Some Bayesian extensions of neural network-based graphon approximations

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Joint work with

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Overview

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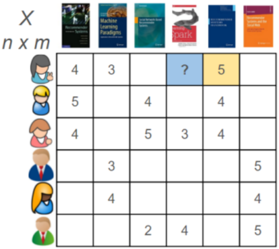
2. Consider variational inference in such a model and why.

3. Implement an infinite stochastic blockmodel, with good reason.

4. Review the pros and cons of being Bayesian here and other lessons learned along the way.

Relational data modeling



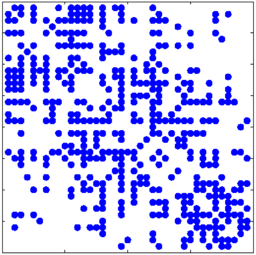


Figure from:
https://buildingrecommenders.wordpress.com/2015/11/18/overview-of-recommender-algorithms-part-2/

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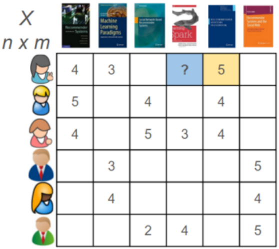

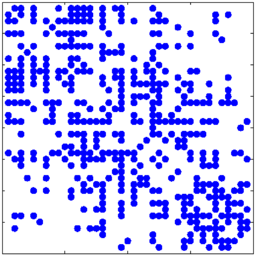

“Minibatch learning” with these two data structures...

- What’s the appropriate minibatch?
- Which entries are missing?

Lee et al. [2017]

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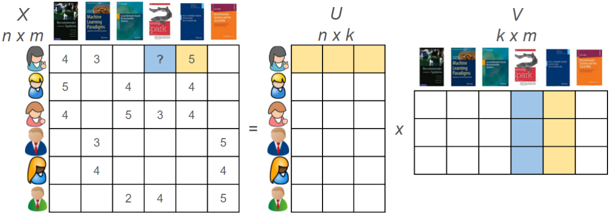
Matrix factorization... linear models



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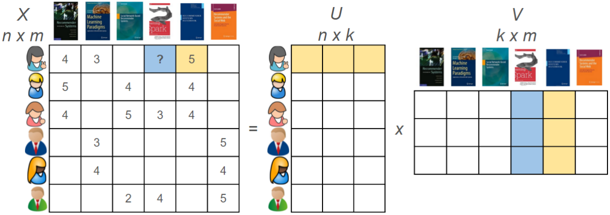

The (n, m)-th entry of the matrix is modeled as

$$X_{n,m} \approx U_n^T V_m = \sum_{d=1}^{D} U_{n,d} V_{m,d}$$

Some $U_n \in \mathbb{R}^D$ and $V_m \in \mathbb{R}^D$, with D small. A linear model.

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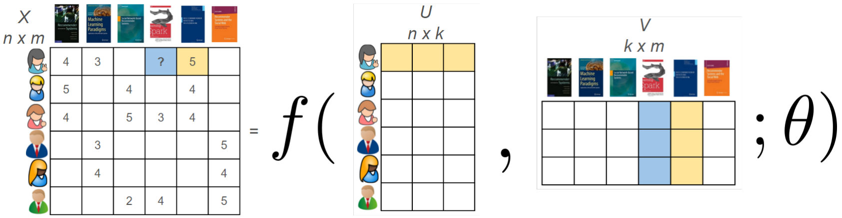
Neural network matrix factorization

(Dziugaite and Roy [2015])



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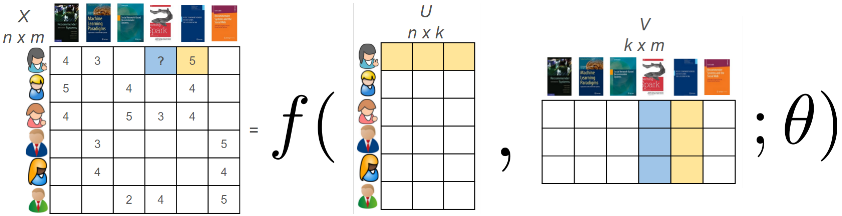

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The (n, m)-th entry of the matrix is modeled as

$$X_{n,m} \approx \cancel{U_n^T V_m = \sum_{d=1}^{D} U_{n,d} V_{m,d}} \;\; f(U_n, V_m; \theta)$$

Generalized to a nonlinear model.

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(Dziugaite and Roy [2015])

Matrix factorization	Network model
$X_{n,m} \approx f(U_n, V_m; \theta)$	$\mathbb{P}\{X_{n,m} = 1\} \approx \sigma(f(U_n, V_m; \theta))$

E.g.,

$$X_{n,m} \approx W_o \sigma(W_h \cdot [U_n, V_m] + b_h) + b_o$$

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Note: Inputs of the nnet are now parameters. (A Bayesian habit?)

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Gradient-based inference targeting, for example,

$$\begin{aligned} \text{Loss } = & \sum_{(n,m)} (X_{n,m} - f(U_n, V_m; \theta))^2 \\ & + \lambda_1 (||U||_F^2 + ||V||_F^2) && \text{regularize inputs (?)} \\ & + \lambda_2 ||\theta||_F^2 && \text{L1/L2 regularization} \end{aligned}$$

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Competitive performance; dominates linear baselines

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Pros:

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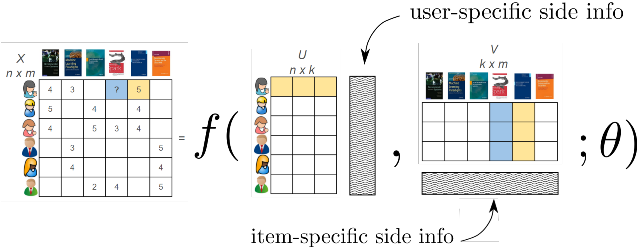

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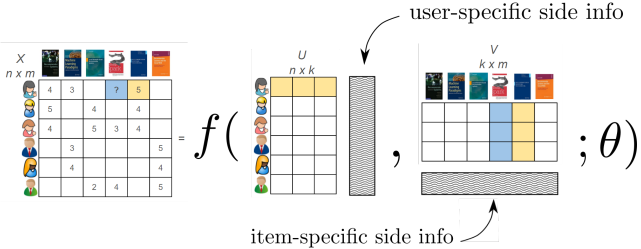

- Gradient-based learning tools (e.g., Tensorflow/Torch/etc.)

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Motivates things like a “stochastic blockmodel”...

- In some (most?) cases, consumers don’t necessarily need to interpret the inferred nnet...
- Will often settle for some interpretable (inferred) components
  - like convincing clusterings of the users.

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- So, reduced N sets of parameters to just K
- ... like clustering the users (rows of the matrix)

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- Straightforward application: "Variational inference for Dirichlet process mixtures" Blei and Jordan [2006]
- Informally, prediction looks like

$$\mathbb{P}\{X^*_{i,j} = 1\} \approx \mathbb{E}_{q(Z)}[\sigma(f(U_{Z_i}, U_{Z_j}; \theta))]$$

$q(Z) \approx p(Z \mid X)$ an approximation to the posterior.

Stick-breaking, mean-field variational inference

Stick-breaking construction:

Let $V_i \sim \text{beta}(1, c)$, $i = 1, 2, \ldots$ and

$$\pi_k = V_k \prod_{\ell=1}^{k-1} (1 - V_\ell), \quad k = 1, 2, \ldots,$$

$$Z_n \mid \pi \sim \text{Discrete}(\pi), \quad n \leq N.$$

Log likelihood is, for example,

$$\sum_{(i,j)} \log p(X_{i,j} \mid f(U_{Z_i}, U_{Z_j}; \theta)) + \log p(Z \mid V) + \log p(V)$$

Stick-breaking, mean-field variational inference

Let q denote a "variational approximation" to the posterior:

$$\begin{aligned} q(V_k) &= \text{beta}(V_k; a_k, b_k), \\ q(Z_n) &= \text{Discrete}(Z_n; \eta_n). \end{aligned}$$

Maximize the following lower bound on the log marginal likelihood

$$\begin{aligned} \log p(X) \geq & \mathbb{E}_{q(Z,V)}\Big[\sum_{(i,j)} \log p(X_{i,j} \mid f(U_{Z_i}, U_{Z_j}; \theta))\Big] \\ & - \mathrm{KL}[q(Z,V) || p(Z,V)] \end{aligned}$$

KL the Kullback–Leibler divergence.

Stick-breaking, mean-field variational inference

Algorithm:

- Initialize q.
- Iterate:
  - Update

$$q(Z_n = k) \propto \exp\Big\{\mathbb{E}_q[\log V_k] + \sum_{\ell \geq k+1} \mathbb{E}_q[\log(1 - V_\ell)] + \mathbb{E}_q\Big[\sum_{(i,j)} \log p(X_{i,j} \mid Z, \{Z_n = k\})\Big]\Big\},$$

  - Take a gradient step

$$\Theta \leftarrow \Theta + \eta \nabla_\Theta \Big\{\mathbb{E}_q\Big[\sum_{(i,j)} \log p(X_{i,j} \mid f(U_{Z_i}, U_{Z_j}; \theta))\Big] - \mathrm{KL}[q(Z, V) || p(Z, V)]\Big\}$$

  some schedule η and all parameters Θ

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  - Score function estimators with control variates Ranganath et al. [2014], Paisley et al. [2012]

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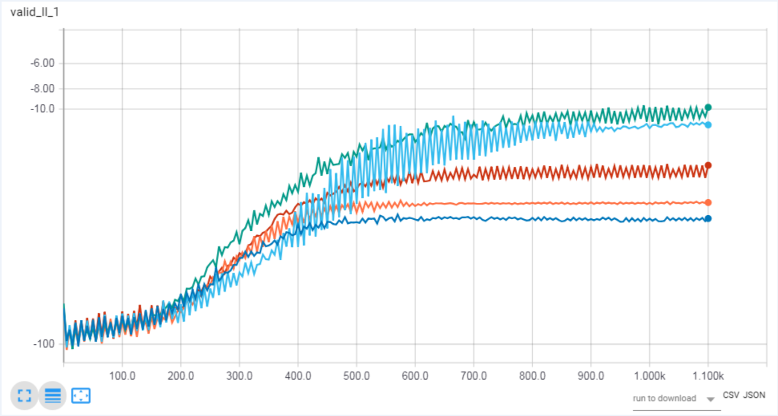
  - Often easy with packages such as Tensorflow Contrib's "distributions"

We can learn the usual cool structure

Some inferred NIPS Coauthorship clusters:

LeCun_Y	Giles_C	Jordan_M	Ferguson_D
Bengio_Y	LeCun_Y	Ghahramani_Z	Jaakola_T
Bottou_L	Liu_S	Bishop_C	Doucet_A
Dayan_P	Zemel_R	Amari_S	Bartlett_P
Frey_B_J	Mueller_P	Chapelle_O	Bartlett_M
Koller_D	Ng_A_Y	Burges_C	Guyon_I
Bishop_C	Opper_M	Edelman_S	Kearns_M
Jackel_L	Pearlmutter_B	Hinton	Burges_C
Graf_H	Rumelhart_D	Buhmann_J	Hinton_G
Doya_K	Poggio_T	Johnson_D	Jung_T

But it's not without pain points...



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- Some evidence layers useful when U contains side information.
  - E.g., Movie genre in Movielens 100K
  - Author word counts across papers in NIPS dataset

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- With Bayesian inference on your deep nnet...
  - You may find all that structure isn't necessary...
  - ...until you add data (not parameters).
- I wish we focused more on (scalable) MCMC inference with deep learning architectures.

D. M Blei and M. I. Jordan. Variational inference for Dirichlet process mixtures. Bayesian Analysis, 1(1): 121–143, 2006.

G. K. Dziugaite and D. M. Roy. Neural network matrix factorization. arXiv preprint arXiv:1511.06443, 2015.

D. P. Kingma and M. Welling. Auto-encoding variational Bayes. In ICLR, 2014.

J. Lee, C. Heaukulani, Z. Ghahramani, L. F. James, and S. Choi. Bayesian inference on random simple graphs with power law degree distributions. In Proceedings of the 34th International Conference on Machine Learning, 2017.

J. Lloyd, P. Orbanz, Z. Ghahramani, and D. M. Roy. Random function priors for exchangeable arrays with applications to graphs and relational data. In Advances in Neural Information Processing Systems 25, 2012.

P. Orbanz and D. M. Roy. Bayesian models of graphs, arrays and other exchangeable random structures. IEEE transactions on pattern analysis and machine intelligence, 37(2):437–461, 2015.

J. Paisley, D. M. Blei, and M. I. Jordan. Variational Bayesian inference with stochastic search. In ICML, 2012.

R. Ranganath, S. Gerrish, and D. M. Blei. Black box variational inference. In AISTATS, 2014.

T. Salimans and D. A. Knowles. Fixed-form variational posterior approximation through stochastic linear regression. Bayesian Analysis, 8(4):837–882, 2013.