

NON-NEGATIVE SPARSE CODING

by P. O. Hoyer, 2002

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Outline

- Non-negative sparse coding
- Estimating the hidden components
- Learning the basis
- Experiments
- Proof of monotonic convergence

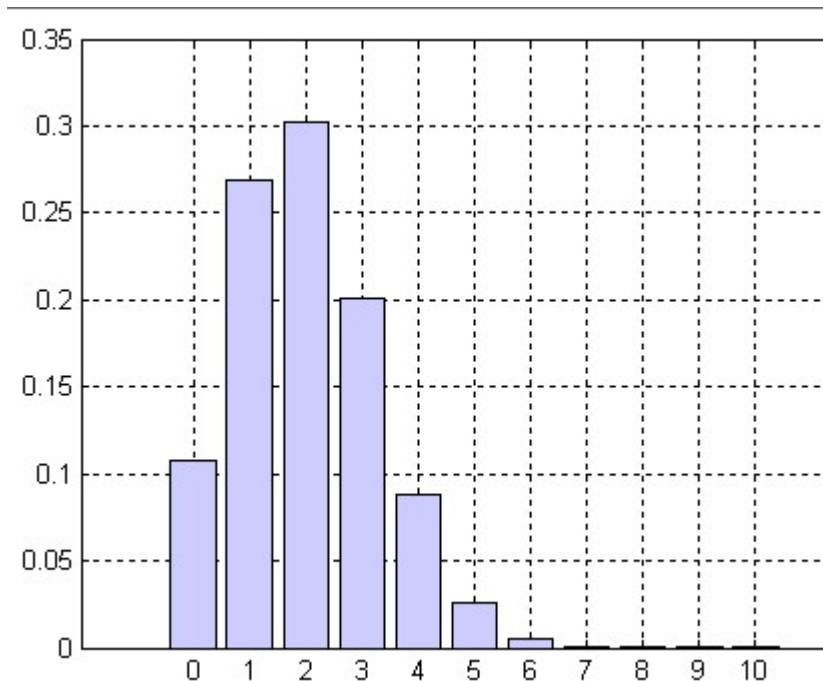
NMF

$$X \approx AS (X \in \mathbb{R}^{n \times m}) \Rightarrow \mathbf{x}_i \approx [\mathbf{a}_1, \mathbf{a}_2 \dots \mathbf{a}_r] \begin{bmatrix} s_{i1} \\ s_{i2} \\ \cdot \\ \cdot \\ \cdot \\ s_{ir} \end{bmatrix}$$

- Linear Decomposition
 1. columns of A contain the basis vector
 2. rows of S contain the corresponding hidden component

Linear Sparse Coding

- Goal-Representing any given input vector using only a few significantly non-zero hidden coefficients.



Non-negative Sparse Coding

- Both NMF and sparseness are important for learning parts-based representations.
- Combining the goal of small reconstruction error of NMF with that of sparseness.

$$\begin{cases} \min_{\mathbf{A}, \mathbf{S}} C(\mathbf{A}, \mathbf{S}) = \frac{1}{2} \|\mathbf{X} - \mathbf{AS}\|^2 + \lambda \sum_{ij} f(s_{ij}) \\ \mathbf{A} \geq 0, \mathbf{S} \geq 0, \forall i: \|\mathbf{a}_i\| = 1, \lambda \geq 0 \end{cases}$$

Estimating the hidden components

- For a given basis A , the objective is convex with respect to S , so the global minimum exists.

- Update rule for S :

$$\mathbf{S}^{t+1} = \mathbf{S}^t \cdot * \left(\mathbf{A}^T \mathbf{X} \right) ./ \left(\mathbf{A}^T \mathbf{A} \mathbf{S} + \lambda \right)$$

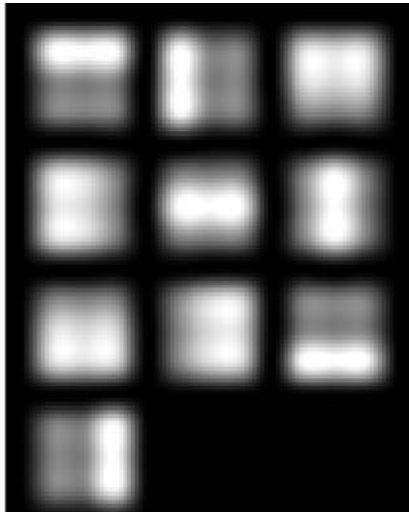
the proof of monotonous convergence is similar to that of NMF

Learning the basis

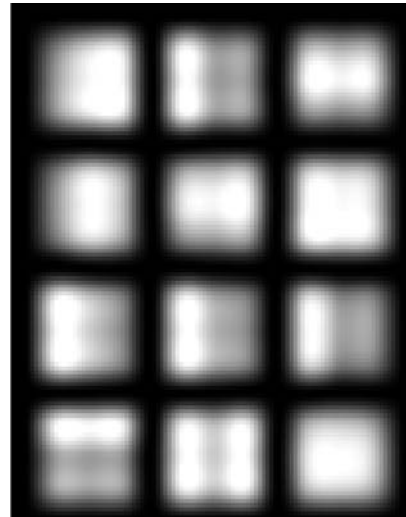
- Consider the optimization of A , holding S fixed
- Updating steps of A :
 - 1. $A^{t+1} = A^t + \mu(X - A^t S) S^T$
 - 2. Set all the negative values in A^{t+1} to zero.
 - 3. Rescale each column of A^{t+1} to unit norm.

Experiments-learning basis

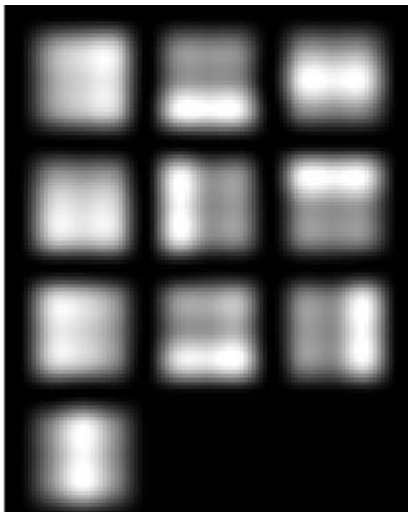
Features



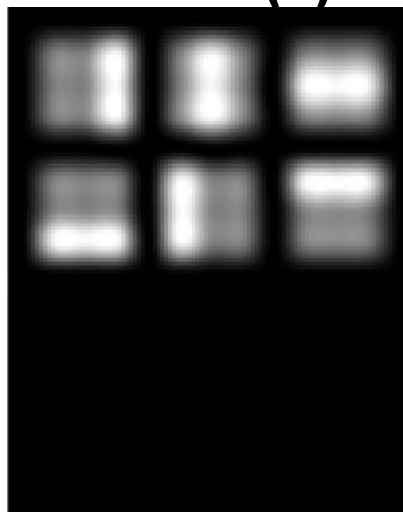
Samples



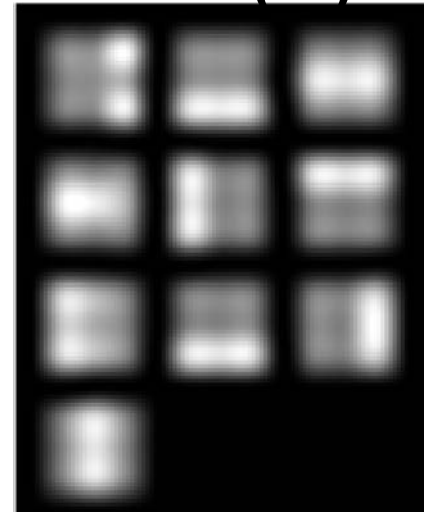
NNSC



NMF(6)



NMF(10)

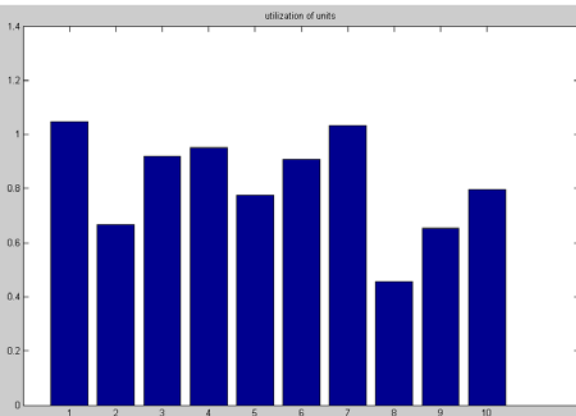
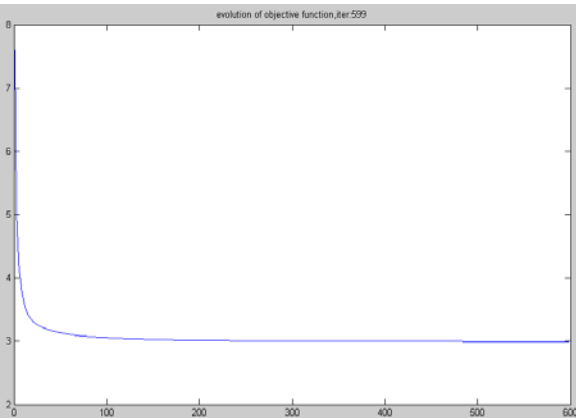


Experiments

convergence and hidden components

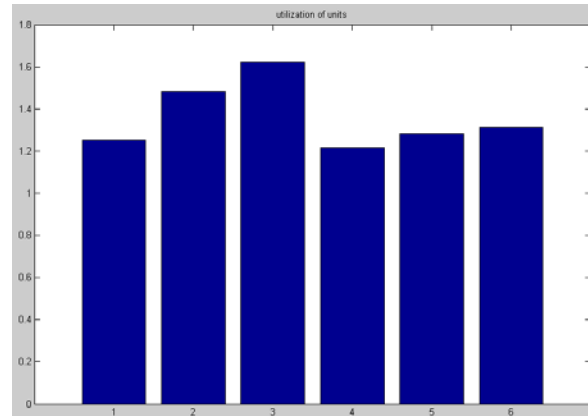
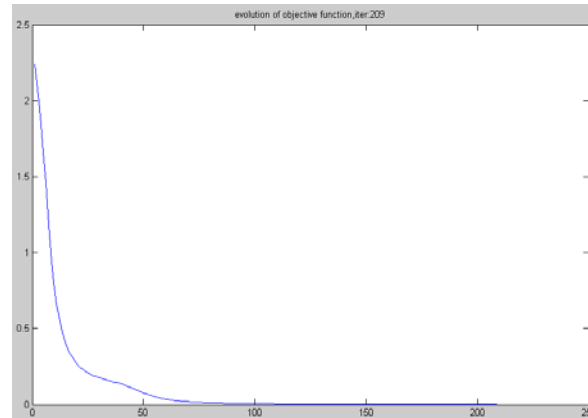
NNSC

[583]:2.94223/4.11878



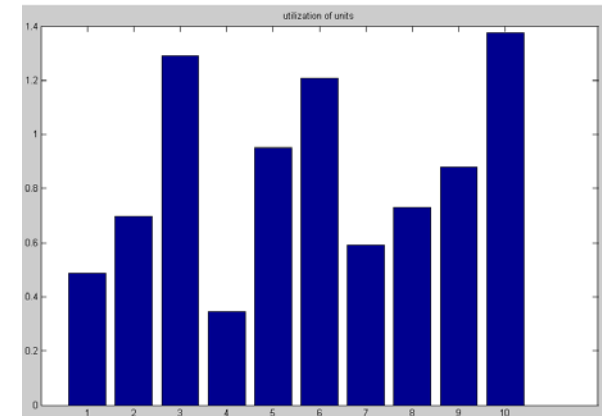
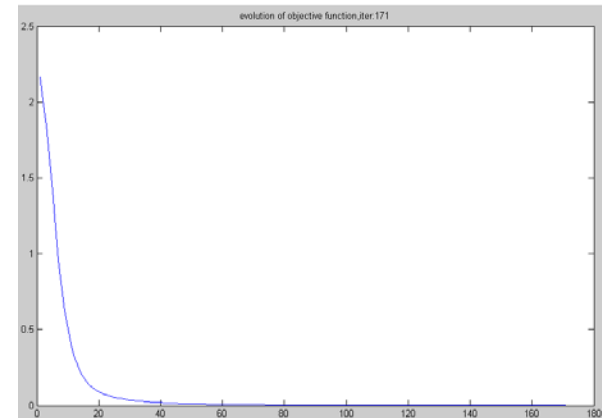
NMF(6)

[209]: 0.00129 / 0.00000



NMF(10)

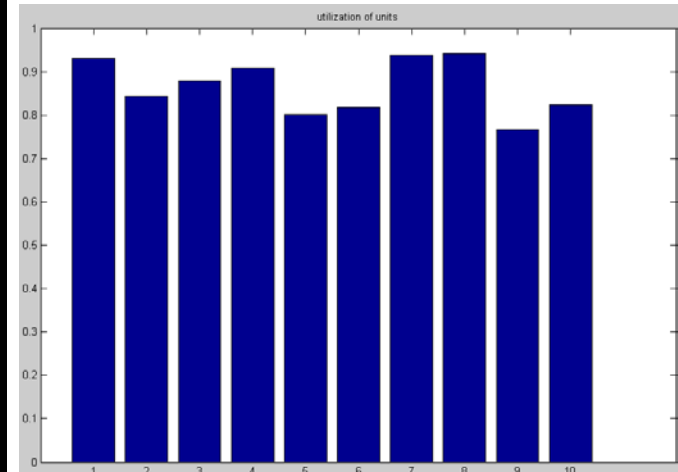
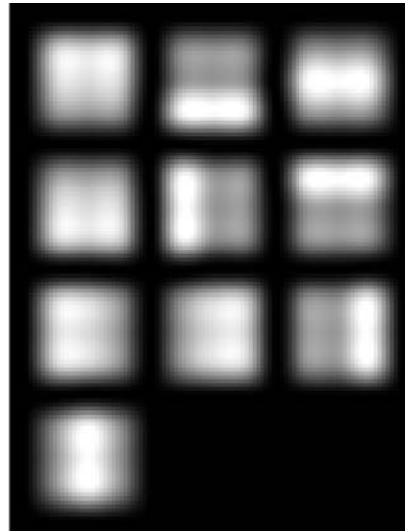
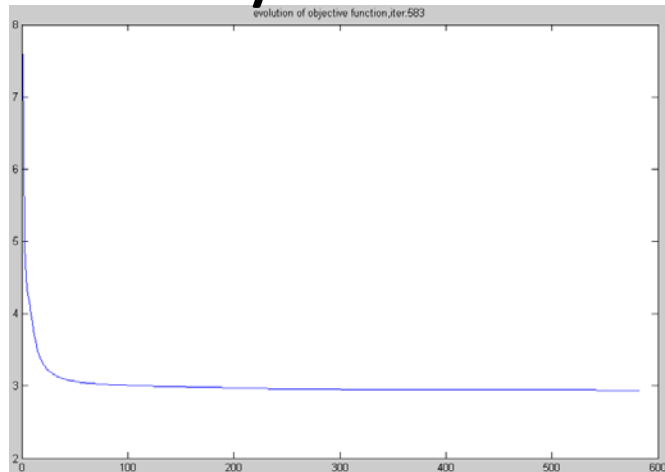
[171]: 0.00097 / 0.00000



Experiments-Change NNSC a little

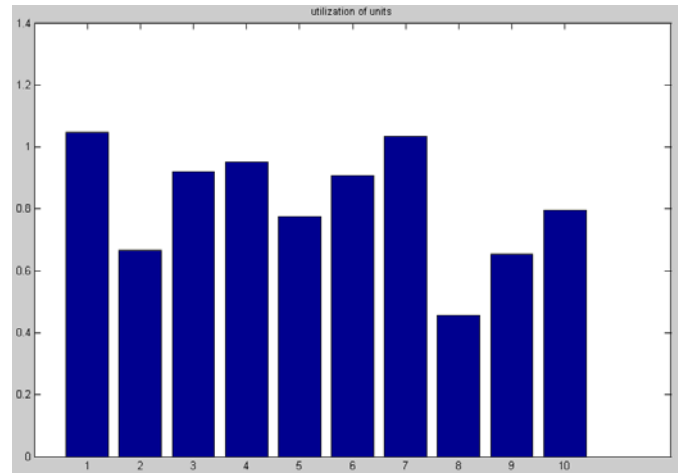
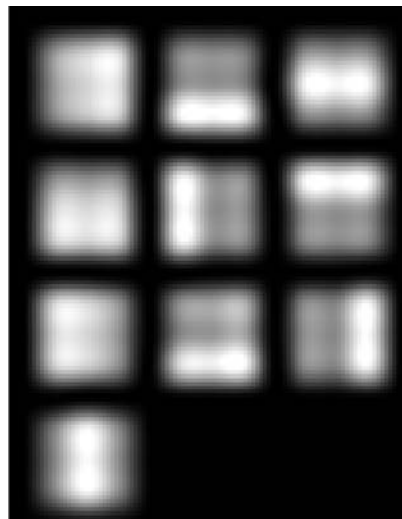
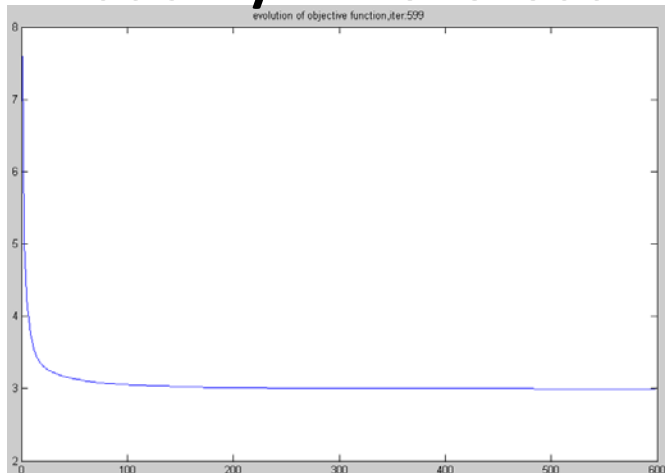
NNSC

2.94223/4.11878 583



Changed NNSC

2.99647/4.11878 599



Three problems remained of NMF

- How to get the step size(numerator and denominator)?
- How to handle the concave case?
- How to construct auxiliary function?

Proof of monotonic convergence(1)

- Objective function:

$$F(\mathbf{h}) = \frac{1}{2} \sum_i \left(\mathbf{v}_i - \sum_a \mathbf{W}_{ia} \mathbf{h}_a \right)^2 = \frac{1}{2} \|\mathbf{v} - \mathbf{W}\mathbf{h}\|^2 = \frac{1}{2} \text{Tr} \left[(\mathbf{v} - \mathbf{W}\mathbf{h})(\mathbf{v} - \mathbf{W}\mathbf{h})^T \right]$$

- Auxiliary function:

$$G(\mathbf{h}, \mathbf{h}^t): \begin{cases} G(\mathbf{h}, \mathbf{h}^t) \geq F(\mathbf{h}) \\ G(\mathbf{h}, \mathbf{h}) = F(\mathbf{h}) \end{cases}$$

$$\mathbf{h}^{t+1} = \arg \min_{\mathbf{h}} G(\mathbf{h}, \mathbf{h}^t)$$

- $F(\mathbf{h})$ is convergent: $F(\mathbf{h}^{t+1}) \leq G(\mathbf{h}^{t+1}, \mathbf{h}^t) \leq G(\mathbf{h}^t, \mathbf{h}^t) = F(\mathbf{h}^t)$
- Does the auxiliary function exists?

Proof of monotonic convergence(2)

- Constructing the auxiliary function for $F(\mathbf{h})$

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

$$\mathbf{K}_{ab}(\mathbf{h}^t) = \delta_{ab} \frac{(\mathbf{W}^T \mathbf{W} \mathbf{h})_a}{h_a^t} = \begin{pmatrix} \frac{(\mathbf{W}^T \mathbf{W} \mathbf{h})_1}{h_1^t} & & 0 \\ & \ddots & \\ 0 & & \frac{(\mathbf{W}^T \mathbf{W} \mathbf{h})_r}{h_r^t} \end{pmatrix}$$

$$\frac{\partial F(\mathbf{h})}{\partial \mathbf{h}} = \mathbf{W}^T \mathbf{W} \mathbf{h}, \quad \frac{\partial^2 F(\mathbf{h})}{\partial \mathbf{h}^2} = \mathbf{W} \mathbf{W}^T$$

- Second-order Taylor expansion of $F(\mathbf{h})$ at \mathbf{h}^t

$$F(\mathbf{h}) = F(\mathbf{h}^t) + (\mathbf{h} - \mathbf{h}^t)^T \nabla F(\mathbf{h}^t) + \frac{1}{2} (\mathbf{h} - \mathbf{h}^t)^T \mathbf{W}^T \mathbf{W} (\mathbf{h} - \mathbf{h}^t)$$

Proof of monotonic convergence(3)

- Proving $G(\mathbf{h}, \mathbf{h}^t)$ is the auxiliary function of $F(\mathbf{h})$

1. $G(\mathbf{h}, \mathbf{h}) = F(\mathbf{h})$ is obvious.

2. $G(\mathbf{h}, \mathbf{h}^t) \geq F(\mathbf{h}) \Leftrightarrow (\mathbf{h} - \mathbf{h}^t)^T [K(\mathbf{h}^t) - \mathbf{W}^T \mathbf{W}] (\mathbf{h} - \mathbf{h}^t) \geq 0$

$$M_{ab}(\mathbf{h}^t) = \mathbf{h}_a^t [K(\mathbf{h}^t) - \mathbf{W}^T \mathbf{W}]_{ab} \mathbf{h}_b^t$$

$$\mathbf{v}^T M \mathbf{v} = \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t K(\mathbf{h}^t)_{ab} \mathbf{h}_b^t \mathbf{v}_b - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \sum_a \mathbf{v}_a \mathbf{h}_a^t K(\mathbf{h}^t)_{aa} \mathbf{h}_a^t \mathbf{v}_a - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \sum_a \mathbf{v}_a^2 (\mathbf{W}^T \mathbf{W} \mathbf{h}^t)_a \mathbf{h}_a^t - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \sum_a \mathbf{v}_a^2 \mathbf{h}_a^t \left(\sum_b (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \right) - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \sum_{ab} \mathbf{v}_a^2 \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \sum_{ab} \mathbf{v}_a^2 \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \frac{1}{2} \sum_{ab} \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t (\mathbf{v}_a^2 + \mathbf{v}_b^2) - \sum_{ab} \mathbf{v}_a \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t \mathbf{v}_b$$

$$= \frac{1}{2} \sum_{ab} \mathbf{h}_a^t (\mathbf{W}^T \mathbf{W})_{ab} \mathbf{h}_b^t (\mathbf{v}_a - \mathbf{v}_b)^2 \geq 0$$

$K(\mathbf{h}^t) - \mathbf{W}^T \mathbf{W}$ is semi-positive definite if and only if \mathbf{M} is semi-positive definite.

$$\mathbf{v}^T [K(\mathbf{h}^t) - \mathbf{W}^T \mathbf{W}] \mathbf{v} = \frac{1}{2} \sum_{ab} (\mathbf{W}^T \mathbf{W})_{ab} (\mathbf{v}_a - \mathbf{v}_b)^2 \geq 0$$

The update rule of \mathbf{h}

$$\mathbf{h}^{t+1} = \arg \min_{\mathbf{h}} G(\mathbf{h}, \mathbf{h}^t)$$

$$\frac{\partial G(\mathbf{h}, \mathbf{h}^t)}{\partial \mathbf{h}} = \nabla F(\mathbf{h}^t) + K(\mathbf{h}^t)(\mathbf{h} - \mathbf{h}^t) = 0$$

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

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

Handle the concave case

- Solution one:

$$G(\mathbf{h}, \mathbf{h}^t): \begin{cases} G(\mathbf{h}, \mathbf{h}^t) \leq F(\mathbf{h}) \\ G(\mathbf{h}, \mathbf{h}) = F(\mathbf{h}) \end{cases}$$

$$\mathbf{h}^{t+1} = \arg \max_{\mathbf{h}} G(\mathbf{h}, \mathbf{h}^t)$$

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

- Solution two:
 - Converting the objective function to convex by multiple it by a negative number.