Approximate Nonconvex Optimization and Treewidth

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Collaborators +

- Gonzalo Muñoz: optimizer
- Sebastian Pokutta: optimizer, ML, algorithms, everything
- Mark Zuckergerg, Nuri Ozbay: ex Ph-D students
- Some of us (me) are not ML experts. Some of us are.
- This talk is about theory, theory, theory.
- But we will also outline a possible realistic application of the methodology.

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- It has been only recently that results regarding the complexity of training deep neural networks have been obtained.
- We will show that large classes of Neural Networks can be trained to proved near optimality using linear programs whose size is linear on the training data.
- SGD has running time linear on the training data, but it does not offer optimality guarantees.

Empirical Risk Minimization problem

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Given:

- D data points $(\hat{x}_i, \hat{y}_i)$, $i = 1, \ldots, D$
- $\hat{x}_i \in \mathbb{R}^n,\ \hat{y}_i \in \mathbb{R}^m$
- A loss function $\ell : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ (not necessarily convex)

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Compute $f : \mathbb{R}^n \to \mathbb{R}^m$ to solve

$$
\begin{aligned}
&\min_f \frac{1}{D} \sum_{i=1}^{D} \ell(f(\hat{x}^i), \hat{y}^i) && \text{(+ optional regularizer } \Phi(f)\text{)} \\
&f \in F && \text{(some class)}
\end{aligned}
$$

Function parameterization

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Using this notation the ERM problem becomes

$$\min_{\theta \in \Theta} \frac{1}{D} \sum_{i=1}^{D} \ell(f(\hat{x}^i, \theta), \hat{y}^i)$$

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Examples:

- Linear Regression. $f(x) \;=\; Ax + b$ with ℓ_2-loss.
- Binary Classification. Varying f families and cross-entropy loss: $\ell(p, y) = -y \log(p) - (1 - y) \log(1 - p)$
- Neural Networks with k layers. $f(x) \;=\; T_{k+1} \circ \sigma \circ T_k \circ \sigma \ldots \circ \sigma \circ T_1(x)$, each T_j affine.

Deep Networks (with 2-norm squared loss)

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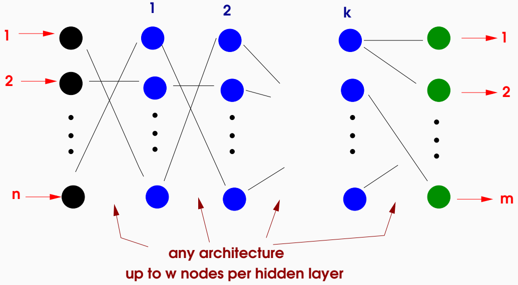
- A_1 is $n \times w$, A_{k+1} is $w \times m$, A_i is $w \times w$ otherwise.



What we know for Neural Nets

Hardness Result

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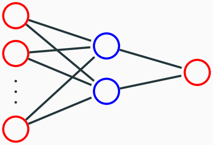
Theorem (Blum and Rivest 1992)

When $\ell \in$ (absolute value, 2-norm squared) training is NP-hard even if $k = 1$ (only 3 nodes), $D \in O(n)$, $m = 1$, $\hat{x}^i \in \{0,1\}^n$, $\hat{y}^i \in \{0,1\}$ and weights are ± 1.



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- *Running time is (more than) doubly exponential in e.g. number of layers.*
- *For two layers, exponential in* $\epsilon^{-\Theta(1)}$ *and polynomial in* D

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$$O\left(2^w \boldsymbol{D}^{\boldsymbol{nw}} poly(D, n, w)\right)$$

*Polynomial in the size **D** of the data set, for fixed n, w.*

$\boldsymbol{n} =$ *dimension of input vectors,*

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Theorem

For every $\epsilon > 0$, ℓ, $\Theta \subseteq [-1, 1]^N$ and D, there is a polytope with variables (θ, x^i, y^i, L_i) of size

$$O\left((2\mathcal{L}/\epsilon)^{N+n+m+1}\, D\right)$$

($\boldsymbol{\mathcal{L}}$ = *largest Lipshitz constant of any* $\boldsymbol{\sigma}$, *and* $\mathbf{N = O(wk)}$)

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s.t. $\forall$ data set $(\hat{X}, \hat{Y}) = (\hat{x}^i, \hat{y}^i)$, $i = 1, \ldots D$, there is a face $\mathcal{F}_{\hat{X},\hat{Y}}$ with

$$\min_{\theta \in \Theta} \frac{1}{D} \sum_{i=1}^{D} L_i$$

$$(\theta, L) \in \mathrm{proj}(\mathcal{F}_{\hat{X},\hat{Y}})$$

provides an ϵ-approximation to ERM with data $\hat{X}, \hat{Y}$.

A uniform ("universal") linear program of size linear in the quantity of training data.

Our main toolset

Treewidth

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- **OLD** concept, but term coined by Robertson and Seymour (1980s).
- Informal definition: graphs with small treewidth are the "simple" graphs
- **Many** equivalent definitions.
- Trees have treewidth 1
- Cycles have treewidth 2
- K_n has treewidth $n - 1$
- the $k \times k$ planar grid has treewidth k

Treewidth

Informal algorithmic definition:

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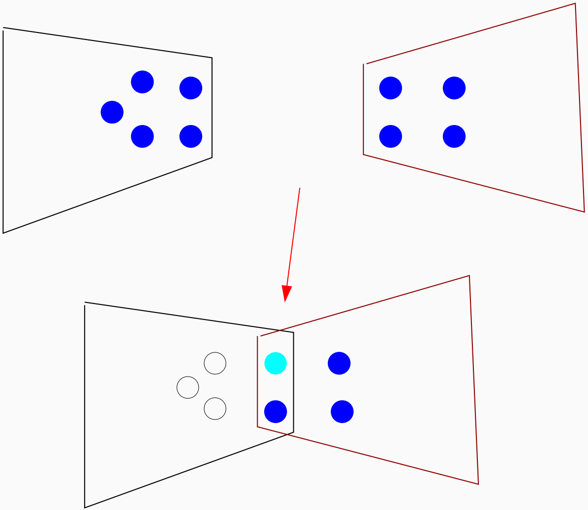
- Start with with m “bags” with up to $\omega + 1$ vertices each, numbered $1, 2, \ldots, m$. “Bag” = graph.
- Each bag includes some edges between vertices in the bag.
- Start of procedure: each bag is a “processed unit”. All vertices are “boundary” vertices.
- Inductive step: take two processed units. Idenfify (“glue”) some of the boundary with the same number of vertices in one unit with same number of boundary vertices of the other, forming a new processing unit.
- The boundary of the new unit will be a subset of the union of the two boundaries, of size $\leq \omega + 1$

Treewidth



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  - Early result: given a planar graph H any graph with no H minor has tree-width at most $f(H)$.

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- Nonserial Dynamic Programming, Nemhauser (1964). Bertele and Brioschi (1972).

Second tool: approximation through digitization

Let $0 \leq z \leq 1$ and let $L > 0$ integral
Then we can approximate

$$z \quad \approx \quad \textstyle\sum_{k=1}^{L} 2^{-k}\, y_k, \quad \text{where each } y_k \text{ binary.}$$

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- $\hat{F}(y) \leq F(x) + m\mathcal{L}\, 2^{-L}$

Final ingredient: lifted formulations

Lovász and Schrijver, Sherali and Adams, ~ 1990

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    then can say: $2x[\{1,2\},\{3\}] + x[\{1,2,4\},\{3\}] \leq x[\{1,2\},\{3\}]$
  - And more, e.g. $x[\{1,2\},\{3\}] + x[\{1\},\{2,3\}] = x[\{1\},\{3\}]$
- "Level-k" formulation: only use monomials with up to k terms

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then "level-k" formulation implies all valid inequalities $c^T x \leq d$

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- $0/1$ integer programming: $\{x \in \{0,1\}^n \ : \ Ax \leq b\}$
- Key idea: **add** new variables that express conjunctions:
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  - Same as monomial $x_1 x_2 (1 - x_3)$
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where the subgraph of the intersection graph of A, induced by c
has **treewidth** $\leq k$

Approximate optimization of well-behaved functions

Prototype problem:

$$\begin{aligned} c^* \ \doteq \ \min\ & c^T x \\ \text{s.t. } & f_i(x) \leq 0, \qquad i = 1, \ldots, m \\ & x \in [0,1]^n \end{aligned}$$

An extension of work in Bienstock and Muñoz (2015).

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$$c^T\hat{x} \ \le \ c^* + O(\epsilon), \quad f_i(\hat{x}) \ \le \ O(\epsilon)\ \forall i$$

Application to ERM problem

We now apply the LP approximation result to:

$$\min_{\theta\in\Theta} \frac{1}{D}\sum_{i=1}^{D} \ell(f(\hat{x}^i,\theta),\hat{y}^i) \quad 1\leq i\leq D$$

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with $\Theta \subseteq [-1,1]^N$, $\hat{x}^i \in [-1,1]^n$ and $\hat{y}^i \in [-1,1]^m$. We use the epigraph formulation:

$$\min_{\theta\in\Theta} \frac{1}{D}\sum_{i=1}^{D} L_i$$

$$L_i \geq \ell(f(\hat{x}^i,\theta),\hat{y}^i) \quad 1 \leq i \leq D$$

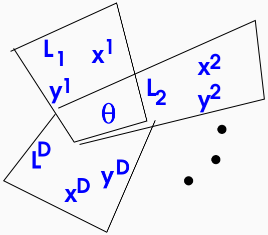
Let $\mathcal{L}$ be the Lipschitz constant for $g(x,y,\theta) \doteq \ell(f(x,\theta),y)$ over $[-1,1]^{n+m+N}$.

Proof Sketch

Every system of constraints of the type

$$L_i \geq \ell(f(x^i, \theta), y^i) \quad 1 \leq i \leq D$$

has an intersection graph with the following structure:



resulting in a formulation with *treewidth* at most $N + n + m + 1$

LP size details

Thus the LP size given by the expression

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Different architectures $\rightarrow$ N and $\mathcal{L}$.

Architecture-Specific Consequences

Theorem (Arora, Basu, Mianjy and Mukherjee 2018)

If $k = 1$ *(one "hidden layer") and* $m = 1$ *there is an exact training algorithm of complexity*

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If $k = 1$ (one "hidden layer") and $m = 1$ there is an exact training algorithm of complexity

$$O\left(\, 2^{w} D^{nw} poly(D, n, w) \,\right)$$

Polynomial in the size of the data set, for fixed n, w.

Consequence of our result

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If the entries of A_i, b_i are required to be in $[-1, 1]$, for any k, n, m, w, ϵ there is a uniform LP of size

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Core of the proof: In a DNN with k hidden layers the Lipschitz constant of $g(x, y, \theta)$ over $[-1, 1]^{n+m+N}$ is $\sim nw^k$.

The Blum-Rivest setup (Binarized Neural Networks)

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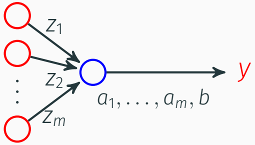
Activation units:



With $z \in \{0,1\}^m$,

$$y = \begin{cases} 1, & \text{if } a^T z > b \\ 0, & \text{otherwise.} \end{cases}$$

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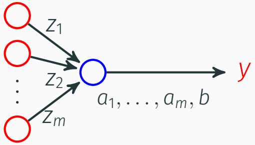

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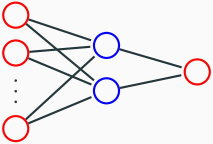
Network with n binary inputs, m binary outputs, k layers

The Blum-Rivest setup (Binarized Neural Networks)

Theorem (Blum and Rivest 1992)

When $\ell \in$ (absolute value, 2-norm squared) training is NP-hard even if $k = 1$ (only 3 nodes), $D \in O(n)$, $m = 1$ and weights are ± 1.



Theorem

Consider a BNN with $m = 1$ and ℓ arbitrary. There is a uniform LP of size

$$O(2^{poly(k,n,w)}D)$$

that solves ERM exactly for any input data.

Concluding comments

- The results can be improved by considering the sparsity of the network itself.
- Training using this approach *generalizes*. Meaning, using *enough*[1] data points we get an approximation to the "true" Risk Minimization problem.

[1] depends on $\mathcal{L}$ and ϵ

Thank you!

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We are solving Linear Programs. There are classical examples of linear programs that are solved **incrementally**.

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- Example 1: Edmonds' weighted matching algorithm (bah, that is theory only)
- Example 2: Solving large set-partitioning LPs (airline industry)
- This requires tricks that exploit LP structure. It only works with LPs that have specific, known structure
- That is the case in the above LPs.