Supporting information for Data driven estimation of imputation error -A strategy for imputation with a reject option

S1 Appendix

Imputation with Probabilistic PCA

We focus on latent variable models for dimensional reduction; in case so-called "probabilistic principal component analysis" (for a general discussion and references to original work see [\[2\]](#page-1-0)). Under the probabilistic PCA model data are generated by the process

$$
\bar{x} = \bar{A}\bar{z} + \bar{\epsilon} \tag{1}
$$

where the latent variables (principal components) are multivariate normal with unit covariance matrix $\bar{z} \sim \mathcal{N}(\bar{0}, I)$, and the additive noise is normal with variance σ^2 , hence, $\bar{\epsilon} \sim \mathcal{N}(\bar{0}, \sigma^2 I)$. The observations are multivariate normal with covariance matrix

$$
\bar{\bar{\Sigma}} = \bar{\bar{A}} \bar{\bar{A}}^T + \sigma^2 I. \tag{2}
$$

Using

$$
p\left(\bar{x},\bar{z}|\bar{A},\sigma_0^2\right) = p\left(\bar{x}|\bar{z}\right)p\left(\bar{z}\right) \propto e^{-\frac{1}{2\sigma^2}||\bar{A}\bar{z}-\bar{x}||^2}e^{-\frac{1}{2}\bar{z}^2},\tag{3}
$$

we get the distribution of the principal components conditioned on observations

$$
\log p(\bar{z}|\bar{x}) = -\frac{1}{2\sigma^2} ||\bar{A}\bar{z} - \bar{x}||^2 - \frac{1}{2}\bar{z}^2 + \text{const.},\tag{4}
$$

$$
= -\frac{1}{2\sigma^2} \bar{z}^T \bar{A} \bar{A}^T \bar{z} + \frac{1}{\sigma^2} \bar{x}^T \bar{A} \bar{z} - \frac{1}{2} \bar{z}^2 + \text{const.} \tag{5}
$$

Hence, the conditional distribution of the principal components is the normal distribution $\mathcal{N}\left(\bar{\mu}_{z|x}, \bar{\bar{\Sigma}}_{z|x}\right)$, with

$$
\bar{\mu}_{z|x} = \frac{1}{\sigma^2} \bar{\bar{\Sigma}}_{z|x} \bar{A}^T \bar{x},
$$

$$
\bar{\bar{\Sigma}}_{z|x}^{-1} = \frac{\bar{\bar{A}} \bar{A}^T}{\sigma^2} + I
$$
 (6)

Inference based on a sample of N complete data points $\bar{x} \in \mathbb{R}^d$ forming the data matrix

$$
\bar{\bar{X}} = [\bar{x}_1, \bar{x}_2, \dots, \bar{x}_N](centered)
$$
\n(7)

is based on the singular value decomposition,

$$
\bar{\bar{X}} = \bar{\bar{U}} \bar{\bar{S}} \bar{\bar{V}}^T. \tag{8}
$$

Let k be the selected subspace dimension, then the subspace of interest is spanned by the columns of the matrix $\overline{\overline{A}}$ estimated by

$$
\hat{\bar{A}} = \bar{\bar{U}}_{1:k}\bar{\bar{S}}_{1:k}.
$$
\n
$$
(9)
$$

The noise variance is estimated from the variance outside the subspace of interest

$$
\widehat{\sigma^2} = \frac{\text{Tr}\,(\bar{\bar{X}}\bar{\bar{X}}^T) - \text{Tr}\,(\bar{\bar{X}}_r \bar{\bar{X}}_r^T)}{N(d-k)}.
$$
\n(10)

where the subspace reconstruction of data is given by

$$
\bar{\bar{X}}_r = \bar{\bar{U}}_{1:k}\bar{\bar{U}}_{1:k}^T \cdot \bar{x}.\tag{11}
$$

Now consider inference based on missing data, i.e., the remaining features indexed by the set $m \bar{x} \longrightarrow \bar{x}_m$. The relevant distribution of principal components conditioned on the features present \bar{x}_m is given simply by $\mathcal{N}\left(\bar{\mu}_{z|\bar{x}_m}, \bar{\bar{\Sigma}}_{z|\bar{x}_m}\right)$, with

$$
\widehat{\bar{\bar{\Sigma}}}_{z|\bar{x}_m} = \frac{\hat{\bar{A}}_m \hat{\bar{A}}_m^T}{\hat{\sigma}^2} + I \tag{12}
$$

$$
\widehat{\bar{\mu}_{z|\bar{x}_{m}}} = \frac{1}{\widehat{\sigma^{2}}} \widehat{\bar{\Sigma}}_{\bar{z}|\bar{x}_{m}} \widehat{\bar{A}}_{m}^{T} \bar{x}_{m}
$$
\n(13)

where $\hat{\bar{A}}_m$ are the rows of subspace spanning vectors corresponding to the features present \bar{x}_m .

References

1. Bishop CM. Pattern Recognition and Machine Learning (Information Science and Statistics). Secaucus, NJ, USA: Springer-Verlag New York, Inc.; 2006.