Learning Neural Networks with Adaptive Regularization

Han Zhao
han.zhao@cs.cmu.edu
Machine Learning Department, Carnegie Mellon University

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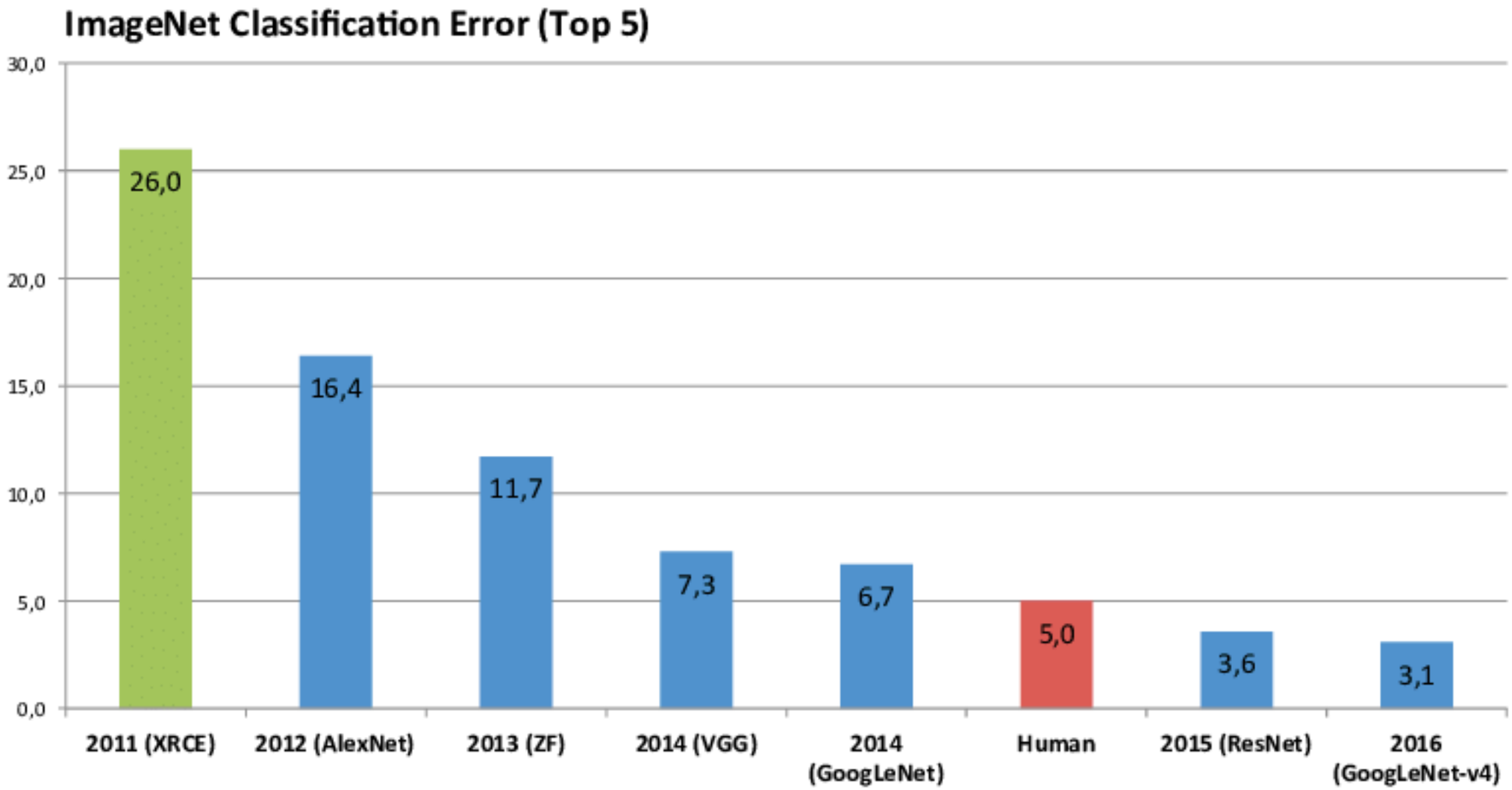
Joint work with Yao-Hung Hubert Tsai, Ruslan Salakhutdinov, and Geoffrey J. Gordon

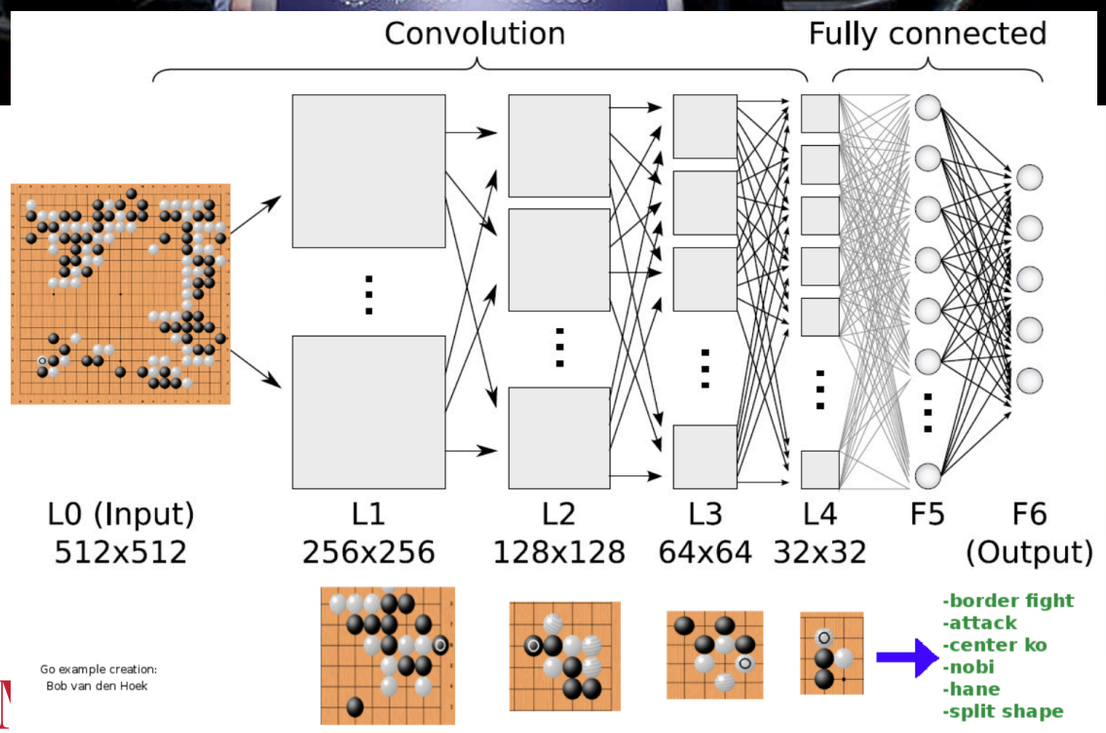
Recent Success of Deep Learning

ImageNet (Top 5) Classification Error:



Recent Success of Deep Learning

Go: AlphaGo vs Seudo Lee and Jie Ke



Go example creation:
Bob van den Hoek

Recent Success of Deep Learning

Dota 2: OpenAI Five

- Beats professional player on One-on-One game, 2017
- Beats amateur and semi-professional teams on Five-on-Five games, 2018

Recent Success of Deep Learning

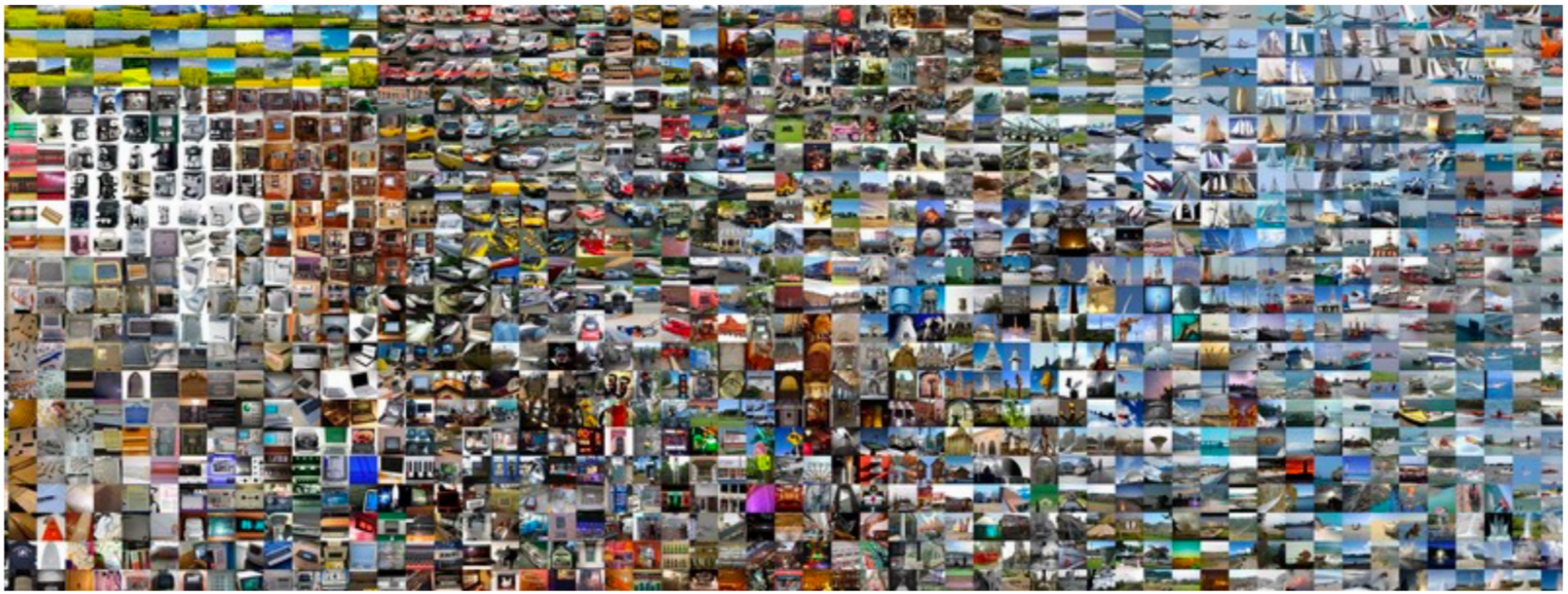
Other application domains:

- Natural Language Processing: Neural Machine Translation (2014)
- Artificial Game Playing: Atari (2015), AlphaGo (2016), StarCraft II (2018)
- Automatic Speech Recognition (2010)
- Computer Vision: Image generation (2014)
- Healthcare: Drug discovery…

Recent Success of Deep Learning

However, successful training of neural networks requires:

- Large-scale datasets
- Powerful computational resources



ImageNet: ~1M images, ~1K classes

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Configuration	Search threads	No. of CPU	No. of GPU	Elo rating
Single[10] p. 10–11	40	48	1	2,181
Single	40	48	2	2,738
Single	40	48	4	2,850
Single	40	48	8	2,890
Distributed	12	428	64	2,937
Distributed	24	764	112	3,079
Distributed	40	1,202	176	3,140
Distributed	64	1,920	280	3,168

Versions	Hardware	Elo rating	Matches
AlphaGo Fan	176 GPUs,[52] distributed	3,144[51]	5:0 against Fan Hui
AlphaGo Lee	48 TPUs,[52] distributed	3,739[51]	4:1 against Lee Sedol
AlphaGo Master	4 TPUs,[52] single machine	4,858[51]	60:0 against professional players; Future of Go Summit

Go: training data ~ almost infinity: simulated self-playing game

Recent Success of Deep Learning

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How to effectively regularize the training of neural networks when there is only few data available?

Outline

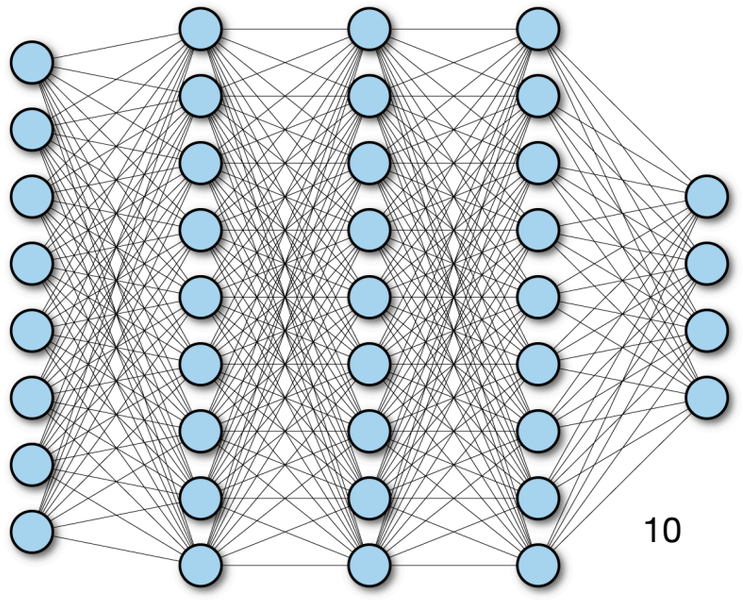
- Deep Learning Preliminary
- Learning with Adaptive Regularization
- Experiments
- Conclusion

Deep Learning Preliminary

A simple fully-connected neural network:

- Data set: $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^n, \quad \mathbf{x}_i \in \mathbb{R}^d, y_i \in \{0, 1\}, \ \forall i \in [n]$
- Model:

$$f(\mathbf{x}; \theta) = \sigma(W_L g(W_{L-1} \cdots W_2 g(W_1 \mathbf{x})))$$



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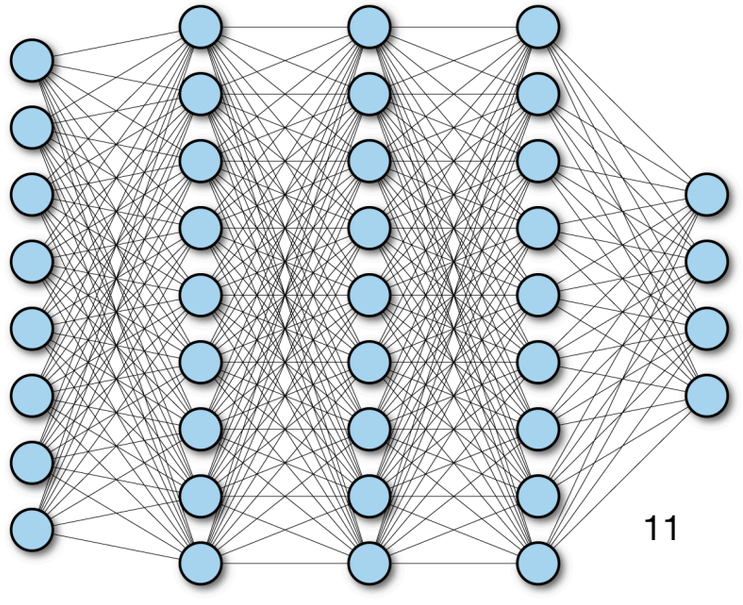

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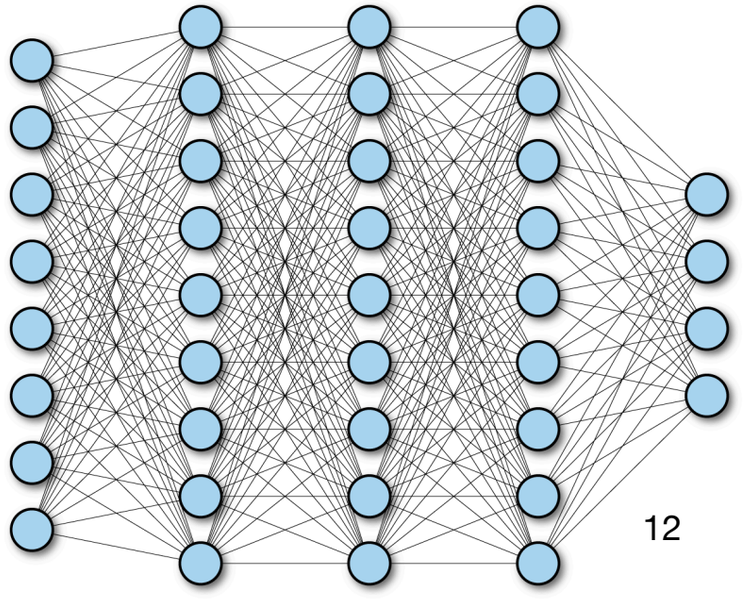

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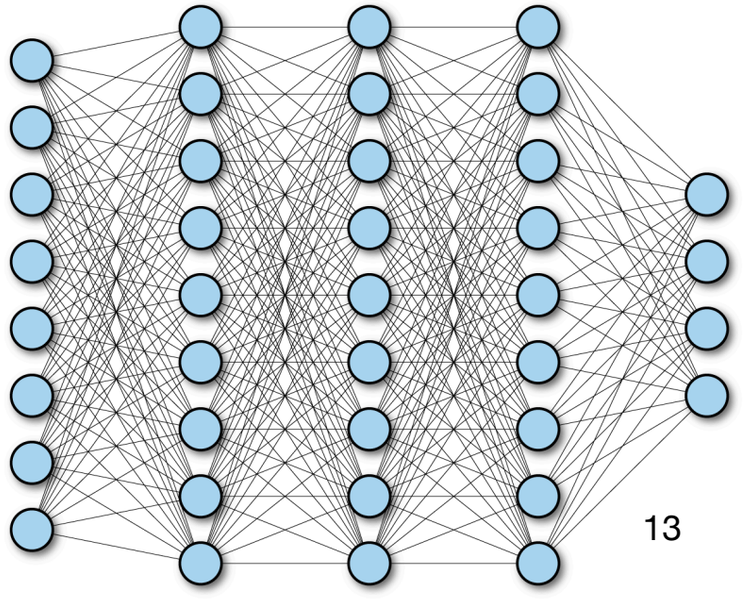
- Essentially: a sequence of affine transformation + component-wise nonlinear activation



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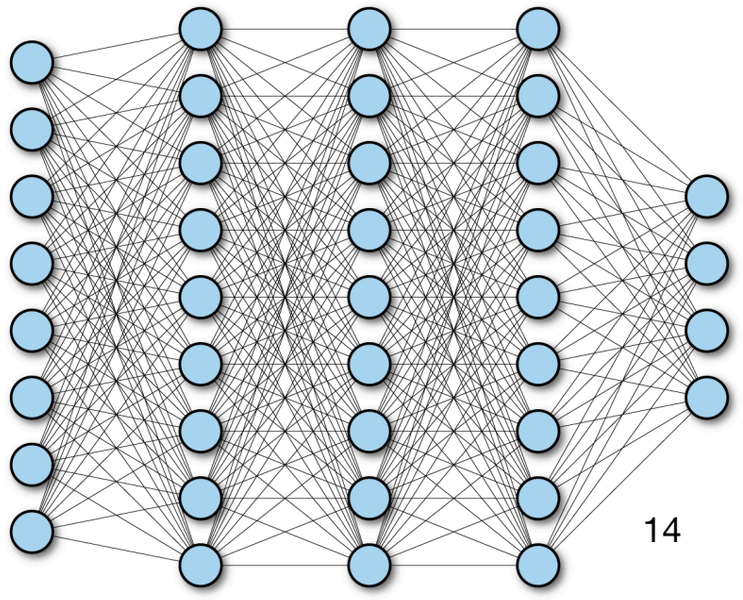
A simple fully-connected neural network:

- Loss function: Maximum Log-likelihood Estimation (MLE)

$$\hat{y} := f(\mathbf{x}; \theta) = \sigma\left(W_L g\left(W_{L-1} \cdots W_2 g\left(W_1 \mathbf{x}\right)\right)\right) \in (0, 1)$$



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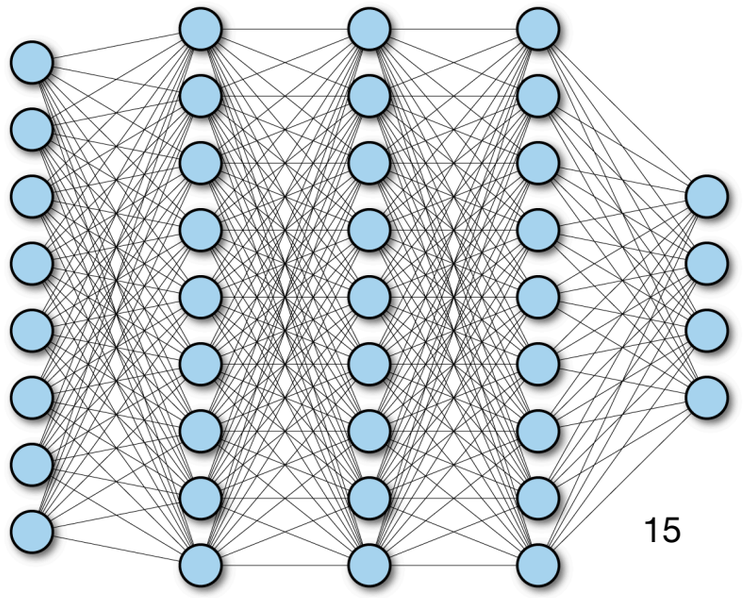
- Optimization: stochastic gradient descent

$$\theta \leftarrow \theta - \gamma \frac{\partial \ell(\theta)}{\partial \theta}$$



Deep Learning Preliminary

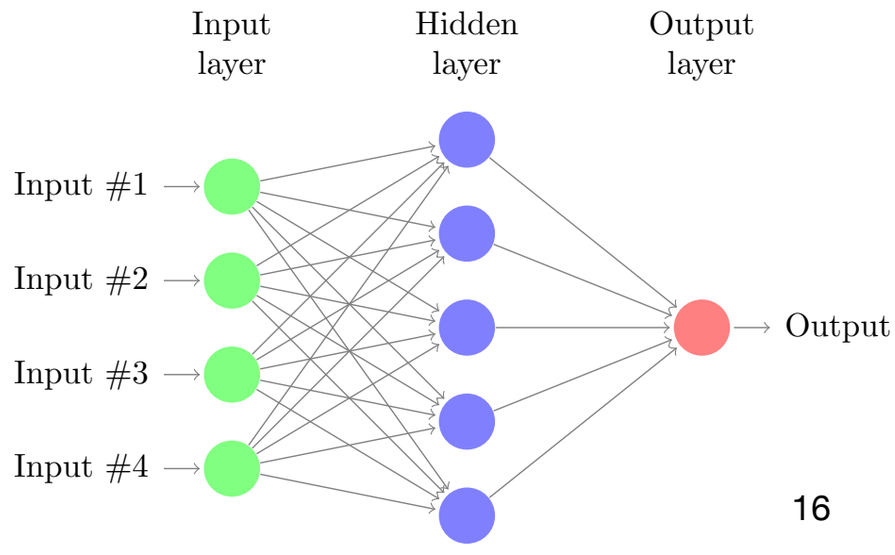
Let's consider a two-layer NN as illustration:

- Hidden layer $\mathbf{h} \in \mathbb{R}^p$ with output $\hat{y} \in \mathbb{R}$ for regression problem:

$$\hat{y} = \mathbf{a}^T \mathbf{h}, \quad \mathbf{h} = g(W\mathbf{x}), \quad W \in \mathbb{R}^{p \times d}$$

- Loss function:

$$\ell(W, \mathbf{a}) = \frac{1}{2}(\hat{y} - y)^2$$



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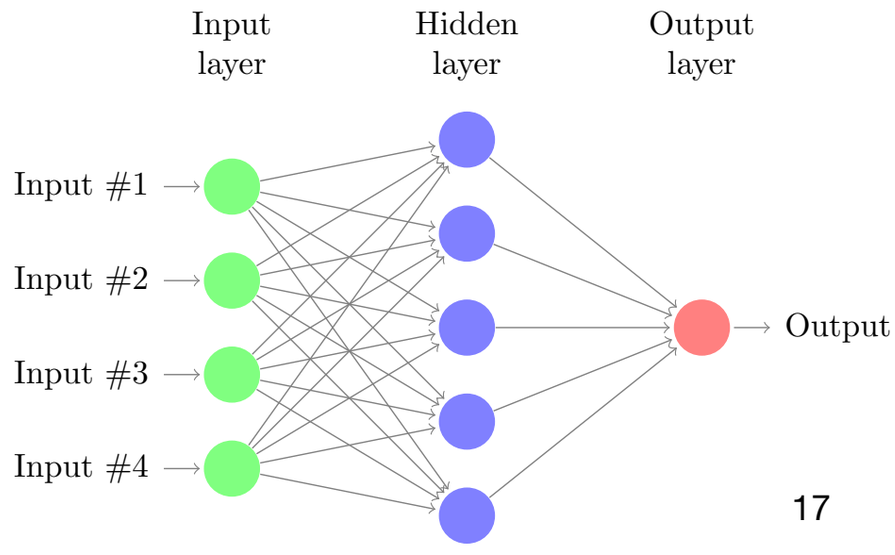

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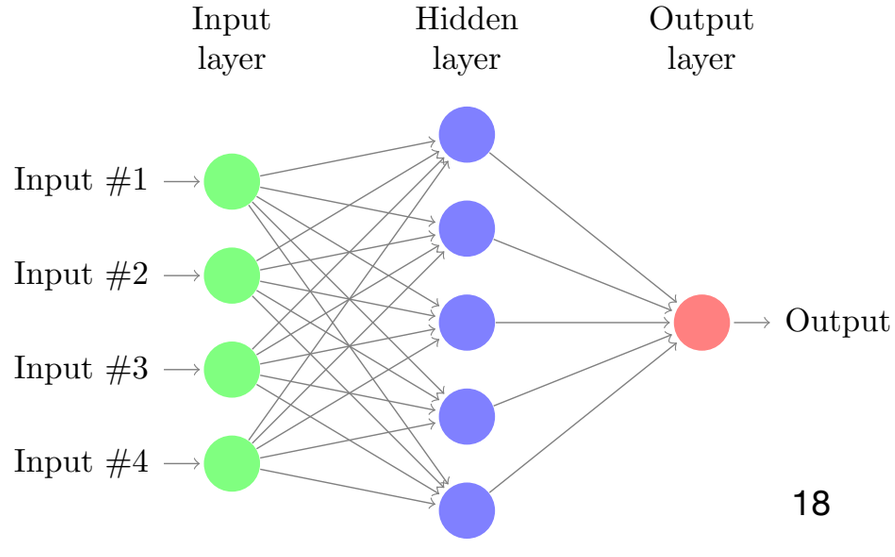

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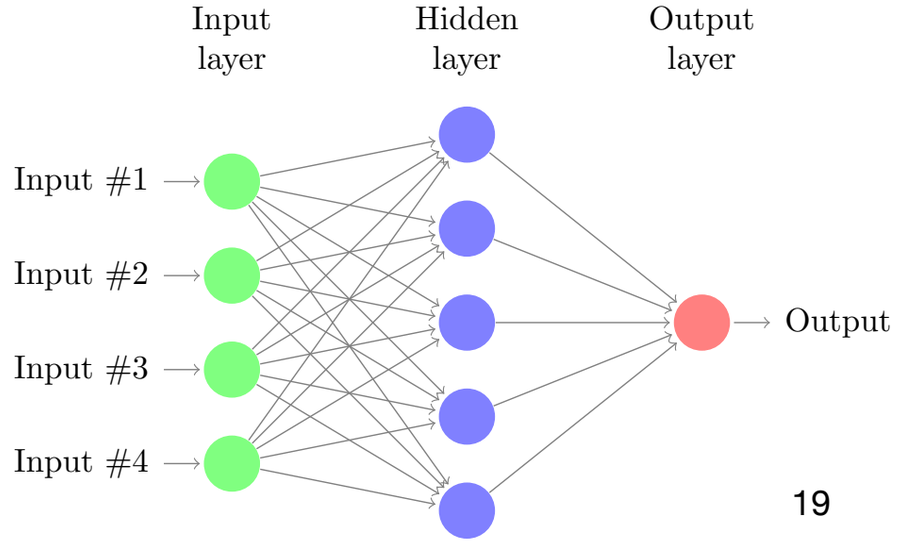

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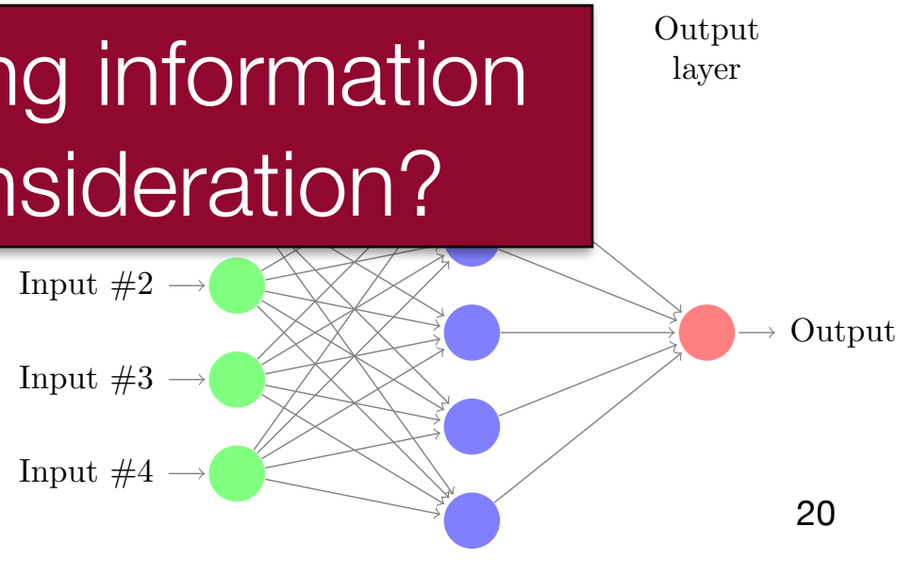
Update each row/column by taking information from other rows/columns into consideration?



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Learning with Adaptive Regularization

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How can we make use of this structure?

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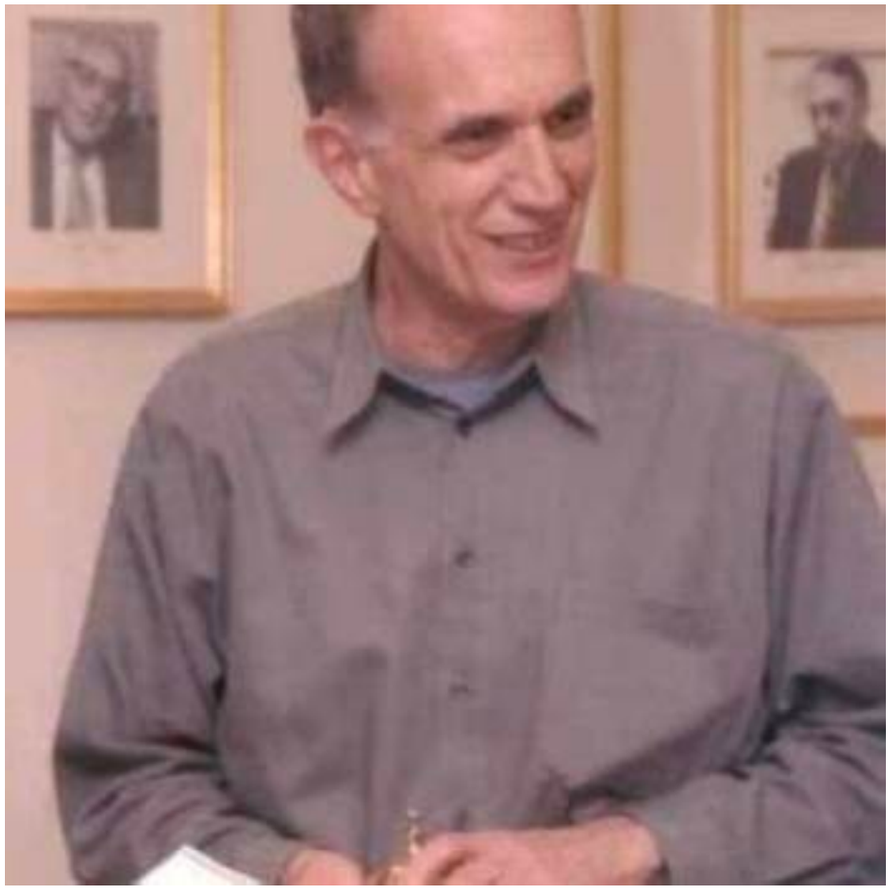

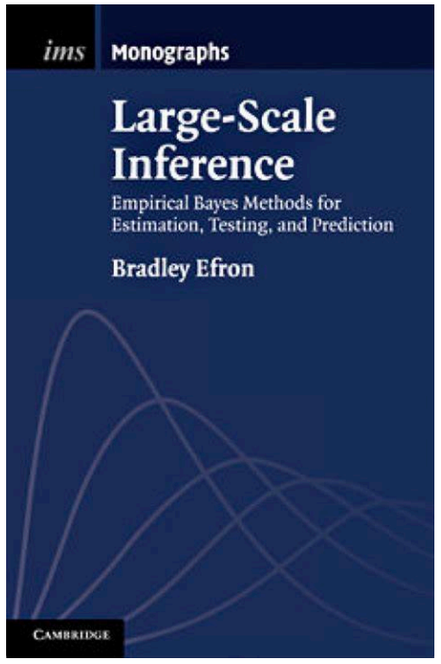

"Learning from the experience of others"

— Prof. Bradley Efron

Learning with Adaptive Regularization

Recall the gradient update formula for W:

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Now consider the following multivariate normal distribution:

$$W \sim \mathcal{MN}(0_{p \times d}, \Sigma_r, \Sigma_c)$$

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- Equivalently, this means

$$\text{vec}(W) \sim \mathcal{N}(0_{p\times d}, \Sigma_c \otimes \Sigma_r)$$

$$p(W \mid \Sigma_r, \Sigma_c) = \frac{\exp\left(-\text{Tr}(\Sigma_r^{-1} W \Sigma_c^{-1} W^T)/2\right)}{(2\pi)^{pd/2}\det(\Sigma_r)^{d/2}\det(\Sigma_c)^{p/2}}$$

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- Or, $\quad W_{i:} \sim \mathcal{N}(\mathbf{0}_d, [\Sigma_r]_{ii} \cdot \Sigma_c), \quad W_{:j} \sim \mathcal{N}(\mathbf{0}_p, [\Sigma_c]_{jj} \cdot \Sigma_r)$

Learning with Adaptive Regularization

OK, but how to determine the parameters in the prior?

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The empirical Bayes method: set the parameters of the prior from data by maximizing the marginal log-likelihood function (Efron and Morris, 1973; Efron and Hastie, 2016)

$$\widehat{\Sigma_r}, \widehat{\Sigma_c} = \underset{\Sigma_r, \Sigma_c}{\arg\max}\ p(\mathcal{D} \mid \Sigma_r, \Sigma_c) = \underset{\Sigma_r, \Sigma_c}{\arg\max} \int p(\mathcal{D} \mid W) \cdot p(W \mid \Sigma_r, \Sigma_c)\ dW$$

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- Example with closed-form solution: the James-Stein estimator

Learning with Adaptive Regularization

Iterative maximization of the joint distribution:

- Given weight matrix W, compute the most likely parameters Σ_r, Σ_c
- Given parameters Σ_r, Σ_c, plug in and update W

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Instantiate the above principle using the matrix-variate normal distribution, we arrive at the following optimization problem:

$$\min_{W, \mathbf{a}} \min_{\Omega_r, \Omega_c} \quad \frac{1}{2n} \sum_{i \in [n]} (\hat{y}(\mathbf{x}_i; W, \mathbf{a}) - y_i)^2 + \lambda ||\Omega_r^{1/2} W \Omega_c^{1/2}||_F^2 - \lambda \big(d \log\det(\Omega_r) + p \log\det(\Omega_c) \big)$$

$$\text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p, \; uI_d \preceq \Omega_c \preceq vI_d$$

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- $\Omega_r := \Sigma_r^{-1},\ \Omega_c := \Sigma_c^{-1}$ are the precision matrices
- The first term corresponds to data fitting term
- The second term corresponds to regularization term
- λ is a trade-off hyper-parameter that only depends on p, d

Learning with Adaptive Regularization

Maximum-A-Posteriori estimation

$$\min_{W,\mathbf{a}} \min_{\Omega_r,\Omega_c} \quad \frac{1}{2n}\sum_{i\in[n]}(\hat{y}(\mathbf{x}_i;W,\mathbf{a})-y_i)^2+\lambda||\Omega_r^{1/2}W\Omega_c^{1/2}||_F^2-\lambda\Big(d\log\det(\Omega_r)+p\log\det(\Omega_c)\Big)$$

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$$||\Omega_r^{1/2}W\Omega_c^{1/2}||_F^2=||\text{vec}(\Omega_r^{1/2}W\Omega_c^{1/2})||_2^2=||(\Omega_c^{1/2}\otimes\Omega_r^{1/2})\ \text{vec}(W)||_2^2$$

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Maximum-A-Posteriori estimation

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$$||\Omega_r^{1/2}W\Omega_c^{1/2}||_F^2=||\mathrm{vec}(\Omega_r^{1/2}W\Omega_c^{1/2})||_2^2=||(\Omega_c^{1/2}\otimes\Omega_r^{1/2})\ \mathrm{vec}(W)||_2^2$$

- Tikhonov regularization imposed on W with the Tikhonov matrix as $\Gamma:=\Omega_c^{1/2}\otimes\Omega_r^{1/2}$

Learning with Adaptive Regularization

Maximum-A-Posteriori estimation

$$\min_{W,\mathbf{a}} \min_{\Omega_r,\Omega_c} \quad \frac{1}{2n}\sum_{i\in[n]}(\hat{y}(\mathbf{x}_i;W,\mathbf{a})-y_i)^2+\lambda||\Omega_r^{1/2}W\Omega_c^{1/2}||_F^2-\lambda\Big(d\log\det(\Omega_r)+p\log\det(\Omega_c)\Big)$$

$$\text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p,\ uI_d \preceq \Omega_c \preceq vI_d$$

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- Tikhonov regularization imposed on W with the Tikhonov matrix as $\Gamma := \Omega_c^{1/2}\otimes\Omega_r^{1/2}$
- The Tikhonov matrix is not predefined, but learned from data adaptively

Learning with Adaptive Regularization

Volume minimization

$\log\det(\cdot)$ is a concave function over the positive-definite cone. For any pair of matrices $A_1, A_2 \in \mathbb{S}^m_{++}$, the following inequality holds:

$$\begin{aligned}\log\det(A_1) &\leq \log\det(A_2) + \langle \nabla \log\det(A_2), A_1 - A_2 \rangle \\ &= \log\det(A_2) + \mathrm{Tr}(A_2^{-1} A_1) - m\end{aligned}$$

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Apply the above inequality twice, we obtain:

$$d\log\det(W\Omega_c W^T/2d) \leq -d\log\det(\Omega_r) + \frac{1}{2}\mathrm{Tr}(\Omega_r W \Omega_c W^T) - dp,$$

$$p\log\det(W^T\Omega_r W/2p) \leq -p\log\det(\Omega_c) + \frac{1}{2}\mathrm{Tr}(\Omega_r W \Omega_c W^T) - dp.$$

Learning with Adaptive Regularization

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which implies:

$$d\log\det(W\Omega_c W^T) + p\log\det(W^T\Omega_r W) \leq ||\Omega_r^{1/2} W \Omega_c^{1/2}||_F^2 - \big(d\log\det(\Omega_r) + p\log\det(\Omega_c)\big) + c$$

Learning with Adaptive Regularization

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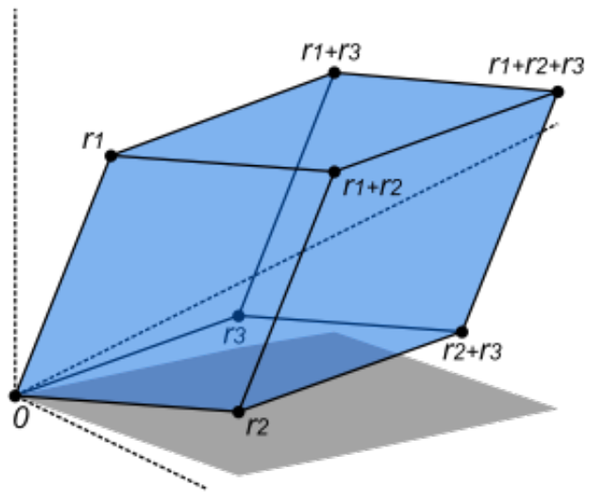
Squared volume of the parallelepiped spanned by row/column vectors of preconditioned W

Our regularizer



Learning with Adaptive Regularization

How to optimize (Ω_r, Ω_c) ?

$$\min_{W,\mathbf{a}} \min_{\Omega_r,\Omega_c} \quad \frac{1}{2n} \sum_{i\in[n]} (\hat{y}(\mathbf{x}_i; W, \mathbf{a}) - y_i)^2 + \lambda ||\Omega_r^{1/2} W \Omega_c^{1/2}||_F^2 - \lambda \big(d \log\det(\Omega_r) + p \log\det(\Omega_c)\big)$$

$$\text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p,\ uI_d \preceq \Omega_c \preceq vI_d$$

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- For fixed W and Ω_c, the objective function is convex in Ω_r

Learning with Adaptive Regularization

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- For fixed W and Ω_r, the objective function is convex in Ω_c

Learning with Adaptive Regularization

How to optimize (Ω_r, Ω_c) ?

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- For fixed W and Ω_c, the objective function is convex in Ω_r
- For fixed W and Ω_r, the objective function is convex in Ω_c
- The objective function is symmetric w.r.t. Ω_r and Ω_c

It suffices if we focus on and solve one of them

Learning with Adaptive Regularization

For fixed W and Ω_c, consider the optimization over Ω_r:

$$\min_{\Omega_r} \quad \mathrm{Tr}(\Omega_r W \Omega_c W^T) - d \log\det(\Omega_r), \qquad \text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p$$

Define the constraint set: $\mathcal{C} := \{A \in \mathbb{S}^p_{++} \mid uI_p \preceq A \preceq vI_p\}$ and indicator function

$$\mathbb{I}_{\mathcal{C}}(A) = \begin{cases} 0 & \text{If } A \in \mathcal{C} \\ \infty & \text{Otherwise} \end{cases}$$

Learning with Adaptive Regularization

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Now we have an equivalent unconstrained convex optimization problem:

$$\min_{\Omega_r} \quad \mathrm{Tr}(\Omega_r W \Omega_c W^T) - d \log\det(\Omega_r) + \mathbb{I}_{\mathcal{C}}(\Omega_r)$$

Learning with Adaptive Regularization

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The first-order optimality condition tells us:

$$0 \in \partial \left(\frac{1}{d} \mathrm{Tr}(\Omega_r W \Omega_c W^T) - \log\det(\Omega_r) + \mathbb{I}_{\mathcal{C}}(\Omega_r) \right) = W\Omega_c W^T/d - \Omega_r^{-1} + \mathcal{N}_{\mathcal{C}}(\Omega_r)$$

Learning with Adaptive Regularization

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$$\min_{\Omega_r} \quad \mathrm{Tr}(\Omega_r W \Omega_c W^T) - d \log\det(\Omega_r), \qquad \text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p$$

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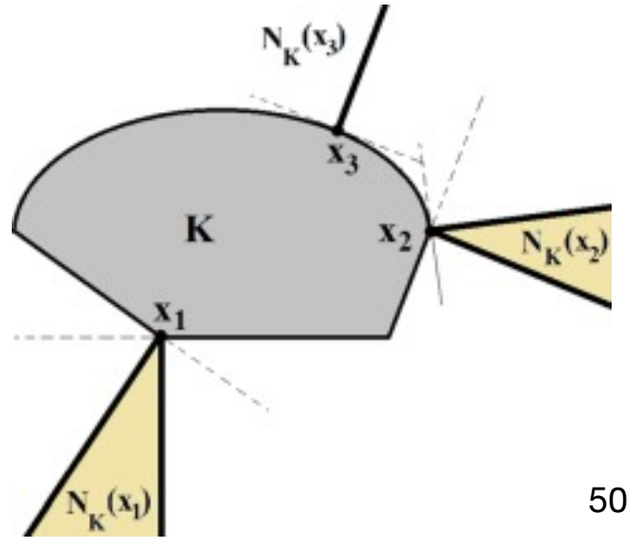
where

$$\mathcal{N}_{\mathcal{C}}(A) := \{B \in \mathbb{S}^p \mid \mathrm{Tr}(B^T(Z - A)) \leq 0, \forall Z \in \mathcal{C}\}$$

is the normal cone w.r.t. the constraint set $\mathcal{C}$ at A.



Learning with Adaptive Regularization

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Lemma: Let $\Omega_r \in \mathcal{C}$, then $\mathcal{N}_{\mathcal{C}}(\Omega_r) = -\mathcal{N}_{\mathcal{C}}(\Omega_r^{-1})$.

Learning with Adaptive Regularization

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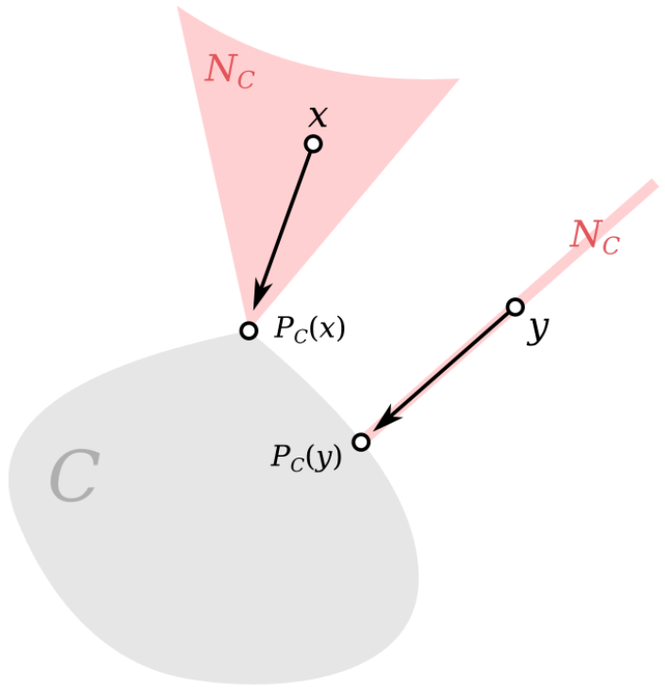
With this lemma, we have:

$$W\Omega_c W^T/d - \Omega_r^{-1} \in \mathcal{N}_{\mathcal{C}}(\Omega_r^{-1})$$

which means the optimal Ω_r^{-1} is the Euclidean projection of $W\Omega_c W^T/d$ onto $\mathcal{C}$.



Learning with Adaptive Regularization

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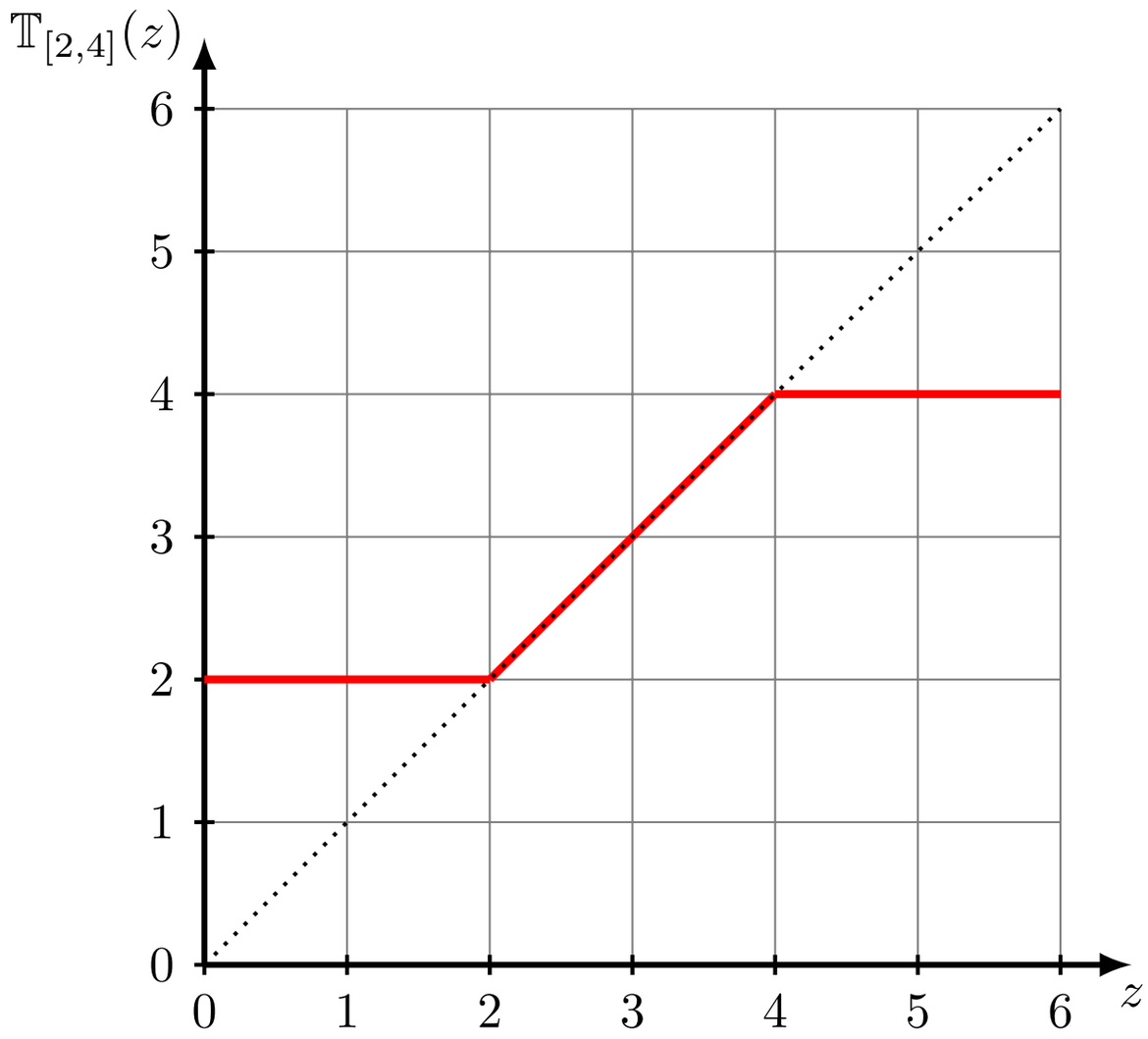
which means the optimal Ω_r^{-1} is the Euclidean projection of $W\Omega_c W^T/d$ onto $\mathcal{C}$. Hence it suffices if we can solve the following problem:

$$\min_{\Omega_r} \quad ||\Omega_r - \widetilde{\Omega_r}||_F^2, \qquad \text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p$$

Learning with Adaptive Regularization

Given a pair of constants $0 < u \leq v$, define the following thresholding operator:

$$\mathbb{T}_{[u,v]}(x) := \max\{u, \min\{v, x\}\}$$



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The Euclidean projection onto $\mathcal{C}$ has the following closed form solution:

Theorem: Let $\widetilde{\Omega_r} \in \mathbb{S}^p$ with eigendecomposition as $\widetilde{\Omega_r} = Q\Lambda Q^T$. Then $\text{Proj}_{\mathcal{C}}(\widetilde{\Omega_r}) = Q\mathbb{T}_{[u,v]}(\Lambda)Q^T$.

Simple: Apply eigendecomposition and then threshold the spectrum

Learning with Adaptive Regularization

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Simple: Apply eigendecomposition and then threshold the spectrum

$$\min_{\Omega_r} \quad \mathrm{Tr}(\Omega_r W \Omega_c W^T) - d \log\det(\Omega_r), \qquad \text{subject to} \quad uI_p \preceq \Omega_r \preceq vI_p$$

Solution: $$\Omega_r^* = Q\mathbb{T}_{[u,v]}(d/\mathbf{r})Q^T$$

where $Q\mathrm{diag}(\mathbf{r})Q^T = W\Omega_c W^T$ is the spectral decomposition of $W\Omega_c W^T$

Learning with Adaptive Regularization

Block Coordinate Descent for Adaptive Regularization:

Algorithm 1 Block Coordinate Descent for Adaptive Regularization

Input: Initial value $\phi^{(0)} := \{\mathbf{a}^{(0)}, W^{(0)}\}$, $\Omega_r^{(0)} \in \mathbb{S}_{++}^p$ and $\Omega_c^{(0)} \in \mathbb{S}_{++}^d$, first-order optimization algorithm $\mathfrak{A}$.

for $t = 1, \ldots, \infty$ until convergence **do**
  Fix $\Omega_r^{(t-1)}$, $\Omega_c^{(t-1)}$, optimize $\phi^{(t)}$ by backpropagation and algorithm $\mathfrak{A}$
  $\Omega_r^{(t)} \leftarrow \textsc{InvThreshold}(W^{(t)}\Omega_c^{(t-1)}W^{(t)T}, d, u, v)$
  $\Omega_c^{(t)} \leftarrow \textsc{InvThreshold}(W^{(t)T}\Omega_r^{(t)}W^{(t)}, p, u, v)$
end for
procedure $\textsc{InvThreshold}(\Delta, m, u, v)$
  Compute SVD: $Q\mathrm{diag}(\mathbf{r})Q^T = \mathrm{SVD}(\Delta)$
  Hard thresholding $\mathbf{r}' \leftarrow \mathbb{I}_{[u,v]}(m/\mathbf{r})$
  return $Q\mathrm{diag}(\mathbf{r}')Q^T$
end procedure

- One SVD in each outer iteration to solve the matrix optimization problem
- Seamlessly work with end-to-end training with back-propagation

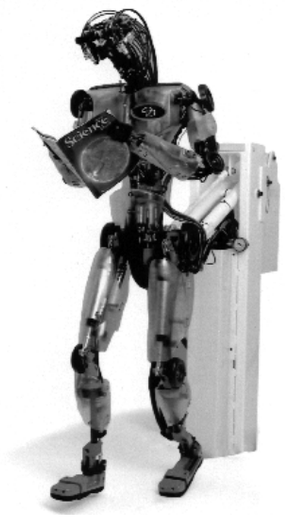
Outline

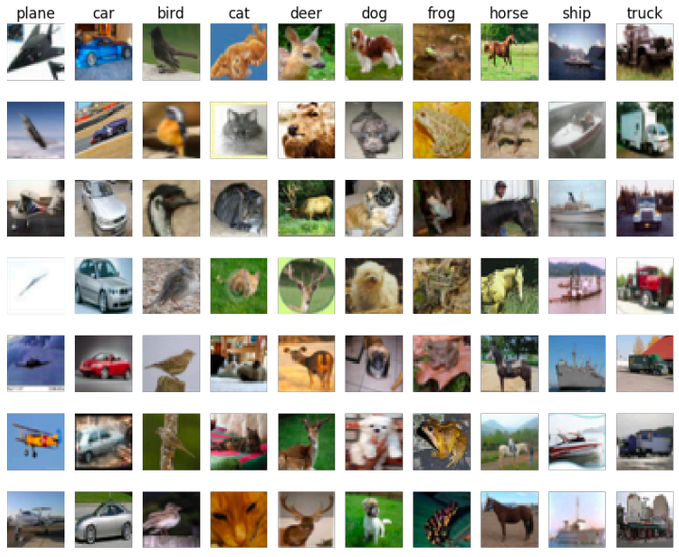
- Deep Learning Preliminary
- Learning with Adaptive Regularization
- Experiments
- Conclusion

Experiments

Multiclass Classification and Multitask Regression

- Multiclass Classification: MNIST and CIFAR10
  - MNIST: $\text{CONV}_{5\times5\times1\times10} - \text{CONV}_{5\times5\times10\times20} - \text{FC}_{320\times50} - \text{FC}_{50\times10}$
  - CIFAR10: $\text{CONV}_{5\times5\times3\times10} - \text{CONV}_{5\times5\times10\times20} - \text{FC}_{500\times500} - \text{FC}_{500\times500} - \text{FC}_{500\times10}$
- Multitask Regression: SARCOS
  - SARCOS: $\text{FC}_{21\times256} - \text{FC}_{256\times100} - \text{FC}_{100\times7}$





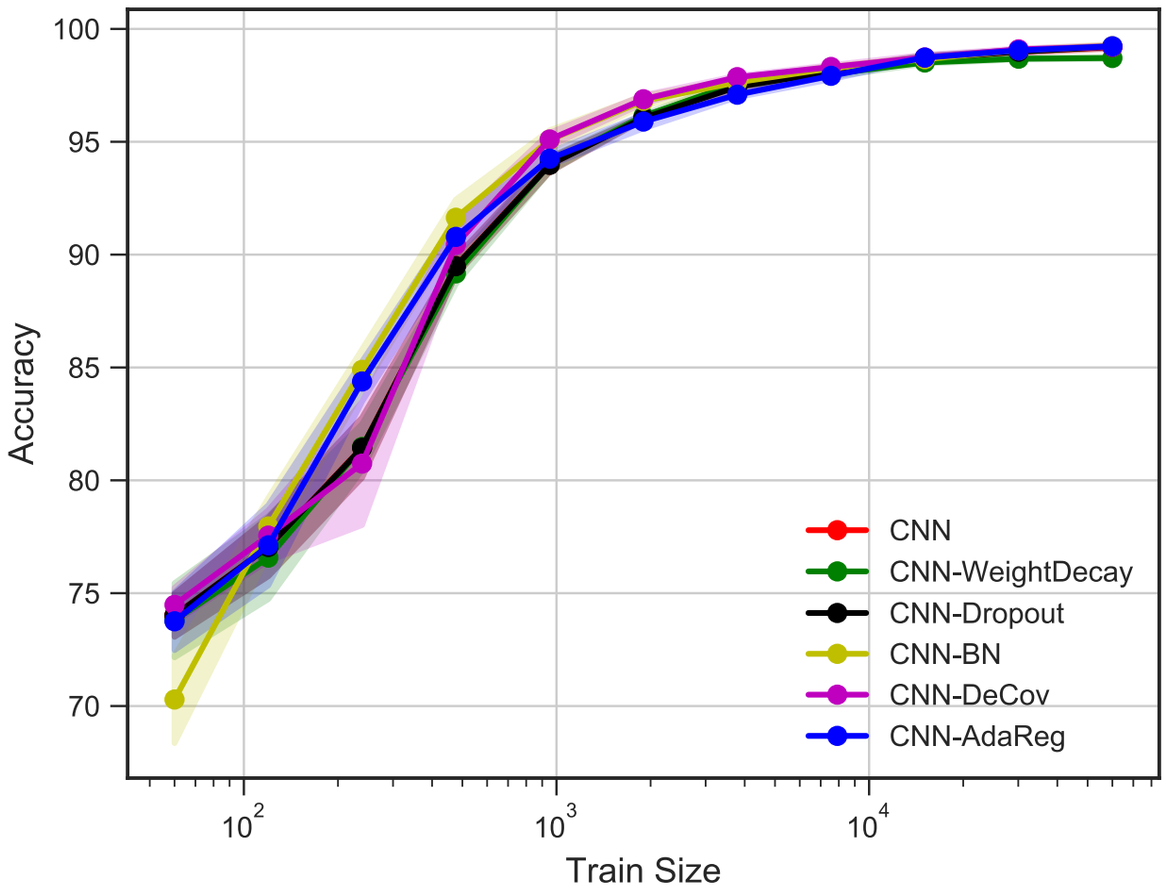
Experiments

Multiclass Classification and Multitask Regression

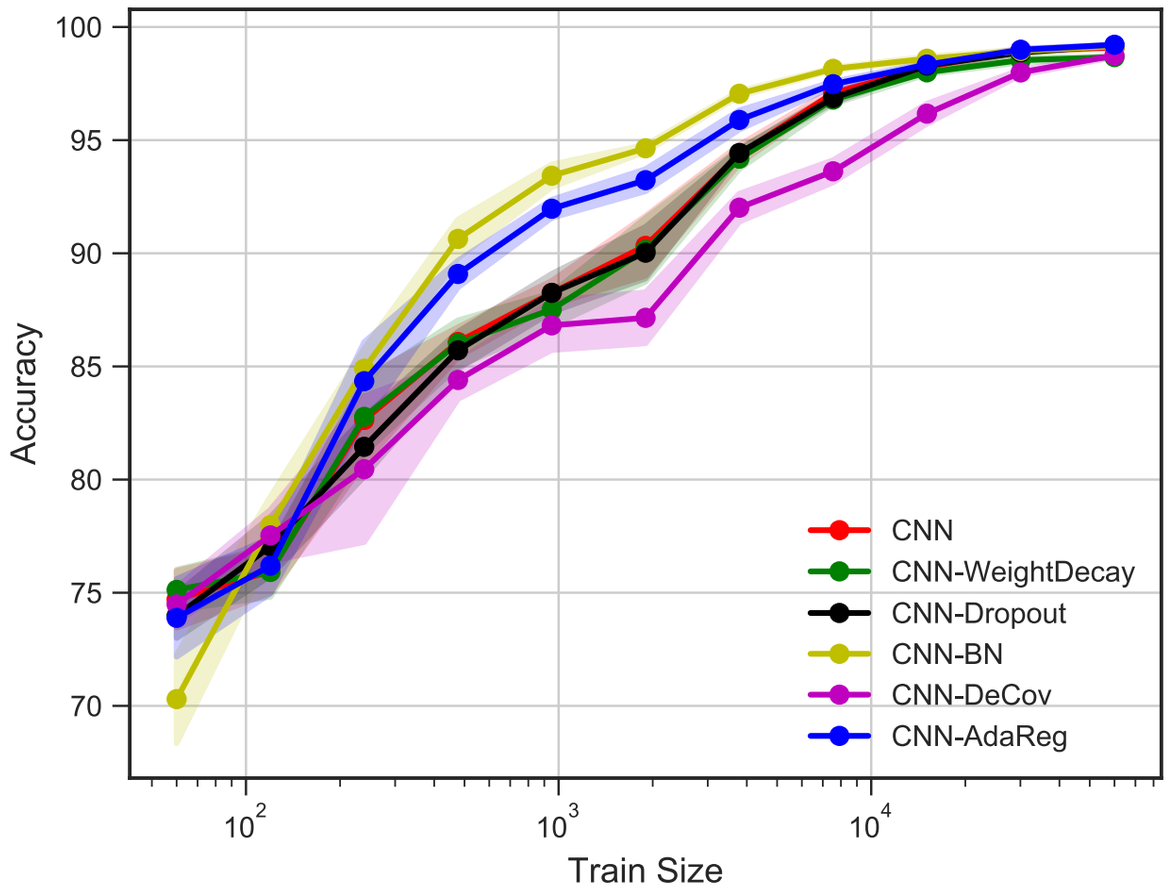
- Dropout: randomly inhibiting hidden activations
- Batch Normalization (BN): maintain and correct internal covariate shift
- Weight Decay: L2 regularization of weight matrix
- DeCov: penalize covariance matrix of hidden representations

Experiments

Generalization performance on MNIST (10 classes)



Batch size = 256

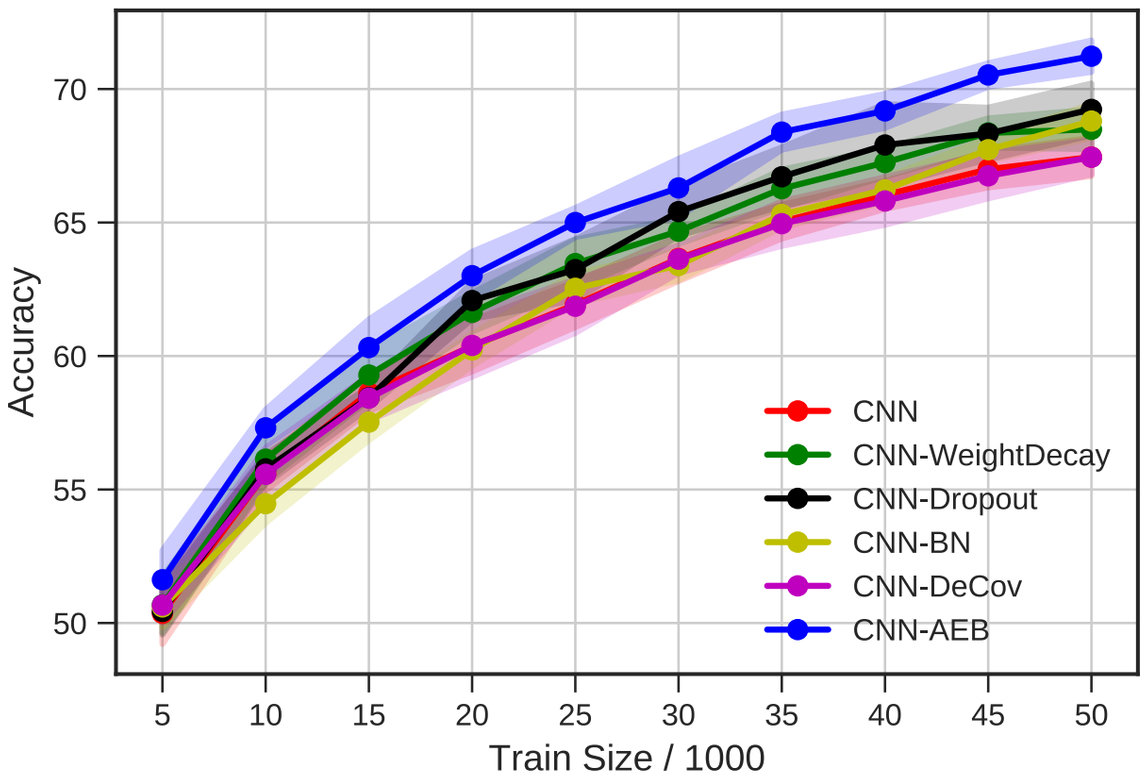


Batch size = 2048

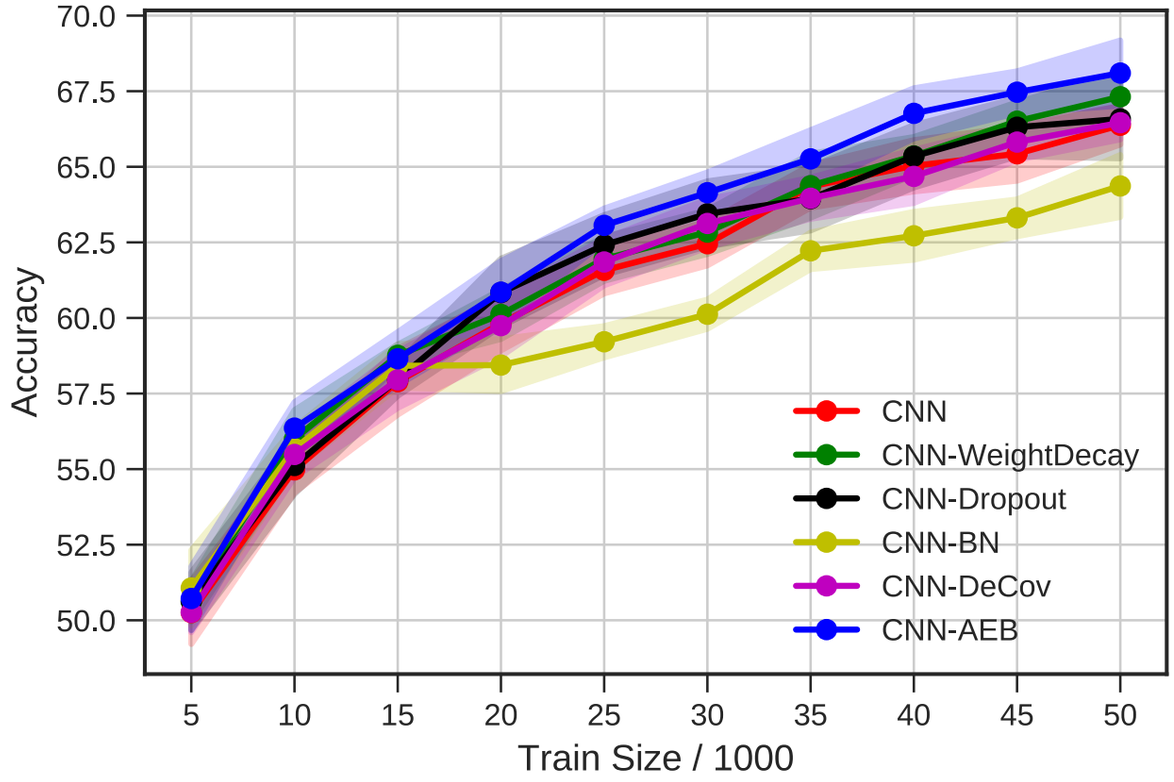
- AdaReg improves generalization with large batch size and small training size on MNIST

Experiments

Generalization performance on CIFAR10 (10 classes)



Batch size = 256

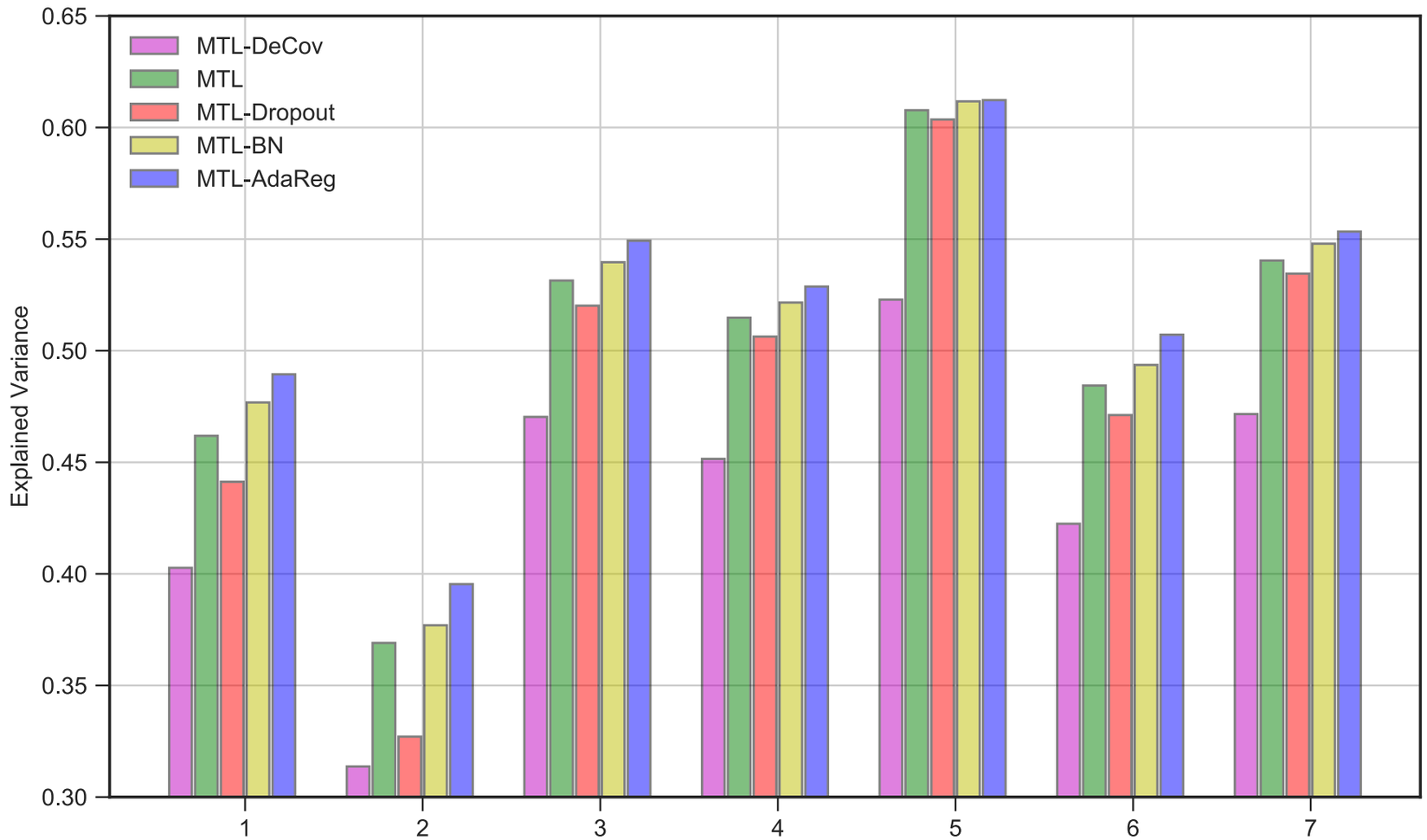


Batch size = 2048

- AdaReg consistently improves generalization on CIFAR10

Experiments

Generalization performance on SARCOS (7 tasks)

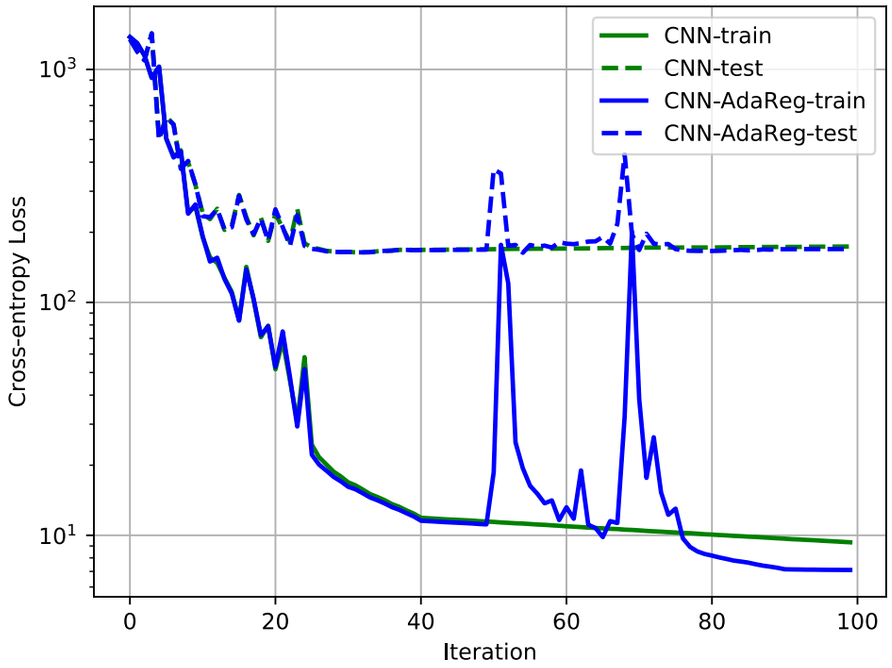


- Explained variance ~ negative MSE
- For regression tasks, AdaReg consistently outperforms other baselines in terms of generalization

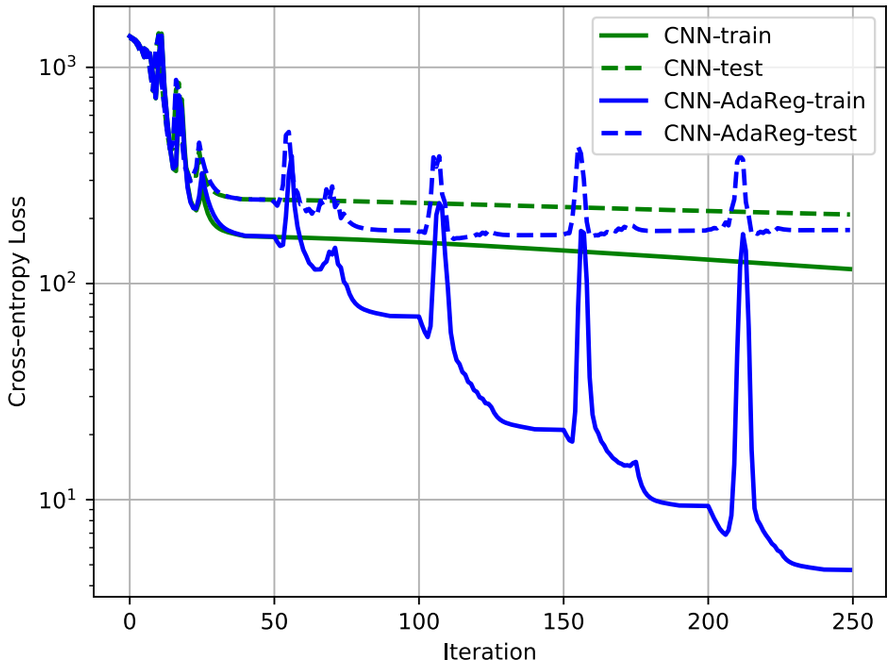
Experiments

AdaReg optimization trajectory on MNIST (train size/batch size)

600/256



600/2048



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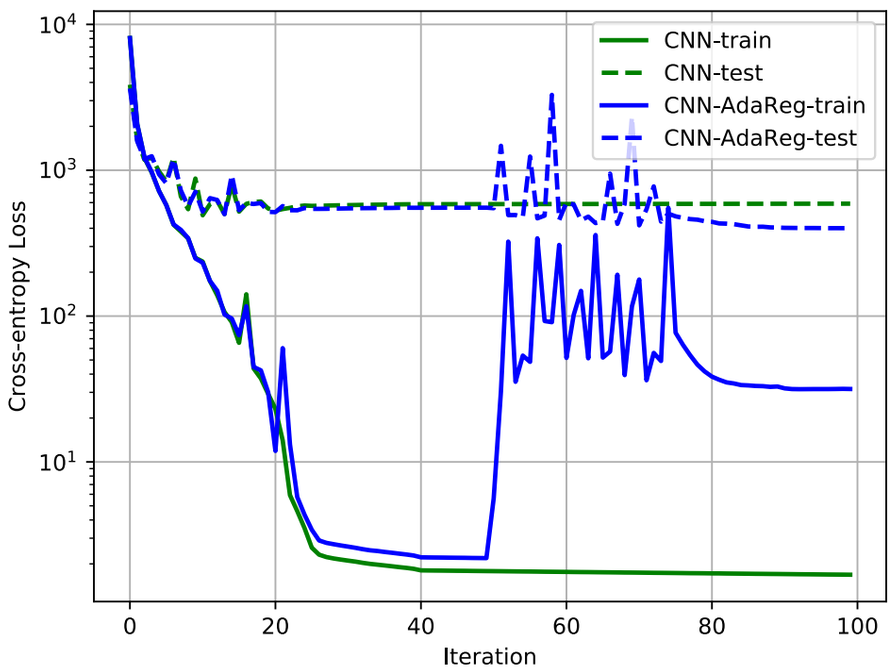
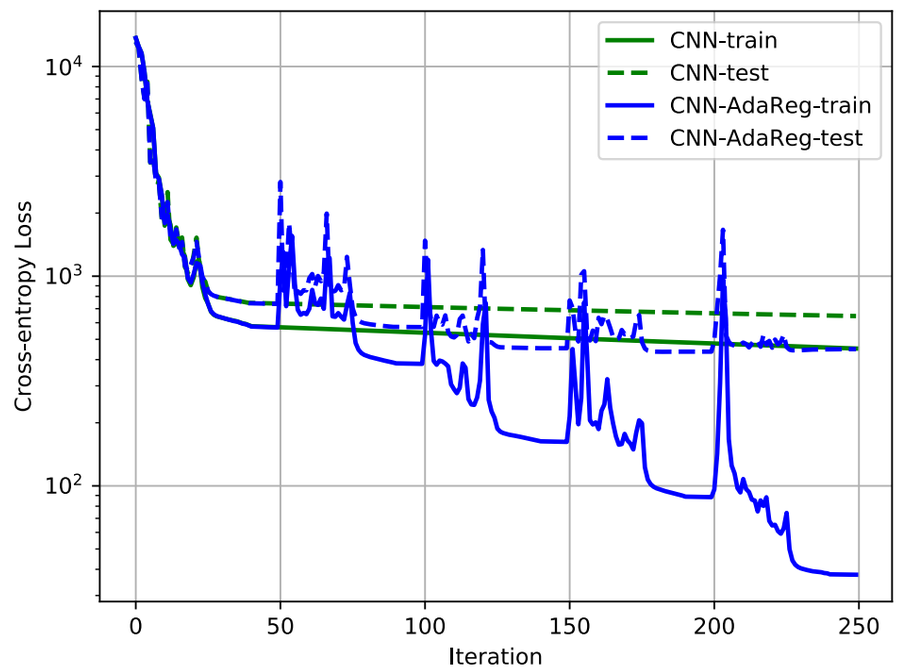


6000/2048



Carnegie M

Experiments

Stable Rank and Spectral Norm:

$$\text{srank}(W) := ||W||_F^2 / ||W||_2^2 \qquad 1 \leq \text{srank}(W) \leq \text{rank}(W)$$

Generalization bound of NNs using spectral norms and stable ranks (Neyshabur et al. ICLR' 17):

$$\text{Generalization Error} = O\left(\sqrt{\prod_{j=1}^{L} ||W_j||_2^2 \sum_{j=1}^{L} \text{srank}(W_j)/n}\right)$$

- Smaller stable rank and spectral norm implies better generalization

Experiments

AdaReg leads to smaller stable ranks and spectral norms

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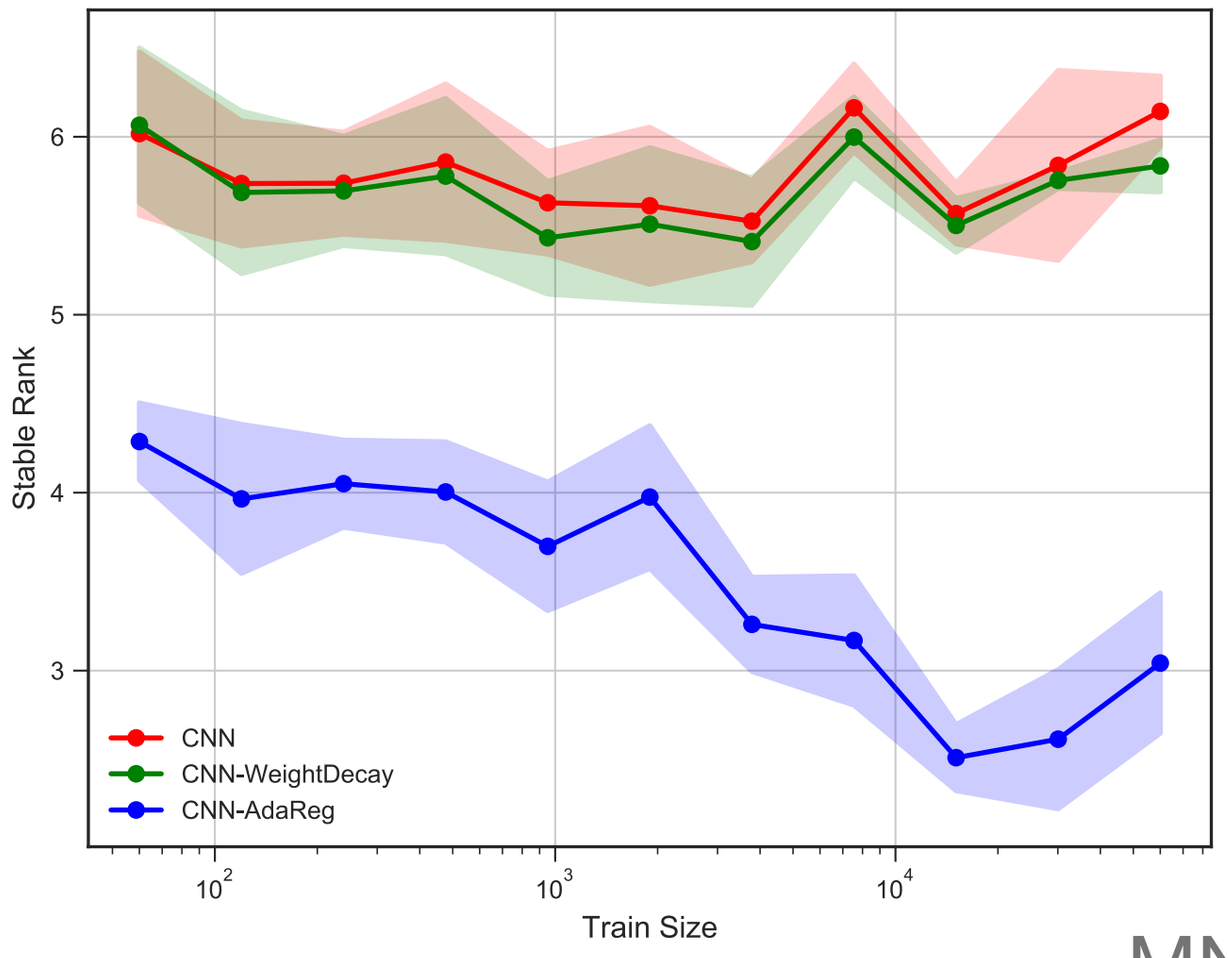
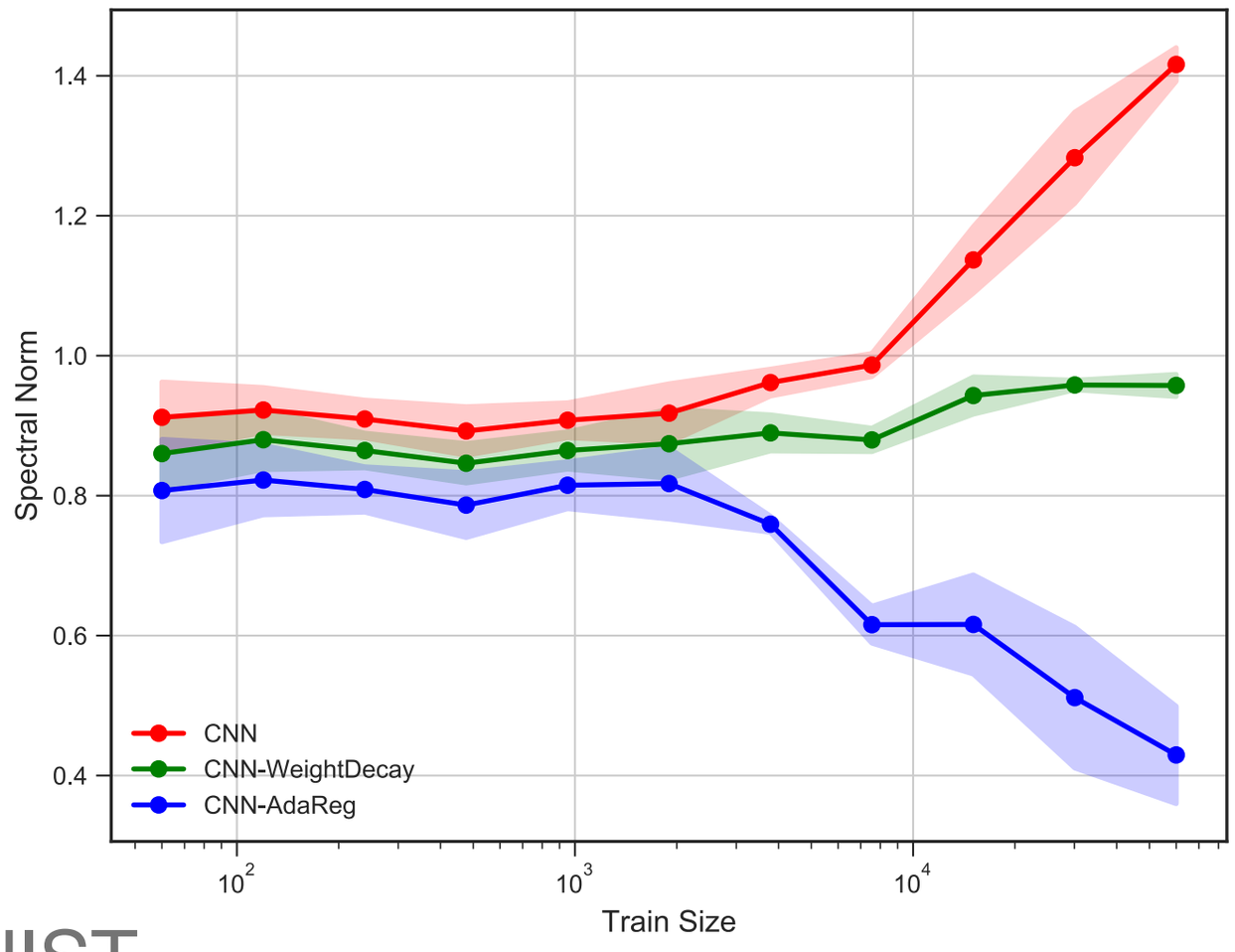


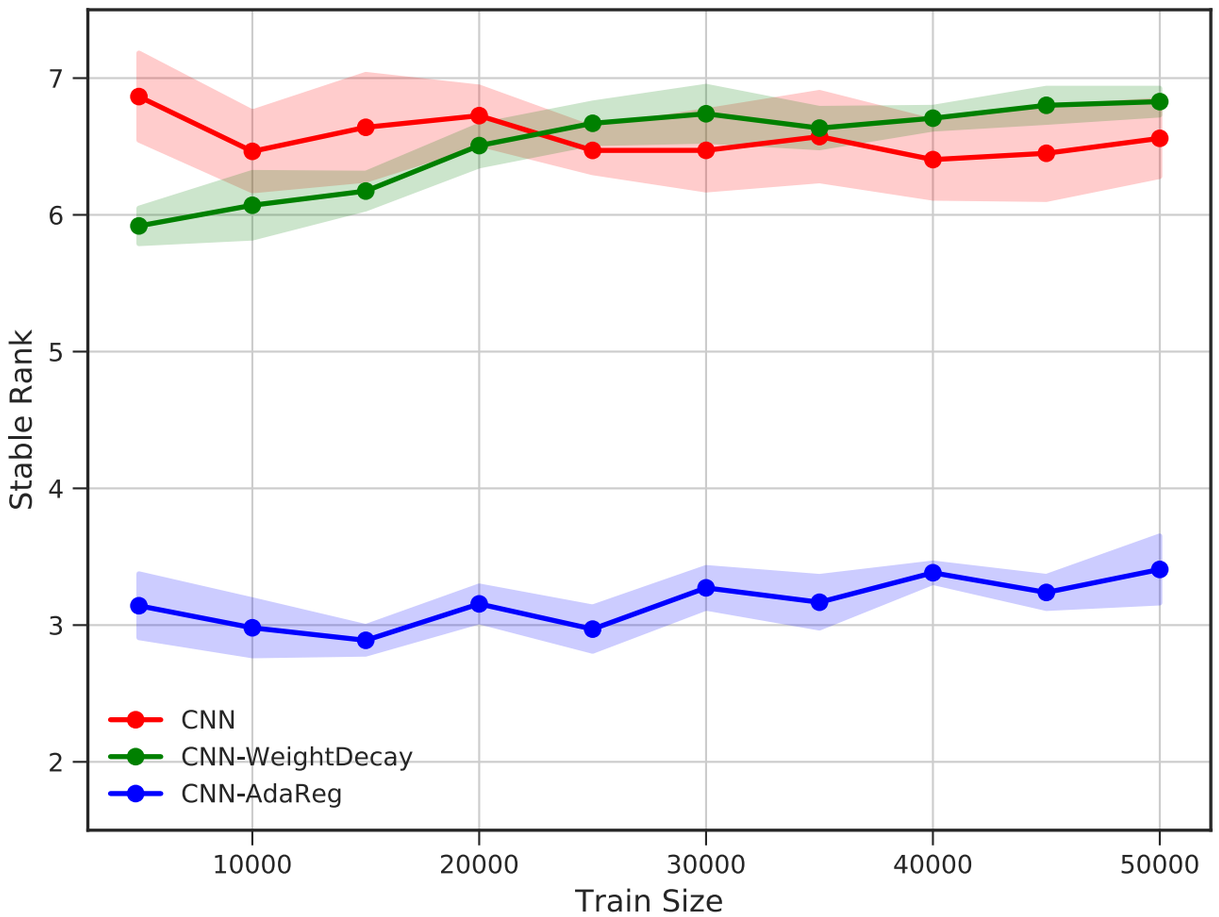


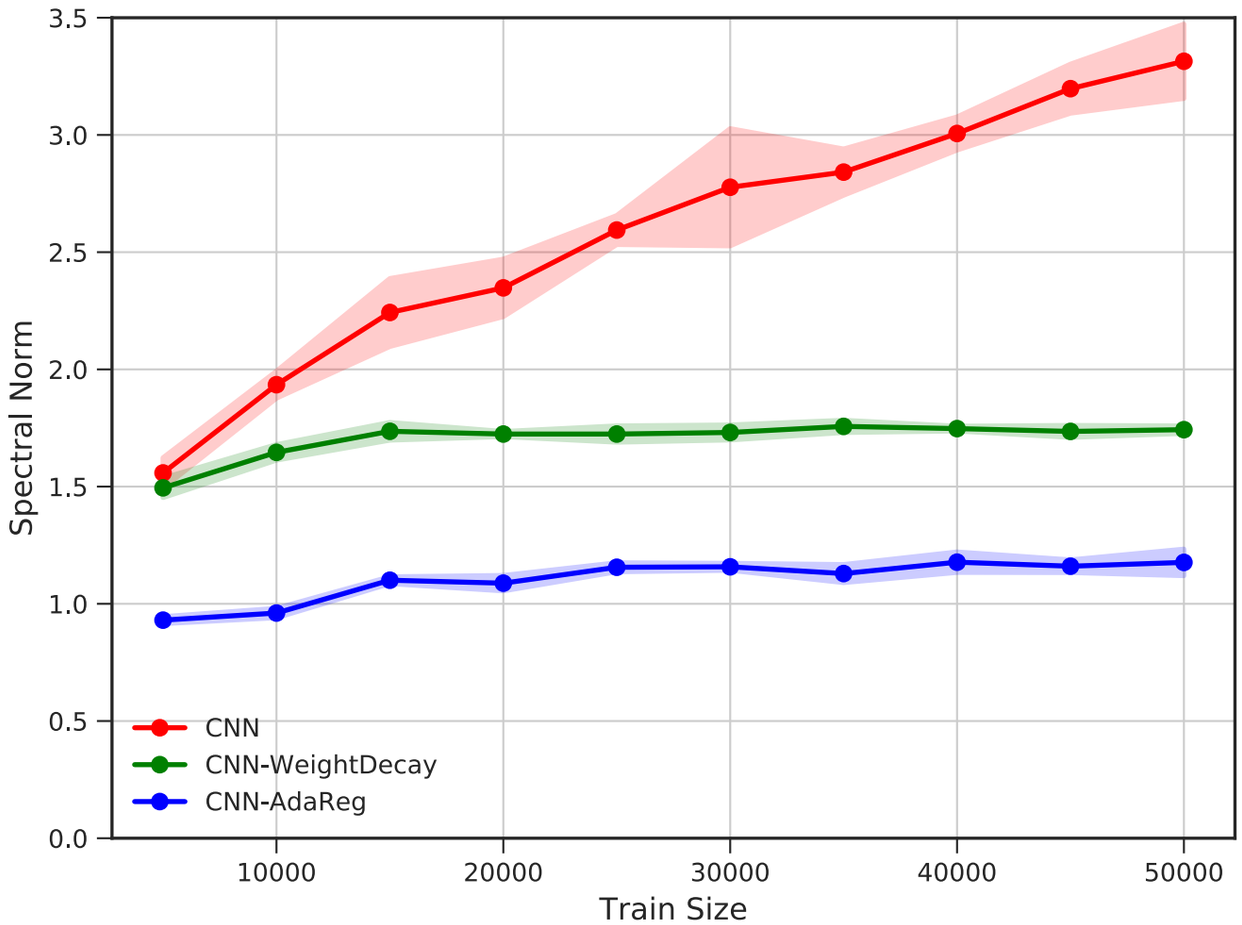
MNIST

Experiments

AdaReg leads to smaller stable ranks and spectral norms

$$\text{Generalization Error} = O\left(\sqrt{\prod_{j=1}^{L} ||W_j||_2^2 \sum_{j=1}^{L} \text{srank}(W_j)/n}\right)$$

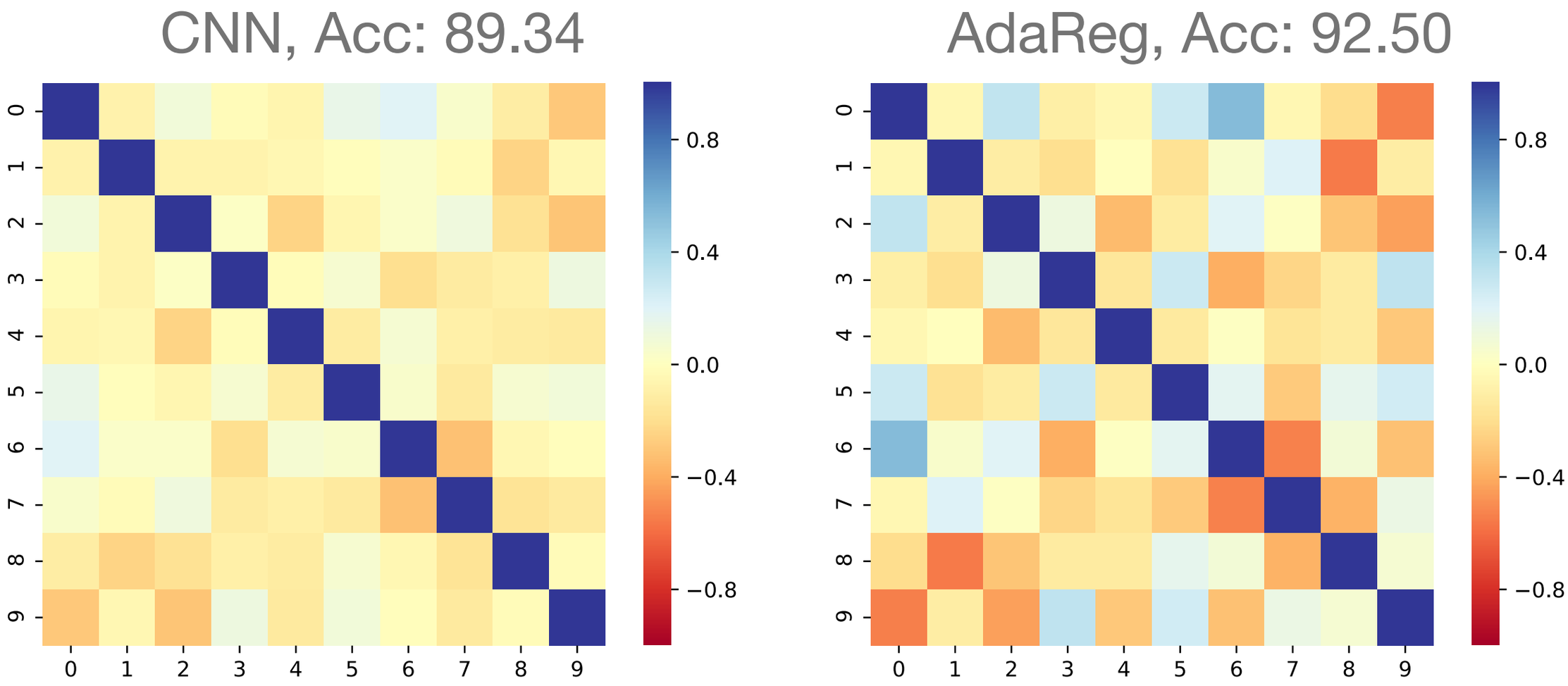




CIFAR10

Experiments

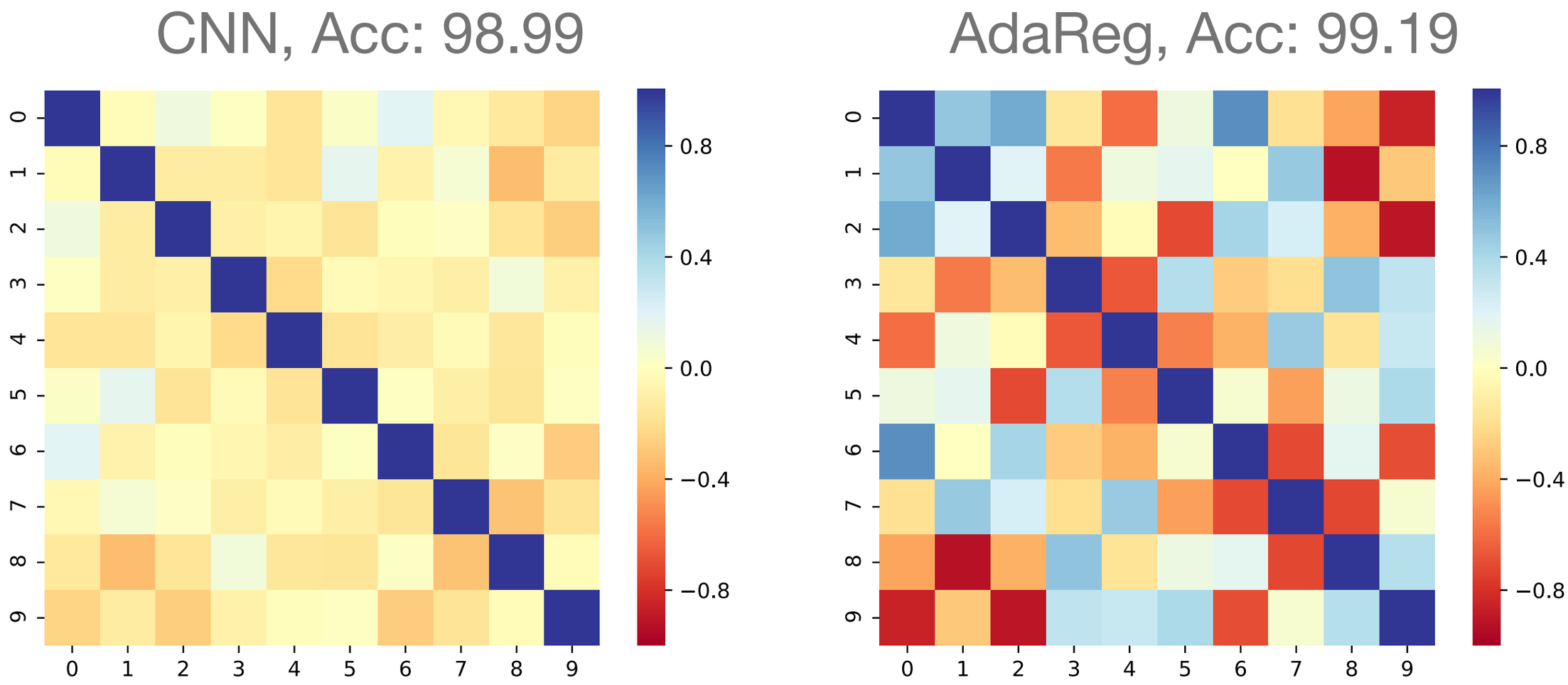
Correlations learned in the weight matrix:



- The effect of sharing statistical strength, i.e., “learning from the experience of others”

Experiments

Correlations learned in the weight matrix:



MNIST, train size = 6,000

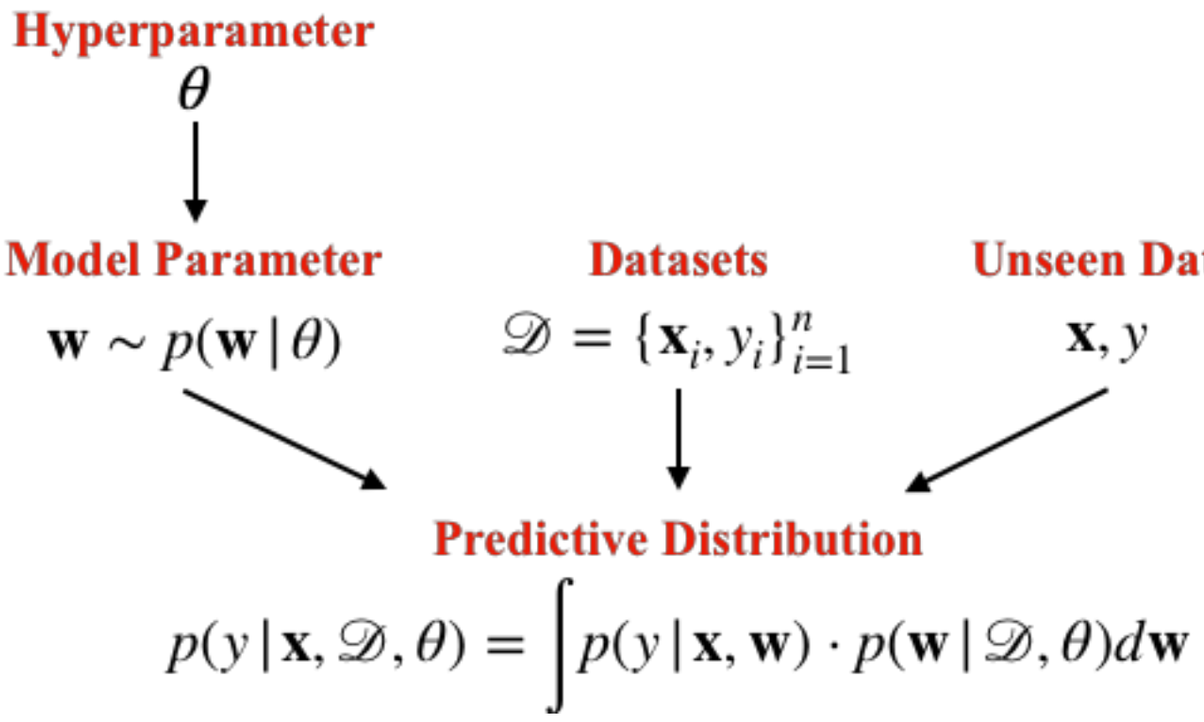
- The effect of sharing statistical strength, i.e., “learning from the experience of others”

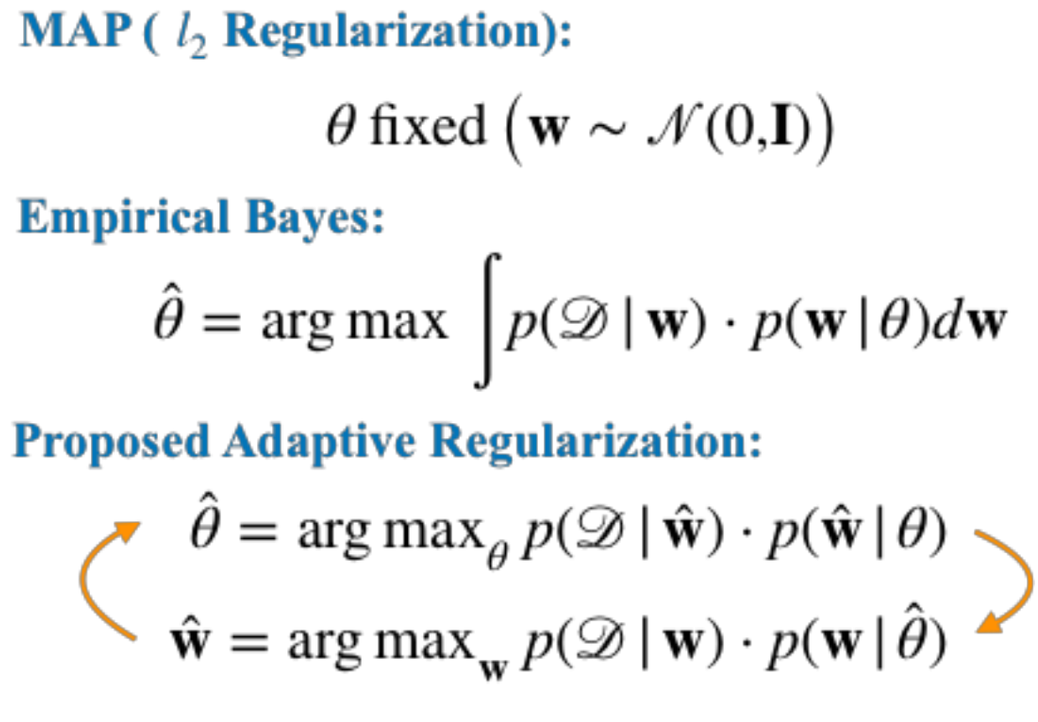
Outline

- Deep Learning Preliminary
- Learning with Adaptive Regularization
- Experiments
- Conclusion

Conclusion

- AdaReg: an approximate empirical Bayes method for regularizing NN training on small datasets





- Learn the preconditioning matrix adaptively from data

- Significant improvement in terms of spectral norm and stable rank, leading to smaller generalization error

Thanks

Q & A

Paper available at: https://arxiv.org/abs/1907.06288
To appear @ NeurIPS-19, code available @ https://github.com/yaohungt/Adaptive-Regularization-Neural-Network