Non-negative Matrix Factorization (NMF)

Problem Motivation

- Soft clustering
  - Clustering where each observation can have partial membership in each cluster
- Identify latent features
  - Identify topics in a corpus of text
  - Identify parts of faces in facial recognition

Example: Baking a Cake

- Given a cake, we cannot directly observe its flour and sugar contents
- But, we can directly measure carbohydrates, fat, and protein
- NMF can learn ingredients and proportions from the final product

Example: Baking a Cake

- Recipe is a linear combination of ingredients
  - **2** cups flour
  - **1** cup sugar

Example: Baking a Cake

- Ingredients are linear combination of carbohydrates, fat, and protein
  - Flour:
    20g carbohydrates, **5**g protein, **1**g fat
  - Sugar:
    10g carbohydrates, **0**g protein, **1**g fat

Example: Baking a Cake

Recipe and ingredients can be represented by vectors/matrices

$$\text{Recipe} = [\text{flour, sugar}] = [2, 1]$$

$$\begin{aligned}\text{Ingredients} &= \begin{bmatrix} f_c & f_p & f_f \\ s_c & s_p & s_f \end{bmatrix} \\ &= \begin{bmatrix} 20 & 5 & 1 \\ 10 & 0 & 1 \end{bmatrix}\end{aligned}$$

Example: Baking a Cake

Cake is product of recipe vector and ingredient matrix

$$\begin{aligned}
\text{Cake} &= (recipe)[Ingredients] \\
&= \begin{pmatrix} 2 & 1 \end{pmatrix} \begin{bmatrix} 20 & 5 & 1 \\ 10 & 0 & 1 \end{bmatrix} \\
&= 2 \begin{pmatrix} 20 & 5 & 1 \end{pmatrix} + 1 \begin{pmatrix} 10 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 50 & 10 & 3 \end{pmatrix}
\end{aligned}$$

Example: Baking a Cake

Many cakes can be represented by product of 2 matrices

$$\begin{bmatrix} c_1 & p_1 & f_1 \\ c_2 & p_2 & f_2 \\ c_3 & p_3 & f_3 \\ \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} w_{1f} & w_{1s} \\ w_{2f} & w_{2s} \\ w_{3f} & w_{3s} \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} f_c & f_p & f_f \\ s_c & s_p & s_f \end{bmatrix}$$

Example: Unbaking a Cake

Finding the recipe

Given cakes and a set of ingredients, can we figure out the recipe?

$$\begin{bmatrix} 30 & 5 & 2 \\ 20 & 5 & 3 \\ 25 & 3 & 3 \\ \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} w_{1f} & w_{1s} \\ w_{2f} & w_{2s} \\ w_{3f} & w_{3s} \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} 20 & 5 & 1 \\ 10 & 0 & 1 \end{bmatrix}$$

Example: Unbaking a Cake

Finding the recipe

Can perform OLS minimization to find the recipe

$$\begin{bmatrix}25 & 3 & 3\end{bmatrix} = \begin{pmatrix}w_f & w_s\end{pmatrix} \begin{bmatrix}20 & 5 & 1 \\ 10 & 0 & 1\end{bmatrix}$$

$$25 \approx \hat{c} = 20w_{3f} + 10w_{3s}$$

$$3 \approx \hat{p} = 5w_{3f} + 0w_{3s}$$

$$3 \approx \hat{f} = 1w_{3f} + 1w_{3s}$$

$$\underset{\vec{w}}{\operatorname{argmin}} \sum_{y \in (c,p,f)} (y - \hat{y})^2$$

Example: Unbaking a Cake

Finding the ingredients

Given cakes and a set of recipes, can we figure out the ingredients?

$$\begin{bmatrix} 30 & 5 & 2 \\ 20 & 5 & 3 \\ 25 & 3 & 3 \\ \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 1 & 2 \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} f_c & f_p & f_f \\ s_c & s_p & s_f \end{bmatrix}$$

Example: Unbaking a Cake

Finding the ingredients

Can perform OLS minimization to find the ingredients

$$\begin{bmatrix}25 & 3 & 3\end{bmatrix} = \begin{pmatrix}1 & 2\end{pmatrix} \begin{bmatrix} f_c & f_p & f_f \\ s_c & s_p & s_f \end{bmatrix}$$

$$25 = \hat{c} \approx 1f_c + 2s_c = 1f_c + 2s_c + 0f_p + 0s_p + 0f_f + 0s_f$$

$$3 = \hat{p} \approx 1f_p + 2s_p = 0f_c + 0s_c + 1f_p + 2s_p + 0f_f + 0s_f$$

$$3 = \hat{f} \approx 1f_f + 2s_f = 0f_c + 0s_c + 0f_p + 0s_p + 1f_f + 2s_f$$

...continued for all observations

Example: Unbaking a Cake

Finding the ingredients and the recipes

What if you don’t know the recipe proportions *or* the ingredients?

$$\begin{bmatrix} 30 & 5 & 2 \\ 20 & 5 & 3 \\ 25 & 3 & 3 \\ \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} w_{1f} & w_{1s} \\ w_{2f} & w_{2s} \\ w_{3f} & w_{3s} \\ \vdots & \vdots \end{bmatrix} \begin{bmatrix} f_c & f_p & f_f \\ s_c & s_p & s_f \end{bmatrix}$$

Alternating Least Squares

$$X = WH$$

1. Initialize* W and H
2. Solve for H holding W constant (minimize OLS) and clip negative values
3. Solve W holding H constant (minimize OLS) and clip negative values
4. Repeat steps 2 and 3 until convergence

**Initialization methods vary. Random initialization and k-means are common.*

Alternating Least Squares

- ALS is “biconvex”
- It is not globally convex, so it will not necessarily find local optima
- Better optima can be found with strategic initializations (like k means) or multiple random initializations

Interpreting NMF Results

$$X = WH$$

X = (observations) x (features)

W = (observations) x (latent features)

H = (latent features) x (observed features)

Interpreting NMF Results

Topic Modeling

X = (documents) x (word counts)

W = (documents) x (?)

H = (?) x (word counts)

→ Latent features correspond to topics. This is explored in today’s assignment.

Interpreting NMF Results

Face Identification

Suppose X is a set of images of faces (all the same size)

X = (images) x (pixel intensities)

W = (image) x (?)

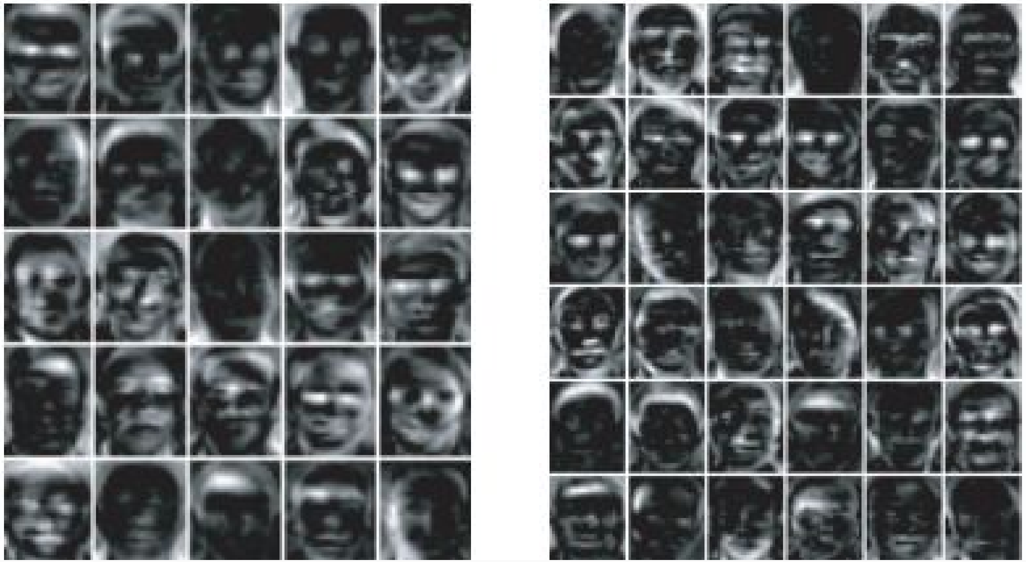
H = (?) x (pixel intensities)

→ Latent features correspond to parts of faces

Interpreting NMF Results

Face Identification

Basis images from NMF on faces http://www.cs.ucsb.edu/~mturk/pubs/IJPRAI05.pdf



NMF Summary

- NMF decomposes feature matrix X (n x m) into W and H
- W is (n x k) - represents strength of each latent feature for each observation
- H is (k x m) - represents strength of each observed feature for each latent feature
- k is the number of latent features
- W and H are learned via alternating least squares

Extensions

- Regularization
  - Can add lasso or ridge term to ALS
- Choosing k
  - See “Rank Selection in Low-rank Matrix Approximations: A Study of Cross-Validation for NMFs” https://www.cs.umd.edu/~bhargav/nips2010.pdf
- Other cost functions
- Other optimization methods
  - Multiplicative update rule