  - though applications need good methodologies, but good methodologies learn a lot from though applications
  - we won't eat your lunch: too many things we will never know, usually more than happy with our minor slice of the glory cake
- Optimization a minority stake in any good application, but at the right moment it can save your day

Thank You

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