Theoretical Connection between Locally Linear Embedding, Factor Analysis, and Probabilistic PCA

Benyamin Ghojogh*, Ali Ghodsi**, Fakhri Karray*, **Mark Crowley***

* Department of Electrical & Computer Engineering
** Department of Statistics and Actuarial Science
University of Waterloo, ON, Canada

June 1, 2022

Twitter: `@compthink`
PubPub (**7eqtuyyc**): `caiac.pubpub.org/pub/7eqtuyyc`

What is Dimensionality Reduction?

- Big Idea: extracting informative low-dimensional features from high-dimensional data.
- Also known as: Manifold Learning, Feature Extraction, Finding a "projection" to a simpler space
- **Useful for:** Data Preprocessing and Reduction, Visualizaton, Improved Performance on high-dimensional data, ML on Embedded Systems, ..., many more.

Dimensonality Reduction methods can be *divided into three broad categories*:

1. Spectral methods:
   - Examples: PCA and LLE
2. Probabilistic methods:
   - Examples: Probabilistic PCA, Factor Analysis
3. Neural network-based methods:
   - Examples: Restricted Boltzmann Machine, Variational Autoencoder

Building a Bridge

In this work we build a bridge between the *spectral* and *probabilistic* approaches to Dimensionality Reduction.
In particular, we look at these three methods:

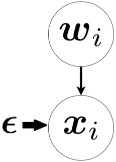
1. Factor Analysis
2. Probabilistic PCA
3. LLE

We show:

- how these methods are all tightly related,
- and how this relationship explains their different properties.

Factor Analysis

Factor analysis [1, 2] assumes that every data point $\boldsymbol{x}_i$ is generated from a latent factor $\boldsymbol{w}_i$ [3].



$$\boldsymbol{x}_i := \boldsymbol{\Lambda}\boldsymbol{w}_i + \boldsymbol{\mu} + \boldsymbol{\epsilon}, \tag{1}$$

$$\mathbb{P}(\boldsymbol{x}_i \,|\, \boldsymbol{w}_i, \boldsymbol{\Lambda}, \boldsymbol{\mu}, \boldsymbol{\Psi}) = \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\Lambda}\boldsymbol{w}_i + \boldsymbol{\mu}, \boldsymbol{\Psi}). \tag{2}$$

Probabilistic PCA

Probabilistic PCA [4, 5] is a special case of factor analysis where the variance of noise is equal in all dimensions of data space with covariance between dimensions, i.e. [3]:

$$\boldsymbol{\Psi} = \sigma^2 \boldsymbol{I}. \tag{3}$$

Therefore:

$$\boldsymbol{x}_i := \boldsymbol{\Lambda} \boldsymbol{w}_i + \boldsymbol{\mu} + \boldsymbol{\epsilon}, \tag{4}$$
$$\mathbb{P}(\boldsymbol{\epsilon}) = \mathcal{N}(\boldsymbol{0}, \sigma^2 \boldsymbol{I}), \tag{5}$$
$$\mathbb{P}(\boldsymbol{x}_i \,|\, \boldsymbol{w}_i, \boldsymbol{\Lambda}, \boldsymbol{\mu}, \sigma^2 \boldsymbol{I}) = \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\Lambda} \boldsymbol{w}_i + \boldsymbol{\mu}, \sigma^2 \boldsymbol{I}). \tag{6}$$

Locally Linear Embedding (LLE)

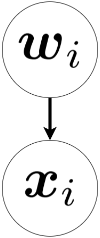
LLE [6, 7] has two main steps [8]:

- linear reconstruction
- linear embedding

Linear reconstruction of LLE can be seen stochastically where every point $\boldsymbol{x}_i$ is conditioned on and generated by its reconstruction weights $\boldsymbol{w}_i$ as a latent factor:

$$\boldsymbol{x}_i = \boldsymbol{X}_i \boldsymbol{w}_i + \boldsymbol{\mu}, \quad (7)$$

$$\mathbb{P}(\boldsymbol{w}_i) = \mathcal{N}(\boldsymbol{w}_i; \mathbf{0}, \boldsymbol{\Omega}_i). \quad (8)$$



The covariance $\boldsymbol{\Omega}_i$ can be learned by Expectation Maximization (EM).

- If $\boldsymbol{\Omega}_i = \sigma_i \boldsymbol{I}$ is assumed (like in Probabilistic PCA), we'll have close-form solution (as in the Probabilistic PCA).
- See our paper at the conference for more details.

Connection of LLE, Factor Analysis, and Probabilistic PCA

- Comparing Eqs. (1) and (7):

$$\boldsymbol{x}_i := \boldsymbol{\Lambda} \boldsymbol{w}_i + \boldsymbol{\mu} + \boldsymbol{\epsilon}, \quad \text{(factor analysis, probabilistic PCA)}$$
$$\boldsymbol{x}_i = \boldsymbol{X}_i \boldsymbol{w}_i + \boldsymbol{\mu}, \quad \text{(LLE)}$$

  shows that data point $\boldsymbol{x}_i$ is conditioned on some latent variable $\boldsymbol{w}_i$ (using a transformation matrix), in all methods of factor analysis, probabilistic PCA, and LLE.
- In factor analysis and probabilistic PCA: $\boldsymbol{x}_i := \boldsymbol{\Lambda} \boldsymbol{w}_i + \boldsymbol{\mu} + \boldsymbol{\epsilon}$.
  - Global matrix $\boldsymbol{\Lambda}$
  - So it is data-independent (it is the same matrix for all data points).
- In LLE: $\boldsymbol{x}_i = \boldsymbol{X}_i \boldsymbol{w}_i + \boldsymbol{\mu}$.
  - local matrix $\boldsymbol{X}_i$
  - So it is data-dependent (it is different for every data point).
- This explains why factor analysis and probabilistic PCA are linear methods and LLE is a nonlinear algorithm.

Thank You

- "Theoretical Connection between Locally Linear Embedding, Factor Analysis, and Probabilistic PCA"
- Benyamin Ghojogh, Ali Ghodsi, Fakhri Karray, **Mark Crowley**
- PubPub (**7eqtuyyc**): `caiac.pubpub.org/pub/7eqtuyyc`

Acknowledgements

- Research funded in part by:
  - NSERC - Discovery Grant Program, CRD Grants on Digital Pathology
  - NRC - Collaboration Centre Programs

References

[1] B. Fruchter, *Introduction to factor analysis.*
Van Nostrand, 1954.

[2] D. Child, *The essentials of factor analysis.*
Cassell Educational, 1990.

[3] B. Ghojogh, A. Ghodsi, F. Karray, and M. Crowley, "Factor analysis, probabilistic principal component analysis, variational inference, and variational autoencoder: Tutorial and survey," *arXiv preprint arXiv:2101.00734*, 2021.

[4] S. Roweis, "EM algorithms for PCA and SPCA," *Advances in neural information processing systems*, vol. 10, pp. 626–632, 1997.

[5] M. E. Tipping and C. M. Bishop, "Probabilistic principal component analysis," *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, vol. 61, no. 3, pp. 611–622, 1999.

[6] S. T. Roweis and L. K. Saul, "Nonlinear dimensionality reduction by locally linear embedding," *Science*, vol. 290, no. 5500, pp. 2323–2326, 2000.

[7] L. K. Saul and S. T. Roweis, "Think globally, fit locally: unsupervised learning of low dimensional manifolds," *Journal of machine learning research*, vol. 4, no. Jun, pp. 119–155, 2003.

[8] B. Ghojogh, A. Ghodsi, F. Karray, and M. Crowley, "Locally linear embedding and its variants: Tutorial and survey," *arXiv preprint arXiv:2011.10925*, 2020.