A note on the instability and degeneracy of deep learning models

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Introduction

- A probability model exhibits instability if small changes in a data outcome result in large changes in probability
- Model degeneracy implies placing all probability on a small portion of the sample space

Goal: Quantify instability for general probability models defined on sequences of observations, where each sequence of length N has a finite number of possible outcomes

Notation

- $\boldsymbol{X} = (X_1, \dots, X_N)$ a set of discrete random variables with a finite sample space, \mathcal{X}^N
- ullet For each N, $P_{oldsymbol{ heta}_N}$ is a probability model on \mathcal{X}^N

FSFS models

Finitely Supported Finite Sequence (FSFS) model class

A series P_{θ_N} of probability models, indexed by a generic sequence of parameters θ_N , to describe data of each length $N \geq 1$ with model support of P_{θ_N} equaling the (finite) sample space \mathcal{X}^N .

- ullet The size and structure of such parameters $heta_N$ are without restriction
- Natural cases include $m{ heta}_N \in \mathbb{R}^{q(N)}$ for some arbitrary integer-valued function $q(\cdot) \geq 1$

Discrete exponential family models

Exponential family model for \boldsymbol{X} with pmf of the form

$$p_{N,\lambda}(\mathbf{x}) = \exp\left[\boldsymbol{\eta}^T(\lambda)\mathbf{g}_N(\mathbf{x}) - \psi(\lambda)\right], \quad \mathbf{x} \in \mathcal{X}^N,$$

for fixed positive dimensions of the parameter, $\lambda \in \Lambda \subset \mathbb{R}^k$ and natural parameter $\eta: \mathbb{R}^k \mapsto \mathbb{R}^L$ spaces, $\boldsymbol{g}_N: \mathcal{X}^N \mapsto \mathbb{R}^L$ a vector of sufficient statistics,

$$\psi(\lambda) = \log \sum_{\mathbf{x} \in \mathcal{X}^N} \exp \left[\boldsymbol{\eta}^T(\lambda) \mathbf{g}_N(\mathbf{x}) \right], \qquad \lambda \in \Lambda,$$

the normalizing function, and $\Lambda = \{ \lambda \in \mathbb{R}^k : \psi(\lambda) < \infty, k \leq q(N) \}$ is the parameter space.

Discrete exponential family models (cont'd)

- Such models arise with
 - Spatial data on a lattice (Besag 1974)
 - Network data (Wasserman and Faust 1994; Handcock 2003)
 - ullet Binomial sampling with N iid Bernoulli random variables
- These models are special cases of the FSFS models
- $P_{ heta_N}(extbf{x}) \equiv p_{N,\lambda_N}(extbf{x})$ with $heta_N = \lambda_N$ a sequence of elements of $\Lambda \subset \mathbb{R}^k$
- $P_{\theta_N}(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathcal{X}^N$
- ullet The dimension of the parameter $heta_N$ is the same for each N (k)
- Schweinberger (2011) considered instability in such exponential models

Restricted Boltzmann machines

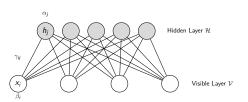


Figure 1: An example restricted Boltzmann machine (RBM). Hidden nodes are indicated by gray filled circles and the visible nodes indicated by unfilled circles.

- $\mathcal{X} = \{-1, 1\}$
- $X = (X_1, ..., X_N)$: N random variables for visibles with support \mathcal{X}^N
- $H = (H_1, ..., H_{N_H})$: N_H random variables for hiddens with support \mathcal{X}^{N_H}
- Parameters $\alpha \in \mathbb{R}^{N_H}$, $\beta \in \mathbb{R}^N$, Γ a matrix of size $N_H \times N$ $(\theta_N = (\alpha, \beta, \Gamma) \in \Theta_N \subset \mathbb{R}^{q(N)}$ with $q(N) = N + N_H + N * N_H)$

Joint pmf:

$$P_{\boldsymbol{\theta}_N}(\tilde{\boldsymbol{x}}) = \exp\left[\boldsymbol{\alpha}^T \boldsymbol{h} + \boldsymbol{\beta}^T \boldsymbol{x} + \boldsymbol{h}^T \Gamma \boldsymbol{x} - \psi(\boldsymbol{\theta}_N)\right], \quad \tilde{\boldsymbol{x}} = (\boldsymbol{h}, \boldsymbol{x}) \in \mathcal{X}^{N+N_H}$$

Restricted Boltzmann machines (cont'd)

• The pmf for the visible variables X_1, \ldots, X_N follows from marginalization:

$$P_{\theta_N}(\mathbf{x}) = \sum_{\mathbf{h} \in \mathcal{X}^{N_H}} P_{\theta_N}(\mathbf{x}, \mathbf{h}), \qquad \mathbf{x} \in \mathcal{X}^N.$$

- Size of θ_N , q(N), increases as a function of sample dimension N
- Can choose the number N_H of hidden variables to change with N (potentially increase)
- The RBM model specification for visibles is a FSFS model
- Models formed by marginalizing a base FSFS model (e.g., a type of exponential family model) is again a FSFS model class

Deep learning

- *M* the number of hidden layers included in the model
- $N_{(H,1)}, \ldots, N_{((H,M))}$ the number of hidden variables within each hidden layer
- $\tilde{\mathbf{X}} = \{H_1^{(1)}, \dots, H_{N_{(H,1)}}^{(1)}, \dots, H_1^{(M)}, \dots, H_{N_{(H,M)}}^{(M)}, \mathbf{X}\}$
 - Hidden variables $\{H_i^{(j)}: i = 1, ..., N_{(H,j)}, j = 1, ..., M\}$
 - Visible variables $\boldsymbol{X} = (X_1, \dots, X_N)$
 - $H_i^{(j)}, X_k \in \mathcal{X} = \{-1, 1\}$ for all i, j, k

Two models with "deep architecture" that contain multiple hidden layers in addition to a visible layer of data

- 1 Deep Boltzmann machine (DBM)
- 2 Deep belief network (DBN)

Deep Boltzmann machine (DBM)

Stacked RBMs with conditional dependence between neighboring layers. Joint pmf:

$$\begin{split} P_{\boldsymbol{\theta}_N}(\tilde{\boldsymbol{x}}) &= \exp\left[\sum_{i=1}^M \boldsymbol{\alpha}^{(i)T} \boldsymbol{h}^{(i)} + \boldsymbol{\beta}^T \boldsymbol{x} + \boldsymbol{h}^{(1)T} \boldsymbol{\Gamma}^{(0)} \boldsymbol{x} + \sum_{i=1}^{M-1} \boldsymbol{h}^{(i)T} \boldsymbol{\Gamma}^{(i)} \boldsymbol{h}^{(i+1)} - \boldsymbol{\psi}(\boldsymbol{\theta}_N)\right], \\ \tilde{\boldsymbol{x}} &= (\boldsymbol{h}^{(1)}, \dots, \boldsymbol{h}^{(M)}, \boldsymbol{x}) \in \mathcal{X}^{N_{(H,1)} + \dots + N_{(H,M)} + N} \end{split}$$

- Let $\theta_N = (\alpha^{(1)}, \dots, \alpha^{(M)}, \beta, \Gamma^{(0)}, \dots, \Gamma^{(M-1)}) \in \Theta_N \subset \mathbb{R}^{q(N)},$ $q(N) = N_{(H,1)} + \dots + N_{(H,M)} + N + N_{(H,1)} * N + N_{H,2} * H_{(H,1)} + \dots + N_{(H,M)} * H_{(H,M)-1}$
- The probability mass function for X_1, \ldots, X_N follows from marginalization of the joint pmf
- The visible DBM model specification is an example of a FSFS model.

Deep belief network (DBN)

- **Similar** to a DBM: Multiple layers of latent random variables stacked in a deep architecture with no conditional dependence between layers
- **Difference**: all but the last stacked layer in a DBN are Bayesian networks (see Pearl 1985)
 - A "weight" parameter is placed on each interaction between visibles, X_1, \ldots, X_N and the first layer of latent variables, $H_1^{(1)}, \ldots, H_{N_{H-1}}^{(1)}$
 - The number q(N) of components in the parameter vector is dependent on the dimension of the visibles
- For visibles X_1, \ldots, X_N with support \mathcal{X}^N , a DBN is also a FSFS model

Instability results

Implications

Thank you

Questions?

- Slides http://bit.ly/kaplan-private
- Contact
 - Email ajkaplan@iastate.edu
 - Twitter http://twitter.com/andeekaplan
 - GitHub http://github.com/andeek

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