Learning and generalization in over-parameterized neural networks, going beyond kernels

Yuanzhi Li

Stanford University

date: Today

A bit of history of machine learning

- Practical machine learning (Phase 1):

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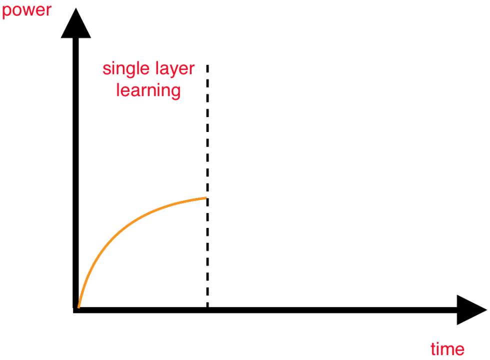

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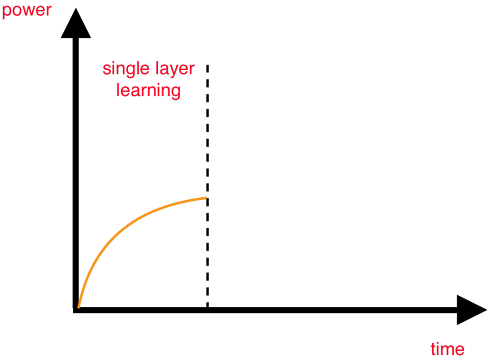

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- Single layer perceptrons (linear regressions, kernel methods, linear regression over feature mappings).

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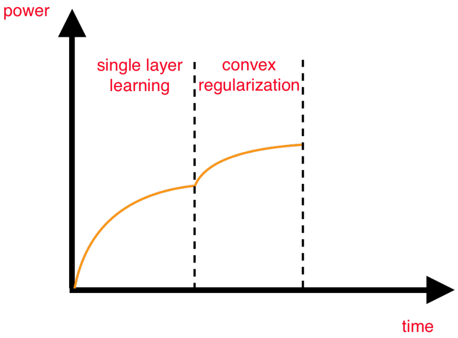

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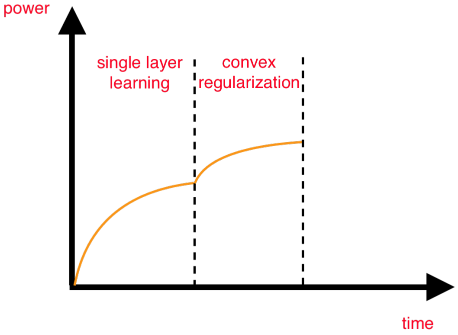

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- Feature mappings with convex regularizations (e.g. ℓ_1 regularizations for Lasso, nuclear norm regularizations for matrix completion, matrix sensing, PSD regularizations for SOS).

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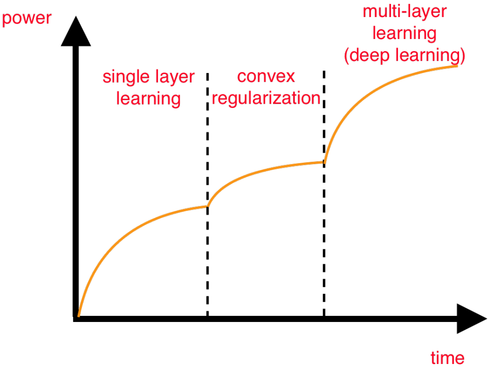

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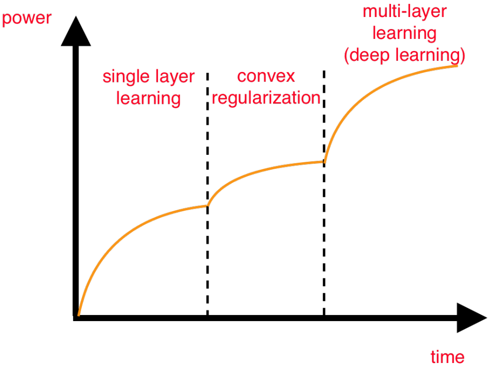

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- Multi-layer perceptrons (Deep learning) and non-convex algorithms.

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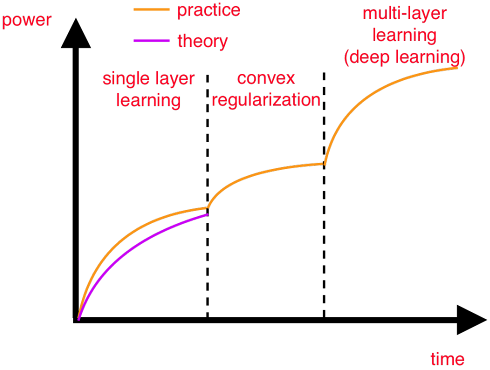

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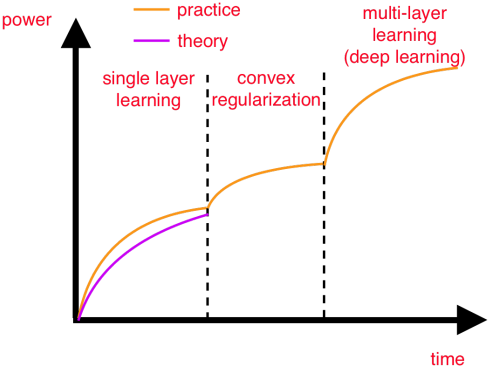

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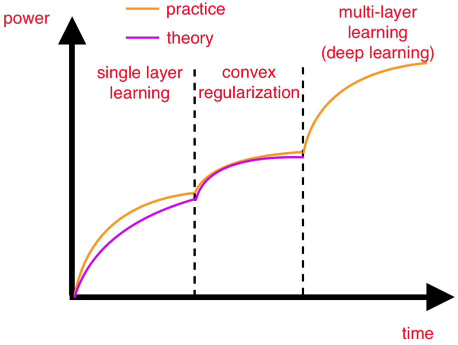

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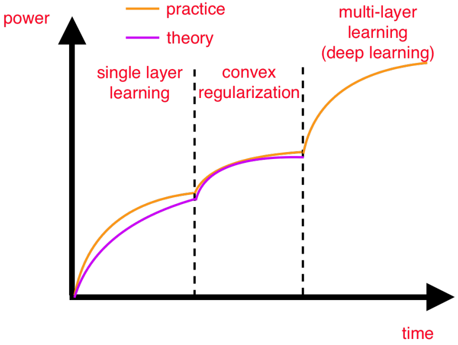

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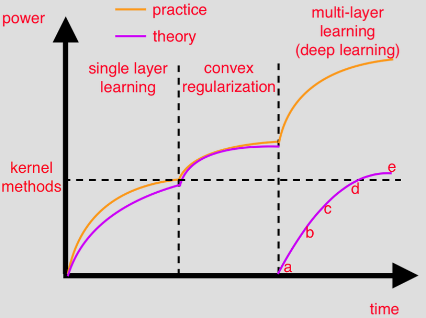

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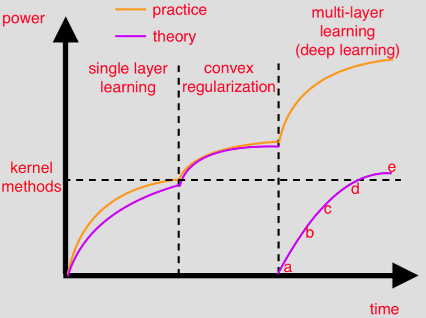

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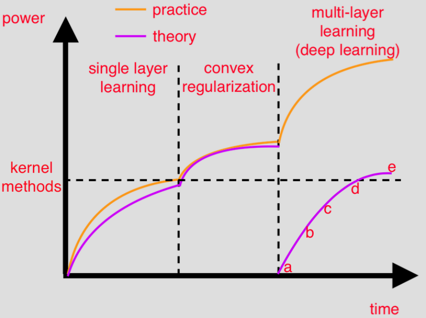

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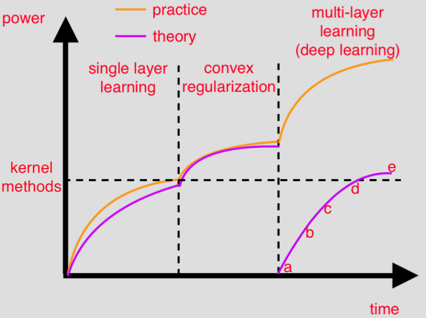

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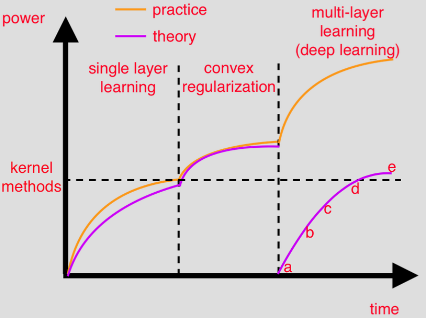

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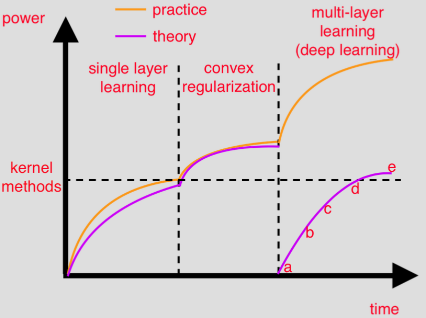

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  - (d). Neural networks can learn functions that are learnable by kernels: The neural tangent kernel (NTK) approach.

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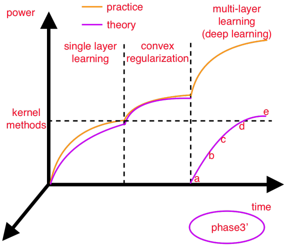

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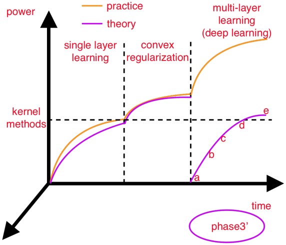

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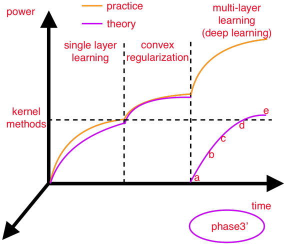

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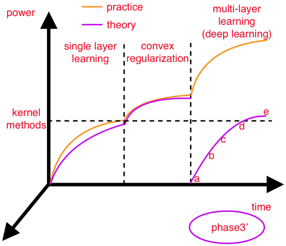

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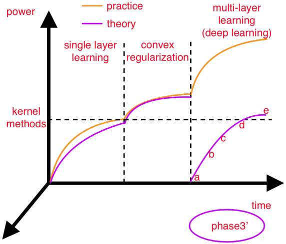

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- This talk focuses on (distribution free) PAC learning.

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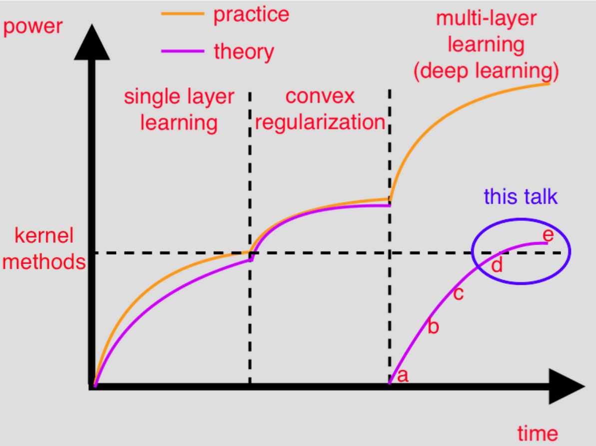
- 

power
practice
theory
multi-layer
learning
(deep learning)
single layer
learning
convex
regularization
this talk
kernel
methods
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time

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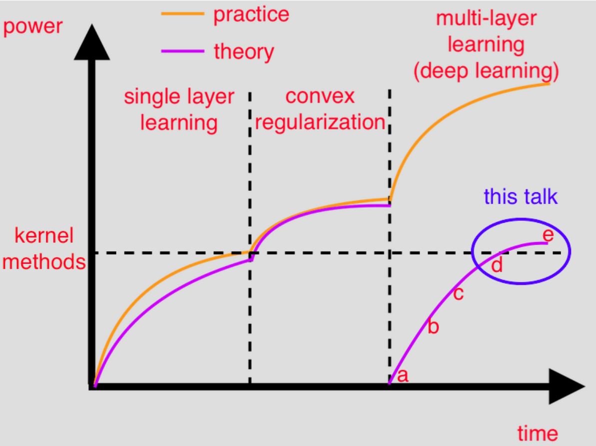
- 

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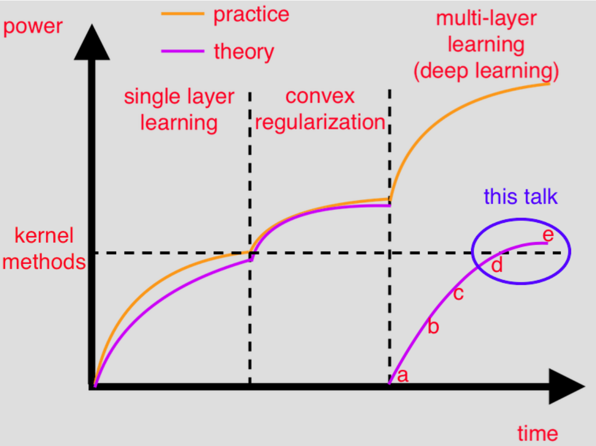
- 

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- In (distribution free) PAC learning setting.

Tangent kernel and neural tangent kernel

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- Neural tangent kernel (NTK) $K(x, y) = \langle \nabla_W f(W_0, x), \nabla_W f(W_0, y) \rangle$ where f is the neural network, W_0 is usually the (random) initialization.

Neural tangent kernel

Theorem (ALS'18, arXiv:1811.03962)

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- *If Oops, then training neural network $f \approx$ linear regression over feature mappings $\phi(x) = \nabla_W f(W_0, x)$.*

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- L-layer network is typically 2^L instead of $\text{poly}(L)$ smooth: Need to use non-worst case bounds.

Neural tangent kernel (proof intuition)

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- $1_{\langle w_i^*, x\rangle \geq 0} \approx 1_{\langle w_i^{(0)}, x\rangle \geq 0}$: The activation pattern does not change too much, network stays close to its NTK.
- The (explicit) two layer proof is originated in [LL'18], arXiv:1808.01204: Learning Overparameterized Neural Networks via Stochastic Gradient Descent on Structured Data.

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- Can we prove that neural networks do better than NTKs in theory?

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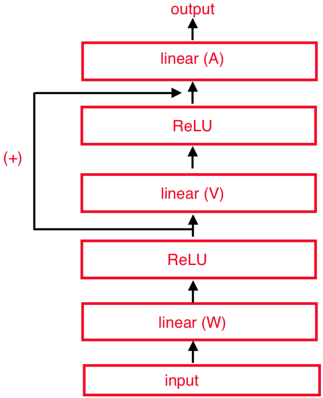

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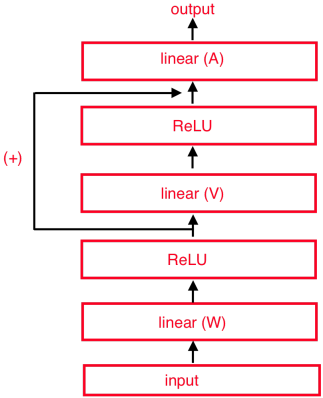

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- The (sample/time) complexity of learning ϕ using kernel methods.

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  - Intuitively, eventually $\mathrm{ReLU}(Wx)$ aligns with A through the signal $A\mathrm{ReLU}(Wx)$, so $\mathbb{E}_x[\mathrm{ReLU}(Wx)\mathrm{ReLU}(Wx)^\top]) \approx AA^\top$.

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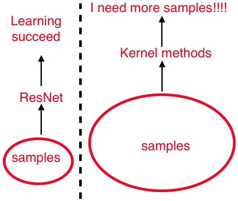
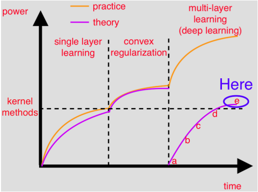
- 



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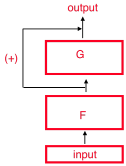

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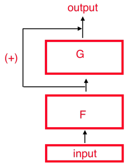
- 

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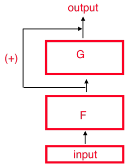
- 

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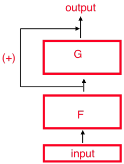
- 

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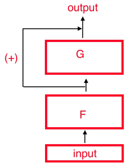
- 

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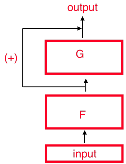
- 

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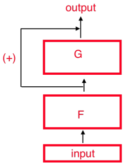
- 

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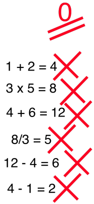
- 

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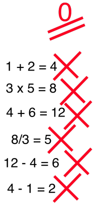
- 

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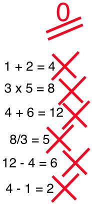
- 

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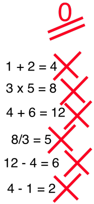
- 

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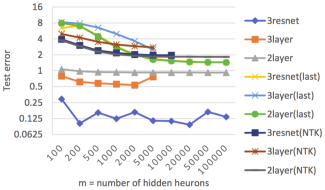

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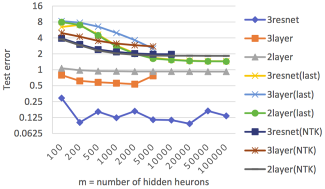

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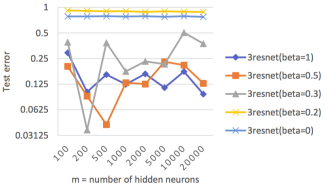
- 

(b) sensitivity test on $\alpha = 0.3$

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- Changing the initialization: Learning ReLU network with over-parameterized ReLU network [LMZ' 19] (to appear).

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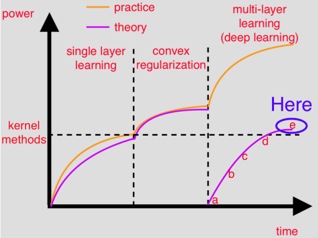
  - 

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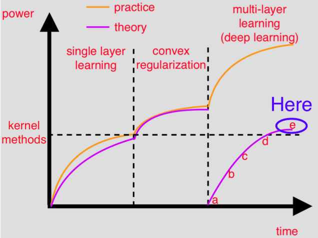
  - 

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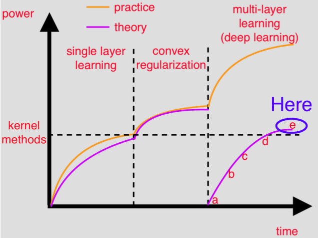
  - 

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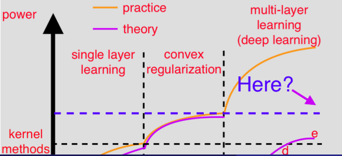

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- Theoretical machine learning: Convex-P/poly v.s. Non-convex-P/poly.

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Definition (Convex circuit)

- A (k-output) circuit C with two inputs $W \in \mathbb{R}^m, x \in \mathbb{R}^d$ is a convex circuit over loss $L : \mathbb{R}^{2k} \to \mathbb{R}$ and a set $\mathcal{S} \in \mathbb{R}^{d+k}$ if given any $(x, y) \in \mathcal{S}$:
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- Question: is non-convex-P/poly better than convex-P/poly?

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Question (Fundamental question)

Is non-convex optimization (training neural networks) provably better than convex/one point convex optimization in efficiently computable regime?