Optimization for Machine Learning

Approximation Theory and Machine Learning

Sven Leyffer

Argonne National Laboratory

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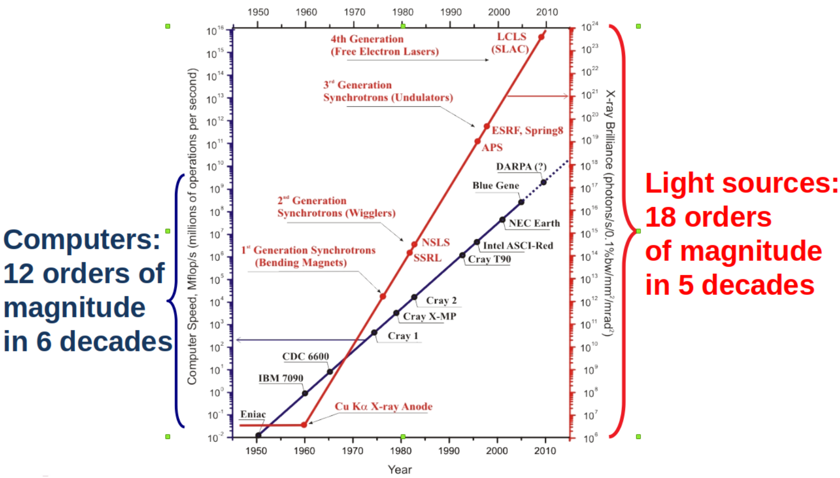
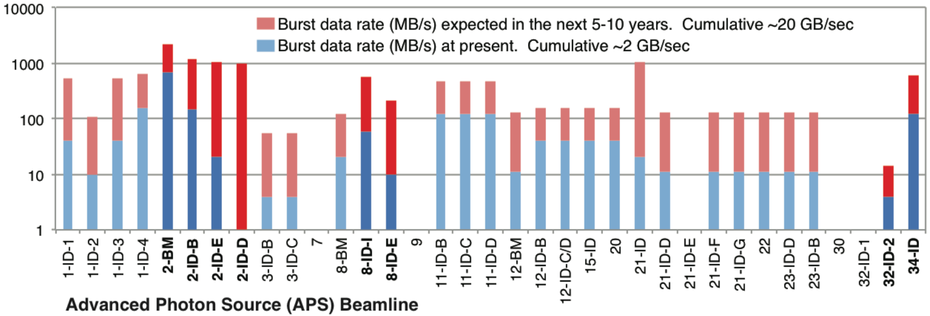
Outline

Motivation: Datanami from DOE Lightsource Upgrades



Data size and speed to outpace Moore's law (source Ian Foster)

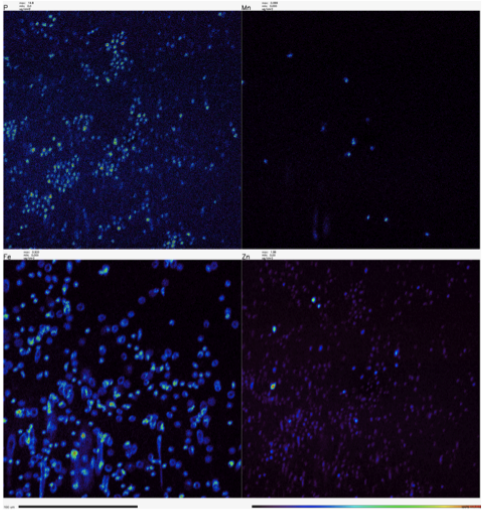
Challenges at DOE Lightsources



Math, Stats, and CS Challenges from APS Upgrade

- 10x increase in data rates and size ⇒ HPC & CS
- Heterogeneous experiments & requirements ⇒ hotchpotch of math/CS solution
- Multi-modal data analysis, movies, ... ⇒ more complex reconstruction
- New experimental design ⇒ less regular data

Example: Learning Cell Identification from Spectral Data



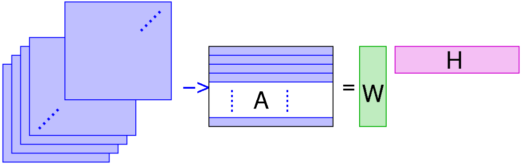
Identify cell-type from concentration maps of P, Mn, Fe, Zn ...

Learning Cell Identification via Nonnegative Matrix Factorization

$$\underset{W,H}{\text{minimize}} \ \|A - WH\|_F^2 \quad \text{subject to } W \geq 0, \ H \geq 0$$

where “data” A is $1,000 \times 1,000$ image $\times 2,000$ channels

- W are weight $\simeq$ additive elemental spectra
- H are images $\simeq$ additive elemental maps

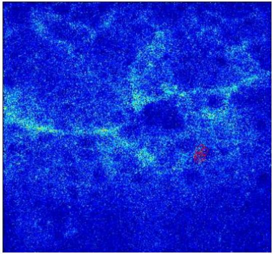


Solve using (cheap) gradient steps ... need good initialization of W!

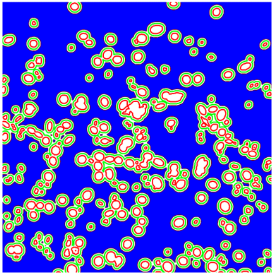
Insight from Data

Repeat analysis hundreds of times to, e.g., classify/identify cancerous cells etc.

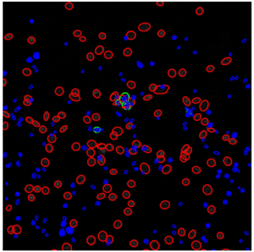
Result: Learning Cell Identification from Spectral Data



Raw data ...



... identify cell ...



... classify cells

Traditional Cell Identification at APS

Ask student/postdoc to "mark" potential cell locations by hand & test

Opportunities for Applied Math & CS Light Sources

ML plus physical/statistical models, large-scale streaming data, ...

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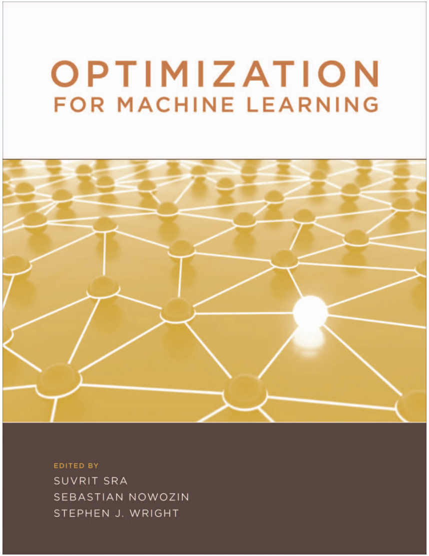
Optimization for Machine Learning [Sra, Nowozin, & Wright (eds.)]



- Convexity & Sparsity-Inducing Norms
- Nonsmooth Optimization: Gradient, Subgradient & Proximal Methods
- Newton & Interior-Point Methods for ML
- Cutting-Pane Methods in ML
- Augmented Lagrangian Methods & ADMM
- Uncertainty & Robust optimization in ML
- (Inverse) Covariance Selection

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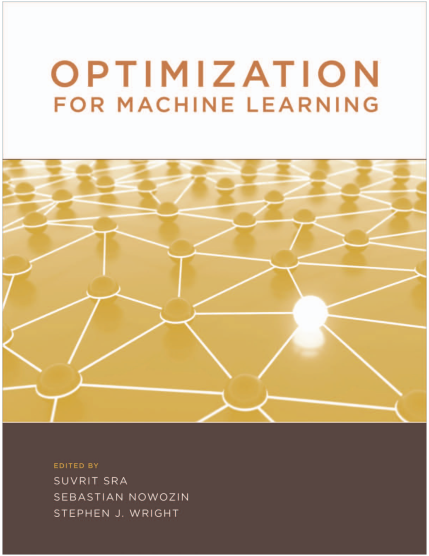

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Important Argonne Legalese Disclaimer

I made zero contributions to this fantastic book!

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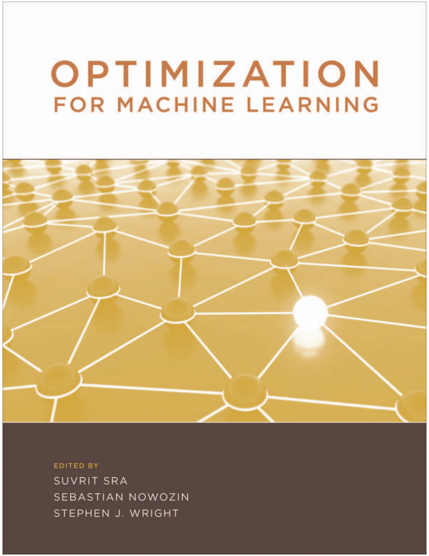

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The Four Lands of Learning [Moritz Hardt, UC Berkeley]

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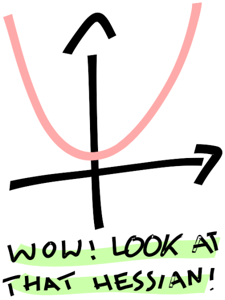
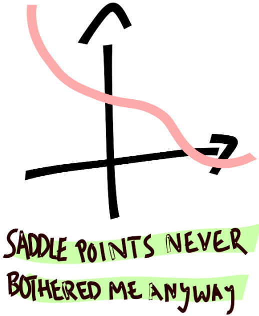


Gradientina



https://mrtz.org/gradientina.html#/

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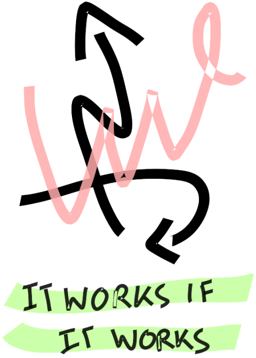

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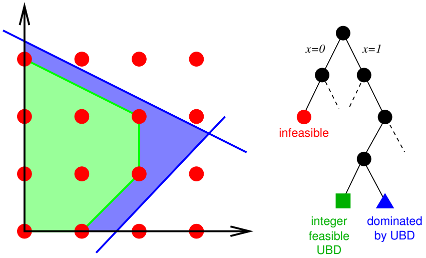
Outline

Mixed-Integer Nonlinear Optimization

Mixed-Integer Nonlinear Program (MINLP)

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \; & c(x) \le 0 \\ & x \in \mathcal{X} \\ & x_i \in \mathbb{Z} \text{ for all } i \in \mathcal{I} \end{aligned}$$

... see survey, [Belotti et al., 2013]



- $\mathcal{X}$ bounded polyhedral set, e.g. $\mathcal{X} = \{x \; : \; l \le A^T x \le u\}$
- $f : \mathbb{R}^n \to R$ and $c : \mathbb{R}^n \to \mathbb{R}^m$ twice continuously differentiable (maybe convex)
- $\mathcal{I} \subset \{1, \ldots, n\}$ subset of integer variables
- MINLPs are NP-hard, see [Kannan and Monma, 1978]
- Worse: MINLP are undecidable, see [Jeroslow, 1973]

Optimal Symbolic Regression

Goal in Optimal Symbolic Regression

Find symbolic mathematical expression that explains dependent variable in terms of independent variables without assuming functional form!

[Austel et al., 2017] propose MINLP model

- Find simplest symbolic mathematical expression ... objective
- Constrain the "grammar" of expressions ... constraints
- Match data (observations) to expression ... continuous variables
- Select "best" possible expression ... binary variables

... model mathematical expressions as a directed acyclic graph (DAG)

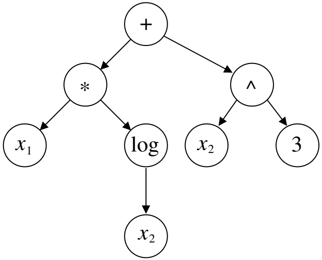
Factorable Functions and Expression Trees

Definition (Factorable Function)

$f(x)$ is factorable iff expressed as sum of products of unary functions of a finite set $\mathcal{O}_{\text{unary}} = \{\sin, \cos, \exp, \log, |\cdot|\}$ whose arguments are variables, constants, or other functions, which are factorable.

- Combination of functions from set of operators $\mathcal{O} = \{+, \times, /, \hat{}, \sin, \cos, \exp, \log, |\cdot|\}$.
- Excludes integrals $\int_{\xi=x_0}^{x} h(\xi) d\xi$ and black-box functions
- Can be represented as expression trees
- Forms basis for automatic differentiation & global optimization of nonconvex functions ... see, e.g. [Gebremedhin et al., 2005]

Expression Tree



$f(x_1, x_2) = x_1 \log(x_2) + x_2^3$

Optimal Symbolic Regression [Austel et al., 2017]

Build and solve optimal symbolic regression as MINLP

- Form "supertree" of all possible expression trees
- Use binary variables to switch parts of tree on/off
- Compute data mismatch by propagating data values through tree
- Minimize complexity (size) of expression tree with bound on data mismatch

$\Rightarrow$ large nonconvex MINLP model ... solved using `Baron`, `SCIP`, `Couenne`

Example: Kepler's Law on planetary motion from NASA data with depth 3

Data	2% Noise	10% Noise	30% Noise
Ex1	$\sqrt[3]{c\tau^2 M}$	$\sqrt[3]{\tau^2}(M+c)$	$\sqrt{c\tau^2}$
Ex2	$\sqrt[3]{c\tau^2 M}$	$\sqrt[3]{\tau^2}c$	$\sqrt{\tau}$
Ex3	$\sqrt[3]{c\tau^2 M}$	$\sqrt[3]{\tau M}+\tau$	$\sqrt{c\tau}+c$

Correct answer: $d = \sqrt[3]{c\tau^2(M+m)}$ major semi-axis of m orbiting M at period τ

Deep Neural Nets (DNNs) as MIPs [Fischetti and Jo, 2018]

Model DNN as MIP

- Model ReLU activation function with binary variables
- Model output of DNN as function of inputs (variable!)
- Solvable for DNNs of moderate size with MIP solvers

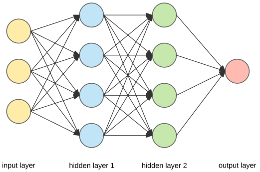


Image from Arden Dertad

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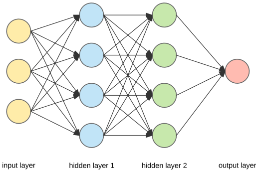

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WARNING: Do not use for training of DNN!

MIP-model is totally unsuitable for training ... cumbersome & expensive to evaluate!

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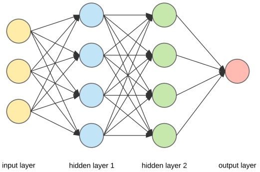

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Where can we use MIP models?

Use MIP for building adversarial examples that fool the DNN ... flexible!

Deep Neural Nets (DNNs) as MIPs [Fischetti and Jo, 2018]

- DNN with $K+1$ layers: input$=0,\ldots,K=$output
- n_k nodes/units per layer `UNIT(j,k)` with output $x_j^k \leftarrow$ `UNIT(j,k)`
- `UNIT(j,k)`, e.g. ReLU: $x^k = \max\left(0, W^{k-1}x^{k-1} + b^{k-1}\right)$,
  where W^k, b^k DNN known parameters (from training)

Key Insight (not new): Use Implication Constraints!

Model $x = \max(0, w^T y + b)$ using implications, or binary variables:

$$x = \max(0, w^T y + b) \;\Leftrightarrow\; \begin{cases} w^T y + b = x - s, \quad x \geq 0,\; s \geq 0 \\ z \in \{0,1\}, \quad \text{with } z = 1 \Rightarrow x \leq 0 \text{ and } z = 0 \Rightarrow s \leq 0 \end{cases}$$

... alternative $0 \leq s \;\perp\; x \geq 0$ complementarity constraint

Also model `MaxPool`: $x = \max(y_1, \ldots, y_t)$ using t binary vars & SOS-1 constraint

Deep Neural Nets (DNNs) as MIPs [Fischetti and Jo, 2018]

Gives MIP model with flexible objective (DNN outputs x^K, binary vars x)

$$\begin{aligned} \underset{x,s,z}{\text{minimize}} \quad & c^T x + d^T z \\ \text{subject to} \quad & \left(w_j^{k-1}\right)^T x^{k-1} + b_j^{k-1} = x_j^k - s_j^k, \quad x_j^k, s_j^k \geq 0 \\ & z_j^k \in \{0,1\}, \quad \text{with } z_j^k = 1 \Rightarrow x_j^k \leq 0 \text{ and } z_j^k = 0 \Rightarrow s_j^k \leq 0 \\ & l^0 \leq x^0 \leq u^0 \end{aligned}$$

... for given input $= x^0$, just compute output $= x^K$ expensive!

Modeling Implication Constraints

$$\begin{aligned} & z \in \{0,1\}, \quad \text{with } z = 1 \Rightarrow x \leq 0 \text{ and } z = 0 \Rightarrow s \leq 0 \\ \Leftrightarrow\ & z \in \{0,1\}, \quad \text{with } x \leq M_x(1-z) \text{ and } s \leq M_s z \end{aligned}$$

Use MIP for Building Adversarial Example

- Fix weights W, b from training data
- Find smallest perturbation to inputs x^0 that results in mis-classification

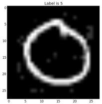
Deep Neural Nets (DNNs) as MIPs [Fischetti and Jo, 2018]

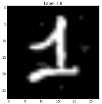
Example: DNN for digit classification as MIP

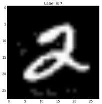
- Misclassify all digits: $\hat{d} = (d + 5) \bmod 10$, i.e. $0 \to 5$, $1 \to 6$, ...
- Require activation of "wrong" digit in final layer is 20% above others
- Need tight bnds M_x, M_s in implications: propagate bnds forward through DNN

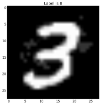
Results with CPLEX Solver and Tight Bounds (300s max CPU)

# Hidden	# Nodes	% Solved	# Nodes	CPU
3	8	100	552	0.6
4	20/8	100	20,309	12.1
5	20/10	67	76,714	171.1









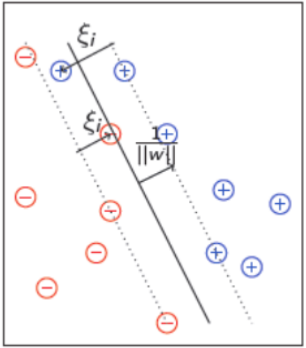
Sparse Support-Vector Machines

Standard SVM Training

- Data $S = \{x_i, y_i\}_{i=1}^m$: features $x_i \in \mathbb{R}^n$ labels $y_i \in \{-1, 1\}$
- $\xi \geq 0$ slacks, b bias, $c > 0$ penalty parameter

$$\begin{aligned} \underset{w,b,\xi}{\text{minimize}} \quad & \tfrac{1}{2}\|w\|_2^2 + c\|\xi\|_1 = \tfrac{1}{2}\|w\|_2^2 + c\mathbf{1}^T\xi \\ \text{subject to} \quad & Y(Xw - b\mathbf{1}) + \xi \geq \mathbf{1} \\ & \xi \geq 0, \end{aligned}$$

where $Y = \text{diag}(y)$ and $X = [x_1, \ldots, x_m]^T$



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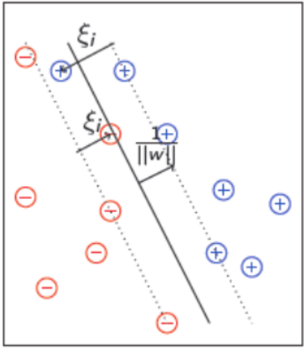


Find MINLP Model for Feature Selection in SVMs

Given labeled training data find maximum margin classifier that minimizes hinge-loss and cardinality of weight-vector, $\|w\|_0$

Sparse Support-Vector Machines

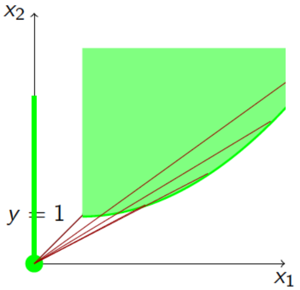
[Guan et al., 2009] consider ℓ_0-norm penalty on w as MINLP

$$\begin{aligned} \underset{w,b,\xi}{\text{minimize}} \quad & \tfrac{1}{2}\|w\|_2^2 + a\|w\|_0 + c\mathbf{1}^T\xi \\ \text{subject to } & Y(Xw - b\mathbf{1}) + \xi \geq \mathbf{1},\ \xi \geq 0, \end{aligned}$$

Model ℓ_0 with Perspective & Binary z_j Counter

$$\begin{aligned} \underset{u,w,b,\xi,z}{\text{minimize}} \quad & \mathbf{1}^T u + a\mathbf{1}^T z + c\mathbf{1}^T\xi \\ \text{subject to } & Y(Xw - b\mathbf{1}) + \xi \geq \mathbf{1},\ \xi \geq 0 \\ & w_j^2 \leq z_j u_j,\ u \geq 0,\ z_j \in \{0,1\} \end{aligned}$$

... conic-MIP, see, e.g. [Günlük and Linderoth, 2008]



... $w_j^2 \leq z_j u_j$ violates CQs $\Rightarrow$ weaker big-M formulation ...

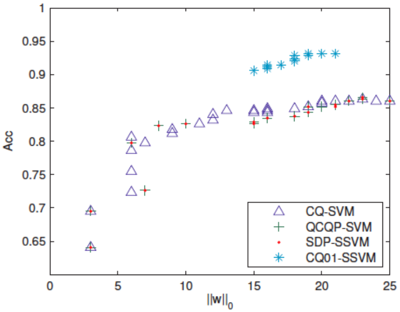
$$0 \leq u_j \leq M_u z_j, \quad w_j^2 \leq u_j$$

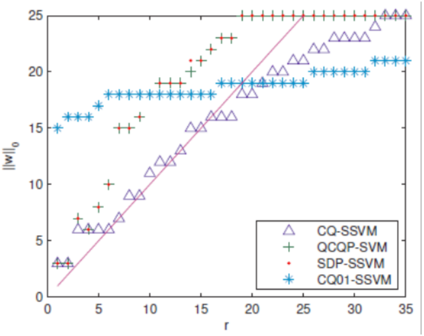
Sparse Support-Vector Machines

[Goldberg et al., 2013] rewrite $w_j^2 \leq z_j u_j$ as

$$\| (2w_j, u_j - z_j) \|_2 \leq u_j + z_j$$

... second-order cone constraint ... and relax integrality ... add $\sum z_j \leq r$





... good classification accuracy & small $\|w\|_0$!

Sparse Support-Vector Machines [Maldonado et al., 2014]

Mixed-Integer Linear SVM

[Maldonado et al., 2014] formulate MILP: min $\|\xi\|_1$ subj. to $\|w\|_0 \leq B$

$$
\begin{aligned}
\underset{w,b,\xi,z}{\text{minimize}} \quad & \mathbf{1}^T \xi && \text{classification error} \\
\text{subject to } & Y(Xw - b\mathbf{1}) + \xi \geq \mathbf{1} && \text{classifier c/s} \\
& L z_j \leq w_j \leq U z_j && \text{on/off } w_j \\
& \sum_j c_j z_j \leq B && \text{budget constraint} \\
& \xi \geq 0, \quad z_j \in \{0, 1\}
\end{aligned}
$$

for bounds $L < U$ and budget $B > 0$

Outline

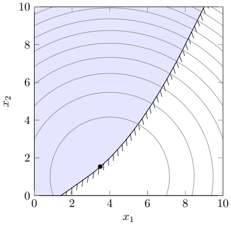
Nonlinear Robust Optimization

Nonlinear Robust Optimization

$$\underset{x}{\text{minimize}} \quad f(x)$$
$$\text{subject to } c(x; u) \geq 0, \quad \forall\, u \in \mathcal{U}$$
$$x \in \mathcal{X}$$

Small Example

$$\underset{x \geq 0}{\text{minimize}} \quad (x_1 - 4)^2 + (x_2 - 1)^2$$
$$\text{subject to } x_1\sqrt{u} - x_2 u \leq 2,$$
$$\ldots \forall u \in \left[\tfrac{1}{4}, 2\right]$$



Assumptions (e.g. [Leyffer et al., 2018]) ... wlog assume $f(x)$ is deterministic

- $u \in \mathcal{U}$ uncertain parameters closed convex set, independent of x
- $c(x; u) \geq 0 \ \forall\, u \in \mathcal{U}$ robust constraints ... semi-infinite optimization problem
- $\mathcal{X} \subset \mathbb{R}^n$ standard (certain) constraints; $f(x)$ and $c(x; u)$ smooth functions

Linear Robust Optimization [Ben-Tal and Nemirovski, 1999]

Robust linear constraints are easy! E.g. $a^T x + b \geq 0, \quad \forall a \in \mathcal{U} := \{B^T a \geq c\}$

... rewrite semi-infinite constraint as a minimum

$$\Leftrightarrow \left\{ \begin{array}{ll} \underset{a}{\text{minimize}} & a^T x + b \\ \text{subject to } B^T a \geq c \end{array} \right\} \geq 0$$

... apply duality: $\mathcal{L}(a, \lambda) := a^T x + b - \lambda^T (B^T a - c)$

$$\Leftrightarrow \left\{ \begin{array}{l} \underset{a,\lambda}{\text{maximize}} \;\; \mathcal{L}(a, \lambda) = b + \lambda^T c \\ \text{subject to } 0 = \nabla_a \mathcal{L}(a, \lambda) = x - B\lambda, \quad \lambda \geq 0 \end{array} \right\} \geq 0$$

... only need feasible point ≥ 0 ... becomes standard polyhedral set

$$b + \lambda^T c \geq 0, \quad x = B\lambda, \quad \lambda \geq 0$$

Duality Trick for Conic and Linear Robust Optimization

Duality trick generalizes to other conic uncertainty sets

$$(P) \quad \underset{x}{\text{minimize}} \ f(x) \quad \text{subject to } c(x;u) \geq 0, \ \forall\, u \in \mathcal{U}, \quad x \in \mathcal{X}$$

... creates classes of tractable extended formulations

Robust Constraints $c(x;u) \geq 0$	Uncertainty Set $\mathcal{U}$	Extended Formulation
Linear	Polyhedral	Linear Program
Linear	Ellipsoidal	Conic QP
Conic	Conic	SDP

Robust Optimization for Support Vector Machines (SVMs)

Standard SVM Training

- Data $S = \{x_i, y_i\}_{i=1}^m$: features $x_i \in \mathbb{R}^n$ labels $y_i \in \{-1, 1\}$
- $\xi \geq 0$ slacks, b bias, $c > 0$ penalty parameter

$$\begin{aligned} \underset{w,b,\xi}{\text{minimize}} \quad & \tfrac{1}{2}\|w\|_2^2 + c\mathbf{1}^T\xi \\ \text{subject to } & Y\left(Xw - b\mathbf{1}\right) + \xi \geq \mathbf{1}, \qquad \xi \geq 0, \end{aligned}$$

where $Y = \text{diag}(y)$ and $X = [x_1, \ldots, x_m]^T$

SVMs with Additive Location Errors

- See survey article [Caramanis et al., 2012] & use duality trick!
- Location errors $x_i^{\text{true}} = x_i + u_i$ & ellipsoid uncertainty $\mathcal{U} = \{u_i \mid u_i^T\Sigma u_i \leq 1\}$:

$$\begin{aligned} y_i\left(w^T(x_i + u_i) - b\right) + \xi \geq 1, \qquad & \forall u_i : u_i^T\Sigma u_i \leq 1 \\ \Leftrightarrow y_i\left(w^Tx_i - b\right) + \xi + \|\Sigma^{1/2}w\|_2 \geq 1 \qquad & \text{SOC constraint} \end{aligned}$$

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General Case of Location Errors: "Worst-Case SVM"

$$\underset{w,b}{\text{minimize}} \ \underset{u \in \mathcal{U}}{\text{maximize}} \left\{ \frac{1}{2}\|w\|_2^2 + c \sum_j \max\left\{1 - y_j\left(w^T(x_j + u_j) - b\right), 0\right\} \right\}$$

for uncertainty set $U = \left\{(u_1, \ldots, u_m) \mid \sum_j \|u_j\| \leq d\right\}$ equivalent to

$$\underset{w,b}{\text{minimize}} \left\{ \frac{1}{2}\|w\|_2^2 + d\|w\|_D + c \sum_j \max\left\{1 - y_j\left(w^T(x_j + u_j) - b\right), 0\right\} \right\}$$

where $\|\cdot\|_D$ is dual norm of $\|\cdot\|$, e.g. $\ell_2 \leftrightarrow \ell_2$ or $\ell_\infty \leftrightarrow \ell_1$, ... follows from duality

[Caramanis et al., 2012] argue that derivation shows that:

- Regularized classifiers are more robust: satisfy worst-case principle
- Provide probabilistic interpretation if viewed as chance constraints

Conclusions and Extension: Optimization for Machine Learning

Conclusions

- Mixed-Integer Optimization for Machine Learning
  - Optimal symbolic regression, expression trees, nonconvex MIP
  - MIPs of deep neural nets for building adversarial examples
  - Support-vector machines & ℓ_0 regularizers & constraints
- Robust Optimization for Machine Learning
  - Best "worst-case" SVM $\Rightarrow$ equivalent tractable formulation

Extensions and Challenges

- Extending use of integer variables into design of DNNs
- Realistic stochastic interpretation of regularizers in SVM, DNN, ...

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