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► **To cite this version:**

| Serge Iovleff. Probabilistic Auto-Associative Models and Semi-Linear PCA. 2012. hal-00734070v1

HAL Id: hal-00734070

<https://hal.science/hal-00734070v1>

Preprint submitted on 20 Sep 2012 (v1), last revised 10 Dec 2014 (v2)

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PROBABILISTIC AUTO-ASSOCIATIVE MODELS AND SEMI-LINEAR PCA

SERGE IOVLEFF

ABSTRACT. Auto-Associative models cover a large class of methods used in data analysis. In this paper, we describe the general properties of these models when the projection component is linear and we propose and test an easy to implement Probabilistic Semi-Linear Auto-Associative model in a Gaussian setting. We show it is a generalization of the PCA model to the semi-linear case. Numerical experiments on simulated datasets and a real astronomical application highlight the interest of this approach.

1. INTRODUCTION

Principal component analysis (PCA) [29, 20, 23] is a well established tool for dimension reduction in multivariate data analysis. It benefits from a simple geometrical interpretation. Given a set of n points $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_n)'$ with $\mathbf{y}_i \in \mathbb{R}^p$ and an integer $0 \leq d \leq p$, PCA builds the d -dimensional affine subspace minimizing the Euclidean distance to the scatter-plot [29]. The application of principal component analysis postulates implicitly some form of linearity. More precisely, one assumes that the data cloud is directed, and that the data points can be well approximated by their projections to the affine hyperplane corresponding to the first d principal components.

Starting from this point of view, many authors have proposed nonlinear extensions of this technique. Principal curves or principal surfaces methods [16, 17, 6] belong to this family of approaches, non-linear transformation of the original data set [7, 3] too. The auto-associative neural networks can also be viewed as a non-linear PCA model [2, 27, 4, 19]. In [13] we propose the auto-associative models (AAM) as candidates to the generalization of PCA using a projection pursuit regression algorithm [9, 25] adapted to the auto-associative case. A common point of these approaches is that they have the intent to estimate an auto-associative model whose definition is given hereafter.

Definition 1.1. *A function g is an auto-associative function of dimension d if it is a map from \mathbb{R}^p to \mathbb{R}^p that can be written $g = R \circ P$ where P*

Date: September 20, 2012.

(the “Projection”) is a map from \mathbb{R}^p to \mathbb{R}^d (generally $d < p$) and R (the “Restoration” or the “Regression”) is a map from \mathbb{R}^d to \mathbb{R}^p .

An auto-associative model (AAM) of dimension d is a manifold \mathcal{M}_g of the form

$$\mathcal{M}_g = \{\mathbf{y} \in \mathbb{R}^p, \mathbf{y} - g(\mathbf{y}) = 0\}$$

where g is an auto-associative function of dimension d .

For example the PCA constructs an auto-associative model using as auto-associative function an orthogonal projector on an affine subspace of dimension d . More precisely we have

$$g(\mathbf{y}) = \mathbf{m} + \sum_{i=1}^d \langle \vec{\mathbf{a}}^i, \mathbf{y} - \mathbf{m} \rangle \vec{\mathbf{a}}^i, \quad \mathbf{y} \in \mathbb{R}^p$$

with $\mathbf{y}, \mathbf{m}, \vec{\mathbf{a}}_i \in \mathbb{R}^p$ and the vectors $\vec{\mathbf{a}}_i$ chosen in order to maximize the projected variance. g can be written $g = R \circ P$ with

$$P(\mathbf{y}) = \left(\langle \vec{\mathbf{a}}^1, \mathbf{y} - \mathbf{m} \rangle, \dots, \langle \vec{\mathbf{a}}^d, \mathbf{y} - \mathbf{m} \rangle \right)$$

and

$$R(\mathbf{x}) = \mathbf{m} + x_1 \vec{\mathbf{a}}^1 + \dots + x_d \vec{\mathbf{a}}^d$$

with $\mathbf{x} = (x_1, \dots, x_d)'$. The AAM is then the affine subspace given by the following equation

$$\mathcal{M}_g = \left\{ \mathbf{y} \in \mathbb{R}^p; \mathbf{y} - \mathbf{m} - \sum_{i=1}^d \langle \vec{\mathbf{a}}^i, \mathbf{y} - \mathbf{m} \rangle \vec{\mathbf{a}}^i = 0 \right\}$$

Interested reader can check that principal curves, principal surfaces, auto-associative neural networks, kernel PCA [31], ISOMAP [36] and local linear embedding [30] have also the intent to estimate an AAM.

In the PCA approach the projection and the restoration function are both linear. It is thus natural to say that the PCA is a *Linear Auto-Associative Model*. In the general case, the manifold \mathcal{M}_g set can be empty (i.e. the auto-associative function g have no fixed point) or very complicated to describe. Our aim in this paper is to study from a theoretical and practical point of view the properties of some Auto-Associative models in an intermediary situation between the PCA model and the general case: we will assume that the projection function is linear and let the regression function be arbitrary. We call the resulting AAM the *Semi-Linear Auto-Associative Models* (SLAAM).

Having restricted our study to the SLAAM, we have to give us some criteria to maximize. As we said previously, the PCA tries to maximize the projected variance or, equivalently, to minimize the residual variance. Common AAM approaches used also the squared reconstruction error as criteria,

or more recently a penalized criteria [17]. However as pointed out by M. E. Tipping and C. M. Bishop [37], one limiting disadvantage of this approach is the absence of a probability density model and associated likelihood measure. The presence of a probabilistic model is desirable as

- the definition of a likelihood measure permits comparison between concurrent models and facilitates statistical testing,
- A single AAM may be extended to a mixture of such models,
- if a probabilistic AAM is used to model the class conditional densities in a classification problem, the posterior probabilities of class membership may be computed.

We propose thus a Gaussian generative model for the SLAAM and try to estimate it using a maximum likelihood approach. In the general case we are faced with a difficult optimization problem and we cannot go further without additional assumptions. It will appear clearly that if \mathbf{P} is *known* then the estimation problem of a SLAAM is very close to an estimation problem in a regression context. There is however some differences we will enlighten. In particular it will appear that in order to get tractable maximum-likelihood estimates, we have to impose some restrictions to the noise. We call the resulting model of all these assumptions/simplifications a Semi-Linear Principal Component Analysis. It does not seem possible to add non-linearity to the PCA and get tractable likelihood estimate for \mathbf{P} . But clearly, the assumption that \mathbf{P} is known is too strong in practice. We propose thus to estimate it in a separate step using either the PCA or a contiguity analysis [26] by extending our previous work on the Auto-Associative models [13]. Finally, even if \mathbf{P} is assumed known it remains to estimate the regression function R which is a non-linear function from \mathbb{R}^d to \mathbb{R}^p . If $d > 1$ and p is moderately high the task become very complicated. Thus we simplify once more the model and assume that R is additive inspired by the Generalized Additive Model (GAM) approach [18].

In view of the experiments we have performed and we present there, it seems we obtain a practical and simple model which generalizes in an understandable way the PCA model to the non-linear case.

The paper is organized as follows. Section 2 introduces the Probabilistic Semi-Linear Auto-Associative Models (PSLAAM) and relate them to the PCA and Probabilistic PCA models. In section 3 we present the Probabilistic Semi-Linear PCA models and the estimation of their parameters conditionally to the knowledge of the projection matrix \mathbf{P} . Section 4 is devoted to the determination of the projection matrix \mathbf{P} using contiguity analysis. Data sets and experiments are detailed in Section 5 with a real astronomical data set. Finally, some concluding remarks are proposed in Section 6.

2. SEMI-LINEAR AUTO-ASSOCIATIF MODELS (SLAAM)

2.1. Geometrical properties of the SLAAM. Let us first consider a general auto-associative model as given in the definition 1.1. We have the following evident property

Proposition 2.1. *Let $H = \{P(\mathbf{y}); \mathbf{y} \in \mathcal{M}_g\} \subset \mathbb{R}^d$. On H the projection function and the regression function verify*

$$(1) \quad P \circ R = \text{Id}_d$$

where Id_d denote the identity function of \mathbb{R}^d .

Proof. Let $\mathbf{y} \in \mathcal{M}_g$ and let $\mathbf{x} = P(\mathbf{y})$, then

$$\mathbf{x} = P(\mathbf{y}) = P(g(\mathbf{y})) = P(R(P(\mathbf{y}))) = P(R(\mathbf{x})).$$

□

As a consequence, we have the following “orthogonality” property verified by an AAM when P is an additive function

Proposition 2.2. *Let $V = \{P(\mathbf{y}); \mathbf{y} \in \mathbb{R}^p\}$ and assume that the property (1) extend on V , let $\mathbf{y} \in \mathbb{R}^p$, $\bar{\mathbf{y}} = R(P(\mathbf{y}))$ and $\bar{\varepsilon} = \mathbf{y} - \bar{\mathbf{y}}$. If P is additive, i.e. $P(\mathbf{y} + \mathbf{y}') = P(\mathbf{y}) + P(\mathbf{y}')$, then*

$$P(\bar{\varepsilon}) = 0.$$

Proof. Using the property (1), we have on one hand $P(\bar{\mathbf{y}}) = P(R(P(\mathbf{y}))) = P(\mathbf{y})$. While on the other hand $P(\bar{\mathbf{y}}) = P(\mathbf{y} - \bar{\varepsilon}) = P(\mathbf{y}) - P(\bar{\varepsilon})$ giving the announced result. □

Clearly we have $H \subset V$ and the assumption given in this proposition seems quite natural. We focus now on the semi-linear case and we assume that

$$(2) \quad P(\mathbf{y}) = \left(\langle \bar{\mathbf{a}}^1, \mathbf{y} \rangle, \dots, \langle \bar{\mathbf{a}}^d, \mathbf{y} \rangle \right) = \mathbf{P}\mathbf{y}.$$

with $\mathbf{P} = (\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^d)'$ a matrix of size (d, p) .

Proposition 2.3. *Let $g = R \circ P$ be an auto-associative function, with P given in (2) and R verifying the property (1). Let $\mathcal{B} = (\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^d, \bar{\mathbf{a}}^{d+1}, \dots, \bar{\mathbf{a}}^p)$ be an orthonormal basis of \mathbb{R}^p with $(\bar{\mathbf{a}}^{d+1}, \dots, \bar{\mathbf{a}}^p)$ chosen arbitrarily. Let*

$\mathbf{y} \in \mathcal{M}_g$, and let $\tilde{\mathbf{y}}$ and \tilde{r} denote respectively the vector \mathbf{y} and the auto-associative function r in the basis \mathcal{B} , then

$$(3) \quad \begin{pmatrix} \tilde{y}_1 \\ \vdots \\ \tilde{y}_d \\ \tilde{y}_{d+1} \\ \vdots \\ \tilde{y}_p \end{pmatrix} = \begin{pmatrix} \tilde{y}_1 \\ \vdots \\ \tilde{y}_d \\ \tilde{r}_{d+1}(\tilde{y}_1, \dots, \tilde{y}_d) \\ \vdots \\ \tilde{r}_p(\tilde{y}_1, \dots, \tilde{y}_d) \end{pmatrix}.$$

Proof. It suffices to notice that the change of basis matrix \mathbf{Q} is given by

$$\mathbf{Q}' = (\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^d, \bar{\mathbf{a}}^{(d+1)}, \dots, \bar{\mathbf{a}}^p),$$

thus the left multiplication of \mathbf{y} and r by \mathbf{Q} , using (1), will give (3). \square

From this last proposition we can see that the Semi-Linear Auto-Associative models have a relatively simple geometrical structure and that we cannot expect to model highly non-linear models with them.

2.2. Probabilistic Semi-Linear Auto-Associative Models (PSLAAM).

In the sequel, we will denote by V the subspace spanned by the set of vectors $(\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^d)$, and give us an arbitrary orthonormal basis of V^\perp denoted by $(\bar{\mathbf{a}}^{d+1}, \dots, \bar{\mathbf{a}}^p)$. We will denote by \mathbf{P} the matrix $(\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^d)'$ and by $\bar{\mathbf{P}}$ the matrix $(\bar{\mathbf{a}}^{d+1}, \dots, \bar{\mathbf{a}}^p)'$. As in proposition 2.3, \mathbf{Q} represents the unitary matrix $(\mathbf{P}|\bar{\mathbf{P}})' = (\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^p)'$.

2.2.1. General Gaussian Setting.

Definition 2.1. Let \mathbf{x} be a d -dimensional Gaussian random vector:

$$(4) \quad \mathbf{x} \sim \mathcal{N}(\mu_{\mathbf{x}}, \Sigma_{\mathbf{x}})$$

and let $\tilde{\varepsilon}$ be a p -dimensional centered Gaussian random vector with a diagonal covariance matrix $\Sigma_{\tilde{\varepsilon}} = \text{Diag}(\sigma_1, \dots, \sigma_p)$.

The p -dimensional vector \mathbf{y} is a Probabilistic Semi-Linear Auto-Associative Model (PSLAAM) if it can be written

$$(5) \quad \mathbf{y} = \mathbf{Q}' \left(\begin{pmatrix} x_1 \\ \vdots \\ x_d \\ \tilde{r}_{d+1}(\mathbf{x}) \\ \vdots \\ \tilde{r}_p(\mathbf{x}) \end{pmatrix} + \tilde{\varepsilon} \right) = R(\mathbf{x}) + \varepsilon,$$

where the $\tilde{r}_j(\mathbf{x})$, $d+1 \leq j \leq p$, are arbitrary real functions from \mathbb{R}^d to \mathbb{R} .

2.2.2. *Link with the Principal Component Analysis.* Assume that:

- (1) $\tilde{r}_j(\mathbf{x}) = \tilde{\mu}_j$ for all $j \in \{d+1, \dots, p\}$,
- (2) the covariance matrix of \mathbf{x} , $\Sigma_x = \text{Diag}(\sigma_1^2, \dots, \sigma_d^2)$ is diagonal with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_d$,
- (3) the Gaussian noise $\tilde{\varepsilon}$ have the following covariance matrix $\Sigma_\varepsilon = \text{Diag}(0, \dots, 0, \sigma^2, \dots, \sigma^2)$ with $\sigma < \sigma_d$.

then the vector \mathbf{y} is a Gaussian random vector

$$\mathbf{y} \sim \mathcal{N}(\mu, \Sigma)$$

with

$$\mu = \mathbf{Q}' \begin{pmatrix} \tilde{\mu}_1 \\ \vdots \\ \tilde{\mu}_d \\ \tilde{\mu}_{d+1} \\ \vdots \\ \tilde{\mu}_p \end{pmatrix} \quad \text{and} \quad \Sigma = \mathbf{Q} \begin{pmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_d & & & \\ & & & \sigma & & \\ & & & & \ddots & \\ 0 & & & & & \sigma \end{pmatrix} \mathbf{Q}'$$

and $\tilde{\mathbf{a}}^1, \dots, \tilde{\mathbf{a}}^d$ are the d first eigenvectors given by the PCA.

2.2.3. *Link with the Probabilistic Principal Component Analysis.* The probabilistic PCA [37] is a model of the form

$$(6) \quad \mathbf{y} = \mu + \mathbf{W}\mathbf{x} + \varepsilon,$$

with \mathbf{W} a (p, d) matrix, \mathbf{x} a d -dimensional isotropic Gaussian vector, i.e. $\mathbf{x} \sim \mathcal{N}(0, I_d)$, and ε a p -dimensional centered Gaussian random vector with covariance matrix $\sigma^2 I_p$. The law of \mathbf{y} is not modified if \mathbf{W} is right multiplied by a (d, d) unitary matrix, it is thus possible to impose to the rows of \mathbf{W} to be orthogonal (assuming that \mathbf{W} is of full rank).

The following proposition is then straightforward

Proposition 2.4. *Assume that $\tilde{\varepsilon}$ (and thus ε) is an isotropic Gaussian noise, i.e. $\Sigma_{\tilde{\varepsilon}} = \sigma^2 I_p$, take $\tilde{r}_j = \tilde{\mu}_j$ for all $d+1 \leq j \leq p$ and set*

$$\mathbf{W} = \mathbf{P}' \begin{pmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \sigma_d \end{pmatrix}.$$

The resulting Probabilistic Semi-Linear Auto-Associative Model is a Probabilistic Principal Component Analysis.

For this simple model there exists a close form of the posterior probability of \mathbf{y} and for the maximum likelihood of the parameters of the model. In

particular, the matrix \mathbf{W} can be estimated up to a rotation and spans the principal subset of the data.

3. SEMI-LINEAR PCA

Our aim is now to generalize the PCA model we present in part (2.2.2) to the semi-linear case. We observe that in the PCA model, if the matrix \mathbf{P} is known, then we are able to know the random variable \mathbf{x} . This observation lead us to formulate the following hypothesis about the noise $\tilde{\varepsilon}$:

N: the Gaussian noise $\tilde{\varepsilon}$ have the following covariance matrix $\Sigma_{\tilde{\varepsilon}} = \text{Diag}(0, \dots, 0, \sigma^2, \dots, \sigma^2)$.

Expressing \mathbf{y} in the basis \mathcal{B} (definition 2.1) we get the following expression for $\tilde{\mathbf{y}}$:

$$(7) \quad \begin{pmatrix} \tilde{y}_1 \\ \vdots \\ \tilde{y}_d \\ \tilde{y}_{d+1} \\ \vdots \\ \tilde{y}_p \end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_d \\ \tilde{r}_{d+1}(\mathbf{x}) \\ \vdots \\ \tilde{r}_p(\mathbf{x}) \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \tilde{\varepsilon}_{d+1} \\ \vdots \\ \tilde{\varepsilon}_p \end{pmatrix}.$$

In other word, the coordinates of $\tilde{\mathbf{y}}$ can be split in two sets. The d first coordinates are the Gaussian random vector \mathbf{x} , while the $p - d$ remaining coordinates are a random vector \mathbf{z} which is conditionally to \mathbf{x} a Gaussian random vector $\mathcal{N}(\tilde{r}(\mathbf{x}), \sigma^2 I_{p-d})$. Observe that the regression functions are dependents of the choice of the vectors $\vec{\mathbf{a}}_{d+1}, \dots, \vec{\mathbf{a}}_p$ and that, as the noise ε lives in the orthogonal of V , we have $\mathbf{x} = \mathbf{P}\mathbf{y}$.

3.1. Maximum Likelihood Estimates. The parameters we have to estimate are the position and correlation parameters μ_x and Σ_x for the \mathbf{x} part and (σ^2, \tilde{r}) for the non-linear part. Given a set of n points $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_n)'$ in \mathbb{R}^p , we get by projection two sets of n points $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)' = \mathbf{Y}\mathbf{P}'$ in \mathbb{R}^d , and $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_n)' = \mathbf{Y}\bar{\mathbf{P}}'$ in \mathbb{R}^{p-d} .

Standard calculation give the maximum likelihood for μ_x and Σ_x

$$(8) \quad \hat{\mu}_x = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i.$$

and

$$(9) \quad \hat{\Sigma}_x = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \hat{\mu}_x)(\mathbf{x}_i - \hat{\mu}_x)'$$

The maximum likelihood of σ^2 is given by

$$(10) \quad \hat{\sigma}^2 = \frac{1}{n(p-d)} \sum_{i=1}^n \left\| \mathbf{z}_i - \hat{\tilde{R}}(\mathbf{x}_i) \right\|^2.$$

It remains to estimate \tilde{R} . We consider two cases : \tilde{R} is a linear function and \tilde{R} is a linear combination of the elements of a B-Spline function basis. The linear case is just a toy example that we will use for comparison with the additive B-Spline case. In the non-linear case, we have to estimate a function from \mathbb{R}^d to \mathbb{R}^{p-d} . As we say in the introduction this is a difficult task and we restrict ourself to a generalized additive model (GAM) by assuming that the function \tilde{R} is additive, i.e.

$$(11) \quad \tilde{R}(\mathbf{x}) = \sum_{j=1}^d \tilde{\mathbf{r}}^j(x_j),$$

where each $\tilde{\mathbf{r}}^j$ is a map from \mathbb{R} into \mathbb{R}^{p-d} .

3.2. Linear Auto-Associative Models. In the linear case, we are looking for a vector μ and a $(d, p-d)$ matrix \mathbf{R} minimizing

$$\sum_{i=1}^n \left\| \mathbf{z}_i - \mu - \mathbf{R}'\mathbf{x}_i \right\|^2.$$

It is easily verified that

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n (\mathbf{z}_i - \mathbf{R}'\mathbf{x}_i) = \hat{\mu}_z - \mathbf{R}'\hat{\mu}_x.$$

Setting $\bar{\mathbf{X}} = \mathbf{X} - \mathbf{1}\hat{\mu}'_x$ and $\bar{\mathbf{Z}} = \mathbf{Z} - \mathbf{1}\hat{\mu}'_z$, where $\mathbf{1}$ represent a vector of size n with 1 on every coordinates. Assuming that the matrix $\bar{\mathbf{X}}'\bar{\mathbf{X}}$ is invertible, standard calculus show that

$$\hat{\mathbf{R}} = (\bar{\mathbf{X}}'\bar{\mathbf{X}})^{-1}\bar{\mathbf{X}}'\bar{\mathbf{Z}}.$$

Finally, using the decomposition in eigenvalues of the covariance matrix of \mathbf{Y} , it is straightforward to verify the following theorem

Theorem 3.1. *If the d orthonormal vectors $\mathbf{a}^1, \dots, \mathbf{a}^d$ are the eigenvectors associated with the d first eigenvalues of the covariance matrix of \mathbf{Y} then the estimated auto-associative model is the on obtain by the PCA.*

3.3. Additive Semi-Linear Auto-Associative Models. In order to estimate the regression functions $\tilde{\mathbf{r}}^j, j = 1 \dots, d$, we express them as a linear combination of m B-Spline functions basis s^{jl} where m is a number chosen by

the user. We have thus to estimate the set of coefficients (α_{jl}) , $j = 1, \dots, d$, $l = 0, \dots, m$ by minimizing

$$\sum_{i=1}^n \left\| \mathbf{z}_i - \alpha_0 - \sum_{j=1}^d \sum_{l=1}^m \alpha_{jl} \mathbf{s}^{jl}(x_{ij}) \right\|^2.$$

Standard regression techniques give then the estimates

$$\hat{R}(\mathbf{x}) = \hat{\alpha}_0 + \sum_{j=1}^d \sum_{l=1}^m \hat{\alpha}_{jl} \mathbf{s}^{jl}(x_{ij}), \quad \text{with } \hat{\alpha} = ((\mathbf{S}'\mathbf{S})^{-1}\mathbf{S}'\mathbf{Z})$$

where \mathbf{S} is the design matrix which depends of the knots position, degree of the B-Spline and the number of control points chosen by the user [14].

The estimated regression function \mathbf{r}^j , for $j = 1, \dots, d$ are then given by the formula

$$\hat{\mathbf{r}}^j = \sum_{l=1}^m \hat{\alpha}_{jl} \mathbf{s}^{jl}.$$

3.4. Estimation in practice. The drawback of the previous maximum likelihood equations is that, given the projection matrix \mathbf{P} , we have to perform a rotation of the original data set and next to perform an inverse rotation of the estimated model. In practice, we avoid such computations by estimating the model using the following steps:

- **(C)** Center and (optionally) standardize the data set \mathbf{Y} : obtain $\bar{\mathbf{Y}}$,
- **(P)** Compute the projected data set $\mathbf{X} = \bar{\mathbf{Y}}\mathbf{P}'$ (\mathbf{X} is centered),
- **(R)** Compute the regression $\bar{\mathbf{Y}} \sim \mathbf{X}$ (without intercept),
- **(S)** Compute the log-likelihood and the BIC criteria.

As we can see the main difference is in the regression step: we estimate directly a function from \mathbb{R}^d to \mathbb{R}^p . In practice, as the non-linear part of the model is in V^\perp , the regression function we obtain numerically give the identity function in the V space.

3.5. Model Selection. Since a Semi-linear PCA model depends highly of the projection matrix \mathbf{P} , model selection allows to select among various candidate the best projection. Several criteria for model selection have been proposed in the literature and the widely used are penalized likelihood criteria. Classical tools for model selection include the AIC [1] and BIC [33] criteria. The Bayesian Information Criterion (BIC) is certainly the most popular and consists in selecting the model which penalizes the likelihood by $\frac{\gamma(\mathcal{M})}{2} \log(n)$ where $\gamma(\mathcal{M})$ is the number of parameters of the model \mathcal{M} and n is the number of observations.

In practice we will fix a set of vectors $\vec{\mathbf{a}}^1, \dots, \vec{\mathbf{a}}^{d_{\max}}$ given either by the contiguity analysis (section 4) or the PCA and select the dimension of the model using the BIC criteria because of its popularity. The projection matrices we compare are thus $\mathbf{P} = (\vec{\mathbf{a}}^1)'$, $\mathbf{P} = (\vec{\mathbf{a}}^1, \vec{\mathbf{a}}^2)'$, ... and so on.

4. CONTIGUITY ANALYSIS

Given $(\vec{\mathbf{a}}^1, \dots, \vec{\mathbf{a}}^d)$ an orthonormal set of vector in \mathbb{R}^p , an index $I: \mathbb{R}^{p \times d} \rightarrow \mathbb{R}_+$ is a functional measuring the interest of the projection of the vector $\vec{\mathbf{y}}$ on $\text{Vec}(\vec{\mathbf{a}}^1, \dots, \vec{\mathbf{a}}^d)$ with a non negative real number. A widely used choice of I is $I(\langle \vec{\mathbf{a}}^1, \vec{\mathbf{y}} \rangle, \dots, \langle \vec{\mathbf{a}}^d, \vec{\mathbf{y}} \rangle) = \text{tr}(\text{Var}[\mathbf{P}\vec{\mathbf{y}}])$, the projected variance. This is the criteria maximized in the usual PCA method [23].

The choice of the index I is crucial in order to find "good" parametrization directions for the manifold to be estimated. We refer to [21] and [24] for a review on this topic in a projection pursuit setting. The meaning of the word "good" depends on the considered data analysis problem. For instance, Friedman *et al* [10, 8], and more recently Hall [15], have proposed an index which measure the deviation from the normality in order to reveal more complex structures of the scatter plot. An alternative approach can be found in [5] where a particular metric is introduced in PCA in order to detect clusters. We can also mention the index dedicated to outliers detection [28].

Our approach generalizes the one we present in [13] and consists in defining a contiguity coefficient similar to Labart one's [26] whose maximization allows to unfold nonlinear structures.

A *contiguity* matrix is a $n \times n$ boolean matrix M whose entry is $m_{ij} = 1$ if data points i and j are "neighbors" and $m_{ij} = 0$ otherwise. Labart proposes to use a threshold r_0 to the set of $n(n-1)$ distances in order to construct this matrix but the choice of r_0 could be delicate. In [13] we propose to use a first order contiguity matrix, i.e. $m_{ij} = 1$ iff i is the nearest neighbor of j in order to construct the proximity graph. In order to get a more robust estimate of the neighbor structure, it is possible to generalize this approach and to use a k -contiguity matrix, i.e. $m_{ij} = 1$ iff i is one of the k -nearest neighbor of j .

The contiguity matrix being chosen, we compute the *local covariance* matrix

$$(12) \quad \mathbf{V}^* = \frac{1}{2kn} \sum_{i=1}^n \sum_{j=1}^n m_{ij} (\mathbf{y}_i - \mathbf{y}_j)(\mathbf{y}_i - \mathbf{y}_j)'$$

and the total variance matrix

$$(13) \quad \mathbf{V} = \frac{1}{n} \sum_{i=1}^n (\mathbf{y}_i - \hat{\boldsymbol{\mu}})(\mathbf{y}_i - \hat{\boldsymbol{\mu}})'$$

The axis of projection are then estimated by maximizing the contiguity index

$$(14) \quad I(\bar{\mathbf{a}}^1, \dots, \bar{\mathbf{a}}^d) = \sum_{i=1}^d \frac{\bar{\mathbf{a}}^{i'} \mathbf{V}^* \bar{\mathbf{a}}^i}{\bar{\mathbf{a}}^{i'} \mathbf{V} \bar{\mathbf{a}}^i}.$$

Using standard optimization techniques, It can be shown that the resulting axis are the d eigenvectors associated with the largest eigenvalues of the matrix $\mathbf{V}^{*-1}\mathbf{V}$.

5. EXAMPLES

We first present two illustrations of the estimation principle of PSLAAM on low dimensional data (Section 5.1 and 5.2). These two simulated examples are very similar from the one we use in our previous article with S. Girard [13]. Second, PSLAAM is applied to an astronomical analysis problem in Section 5.3.

Similarly, we always use an additive B-Spline regression model for the estimation of the regression function \tilde{R} (section 3.3). The B-Spline are of degree 3 and we select the number of control points using the BIC .

5.1. First example on simulated data. The data are simulated using a one-dimensional regression function in \mathbb{R}^3 . The equation of the AA model is given by

$$(15) \quad x \rightarrow (x, \sin x, \cos x),$$

and thus $P(x, y, z) = x$. The first coordinate of the random vector is sampled from a centered Gaussian distribution with standard deviation $\sigma_x = 3$ a thousand times. An independent noise with standard deviation $\sigma = 1$ has then been added to the y and z coordinates.

The axis of projection have been computed thanks to the contiguity analysis (section 4) using the 3 nearest neighbors for the proximity graph. The correlations between the projected data set and the original data set are

	X	Y	Z
Proj ₁	0.9999680850	-0.0005794581	0.0089238830

which show that the first axis given by the contiguity analysis is very close from the x -axis as it was expected. The result of the contiguity analysis can be visualized in the figure 1.

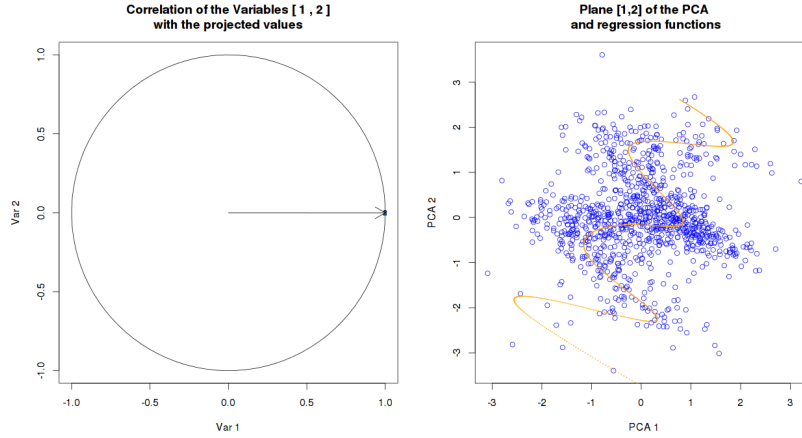


FIGURE 1. Correlation of the first axis obtain using a contiguity analysis with the X and Y variables and representation of the scatter-plot and regression function in the main PCA plan. This graphic has been obtained with R using the *plot* command of the *aam* library.

The projected variance on the first axis is 9.20496 which is also very close from 9. We use the BIC criteria in order to select the dimension of the model and the number of control points. A summary of the tested model is given in the table 1

Finally the result of the regression is drawn in the figure 2.

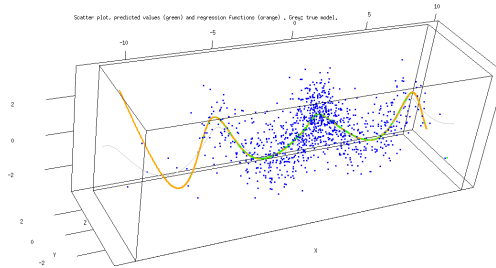


FIGURE 2. The simulated scatter-plot (blue), the estimated AAM (orange) and the true AAM (grey). This graphic is obtained with R using the *draw3d* command of the *aam* library.

		Contiguity Analysis		PCA	
	dim	BIC	Residual Variance	BIC	Residual Variance
linear	1	9987,13(5)	1.439	11495.8	1.43864
	2	10609.7(10)	1.40815		
9	1	11247.6(29)	1.06557	11058.4	1.06407
	2	11621(58)	1.1086		
10	1	11060.7(32)	0.986316	10926.3	0.985777
	2	11469(64)	0.913605		
11	1	10853.7(35)	0.941064	10855	0.92711
	2	11503(70)	0.90682		
12	1	10844.6(38)	0.92717	10845(38)	0.941661
	2	11525(76)	0.892669		
13	1	10871.4(41)	0.929965	10871.6	0.927976
	2	11568.4(82)	0.891119		
14	1	10888.5(44)	0.927834	10888.3	0.927976
	2	11604(88)	0.885939		

TABLE 1. Values of the BIC criteria for $d = 1$ and $d = 2$ and for various number of control points (given in the first column). The number of free parameters of each model is given in parenthesis. The BIC criteria selects the model of dimension 1 with 11 control points. The axis of projection can be either the one obtained by contiguity analysis or the one obtained using the PCA.

5.2. **Second example on simulated data.** In our second example the AAM is given by

$$(16) \quad (x, y) \rightarrow (x, y, \cos(\pi r/3)(1 - \exp(-64r^2)) \exp(0.2r))$$

with $r = \sqrt{x^2 + y^2}$ and thus $P(x, y, z) = (x, y)$. The first two coordinates of the random vector are sampled from a centered Gaussian distribution with covariance matrix

$$\Sigma_x = \begin{pmatrix} 1.8 & 0 \\ 0 & 1.5 \end{pmatrix}$$

and $n = 1000$ points are simulated. An independent noise with standard deviation $\sigma = 0.5$ has then been added to the z coordinate.

The correlations between the projected data set and the original data are

	X	Y	Z
Proj ₁	0.99924737	-0.1488330	0.0179811
Proj ₂	-0.14239437	0.98532966	0.01396622

which show that the (x, y) -plan is the plan essentially chosen by the contiguity analysis. The result of the contiguity analysis is displayed in the figure 3.

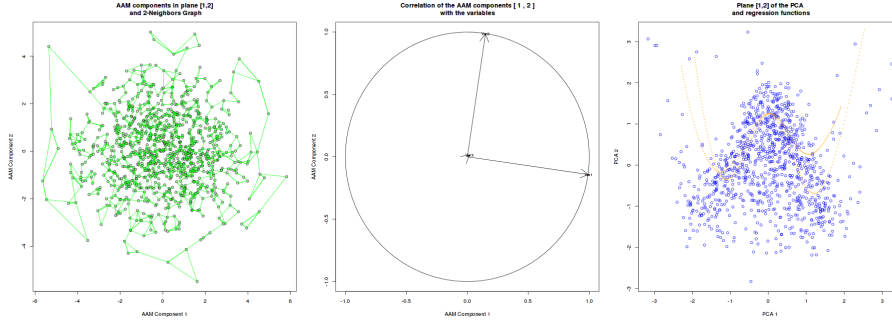


FIGURE 3. The AAM components and the 2-neighbors graph, the correlation circle of the AAM components with the variables and representation of the scatter-plot in the PCA plan. These pictures have been obtained using the *plot* command of the *aam* library.

The BIC criteria select 7 control points. A summary of the tested model is given in the table 2. The selected model over-estimate the residual variance by a factor 2. It is not a surprising result as the original model is not additive and we cannot expect to reconstruct it exactly. We don't show the results with the PCA as the first axis this method select is the Z -axis which is clearly the wrong parametrization.

The true model and the estimated model obtained with an additive B-Spline regression are given in the figure 5.2.

5.3. Example in spectrometry analysis. Finally we illustrate the performance of the semi-linear PCA on a real data set. The data consists of 19-dimensional spectral information of 487 stars [34, 12, 35, 11] and they have been classified in 6 groups. They have been modeled by [32] using an auto-associative neural networks based on a 19-30-10-30-19 network. Using the terminology of this article the model proposed by M. Scholz and its co-authors is an auto-associative model of dimension 10. We select the model using the BIC criteria. The main results are the following:

- (1) The axis of projection given by the PCA outperform largely the results we obtain with the contiguity analysis, for any choice of control point.

	dim	BIC	Residual Variance
linear	1	11024.7(5)	1.78335
	2	10.832.7(10)	1.20314
	2	10654.2(34)	0.852753
6	1	11072.6(20)	1.68675
	2	10716.1(40)	0.870381
7	1	11014.2(23)	1.55841
	2	10.213.6(46)	0.505186
8	1	11.031.6(26)	1.55334
	2	10.216.6(52)	0.486137
9	1	11051.7(29)	1.55229
	2	10255(58)	0.484644

TABLE 2. Values of the BIC criteria for $d = 1$ and $d = 2$ and for various number of control points (given in the first column). The number of free parameters of each model is given in parenthesis. The BIC criteria selects the model of dimension 2 with 7 control points.

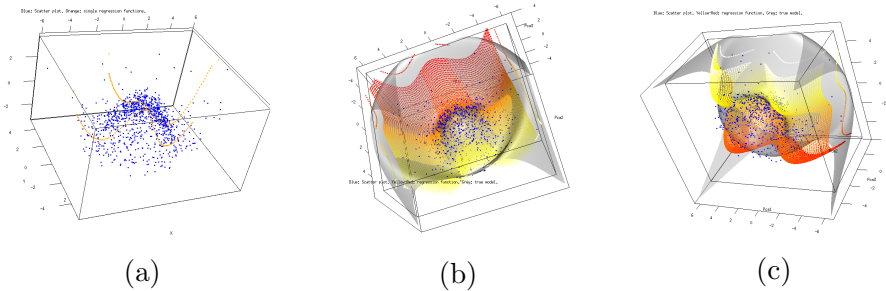


FIGURE 4. (a) the original data set (blue) and the individual regression functions. (b)-(c) two views of the original manifold (grey) and of the extrapolated manifold using an additive B-Spline regression (yellow-red). These images have been obtained using the *draw3d* function of the *aam* library.

- (2) The BIC criteria retains a model of dimension 5 with 9 Control Points (871 parameters) when we use a non-linear regression step. The residual variance is $\sigma^2 = 0.0080763$ while the total variance (inertia) of the data was 26.59832.
- (3) The BIC criteria retains a model of dimension 12 (307 parameters) when we use a linear regression step. Observe that in this case, we are performing an usual PCA (theorem 3.1).

The data cloud in the main PCA space with the values predicted by the model is displayed in the figure 5.

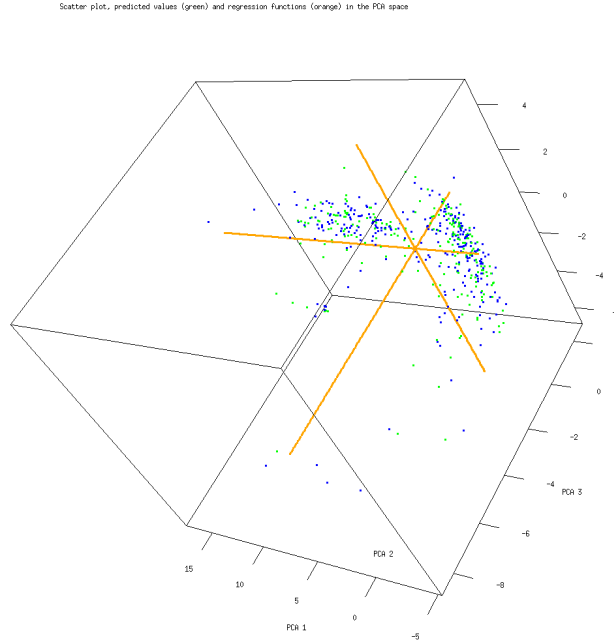


FIGURE 5. Data cloud in the main PCA space with the predicted values (green).

A summary of some tested model are given in the table 3 and some planes of projection are displayed in the picture 6. We visualize each components of the regression functions by setting all, except one, predictors to zero and we represent the evolution of the regression function in the \mathbb{R}^{14} space in the graphic 7.

PCA			
Control Points	BIC value	dim	Residual variance
Linear	1829,95(307)	12	0,0049702
7	1187,26(820)	6	0,00727521
8	1147,62(776)	5	0,00975073
9	453,387(871)	5	0,0080763
10	701,769(966)	5	0,00768342
11	1333,45(1061)	5	0,00773327

TABLE 3. Values of the BIC criteria for various number of control points (given in the first column). The BIC criteria select the model of dimension 5 with 9 control points using as projection matrix the 5 axis given by the PCA. The total variance (inertia) of the data set was 26.59832.

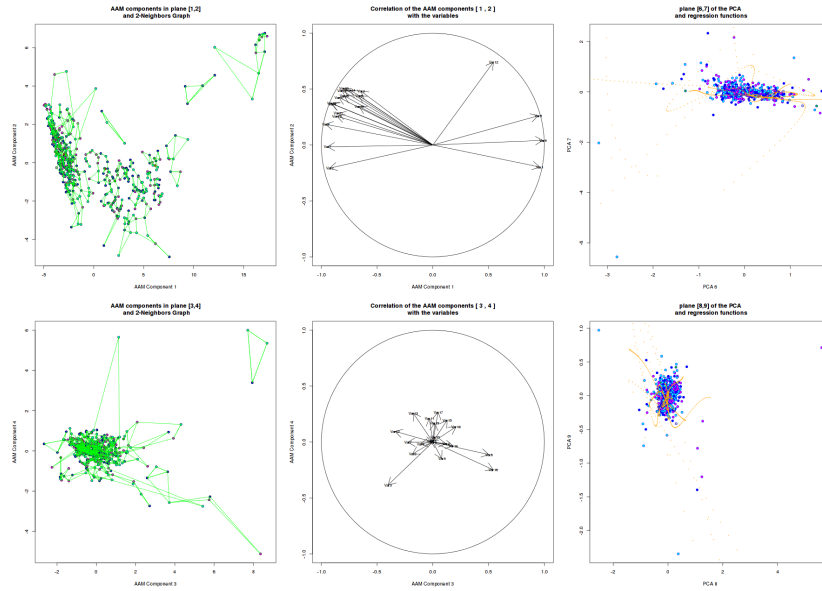


FIGURE 6. Some plans of projection of the PCA with the 2-neighbors graph (left) and with the single regression functions (right). As we use the PCA for the projection matrix, the AAM components are the PCA components. The colors of the points represent the classification of the stars.

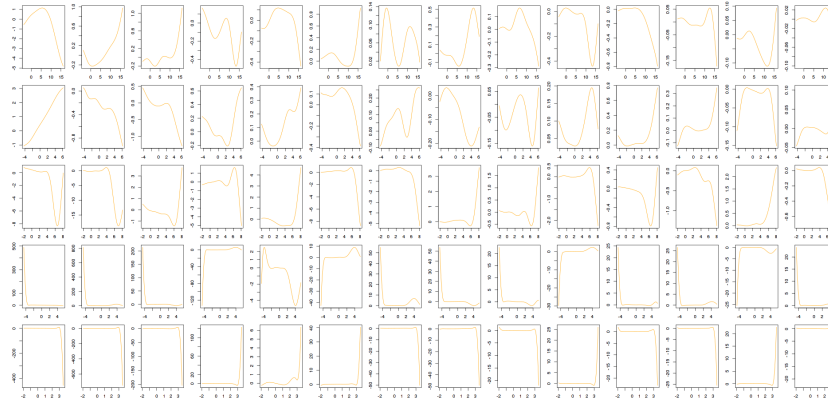


FIGURE 7. The individual regression functions from \mathbb{R}^5 to \mathbb{R}^{14} . In each row we have the non-zero predictor sampled in the range $[\min, \max]$, and in each column the evolution of the functions in the dimension 6,...,19. The system of coordinates is the one given by the PCA.

6. CONCLUSION

We have presented a class of auto-associative model for data modeling and visualization called semi-linear auto-associative models. We provided theoretical groundings for these models by proving that the principal component

analysis and the probabilistic principal component analysis are special cases. Our model allows to models data set with a simple non-linear component and is truly generative with an underlying probabilistic interpretation. However it does not allow to models data with a strong non-linear component and it depends highly on the choice of the projection matrix.

The Semi-Linear PCA have been implemented in C++ using the *stk++* library [22] and is available at: <https://sourcesup.renater.fr/projects/aam/>.

The program is accompanied with a set of *R* scripts which allows to simulate and display the results of the *aam* program.

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