Algorithms for Non-negative Matrix Factorization

content

Introduction

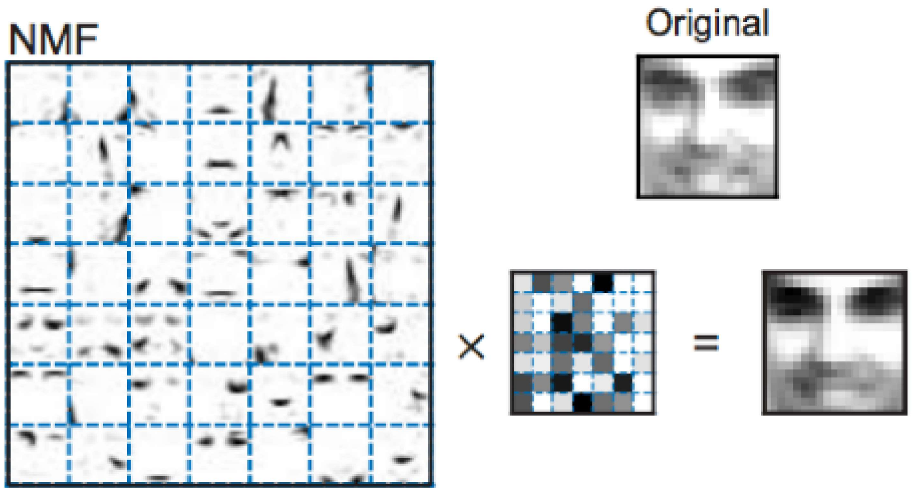
Daniel D. Lee Bell Laboratories Lucent Technologies.

H. Sebastian Seung Dept.of Brain and Cog. Sci. Massachusetts Institute of Technology Cambridge

Introduction

Non-negative matrix factorization (NMF)

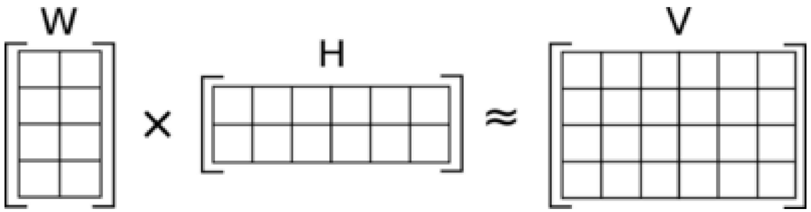
- Nonnegativity is useful constraint for matrix factorization that can learn a parts representation of the data.
- Sparse combinations to generate expressiveness in the reconstructions



Non-negative matrix factorization

Non-negative matrix factorization (NMF): Given a non-negative matrix V, find non-negative matrix factors W and H such that:

$$V \approx WH$$



- V is an $n \times m$ matrix: m examples, n features.
- $W_{n \times r}$, $H_{r \times m}$, where $r < m, r < n$. **Compressed** !
- $v_{*j} \approx W h_{*j}$, v is approximated by a linear combination of the columns of W, weighted by the components of h.

How to find: NP-hard. Alternating iterative method.

Two algorithms will be discussed.

Cost functions

1. Euclidean distance

$$\|A - B\|^2 = \Sigma_{ij}(A_{ij} - B_{ij})^2$$

lower bounded by zero, vanishes if $A = B$

2. Divergence

$$D(A\|B) = \Sigma_{ij}(A_{ij} \log \frac{A_{ij}}{B_{ij}} - A_{ij} + B_{ij})$$

- lower bounded by zero.
- not symmetric, not distance.
- reduces to the Kullback-Leibler divergence when $\Sigma_{ij}A_{ij} = \Sigma_{ij}B_{ij} = 1$

Kullback-Leibler divergence(relative entropy)

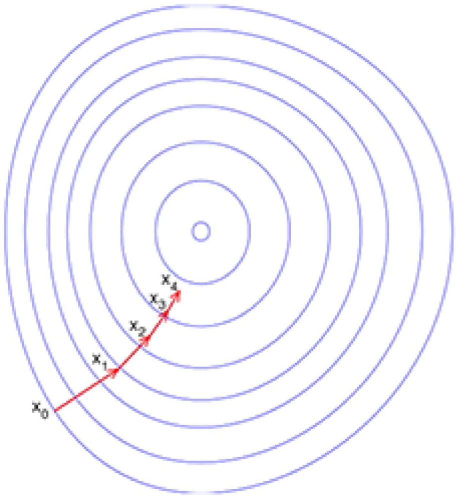
$$D(p\|q) = \Sigma_{i=1}^{n} p(x) \log \frac{p(x)}{q(x)}$$

Cost functions

Problem1 Minimize $||V - WH||^2$ with respect to W and H, subject to the constraints $W, H \geq 0$.

Problem2 Minimize $D(A||B)$ with respect to W and H, subject to the constraints $W, H \geq 0$.

Gradient descent



Multiplicative update rules

Theorem 1 The Euclidean distance $\|V - WH\|$ is nonincreasing under the update rules

$$H_{a\mu} \leftarrow H_{a\mu} \frac{(W^T V_{a\mu})}{(W^T W H)_{a\mu}} \quad W_{ia} \leftarrow W_{ia} \frac{(V H^T)_{ia}}{(W H H^T)_{ia}}$$

invariant if and only if W and H are at a stationary point of the distance.

Theorem 2 The divergence $D(A\|B)$ is nonincreasing under the update rules

$$H_{au} \leftarrow \frac{\Sigma_i W_{ia} V_{i\mu}/(WH)_{i\mu}}{\Sigma_k W_{ka}} \quad W_{ia} \leftarrow W_{ia} \frac{\Sigma_\mu H_{a\mu} V_{i\mu}/(WH)_{i\mu}}{\Sigma_v H_{av}}$$

invariant if and only if W and H are at a stationary point of the distance.

multiplicative factor is unity when $V = WH$, so that perfect reconstruction is necessarily a fixed point of the update rules.

Multiplicative versus additive update rules

Gradient descent

1. Euclidean distance

$$H_{a\mu} \leftarrow +\eta_{a\mu}[(W^TV)_{a\mu} - (W^TWH)_{a\mu}] \text{ set: } \eta_{a\mu} = \frac{H_{a\mu}}{(W^TWH)_{a\mu}}$$

$$\Downarrow$$

$$H_{a\mu} \leftarrow H_{a\mu}\frac{(W^TV_{a\mu})}{(W^TWH)_{a\mu}}(\text{in Theory 1})$$

2.Divergence

$$H_{a\mu} \leftarrow +\eta_{a\mu}[\Sigma_i W_{ia}\frac{V_{i\mu}}{(WH)_{i\mu} - \Sigma_i W_{ia}}] \text{ set: } \eta_{a\mu} = \frac{H_{a\mu}}{\Sigma_i W_{ia}}$$

$$\Downarrow$$

$$H_{au} \leftarrow \frac{\Sigma_i W_{ia}V_{i\mu}/(WH)_{i\mu}}{\Sigma_k W_{ka}}(\text{in Theory 2})$$

Proofs of convergence

Definition 1 $G(h, h')$ is an auxiliary function for $F(h)$ if the conditions

$$G(h, h') \geq F(h), G(h, h) = F(h)$$

are satisfied.

Lemma 1 If G is an auxiliary function, then F is nonincreasing under the update $h^{t+1} = arg\min_h G(h, h^t)$

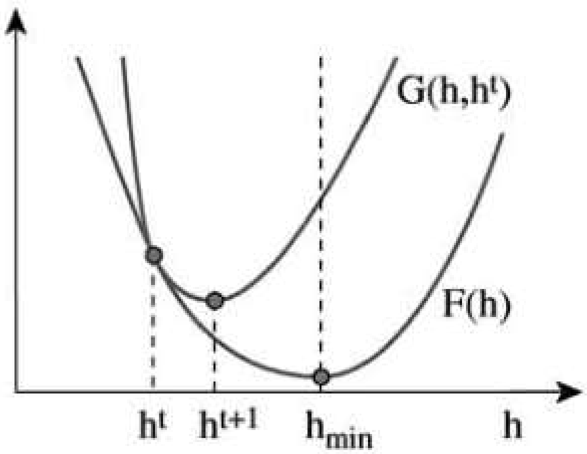


Figure 1: Minimizing the auxiliary function $G(h, h^t) \geq F(h)$ guarantees that $F(h^{t+1}) \leq F(ht)$ for $h^{n+1} = arg\min_h G(h, h^t)$.

Proofs of convergence

Lemma 2 If $K(h^t)$ is the diagonal matrix

$$K_{ab}(h^t) = \delta_{ab}(W^T W h^t)_a / h_a^t$$

then

$$G(h, h^t) = F(h^t) + (h - h^t)^T \nabla F(h^t) + \frac{1}{2}(h - h^t)^T K(h^t)(h - h^t)$$

is an auxiliary function for

$$F(h) = \frac{1}{2}\Sigma_i (v_i - \Sigma_a W_{ia} h_a)^2$$

Proof of Theorem 1

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

$$h_a^{t+1} = h_a^t \frac{(W^T v)_a}{(W^T W h^t)_a}$$

reversing the roles of W and H, F can similarly be shown to be nonincreasing under the update rules for W.

Proofs of convergence

Lemma 3 Define

$$\begin{aligned} G(h, h^t) = \quad & \Sigma_i (v_i \log v_i - v_i) + \Sigma_{ia} W_{ia} h_a \\ & -\Sigma_{ia} v_i \tfrac{W_{ia} h_a^t}{\Sigma_b W_{ib} h_b^t} (\log W_{ia} h_a - \log \tfrac{W_{ia} h_a^t}{\Sigma_b W_{ib} h_b^t}) \end{aligned}$$

this is an auxiliary function for

$$F(h) = \Sigma_i v_i \log(\frac{v_i}{\Sigma_a W_{ia} h_a}) - v_i + \Sigma_a W_{ia} h_a$$

Proof of Theorem 2 The minimum of $G(h, h^t)$ with respect to h is determined by setting the gradient to zero:

$$\frac{dG(h, h^t)}{dh_a} = -\Sigma_i v_i \frac{W_{ia} h_a^t}{\Sigma_b W_{ib} h_b^t} \frac{1}{h_a} + \Sigma_i W_{ia} = 0$$

update rule:

$$h_a^{t+1} = \frac{h_a^t}{\Sigma_b W_{kb}} \Sigma_i \frac{v_i}{\Sigma_b W_{ib} h_b^t} W_{ia}$$

Rewriten in matrix form, it is equivalent to the update rule.

Discussion

- The update rules guaranteed to find **at least locally optimal solutions** of Problems 1 and 2.
- The convergence proofs rely upon **defining an appropriate auxiliary function**, more generalize?
- Easy to implement computationally, utilized by other applications?

Thank you!