#### Trimming the $\ell_1$ Regularizer: Statistical Analysis, Optimization, and Applications to Deep Learning

Jihun Yun<sup>1</sup>, Peng Zheng<sup>2</sup>, Eunho Yang<sup>1,3</sup>, Aurélie C. Lozano<sup>4</sup>, Aleksandr Aravkin<sup>2</sup>

<sup>1</sup>KAIST <sup>2</sup>University of Washington <sup>3</sup>AITRICS <sup>4</sup>IBM T.J. Watson Research Center

arcprime@kaist.ac.kr

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Introduction and Setup

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## $\ell_1$ Regularization is Popular

• High-dimensional data with  $\ell_1$  regularization ( $n \ll p$ )

• Genomic Data, Matrix Completion, Deep Learning, etc.



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Trimmed  $\ell_1$  Penalty

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### Concrete Example 1

Lasso

#### Example 1: Lasso\* (Sparse Linear Regression)

$$\widehat{\boldsymbol{\theta}} \in \operatorname*{argmin}_{\boldsymbol{\theta} \in \Omega} \ \frac{1}{2n} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|_2^2 + \lambda_n \|\boldsymbol{\theta}\|_1$$



\* R. Tibshirani. Regression shrinkage and selection via the lasso. JRSS, Series B,1996.

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### Concrete Example 2

Graphical Lasso

Example 2: Graphical Lasso\* (Sparse Concentration Matrix)

$$\widehat{\Theta} \in \operatorname*{argmin}_{\Theta \in \mathcal{S}_{++}^p} \operatorname{trace}(\widehat{\Sigma}\Theta) - \log \det(\Theta) + \lambda_n \|\Theta\|_{1, \mathrm{off}}$$

where  $\widehat{\Sigma}$  is a sample covariance matrix,  $\mathcal{S}_{++}^p$  the symmetric and strictly positive definite matrices, and  $\|\Theta\|_{1,\text{off}}$  the  $\ell_1$ -norm on the off-diagonal elements of  $\Theta$ .



\*P. Ravikumar, M. J. Wainwright, G. Raskutti, and B. Yu. High-dimensional covariance estimation by minimizing 11-penalized log-determinant divergence. EJS, 2011

# Concrete Example 3

Group  $\ell_1$  on Network Pruning Task

#### Example 3: Group $\ell_1^*$ (Structured Sparsity of Weight Parameters)

$$\widehat{\boldsymbol{\theta}} \in \operatorname*{argmin}_{\boldsymbol{\theta} \in \Omega} \ \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) + \lambda_n \|\boldsymbol{\theta}\|_{\mathcal{G}}$$

where  $\hat{\theta}$  is a collection of weight parameters of neural networks,  $\mathcal{L}$  the neural network loss (ex. softmax), and  $\|\theta\|_{\mathcal{G}}$  the group sparsity regularizer.



\* W. Wen, C. Wu, Y. Wang, Y. Chen, and H. Li. Learning Structured Sparsity in Deep Neural Networks. NIPS, 2016

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- As parameter size gets larger, the shrinkage bias effect also tends to be larger.
  - The  $\ell_1$  penalty is proportional to the size of parameters.

## Despite the popularity of $\ell_1$ penalty (and also strong statistical guarantees), Is it really good enough?

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## Non-convex Regularizers

**Previous Work** 

- For *amenable* non-convex regularizers (such as SCAD\* and MCP\*\*),
  - ▷ Amenable regularizer: Resembles l₁ at the origin and has vanishing derivatives at the tail.
     → coordinate-wise decomposable.
  - (Loh & Wainwright)\*\*\* provide the statistical analysis on amenable regularizers.



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#### What about more structurally complex regularizer?

\*\*\* P. Loh and M. J. Wainwright. Support recovery without incoherence: A case for nonconvex regularization. The Annals of Statistics, 2017.

<sup>\*</sup> J. Fan and R. Li. Variable selection via non-concave penalized likelihood and its oracle properties. Jour. Amer. Stat. Ass., 96(456):1348-1360, December 2001.

<sup>\*\*</sup> Cun-Hui Zhang et al. Nearly unbiased variable selection under minimax concave penalty. The Annals of statistics, 38(2):894-942, 2010.

<sup>\*\*\*</sup> P. Loh and M. J. Wainwright. Regularized M-estimators with non-convexity: statistical and algorithmic theory for local optima and algorithmic. JMLR, 2015.

Definition

- In this paper, we study the Trimmed  $\ell_1$  penalty.
  - New class of regularizers.

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#### • Definition:

For a parameter vector  $\theta \in \mathbb{R}^p$ , we only  $\ell_1$ -penalize each entry except largest h entries (We call h the trimming parameter).

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First Formulation



• We can *formalize* by defining the order statistics of the parameter vector  $|\theta_{(1)}| > |\theta_{(2)}| > \cdots > |\theta_{(p)}|$ , the *M*-estimation with the Trimmed  $\ell_1$  penalty is

$$\underset{\boldsymbol{\theta}\in\Omega}{\operatorname{minimize}} \ \mathcal{L}(\boldsymbol{\theta};\mathcal{D}) + \lambda_n \mathcal{R}(\boldsymbol{\theta};h)$$

where the regularizer  $\mathcal{R}(\theta; h) = \sum_{j=h+1}^{p} |\theta_{(j)}|$  (sum of smallest p - h entries in absolute values).

• Importantly, the Trimmed  $\ell_1$  is not amenable nor coordinate-wise separable.

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# M-estimation with the Trimmed $\ell_1$ penalty $_{\text{Second Formulation}}$

• We can rewrite the *M*-estimation with the Trimmed  $\ell_1$  penalty by introducing additional variable *w*:

$$\begin{array}{l} \underset{\boldsymbol{\theta} \in \Omega, \boldsymbol{w} \in [0,1]^p}{\text{minimize}} \ \mathcal{F}(\boldsymbol{\theta}, \boldsymbol{w}) \coloneqq \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) + \lambda_n \sum_{j=1}^p w_j |\theta_j| \\ \\ \text{such that } \mathbf{1}^T \boldsymbol{w} \geq p - h \end{array}$$

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- The variable w encodes the sparsity pattern and order information of  $\theta$ . As an ideal case,
  - $w_j = 0$  for largest h entries
  - $w_j = 1$  for smallest p h entries

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- The variable w encodes the sparsity pattern and order information of  $\theta$ . As an ideal case,
  - $w_j = 0$  for largest h entries
  - $w_j = 1$  for smallest p h entries
- If we set the trimming parameter h = 0, it is just a standard  $\ell_1$ .

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#### *M*-estimation with the Trimmed $\ell_1$ penalty

Second Formulation: Important Properties

$$\begin{array}{l} \underset{\boldsymbol{\theta} \in \Omega, \boldsymbol{w} \in [0,1]^p}{\text{minimize}} \ \mathcal{F}(\boldsymbol{\theta}, \boldsymbol{w}) \coloneqq \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) + \lambda_n \sum_{j=1}^p w_j |\theta_j| \\ \\ \text{such that } \mathbf{1}^T \boldsymbol{w} \geq p - h \end{array}$$

- $\bullet$  The objective function  ${\cal F}$  is
  - Weighted  $\ell_1$ -regularized if we fix w.
  - Linear in w with fixing  $\theta$ .
  - However,  $\mathcal{F}$  is **non-convex** in jointly  $(\theta, w)$  because of coupling of  $\theta$  and w.
- We use this second formulation for an optimization.
  - Since we don't need to sort the parameter.

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Unit Balls Visualization

• Trimmed  $\ell_1$  Unit balls of  $\theta = (\theta_1, \theta_2, \theta_3)$  in the 3-dimensional space.

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Unit Balls Visualization

• Trimmed  $\ell_1$  Unit balls of  $\theta = (\theta_1, \theta_2, \theta_3)$  in the 3-dimensional space.



- For h = 0, the shape is the same as standard  $\ell_1$  unit ball.
- For h > 0, the penalty could be unbounded.
  - Since the largest *h* entries are not penalized, the unit ball could extend to infinity in these directions.
  - $\bullet\,$  As h increases, the penalty would be more complicated.

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#### Assumptions:

(C1) The loss  $\mathcal{L}$  is differentiable and convex.

(C2) Restricted Strong Convexity on  $\theta$ : Let  $\mathbb{D}$  be the set of all possible error vectors for  $\theta$ . Then, for all  $\theta - \theta^* \in \mathbb{D}$ ,

$$\langle \nabla \mathcal{L}(\boldsymbol{\theta}^*, \Delta) - \nabla \mathcal{L}(\boldsymbol{\theta}^*), \Delta \rangle \geq \kappa_l \|\Delta\|_2^2 - \tau_1 \frac{\log p}{n} \|\Delta\|_1^2,$$

where  $\kappa_l$  is a "curvature" parameter, and  $\tau_1$  a "tolerance".

- Allowing a small loss difference to be translated to a small error  $\theta \theta^*$ .
- RSC condition is a standard one in this line of work.

Quantity:

• Let 
$$\widehat{Q} = \int_0^1 \nabla^2 \mathcal{L}(\boldsymbol{\theta}^* + t(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)) dt.$$

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# Statistical Analysis Theorem 1: General $\ell_{\infty}$ -error Bound and Variable Selection

- Consider an M-estimation problem with the Trimmed  $\ell_1$  penalty.
- Under (C1)&(C2) and standard conditions, for *any* local minimum  $\tilde{\theta}$ , we have
  - For every pair  $j_1 \in S$ ,  $j_2 \in S^c$ , we have  $|\tilde{\theta}_{j_1}| > |\tilde{\theta}_{j_2}|$

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**Theorem 1**: General  $\ell_{\infty}$ -error Bound and Variable Selection

• For every pair  $j_1 \in S$ ,  $j_2 \in S^c$ , we have  $|\tilde{\theta}_{j_1}| > |\tilde{\theta}_{j_2}|$ • If h < k, all  $j \in S^c$  are successfully estimated as zero and

$$\|\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\|_{\infty} \leq \left\| (\widehat{Q}_{SS})^{-1} \nabla \mathcal{L}(\boldsymbol{\theta}^*)_S \right\|_{\infty} + \lambda_n \left\| (\widehat{Q}_{SS})^{-1} \right\|_{\infty}$$

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● If  $h \ge k$ , at least the smallest (in absolute) p - h entries in  $S^c$  are exactly zero and  $\|\tilde{\theta} - \theta\|_{\infty} \le \|(\hat{Q}_{\hat{U}\hat{U}})^{-1} \nabla \mathcal{L}(\theta^*)_{\hat{U}}\|_{\infty}$  where  $\hat{U}$  is defined as the h largest absolute entries of  $\tilde{\theta}$  including S.

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**Theorem 1**: General  $\ell_{\infty}$ -error Bound and Variable Selection

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**Theorem 2:** General  $\ell_2$ -error Bound

#### Theorem 2

- Consider an M-estimation problem with Trimmed  $\ell_1$  regularization where all conditions in Theorem 1 hold.
- For any local minimum  $\hat{\theta}$ , the parameter estimation error in terms of  $\ell_2$ -norm is upper bounded as:

$$\|\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\|_2 = \begin{cases} C\lambda_n \left(\sqrt{k}/2 + \sqrt{k-h}\right) & \text{ if } h < k\\ C\lambda_n \sqrt{h}/2 & \text{ otherwise} \end{cases}$$

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• From our bound, h = k is the best case!

• We can choose  $h \asymp k$  via cross-validation.

Table:  $\ell_2$ -error bound for different h values.

**Remarks:** Other alternative penalties vs. Trimmed  $\ell_1$ 

$$\|\widetilde{\boldsymbol{\theta}} - \boldsymbol{\theta}^*\|_2 = \begin{cases} C\lambda_n \left(\sqrt{k}/2 + \sqrt{k-h}\right) & \text{ if } h < k \\ C\lambda_n \sqrt{h}/2 & \text{ otherwise} \end{cases}$$

•  $\rho_{\lambda}(t)$ :  $(\mu, \gamma)$ -amenable •  $\rho_{\lambda}(t) + \frac{1}{2}\mu t^2$  is convex. •  $\rho'_{\lambda}(t) = 0$  for  $|t| > \gamma$ .

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Table:  $\ell_2$ -error bound comparison with universal constant  $c_0$  in sub-Gaussian tail bounds.

	Standard $\ell_1$ ( $h=0$ )	$(\mu,\gamma)$ -amenable	Trimmed $\ell_1$ $(h=k)$
$\ \widetilde{oldsymbol{ heta}}-oldsymbol{ heta}^*\ _2$	$\frac{3c_0}{\kappa_l}\frac{\lambda_n\sqrt{k}}{2}$	$\frac{c_0}{\kappa_l - \frac{3}{2}\mu} \frac{\lambda_n \sqrt{k}}{2}$	$rac{c_0}{\kappa_l}rac{\lambda_n\sqrt{k}}{2}$

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• Trimmed  $\ell_1$  can achieve three times smaller bound than standard one.

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• Also, we have a smaller bound than non-convex regularizers since  $(\mu, \gamma)$ -amenable regularizers have (possibly large)  $\mu$  in the denominator.

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#### Statistical Analysis Corollary 1: General $\ell_{\infty}$ -error Bound for Linear Regression

- Consider a linear regression problem with sub-Gaussian error  $\epsilon$ .
- Under standard conditions as in **Theorem 1** and incoherence condition on sample covariance, with high probability, *any* local minimum  $\tilde{\theta}$  satisfies



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### Optimization for Trimmed $\ell_1$ Regularized Program

• For an optimization, we use our **second formulation** of trimmed regularization problem

$$\min_{\boldsymbol{\theta} \in \Omega, \boldsymbol{w} \in [0,1]^p} \mathcal{F}(\boldsymbol{\theta}, \boldsymbol{w}) \coloneqq \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) + \lambda \sum_{j=1}^p w_j |\theta_j| \quad \text{s.t.} \quad \mathbf{1}^T \boldsymbol{w} \ge p - h$$

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• We update  $(\theta, w)$  in an alternating manner.

$$\begin{aligned} & \boldsymbol{\theta}^{k+1} \leftarrow \mathrm{prox}_{\eta \lambda \mathcal{R}(\cdot, \boldsymbol{w}^k)} [\boldsymbol{\theta}^k - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}^k)] \\ & \boldsymbol{w}^{k+1} \leftarrow \mathrm{proj}_{\mathcal{S}} [\boldsymbol{w}^k - \tau \boldsymbol{r}(\boldsymbol{\theta}^{k+1})] \end{aligned}$$

- Fixing w, prox operator is weighted  $\ell_1$  norm.
- By fixing  $\theta$ , the objective function  $\mathcal{F}$  is linear in w.
- proj<sub>S</sub> is a projection onto the constraint set S = {w ∈ [0,1]<sup>p</sup> | 1<sup>T</sup>w = p − h}.

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### Optimization: Comparison with DC-based Approach

- Convergence history our algorithm vs. Algorithm 2 of (Khamaru & Wainwright, 2018)\*.
  - Algorithm 2 of (Khamaru & Wainwright, 2018) is an optimization method for (non-convex and non-smooth) objective functions of the form difference of convex functions ( $f := g + \phi h$ ).
  - Trimmed regularized problem can be formulated as a DC.



Figure: Algorithm comparison with  $\lambda \in \{0.5, 5, 10, 20\}$ .

\*K. Khamaru and M. J. Wainwright. Convergence guarantees for a class of non-convex and non-smooth optimization problems. ICML, 2018

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Incoherent Case: Support Recovery

#### • Scenario 1: Incoherence condition is satisfied



• Probability of successful support recovery for Trimmed Lasso, SCAD, MCP, and standard Lasso with (p,k) = (128,8), (256,16), (512,32).

Image: A matched a matc

Incoherent Case: Stationary &  $\log \ell_2$ -error Comparison

• Scenario 1: Incoherence condition is satisfied



(Left) 50 random initializations for a setting with (n, p, k) = (160, 256, 16).
(Right) log ℓ<sub>2</sub>-error comparison.

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Nonincoherent Case: Support Recovery

- Scenario 2: Incoherence condition violated
  - Note that we need an incoherence condition in our Corollary 1.
  - Interestingly, the Trimmed Lasso outperforms all the other comparison regularizers even in this regime.



• Probability of successful support recovery for Trimmed Lasso, SCAD, MCP, and standard Lasso with (p,k) = (128,8), (256,16), (512,32).

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Nonincoherent Case: Stationary &  $\log \ell_2$ -error Comparison

• Scenario 2: Incoherence condition violated



- (Left) 50 random initializations for a setting with (n, p, k) = (160, 256, 16).
- (**Right**)  $\log \ell_2$ -error comparison.

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Nonincoherent Case: Stationary

- Scenario 3
  - (Left) True signals and regularization parameter  $\lambda$  are both small (Small regime)
  - Investigating the choice of the trimming parameter *h* (Middle: Incoherent case, **Right**: Non-incoherent case).



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Input Structure Recovery of Compact Neural Networks

- We apply trimmed regularization to recover the weight structure of neural networks as parameter support recovery.
- Motivated by the recent work of Oymak (2018)\*, we consider



- The regression model,  $y_i = \boldsymbol{o}^T \operatorname{ReLU}(\boldsymbol{W}^* \boldsymbol{x}_i)$  with  $\boldsymbol{o} = \boldsymbol{1}$ .
- Each hidden node is connected to only 4 input features.

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\* Samet Oymak. Learning Compact Neural Networks with Regularization. ICML, 2018.

# Applications to Deep Learning 1

Input Structure Recovery of Compact Neural Networks: Results

• With good initialization (small perturbation from true weight)



• With random initialization



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## Applications to Deep Learning 2: Pruning Deep Networks



• **Pruning neurons** is more computationally efficient than edge-wise pruning.

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Trimmed Group  $\ell_1$  Regularization on Deep Networks

To encourage group sparsity on neural networks, we consider two cases:

- Neuron sparsity (for fully-connected layers)
  - Let  $\theta_l \in \mathbb{R}^{n_{\text{in}} \times n_{\text{out}}}$  be a weight parameter, then we can enforce group-wise sparsity via Trimmed group  $\ell_1$  penalty as

$$\mathcal{R}_l(oldsymbol{ heta}_l,oldsymbol{w}) = \lambda_l \sum_{j=1}^{n_{\mathsf{in}}} w_j \sqrt{ heta_{j,1}^2 + heta_{j,2}^2 + \cdots + heta_{j,n_{\mathsf{out}}}}$$

- Activation map sparsity (for convolutional layers)
  - Similarly, let  $oldsymbol{ heta}_l \in \mathbb{R}^{C_{\mathsf{out}} imes C_{\mathsf{in}} imes H imes W}$  be a weight parameter, then

$$\mathcal{R}_l(\boldsymbol{\theta}, \boldsymbol{w}) = \lambda_l \sum_{j=1}^{C_{\text{out}}} w_j \sqrt{\sum_{m,n,k} \theta_{j,m,n,k}^2}$$

for all possible indices (m, n, k).

with the constraint  $\mathbf{1}^T \boldsymbol{w} = n_{in} - h_l$  or  $C_{out} - h_l$  respectively.

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#### Applications to Deep Learning: Pruning Deep Networks Results on MNIST dataset

• Comparison with vanilla group  $\ell_1$  penalty vs. Trimmed group  $\ell_1$  penalty on LeNet-300-100 structure

Method	Pruned Model	Error (%)
No Regularization	784-300-100	1.6
grp $\ell_1$	784-241-67	1.7
$\operatorname{grp} \ell_{1_{\operatorname{trim}}}, h = \operatorname{half} \operatorname{of} \operatorname{original}$	392-150-50	1.6

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#### Applications to Deep Learning: Pruning Deep Networks Bayesian Neural Networks with Trimmed *l*<sub>1</sub> Regularization

• Most modern algorithms for network pruning are based on **Bayesian** variational framework. We propose a Bayesian neural network with Trimmed  $\ell_1$  regularization regarding only  $\theta$  as Bayesian.

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#### Applications to Deep Learning: Pruning Deep Networks Bayesian Neural Networks with Trimmed l<sub>1</sub> Regularization

- Most modern algorithms for network pruning are based on **Bayesian** variational framework. We propose a Bayesian neural network with Trimmed  $\ell_1$  regularization regarding only  $\theta$  as Bayesian.
- By relationship between **Bayesian neural networks** and variational dropout, we choose  $q_{\theta,\alpha}(\theta_{i,j}) = \mathcal{N}(\phi_{i,j}, \alpha_{i,j}\phi_{i,j}^2)$  as a variational distribution.

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- Most modern algorithms for network pruning are based on **Bayesian** variational framework. We propose a Bayesian neural network with Trimmed  $\ell_1$  regularization regarding only  $\theta$  as Bayesian.
- By relationship between **Bayesian neural networks** and variational dropout, we choose  $q_{\theta,\alpha}(\theta_{i,j}) = \mathcal{N}(\phi_{i,j}, \alpha_{i,j}\phi_{i,j}^2)$  as a variational distribution.
- $\bullet$  Combined with Trimmed  $\ell_1$  regularization, the objective is

$$\underbrace{\mathbb{E}_{q_{\phi,\alpha}(\boldsymbol{\theta})}\Big[-\mathcal{L}(\mathcal{W};\mathcal{D})\Big] + \mathbb{KL}(q_{\phi,\alpha}(\mathcal{W})\|p(\mathcal{W}))}_{\mathsf{ELBO}} + \underbrace{\mathbb{E}_{q_{\phi,\alpha}(\boldsymbol{\theta})}\Big[\sum_{l=1}^{L+1} \lambda_{l}\mathcal{R}_{l}(\boldsymbol{\theta}_{l},\boldsymbol{w}_{l})\Big]}_{\mathsf{Expected Trimmed group }\ell_{1} \text{ penalty}}$$

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#### Applications to Deep Learning: Pruning Deep Networks Results on MNIST dataset (Cont' d)

- With Bayesian extensions on LeNet-300-100
  - We compare with a smoothed  $\ell_0$ -norm under Bayesian variational framework proposed by Louizos et al. (2018)\*

Method	Pruned Model	Error (%)
$\ell_0$ (Louizos et al., 2018)	219-214-100	1.4
$\ell_0$ , $\lambda$ sep. (Louizos et al., 2018)	266-88-33	1.8
Bayes grp $\ell_{1_{\text{trim}}}, h = \ell_0$	219-214-100	1.4
Bayes grp $\ell_{1_{\text{trim}}}$ , $h = \ell_0$ , $\lambda$ sep.	266-88-33	1.6
Bayes grp $\ell_{1_{\mathrm{trim}}}$ , $h < \ell_0$ , $\lambda$ sep.	245-75-25	1.7

• With Bayesian extensions on LeNet-5-Caffe

Method	Pruned Model	Error (%)
$\ell_0$ (Louizos et al., 2018)	20-25-45-462	0.9
$\ell_0, \lambda$ sep. (Louizos et al., 2018)	9-18-65-25	1.0
Bayes grp $\ell_{1_{\text{trim}}}, h < \ell_0$	20-25-45-150	0.9
Bayes grp $\ell_{1_{\text{trim}}}$ , $h = \ell_0$ , $\lambda$ sep.	9-18-65-25	1.0
Bayes grp $\ell_{1_{\text{trim}}}$ , $h < \ell_0$ , $\lambda$ sep.	8-17-53-19	1.0

\*Louizos et al. Learning Sparse Neural Networks through  $\ell_0$  Regularization. ICLR, 2018

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- High-dimensional *M*-estimators with Trimmed  $\ell_1$  penalty: Alleviate the bias incurred by the vanilla  $\ell_1$  penalty by leaving the *h* largest parameter entries penalty-free.
- Theoretical Results on support recovery and  $\ell_2$ -error hold for any local optima and are competitive with other non-convex regularizers.
- **Simulation experiments** demonstrated the value of approach compared to Lasso and non-convex penalties.
- Future work:
  - Trimming for other standard regularizers beyond sparsity
  - Bypassing incoherence condition in corollaries
  - More experiments and theories when RSC does not hold
  - Investigating the use of trimmed regularization in deep models.

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## THANK YOU! Any Questions?

## Poster Session at Pacific Ballroom #186 6:30pm – 9:00pm

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