The Hidden Convex Optimization Landscape of Deep Neural Networks

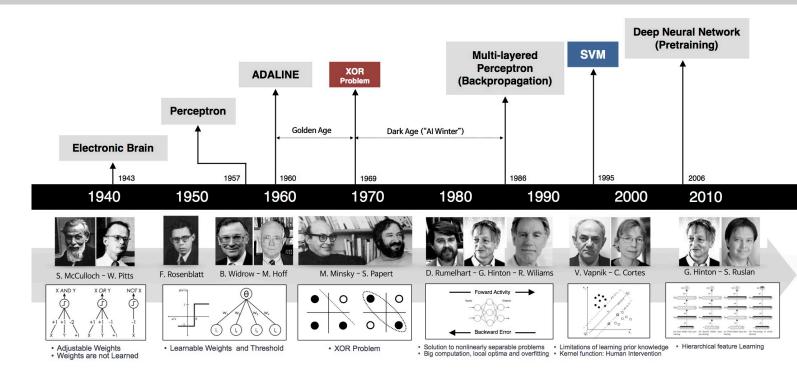
One World Optimization Seminar

Mert Pilanci

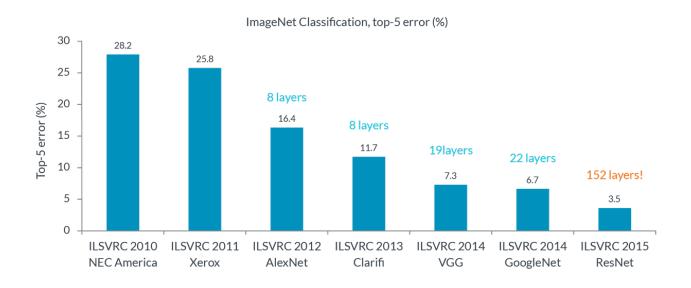
Electrical Engineering Stanford University

joint work with Tolga Ergen, Jonathan Lacotte and Yifei Wang

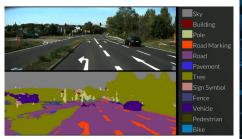
History of Artificial Neural Networks



Deep learning revolution



The Impact of Deep Learning

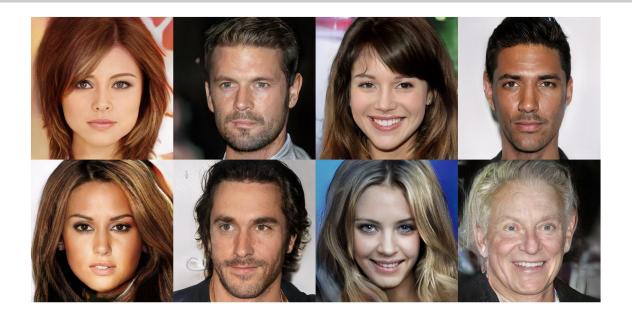






Y. LeCun, Y. Bengio, G. Hinton (2015)

The Impact of Deep Learning



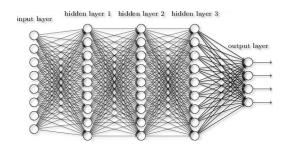
these are not real people

Generative Adversarial Networks, Goodfellow et al. (2014), Karras et al. (2018)

Outline

- Challenges in neural networks
- ReLU neural networks are convex models
- Role of the architecture
- Generative Adversarial Networks
- Deeper ReLU networks

Deep Neural Networks



- non-convex (stochastic) gradient descent
- extremely high-dimensional problems

152 layer ResNet-152: 60.2 Million parameters (2015)

GPT¹-3 language model: 175 Billion parameters (May 2020)

BAAI² multi-modal model: 1.75 Trillion parameters (June 2021)

¹OpenAl General Purpose Transformer

²The Beijing Academy of Artificial Intelligence

- often provide the best performance due to their large capacity
 - \rightarrow challenging to train

GPT-3 is estimated to cost \$12 Million for a single training run requires large non-public datasets

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

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 - ightarrow hard to interpret what the model is actually learning

nature

Letter | Published: 29 August 2018

Deep learning of aftershock patterns following large earthquakes

Phoebe M. R. DeVries ⊡, Fernanda Viégas, Martin Wattenberg & Brendan J. Meade

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

one year later, another paper logistic regression performs just as good as the 6 layer NN

nature

Matters Arising | Published: 02 October 2019

One neuron versus deep learning in aftershock prediction

Interpretability is important

Example: Deep networks for MR image reconstruction (FastMRI Challenge, 2020)

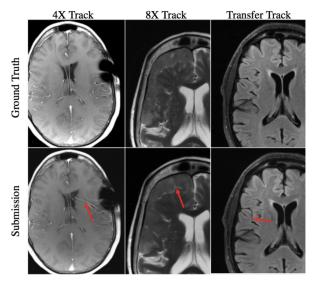


Figure 7: Examples of reconstruction hallucinations among challenge submissions. (*left*) A 4X submission from Neurospin generated a false vessel, possibly related to susceptibilities introduced by surgical staples. (*center*) An 8X submission from ATB introduced a linear bright signal mimicking a cleft of cerebrospinal fluid, as well as blurring of the boundaries of the extra-axial mass. (*right*) A submission from ResoNNance introduced a false sulcus or prominent vessel.

Adversarial examples



"panda" 57.7% confidence



+.007 ×

"nematode" 8.2% confidence



"gibbon"
99.3 % confidence





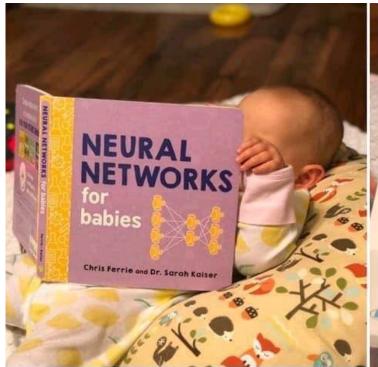
- o adversarial examples, Szegedy et al., 2014, Goodfellow et al., 2015
- o stop sign recognized as speed limit sign, Evtimov et al, 2017

Questions

- What are neural networks actually doing?
- Are they automatically finding the 'best' features?
- Is it possible to establish optimality?
- Is there a more efficient way?

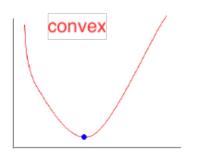
deep convnet (2012), transformer (2017), fully connected mixer (May 2021), ...?

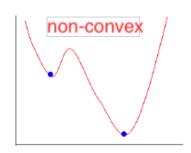
How neural networks work?





How neural networks work?





- least-squares, logistic regression, support vector machines etc. are understood extremely well
- the choice of the solver does not matter
- insightful theorems for neural networks?

Least Squares

$$\min_{x} \|Ax - b\|_2^2$$

convex optimality condition: $A^TAx = A^Tb$ efficient solvers: conjugate gradient (CG), preconditioned CG, QR, Cholesky...

Least Squares with L1 Regularization

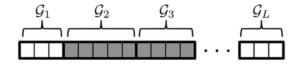
$$\min_{x} ||Ax - y||_{2}^{2} + \lambda ||x||_{1}$$

Lasso

• L1 norm $||x||_1 = \sum_{i=1}^d |x_i|$ encourages sparsity in the solution x^*

Least Squares with Group L1 regularization

$$\min_{x} \| \sum_{i=1}^{k} A_i x_i - y \|_2^2 + \lambda \sum_{i=1}^{k} \| x_i \|_2$$



Group Lasso

- \circ encourages group sparsity in the solution x^* , i.e., most blocks x_i are zero
- o convex optimization and convex regularization methods are well understood

Yuan & Lin (2007), Cevher et al. (2009, 2013, 2016)

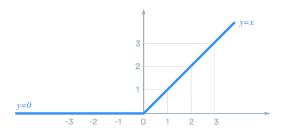
Two-Layer Neural Networks with Rectified Linear Unit (ReLU) activation

$$p_{\text{non-convex}} := \min \min L \left(\phi(XW_1)W_2, y \right) + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$

$$W_1 \in \mathbb{R}^{d \times m}$$

$$W_2 \in \mathbb{R}^{m \times 1}$$

where
$$\phi(u) = \text{ReLU}(u) = (u)_+$$



Neural Networks are Convex Regularizers

$$\begin{aligned} p_{\mathsf{non-convex}} &:= & \min\!\min\! \ L\left(\phi(XW_1)W_2,y\right) + \lambda\left(\|W_1\|_F^2 + \|W_2\|_F^2\right) \\ & W_1 \in \mathbb{R}^{d \times m} \\ & W_2 \in \mathbb{R}^{m \times 1} \\ p_{\mathsf{convex}} &:= & \min\!\min\! \ L\left(Z,y\right) + \lambda \underbrace{R(Z)}_{\mathsf{convex}} \end{aligned}$$

 $Z \in \mathcal{K} \subseteq \mathbb{R}^{d \times p}$

$$p_{\text{non-convex}} := \min \sum_{L \ (\phi(XW_1)W_2, y) + \lambda \ (\|W_1\|_F^2 + \|W_2\|_F^2)} W_1 \in \mathbb{R}^{d \times m}$$

$$W_2 \in \mathbb{R}^{m \times 1}$$

 $p_{\mathsf{Convex}} := \mathsf{minimize} \quad L\left(Z,y\right) + \lambda R(Z)$

$$Z\in\mathcal{K}\subseteq\mathbb{R}^{d\times p}$$
 Theorem $p_{\text{non-convex}}=p_{\text{convex}},$ and an optimal solution to $p_{\text{non-convex}}$

can be obtained from an optimal solution to p_{CONVeX} .

M. Pilanci, T. Ergen **Neural Networks are Convex Regularizers: Exact**

18

Polynomial-time Convex Optimization Formulations for Two-Layer Networks, ICML 2020

Squared Loss: ReLU Neural Networks are Convex Group Lasso Models

data matrix $X \in \mathbb{R}^{n imes d}$ and label vector $y \in \mathbb{R}^n$

$$X = \begin{bmatrix} x_1^t \\ \vdots \\ x_n^T \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$\left[\begin{array}{c} x_n^T \end{array}\right] \left[\begin{array}{c} y_n \end{array}\right]$$

$$p_{\mathsf{non-convex}} = \ \mathsf{minimize}_{W_1,W_2} \ \left\| \sum_{i=1}^m \phi(XW_{1j})W_{2j} - y \right\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$

$$p_{\mathsf{CONVEX}} = \mathsf{minimize}_{u_1, v_1 \dots u_p, v_p \in \mathcal{K}} \left\| \sum_{i=1}^p D_i X(u_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|u_i\|_2 + \|v_i\|_2 \right)$$

$$D_1, \dots, D_p \text{ are fixed diagonal matrices}$$

Theorem $p_{\text{non-convex}} = p_{\text{convex}}$, and an optimal solution to $p_{\text{non-convex}}$ can be recovered from optimal non-zero u_i^*, v_i^* , i = 1, ..., p as $W_{1i}^* = \frac{u_i^*}{\sqrt{||u_i^*||_2}}$, $W_{2i} = \sqrt{||u_i^*||_2}$ or $W_{1i}^* = \frac{v_i^*}{\sqrt{||v_i^*||_2}}$, $W_{2i} = -\sqrt{||v_i^*||_2}$.

Regularization Path

$$p_{\mathsf{convex}} = \mathsf{minimize}_{u_1, v_1 \dots u_p, v_p \in \mathcal{K}} \left\| \sum_{i=1}^p D_i X(u_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|u_i\|_2 + \|v_i\|_2 \right)$$

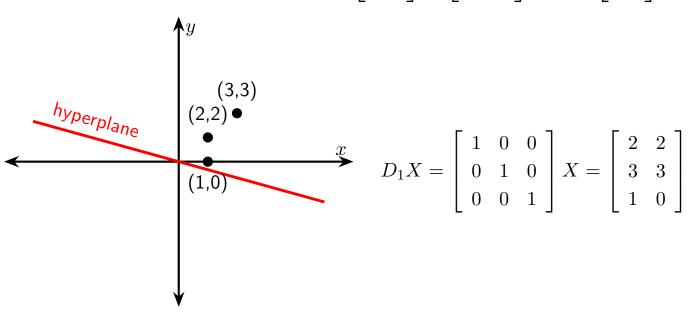
• As $\lambda \in (0, \infty)$ increases, the number of non-zeros in the solution decreases

Corollary

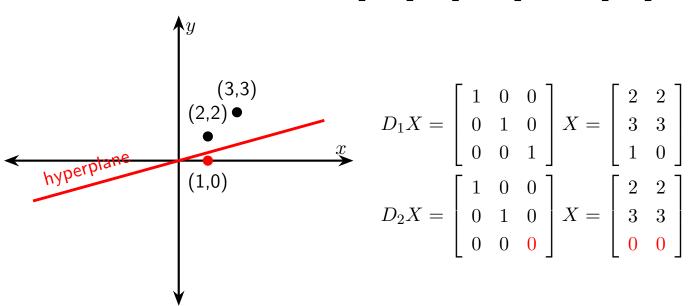
Optimal solutions of p_{CONVeX} generates the entire set of optimal architectures $f(x) = W_2\phi(W_1x)$ with m neurons for m=1,2,..., where $W_1 \in \mathbb{R}^{d \times m}$, $W_2 \in \mathbb{R}^{m \times 1}$

non-convex NN models correspond to regularized convex models

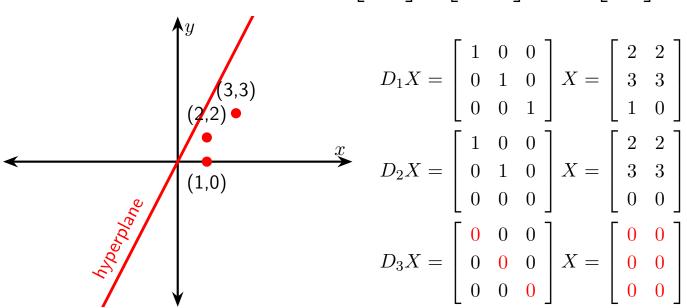
$$n=3$$
 samples in \mathbb{R}^d , $d=2$ $X=\left[egin{array}{c} x_1^T \ x_2^T \ x_3^T \end{array}
ight]=\left[egin{array}{c} 2 & 2 \ 3 & 3 \ 1 & 0 \end{array}
ight], \quad y=\left[egin{array}{c} y_1 \ y_2 \ y_3 \end{array}
ight]$



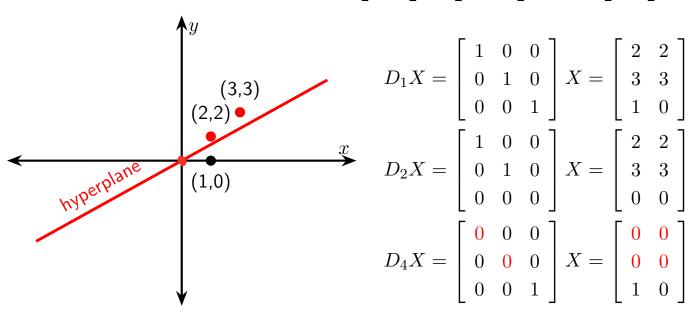
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ight]$



Example: Convex Program for n = 3, d = 2

$$n=3 \text{ samples} \quad X=\left[egin{array}{c} x_1^T \ x_2^T \ x_3^T \end{array}
ight], \quad y=\left[egin{array}{c} y_1 \ y_2 \ y_3 \end{array}
ight]$$

$$\min \left\| \begin{bmatrix} x_1^T \\ x_2^T \\ x_3^T \end{bmatrix} (u_1 - v_1) + \begin{bmatrix} x_1^T \\ x_2^T \\ 0 \end{bmatrix} (u_2 - v_2) + \begin{bmatrix} 0 \\ 0 \\ x_2^T \end{bmatrix} (u_3 - v_3) - y \right\|^2$$

$$D_1Xu_1 > 0, D_1Xv_1 > 0$$

$$D_2Xu_2 \ge 0, D_2Xv_2 \ge 0$$

$$D_4Xu_3 \ge 0, D_4Xv_3 \ge 0$$

 $+ \lambda \Big(\sum_{i=1}^{3} \|u_i\|_2 + \|v_i\|_2 \Big)$

Neural Networks as High-dimensional Variable Selectors

$$X = \left[\begin{array}{c} x_1^T \\ \vdots \\ x_n^T \end{array}\right] \in \mathbb{R}^{n \times d} \xrightarrow{\text{neural } \\ \text{network}} \bar{X} = [D_1 X, ..., D_p X] \in \mathbb{R}^{n \times p}$$

neural network = convex regularization applied to \bar{X}

Computational Complexity

Learning two-layer ReLU neural networks with m neurons

$$f(x) = \sum_{j=1}^{m} W_{2j} \phi(W_{j1}x)$$

Previous result: \circ Combinatorial $O(2^m n^{dm})$ (Arora et al., ICLR 2018)

Convex program $O((\frac{n}{r})^r)$ where $r = \operatorname{rank}(X)$

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$$O((\frac{n}{r})^r)$$
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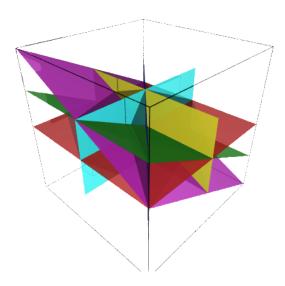
- n: number of samples, d: dimension
- (i) polynomial in n and m for fixed rank r
- (ii) exponential in d for full rank data r = d. This can not be improved unless P = NP even for m = 1.

Hyperplane Arrangements

Let
$$X \in \mathbb{R}^{n \times d}$$

$$\{\mathbf{sign}(Xw): w \in \mathbb{R}^d\}$$

at most $2\sum_{k=0}^{r-1} \binom{n}{k} \leq O\left((\frac{n}{r})^r\right)$ patterns where $r = \mathbf{rank}(X)$.

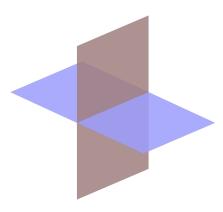


Convolutional Hyperplane Arrangements

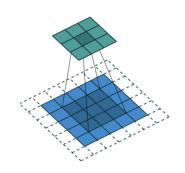
Let $X \in \mathbb{R}^{n \times d}$ be partitioned into patch matrices $X = [X_1,...,X_K]$ where $X_k \in \mathbb{R}^{n \times h}$

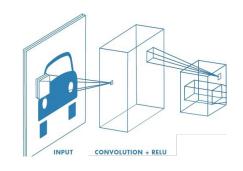
$$\{\mathbf{sign}(X_k w) : w \in \mathbb{R}^h\}_{k=1}^K$$

at most $O((\frac{nK}{h})^h)$ patterns where h is the filter size.



Convolutional Neural Networks can be optimized in fully polynomial time





o $f(x) = W_2\phi(W_1x)$, $W_1 \in \mathbb{R}^{d \times m}$, $W_2 \in \mathbb{R}^{m \times 1}$ m filters (neurons), h filter size typical example: 1024 filters of size 3×3 (m = 1024, h = 9) convex optimization complexity: polynomial in all parameters n, m and d

M. Pilanci, T. Ergen Implicit Convex Regularizers of CNN Architectures, ICLR 2021

Approximating the Convex Program

$$p_{\mathsf{CONVEX}} = \mathsf{minimize}_{u_1, v_1 \dots u_p, v_p \in \mathcal{K}} \left\| \sum_{i=1}^p D_i X(u_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|u_i\|_2 + \|v_i\|_2 \right)$$

- Sample $D_1,...,D_p$ as $\mathsf{Diag}(Xu \geq 0)$ where $u \sim N(0,I)$
- Low rank approximation of $X \approx X_r$ where $\|X X_r\|_2 \le \sigma_{r+1}$ $(1 + \frac{\sigma_{r+1}}{\lambda})$ approximation in $O\left((\frac{n}{r})^r\right)$ complexity
- Backpropagation (gradient descent) on the non-convex loss
 is a heuristic for the convex program

An Exact Characterization of All Optimal Solutions

$$p_{\text{non-convex}} := \underset{}{\text{minimize}} \quad L\left(\phi(XW_1)W_2, y\right) + \lambda\left(\|W_1\|_F^2 + \|W_2\|_F^2\right)$$

$$W_1 \in \mathbb{R}^{d \times m}$$

$$W_2 \in \mathbb{R}^{m \times 1}$$

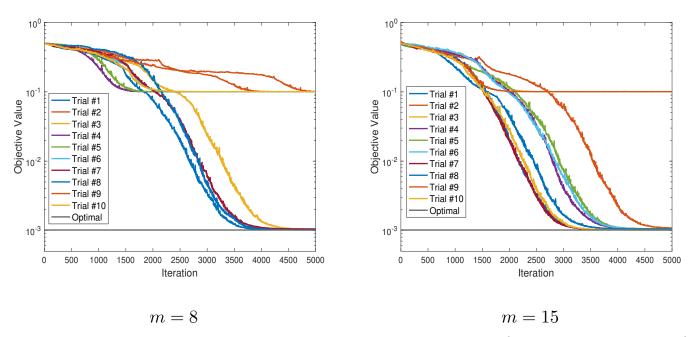
$$p_{\mathsf{Convex}} := \mathsf{minimize} \quad L\left(Z,y\right) + \lambda R(Z)$$

$$Z \in \mathcal{K} \subseteq \mathbb{R}^{d \times p}$$

Theorem All optimal solutions of $p_{\text{non-convex}}$ can be found from the optimal solutions of p_{convex} up to permutation and neuron splitting. Hence, the optimal set of $p_{\text{non-convex}}$ is convex up to equivalence.

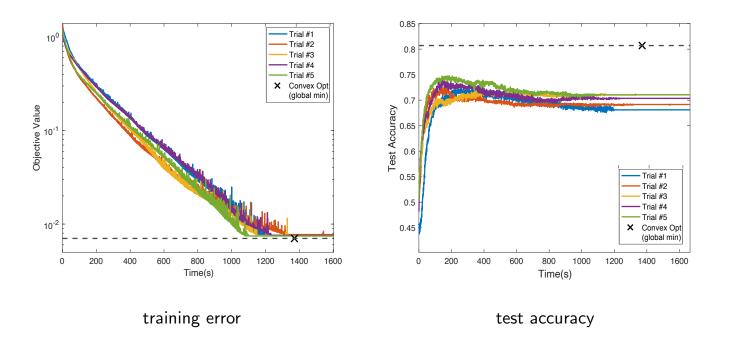
Y. Wang, J. Lacotte, M. Pilanci, **The Hidden Convex Optimization Landscape of Two-Layer ReLU Neural Networks, ICLR 2022**

Numerical Experiment: Two-Layer Fully Connected ReLU



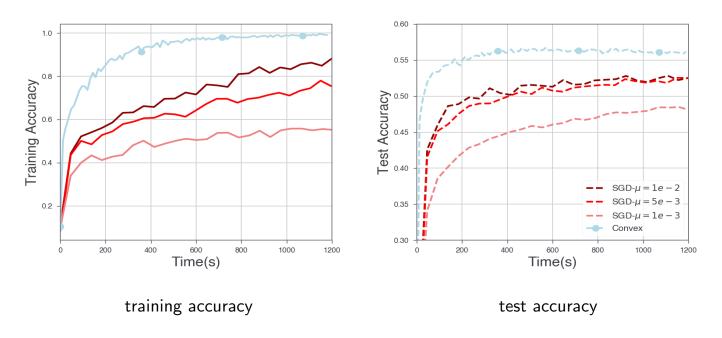
Training cost of a two-layer ReLU network trained with SGD (10 initialization trials) and the convex program on a toy dataset (d=2)

Numerical Experiment: Two-Layer Convolutional Network on CIFAR



binary classification on a subset of the CIFAR Dataset

SGD for the Convex Program vs SGD for the Non-convex Problem



10-class classification on the CIFAR Dataset ($n=50,000,\,d=3072$) with randomly sampled arrangement patterns for the convex program

Plan for the rest of the talk

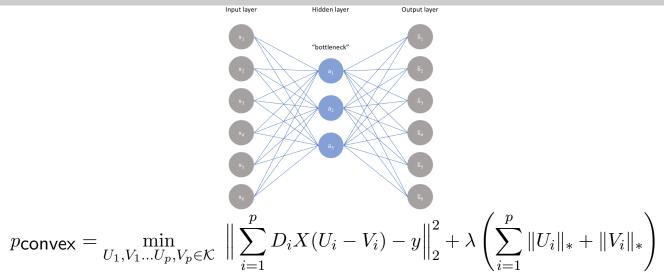
 Are all neural network problems convex? What is the role of the network architecture? What does gradient descent with no regularization do?
 vector output networks, e.g., autoencoders
 batch normalization layers
 gradient flow

Generative Adversarial Networks (GANs) deeper networks

Numerical results

convex vs non-convex neural networks convex GANs

Vector Output Two-layer ReLU Networks: Nuclear Norm Regularization



Theorem $p_{\text{non-convex}} = p_{\text{convex}}$, and an optimal solution to $p_{\text{non-convex}}$ can be recovered from optimal non-zero U_i^*, V_i^* , i = 1, ..., p.

A. Sahiner, T. Ergen, J. Pauly, M. Pilanci Vector-output ReLU Neural Network Problems are Copositive Programs, ICLR 2021

ReLU Networks with Batch Normalization (BN)

 \circ BN transforms a batch of data to zero mean and standard deviation one, and has two trainable parameters α,γ

$$\mathbf{BN}_{\alpha,\gamma}(x) = \frac{(I - \frac{1}{n}\mathbf{1}\mathbf{1}^T)x}{\|(I - \frac{1}{n}\mathbf{1}\mathbf{1}^T)x\|_2}\gamma + \alpha$$

where $U_i \Sigma_i V_i^T = D_i X$ is the SVD of DX_i , i.e., BatchNorm whitens local data

T. Ergen, A. Sahiner, B. Ozturkler, J. Pauly, M. Mardani, M. Pilanci **Demystifying Batch Normalization in ReLU Networks, ICLR 2022**

Unregularized Gradient Flow Converges to the Optimum of the Convex Program

Consider the **unregularized** problem

$$\min_{\theta} \mathcal{L}(\theta) = \min_{\theta = \{w_{11}, w_{21}, \dots, w_{1p}, w_{2p}\}} \ell \left(\sum_{j=1}^{m} (Xw_{1j})_{+} w_{2j}, y \right)$$

and corresponding non-convex gradient flow

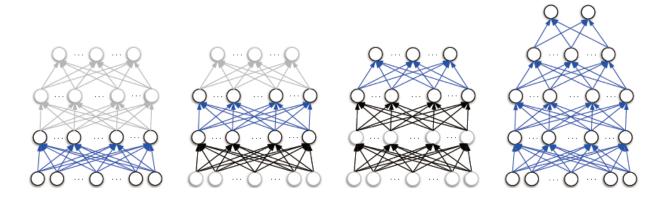
$$\frac{d}{dt}\theta(t) \in -\partial \mathcal{L}(\theta(t))$$

Theorem: Suppose that X is linearly separable, and ℓ is log loss. Then, $\theta(t)$ converges to the solution of the convex program

$$\text{minimize}_{u_1,v_1...u_p,v_p \in \mathcal{K}} \sum_{i=1}^p \|u_i\|_2 + \|v_i\|_2 \text{ s.t. } Diag(y) \sum_{i=1}^p D_i X(u_i - v_i) \geq 1$$

Y. Wang, M. Pilanci, The Convex Geometry of Backpropagation: Neural Network Gradient Flows Converge to Extreme Points of the Dual Convex Program, ICLR 2022

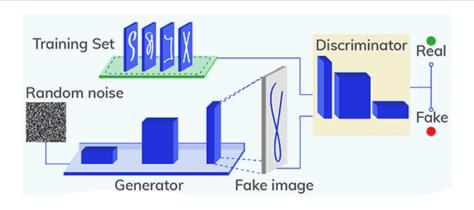
Layer-Wise Learning Deep Networks



16 Layer NN (VGG16) (Simonyan et al. 2015) Layerwise (2-Layer \times 15) (Belilovsky et al. 2019)

CIFAR-10 Imagenet 92% 90.9% 90.4% 88.7%

Convex Generative Adversarial Networks (GANs)



Wasserstein GAN parameterized with neural networks

$$p^* = \min_{\theta_g} \max_{D: \text{1-Lipschitz}} \mathbb{E}_{x \sim p_x}[D(x)] - \mathbb{E}_{z \sim p_z}[D(G_{\theta_g}(z))]$$

$$\cong \min_{\theta_g} \max_{\theta_d} \mathbb{E}_{x \sim p_x}[D_{\theta_d}(x)] - \mathbb{E}_{z \sim p_z}[D_{\theta_d}(G_{\theta_g}(z))]$$

Theorem Two layer generator two layer discriminator WGAN problems are convex-concave games.

- two-layer ReLU-activation generator $G_{\theta_a}(Z) = (ZW_1)_+ W_2$
- \circ two-layer quadratic activation discriminator $D_{\theta_d}(X)=(XV_1)^2V_2$ Wasserstein GAN problem is equivalent to a convex-concave game, which can be solved via convex optimization

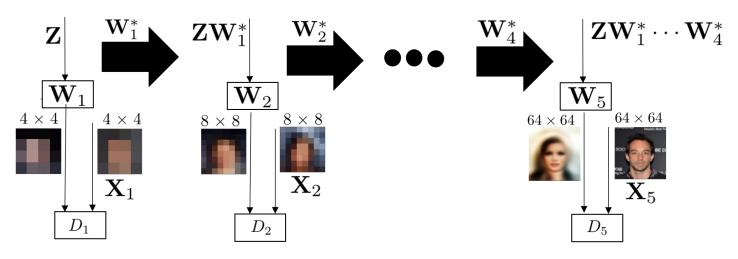
$$G^* = \operatorname{argmin}_G \|G\|_F^2 \text{ s.t. } \|X^\top X - G^\top G\|_2 \le \lambda$$

$$W_1^*, W_2^* = \operatorname{argmin}_{W_1, W_2} ||W_1||_F^2 + ||W_2||_F^2 \text{ s.t. } G^* = (ZW_1)_+ W_2,$$

- the first problem can be solved via singular value thresholding as $G^* = U(\Sigma^2 \lambda I)^{1/2}_+ V^\top$ where $X = U\Sigma V^\top$ is the SVD of X.
- o the second problem can be solved via convex optimization as shown earlier

Progressive GANs

deeper architectures can be trained layerwise



Numerical Results

real faces from the CelebA dataset



fake faces generated using convex optimization



two-layer quadratic activation discriminator and linear generator trained via closed form optimal solution progressively for a total of 4 layers

A. Sahiner et al. Hidden Convexity of Wasserstein GANs, ICLR 2022

Three-layer Neural Networks: Double Hyperplane Arrangements

$$p_{3}^{*} = \min_{\substack{\{W_{j}, u_{j}, w_{1j}, w_{2j}\}_{j=1}^{m} \\ u_{j} \in \mathcal{B}_{2}, \forall j}} \frac{1}{2} \left\| \sum_{j=1}^{m} \left((\mathbf{X}W_{j})_{+} w_{1j} \right)_{+} w_{2j} - y \right\|_{2}^{2} + \frac{\beta}{2} \sum_{j=1}^{m} \left(\|W_{j}\|_{F}^{2} + \|w_{1j}\|_{2}^{2} + w_{2j}^{2} \right),$$

Theorem

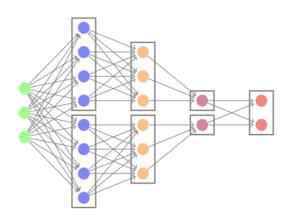
The equivalent convex problem is

$$\min_{\{W_i, W_i'\}_{i=1}^p \in \mathcal{K}} \frac{1}{2} \left\| \sum_{j=1}^p \sum_{j=1}^P D_i D_j \tilde{\mathbf{X}} \left(W_{ij}' - W_{ij} \right) - y \right\|^2 + \frac{\beta}{2} \sum_{j=1}^p \|W_{ij}\|_F + \|W_{ij}'\|_F$$

T. Ergen, M. Pilanci Global Optimality Beyond Two Layers: Training Deep ReLU Networks via Convex Programs, ICML 2021

Deep ReLU Networks

Input Layer 1 Layer 2 Layer 3 Layer 4



arbitrarily deep ReLU neural networks with parallel architecture

Theorem There is a convex program such that $p_{\text{non-convex}} = p_{\text{convex}}$ Y. Wang, T. Ergen, M. Pilanci, **Parallel Deep Neural Networks Have Zero Duality Gap, arXiv 2021**.

Conclusion and Open Problems

- we can **train** ReLU and polynomial NNs in polynomial time
- convex optimization theory & solvers can be applied
- multi layer ReLU neural network problems are convex in higher dimensions
- neural networks seek sparsity
- \circ architecture search = regularizer search (block ℓ_2 - ℓ_1 , nuclear norm,...)
- we need faster algorithms to solve high-dimensional convex programs whose solutions are sparse and better layer-wise learning strategies

CODE: github.com/pilancilab

References

stanford.edu/~pilanci CODE: github.com/pilancilab

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