

Larson Hogstrom  
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$$H_{aj} \leftarrow H_{aj} \frac{(W^T A)_{aj}}{(W^T W H)_{aj}} \quad W_{ia} \leftarrow W_{ia} \frac{(W^T A)_{ia}}{(W^T W H)_{ia}} \quad (1)$$

## Outline

- Introduction + definition
- cost functions: Euclidian distance, Frobenius norm, KL divergence, Renyi's divergence. Can you construct a situation in which certain norms are better than others?
- update rules: multiplicative update, ALS method, gradient methods
- computational comparison: flop counts, accuracy, size of inputs
- applications to calculating metagenes

## Introduction

This report introduces the framework for parts-based representations using NMF and focuses on the algorithms and numerical aspects of computation.

**definition** For a nonnegative matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$ , select a low-rank approximation of size  $k$  such that there are two nonnegative matrices  $\mathbf{W} \in \mathbb{R}^{m \times k}$  and  $\mathbf{H} \in \mathbb{R}^{k \times n}$  which minimizes a function such as

$$f(\mathbf{W}, \mathbf{H}) = \frac{1}{2} \|\mathbf{A} - \mathbf{WH}\|_F^2$$

Other commonly used objective functions include Euclidian distance and Kullback-Leibler (KL) divergence. KL can be extended to a more general information-based framework using Renyi's divergence. (Devarajan, 2005). Here, a single parameter  $\alpha$  is used to represent a continuum of distance measures and KL arises as a special case as  $\alpha \rightarrow 1$ .

$$KL(V||WH) = \sum_{ij} [V_{ij} \log \frac{V_{ij}}{(WH)_{ij}} - V_{ij} + (WH)_{ij}]$$

more text

## Fundamental Algorithms

One of the first and most widely adopted algorithms for NMF is the multiplicative update rule. This takes the general form:

**Data:** Input data matrix:  $\mathbf{A} \in \mathbb{R}^{m \times n}$

**Result:** nonnegative factorization of  $\mathbf{A}$  using  $k$  components, creating matrices  $\mathbf{W} \in \mathbb{R}^{m \times k}$  and  $\mathbf{H} \in \mathbb{R}^{k \times n}$

initialization;

$\mathbf{W} \leftarrow$  random dense ( $m \times k$ ) matrix

$\mathbf{H} \leftarrow$  random dense ( $k \times n$ ) matrix

**for**  $i = 1$  to *maxiter* **do**

$\mathbf{H} = \mathbf{H} \cdot (\mathbf{W}^T \mathbf{A}) ./ (\mathbf{W}^T \mathbf{W} \mathbf{H})$

$\mathbf{W} = \mathbf{W} \cdot (\mathbf{A} \mathbf{H}^T) ./ (\mathbf{W} \mathbf{H} \mathbf{H}^T)$

**end**

**Algorithm 1:** multiplicative update

Often the  
requires  $O(mnk)$  work per iteration

Figure 1: A picture of a gull.

