The Hidden Convex Optimization Landscape of Deep Neural Networks

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The Impact of Deep Learning







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

Deep Neural Networks



- non-convex (stochastic) gradient descent
- o 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)

GPT-4 (March 2023)

¹OpenAl General Purpose Transformer ²The Beijing Academy of Artificial Intelligence

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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

Nature 560, 632–634(2018) | Cite this article 19k Accesses | 20 Citations | 1018 Altmetric | Metrics

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one year later, another paper **Nature**

Matters Arising | Published: 02 October 2019

One neuron versus deep learning in aftershock prediction

Arnaud Mignan 🖂 & Marco Broccardo 🖂

Nature 574, E1–E3(2019) | Cite this article

6210 Accesses 2 Citations 367 Altmetric Metrics

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logistic regression (1 layer) has the same performance as the 6 layer NN for this task



Sensitive to perturbations



- o adversarial examples, Szegedy et al., 2014, Goodfellow et al., 2015
- $\circ~({\sf left})$ traffic light is classified as 'oven' when 11 pixels are changed
- o (right) stop sign recognized as speed limit sign, Evtimov et al, 2017

Deep networks can hallucinate!

Fast MRI Challenge, 2020 model generates a false vessel (Muckley et al.)



- what are neural networks actually doing?
- o can we make neural network models more reliable?
- o can we make training energy/memory/data efficient?

How neural networks work?



- Least-Squares, Logistic Regression, Support Vector Machines etc. are understood extremely well
- Insightful theorems for neural networks?



- optimality condition: $A^T(Ax b) = 0$
- solvers: Cholesky/QR, Conjugate Gradient,...

Least Squares with L1 regularization

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

• L1 norm
$$||x||_1 = \sum_{i=1}^d |x_i|$$

encourages solution x^* to be sparse

L1 regularization: mechanical interpretation with large λ

$$\begin{array}{l} \min_{x} \quad \underbrace{\frac{1}{2}(x-y)^{2}}_{\text{elastic energy}} + \underbrace{\lambda |x|}_{\text{potential energy}}\\ \text{red spring constant} = 1\\ \text{blue ball mass} = \lambda \text{ (large)} \end{array}$$

Least Squares with group L1 regularization



$$\min_{x} \left\| \sum_{i=1}^{L} A_{i} x_{i} - y \right\|_{2}^{2} + \lambda \sum_{i=1}^{L} \|x_{i}\|_{2}$$

$$\|x_i\|_2 = \sqrt{\sum_{j=1}^d x_{ij}^2}$$

encourages solution x^* to be group sparse, i.e., most blocks x_i are zero

Training two-layer neural networks: Non-convex optimization

$$p_{\text{non-convex}} := \min \min \mathbb{L} \left(\phi(XW_1)W_2, y \right) + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$
$$W_1 \in \mathbb{R}^{d \times m}$$
$$W_2 \in \mathbb{R}^{m \times 1}$$

where $\phi(u)$ is the activation function



$$p_{\text{non-convex}} := \min \min L \left(\phi(XW_1)W_2, y \right) + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$
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where $\phi(u) = \text{ReLU}(u) = \max(0, u)$ or $\phi(u) = \text{sign}(u)$ $p_{\text{non-convex}} := \text{minimize} \quad L(\phi(XW_1)W_2, y) + \lambda(||W_1||_F^2 + ||W_2||_F^2)$ $W_1 \in \mathbb{R}^{d \times m}$ $W_2 \in \mathbb{R}^{m \times 1}$ $p_{\text{convex}} := \text{minimize} \quad L(Z, y) + \lambda$ R(Z)convex regularization $Z \in \mathcal{K} \subseteq \mathbb{R}^{d \times p}$

 $p_{\text{non-convex}} := \min \sum_{k=1}^{m} L\left(\phi(XW_1)W_2, y\right) + \lambda\left(\|W_1\|_F^2 + \|W_2\|_F^2\right)$ $W_1 \in \mathbb{R}^{d \times m}$ $W_2 \in \mathbb{R}^{m \times 1}$

$$p_{\mathsf{convex}} := \min \min L (Z, y) + \lambda R(Z)$$
$$Z \in \mathcal{K} \subseteq \mathbb{R}^{d \times p}$$

Theorem $p_{non-convex} = p_{convex}$, and an optimal solution to $p_{non-convex}$ can be obtained from an optimal solution to p_{convex} .

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M. Pilanci, T. Ergen, Neural Networks are Convex Regularizers: Exact Polynomial-time Convex Optimization Formulations for Two-Layer Networks. ICML 2020, T. Ergen, I. Gulluk, J. Lacotte, M. Pilanci, ICLR 2023

ReLU Network using squared loss = group Lasso using fixed features

data matrix
$$X \in \mathbb{R}^{n \times d}$$
 and label vector $y \in \mathbb{R}^n X = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix}$, $y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$
 $p_{\text{non-convex}} = \text{minimize}_{W_1, W_2} \left\| \sum_{j=1}^m \phi(XW_{1j})W_{2j} - y \right\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$
 $p_{\text{convex}} = \text{minimize}_{u_1, v_1 \dots u_p, v_p \in \mathcal{K}} \left\| \sum_{i=1}^p D_i X(u_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|u_i\|_2 + \|v_i\|_2 \right)$

 $D_1, ..., D_p$ are fixed diagonal matrices

Theorem $p_{non-convex} = p_{convex}$, and an optimal solution to $p_{non-convex}$ can be recovered from optimal non-zero u_i^*, v_i^* , i = 1, ..., p as

$$W_{1j}^* = rac{u_i^*}{\sqrt{\|u_i^*\|_2}}$$
, $W_{2j} = \sqrt{\|u_i^*\|_2}$ or $W_{1j}^* = rac{v_j^*}{\sqrt{\|v_j^*\|_2}}$, $W_{2j} = -\sqrt{\|v_j^*\|_2}$.

$$n = 3 \text{ samples in } \mathbb{R}^{d}, d = 2 \quad X = \begin{bmatrix} x_{1}^{T} \\ x_{2}^{T} \\ x_{3}^{T} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} y_{1} \\ y_{2} \\ y_{3} \end{bmatrix}$$

$$(3,3)$$

$$(2,2) \bullet$$

$$(1,0) \quad D_{1}X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}$$

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$$\begin{pmatrix} y \\ (3,3) \\ (2,2) \bullet \\ \bullet \\ (1,0) \end{pmatrix}$$

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$$L_{1}X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}$$

$$D_{2}X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 0 & 0 \end{bmatrix}$$

$$D_{4}X = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \end{bmatrix}$$

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

 $D_1 X u_1 \ge 0, D_1 X v_1 \ge 0$ $D_2 X u_2 \ge 0, D_2 X v_2 \ge 0$ $D_4 X u_3 \ge 0, D_4 X v_3 \ge 0$

equivalent to the non-convex two-layer NN problem

Computational Complexity

Learning two-layer ReLU neural networks with m neurons $f(x) = \sum_{j=1}^m W_{2j} \phi(W_{j1}x)$

Previous results: \circ Combinatorial $O(2^m n^{dm})$ (Arora et al., ICLR 2018) \circ Approximate $O(2^{\sqrt{m}})$ (Goel et al., COLT 2017)

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

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

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

Number of variables = number of hyperplane arrangements

• convex program has at most $\left(\left(\frac{n}{r}\right)^r\right)$ variables

#activation patterns of a **one neuron**

 $= \left| \{ \operatorname{sign}(Xw) : w \in \mathbb{R}^d \} \right| \le O((\frac{n}{r})^r) \text{ where } r = \operatorname{rank}(X).$



o rank is constant for convolutional networks

e.g., $3 \times 3 \times 1024$ convolution $\implies r = 9 \implies$ polynomial-time 23

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 $\alpha,\gamma\,$

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

$$p_{\text{non-convex}} = \min_{W_1, W_2, \alpha, \gamma} \left\| \mathbf{BN}_{\alpha, \gamma}(\phi(XW_1))W_2 - y \right\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$
$$\| \\ p_{\text{convex}} = \min_{w_1, v_1 \dots w_p, v_p \in \mathcal{K}} \left\| \sum_{i=1}^p U_i(w_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|w_i\|_2 + \|v_i\|_2 \right)$$

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**

Vector Output Two-layer ReLU: equivalent to nuclear norm penalty

$$p_{\mathsf{non-convex}} = \min_{W_1 \in \mathbb{R}^{d \times m}, W_2 \in \mathbb{R}^{m \times c}} \left\| \sum_{j=1}^m \phi(XW_{1j}) W_{2j} - Y \right\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$
$$p_{\mathsf{convex}} = \min_{U_1, V_1 \dots U_p, V_p \in \mathcal{K}} \left\| \sum_{i=1}^p D_i X(U_i - V_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|U_i\|_* + \|V_i\|_* \right)$$

 $D_1, ..., D_p$ 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.

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

Three layer NN: FC-Relu-FC-Relu-FC is equivalent to a convex program with 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

$$\min_{\{W_i, W_i'\}_{i=1}^p \in \mathcal{K}} \frac{1}{2} \left\| \sum_{i=1}^p \sum_{j=1}^P D_i D_j \tilde{\mathbf{X}} \left(W_{ij}' - W_{ij} \right) - y \right\|_2^2 + \frac{\beta}{2} \sum_{i,j=1}^p \|W_{ij}\|_F + \|W_{ij}'\|_F$$

Reducing Complexity: Approximating Convex Programs by Sampling

$$\tilde{p}_{\mathsf{sampled-cvx}} = \mathsf{minimize}_{u_1, v_1 \dots u_{\tilde{p}}, v_{\tilde{p}} \in \mathcal{K}} \left\| \sum_{i=1}^p D_i X(u_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^p \|u_i\|_2 + \|v_i\|_2 \right) \right\|_2^2$$

- sampled convex model: sample $D_1, ..., D_{\tilde{p}}$ as $\text{Diag}(Xu \ge 0)$ where $u \sim N(0, I)$
- guarantee for two-layer ReLU NNs: $(1 + \frac{\sigma_{k+1}(X)}{\lambda})$ relative objective value approximation using $O((\frac{n}{k})^k)$ samples



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

Theorem Stationary points
$$\left\{x : 0 \in \operatorname{conv}\left\{\lim_{k \to \infty} \nabla f(x_k) \mid \lim_{k \to \infty} x_k = x, x_k \in D\right\}\right\}$$

of $p_{\sf non-convex}$ are optimal solutions of the sampled convex program $p_{\sf sampled-cvx}$

Y. Wang, J. Lacotte, M. Pilanci. The Hidden Convex Optimization Landscape of Two-Layer ReLU Neural Networks: an Exact Characterization of the Optimal Solutions ICLR, 2022

Exact Convex Program: Two-Layer ReLU NN



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

Exact Convex Program: Classifying a subset of CIFAR-10



Figure: Two-layer ReLU network trained with SGD (10 initialization trials) and the convex program on a subset of CIFAR-10 for binary classification (n = 195)

Sampled Convex Model vs Non-convex Model (Stochastic Gradient Descent)



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

Re-training Final Convolutional Layers of Pretrained Deep Nets



Person detection task on the COCO Dataset containing 110,000 images of median resolution 640 x 480. Two-layer ReLU CNN trained on pretrained MobileNetV3 features (convex PyTorch model: https://github.com/pilancilab/convex_nn)

Specialized Convex Solver: Performance Profile

- baseline: gradient based nonconvex optimization: SGD, ADAM (best of 10 random initializations and 10 learning rates)
- convex: proximal gradient with adaptive acceleration

 ${\cal O}(1/T^2)$ convergence rate



Performance profile showing the percentage of problems solved over a collection of 400 UC Irvine datasets up to 10^{-3} training error vs time ⁴

⁴A. Mishkin, A. Sahiner, M. Pilanci. **Fast Convex Optimization for Two-Layer ReLU Networks, ICML 2022**. github.com/pilancilab/scnn

Interpreting Neural Networks via Convexity: Time Series Prediction



Interpreting Neural Networks via Convexity: Time Series Prediction

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

• sampled convex program: $D_i = \text{diag}(Xu_i \ge 0), u_i \sim \mathcal{N}(0, I)$ forms a Locality Sensitive Hash (Charikar, 2002)

Layer-Wise Training of Deep Networks



- (i) train a two-layer network convex optimization
- (ii) fix the hidden layer to use as feature embedding
- (ii) repeat two-layer network training on these features
 - o ideal for edge AI: low memory and low communication between blocks
 - o modular: networks can keep evolving, can terminate early during inference
 - each convex model is trained to global optimality efficiently with no hyperparameter tuning

Numerical results for layer-wise convex learning: CIFAR-10 image classification



• end-to-end trained 5 layer CNN accuracy: 89%, 16 layer VGG accuracy: 92%

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. Saddle-points exists and globally solvable under convex parameterization. (Sahiner et al. **Hidden Convexity of Wasserstein GANs, ICLR 2022.)**

Conclusion and Open Problems

- neural networks are high-dimensional convex models. Convex optimization theory & solvers can be applied.
- we can have better specialized solvers (e.g., accelerated proximal gradient)
- Extensions: autoencoders, transformers, diffusion models
- o Open problems: improving the sampler
- Ref 1 M. Pilanci, T. Ergen, Neural Networks are Convex Regularizers: Exact Polynomial-time Convex Optimization Formulations for Two-Layer Networks. ICML 2020
- Ref 2 T. Ergen, M. Pilanci, Convex Geometry and Duality of Over-parameterized Neural Networks. JMLR 2021

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

$$G^* = \operatorname{argmin}_G \|G\|_F^2$$
 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



deeper architectures can be trained layerwise

Numerical Results

• real faces from the CelebA dataset



o 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, preprint 2021** based on the attention module

$$f(X) = \sigma(XQ^T K X) X V$$

- $\circ \ Q, K, V$ are trainable parameters: Q : query, K : key, V : value
- o used in transformers, vision transformers, mixer models...
- There is a convex formulation¹

¹A. Sahiner, T. Ergen, B. Ozturkler, M. Mardani, J. Pauly, M. Pilanci, ICML 2022

- transfer learning without fine-tuning existing weights of the backbone network
- o generate embeddings from an ImageNet pre-trained deep transformer model
- then finetune by training a two-layer attention block using convex optimization to classify images from CIFAR-100, while leaving the pre-trained backbone fixed

- transfer learning without fine-tuning existing weights of the backbone network
- o generate embeddings from an ImageNet pre-trained deep transformer model
- then finetune by training a two-layer attention block using convex optimization to classify images from CIFAR-100, while leaving the pre-trained backbone fixed
- **unified architecture:** can be applied to any data (text, images, time series, tabular data, multimodal data...)
- ideal for fine-tuning edge devices

Two layer CNN with pooling: Conv-Pooling-Relu-FC is equivalent to ℓ_1 penalty, i.e., constrained Lasso $\min_{w \in \mathcal{K}} \|\Phi w - y\|_2^2 + \lambda \|w\|_1$

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

Theorem

Let $ilde{\mathbf{X}} = \mathbf{X}F$ and $F \in \mathbb{C}^{d imes d}$ be the DFT matrix. The equivalent convex problem is

$$\begin{split} & \min_{\substack{\{w_i, w_i'\}_{i=1}^p \\ w_i, w_i' \in \mathbb{C}^d, \forall i}} \frac{1}{2} \left\| \sum_{i=1}^p \text{diag}(S_i) \tilde{\mathbf{X}} \left(w_i' - w_i \right) - y \right\|_2^2 + \frac{\beta}{\sqrt{d}} \sum_{i=1}^p \left(\|w_i\|_1 + \|w_i'\|_1 \right) \\ & \text{s.t.} \ (2\text{diag}(S_i) - I_n) \tilde{\mathbf{X}} w_i \ge 0, \ (2\text{diag}(S_i) - I_n) \tilde{\mathbf{X}} w_i' \ge 0, \forall i, \end{split}$$

Sampled Convex Model vs Non-convex Model for fine-tuning



Person detection task on the Common Objects in Context Dataset (110,000 images of median resolution 640 x 480).

Fine-tuning all layers of MobileNetV3 + convex and non-convex CNN head