7.Nonlinear Programming and MIP Technology

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From Linear to Nonlinear

- Some problems can be easily encoded in standard LP form
- For some others is not trivial to get a linear formulation, they may involve constraints like:
  - $y = x^2 + \frac{1}{z}$
  - $c > 10 \implies a \geq b \vee d \neq e$
  - $allDifferent(x_1, \ldots, x_n)$
- Mathematical methods for handling these problems either:
  - Use a specific Nonlinear Programming approach, or
  - Encode the problem into an equisatisfiable linear problem

Nonlinear programming

- Nonlinear Programming (NLP) problems have generic form:

$$\begin{array}{ll} \min & f(x) \\ s.t. & g_i(x) \leq 0 \quad i = 1, \ldots, m \end{array}$$

  where one function among $f, g_1, \ldots, g_m$ is non-linear

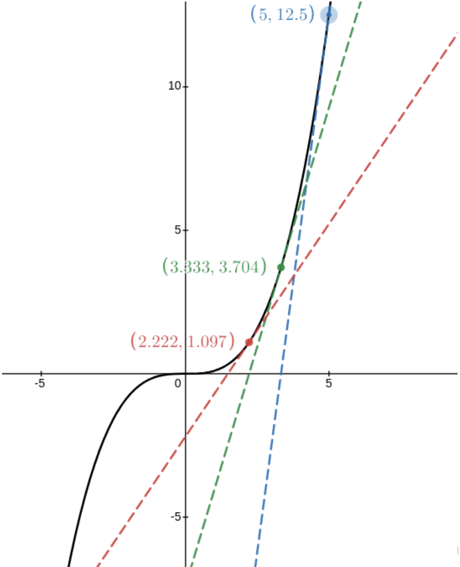
- Different NLP methods exist based on the problem type
  - E.g., Quadratic programming (QP): min $\frac{1}{2}x^t\, Q\, x + c^t x$ s.t $Ax \leq b$
  - Newton's method
  - Steepest descent
  - Lagrange multipliers
  - ...

Newton-Raphson's method (root finding)

- Let $f : X \to \mathbb{R}$ be a function, f' its derivative and $x_0 \in X$
- The tangent of f at $(x_0, f(x_0))$ is $t_0(x) = f'(x_0)(x - x_0) + f(x_0)$
  - We can use t_0 as linear approximation of f
- The intersection of t_0 with x-axis is a point x_1 such that $t_0(x_1) = 0$, hence $f'(x_0)(x_1 - x_0) + f(x_0) = 0$ so $x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$
- We can iterate to get $x_2 = x_1 - \dfrac{f(x_1)}{f'(x_1)}, \ldots, x_{k+1} = x_k - \dfrac{f(x_k)}{f'(x_k)}$
- Under some conditions (...) we converge to a x_k such that $f(x_k) = 0$

Example

E.g. if $f(x) = \frac{x^3}{10}$ and $x_0 = 5$:

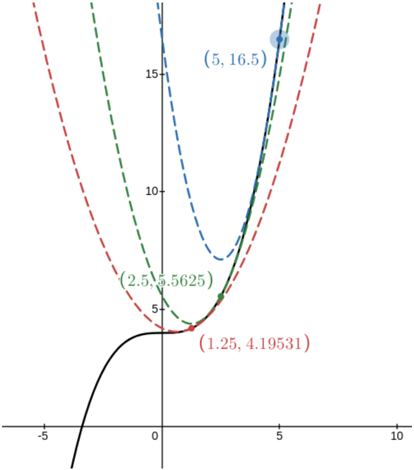


Newton-Raphson's method (optimization)

- If f is twice-differentiable, this method is applicable to find the roots of f' too: $f'(x) = 0 \implies$ stationary points
  - Either a minimum, maximum or inflection (saddle) point
- At k-th iteration, instead of tangent t_k we consider the parabola $p_k(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2$ with same slope and curvature of $f(x_k)$ and then proceed with $x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$
- If $f(x) = ax^2 + bx + c$ then only one step needed to converge: $x_1 = x_0 - \frac{2ax_0 + b}{2a} = -\frac{b}{2a}$ and $f'(x_1) = 2a \cdot \frac{b^2}{4a^2} - b \cdot \frac{b}{2a} = 0$

Example

E.g. if $f(x) = \dfrac{x^3}{10} + 4$ and $x_0 = 5$:

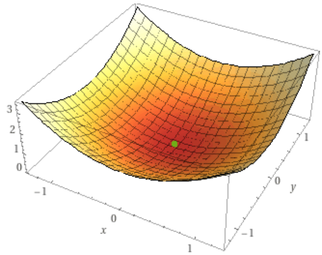


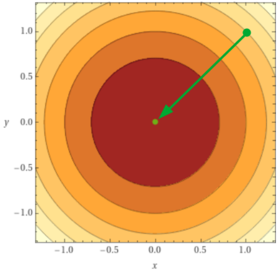
Newton-Raphson's method (multivariable minimization)

- If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ with $n > 1$, we use the gradient instead of f':
  $\nabla f(x) = \left\{ \left(\frac{\partial f}{\partial x_1}(x), \ldots, \frac{\partial f}{\partial x_n}(x) \right) \mid x \in \mathbb{R}^n \right\}$
  - ∇f is a vector in $\mathbb{R}^n$ denoting the direction of steepest ascent
- Instead of f'' we use Hessian $\nabla^2 f(x) = H_f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ & \cdots & \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$
  - $\nabla^2 f$ is a matrix in $\mathbb{R}^{n \times n}$ denoting the curvature of f
- We start with $\mathbf{x_0} \in \mathbb{R}^n$ and $\mathbf{x_{k+1}} = x_k - (\nabla^2 f(\mathbf{x_k}))^{-1} \cdot \nabla f(\mathbf{x_k})$
  - $\nabla f(x_k)$ points "uphill" $\rightarrow -\nabla f(x_k)$ points "downhill"
  - H_f "adjusts" the direction according to "how sharp" the surface is

Example

- E.g., if $f(x, y) = x^2 + y^2$ then $\nabla f = (2x, 2y)$ and $\nabla^2 f = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$
- If $x_0 = (1, 1)$ we have $\nabla f(x_0) = (2, 2)$ and $\nabla^2 f(x_0) = \nabla^2 f$
- $x_1 = x_0 - (\nabla^2 f(\mathbf{x_0}))^{-1} \cdot \nabla f(\mathbf{x_0}) = (1, 1) - \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \begin{pmatrix} 2 \\ 2 \end{pmatrix} = (0, 0)$
- $\nabla f(x_1) = (0, 0)$: we found a local minimum
  - $\nabla f(x) = (0, \ldots, 0)$ is necessary but not sufficient condition for x be a global optimum





Newton-Raphson's method

- Interior point approaches can exploit Newton-Raphson's method to traverse the feasible region of constrained (N)LP problems
  - E.g., primal-dual interior-point method
- This is a second-order method: 2^{nd}-order derivatives used to compute the optimization trajectory (Hessian)
  - While first-order methods are based on 1^{st} order derivatives (gradient)
  - Derivatives-free methods also exist (e.g. dichotomic search)
- Computing and inverting Hessian matrix is expensive
  - Also no guarantee of convergence if not positive definite

Local Search

- Newton-Raphson's method is a form of Local Search (LS):
  - It starts from an initial state
  - It moves from one state to another one
  - Each move uses local information only (neighborhood states)
  - Each move should improve the current state
  - Global optimality not guaranteed in general
- Other well known LS methods are: simulated annealing, hill climbing, steepest descent, tabu search, LNS...
- Gradient descent: steepest descent method using the negative gradient to decide direction of next move

Gradient descent

- Gradient descent (GD) is a well-known 1st order approach that gained popularity with the rise of ML and (deep) neural networks
- GD often used for training ML models: a loss function $L(x, \theta)$ over input data $x = (x_1, \dots, x_n)$ and model parameters $\theta = (\theta_1, \dots, \theta_m)$ is iteratively minimized starting from an initial state $\theta^{(0)}$
- GD computes $\theta^{(k+1)} = \theta^{(k)} - \lambda \nabla L(\theta^{(k)})$ for $k = 0, 1, 2, \dots$
- Step $k + 1$ depends on direction $-\nabla L(\theta^k)$ and learning rate λ
  - $-\nabla L(\theta^k)$ specifies "where to go" to minimize the loss
  - λ is the "size of a step" towards minimum loss (typically small)

Gradient descent

- GD can be used in different modes:
  - Batch: model updated after evaluating all training set (training epoch)
  - Stochastic: subset of N samples randomly selected from training set
    - If $N > 1$ is small, sometimes referred as mini-batch
- Apart from neural networks, GD can be used to train linear classifiers
  - Less robust than SVMs
  - Nonlinear logistic classifiers better for binary classification
- Newton's can converge in fewer steps than GD but computing and inverting the Hessian might make it slower in practice

Lagrange multipliers

- Instead of solving $\min f(x)$ s.t. $g_i(x) \leq 0$, unconstrain the problem and only keep a new loss function: $\min \left(L(x, \Lambda) = f(x) + \Lambda_i p_i(x) \right)$
  - Weights $\Lambda_i \geq 0$ are called Lagrangian multipliers
  - Terms $p_i(x) \geq 0$ are penalty functions such that $g_i(x) \leq 0 \Leftrightarrow p(x) = 0$
- Penalties $p_i(x)$ should reflect "how far" x is from satisfying $g_i(x) \leq 0$
  - E.g., $p_i(x) = \max(0, g_i(x))$ better than $p_i(x) = \begin{cases} 0 & \text{if } g_i(x) \leq 0 \\ 1 & \text{if } g_i(x) > 0 \end{cases}$
- Lagrangian-based LS can be applied for any constraint $c_i(x)$ by using steepest descent to iteratively update weights Λ_i at each step
  - To use gradient descent, penalties $p_i(x)$ should be differentiable

Linearization

- An alternative approach, suitable for combinatorial problems, is to linearize nonlinear constraints to get an equisatisfiable MIP problem
- This approach works if the variables are bounded
- E.g., nonlinear constraint $5x \leq 18 \lor -y + 2z < 3$
  - i.e., $f(x, y, z) \geq 1$ with $f(x, y, z) = \begin{cases} 1 & \text{if } 5x \leq 18 \text{ or } -y + 2z < 3 \\ 0 & \text{otherwise} \end{cases}$

Reification

- Logical combinations of constraints can be handled via reification
- Given constraint $C(x_1, \ldots, x_k)$ a (full) reification of C is a Boolean variable b s.t. $b = true \iff C(x_1, \ldots, x_k)$
  - An integer reification is s.t. $b \in \{0, 1\}$ and $b = 1 \iff C(x_1, \ldots, x_k)$
  - An integer half-reification is s.t. $b \in \{0, 1\}$ and $b = 1 \Rightarrow C(x_1, \ldots, x_k)$
    - $b = 0 \ \vee \ C(x_1, \ldots, x_k)$
- Easy case: integer reification of Boolean operations. If C, C_1, C_2 are Boolean variables (i.e., propositions or 0-arity predicates):
  - $C = C_1 \vee C_2$ becomes $b_1 \leq b \wedge b_2 \leq b \wedge b \leq b_1 + b_2$
  - $C = C_1 \wedge C_2$ becomes $b \leq b_1 \wedge b \leq b_2 \wedge b_1 + b_2 \leq b + 1$
  - $C = \neg C_1$ becomes $b = 1 - b_1$

  with $b, b_1, b_2 \in \{0, 1\}$

Reification

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  - An integer half-reification is s.t. $b \in \{0, 1\}$ and $b = 1 \Rightarrow C(x_1, \ldots, x_k)$
    - $b = 0 \ \vee \ C(x_1, \ldots, x_k)$
- Common case: $C_1 \vee \cdots \vee C_m$ where C_i are linear inequalities: $C_i \equiv \sum_j \alpha_{i,j} x_j \leq \beta_i$ for $i = 1, \ldots, m$ and $j = 1, \ldots, n$
  - At least one inequality must hold
  - How to linearize it via integer reification?

Big-M trick

- We introduce integer reifications $b_1, \ldots, b_m \in \{0,1\}$, impose $\sum_{i=1}^{m} b_i \geq 1$ and for each inequality $\sum_j \alpha_{i,j} x_j \leq \beta_i$ we enforce $\sum_j \alpha_{i,j} x_j - \beta_i \leq M \cdot (1 - b_i)$ where M is a *"big enough"* constant:
  - $b_i = 0 \implies \sum_j \alpha_{i,j} x_j - \beta_i \leq M$: always satisfied
  - $b_i = 1 \implies \sum_j \alpha_{i,j} x_j \leq \beta_i$: original inequality C_i must be satisfied
- M is called a Big-M number. If $x_j \in [l_j..u_j]$ we can define a specialized Big-M for each equation: $M_i = -\beta_i + \sum_j \max\{\alpha_{i,j} l_j, \alpha_{i,j} u_j\}$
- E.g., if $5x \leq 18 \vee -y + 2z \leq 3$ with $x \in [0..30]$, $y \in [-5..-2]$, $z \in [-6..7]$ we introduce $b_1, b_2 \in \{0,1\}$ and we impose:
  - $b_1 + b_2 \geq 1$
  - $5x \leq 18 + (\max\{5 \cdot 0, 5 \cdot 30\} - 18) \cdot (1 - b_1) = 18 + 132 \cdot (1 - b_1)$
  - $-y + 2z \leq ((-1) \cdot (-5) + 2 \cdot 7 - 3) \cdot (1 - b_2) = 3 + 16 \cdot (1 - b_2)$

Min/max constraints

- To linearize $y = \min\{x_1, x_2\}$ with $x_1 \in [l_1..u_1], x_2 \in [l_2..u_2]$ we could linearize $(x_1 \leq x_2 \Rightarrow y = x_1) \wedge (x_2 < x_1 \Rightarrow y = x_2)$ as above
  - 4 binary variables introduced
- ...Or simply add 1 new variable $b \in \{0, 1\}$ and impose:
  - $y \leq x_1$
  - $y \leq x_2$
  - $y \geq x_1 - (u_1 - l_2) \cdot (1 - b)$
  - $y \geq x_2 - (u_2 - l_1) \cdot b$
- In this way:
  - $b = 0 \implies y \geq \overbrace{x_1 - u_1}^{\leq 0} + l_2 \ \wedge \ y \geq x_2 \implies y = x_2$
  - $b = 1 \implies y \geq \underbrace{x_2 - u_2}_{\leq 0} + l_1 \ \wedge \ y \geq x_1 \implies y = x_1$

Min/max constraints

- If $y = \min\{x_1, \dots, x_k\}$, we introduce $b_1, \dots, b_k \in \{0, 1\}$ and impose $\sum_{i=1}^{k} b_i = 1 \quad \wedge \quad y \leq x_i \quad \wedge \quad y \geq x_i - (u_i - l_{min})(1 - b_i)$
  - $l_{min} = \min\{l_1, \dots, l_k\}$, so $b_i = 1 \implies x_i = \min\{x_1, \dots, x_k\}$
- If $y = \max\{x_1, \dots, x_k\}$, $y \geq x_i \;\wedge\; y \leq x_i + (u_{max} - l_i)(1 - b_i)$
  - $u_{max} = \max\{u_1, \dots, u_k\}$ and $b_i = 1 \implies x_i = \max\{x_1, \dots, x_k\}$
- This approach can be used for other nonlinear constraints
  - E.g. $y = |x|$, $x \neq y$ or $y = kx$ with $k \in \{0, 1\}$. Try as exercise!

Unary encoding

- Alternative approach: unary encoding. If $D(x)$ is the domain of x we introduce $|D(x)|$ binary variables $b_k^x \in \{0,1\}$ and impose:

$$\sum_{k \in D(x)} b_k^x = 1 \;\wedge\; \sum_{k \in D(x)} k \cdot b_k^x = x \qquad (1)$$

- In this way $b_k^x = 1 \iff x = k$
  - E.g., $x \in [4..6]$ encoded as $b_4^x + b_5^x + b_6^x = 1 \;\wedge\; 4b_4^x + 5b_5^x + 6b_6^x = x$
- Pros: tighter linear relaxation, better encoding of global constraints
- Cons: lots of binary variables if the domain is big

Unary encoding

- E.g., for *allDifferent*$(x_1, \ldots, x_n)$ we impose (1) and $\sum_{i=1}^{n} \alpha_{i,j} b_j^{x_i} \leq 1$ for $j \in \bigcup_{1 \leq h < k \leq n} (D(x_h) \cap D(x_k))$ and $\alpha_{i,j} = \begin{cases} 1 & \text{if } j \in D(x_i) \\ 0 & \text{otherwise} \end{cases}$

- E.g., if $x \in [2..11]$, $y \in [-5..4]$, $z \in [3..5]$ we impose (1) for x, y, z and we constrain variables b_j for $j \in [2..4] \cup [3..5] \cup [3..5] = [2..5]$:

$$\begin{array}{ccccccc} b_2^x & + & b_2^y & + & 0\cancel{b_2^z} & \leq & 1 \\ b_3^x & + & b_3^y & + & b_3^z & \leq & 1 \\ b_4^x & + & b_4^y & + & b_4^z & \leq & 1 \\ b_5^x & + & 0\cancel{b_5^y} & + & b_5^z & \leq & 1 \end{array}$$

Unary encoding

- Easy encoding of element: $z = [x_1, \ldots, x_n][y]$ as $z = \sum_{i=1}^{n} b_i^y x_i$
  - Not linear, but easy to linearize
- Multiplication harder! E.g., $z = xy$ with $y \in [l_y..u_y]$ can be defined as $z = [xl_y, \ldots, xu_y][y - l_y + 1]$
  - E.g., $z = xy$ with $y \in [2..3]$ becomes $z = [2x, 3x][y - 1]$
- Particular case: $y = x^n$ with n constant
- E.g., $y = x^3$ with $x \in [-2..1]$ becomes $y = [-8, -1, 0, 1][x + 3]$

MiniZinc encoding

- MiniZinc allows one to compile a CP model with finite domains into an equisatisfiable FlatZinc instance with linear constraints only
  - So any MIP solver supporting FlatZinc can solve it!
  - Useful, not necessarily efficient...
- See `share/minizinc/linear/domain_encodings.mzn` where function `eq_encode(var int:x)` enforces (1) for integer variable x
  - MiniZinc common subexpression elimination ensures that binary variables b_i^x are reused if x is encoded again
- More details in: Belov, Gleb, et al. *"Improved linearization of constraint programming models."* CP 2016.

MiniZinc solvers

MiniZinc bundle contains different MIP solvers. Some of them are directly usable, without further installations:

- COIN-BC (a.k.a. CBC)
  - Based on Branch-and-Cut `https://github.com/coin-or/Cbc`
  - Part of open-source COIN-OR initiative
  - Default solver of PuLP Python module for LP
- HiGHS
  - Based on high performance dual revised simplex implementation (HSOL) and its parallel variant (PAMI) by Q. Huangfu*
  - Freely available `https://highs.dev`

*Parallelizing the dual revised simplex method, Q. Huangfu and J. A. J. Hall, Mathematical Programming Computation, 10 (1), 119-142, 2018.

MiniZinc solvers

Other MIP solvers need external plugins/licenses:

- IBM ILOG CPLEX (commercial, free licenses available)
  - https://www.ibm.com/products/ilog-cplex-optimization-studio
- Gurobi (commercial, free licenses available)
  - https://www.gurobi.com/
- SCIP (non-commercial)
  - https://www.scipopt.org/)
- FICO Xpress (commercial, free licenses available)
  - https://www.fico.com/en/products/fico-xpress-solver

MIP Technology

- MiniZinc is a "CP-oriented" modeling language. More "mathematical programming"-oriented languages exist
  - E.g., AMPL
- Alternatively, one can use LP libraries or add-in
  - E.g., PuLP or Excel solver
- Or simply the APIs provided by a particular solver
  - E.g., Gurobipy

AMPL

- AMPL (*A Mathematical Programming Language*) is an algebraic modeling language developed by Fourer, Gay, Kernighan in 1985
- It supports separation between model and data (*high-level*)
- Problems are passed to solvers as .nl files (*low-level*)
- Supported by many open-source and commercial solvers
- `https://ampl.com/`

Brewery example with AMPL

beer.dat

```
set PROD := beer ale;
set INGR := corn hops malt;

param: profit :=
ale  13
beer 23;

param: supply :=
corn  480
hops  160
malt 1190;

param amt: ale beer :=
corn          5  15
hops          4   4
malt         35  20;
```

beer.mod

```
set INGR;
set PROD;
param profit {PROD};
param supply {INGR};
param amt {INGR, PROD};
var x {PROD} >= 0;

maximize total_profit:
   sum {j in PROD} x[j] * profit[j];

subject to constraints {i in INGR}:
   sum {j in PROD} amt[i,j] * x[j] <= supply[i];
```

```
[cos226:tucson] ~> ampl
AMPL Version 20010215 (SunOS 5.7)
ampl: model beer.mod;
ampl: data beer.dat;
ampl: solve;
CPLEX 7.1.0: optimal solution; objective 800
ampl: display x;
x [*] :=  ale 12  beer 28;
```

From https://www.cs.princeton.edu/courses/archive/spr07/cos226/lectures/22LinearProgramming.pdf

Brewery example with GurobiPy

```python
import gurobipy as gp

# Create a new model
m = gp.Model()

# Create variables
A = m.addVar(vtype='I', name="Ale")
B = m.addVar(vtype='I', name="Beer")
# Set objective function
m.setObjective(13 * A + 23 * B, gp.GRB.MAXIMIZE)

# Add constraints
m.addConstr(5*A + 15*B <= 480)
m.addConstr(4*A +  4*B <= 160)
m.addConstr(35*A + 20*B <= 1190)

# Solve it!
m.optimize()

print(f"Optimal profit: {m.objVal}: {A.X} ale(s) and {B.X} beer(s)")
```

`brewery.py`

Brewery example with PULP

```
from pulp import *

prob = LpProblem("Brewery Problem", LpMaximize)

A = LpVariable("Ale", 0, None, LpInteger)
B = LpVariable("Beer", 0, None, LpInteger)

prob += 13*A + 23*B, "Profit"
prob += 5*A + 15*B <= 480, "Corn"
prob += 4*A + 4*B <= 160, "Hop"
prob += 35*A + 20*B <= 1190, "Malt"

# We can specify the solver to use as a parameter of solve
prob.solve()
```

brewery2.py

Take-home messages

- Nonlinear programming (NLP) involves nonlinear constraints and/or objective function
- One can tackle general NLP problems with ad hoc techniques...
  - Quadratic programming, Newton's method, Gradient descent, Lagrange multipliers, item ...
- ...or linearize nonlinear constraints to get an equisatisfiable linear problem
  - Big-M
  - Unary encoding
  - ...
- Plenty of MIP technology available (e.g., AMPL language)

Resources

- CDMO course a.y. 2020/21
- Belov, Gleb, et al. ”*Improved linearization of constraint programming models.*” CP 2016