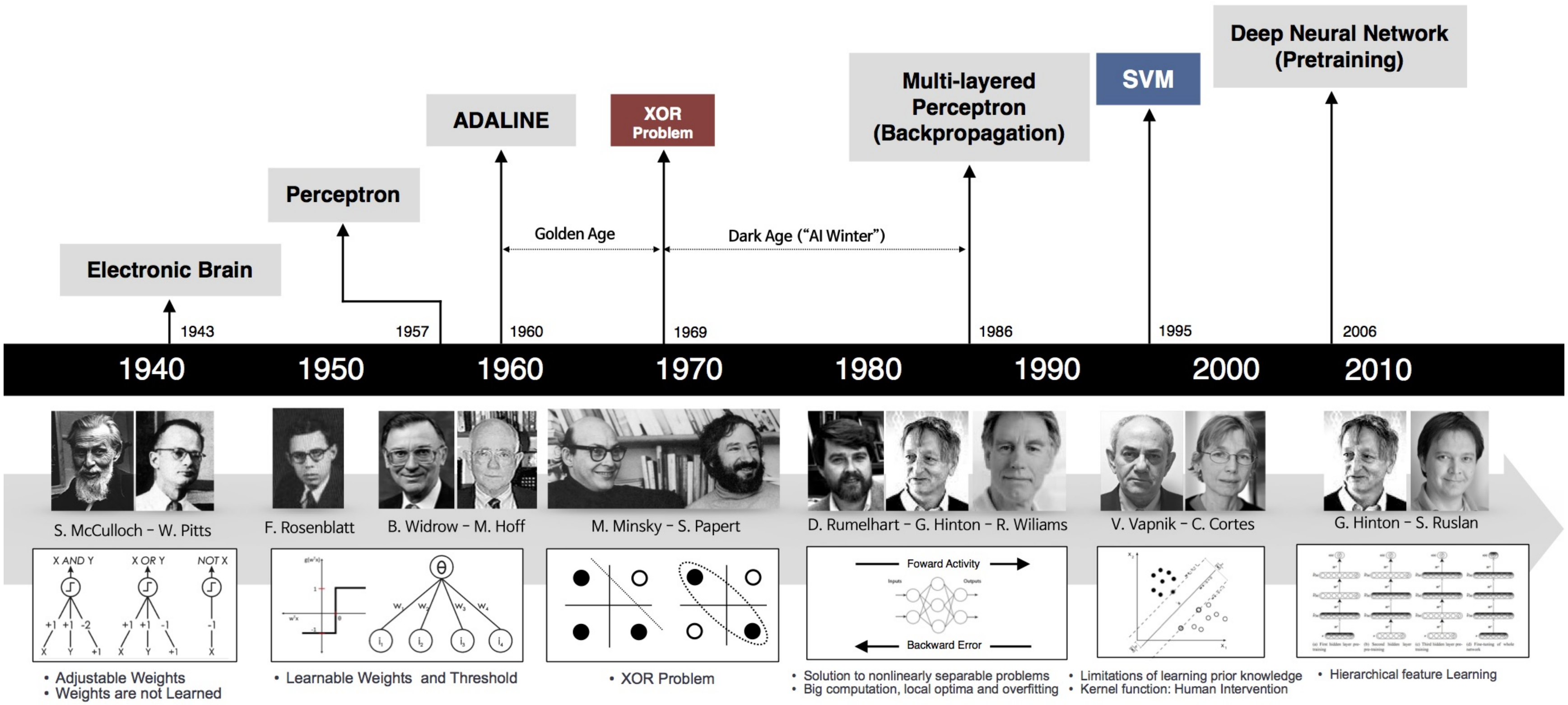
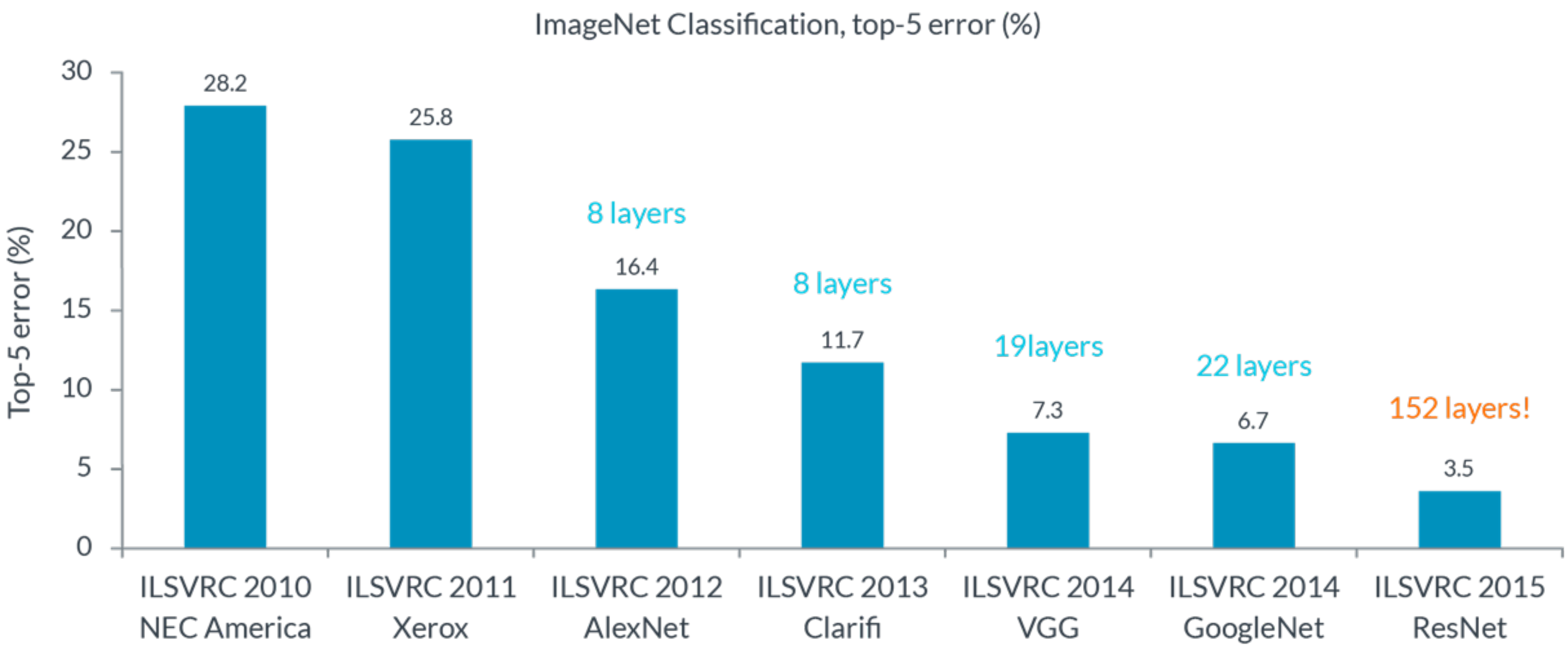
Convex Optimization for Neural Networks

- neural networks
- convex optimization formulations of neural networks
- semi-infinite optimization problems
- numerical examples

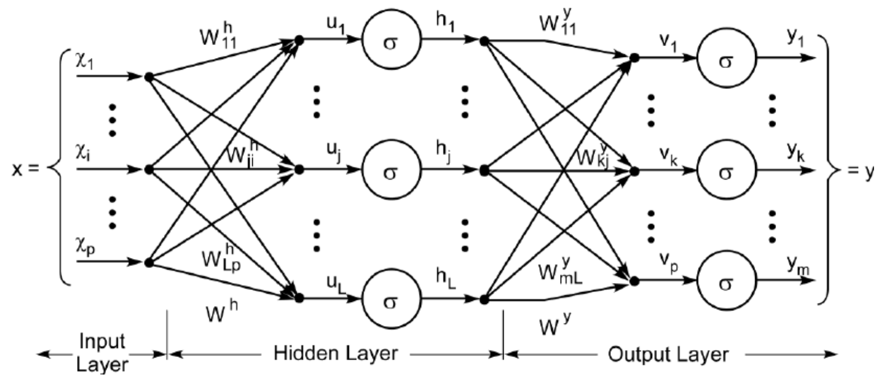
Neural Network Timeline



Deep learning revolution



Multilayer Neural Networks



$$z^{(0)} = x \quad \text{(input)}$$

$$a_j^{(l)} = \sum_i W_{ij}^{(l)} z_i^{(l-1)} \qquad l = 1, ..., L$$

$$z_j^{(l)} = \sigma(a_j^l) \qquad l = 1, ..., L$$

- $\sigma(\cdot)$: activation function, a_j^l : pre-activation of neuron j at layer l

Training Multilayer Neural Networks

- parameters $\Theta = (W^{(1)}, W^{(2)}, ..., W^{(L)})$

  regression (squared loss) vs classification (cross-entropy loss)

$$\min_{\Theta} \sum_{n=1}^{N} \underbrace{(y_n - f(x_n))^2}_{R_n(\Theta)} \qquad \min_{\Theta} - \sum_{n=1}^{N} \underbrace{\sum_{k=1}^{K} y_{nk} \log f_k(x_n)}$$

- (Stochastic) Gradient Descent

  $\Theta_{t+1} = \Theta_{t+1} - \sum_{i \in B} \frac{\partial}{\partial \Theta} R_n(\Theta)$

- non-convex optimization problem

Computing derivatives: Backpropagation Algorithm

$$\min_{\Theta} \sum_{n=1}^{N} \underbrace{(y_n - f(x_n))^2}_{R_n(\Theta)}$$

define $\delta_{nj}^{(l)} \triangleq \frac{\partial R_n(\Theta)}{\partial a_j^{(l)}}$, which are the derivatives of the loss with respect to the pre-activations

then gradients can be computed from

$$\frac{\partial R_n(\Theta)}{\partial W_{ij}^{(l)}} = \frac{\partial R_n(\Theta)}{\partial a_j^{(l)}} \frac{\partial a_j^{(l)}}{\partial W_{ij}^{(l)}} = \delta_{nj}^{(l)} z_i^{(l-1)}$$

Computing derivatives: Backpropagation Algorithm

$$\delta_{nj}^{(l)} \triangleq \frac{\partial R_n(\Theta)}{\partial a_j^{(l)}} = \sum_k \frac{\partial R_n(\Theta)}{\partial a_j^{(l+1)}} \frac{\partial a_j^{(l+1)}}{\partial a_j^{(l)}}$$

$$= \sum_k \delta_{nk}^{(l+1)} W_{jk}^{(l+1)} \sigma'(a_j^{(l)})$$

last term follows from the definition

$$a_k^{(l+1)} = \sum_r W_{rk}^{(l+1)} z_r^{(l)} = \sum_r W_{rk}^{(l+1)} \sigma(a_r^{(l)})$$

- at the output layer $\delta_{nj}^{(L)} = 2(a^{(L)} - y_n)$ since $R_n(\Theta) = ||a^{(L)} - y_n||^2$

Other Optimization Methods

▶ Stochastic Gradient Descent with momentum

$$d_{t+1} = \rho d_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha d_{t+1}$$

- α is the step size (learning rate), e.g., $\alpha = 0.1$ and ρ is the momentum parameter, e.g., $\rho = 0.9$
- $\nabla f(x_t)$ can be replaced with a subgradient for non-differentiable functions
- slow progress when the condition number is high

Diagonal Hessian Approximations

- H_t: a diagonal approximation of the Hessian $\nabla^2 f(x)$

$$x_{t+1} = x_t - \alpha H_t^{-1} \nabla f(x_t)$$

$$H_{t+1} = \text{ update using previous gradients}$$

- AdaGrad - adaptive subgradient method (Duchi et al., 2011)

$$[H_t]_{jj} = \mathsf{diag}\Big(\big(\textstyle\sum_{i=1}^t g_j^2 \big)^{1/2} + \delta \Big)$$

where $g_j := [\nabla f(x_t)]_j$, and $\delta > 0$ small to avoid numerical issues in inversion, e.g., $\delta = 10^{-7}$

effectively uses different learning rates for each coordinate

Other Variations of Diagonal Hessian Approximations

- RMSProp, Tieleman and Hinton, 2012

$$H_{t+1} = \mathrm{diag}((s_{t+1} + \delta)^{1/2})$$

  weighted gradient squared update

  $s_{t+1} = \gamma s_t + (1 - \gamma) g_t^2$ where $g_j := [\nabla f(x_t)]_j$

- ADAM, Kingma and Ba, 2015

  includes momentum and keeps a weighted sum of $[\nabla f(x_t)]_j^2$ and $[\nabla f(x_t)]_j$

Second Order Non-convex Optimization Methods

$$\min_x \sum_{i=1}^{n} (f_x(a_i) - y_i)^2$$

- Gauss-Newton method

$$x_{t+1} = \arg\min_x \; \| \underbrace{f_{x_t}(A) + J_t x}_{\text{Taylor's approx for } f_x} - y\|_2^2 = J_t^\dagger (y - f_{x_t}(A))$$

where $(J_t)_{ij} = \frac{\partial}{\partial x_j} f_x(a_i)$ is the Jacobian matrix

Jacobian Approximations

- Block-diagonal approximations
- Kronecker-factored Approximate Curvature (KFAC), Martens and Grosse, 2015
- Uniform or weighted sampling
- Conjugate Gradient can be used to approximate the Gauss-Newton step

Limitations of Neural Networks and Non-convex Training

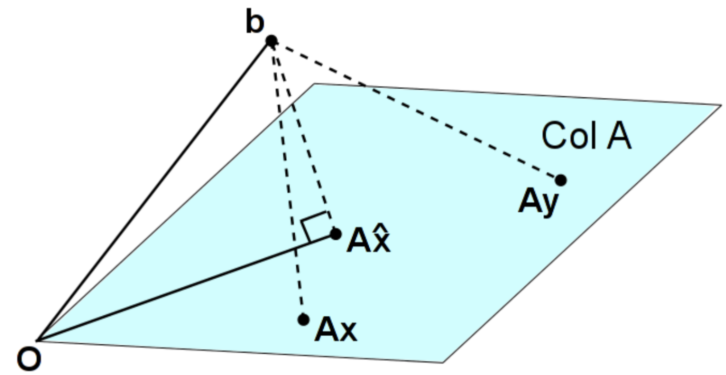
- sensitive to initialization, step-sizes, mini-batching, and the choice of the optimizer
- challenging to train and requires babysitting
- neural networks are complex black-box systems
- hard to interpret what the model is actually learning

Advantages of Convex Optimization

- Convex optimization provides a globally optimal solution
- Reliable and efficient solvers
- Specific solvers and internal parameters, e.g., initialization, step-size, batch-size does not matter
- We can check global optimality via KKT conditions
- Dual problem provides a lower-bound and an optimality gap
- Distributed and decentralized methods are well-studied

Example: Least Squares

$$\min_x \|Ax - b\|_2^2$$



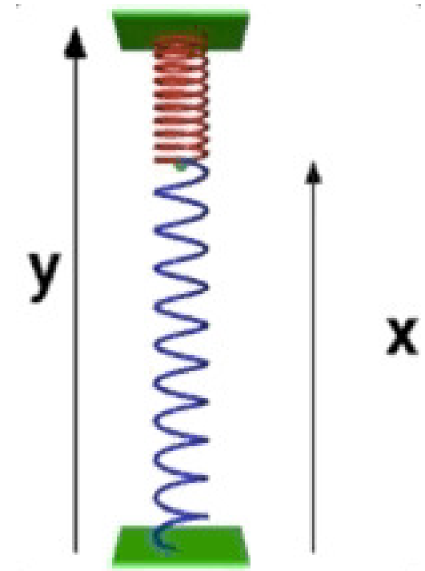
- well-studied convex optimization problem
- many efficient numerical procedures exist: Conjugate Gradient (CG), Preconditioned CG, QR, Cholesky, SVD
- regularized form $\min_x \|Ax - b\|_2^2 + \lambda\|x\|_2^2$, i.e., Ridge Regression is widely used

L2 regularization: mechanical model

$$\min_x \quad \underbrace{\frac{1}{2}(x-y)^2}_{\text{elastic energy}} \quad + \quad \underbrace{\frac{1}{2}\lambda x^2}_{\text{elastic energy}}$$

red spring constant $=1$

blue spring constant $= \lambda$

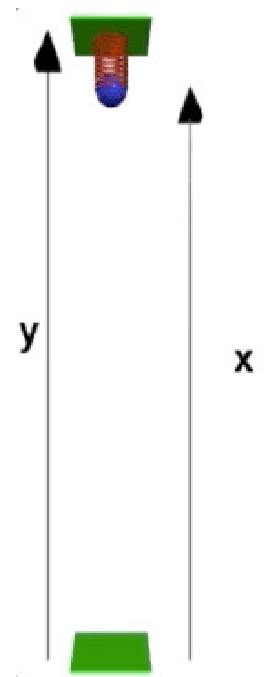


L1 regularization: mechanical model

$$\min_x \quad \underbrace{\frac{1}{2}(x-y)^2}_{\text{elastic energy}} \quad + \quad \underbrace{\lambda|x|}_{\text{potential energy}}$$

red spring constant $=1$

blue ball mass $= \lambda$ (small)

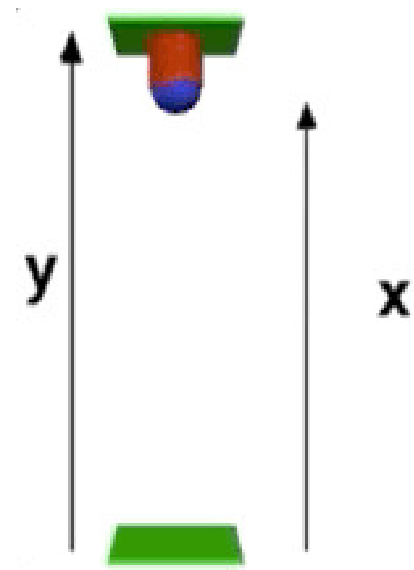


L1 regularization: mechanical model with large λ

$$\min_x \quad \underbrace{\frac{1}{2}(x-y)^2}_{\text{elastic energy}} \quad + \quad \underbrace{\lambda|x|}_{\text{potential energy}}$$

red spring constant $=1$

blue ball mass $= \lambda$ (large)



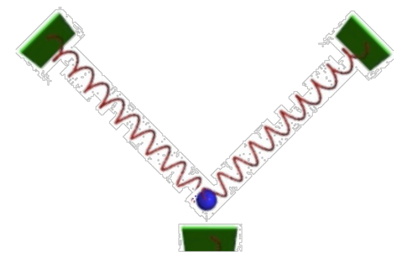
Least Squares with L1 regularization

$$\min_x \|Ax - y\|_2^2 + \lambda \|x\|_1$$

- L1 norm $\|x\|_1 = \sum_{i=1}^d |x_i|$ encourages sparsity of the solution x^*
- many efficient algorithms exist: proximal gradient (PG), accelerated PG, interior point, ADMM

Least Squares with group L1 regularization

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



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

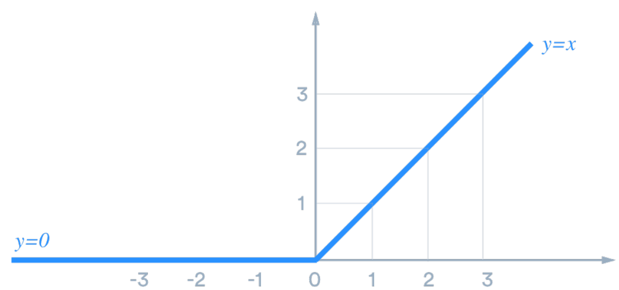
encourages group sparsity in the solution x^*, i.e., most blocks x_i are zero

- convex optimization and convex regularization methods are well understood and widely used in machine learning and statistics

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

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

- $\sigma(u) = \text{ReLU}(u) = \max(0, u)$



Neural Networks are Convex Regularizers

$$
\begin{aligned}
p_{\text{non-convex}} := \min_{\substack{W_1 \in \mathbb{R}^{d\times m} \\ W_2 \in \mathbb{R}^{m\times 1}}} \quad & L\left(\sigma(XW_1)W_2, y\right) + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2\right) \\
p_{\text{convex}} := \min_{Z \in \mathcal{K} \subseteq \mathbb{R}^{d\times p}} \quad & L\left(Z, y\right) + \lambda \underbrace{R(Z)}_{\text{convex regularization}}
\end{aligned}
$$

Neural Networks are Convex Regularizers

$$
\begin{aligned}
p_{\text{non-convex}} := \min \quad & L\left(\sigma(XW_1)W_2, y\right) + \lambda\left(\|W_1\|_F^2 + \|W_2\|_F^2\right) \\
& W_1 \in \mathbb{R}^{d\times m} \\
& W_2 \in \mathbb{R}^{m\times 1} \\
p_{\text{convex}} := \min \quad & L\left(Z, y\right) + \lambda R(Z) \\
& Z \in \mathcal{K} \subseteq \mathbb{R}^{d\times p}
\end{aligned}
$$

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 Polynomial-time Convex Optimization Formulations..., ICML 2020

Two Layer Networks Trained with Squared Loss

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

$$p_{\text{non-convex}} = \min_{W_1,W_2} \Big\| \sum_{j=1}^{m} \sigma(XW_{1j})W_{2j} - y \Big\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$

$$p_{\text{convex}} = \min_{u_i,v_i\in\mathcal{K}} \Big\| \sum_{i=1}^{p} D_i X(u_i - v_i) - y \Big\|_2^2 + \lambda \sum_{i=1}^{p} \|u_i\|_2 + \|v_i\|_2$$

here $D_1, ..., D_p$ 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^* 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

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

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

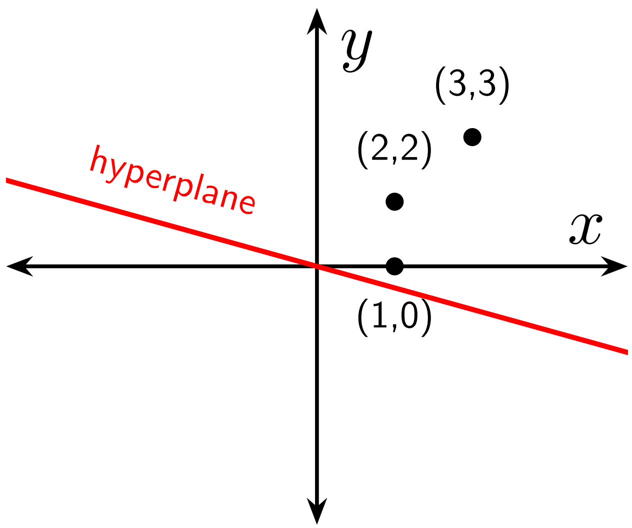
- optimal solutions of p_{convex} generates the entire set of optimal architectures $f(x) = W_2 \sigma(W_1 x)$ with m neurons for $m = 1, 2, ...,$

  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!

Simple Example

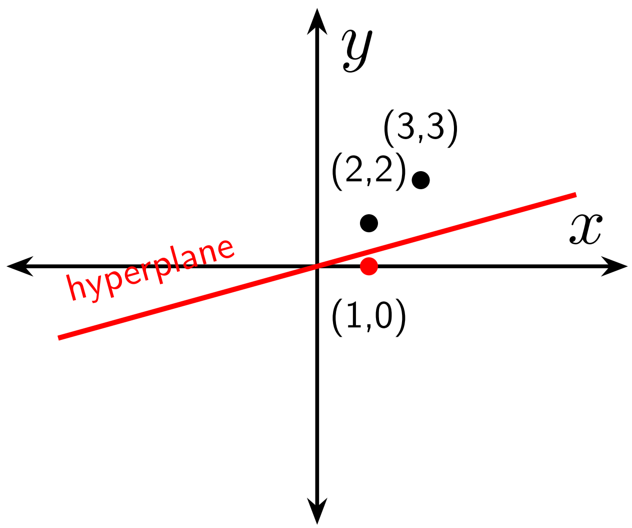
$n = 3$ samples in $\mathbb{R}^d$, $d = 2$ $\quad X = \begin{bmatrix} x_1^T \\ x_2^T \\ x_3^T \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$



$$D_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}$$

Simple Example

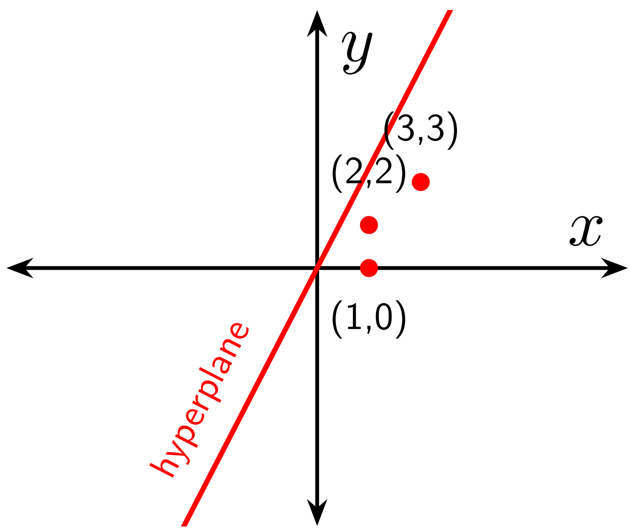
$n = 3$ samples in $\mathbb{R}^d$, $d = 2$ $\quad X = \begin{bmatrix} x_1^T \\ x_2^T \\ x_3^T \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$



$$D_1 X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}$$

$$D_2 X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 0 & 0 \end{bmatrix}$$

Simple Example

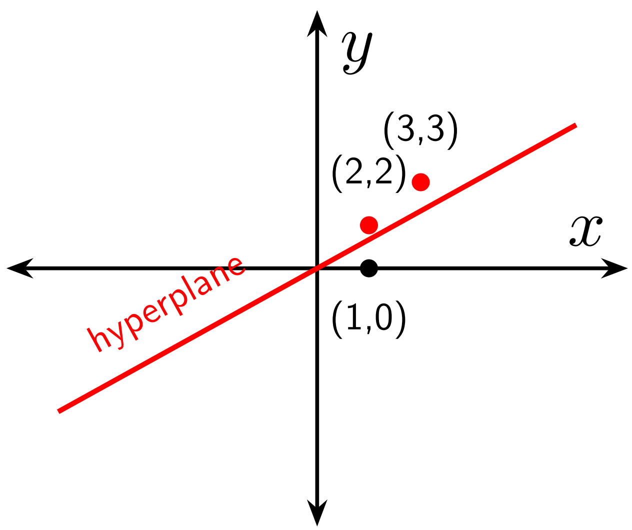


$$D_1X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}$$

$$D_2X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 0 & 0 \end{bmatrix}$$

$$D_3X = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Simple Example



$$D_1X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 1 & 0 \end{bmatrix}$$

$$D_2X = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 2 & 2 \\ 3 & 3 \\ 0 & 0 \end{bmatrix}$$

$$D_3X = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$D_4X = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} X = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \end{bmatrix}$$

Convex Program for $n = 3, d = 2$

$$\min \left\| \begin{bmatrix} x_1^T \\ x_2^T \\ x_3^T \end{bmatrix} (u_1 - v_1) + \begin{bmatrix} x_1^T \\ x_2^T \\ 0 \end{bmatrix} (u_2 - v_2) + \begin{bmatrix} 0 \\ 0 \\ x_3^T \end{bmatrix} (u_3 - v_3) - y \right\|_2^2$$

subject to

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

$D_1 X u_1 \geq 0, D_1 X v_1 \geq 0$

$D_2 X u_2 \geq 0, D_2 X v_2 \geq 0$

$D_4 X u_3 \geq 0, D_4 X v_3 \geq 0$

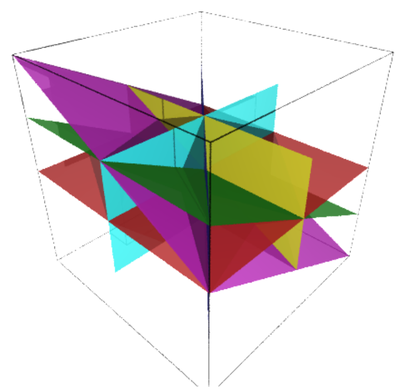
equivalent to the non-convex two-layer NN problem

Hyperplane Arrangements

- consider $X \in \mathbb{R}^{n \times d}$
- $D_1, \ldots, D_P$ are diagonal $0-1$ matrices that encode patterns

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

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



Computational Complexity

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

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

◦ Approximate $O(2^{\sqrt{m}})$ (Goel et al., COLT 2017)

$$\boxed{\text{Convex program } O((\tfrac{n}{r})^r) \text{ where } r = \mathrm{rank}(X)}$$

n : number of samples, d : dimension

(i) polynomial in n and m for fixed rank r

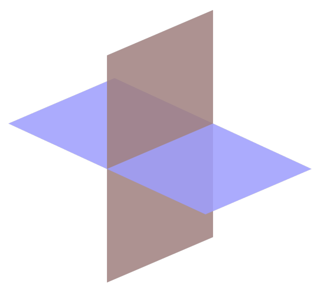
(ii) exponential in d for full rank data $r = d$. This can not be improved unless $P = NP$ even for $m = 1$.

Convolutional Hyperplane Arrangements

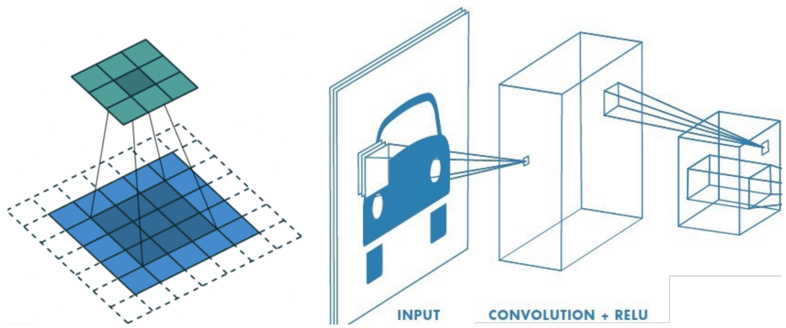
Let $X \in \mathbb{R}^{n \times d}$ be partitioned into patch matrices $X = [X_1, ..., X_K]$ where $X_k \in \mathbb{R}^{n \times h}$

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

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



Convolutional Neural Networks can be optimized in fully polynomial time



- $f(x) = W_2\sigma(W_1x)$, $W_1 \in \mathbb{R}^{d\times m}$, $W_2 \in \mathbb{R}^{m\times 1}$

- m filters (neurons), h filter size, e.g., 1024 filters of size 3×3 $(m = 1024, h = 9)$

- convex optimization complexity is polynomial in all parameters n, m and d

Approximating the Convex Program

$$\min_{u_1,v_1\ldots u_p,v_p\in\mathcal{K}} \Big\| \sum_{i=1}^{p} D_i X(u_i - v_i) - y \Big\|_2^2 + \lambda\Big(\sum_{i=1}^{p} \|u_i\|_2 + \|v_i\|_2\Big)$$

- sample $D_1, ..., D_p$ as Diag$(Xu \geq 0)$ where $u \sim N(0, I)$
- Backpropagation (gradient descent) on the non-convex loss

  is a **heuristic** for the convex program

Numerical Results

- backpropagation converges to a stationary point of the loss
- convex optimization formulation returns the globally optimal neural network
- note that the number of variables is larger in the convex formulation
- interior point method, proximal gradient and ADMM are very effective
- proximal map of the group ℓ_1 regularizer is closed-form

Interior Point Method vs Non-convex SGD

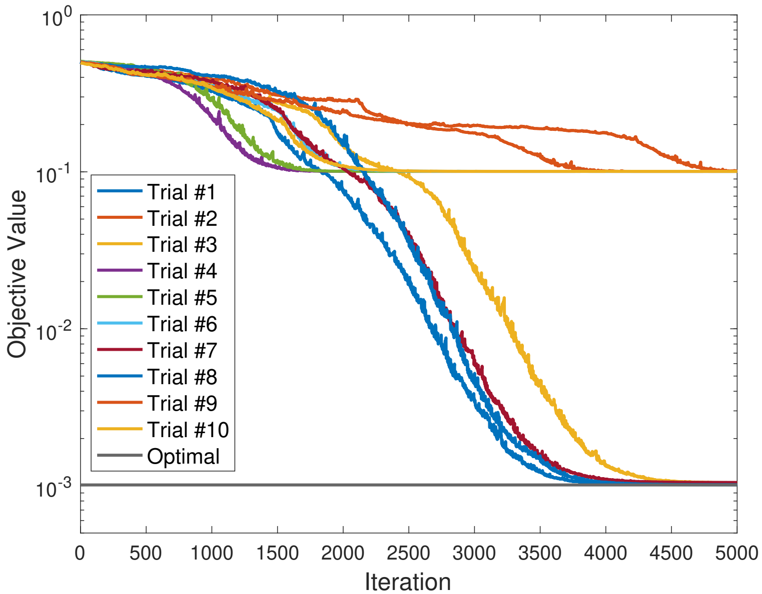


Figure 1: $m = 8$

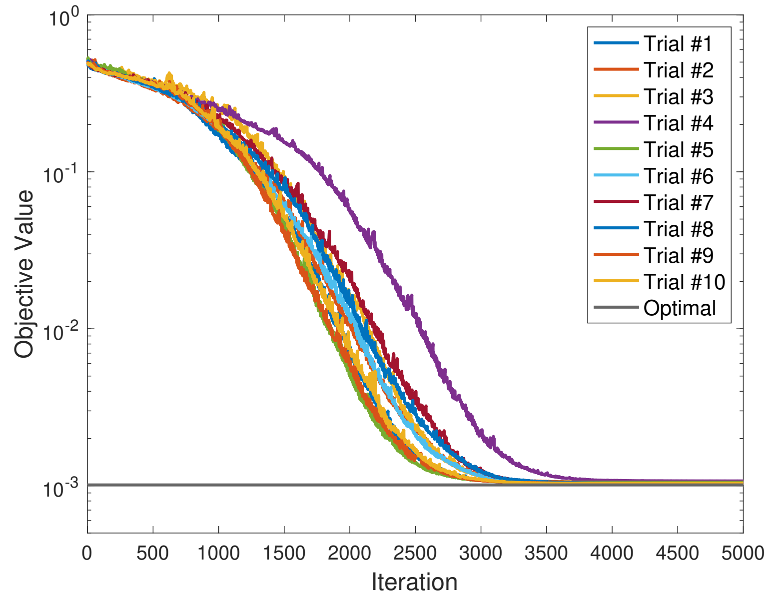


Figure 2: $m = 50$

SGD (10 different initializations) vs the convex program solved with interior point method (optimal) on a toy dataset ($d = 2$)

Convex SGD vs Non-convex SGD and ADAM

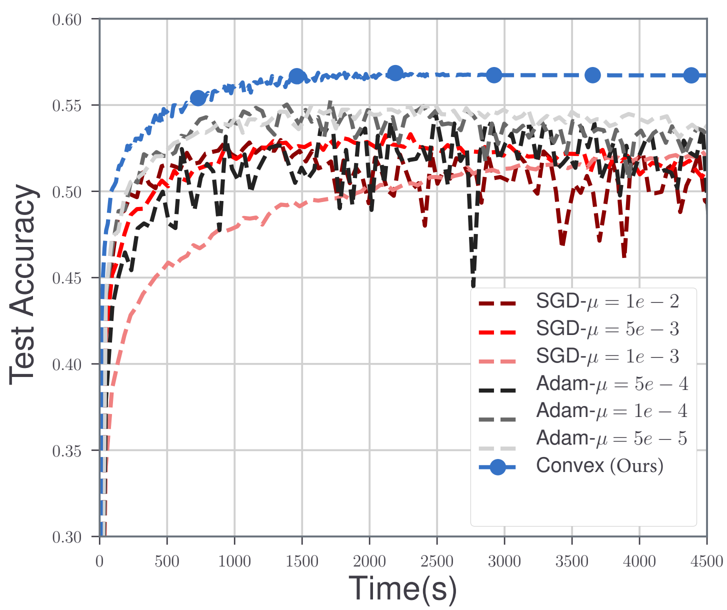


Figure 3: CIFAR-10

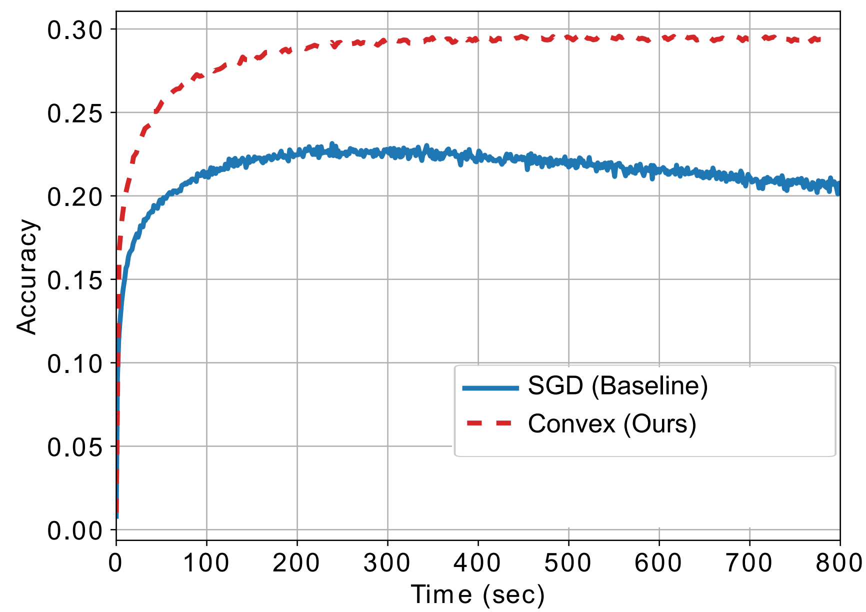


Figure 4: CIFAR-100

CIFAR image classification task $(n = 50000, d = 3072)$

Polynomial Activation Networks

- polynomial activation function $\sigma(t) = at^2 + bt + c$

$$p_{\text{non-convex}} := \min_{\|W_{1i}\|_2 = 1, \forall i} \quad L\left(\sigma(XW_1)W_2, y\right) + \lambda \|W_2\|_1$$

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

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

$$p_{\text{convex}} := \min_{Z} \quad L\left(Z, y\right) + \lambda \underbrace{R(Z)}_{\text{convex regularization}}$$

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

- **Theorem:** $p_{\text{convex}} = p_{\text{non-convex}}$ and can be solved via a convex semidefinite program in polynomial-time with respect to (n, d, m).
  B. Bartan, M. Pilanci Neural Spectrahedra and Semidefinite Lifts 2021

Polynomial Activation Networks

- special case: quadratic activation $\sigma(t) = t^2$

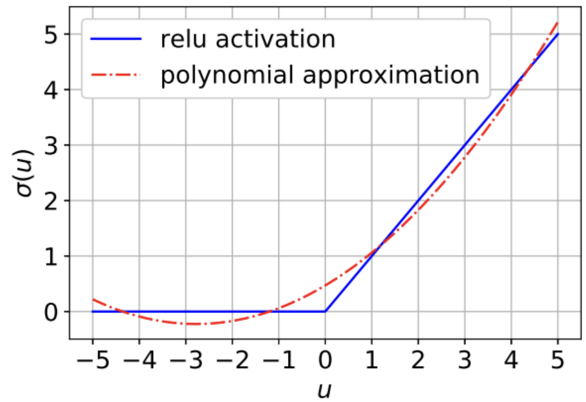
$$p_{\text{convex}} := \min_{Z} \quad L\left(Z, y\right) + \lambda \|Z\|_* \qquad\qquad Z \in \mathcal{K} \subseteq \mathbb{R}^{d \times p}$$

- $\|Z\|_*$ is the nuclear norm
- promotes low rank solutions
- first and second layer weights can be recovered via Eigenvalue Decomposition $Z = \sum_{i=1}^{m} \alpha_i u_i u_i^T$

Polynomial Activation Networks

- polynomial activation function

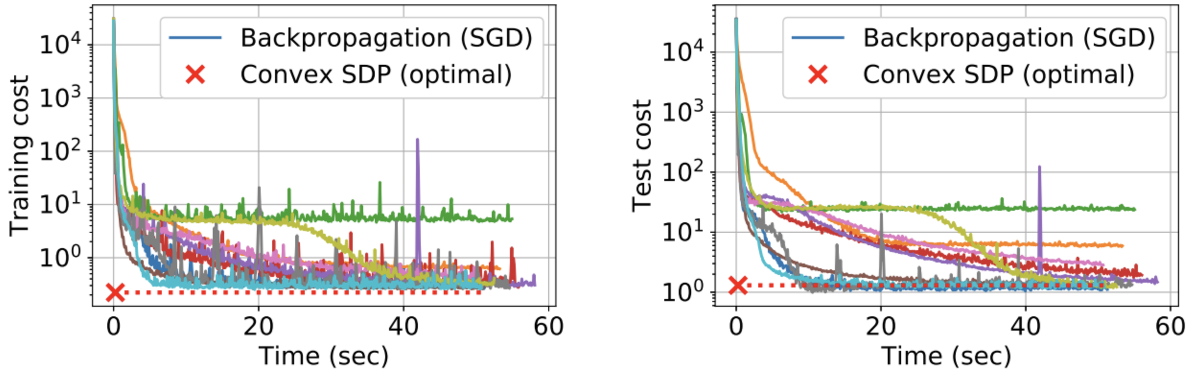
$$\phi(t) = at^2 + bt + c$$



$$\begin{array}{ll} \min\limits_{Z} & L(\hat{y}, y) + \lambda Z_4 \\ \text{s.t.} & \hat{y}_i = a x_i^T Z_1 x_i + b x_i^T Z_2 + c Z_4, i \in [n] \\ & Z = \begin{bmatrix} Z_1 & Z_2 \\ Z_2^T & Z_4 \end{bmatrix} \succeq 0,\ \mathrm{tr}(Z_1) = Z_4, \end{array}$$

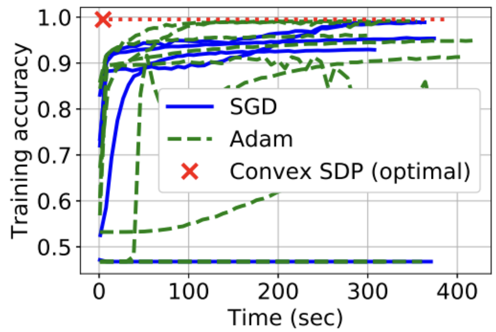
Numerical Results: Quadratic Activation

- toy dataset $n = 100, d = 10$
- $m = 10$ planted neurons

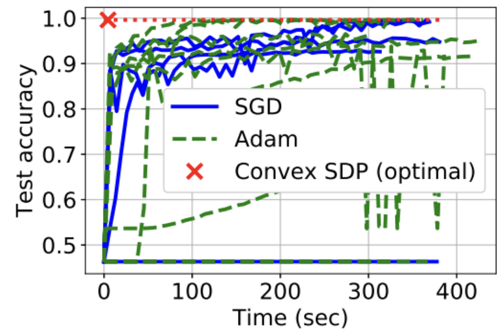


- red cross marker shows the time taken by the convex solver

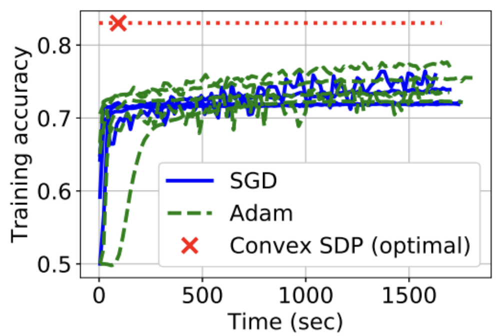
Numerical Results: Polynomial Activation



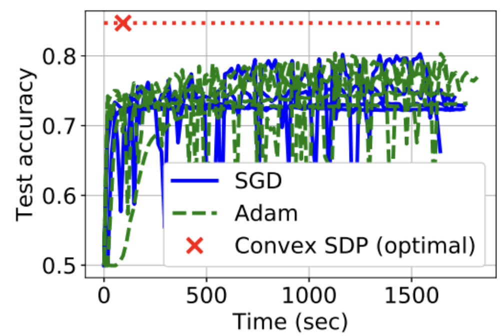
(a) CNN, MNIST, training accuracy



(b) CNN, MNIST, test accuracy



(c) CNN, CIFAR, training accuracy



(d) CNN, CIFAR, test accuracy

Deriving the convex program

- ReLU activation $\sigma(t) = (t)_+$ and weight decay regularization

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

- nested minimization problems
- inner minimization over W_2 is convex for fixed W_1
- not jointly convex in (W_1, W_2)

Scaling Variables

- **Lemma:** The weight decay (ℓ_2^2) regularized non-convex program is equivalent to an ℓ_1 penalized non-convex program

$$
\begin{aligned}
p_{\text{non-convex}} &= \min_{W_1, W_2} \frac{1}{2}\Big\| \sum_{j=1}^{m} \phi(XW_{1j})W_{2j} - y \Big\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right) \\
&= \min_{\|W_{1_j}\|_2 = 1, W_2} \frac{1}{2}\Big\| \sum_{j=1}^{m} \phi(XW_{1j})W_{2j} - y \Big\|_2^2 + \lambda \sum_{j=1}^{m} |W_{2j}|
\end{aligned}
$$

Scaling Variables

$$p_{\text{non-convex}} = \min_{W_1, W_2} \frac{1}{2} \Big\| \sum_{j=1}^{m} \phi(XW_{1j}) W_{2j} - y \Big\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$

- we define

$$\tilde{W}_{1j} := W_{1j}/\alpha_j$$
$$\tilde{W}_{2j} := W_{2j}\alpha_j$$

- neural network output does not change, regularization term changes

Scaling Variables

- plugging-in we get

$$\min_{\alpha_j} \min_{W_1, W_2} \frac{1}{2} \Big\| \sum_{j=1}^m \phi(XW_{1j}) W_{2j} - y \Big\|_2^2 + \lambda \left(\sum_{j=1}^m \|W_{1j}\|_2^2 / \alpha_j^2 + |W_{2j}| \alpha_j^2 \right)$$

- optimize with respect to $\alpha_1, \ldots \alpha_m$
- we obtain

$$\min_{\|W_{1j}\|_2 = 1, W_2} \frac{1}{2} \Big\| \sum_{j=1}^m \phi(XW_{1j}) W_{2j} - y \Big\|_2^2 + \lambda \sum_{j=1}^m |W_{2j}|$$

Convex Duality of Neural Networks

- Replace the inner minimization problem by it's convex dual

$$
\begin{aligned}
p_{\text{non-convex}} &= \min_{\|W_{1j}\|_2=1} \min_{W_2} \frac{1}{2}\Big\| \sum_{j=1}^m \phi(XW_{1j})W_{2j} - y \Big\|_2^2 + \lambda \sum_{j=1}^m |W_{2j}| \\
&= \min_{\|W_{1j}\|_2=1} \max_{v:\, |v^T(XW_{1j})_+| \le \lambda\, \forall j} -\frac{1}{2}\|v-y\|_2 \\
&= \min_{\|W_{1j}\|_2=1} \max_{v} -\frac{1}{2}\|v-y\|_2 + I\big(\, |v^T(XW_{1j})_+| \le \lambda\, \forall j\big)
\end{aligned}
$$

- $I(\cdot)$ is the $-\infty/0$ valued indicator function

- interchange the order of $\min$ and $\max$

Convex Duality of Neural Networks

- by weak duality

$$p_{\text{non-convex}} \geq \max_{v:\, |v^T(XW_{1j})_+| \leq \lambda\, \forall W_{1j}:\, \|W_{1j}\|_2 = 1,\, \forall j} -\frac{1}{2}\|v - y\|_2$$
$$= \max_{v:\, |v^T(XW)_+| \leq \lambda\, \forall W:\, \|W\|_2 = 1} -\frac{1}{2}\|v - y\|_2$$

- note that this is a convex optimization problem

- semi-infinite program: infinitely many constraints and finitely many variables

- it turns out that **strong duality holds** (Pilanci and Ergen, ICML 2020), i.e., the inequality is in fact an equality

Representing constraints

- finally, we can represent the constraints as

$$
\begin{aligned}
|v^T(XW)_+| \leq \lambda \iff |v^T D_k X W_k| &\leq \lambda \\
D_k X W_k &\geq 0 \\
(I - D_k) X W_k &\geq 0
\end{aligned}
$$

D_k are diagonal 0/1 matrices that encode hyperplane arrangements, i.e., sign patterns that can be obtained by $\mathbf{sign}(XW)$ for $W \in \mathbb{R}^d$

Bidual Problem

- the dual of the dual yields claimed convex neural network problem

$$p_{\text{convex}} = \min_{u_i, v_i \in \mathcal{K}} \Big\| \sum_{i=1}^{p} D_i X(u_i - v_i) - y \Big\|_2^2 + \lambda \sum_{i=1}^{p} \|u_i\|_2 + \|v_i\|_2$$

- exact representation since strong duality holds

$$p_{\text{convex}} = p_{\text{non-convex}}$$

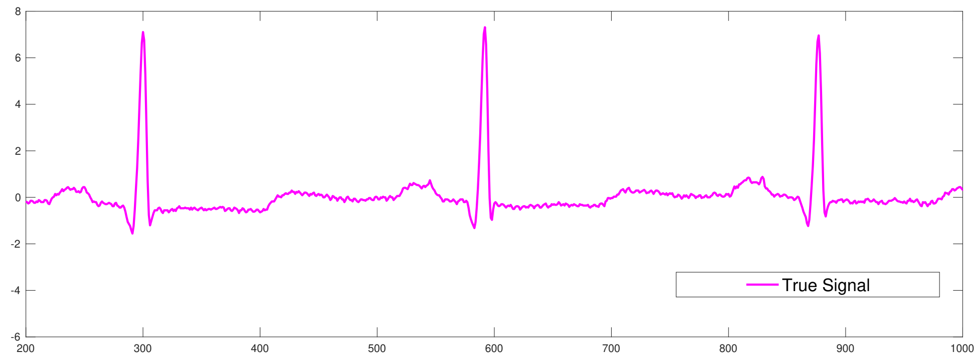
Conclusions

- neural networks can be trained via convex optimization
- global optimality is guaranteed
- higher-dimensional optimization problems
- convex models are transparent and interpretable

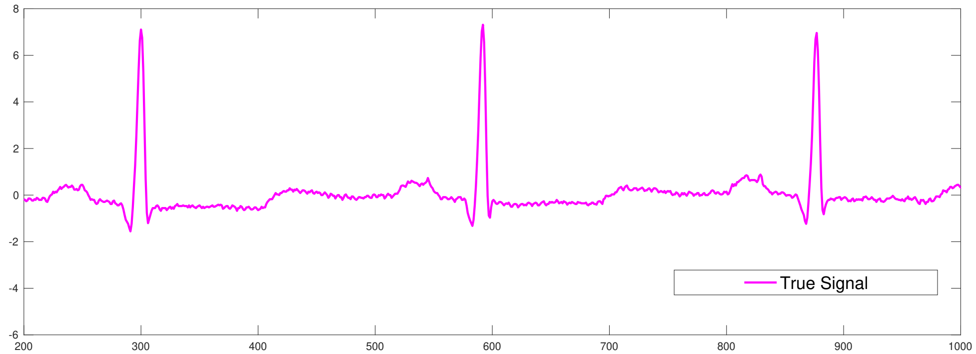
Extra Slides

- convex neural networks for signal processing
- interpreting and explaining neural networks based on the convex formulations
- batch normalization
- convex three-layer ReLU neural networks
- convex Generative Adversarial Networks (GANs)

Electrocardiogram (ECG) Prediction

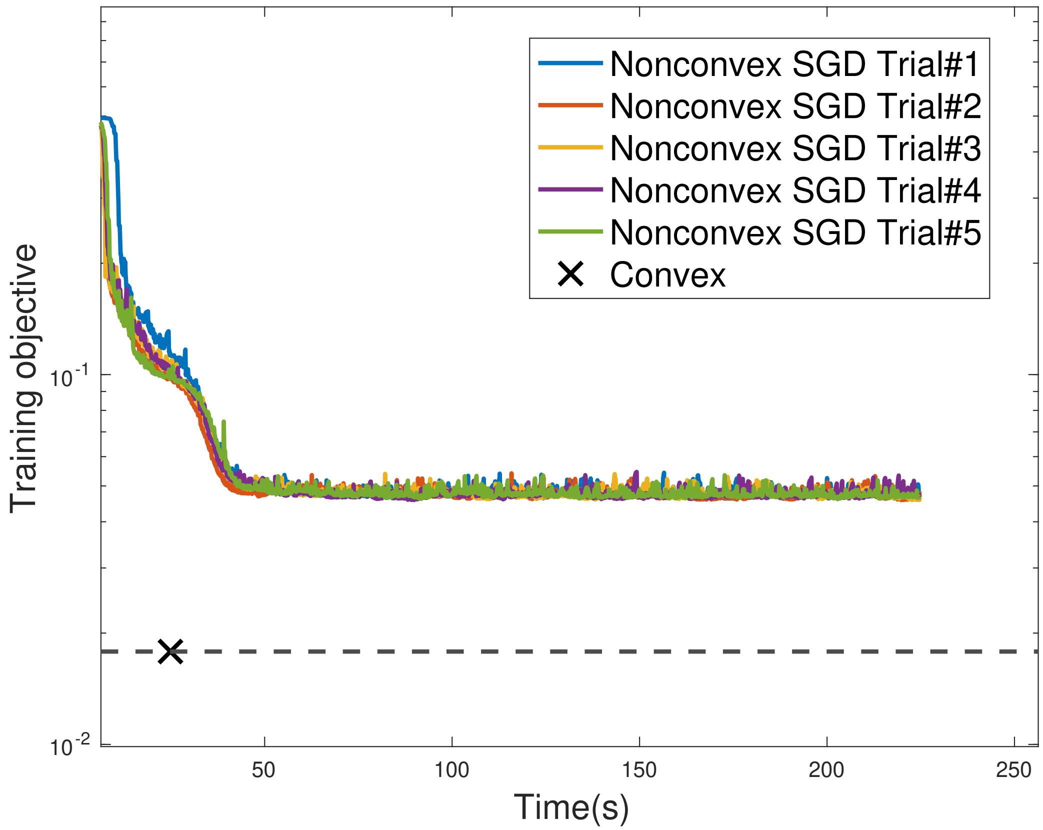


- window size: 15 samples
- training and test set

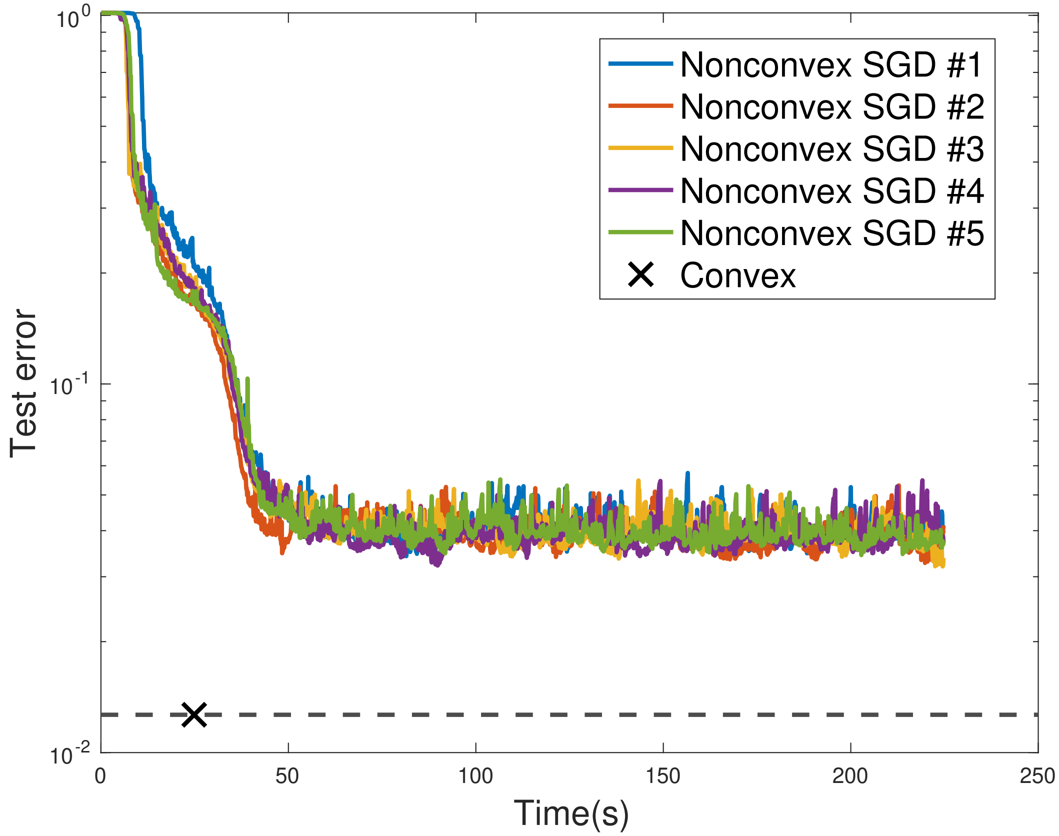


$$X = \begin{bmatrix} x[1] & \dots & x[d] \\ x[2] & \dots & x[d+1] \\ \vdots & & \\ x[n] & \dots & x[d+n-1] \end{bmatrix}, \quad y = \begin{bmatrix} x[d+1] \\ x[d+2] \\ \vdots \\ x[d+n] \end{bmatrix}$$

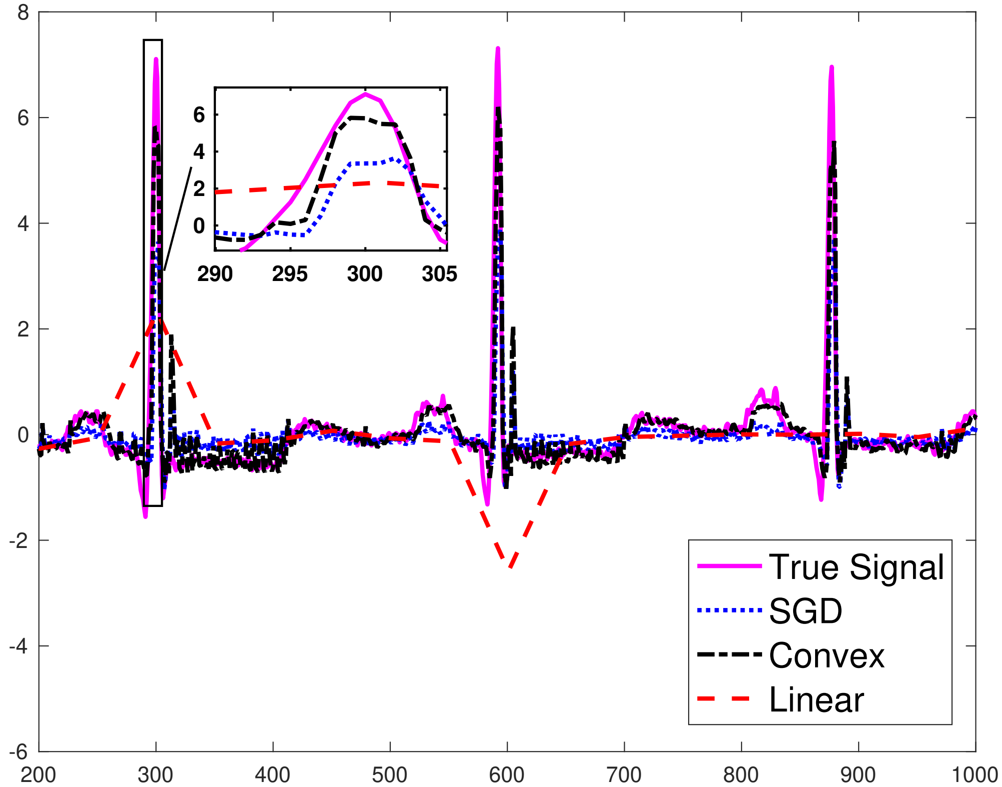
Signal Prediction: Training



Signal Prediction: Test Accuracy

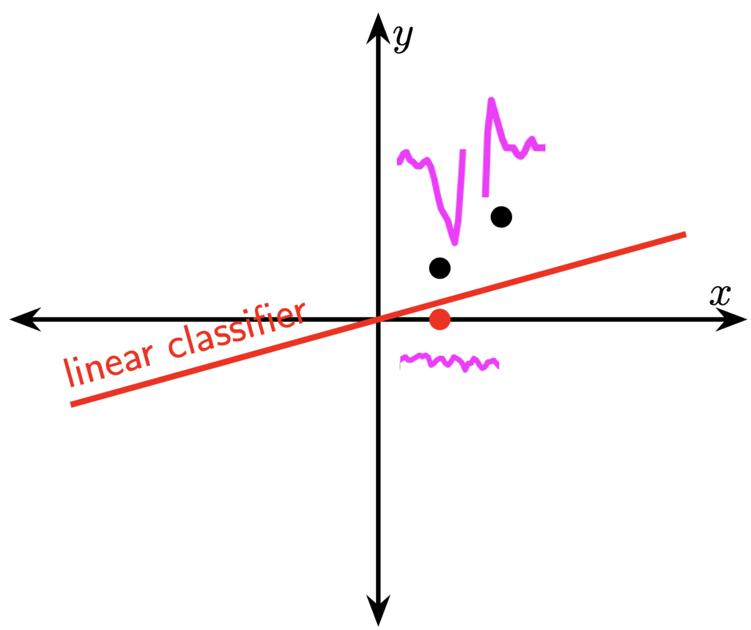


Signal Prediction: Test Accuracy



Interpreting Neural Networks

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



ReLU Networks with Batch Normalization (BN)

- BN layer transforms a batch of input data to have a mean of zero and a standard deviation of one and has two trainable parameters α, γ

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

$$p_{\text{non-convex}} = \min_{W_1, W_2, \alpha, \gamma} \left\| \mathbf{BN}_{\alpha,\gamma}(\phi(XW_1))W_2 - y \right\|_2^2 + \lambda \left(\|W_1\|_F^2 + \|W_2\|_F^2 \right)$$

$$p_{\text{convex}} = \min_{w_1, v_1 \ldots w_p, v_p \in \mathcal{K}} \left\| \sum_{i=1}^{p} U_i(w_i - v_i) - y \right\|_2^2 + \lambda \left(\sum_{i=1}^{p} \|w_i\|_2 + \|v_i\|_2 \right)$$

- where $U_i \Sigma_i V_i^T = D_i X$ is the SVD of DX_i, i.e., BatchNorm extracts singular vectors (T. Ergen et al. Demystifying Batch Normalization in ReLU Networks, 2021)

Three layer ReLU Networks

$$\min_{\substack{\{W_j,\vec{u}_j,\vec{w}_{1j},w_{2j}\}_{j=1}^m \\ \vec{u}_j\in\mathcal{B}_2,\forall j}} \left\|\sum_{j=1}^m \left((\mathbf{X}\vec{W}_j)_+\vec{w}_{1j}\right)_+ w_{2j} - \vec{y}\right\|_2^2 + \beta\sum_{j=1}^m \|\vec{W}_j\|_F^2 + \|\vec{w}_{1j}\|_2^2 + w_{2j}^2$$

- the equivalent convex problem is

$$\min_{\{\vec{W}_i,\vec{W}_i'\}_{i=1}^p\in\mathcal{K}} \frac{1}{2}\left\|\sum_{i=1}^p\sum_{j=1}^P D_iD_j\mathbf{X}\left(\vec{W}_{ij}'-\vec{W}_{ij}\right)-\vec{y}\right\|_2^2 + \frac{\beta}{2}\sum_{i,j=1}^p \|\vec{W}_{ij}\|_F + \|\vec{W}_{ij}'\|_F$$

T. Ergen, M. Pilanci, Convex Optimization of Two- and Three-Layer Networks in Polynomial Time, ICLR 2021

Convex Generative Adversarial Networks (GANs)

- Wasserstein GAN

$$p^* = \min_{\theta_g} \max_{\theta_d} \mathbb{E}_{\vec{x} \sim p_x}[D_{\theta_d}(\vec{x})] - \mathbb{E}_{\vec{z} \sim p_z}[D_{\theta_d}(G_{\theta_g}(\vec{z}))]. \tag{1}$$

- generative model for the data
- discriminator and generator are neural networks

- consider a two-layer ReLU-activation generator $G_{\theta_g}(\vec{Z}) = (\vec{Z}\vec{W}_1)_+\vec{W}_2$ and quadratic activation discriminator $D_{\theta_d}(\vec{X}) = (\vec{X}\vec{V}_1)^2\vec{V}_2$
- Wasserstein GAN problem is equivalent to a convex-concave game
- can be solved via convex optimization as follows

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

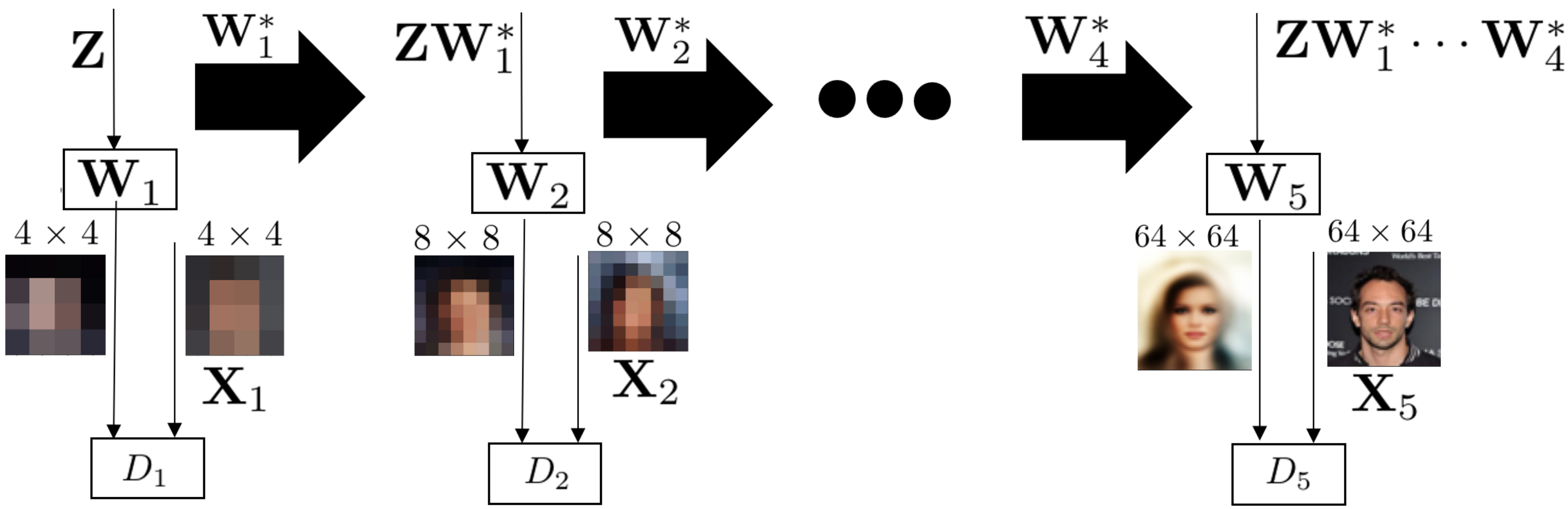
$$\vec{W}_1^*, \vec{W}_2^* = \underset{\vec{W}_1,\vec{W}_2}{\operatorname{argmin}} \|\vec{W}_1\|_F^2 + \|\vec{W}_2\|_F^2 \text{ s.t. } \vec{G}^* = (\vec{Z}\vec{W}_1)_+\vec{W}_2,$$

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

- the second problem can be solved via convex optimization as shown earlier

Progressive GANs

- deeper architectures can be trained layerwise



Numerical Results

- fake faces generated from CelebA dataset
- two-layer quadratic activation discriminator and linear generator
- convex optimization with closed form optimal solution