Global Optimality Beyond Two Layers: Training Deep ReLU Networks via Convex Programs

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Tolga Ergen & Mert Pilanci

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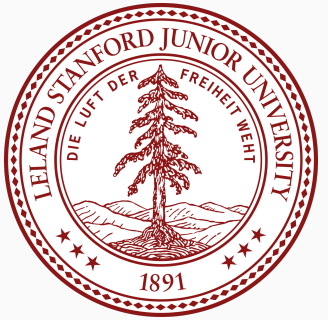
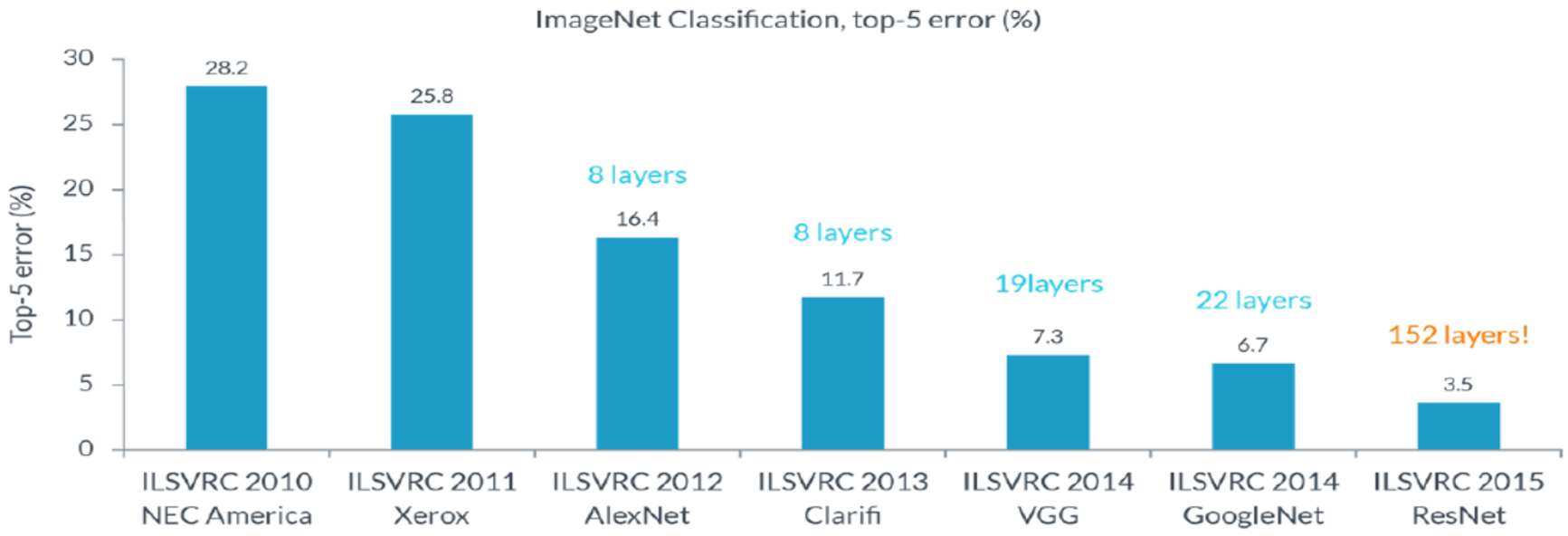
Stanford University



Deep Learning Revolution



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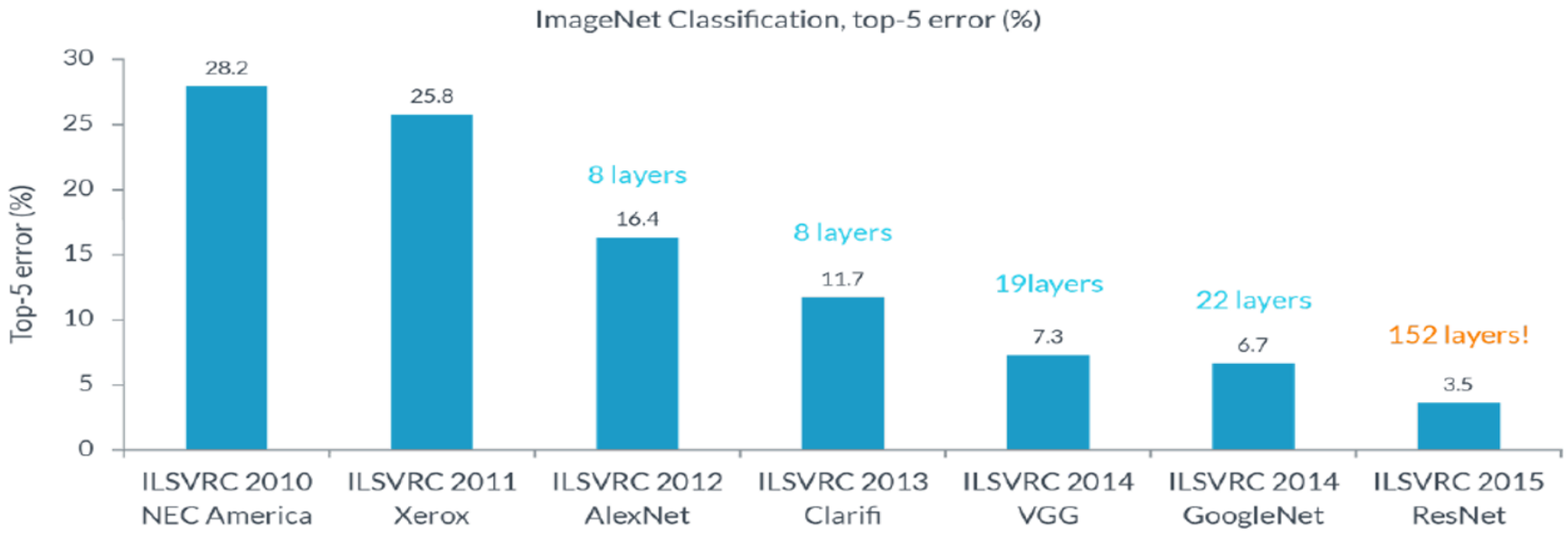

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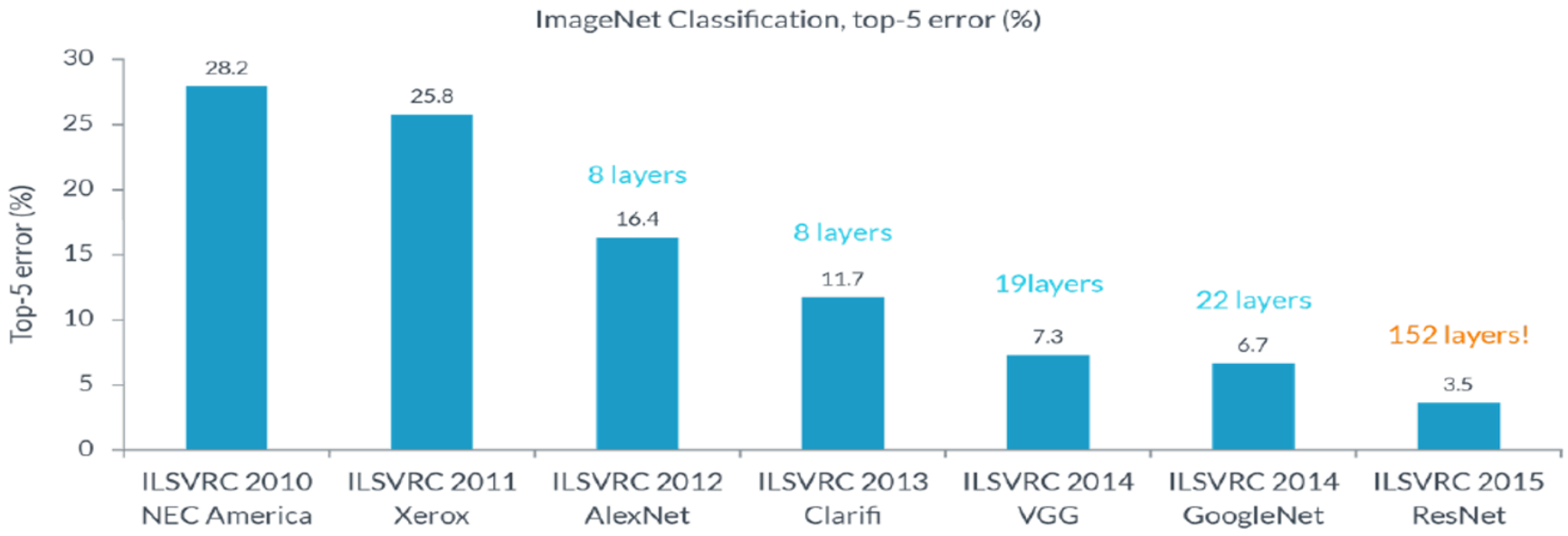

Deep learning models:

- often provide the best performance due to their large capacity
  - challenging to train
- are complex black-box systems based on non-convex optimization
  - hard to interpret what the model is actually learning

Problem Formulation

Model:

Notation:

$\mathbf{X}\ 2\ \mathrm{R}^{n\ \ d}$: Data matrix

$\mathbf{y}\ 2\ \mathrm{R}^{n}$: Label vector

$L(\ ;\ )$: Convex loss function

$R(\ )$: Regularization function

$\ > 0$: Regularization coe cient

: All parameters

l and k : Layer and sub-network indices

$\mathbf{W}_{lk}\ 2\ \mathrm{R}^{m_{l\ \ 1}\ \ m_l}$: Weights

$f_{\ ;k}(\mathbf{X}) := \ (\mathbf{X}\mathbf{W}_{1k})_{+} : : : \mathbf{w}_{(L\ \ 1)k\ \ +} w_{Lk}$

Optimization problem:

$$\min L \left(\sum_{k=1}^{K} f_{\ ;k}(\mathbf{X}); \mathbf{y} \right) + \sum_{k=1}^{K} R_k(\ )$$

Prior Work

- (Haeffele and Vidal, 2017) provided conditions to guarantee that each local minimum is a global optimum
  - require all local minima to be rank-deficient

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- (Pilanci and Ergen, 2020) introduced convex representations for ReLU networks
  - valid only for two-layer networks

Convex Duality for Deep Neural Networks

Lemma

The following problems are equivalent

$$P := \min_{\theta \in \Theta} L\left(\sum_{k=1}^{K} f_{\theta,k}(\mathbf{X}), \mathbf{y}\right) + \frac{\beta}{2} \sum_{k=1}^{K} \sum_{l=L_1}^{L} \|\mathbf{W}_{lk}\|_F^2 = \min_{\theta \in \Theta_p} L\left(\sum_{k=1}^{K} f_{\theta,k}(\mathbf{X}), \mathbf{y}\right) + \beta \sum_{k=1}^{K} |w_{Lk}|,$$

where $\Theta_p := \{\theta : \|\mathbf{W}_{lk}\|_F \leq 1, \forall l \in [L_1, L-2], \|\mathbf{w}_{(L-1)k}\|_2 \leq 1, \forall k\}$.

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$$P^* := \min_{\beta \in \Theta} L\left(\sum_{k=1}^{K} f_{:,k}(\mathbf{X}) \beta_k, \mathbf{y} \right) + \frac{\beta}{2} \sum_{k=1}^{K} \sum_{l=L-1}^{L} \|\mathbf{W}_{lk}\|_F^2 = \min_{\beta \in \Theta_p} L\left(\sum_{k=1}^{K} f_{:,k}(\mathbf{X}) \beta_k, \mathbf{y} \right) + \beta \sum_{k=1}^{K} |w_{Lk}|,$$

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Dual problem with respect to w_{Lk}:

$$P^* \geq D := \max_{\mathbf{v}} -L^*(\mathbf{v}) \text{ s.t. } \max_{\beta \in \Theta_p} |\mathbf{v}^T (\mathbf{X}\mathbf{W}_1)_+ \cdots \mathbf{w}_{(L-1)+}| \leq \beta,$$

where L^* is the Fenchel conjugate function

$$L^*(\mathbf{v}) := \max_{\mathbf{z}} \mathbf{z}^T \mathbf{v} - L(\mathbf{z}, \mathbf{y})$$

Our contribution: We first prove strong duality, i.e., $P^* = D^*$ and then derive convex formulations

Convex Program for Three-layer Networks

Theorem

The non-convex training problem can be equivalently stated as

$$\min_{\mathbf{w};\mathbf{w}^0 \in C} \frac{1}{2} \left\| \mathbf{X}(\mathbf{w}^0 \quad \mathbf{w}) \quad \mathbf{y} \right\|_2^2 + \quad (k\mathbf{w}k_{2;1} + k\mathbf{w}^0 k_{2;1})$$

where $k \quad k_{2;1}$ *is d dimensional group norm:* $k\mathbf{w}k_{2;1} := \sum_{i=1}^{P} k\mathbf{w}_i k_2$

$$\mathbf{X} := \begin{bmatrix} \mathbf{X}_s & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_s \end{bmatrix}; \quad \mathbf{X}_s := \begin{bmatrix} \mathbf{D}_1\mathbf{X} & \mathbf{D}_2\mathbf{X} & \vdots & \mathbf{D}_P\mathbf{X} \end{bmatrix} :$$

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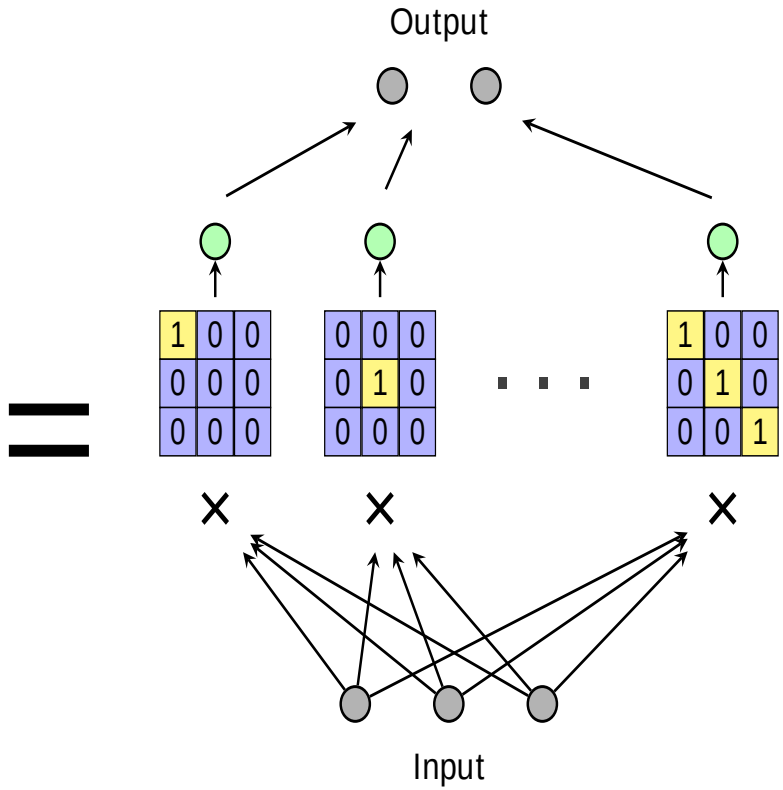
Diagonal matrices (D):

$$(\mathbf{X}\mathbf{w})_+ = \mathbf{D}\mathbf{X}\mathbf{w} \quad ( ) \quad \begin{matrix} \mathbf{D}\mathbf{X}\mathbf{w} & 0 \\ (\mathbf{I}_n & \mathbf{D})\mathbf{X}\mathbf{w} \quad 0 \end{matrix} \quad ( ) \quad (2\mathbf{D} \quad \mathbf{I}_n)\mathbf{X}\mathbf{w} \quad 0;$$

where $\mathbf{D} \in \mathrm{R}^{n \quad n}$ is a diagonal matrix of zeros and ones, i.e., $\mathbf{D}_{ii} \in \{0; 1\}$

Training Complexity

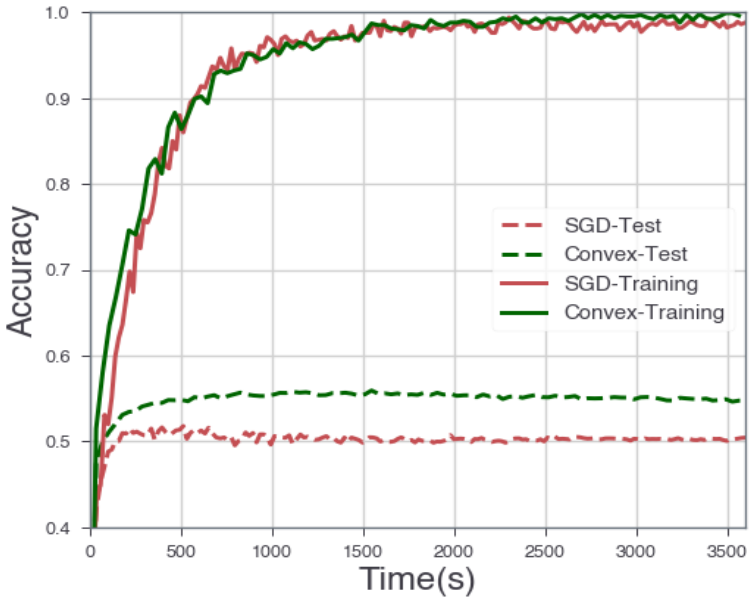
Architecture with three sub-networks ($K = 3$) and ReLU layers ($L = 3$):



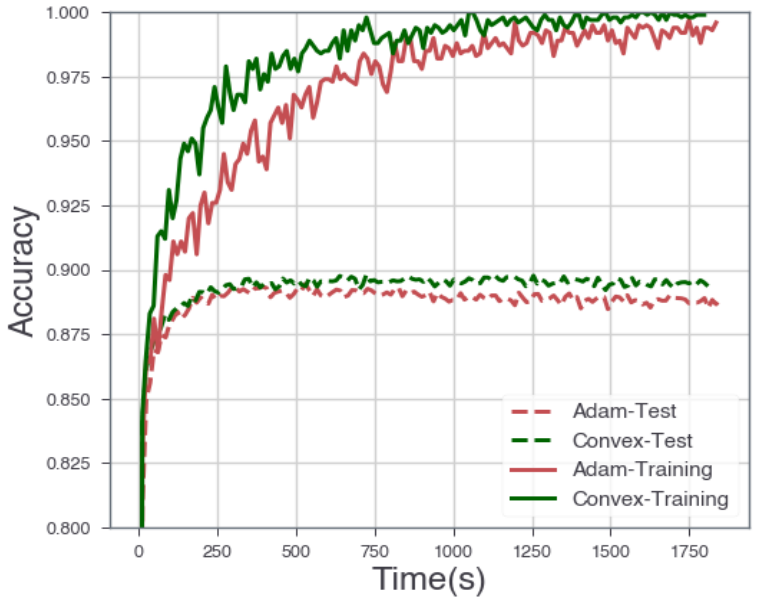
Non-convex **Convex**

Convex program can be globally optimized by standard interior-point solvers with complexity $O(poly(n; d))$

Numerical Results



(a) CIFAR-10



(b) Fashion-MNIST

Figure 1: Test accuracy of a three-layer architecture trained using the non-convex formulation and the convex program

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- **Limitations:**
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  - we put unit `$_2$-norm constraints on the first L 2 layer weights (weight decay may not be the right way to regularize?)
  - when the data matrix is full rank, our approach has exponential-time complexity, which is unavoidable unless P = NP

References

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