Learning in Gated Neural Networks

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Gated Recurrent Neural Networks

- Well-known examples: LSTM and GRU
- State-of-the-art results in many challenging ML tasks

Figure: Google Duplex

Demo

Siri, Alexa and more...

• Language translation

• Speech recognition

• Phrase completion

Google Translate

Break through language barriers

NNs and RNNs

• Feed-forward neural networks

Recurrent neural networks (Vanilla)

Gated RNNs

Figure: Gated Recurrent Unit (GRU)

Key features:

- **Gating mechanism**
- Non-linear 'switching' dynamical systems
- **o** Long term memory

Gates: z_t , $r_t \in [0,1]^d$ depend on the input x_t and the past h_{t-1} States: $h_t, \tilde{h}_t \in \mathbb{R}^d$

Update equations for each t :

$$
h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \widetilde{h}_t
$$

$$
\widetilde{h}_t = f(Ax_t + r_t \odot Bh_{t-1})
$$

Building blocks of GRU

 $h_t = (1 - z_t) \odot h_{t-1} + z_t \odot (1 - r_t) \odot f(Ax_t) + z_t \odot r_t \odot f(Ax_t + Bh_{t-1})$

Building blocks of GRU

 $h_t = (1 - z_t) \odot h_{t-1} + z_t \odot (1 - r_t) \odot f(Ax_t) + z_t \odot r_t \odot f(Ax_t + Bh_{t-1})$

Mixture-of-Experts: Building blocks of GRU

Jacobs, Jordan, Nowlan and Hinton, 1991

 $f =$ sigmoid, $g =$ linear, tanh, ReLU

MoE as gated feed-forward network

MoE: Modern relevance

• Outrageously large neural networks

Figure 1: A Mixture of Experts (MoE) layer embedded within a recurrent language model. In this case, the sparse gating function selects two experts to perform computations. Their outputs are modulated by the outputs of the gating network.

What is known about MoE?

• No provable learning algorithms for parameters¹ \circledcirc

 1 20 years of MoE, MoE: a literature survey

Open problem for 25+ years

$$
\Leftrightarrow P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y | g(\mathbf{a}_1^{\top}\mathbf{x}), \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y | g(\mathbf{a}_2^{\top}\mathbf{x}), \sigma^2)
$$

Open question

Given n i.i.d. samples $(\boldsymbol{x}^{(i)}, y^{(i)})$, does there exist an efficient learning algorithm with provable theoretical guarantees to learn the regressors a_1 , a_2 and the gating parameter w?

Traditional loss functions

Loss functions:

· Log-likelihood loss

$$
L = \log \left(f(\boldsymbol{w}^\top \boldsymbol{x}) \cdot e^{-\frac{\|\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{a}_1^\top \boldsymbol{x})\|^2}{2\sigma^2} } + (1 - f(\boldsymbol{w}^\top \boldsymbol{x})) \cdot e^{-\frac{\|\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{a}_2^\top \boldsymbol{x})\|^2}{2\sigma^2}} \right)
$$

$$
\bullet \ \ L_2\text{-loss}
$$

$$
L = \left(y - \left(f(\mathbf{w}^\top \mathbf{x})g(\mathbf{a}_1^\top \mathbf{x}) + (1 - f(\mathbf{w}^\top \mathbf{x}))g(\mathbf{a}_2^\top \mathbf{x})\right)\right)^2
$$

Traditional algorithms

Algorithms: EM, Gradient descent, and their variants

- **Practical: Often get stuck in local optima**
- Theoretical: Loss surface is hard to analyze because of coupling of w and (a_1, a_2) . Just understood for far simpler problem of Gaussian mixtures

Modular structure

Mixture of classification (w) and regression (a_1, a_2) problems

Key observation

Key observation

If we know the regressors, learning the gating parameter is easy and vice-versa. How to break the gridlock?

Focus of this talk: Breaking the gridlock

- **First learning guarantees for MoE**
- Two novel approaches to learn the parameters:

Method 1: Algorithms

We propose a novel algorithm with first recoverable guarantees

Method 2: Optimization framework

We design a non-trivial loss function on which traditional algorithms like GD converge to true parameters

- **•** Both approaches work with **global initializations**
	- \triangleright restriction: x is Gaussian

Generalizability

k-MoE

Generalizability

Hierarchical mixture of experts (HME)

Figure 2: A two-level hierarchical mixture of experts

Method 1: Design of algorithms

Algorithmic approach: An overview

Recall the model for MoE:

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y|g(\mathbf{a}_1^{\top}\mathbf{x}), \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y|g(\mathbf{a}_2^{\top}\mathbf{x}), \sigma^2)
$$

- We learn (a_1, a_2) and w separately
- First recover (a_1, a_2) without knowing w at all
- **•** Later learn **w** using traditional methods like EM
- Global consistency guarantees (population setting)

Learning regressors without gating

Model for MoE:

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y|g(\mathbf{a}_1^{\top}\mathbf{x}), \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y|g(\mathbf{a}_2^{\top}\mathbf{x}), \sigma^2)
$$

Without gating:

$$
P_{y|\mathbf{x}} = p \cdot \mathcal{N}(y | g(\mathbf{a}_1^{\mathsf{T}} \mathbf{x}), \sigma^2) + (1-p) \cdot \mathcal{N}(y | g(\mathbf{a}_2^{\mathsf{T}} \mathbf{x}), \sigma^2)
$$

- Mixture of generalized linear models (GLMs)!
	- \rightarrow How do we learn a_1 and a_2 without knowing p?
	- ▸ Method of moments

Tensor methods in latent variable models

Anandkumar, Ge, Hsu, Kakade, and Telgarsky 2014

Multiview and Topic Models

Tensor methods in GLMs

Main approach

Basic idea: Construct a third-order super-symmetric tensor from data such that

$$
\mathbb{E}(\psi(X, Y)) = \sum_i \mathbf{a}_i \otimes \mathbf{a}_i \otimes \mathbf{a}_i \Rightarrow \mathbf{a}_i \text{ can be recovered}
$$

- How do we construct ψ ?
	- ▸ Stein's lemma

Stein's lemma 101

Stein's lemma For $f:\mathbb{R}^d\to\mathbb{R}$ and $\mathbf{x}\sim\mathcal{N}(0,I_d)$, $\mathbb{E}[f(\mathbf{x}) \cdot \mathbf{x}] = \mathbb{E}[\nabla_{\mathbf{x}} f(\mathbf{x})] \in \mathbb{R}^d$.

Non-linear regression using Stein's lemma: If $y = g(a_X^{\mathsf{T}}x) + N$, then

$$
\begin{aligned}\n&\underbrace{\mathbb{E}[y \cdot x]}_{\text{Estimated from samples}} &= \mathbb{E}[g(a_1^\top x) \cdot x] + \underbrace{\mathbb{E}[N \cdot x]}_{=0} \\
&= \mathbb{E}[\nabla_x g(a_1^\top x)] \\
&\propto a_1\n\end{aligned}
$$

Mixture of GLMs: Stein's lemma 101

• Recall, for mixture of GLMs:

$$
P_{y|\mathbf{x}} = p \cdot \mathcal{N}(y|g(\mathbf{a}_1^{\mathsf{T}}\mathbf{x}), \sigma^2) + (1-p) \cdot \mathcal{N}(y|g(\mathbf{a}_2^{\mathsf{T}}\mathbf{x}), \sigma^2)
$$

• From Stein's lemma,

$$
\mathbb{E}[y\cdot \pmb{x}]\propto p\cdot \pmb{a}_1+(1-p)\cdot \pmb{a}_2.
$$

- Not unique in a_1 and a_2
- How can we ensure uniqueness?

Stein's lemma 102

2nd order Stein's lemma

$$
\mathbb{E}[f(\mathbf{x}) \cdot \underbrace{(\mathbf{x}\mathbf{x}^{\top} - I)}_{\mathcal{S}_2(\mathbf{x})}] = \mathbb{E}[\nabla_{\mathbf{x}}^{(2)} f(\mathbf{x})] \in \mathbb{R}^{d \times d}.
$$

Mixture of GLMs:

$$
P_{y|\mathbf{x}} = p \cdot \mathcal{N}(y | g(\mathbf{a}_1^T \mathbf{x}), \sigma^2) + (1 - p) \cdot \mathcal{N}(y | g(\mathbf{a}_2^T \mathbf{x}), \sigma^2)
$$

\n
$$
\Rightarrow \mathbb{E}[y \cdot (\mathbf{x} \mathbf{x}^T - I)] \propto 2p \cdot \mathbf{a}_1 \mathbf{a}_1^T + 2(1 - p) \cdot \mathbf{a}_2 \mathbf{a}_2^T.
$$

- Not unique!
- How can we ensure uniqueness?

Stein's lemma 103

3rd order Stein's lemma

$$
\mathbb{E}[f(\mathbf{x})\cdot\mathcal{S}_3(\mathbf{x})]=\mathbb{E}[\nabla_{\mathbf{x}}^{(3)}f(\mathbf{x})]\in\mathbb{R}^{d\times d\times d}
$$

Score transformation $\mathcal{S}_3(\mathbf{x}) = \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x} - \sum_{i \in [d]} \text{sym}(\mathbf{x} \otimes \mathbf{e}_i \otimes \mathbf{e}_i)$

• Mixture of GLMs:

$$
P_{y|\mathbf{x}} = p \cdot \mathcal{N}(y | g(\mathbf{a}_1^\top \mathbf{x}), \sigma^2) + (1 - p) \cdot \mathcal{N}(y | g(\mathbf{a}_2^\top \mathbf{x}), \sigma^2)
$$

\n
$$
\Rightarrow \mathbb{E}[y \cdot S_3(\mathbf{x})] \propto p \cdot \mathbf{a}_1 \otimes \mathbf{a}_1 \otimes \mathbf{a}_1 + (1 - p) \cdot \mathbf{a}_2 \otimes \mathbf{a}_2 \otimes \mathbf{a}_2.
$$

- Unique! (by Kruskal's theorem)
- Can we extend this to MoE?

MoE: Stein's lemma

• For MoE,
$$
p = p(x) = f(w^{\top}x)
$$
 since

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y|g(\mathbf{a}_1^{\top}\mathbf{x}), \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y|g(\mathbf{a}_2^{\top}\mathbf{x}), \sigma^2)
$$

- Can we use Stein's lemma to learn a_1 and a_2 ?
- Natural attempt:

$$
\mathbb{E}[y \cdot S_3(x)] = a_1 \otimes a_1 \otimes a_1 + w \otimes a_1 \otimes w + \ldots + a_1 \otimes a_1 \otimes w + \ldots
$$

Not a super-symmetric tensor

• Can we construct a super-symmetric tensor for MoE?

Key insight: Hermite polynomial transformation

Suppose $g =$ linear and $\sigma = 0$. Then

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathbb{1}\{y = \mathbf{a}_1^{\top}\mathbf{x}\} + (1 - f(\mathbf{w}^{\top}\mathbf{x}))\mathbb{1}\{y = \mathbf{a}_1^{\top}\mathbf{x}\}
$$

\n
$$
\Rightarrow \mathbb{E}[y^3 - 3y|\mathbf{x}] = \sum_{i \in \{1,2\}} f(\mathbf{w}_i^{\top}\mathbf{x})((\mathbf{a}_i^{\top}\mathbf{x})^3 - 3(\mathbf{a}_i^{\top}\mathbf{x})), \quad \mathbf{w}_2 = -\mathbf{w}_1
$$

Key insight: Hermite polynomial transformation

Suppose $g =$ linear and $\sigma = 0$. Then

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathbb{1}\{y = \mathbf{a}_1^{\top}\mathbf{x}\} + (1 - f(\mathbf{w}^{\top}\mathbf{x}))\mathbb{1}\{y = \mathbf{a}_1^{\top}\mathbf{x}\}
$$

\n
$$
\Rightarrow \mathbb{E}[y^3 - 3y|\mathbf{x}] = \sum_{i \in \{1,2\}} f(\mathbf{w}_i^{\top}\mathbf{x})((\mathbf{a}_i^{\top}\mathbf{x})^3 - 3(\mathbf{a}_i^{\top}\mathbf{x})), \quad \mathbf{w}_2 = -\mathbf{w}_1
$$

Now applying Stein's lemma,

$$
\mathbb{E}[(y^3-3y)\cdot S_3(\boldsymbol{x})]=\mathbb{E}[\nabla_{\boldsymbol{x}}^3\mathbb{E}[y^3-3y|\boldsymbol{x}]]=3\sum_{i\in\{1,2\}^s}\boldsymbol{a}_i\otimes \boldsymbol{a}_i\otimes \boldsymbol{a}_i
$$

How do cross terms like $a_i \otimes a_i \otimes w$ disappear?

- Reason: $\mathbb{E}[H'_{3}(Z)] = \mathbb{E}[H''_{3}(Z)] = \mathbb{E}[H'''_{3}(Z)] = 0$
- $H_3(z) = z^3 3z$ is third-Hermite polynomial

Does this work for $\sigma \neq 0$?

Linear experts: Hermite-like-polynomials

Suppose $g =$ linear and $\sigma \neq 0$:

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y|\mathbf{a}_1^{\top}\mathbf{x}, \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y|\mathbf{a}_2^{\top}\mathbf{x}, \sigma^2)
$$

Super-symmetric tensor

$$
\mathcal{T}_3 = \mathbb{E}[(y^3 - 3y(1 + \sigma^2)) \cdot S_3(\boldsymbol{x})] = 3(a_1 \otimes a_1 \otimes a_1 + a_2 \otimes a_2 \otimes a_2)
$$

This very much needs special linear structure. What about other non-linearities for g ?

Generalization: Cubic polynomial transformations

• For a wide class of non-linearities such as $g=$ linear, sigmoid, ReLU, etc.

$$
\mathcal{T}_3 = \mathbb{E}[(y^3 + \alpha y^2 + \beta y) \cdot S_3(\boldsymbol{x})] = c(\boldsymbol{a}_1 \otimes \boldsymbol{a}_1 \otimes \boldsymbol{a}_1 + \boldsymbol{a}_2 \otimes \boldsymbol{a}_2 \otimes \boldsymbol{a}_2)
$$

• How do we choose α and β ?

- ▸ Solving a linear system
- ▸ Example: For sigmoid,

$$
\begin{bmatrix} 0.2067 & 0.2066 \\ 0.0624 & -0.0001 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} -0.1755 - 0.6199 \sigma^2 \\ -0.0936 \end{bmatrix}
$$

• Key idea: Acts like a 'Hermite' like polynomial for general g and cancels cross terms

Learning regressors: Spectral decomposition

Algorithm

- Input: Samples (\mathbf{x}_i, y_i)
- Compute $\hat{\mathcal{T}}_3 = (1/n) \sum_i H_3(y_i) \cdot \mathcal{S}_3(\mathbf{x}_i)$
- \hat{a}_1 , \hat{a}_2 = Rank-2 decomposition on \mathcal{T}_3

Learning the gating

• Recall

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y|\mathbf{a}_1^{\top}\mathbf{x}, \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y|\mathbf{a}_2^{\top}\mathbf{x}, \sigma^2)
$$

- **If** we know a_1 and a_2 , learning w is a classification problem!
- **o** Traditional methods:
	- ▸ EM algorithm
	- ▸ Gradient descent on log-likelihood

Theoretical contributions

- Show global convergence for existing methods
- Provide convergence rate
- **•** Finite sample complexity
- **o** First theoretical guarantees

Learning the gating parameters

Suppose spectral methods give $\hat{\bm{a}}_i$ with $\|\hat{\bm{a}}_i - \bm{a}_i\|_2 \leq \sigma^2\varepsilon$

For high SNR, i.e. $\sigma < \sigma_0$, σ_0 is a dimension independent constant:

- EM iterates converge geometrically to \hat{w}
- Convergence rate is a dimension-independent constant depending on σ and $\|\boldsymbol{a}_1 - \boldsymbol{a}_2\|$
- $\hat{\mathbf{w}}$ is ε -close to the ground truth

Comparison with EM

Figure: Plot of parameter estimation error

Method 2: Optimization framework-loss function design

Regressors: Loss function design

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y | g(\mathbf{a}_1^{\top}\mathbf{x}), \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y | g(\mathbf{a}_2^{\top}\mathbf{x}), \sigma^2)
$$

• Traditional approaches: l_2 -loss, log-likelihood loss

- ▸ Get stuck in local minima
- ▸ No theoretical analysis
- \rightarrow Single loss function for both (a_1, a_2) and w
- Formulation of right loss function is critical (Jacobs et. al 1991)

Theoretical contributions

• Separate loss functions L_4 and L_{log} to learn (a_1, a_2) and w

• Gradient descent on both L_4 and L_{log} . What are they?

Tensor based loss function for regressors

• For linear experts,

$$
P_{y|\mathbf{x}} = f(\mathbf{w}^{\top}\mathbf{x}) \cdot \mathcal{N}(y|\mathbf{a}_1^{\top}\mathbf{x}, \sigma^2) + (1 - f(\mathbf{w}^{\top}\mathbf{x})) \cdot \mathcal{N}(y|\mathbf{a}_2^{\top}\mathbf{x}, \sigma^2)
$$

• Stein's lemma+ 4-Hermite polynomial implies

$$
\mathcal{T}_4 = \mathbb{E}\big[\big(y^4-6y^2\big(1+\sigma^2\big)\big)\cdot \mathcal{S}_4\big(\textbf{x}\big)\big] = 12\big(\textbf{a}_1^{\otimes 4}+\textbf{a}_2^{\otimes 4}\big)
$$

• If $\hat{\boldsymbol{a}}_1$ and $\hat{\boldsymbol{a}}_2$ are parameters,

$$
L_4(\hat{\boldsymbol{a}}_1, \hat{\boldsymbol{a}}_2) \triangleq \sum_{j \neq k} \mathcal{T}_4(\hat{\boldsymbol{a}}_j, \hat{\boldsymbol{a}}_j, \hat{\boldsymbol{a}}_k, \hat{\boldsymbol{a}}_k) - \mu \sum_{j \in \{1, 2\}} \mathcal{T}_4(\hat{\boldsymbol{a}}_j, \hat{\boldsymbol{a}}_j, \hat{\boldsymbol{a}}_j, \hat{\boldsymbol{a}}_j) + \lambda \sum_{j \in \{1, 2\}} (\|\hat{\boldsymbol{a}}_j\|^2 - 1)^2
$$

Landscape of L_4

Properties

- No spurious local minima: All local minima are global
- Global minima are ground truth (upto permutation and sign-flip)
- All saddle points have negative curvature
- SGD converges to approximate global minima

Why L_4 ?

Why L_4 ?

- We provide a non-trivial connection to tensor based losses
- We can show that

$$
L_4(\hat{\boldsymbol{a}}_1, \hat{\boldsymbol{a}}_2) = 12 \sum_i \sum_{j \neq k} \langle \boldsymbol{a}_i, \hat{\boldsymbol{a}}_j \rangle^2 \langle \boldsymbol{a}_i, \hat{\boldsymbol{a}}_k \rangle^2 - 12 \mu \sum_i \sum_j \langle \boldsymbol{a}_i, \hat{\boldsymbol{a}}_j \rangle^4 + \lambda \sum_j (\|\boldsymbol{a}_j\|^2 - 1)^2
$$

- **4-order tensor loss**
	- ▸ Landscape analysis in (Ge et. al 2018)

Empirical performance

Figure: Plot of parameter estimation error

Summary

- Algorithmic innovation: First provably consistent algorithms for MoE in $25+$ years
- Loss function innovation: First SGD based algorithm on novel loss functions with provably nice landscape properties
- Sample complexity: First sample complexity results for MoE
- Global convergence: Our algorithms work with global initializations

Open questions-I

Conjecture

EM algorithm recovers both the regression parameters a_1 , a_2 and gating parameter w globally for 2-MoE

It is known that EM learns the true parameters globally for

- 2-symmetric mixture of Gaussians (Xu 2016, Daskalakis 2017)
- 2-symmetric mixture of linear regressions

Open questions-II

- Minimax rates and optimal algorithms
- Learning algorithms for time-series?
- **•** Generalizing to non-Gaussian inputs
	- ▸ Results: In the absence of gating, we have a loss function framework to provably learn the regressors
	- ▸ With gating?

- **•** Breaking the gridlock in Mixture-of-Experts: Consistent and Efficient Algorithms
- Learning One-hidden-layer Neural Networks under General Input **Distributions**
- Learning in Gated Neural Networks

Conclusion

- 1. Theoretical understanding \checkmark
- 2. Novel algorithms \checkmark
- 1. Theoretical understanding?
- 2. Algorithms?

Thank you!