Recommendation Systems theory

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What is a Recommendation System?

- A hypothetical example of an online survey asking people to give rating of M movies with a score $1-5$:

	$Item_1$	$Item_2$	$Item_3$	$Item_4$	$Item_5$	$Item_6$	$\ldots$	$Item_{M-1}$	$Item_M$
User 1	0	5	0	0	0	0	$\ldots$	0	0
User 2	0	0	1	0	0	0	$\ldots$	0	0
User 3	1	4	0	0	0	0	$\ldots$	0	0
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$
User N	0	0	5	0	0	0	$\ldots$	0	0

- **zeros** doesn't mean a zero score, it means the User has not scored this public service yet.
- Extremely sparse and very large Utility matrix
- In most literature, Columns called "User" and Rows are called "Items"
- **The question is what would the score be, if the User is to score these zero entries.**

The previous example is too futuristic, so let's get back to the movie and rating example from now:

For example, **User 101** has the following rating:

	$Item_1$	$Item_2$	$Item_3$	$Item_4$	$Item_5$	$Item_6$	...	$Item_{M-1}$	$Item_M$
User 101	0	**5**	0	0	**3**	0	...	**2**	0

- **User 101** has ONLY rated three items ($Item_2 = 5$), ($Item_5 = 3$) and ($Item_{M-1} = 2$)
- From these existing ratings, system needs to decide **"recommended"** ratings for the rest $M - 3$ items
- The question is how does $Item_2$, $Item_5$ and $Item_{M-1}$ each contribute to these decisions?

Needless to say **statistics from ALL users** needed for recommendation decision for **individual User**

In Collaborative Filtering, for each pair of items (x, y):

- First obtain statistics $r_{x,y}$, for example:

	$Item_{56}$	$Item_{78}$
User 102	1	5
User 202	2	5
User 376	5	1
...	...	
User 2121	4	1

	$Item_{56}$	$Item_{78}$
User 2321	4	5
User 1232	4	4
User 3533	1	1
...	...	
User 8839	5	4

- Then compute $S_{x,y}$, which similarity measure between item x and y.
- Then recommendation for each item becomes the weighted average of these similarities measures

Pearson correlation similarity of ratings:

$$S_{x,y} = \frac{\sum_{i \in I_{xy}} (r_{x,i} - \bar{r_x})(r_{y,i} - \bar{r_y})}{\sqrt{\sum_{i \in I_{xy}} (r_{x,i} - \bar{r_x})^2 \sum_{i \in I_{xy}} (r_{y,i} - \bar{r_y})^2}}$$

cosine-based approach of ratings:

$$S_{x,y} = \frac{\sum_{i \in I_{xy}} r_{x,i} r_{y,i}}{\sqrt{\sum_{i \in I_x} r_{x,i}^2} \sqrt{\sum_{i \in I_y} r_{y,i}^2}}$$

Recommendation System: A Collaborative Filtering Approach (2)

	$Item_1$	$Item_2$	$Item_3$	$Item_4$	$Item_5$	$Item_6$	$\dots$	$Item_{M-1}$	$Item_M$
User 101	0	**5**	0	0	**3**	0	$\dots$	**2**	0

- Weighted average of these contributions is then applied
- Sometimes, clustering of users may be needed and recommendation is user-group specific. For example, Netflix users.

Recommendation System: what if it's not "ratings", but "counts"?

- Another hypothetical example of number of "views" people looking at the VET Users :

	$Course_1$	$Course_2$	$Course_3$	$Course_4$	$Course_5$	$Course_6$	...	$Course_{M-1}$	$Course_M$
student 1	0	5	0	0	0	0	...	0	0
student 2	0	0	16	0	32	0	...	0	0
student 3	1	4	0	0	0	0	...	0	0
...	...	...	...	...	...	...	...	...	...
student N	0	0	5	0	0	0	...	0	0

- The counts are unbounded.
- "Ratings of 1" means negativity rating, but "Views of 1" does NOT necessarily mean negativity.
- Negative correlation doesn't make sense; We only have "how strong" the positive correlation is.
- Recently latent Poisson Model may be used.

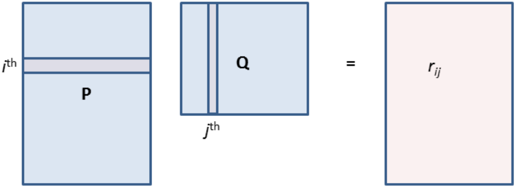
Content-based recommendations with Poisson factorization

An example of a probabilistic approach: (Gopalan, Charlin, Blei, 2014):

- Draw Item intensities $\theta_{dk} \sim \text{Gamma}(c, d)$
- Draw User preferences $\eta_{uk} \sim \text{Gamma}(e, f)$
- Draw Item topic offsets $\epsilon_{dk} \sim \text{Gamma}(g, h)$
- Draw $r_{ud} \sim \text{Poisson}(\eta_u^\top (\theta_d + \epsilon_d))$.

Recommendation System: Matrix factorisation approach, why it works?

$$\mathbf{R} \approx \mathbf{P} \times \mathbf{Q}^T = \hat{\mathbf{R}} \qquad \hat{r}_{ij} = p_i^T q_j = \sum_{k=1}^{K} p_{ik} q_{kj}$$



- number of columns of P and number of rows of Q must **agree**. However, this number K is somewhat arbitrary.
- each row of a user matrix represent a latent "user" feature vector
- each column of a item matrix represent a latent "item" feature vector
- In words, try to find matrices **P** and **Q**, such that when they multiply together the **existing ratings** have minimum changes
- The rest of zeros are replaced by non-zero numbers through matrix multiplication (think about why)
- See demo

Objective function in Matrix factorisation

- **The objective function**: what are we try to minimise?
- We just said in the previous slide that, "such that when they multiply together the **existing ratings** have minimum changes":

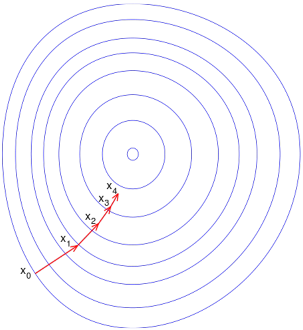
$$e_{ij}^2 = (r_{ij} - \hat{r}_{ij})^2 = \left(r_{ij} - \sum_{k=1}^{K} p_{ik} q_{kj} \right)^2 \qquad E = \sum {e_{ij}}^2 = \sum \left(r_{ij} - \sum_{k=1}^{K} p_{ik} q_{kj} \right)^2$$

We want to find all $\{p_{ik}\}$ and $\{q_{kj}\}$ which minimize E

- Note that $\arg\min(p_{ik})$ depends on one row of $\mathbf{P}$ and one column of $\mathbf{Q}$.
- We can't just let every $\frac{\partial}{\partial p_{ik}} e_{ij}^2 = 0$ and solve them at once.
- We need iterative algorithm, called **Gradient Descent** - and let's take a look:

Gradient Descend in matrix factorisation

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \nabla f(\mathbf{x}_n),\ n \geq 0$$



In the case of recommendation system, we have (remember **Chain rule** from high school?)

$$\frac{\partial}{\partial p_{ik}} e_{ij}^2 = -2(r_{ij} - \hat{r}_{ij})(q_{kj}) = -2e_{ij}q_{kj}$$
$$\frac{\partial}{\partial q_{kj}} e_{ij}^2 = -2(r_{ij} - \hat{r}_{ij})(p_{ik}) = -2e_{ij}p_{kj}$$

$$\begin{aligned} p'_{ik} &= p_{ik} - \alpha_n \underbrace{(-2e_{ij}q_{kj})}_{\nabla f(\mathbf{x}_n)} \\ &= p_{ik} + \alpha_n (2e_{ij}q_{kj}) \end{aligned}$$

$$\begin{aligned} q'_{kj} &= q_{kj} - \alpha_n \underbrace{(-2e_{ij}p_{kj})}_{\nabla f(\mathbf{x}_n)} \\ &= q_{kj} + \alpha_n (2e_{ij}p_{ik}) \end{aligned}$$

- There is this so-called, "identifiability" problem in solving $\arg\min_{A,B} f(AB)$
- Hence let's put a "regulariser" and obtain a new objective function for e_{ij}

$$e_{ij}^2 = (r_{ij} - \sum_{k=1}^{K} p_{ik} q_{kj})^2 + \frac{\beta}{2} \sum_{k=1}^{K} (||P||^2 + ||Q||^2)$$

- Then, the new gradient descent algorithm becomes that of:

$$p'_{ik} = p_{ik} + \alpha \frac{\partial}{\partial p_{ik}} e_{ij}^2 = p_{ik} + \alpha(2e_{ij} q_{kj} - \beta p_{ik})$$

$$q'_{kj} = q_{kj} + \alpha \frac{\partial}{\partial q_{kj}} e_{ij}^2 = q_{kj} + \alpha(2e_{ij} p_{ik} - \beta q_{kj})$$

Recommendation System: A Matrix factorization approach (4)

- An important extension is the requirement that all the elements of the factor matrices $\mathbf{P}$ and $\mathbf{Q}$ should be non-negative.
- Some of my researches are to add **prior probabilities** to the factor matrix, not only make them non-negative, but also enjoy other properties, such as sparsity etc.
- How we choose the optimal K? A lot of my research is in this area.
- Cold Start Problem - where no rating has been given by the user - clustering helps.
- One thing to note is that matrix factorization is very computational expensive. Stochastic Gradient Descent methods are used recently
- **Stochastic** is a buzz word of machine learning in BIG DATA era.

- In Ordinary Least Squares (OLS) **without** regulariser, we solve for β by minimizing the squared error $||y - X\beta||_2$:

$$\textbf{Solution} \qquad \beta = \left(X^T X\right)^{-1} X^T y$$

- In Ordinary Least Squares (OLS) **with** regulariser, we solve for β by minimizing the squared error $||y - X\beta||_2 + \lambda||\beta||_2$:

$$\textbf{Solution} \qquad \beta = \left(X^T X + \lambda I\right)^{-1} X^T y$$

Alternating least squares

$$\beta^* = \arg\max_{\beta} \left(\|y - X\beta\|_2 + \lambda \|\beta\|_2 \right) \implies \beta = \left(X^T X + \lambda I \right)^{-1} X^T y$$

- If we fix Q and optimize for P alone, the problem reduced to linear regression:

$$\forall p_i : J(p_i) = \|R_i - p_i Q^T\|_2 + \lambda \cdot \|p_i\|_2$$
$$\forall q_j : J(q_j) = \|R_j - P q_j^T\|_2 + \lambda \cdot \|q_j\|_2$$

  Matching solutions for p_i and q_j are:

$$p_i = \left(Q^T Q + \lambda I \right)^{-1} Q^T R_i$$
$$q_j = \left(P^T P + \lambda I \right)^{-1} P^T R_j$$

- Since each p_i doesn't depend on other $p_{j \neq i}$, each step can potentially be introduced to massive parallelization.

Bounded approach to NNMF

- In here, we want to assign similarities, i.e., $(-1, \dots 1)$ in each entry:

	$Item_1$	$Item_2$	$Item_3$	$Item_4$	$Item_5$	$Item_6$	...	$Item_{M-1}$	$Item_M$
User 1	0	0.6	0	0	0.4	0	...	0	0
User 2	0	0.9	0.3	0.2?	0	0.5	...	0	0
User 3	0.1	0.4?	0.2	0	0.7	0	...	0.2	0
User 4	0	?	0	?	0	0	...	0	0
...	...	...	...	...	...	...	...	...	...
User N	0.5	0	0.6	0	0	0	...	0	0

- This is part of our **new** research
- We can also set the upper bound to each of the ratings (think about why this is useful?)

Bounded approach to NNMF: Taking in the Popularities

- Looking at the following "viewing" scores:

	$Item_1$	$Item_2$	$Item_3$	$Item_4$	$Item_5$	$Item_6$	$\ldots$	$Item_{M-1}$	$Item_M$
User 1	3	0	15	0	4	0	$\ldots$	6	0
User 2	12	24	20	0	0	0	$\ldots$	0	0
User 3	1	3	12	0	7	0	$\ldots$	2	0
User 4	0	1	0	1	0	0	$\ldots$	0	0
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$
User N	5	0	6	0	0	0	$\ldots$	0	0

- Some items are just **popular**!
- And some users may tend to have **lot of views**
- So can we create individual bounds for each (user, item) pairs?

Factorization Machines

Feature vector **x** / Target y

	User A	User B	User C	User ...	Movie TI	Movie NH	Movie SW	Movie ST	Movie ...	Other Movies rated TI	Other Movies rated NH	Other Movies rated SW	Other Movies rated ST	Other Movies rated ...	Time	Last Movie rated TI	Last Movie rated NH	Last Movie rated SW	Last Movie rated ST	Last Movie rated ...	Target y	
$\mathbf{x}^{(1)}$	1	0	0	...	1	0	0	0	...	0.3	0.3	0.3	0	...	13	0	0	0	0	...	5	$y^{(1)}$
$\mathbf{x}^{(2)}$	1	0	0	...	0	1	0	0	...	0.3	0.3	0.3	0	...	14	1	0	0	0	...	3	$y^{(2)}$
$\mathbf{x}^{(3)}$	1	0	0	...	0	0	1	0	...	0.3	0.3	0.3	0	...	16	0	1	0	0	...	1	$y^{(2)}$
$\mathbf{x}^{(4)}$	0	1	0	...	0	0	1	0	...	0	0	0.5	0.5	...	5	0	0	0	0	...	4	$y^{(3)}$
$\mathbf{x}^{(5)}$	0	1	0	...	0	0	0	1	...	0	0	0.5	0.5	...	8	0	0	1	0	...	5	$y^{(4)}$
$\mathbf{x}^{(6)}$	0	0	1	...	1	0	0	0	...	0.5	0	0.5	0	...	9	0	0	0	0	...	1	$y^{(5)}$
$\mathbf{x}^{(7)}$	0	0	1	...	0	0	1	0	...	0.5	0	0.5	0	...	12	1	0	0	0	...	5	$y^{(6)}$

$$
\begin{aligned}
\hat{y}(\mathbf{x}) &= w_0 + \sum_{i}^{n} w_i x_i + \mathbf{x}^\top \mathrm{triu}(\mathbf{W})\mathbf{x} \\
&= w_0 + \sum_{i}^{n} w_i x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \mathbf{W}_{i,j} x_i x_j \\
&= w_0 + \sum_{i}^{n} w_i x_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \langle \mathbf{v}_i, \mathbf{v}_j \rangle x_i x_j
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{i}^{n} \sum_{j=i+1}^{n} \langle \mathbf{v}_i, \mathbf{v}_j \rangle x_i x_j \\
=&\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \langle \mathbf{v}_i, \mathbf{v}_j \rangle x_i x_j - \frac{1}{2} \sum_{i=1}^{n} \langle \mathbf{v}_i, \mathbf{v}_i \rangle x_i x_i \\
=&\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{f=1}^{k} v_{i,f} v_{j,f} x_i x_j - \frac{1}{2} \sum_{i=1}^{n} \sum_{f=1}^{k} v_{i,f} v_{i,f} x_i x_i \\
=&\frac{1}{2} \sum_{f=1}^{k} \left(\sum_{i=1}^{n} \sum_{j=1}^{n} v_{i,f} v_{j,f} x_i x_j - \sum_{i=1}^{n} v_{i,f} v_{i,f} x_i x_i \right) \\
=&\frac{1}{2} \sum_{f=1}^{k} \left(\left(\sum_{j=1}^{n} v_{j,f} x_j \right) \left(\sum_{i=1}^{n} v_{i,f} x_i \right) - \sum_{i=1}^{n} \left(v_{i,f} x_i \right)^2 \right) \\
=&\frac{1}{2} \sum_{f=1}^{k} \left(\left(\sum_{i=1}^{n} v_{i,f} x_i \right)^2 - \sum_{i=1}^{n} \left(v_{i,f} x_i \right)^2 \right)
\end{aligned}
$$

computational complexity is $O(kn)$

Faster NNMF convergence: Multiplicative Update Rule

- NNMF using Gradient Descend can be prohibitively slow when matrix is large
- A much faster (convergence) approach is to use "**Multiplicative Update Rule**".
- A "nature" publication and popular since Year 2000.

Faster NNMF convergence: Multiplicative Update Rule

- **Apologies** for the notations (this is to inline with each paper) $P \to W$ and $Q \to H$
- **Task:** Minimize $\|V - WH\|_2$ with respect to W and H, subject to the constraints $W, H \geq 0$.
- The Euclidean distance $\|V - WH\|$ is non-increasing under the update rules:

$$H_{a\mu} \leftarrow H_{a\mu} \frac{(W^\top V)_{a\mu}}{(W^\top WH)_{a\mu}} \qquad W_{ia} \leftarrow W_{ia} \frac{(VH^\top)_{ia}}{(WHH^\top)_{ia}}$$

- It looks so easier, but why this update rule works?

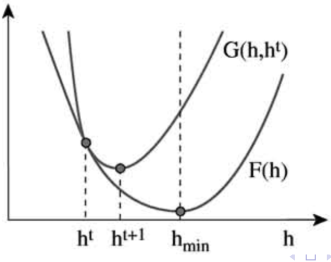
Multiplicative Update Rule

- Let's assume it's **hard** to minimize $F(h)$
- and it's easier to minimize $G(h, h^t)$. Let's find some **auxiliary function** $G(h, h^t)$ s.t.,:

$$G(h, h^t) \geq F(h), \qquad G(h, h) = F(h)$$

$$\text{Let} \qquad h^{t+1} = \arg\min_h G(h, h^t)$$

$$F(h^t) = G(h^t, h^t) \geq \underbrace{G(h^{t+1}, h^t) \geq F(h^{t+1})}_{\text{true for all } h \text{ include } h^{t+1}}$$



Faster NNMF convergence

- How are we going to prove:

$$F(h^t) = G(h^t, h^t) \geq G(h^{t+1}, h^t) \geq F(h^{t+1})$$

- $F(h^t)$ in the context of non-negative matrix factorization is:

$$\begin{aligned}
F(h) &= \frac{1}{2}\|v - Wh\|^2 \\
&= \frac{1}{2}\left(v^\top v - v^\top Wh - h^\top W^\top v + h^\top W^\top Wh\right) = \frac{1}{2}\left(v^\top v - 2v^\top Wh + h^\top W^\top Wh\right) \\
&\text{where } \triangledown F(h) = W^\top Wh - W^\top v \\
&= F(h^t) + (h - h^t)^\top \triangledown F(h^t) + \frac{1}{2}(h - h^t)^\top \underline{(W^\top W)}(h - h^t) \qquad \text{taylor expansion} \\
G(h, h^t) &= F(h^t) + (h - h^t)^\top \triangledown F(h^t) + \frac{1}{2}(h - h^t)^\top \underline{K(h^t)}(h - h^t) \\
&\text{where } K_{a,b}(h^t) = \frac{\delta_{a,b}(W^\top Wh^t)_a}{h^t_a}
\end{aligned}$$

$$
\begin{aligned}
G(h,h^t) \ge F(h) \implies & \frac{1}{2}(h-h^t)^\top \underline{K(h^t)}(h-h^t) \ge \frac{1}{2}(h-h^t)^\top \underline{(W^\top W)}(h-h^t) \ge 0 \\
\implies & \frac{1}{2}(h-h^t)^\top \big(K(h^t) - W^\top W\big)(h-h^t) \ge 0 \\
\implies & \big(K(h^t) - W^\top W\big) \text{ is a positive definite matrix } \textbf{need to prove it}
\end{aligned}
$$

- At each iteration, we just need to find: we simplify $K(h)$ with K:

$$
\begin{aligned}
G(h,h^t) =& F(h^t) + (h-h^t)^\top \nabla F(h^t) + \frac{1}{2}(h-h^t)^\top K(h-h^t) \\
=& F(h^t) + (h-h^t)^\top \nabla F(h^t) + \frac{1}{2}(h^\top Kh \underbrace{-h^{t\top} Kh - h^\top Kh^t}_{=-2h^\top Kh^t} + h^{t\top} Kh^t)
\end{aligned}
$$

$$
\begin{aligned}
\nabla G(h,h^t) &= \nabla F(h^t) + Kh - Kh^t = 0 \\
\implies Kh &= Kh^t - \nabla F(h^t) \\
h &= h^t - K^{-1}\nabla F(h^t)
\end{aligned}
$$

- writing it properly:

$$
h^{(t+1)} \leftarrow h^t - K^{-1}(h^t)\nabla F(h^t)
$$

Faster NNMF convergence

- We need to put the following:

$$h^{(t+1)} \leftarrow h^t - K^{-1}(h^t)\nabla F(h^t)$$

in the form of:

$$H_{a\mu} \leftarrow H_{a\mu}\frac{(W^\top V)_{a\mu}}{(W^\top WV)_{a\mu}} \qquad \text{or} \qquad h_a \leftarrow h_a\frac{(W^\top V)_a}{(W^\top WV)_a}$$

$$K_{a,b}(h^t) = \frac{\delta_{a,b}(W^\top Wh^t)_a}{h_a^t} \implies K(h^t) = \begin{bmatrix} \frac{(W^\top Wh^t)_1}{h_1^t} & \cdots \\ \cdots & \frac{(W^\top Wh^t)_N}{h_N^t} \end{bmatrix}$$

$$\implies K^{-1}(h^t) = \begin{bmatrix} \frac{h_1^t}{(W^\top Wh^t)_1} & \cdots \\ \cdots & \frac{h_N^t}{(W^\top Wh^t)_N} \end{bmatrix}$$

Faster NNMF convergence

- therefore,

$$
\begin{aligned}
h_a^t - \big(K^{-1}(h^t)\underbrace{\nabla F(h^t)}_{W^\top Wh - W^\top v}\big)_a &= h_a^t - \frac{h_a^t}{(W^\top Wh^t)_a}(W^\top Wh^t - W^\top v)_a \\
&= h_a^t - \frac{h_a^t (W^\top Wh^t - W^\top v)_a}{(W^\top Wh^t)_a} \\
&= \frac{h_a^t (W^\top Wh^t)_a - h_a^t (W^\top Wh^t)_a - h_a^t (W^\top v)_a}{(W^\top Wh^t)_a} \\
&= h_a^t \frac{(W^\top v)_a}{(W^\top Wh^t)_a}
\end{aligned}
$$

- One can obtain update for W in a similar fashion.

Lastly, how do we know $\left(K(h^t) - W^\top W\right)$ is a positive definite matrix?

$$K_{a,b}(h^t) = \frac{\delta_{a,b}(W^\top W h^t)_a}{h^t_a} = \frac{\delta_{a,b}\sum_i (W^\top W)_{a,i} h^t_i}{h^t_a}$$

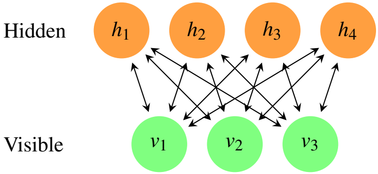
Therefore,

$$\begin{aligned}
&\sum_{a,b} v_a \left[h^t_a K_{a,b}(h^t) h^t_b\right] v_b \\
&= \sum_{a,b} v_a h^t_a \left(\frac{\delta_{a,b}\sum_i (W^\top W)_{a,i} h^t_i}{h^t_a}\right) h^t_b v_b \\
&= \sum_{a} v_a h^t_a \left(\frac{\sum_i (W^\top W)_{a,i} h^t_i}{h^t_a}\right) h^t_a v_a \\
&= \sum_{a} \left(\sum_i (W^\top W)_{a,i} h^t_i\right) h^t_a v_a^2 \\
&= \sum_{a,b} (W^\top W)_{a,b} h^t_b h^t_a v_a^2
\end{aligned}$$

Lastly, how do we know $\left(K(h^t) - W^\top W\right)$ is a positive definite matrix?

$$
\begin{aligned}
v^\top M v &= \sum_{ab} v_a M_{a,b}(h^t) v_b = \sum_{a,b} v_a \underbrace{\left[h^t_a (K(h^t) - W^\top W)_{a,b} h^t_b\right]}_{M_{a,b}(h^t)} v_b \\
&= \sum_{a,b} v_a \left[h^t_a K_{a,b}(h^t) h^t_b\right] v_b - \sum_{a,b} v_a \left[h^t_a (W^\top W)_{a,b} h^t_b\right] v_b \\
&= \sum_{a,b} \left[(W^\top W)_{a,b} h^t_b h^t_a v_a^2\right] - \left[v_a h^t_a (W^\top W)_{a,b} h^t_b v_b\right] \qquad \text{see previous slide} \\
&= \sum_{a,b} (W^\top W)_{a,b} h^t_a h^t_b \left[v_a^2 - v_a v_b\right] \\
&= \frac{1}{2}\left(\sum_{a,b} (W^\top W)_{a,b} h^t_a h^t_b \left[v_a^2 - v_a v_b\right] + (W^\top W)_{a,b} h^t_a h^t_b \left[v_a^2 - v_a v_b\right]\right) \\
&= \frac{1}{2}\left(\sum_{a,b} (W^\top W)_{a,b} h^t_a h^t_b \left[v_a^2 - v_a v_b\right] + \underbrace{(W^\top W)_{b,a} h^t_b h^t_a \left[v_b^2 - v_b v_a\right]}_{\text{swap } a \text{ and } b}\right) \\
&= \frac{1}{2}\left(\sum_{a,b} (W^\top W)_{a,b} h^t_a h^t_b \left[v_a^2 - v_a v_b\right] + (W^\top W)_{b,a} h^t_b h^t_a \left[v_b^2 - v_b v_a\right]\right) \\
&= \frac{1}{2}\left(\sum_{a,b} (W^\top W)_{a,b} h^t_a h^t_b \left[v_a^2 - v_a v_b + v_b^2 - v_b v_a\right]\right) \\
&= \frac{1}{2} \sum_{a,b} (W^\top W)_{a,b} h^t_a h^t_b \left[v_a - v_b\right]^2 \qquad \text{since } W, h^t \text{ are all non-negative}
\end{aligned}
$$

Restrictive Botzmann Machine



Define:
$$
\begin{aligned}
E(\mathbf{v},\mathbf{h}) &= -b^\top \mathbf{v} - c^\top \mathbf{h} - \mathbf{v}^\top W \mathbf{h} \\
&= -\sum_j b_j v_j - \sum_i c_i h_i - \sum_i \sum_j v_j W_{ij} h_i
\end{aligned}
$$

$$
p(\mathbf{v},\mathbf{h}) = \exp(-E(\mathbf{v},\mathbf{h})) = \exp\left(b^\top \mathbf{v} + c^\top \mathbf{h} + \mathbf{v}^\top W \mathbf{h}\right)
$$

- There are two separate offset parameters: b and c, associated with $\mathbf{v}$ and $\mathbf{h}$ respectively.
- Note that there is no interconnecting terms between elements of $\mathbf{v}$ and $\mathbf{h}$. Otherwise, there will be a term $\mathbf{v}^\top W_v \mathbf{v}$ and $\mathbf{h}^\top W_h \mathbf{h}$
- In this presentation, $\mathbf{v}$ and $\mathbf{h}$ are binary arrays.
- $\mathbf{v}$ and $\mathbf{h}$ can take other values, for example Softmax and Gaussian.

RBM Marginal

$$p(\mathbf{v},\mathbf{h}) = \exp(-E(\mathbf{v},\mathbf{h})) = \exp\left(b^\top \mathbf{v} + c^\top \mathbf{h} + \mathbf{v}^\top W\mathbf{h}\right) = \exp\left(\sum_j b_j v_j + \sum_i c_i h_i + \sum_i \sum_j v_j W_{ij} h_i\right)$$

$$\begin{aligned}
p(\mathbf{v}) &= \frac{1}{Z}\sum_{\mathbf{h}} p(\mathbf{v},\mathbf{h}) = \frac{1}{Z}\sum_{\mathbf{h}} \exp\left(b^\top \mathbf{v} + c^\top \mathbf{h} + \mathbf{v}^\top W\mathbf{h}\right) \\
&= \frac{1}{Z}\exp(b^\top \mathbf{v})\sum_{\mathbf{h}} \exp\left(c^\top \mathbf{h} + \mathbf{v}^\top W\mathbf{h}\right) \\
&= \frac{1}{Z}\exp(b^\top \mathbf{v})\sum_{h_1}\sum_{h_2}\cdots\sum_{h_N} \exp^{\sum_i c_i \underbrace{h_i} + \sum_i \sum_j v_j W_{ij} \underbrace{h_i}} \\
&= \frac{1}{Z}\exp(b^\top \mathbf{v})\sum_{h_1}\sum_{h_2}\cdots\sum_{h_N} \exp^{\sum_i \underbrace{h_i} \left(c_i + \sum_j v_j W_{ij}\right)} \\
&= \frac{1}{Z}\exp(b^\top \mathbf{v})\sum_{h_1} \exp^{h_1\left(c_1+\sum_j w_{1j}v_j\right)} \sum_{h_2} \exp^{h_2\left(c_i+\sum_j w_{2j}v_j\right)} \ldots \sum_{h_N} \exp^{h_N\left(c_N+\sum_j w_{Nj}v_j\right)} \\
&= \frac{1}{Z}\exp^{\sum_j b_j v_j} \prod_{i=1}^{N} \sum_{h_i} \exp^{h_i\left(c_i+\sum_j w_{ij}v_j\right)} \\
&= \frac{1}{Z}\prod_j \exp^{b_j v_j} \prod_{i=1}^{N}\left(1+\exp^{c_i+\sum_j w_{ij}v_j}\right)
\end{aligned}$$

RBM conditional

$$p(\mathbf{v},\mathbf{h}) = \exp(-E(\mathbf{v},\mathbf{h})) = \exp\left(b^\top \mathbf{v} + c^\top \mathbf{h} + \mathbf{v}^\top W\mathbf{h}\right) = \exp\left(\sum_j b_j v_j + \sum_i c_i h_i + \sum_i \sum_j v_j W_{ij} h_i\right)$$

$$\begin{aligned}
p(V_l = 1|\mathbf{h}) &= \frac{p(V_l = 1, \mathbf{h})}{p(\mathbf{h})} = \frac{p(V_l = 1, \mathbf{h})}{\sum_{v_l} p(V_l = 1, \mathbf{h})} \\
&= \frac{\exp\left(1 \times b_l + \sum_i 1 \times W_{il} h_i\right)}{\sum_{v_l} \exp\left(b_l v_l + \sum_i v_l W_{il} h_i\right)} \qquad \text{reduce } \sum_j \text{ into a single term} \\
&= \frac{\exp\left(b_l + \sum_i W_{il} h_i\right)}{\underbrace{1}_{v_l=0} + \underbrace{\exp\left(b_l + \sum_i W_{il} h_i\right)}_{v_l=1}} \\
&= \sigma\left(b_l + \sum_i W_{il} h_i\right)
\end{aligned}$$

By symmetry,

$$p(H_i = 1|\mathbf{v}) = \sigma\left(c_i + \sum_j v_j W_{ij}\right)$$

The **derivative** of general Markov Random Field Likelihood

- In here, we did NOT use the structure of RBM, i.e.,
  $p(\mathbf{v}, \mathbf{h}) = \exp\left(b^\top \mathbf{v} + c^\top \mathbf{h} + \mathbf{v}^\top W\mathbf{h}\right) = \exp\left(\sum_j b_j v_j + \sum_i c_i h_i + \sum_i \sum_j v_j W_{ij} h_i\right)$:

$$
\begin{aligned}
\mathcal{L}_{\mathbf{v}}(\theta) &= \log(p(\mathbf{v})) = \log\left(\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}\right) - \log(Z) \\
&= \log\left(\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}\right) - \log\left(\sum_{\mathbf{h},\mathbf{v}} \exp^{-E(\mathbf{v},\mathbf{h})}\right) \\
\Longrightarrow \frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial \theta} &= \frac{1}{\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}} \sum_{\mathbf{h}} \frac{\partial \exp^{-E(\mathbf{v},\mathbf{h})}}{\partial \theta} - \frac{1}{\sum_{\mathbf{h},\mathbf{v}} \exp^{-E(\mathbf{v},\mathbf{h})}} \sum_{\mathbf{h},\mathbf{v}} \frac{\partial \exp^{-E(\mathbf{v},\mathbf{h})}}{\partial \theta} \\
&= -\frac{1}{\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}} \sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})} \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} + \frac{1}{\sum_{\mathbf{h},\mathbf{v}} \exp^{-E(\mathbf{v},\mathbf{h})}} \sum_{\mathbf{h},\mathbf{v}} \exp^{-E(\mathbf{v},\mathbf{h})} \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} \\
&= -\sum_{\mathbf{h}} \frac{\exp^{-E(\mathbf{v},\mathbf{h})}}{\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}} \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} + \sum_{\mathbf{h},\mathbf{v}} \frac{\exp^{-E(\mathbf{v},\mathbf{h})}}{\sum_{\mathbf{h},\mathbf{v}} \exp^{-E(\mathbf{v},\mathbf{h})}} \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} \\
&= -\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} + \sum_{\mathbf{h},\mathbf{v}} p(\mathbf{v},\mathbf{h}) \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta}
\end{aligned}
$$

$$
p(\mathbf{h}|\mathbf{v}) = \frac{p(\mathbf{v},\mathbf{h})}{p(\mathbf{v})} = \frac{\frac{1}{Z}\exp^{-E(\mathbf{v},\mathbf{h})}}{\frac{1}{Z}\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}} = \frac{\exp^{-E(\mathbf{v},\mathbf{h})}}{\sum_{\mathbf{h}} \exp^{-E(\mathbf{v},\mathbf{h})}}
$$

note that the two Z are equal

The **derivative** of RBM Likelihood

$$p(\mathbf{v},\mathbf{h}) = \exp(-E(\mathbf{v},\mathbf{h})) = \exp\left(b^\top \mathbf{v} + c^\top \mathbf{h} + \mathbf{v}^\top W\mathbf{h}\right) = \exp\left(\sum_j b_j v_j + \sum_i c_i h_i + \sum_i \sum_j v_j W_{ij} h_i\right)$$

$$E(\mathbf{v},\mathbf{h}) = -b^\top \mathbf{v} - c^\top \mathbf{h} - \mathbf{v}^\top W\mathbf{h}$$

$$\begin{aligned}
\frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial \theta} &= -\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} + \sum_{\mathbf{h},\mathbf{v}} p(\mathbf{v},\mathbf{h}) \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial \theta} \\
\Longrightarrow \frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial w_{ij}} &= -\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial w_{ij}} + \sum_{\mathbf{h},\mathbf{v}} p(\mathbf{v},\mathbf{h}) \frac{\partial E(\mathbf{v},\mathbf{h})}{\partial w_{ij}} \\
&= +\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) v_j h_i - \sum_{\mathbf{h},\mathbf{v}} p(\mathbf{v},\mathbf{h}) v_j h_i \qquad \text{note the sign change} \\
&= \underline{\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) v_j h_i} - \sum_{\mathbf{v}} p(\mathbf{v}) \underline{\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) v_j h_i} \\
&= p(H_i = 1|\mathbf{v}) v_j - \sum_{\mathbf{v}} p(\mathbf{v}) p(H_i = 1|\mathbf{v}) v_j
\end{aligned}$$

Because: $\underline{\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) v_j h_i} = \sum_{h_1} \cdots \sum_{h_N} \prod_{k=1}^{N} p(h_k|\mathbf{v}) v_j h_i = \sum_{h_i} p(h_i|\mathbf{v}) v_j h_i \times \underbrace{\sum_{\mathbf{h}_{k\neq i}} \prod_{k\neq i}^{N} p(h_k|\mathbf{v})}_{=1}$

$$= \sum_{h_i} p(h_i|\mathbf{v}) v_j h_i = p(H_i = 1|\mathbf{v}) v_j = \sigma\left(c_i + \sum_j v_j W_{ij}\right) v_j$$

Average derivative of RBM Likelihood over data

$$\frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial w_{ij}} = \sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) v_j h_i - \sum_{\mathbf{h},\mathbf{v}} p(\mathbf{v},\mathbf{h}) v_j h_i$$
$$= p(H_i = 1|\mathbf{v}) v_j - \sum_{\mathbf{v}} p(\mathbf{v}) p(H_i = 1|\mathbf{v}) v_j$$

- when we are given a set of observed $\mathbf{v}$:

$$\frac{1}{N}\sum_{\mathbf{v}\in S} \frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial w_{ij}} = \frac{1}{N}\sum_{\mathbf{v}\in S}\sum_{\mathbf{h}} p(\mathbf{h}|\mathbf{v}) v_j h_i - \sum_{\mathbf{h},\mathbf{v}} p(\mathbf{v},\mathbf{h}) v_j h_i$$
$$= \frac{1}{N}\sum_{\mathbf{v}\in S}\left(\mathbb{E}_{p(\mathbf{h}|\mathbf{v})}[v_j h_i] - \mathbb{E}_{p(\mathbf{h},\mathbf{v})}[v_j h_i]\right)$$
$$= \langle v_j h_i \rangle_{p(\mathbf{h}|\mathbf{v})q(\mathbf{v})} - \langle v_j h_i \rangle_{p(\mathbf{h},\mathbf{v})}$$

where $q(\mathbf{v})$ is the sample distribution

- without going through the normal **contrast divergence equation**, we put RBM in the CD form above:

$$\frac{\partial - \mathcal{L}_{\mathbf{v}}(\theta)}{\partial w_{ij}} \propto \langle v_j h_i \rangle_{p(\mathbf{h},\mathbf{v})} - \langle v_j h_i \rangle_{p(\mathbf{h}|\mathbf{v})q(\mathbf{v})}$$

- **Exercise** how complex is $\langle v_j h_i \rangle_{p(\mathbf{h}|\mathbf{v})q(\mathbf{v})}$? say $\mathbf{h}$ and $\mathbf{v}$ each have 100 nodes?
- **Exercise** how can we deal with such complexity?

RBM LLE via Contrast Divergence

the **answer** is to use Gibbs sampling: In each step of Gradient Descend, one performs the following:

- Let $\mathbf{v}^{(0)} = \mathbf{v}$
- Obtain a new set of Monte-Carlo sampled $\mathbf{v}$ iteratively:
  - sample $h^{(t)} \sim p(h_i|\mathbf{v}^{(t)})$ sample $v_j^{(t+1)} \sim p(v_j|\mathbf{h}^{(t)})$
  - until we obtain $\mathbf{v}^{(k)}$
- Update parameters $\{W_{i,j}\}$, $\{b_j\}$ and $\{c_i\}$ as the gradients:

$$
\begin{aligned}
\frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial W_{i,j}} &\approx p(H_i = 1|\mathbf{v}^{(k)})v_j^{(k)} - p(H_i = 1|\mathbf{v}^{(0)})v_j^{(0)} \\
\frac{\partial \mathcal{L}_{\mathbf{v}}(\theta)}{\partial b_j} &\approx v_j^{(k)} - v_j^{(0)} \\
\frac{\partial \mathcal{L}_{\mathbf{v}}(\theta))}{\partial c_i} &\approx p(H_i = 1|\mathbf{v}^{(k)}) - p(H_i = 1|\mathbf{v}^{(0)})
\end{aligned}
$$

RBM Collaborative Filtering

- **each user** can rate one of the m available movies, with a score between $\{1 \ldots K\}$
- therefore, **each user** has a V, observed binary indicator matrix sized $K \times m$
- with $v_i^k = 1$ if a user rated movie i as k and 0 otherwise.
- it's a **softmax** function with $\sum_{k=1}^{K} p(v_i^k = 1|\mathbf{h}) = 1$:

$$p(v_i^k = 1|\mathbf{h}) = \frac{\exp\left(b_i^k + \sum_{j=1}^{F} h_j W_{ij}^k\right)}{\sum_{k=1}^{K} \exp\left(b_i^k + \sum_{j=1}^{F} h_j W_{ij}^k\right)} = \frac{\exp\left(b_i^k + W_{i,:}^k \mathbf{h}\right)}{\sum_{k=1}^{K} \exp\left(b_i^l + W_{i,:}^k \mathbf{h}\right)}$$

- **each user** has $\mathbf{h} \in \{0, 1\}^F$, a binary values of hidden variables
- thought of as representing stochastic binary features that have different values for different users:

$$p(h_j = 1|\mathbf{V}) = \sigma\left(b_j + \sum_{i=1}^{m} \sum_{k=1}^{K} v_i^k W_{ij}^k\right) = \sigma\left(b_j + \sum_{k=1}^{K} (W_{:,j}^k)^\top \mathbf{v}^k\right)$$

Recommendation via RBM

- traditional RBM joint energy

$$E(\mathbf{v}, \mathbf{h}) = -\sum_{i}^{m} b_i v_i - \sum_{j}^{F} b_j h_j - \sum_{i}^{m} \sum_{j}^{F} v_i W_{ij} h_j$$

- **Exercise** in terms of recommendation engine, how is traditional RBM useful?
- In recommendation setting with a rating range, it has changed to:

$$E(\mathbf{v}, \mathbf{h}) - \sum_{i}^{m} \sum_{k=1}^{K} b_i v_i^k - \sum_{j}^{F} b_j h_j - \sum_{i}^{m} \sum_{j}^{F} \sum_{k=1}^{K} v_i W_{ij}^k h_j v_i^k$$