When Does Non-Negative Matrix Factorization Give a Correct Decomposition into Parts?

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Letters to Nature

Juvenile collected and only in the field (2°48.12′ N, 1°40.53′ E) by SCUBA. Between 5 and 16 juveniles were recruited successfully in each of 15, 11 polycarbonate containers (n=25), the bottom of which was covered with an acetate sheet that served as sand for sponge attachment. Containers were then randomly distributed in 3 groups, and sponges in each group were cultured for 14 weeks in 5 different concentrations of {\(\text{SiO}_2\)}: 0.741 ± 0.133, 32.36 ± 0.007 and 100.041 ± 0.860 μM (mean ± s.e.). All cultures were prepared using a 55 μm polycarbonate film, which was collected from the sponge habitat, handled according to standard methods to prevent Si contamination and enriched in dissolved silica, when treatments required, by using Na2SiF6. During the experiment, all sponges were fed weekly addition of 1% of a bacterial culture (50-60 × 10^8 bacteria/ml) to each container. The seawater was replaced weekly, with regeneration of initial food and SiO2 levels. The concentration of SiO2 in culture water was determined on 3 replicate of 1 ml seawater samples per container by using a Bran-Luebbe TRAAKS 200 nutrient automatics. After week 5, the accidental contamination of some culture containers by dinoflagellate subsequent estimates of Si uptake by sponges unreliable, so we discarded them for the study.

For the study of the skeletons, sponges were treated according to standard methods and examined in a Hitachi S-2000 scanning electron microscope (SEM).

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Learning the parts of objects by non-negative matrix factorization

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Is perception of the whole based on perception of its parts? There is psychological and physiological evidence for parts-based representations in the brain, and certain computational theories of object recognition rely on such representations. But little is known about how brains or computers might learn the parts of objects. Here we demonstrate an algorithm for non-negative matrix factorization that is able to learn parts of faces and semantic features of text. This is in contrast to other methods, such as principal components analysis and vector quantization, that learn holistic, not parts-based, representations. Non-negative matrix factorization is distinguished from the other methods by its use of non-negativity constraints. These constraints lead to a
Claim

Their Paper:
• Vague relation between NMF and “Decomposing into Parts.”
• NMF a vague idea.

Our talk:
• Gives a theoretical framework that validates NMF in specific settings.
• Identifies under what conditions NMF works.
The Problem:

\[ X = A \Psi \]

- \( X \) is \( n \times p \)
- \( A \) is \( n \times r \)
- \( \Psi \) is \( r \times p \)
- \( A \geq 0, \Psi \geq 0 \)
Does this make sense?

- When is the factorization *unique*?
- When does NMF find the *correct* decomposition?

- Plumbley (2001) proposed an ICA model that solves the NMF problem, where $n >> p = r$, the $A_{ij}$ are *independent* random variables, and the basis functions are non-negative and linearly independent.
- Parts-articulation models behind the Lee & Seung proposal do not have independent components.
Geometric Reinterpretation

An image in $p$-dimensional space

Positive Orthant
Geometric Reinterpretation

Convex Hull
Geometric Interpretation of NMF

Extreme Rays

Simplicial Cone
Not Unique!
Not Unique!

Positive Orthant is a Simplicial Cone
Example of Uniqueness I

Positive Orthant is a Simplicial Cone
Example of Uniqueness II

\[ C = \{ x : x'1 \geq \sqrt{p-1} \| x \| \} \]

Cone tangent to the planes of the positive orthant.
Convex Duality

- Notion of primal space and dual space.
- Points in one space map to hyperplanes in the other.
- Convex cones map to convex cones.
- Inclusions reverse under duality.
Reinterpretation using Duality

Primal Space

Dual Space

P

C

C*

P*
Theorem

Given a Separable Factorial Articulation Database, there is a unique simplicial hull with $r=AP$ generators which contains all the data points and is contained in the intersection of the positive orthant and the linear span of the generators.

This unique NMF solution is visibly a correct decomposition into parts.
Separable Factorial Articulation Families

Definition:

• A structured family of images, $X_i$, where $P$ is the number of parts and $A$ is the number of articulations.
• Each image, $X_i$, equals a superposition of every part in only one of its articulations.
• Existence of tell-tale pixel for each part/articulation.
• Every possible combination of every part and every articulation occurs.

Consequence: each part can only appear in one articulation at a time, implying negative dependence.
Example: Swimmer
NMF Parts Recovery
Conclusions

- The geometric viewpoint explains the non-well-posedness of NMF in general, and the well-posedness in a specific setting.
- NMF makes sense, in theory, for Separable Factorial Articulation Families.
- The theory correctly predicts the success of non-negative matrix factorization.