Bayesian Sparse Factor Analysis with Kernelized Observations

Carlos Sevilla-Salcedo, Alejandro Guerrero-López, Pablo M. Olmos, Vanessa Gómez-Verdejo
Department of Signal Processing and Communications, Universidad Carlos III de Madrid Leganés, 28911 Spain

Abstract

Latent variable models for multi-view learning attempt to find low-dimensional projections that fairly capture the correlations among multiple views that characterise each datum. High-dimensional views in medium-sized datasets and non-linear problems are traditionally handled by kernel methods, inducing a (non)-linear function between the latent projection and the data itself. However, they usually come with scalability issues and exposure to overfitting. To overcome these limitations, instead of imposing a kernel function, here we propose an alternative method. In particular, we combine probabilistic factor analysis with what we refer to as kernelized observations, in which the model focuses on reconstructing not the data itself, but its correlation with other data points measured by a kernel function. This model can combine several types of views (kernelized or not), can handle heterogeneous data and work in semi-supervised settings. Additionally, by including adequate priors, it can provide compact solutions for the kernelized observations (based in a automatic selection of bayesian support vectors) and can include feature selection capabilities. Using several public databases, we demonstrate the potential of our approach (and its extensions) w.r.t. common multi-view learning models such as kernel canonical correlation analysis or manifold relevance determination gaussian processes latent variable models.

1 Introduction

Given a set of observable data, Latent Variable Models (LVMs) aim to extract a reduced set of hidden variables able to summarise the information into a low dimensional space. These models have become crucial in multi-view problems [1,2,3], where data are represented by different modalities or views, since LVMs are able to explain the common information among all the modalities.

Classical MultiVariate Analysis (MVA) methods, such as Principal Component Analysis (PCA) and Canonical Correlation Analysis (CCA) [4,5], aim to exploit the data correlation to obtain a low dimensional latent representation of the data. Its usage has been generalised due to its easy non-linear extension by means of kernel methods. [6,7]. The fact of supporting a kernel formulation allows these methods to learn arbitrarily complex non-linear models with a complexity determined by the number of training points [8] and make them highly convenient in scenarios with high dimensional data.

Factor Analysis (FA) [9] emerges as a linear bayesian framework where one can obtain the desired latent representation together with a measure of the uncertainty. Among their many variants, such as Probabilistic PCA [10], Supervised PCA [11], Bayesian Factor Regression [12] or Bayesian CCA [13], Inter-Battery FA models [13] stand out for their capability of handling not only latent

*Corresponding author. Email address: sevisal@tsc.uc3m.es
†Pablo M. Olmos is also with the Gregorio Marañón Health Research Institute.

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variables associated to the common information among all the views, but also for being able to model the intra-view information. This model has been recently extended in [14], named as Sparse Semi-supervised Inter-Battery Bayesian Analysis (SSHIBA), to incorporate both missing attributes, feature sparsity/selection, and the ability to handle heterogeneous data such as categorical or multi-dimensional binary data.

The use of kernel methods in bayesian approaches has been mostly developed with Gaussian Processes [15] and their non-supervised version to perform dimensionality reduction (GP latent variable models, GPLVMs) [16]. These approaches combine the advantages of the kernels methods, exploiting the non-linear relationships among the data, with that of a probabilistic framework. In [17], the authors propose a shared GPLVMs approach, called Manifold Relevance Determination (MRD), to provide a non-linear latent representation for multi-view learning problems. This model is extended in [18], including an Automatic Relevance Determination (ARD) prior [19] over the kernel formulation, to endow it with feature selection capabilities.

GPLVMs come with practical scalability drawbacks that need to be addressed. The cubic complexity with the number of training points requires the use of inducing points and variational approaches [20]. Selecting the number of inducing points to use, and where to place them in the latent space, is still a challenging problem, being a common solution to place them in a regular basis along the latent space and only optimize the pseudo-observation at those points [21]. Furthermore, up to our knowledge, there is no versatile implementation in the state-of-the-art of a multi-view GPLVM able to handle heterogeneous observations (integer, categorical, real and positive observations) and missing values.

In this paper we propose a novel method to implement non-linear probabilistic LVMs that still builds upon a linear generative model, hence inheriting their computational and scalability properties. Instead of implementing a kernel method, i.e. a GP, to move from the latent representation to the observed data, we propose to reformulate probabilistic FA so that it generates kernel relationships instead of data observations. In the same way that Kernelized PCA (KPCA) or Kernelized CCA (KCCA) are able to generate non-linear latent variables by linearly combining element of a kernel vector, here, from a bayesian generative point of view, we first i.i.d. sample latent representations and project on an $N$-dimensional space (being $N$ the number of points) using a weight matrix representing the dual parameters. We apply this trick over the SSHIBA formulation [14] to exploit their functionalities over this kernelized formulation. Thanks to that, we can efficiently face semi-supervised heterogeneous multi-view problems combining linear and non-linear data representations; in this way, one can combine kernelized views to deal with non-linear relationships with linearly kernelized to work with high dimensional problems. Besides, we can force the automatic selection of Support Vectors (SVs) to obtain a scalable solution as well as include an ARD prior over the kernel to obtain feature selection capabilities.

2 Bayesian sparse factor analysis with kernelized observations

Let's consider a multi-view problem where we have $N$ data samples represented in $M$ different modalities, $\{X^{(m)}\}_{m=1}^{M}$, and our goal is to find an inter and intra-view non-linear latent representation, $Z$. That is, given that $x^{(m)}_{n,:} \in \mathbb{R}^{D_{m}}$ is the $n$-th data of the $m$-th view, $z_{n,:}$ has to compress, in a low dimensional space of size $K_{c} << (D_{1}, \ldots, D_{M})$, both the common and particular information of $x^{(m)}_{n,:}$ over all the views exploiting the correlations among the data.

Whereas kernel LVMs obtain this latent representation as a linear combination, by some dual variables, of the kernel representation of the $n$-th data, here we propose to reformulate this idea from a generative point of view. In particular, we start from the SSHIBA algorithm formulation [14] and consider that there exist some latent variables $z^{(m)}_{n,:} \sim \mathcal{N}(0, I_{K_{c}})$ which are linearly combined with a set of dual variables $A^{(m)} \in \mathbb{R}^{N \times K_{c}}$ to generate a kernel vector, $k^{(m)}_{n,:}$, as:

$$ k^{(m)}_{n,:} = z^{(m)}_{n,:} A^{(m)T} + \tau^{(m)} $$

(1)

where $\tau^{(m)}$ is zero-mean gaussian noise, with noise power following a Gamma distribution of parameters $a^{(m)}$ and $b^{(m)}$, and $k^{(m)}_{n,:}$ is the kernel representation of the $n$-th data; that is, given a mapping function $\phi(\cdot)$ and its associated kernel function $K(x, x') = \phi(x)^{T} \phi(x')$, $k^{(m)}_{n,:}$ is a vector

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1 Given a matrix $B$, we denote the $i$-th row by $b_{i,:}$ and the $j$-th column by $b_{:,j}$. 

with the kernel between $x_{n,m}$ and all the training data $k_{n,m} = [K(x_{n,m}, x_{1,m}), \ldots, K(x_{n,m}, x_{N,m})]$. 

The dual variable matrix $A^{(m)}$ plays the role of the linear projection matrix and is defined using the same structured ARD prior considered in both [13] and [14]. Namely, an ARD prior that promotes that full rows of this matrix are cancelled, i.e. $a_{n,k}^{(m)} \sim N(0, (\alpha_k^{(m)})^{-1} I_{K_c})$ with $\alpha_k^{(m)} \sim \Gamma(\alpha^{(m)}_0, \beta^{(m)}_0)$, so that in the product in (1) the appropriate set of latent factors is selected.

Figure 1 shows the graphical model of KSSHIBA. Following [13], for the data views that are directly explained given the latent projection we have $x_{n,m} = z_n : W(m)^T + \tau(m)$, where the weight matrix $W^{(m)}$ follows the same structured ARD prior mentioned above. We can refer to these as primal observations. For some other views we might be interested in explaining them indirectly through a kernelized observation following (1). This conversion can be of interest when the view’s dimensionality is much larger than the number of data points $N$. When both primal and kernelized observations are used, the learned latent projection $z_n$ attempts to faithfully reconstruct each of the primal views, and the joint relation between each pair of data points through the reconstruction of the kernel matrix.

The posterior distribution of all model parameters and latent projections is approximated using variational inference with a fully factorized posterior, as detailed in the Supplementary Material, where it can be noted that each update has a computational cost of $O(N^2 K_c + K^3)$.

Note that sampling from the model in (1) does not ensure a valid kernel positive semi-definite matrix. The kernel matrix is simply treated as an observation (a kernelized observation) and, as such, the model parameters will be chosen to minimize the reconstruction error. Experimental results were also shocking for the authors, as fairly good kernel matrices are typically reconstructed after model training. In Figure 2 we include a graphical representation of both a kernelized observation and the map reconstruction through (1) using the mean of the posterior distribution of $z_n$. Certainly, more appropriate models could be used to adapt the observation model (given $z_{n,m}$) to the properties of a kernelized observation. To address this issue, we have explored alternative formulations based in non-independent noise; for example, defining the noise distribution as an inverse-wishart to have a full rank covariance noise or modelling its covariance as the product of two low rank matrices. However, these schemes led to considerably more complicated (less flexible) formulation which limited the rest of the properties of this proposal (as the ones proposed in the following sections). Henceforth, we restrict to the model in (1), and leave this line of work open for future research.

2.1 Automatic bayesian support vector selection

On the basis of a full $N \times N$ kernel, with a more structured ARD prior we can achieve not only the shrinkage of the number of effective latent factors, but also a more compact representation of the data by means of a reduced kernel matrix in which only a reduced set of support vectors (SVs) are kept.

For this purpose, the proposed formulation can introduce a double ARD prior over the dual variables $A^{(m)}, a_{n,k}^{(m)} \sim N(0, (\gamma_n^{(m)} \alpha_k^{(m)})^{-1})$. This way, $\alpha_k^{(m)}$ continues forcing row-wise sparsity to
automatically select the number of latent factors and, additionally, \( \gamma^{(m)} \) induces column-wise sparsity in the columns weight matrix to learn the set of bayesian SVs. This process can be carried out during the inference process, removing the least relevant SVs (and their corresponding columns in \( \Lambda^{(m)} \)) by setting a threshold, providing additional computational improvement.

### 2.2 Automatic feature selection

Furthermore, we can additionally endow the proposed kernelized data representation with feature selection capabilities. If by using the double ARD structured we can cancel full rows or columns, equivalently, by using an ARD kernel we can perform feature selection. In the ARD kernel, each feature of the original observations is multiplied by a variable \( \lambda^{(m)}_d \) in the kernel definition. For example, for a RBF kernel, \( k^{(m)}_{n,u} = \exp\left(-\sum_{d=1}^{D_m} (x^{(m)}_{n,d} - x^{(m)}_{u,d})^2 \lambda^{(m)}_d \right) \), we can optimise \( \lambda^{(m)} = [\lambda^{(m)}_1, \ldots, \lambda^{(m)}_{D_m}] \) by maximising the lower bound of our mean field approach given by direct optimisation over the variational lower bound. In our model, if the \( m \)-th view is kernelized then the only terms in the lower bound where the ARD kernel kicks in are (see Supplementary Material for details):

\[
LB = - \frac{1}{2} \sum_{n=1}^{N} \sum_{u=1}^{N} \left( k^{(m)}_{n,u}^2 - 2 k^{(m)}_{n,u} \langle \alpha^{(m)}_{u:}, \langle \alpha^{(m)}_{u:} \rangle \rangle \langle z^{T}_{n:} \rangle + \langle \alpha^{(m)}_{u:}, \langle \alpha^{(m)}_{u:} \rangle \rangle \langle z^{T}_{n:}, z^{T}_{n:} \rangle \right)
\]

We alternate between mean-field updates over the variational bound with direct maximization of (2) w.r.t. \( \lambda^{(m)} \) using any gradient ascend method (we use Pytorch and Adam for such updates). Finally, by setting a threshold for \( \lambda^{(m)} \) the feature selection can be done while training.

### 3 Results

Throughout this section the presented model is analysed in terms of performance and interpretability of the inferred model parameters and latent projections. Results on some other baselines as well as a more extensive description of the experimental setup and databases are available in the Supplementary Material. Furthermore, an exemplary notebook with the library will be uploaded to an open github repository.\(^2\)

\(^2\)This notebook has been uploaded with the rest of files to the review system.
3.1 Performance evaluation of KSSHIBA for multi-dimensional regression

KSSHIBA can be trained in a semi-supervised way, being capable of predicting by either sampling from the posterior or simply using the mean, as we will do. This section aims to analyse the performance of KSSHIBA for semi-supervised multi-dimensional regression in comparison with some state-of-the-art baselines. To do so, we used some multitask datasets from the Mulan repository \[22, 23, 24\]. Table 1 shows the results obtained on the databases comparing the proposed model with: (1) reference regression methods, such as a Support Vector Regression machine with Gaussian RBF kernel (SVR-RBF) and a MultiLayer Perceptron (MLP); (2) a KCCA+LR and KPCA+LR approach where KCCA/KPCA is used for feature extraction and a Linear Regressor (LR) for prediction purposes. In this case, the number of latent factors has been fixed to the maximum possible, \( C - 1 \) (where \( C \) is the number of tasks) in KCCA and to those which explain 95\% of the variance in KPCA; (3) Multi-view GPLVM (MRD), the number of latent factors is set to twice \( C \). Two versions of KSSHIBA are included. One in which the number of latent factors \( K_c \) is automatically learnt, and one in which we set \( K_c \) to \( C - 1 \).

We calculated the reported results with a nested 10-folds cross-validation (CV). The outer CV is used to divide the dataset into training and test partitions, while the inner CV is in charge of validation and, therefore, it divides the training partition into a second training set and a validation set. This way we were able to estimate the performance of the whole framework and, additionally, validate the model parameters. We used R2 score to measure the performance of the methods.

Table 1: Results on multitask databases of KSSHIBA and the baselines. The white subrow represents the mean and standard deviation of R2 score and the gray subrow the number of effective latent factors found.

| Database | KSSHIBA \( K_c = C - 1 \) | KSSHIBA MRD | KPCA + LR | KCCA + LR | SVR-RBF | MLP |
|----------|--------------------------|----------------|-------------|------------|---------|-----|
| at1pd    | 0.77 ± 0.09              | 0.76 ± 0.10    | 0.67 ± 0.07 | 0.67 ± 0.12 | 0.76 ± 0.10 | 0.01 | 0.77  |
|          | 53 ± 8                   | 5              | 12          | 22 ± 10    | 5        | ±0.05 | ±0.12 |
| at7pd    | 0.48 ± 0.26              | **0.49 ± 0.15** | 0.48 ± 0.12 | 0.39 ± 0.19 | 0.47 ± 0.19 | 0.01 | 0.35  |
|          | 53 ± 11                  | 5              | 12          | 21 ± 1     | 5        | ±0.03 | ±0.69 |
| oes97    | **0.63 ± 0.16**          | **0.63 ± 0.17** | 0.34 ± 0.07 | 0.45 ± 0.20 | 0.42 ± 0.22 | 0.01 | 0.58  |
|          | 108 ± 11                 | 15             | 32          | 12 ± 7     | 15 ± 0   | ±0.10 | ±0.21 |
| oes10    | **0.79 ± 0.08**          | 0.76 ± 0.10    | 0.38 ± 0.07 | 0.59 ± 0.15 | 0.60 ± 0.14 | 0.01 | 0.76  |
|          | 104 ± 22                 | 15             | 32          | 14 ± 7     | 15       | ±0.12 | ±0.08 |
| edm      | 0.37 ± 0.19              | 0.16 ± 0.08    | -0.17 ± 0.45 | **0.38 ± 0.19** | 0.15 ± 0.33 | 0.01 | 0.26  |
|          | 17 ± 2                   | 1              | 16 ± 5     | 1          | ±0.19 | ±0.21 |
| jura     | **0.61 ± 0.10**          | 0.22 ± 0.14    | 0.57 ± 0.06 | 0.38 ± 0.11 | -0.56 ± 0.44 | 0.01 | 0.61  |
|          | 64 ± 7                   | 2              | 6          | 23 ± 1     | 2       | ±0.05 | ±0.06 |
| wq       | 0.12 ± 0.01              | 0.12 ± 0.01    | -0.35 ± 0.08 | 0.09 ± 0.02 | -1.43 ± 0.36 | 0.01 | **0.13** |
|          | 48 ± 3                   | 13             | 28         | 29 ± 1     | 13      | ±0.02 | ±0.03 |
| enb      | **0.99 ± 0.01**          | 0.69 ± 0.04    | 0.91 ± 0.01 | 0.86 ± 0.01 | 0.91 ± 0.03 | 0.01 | **0.99** |
|          | 118 ± 4                  | 1              | 4          | 13 ± 1     | 1       | ±0.01 | ±0.08 |

In particular, we can see that KSSHIBA outperforms most methods in terms of R2 score while providing dimensionality reduction. At the same time, the results obtained by KSSHIBA with \( K_c = C - 1 \) imply that a less restrictive pruning would not deteriorate the results (except for edm, jura and enb where \( C - 1 \) is 1 or 2). Besides providing dimensionality reduction, KSSHIBA proves to be able to perform as well as MLP or even outperform it in terms of R2.

3.2 Evaluation of the solution in terms of SVs

Now, we want to test the capabilities of the KSSSHIBA approach to automatically select a subset of training points. For this purpose, we use the same databases and setup as the previous evaluation to compare to KPCA+LR and KCCA+LR. In these last two models, in order to decide the number
of SVs used to build the kernel matrix, a cross-validation has been done following a Nyström \[25\] subsampling technique.

Table 2 shows that the inclusion of the automatic SV selection on KSSHIBA keeps the original model performance for most databases, even improving it for oes97 and edm. This is done while drastically reducing the model complexity; in fact, analysing this in detail, it is observed that the fact of reducing the number of SVs favours an additional reduction in the final number of latent factors. When comparing to KPCA+LR and KCCA+LR, KSSHIBA mostly shows a lower percentage of SVs needed to describe the kernel. This is due to the fact that KSSHIBA learns the relevance of each element and eliminates them accordingly, whereas KPCA and KCCA obtain this compact solutions with a random selection of SVs.

Table 2: Results on the multitask databases for the automatic SV selection. The first subcolumn shows on the white subrow the mean and standard deviation of the R2 score and on the gray subrow the number of effective latent factors (\(K_c\)), the second subcolumn includes the number of selected SVs (#SVs).

|          | Sparse KSSHIBA | KPCA + LR | KCCA + LR |
|----------|----------------|-----------|-----------|
|          | R2 - \(K_c\)  | #SVs      | R2 - \(K_c\) | #SVs | R2 - \(K_c\) | #SVs |
| at1pd    | 0.77 ± 0.09    | 62 ± 81   | 0.78 ± 0.09 | 87 ± 35 | 0.80 ± 0.09 | 5     |
|          | 41 ± 11        |           |           | 235 ± 111 | 209 ± 105 |
| at7pd    | 0.55 ± 0.15    | 55 ± 78   | 0.56 ± 0.18 | 90 ± 37 | 0.55 ± 0.18 | 5     |
|          | 70 ± 27        |           |           | 236 ± 94 | 207 ± 109 |
| oes97    | 0.58 ± 0.15    | 129 ± 82  | 0.52 ± 0.24 | 124 ± 34 | 0.39 ± 0.37 | 15 |
|          | 61 ± 7         |           |           | 273 ± 93 | 93 ± 80 |
| oes10    | 0.77 ± 0.11    | 179 ± 155 | 0.71 ± 0.12 | 132 ± 53 | 0.66 ± 0.14 | 15 |
|          | 74 ± 6         |           |           | 290 ± 47 | 201 ± 110 |
| edm      | 0.42 ± 0.21    | 83 ± 44   | 0.41 ± 0.26 | 29 ± 14 | 0.22 ± 0.12 | 1 |
|          | 13 ± 4         |           |           | 81 ± 47 | 59 ± 51 |
| jura     | 0.58 ± 0.14    | 175 ± 138 | 0.57 ± 0.10 | 59 ± 14 | 0.37 ± 0.10 | 2 |
|          | 30 ± 4         |           |           | 218 ± 104 | 80 ± 23 |
| enb      | 0.12 ± 0.01    | 616 ± 352 | 0.12 ± 0.02 | 96 ± 49 | 0.10 ± 0.02 | 13 |
|          | 21 ± 2         |           |           | 243 ± 169 | 63 ± 31 |
|          | 78 ± 8         |           |           | 376 ± 253 | 395 ± 54 |
|          | 150 ± 99       |           |           | 376 ± 253 | 395 ± 54 |
|          | 28 ± 1         |           |           | 376 ± 253 | 395 ± 54 |
|          | 91 ± 0.01      |           |           | 91 ± 0.01 | 1 |
|          | 78 ± 8         |           |           | 91 ± 0.01 | 1 |
|          | 150 ± 99       |           |           | 91 ± 0.01 | 1 |
|          | 28 ± 1         |           |           | 91 ± 0.01 | 1 |

To complete this analysis, Figure 3 depicts the mean R2 over 10 folds of the analysed algorithms for the databases where KSSHIBA is outperformed in Table 2. For the sake of comparison, we also included the MRD results when its percentage of inducing points is varied. Whereas MRD, KPCA+LR and KCCA+LR present fluctuations in their performance requiring to adjust the number of SVs to obtain an accurate performance, KSSHIBA has a relatively constant R2 value. This phenomenon occurs because KSSHIBA learns the relevance of each SV and weight their influence on the update of the parameters during all the model inference.

### 3.3 Analysis of the feature selection

In order to test the feature selection extension (see Section 2.2), we now study KSSHIBA on different classification databases where the input view is an image, and the output view is the category label. We used the faces dataset Labeled Faces in the Wild (LFW) [26] and warpAR10P, Yale and Olivetti, which can be found from the Feature Selection Repository.\[8\] We applied over the input view the feature selection extension, obtaining the masks in Figure 4. Despite having different image resolution in each database, we can see how the proposed extension is capable of focusing on the most relevant features (white). For instance, Figures 4a and 4b learn to focus on the area related to glasses, while Figures 4c and 4d are learning the general face features of the images.

[http://featureselection.asu.edu/datasets.php](http://featureselection.asu.edu/datasets.php)
Figure 3: R2 results with different percentages of SVs in KSSHIBA, KCCA+LR and KPCA+LR or inducing points in MRD.

(a) LFW  (b) warpAR10P  (c) Yale  (d) Olivetti

Figure 4: Feature masks learnt by the feature selection extension of KSSHIBA for different face recognition problems. The mask represent the importance of each pixel: lighter colours imply the pixel is more relevant while darker ones represent the pixel is less relevant.

3.4 Analysis of the extracted latent factors

In this section we want to evaluate the interpretability of the extracted latent factors obtained by the proposed model in comparison to the MRD approach based on shared GPLVMs. We used their available library [17] to compare it with KSSHIBA on the Oil classification database [27]. For this purpose we have trained both models with 15 latent factors combined with ARD latent factors selection. KSSHIBA uses a RBF kernel for the input view and MRD uses it for both their input and output views. Under this conditions, the accuracy in the prediction of the labels for the MRD was of 99.0% and KSSHIBA achieved a 99.4%. With the available MRD implementation (Matlab), the computational time is not scalable for the number of data. As seen in the Supplementary Material, there is a difference of two orders of magnitude in computational time.

Figure 5 shows the relevance parameter for each of the learnt latent factors for both models. MRD does not find any view dependent latent factor and all latents are shared by both views (Figure 5a shows the relevance for all these common factors) and, besides, it mainly focuses on latents 12, 13 and 14. On the other hand, KSSHIBA presents independent weights for each view (see Figures 5b and 5c); these results indicate there are certain latent factors that are not relevant and could be pruned (latent 7), some that are only relevant for the input view (latents 5 and 14) and the remaining are common (highlighting latents 0, 2 and 8).

3.5 Multi-view KSSHIBA

One of the main functionalities of KSSHIBA is its capacity to combine multiple views into a single model. We can take advantage of this property when reconstructing kernel representations to combine different types of kernels (one per view). To prove the possibilities of this formulation we used a subset of 1.000 samples from the MNIST database [28] and trained the model in three two-view
scenarios for different kernel types in the input kernelized view: a linear kernel, a gaussian one and second degree polynomial kernel, and using the labels as output view; and, additionally, we include a fourth scenario with four views where each kernel is in an input view and the categories are in the output view. The obtained results show that using the linear kernel has an accuracy of 72.33%, the gaussian has 73.00%, the polynomial 68.67% and their combination increases the performance up to 80.67%.

Figure 6 shows the relevance of each latent factor in the joint scenario (all kernels used). From the original 100 latent factors, the output view only uses 22, being most of them private; in fact, we can observe that the improved performance of the model is obtained using only three common factors to all the views, two additional latents shared with RBF kernel and other two shared by linear and polynomial kernel. Besides, the polynomial and linear kernels share all their latent factors; although this may imply a possible redundancy in their information, we have checked that this is actually reinforcing the latent learning since removing any of these views degrades the model performance.

Figure 6: Measure of relevance on multiple views for each latent factor combining different kernels on MNIST database.

4 Conclusions

We propose a novel probabilistic latent variable model to generate kernel relationships, instead of data observations, based on a linear generative model. We introduce this model using the Bayesian inter-battery factor analysis approach proposed in [14] to show its capabilities to efficiently face semi-supervised heterogeneous multi-view problems combining linear and non-linear data representations. Besides, we extend the model formulation to provide the automatic selection of SVs, obtaining scalable solutions, as well as include an ARD prior over the kernel to obtain feature selection capabilities. The model performance is evaluated in multi-dimensional regression, feature selection over images and multiple-kernel learning problems demonstrating that the inclusion of kernelized observations provide fruitful results.
Appendices

A Mean field

In this section we want to expand some information about the model. In Figure 7 we can see the graphical model for the proposed version of KSSHIBA. Specifically, in this figure we also included the variables associated to every view, not only the kernel view.

![Graphical Model of SSHIBA with Kernelized Views (KSSHIBA)](image)

Figure 7: Complete graphical model of SSHIBA with kernelized views (KSSHIBA).

Table 3 shows the KSSHIBA mean-field factor update rules. For a compact notation, we stuck in matrix $Z$, of dimension $N \times K_c$, the latent projection of all data points and $<>$ represents the mean value of the rv. The derivation of these equations can be found in [14], where the data matrix $X^{(m)}$ is now $K^{(m)}$ and $W^{(m)}$ is now $A^{(m)}$ due to the change to the dual formulation.

| Variable | $q^*$ distribution | Parameters |
|----------|--------------------|------------|
| $z_{n,:}$ | $N(z_{n,:} ; \mu_{z_{n,:}}, \Sigma_Z)$ | $\mu_{z_{n,:}} = \sum_{m=1}^{M} (\langle \tau^{(m)} \rangle_K (A^{(m)}) \Sigma_Z)$ |
| $\Sigma^{-1}_Z = (I + \sum_{m=1}^{M} (\langle \tau^{(m)} \rangle (A^{(m)})^T A^{(m)}) \Sigma_Z)$ |
| $A^{(m)} = \prod_{n=1}^{N} \left( N \left( a^{(m)}_{n,:} ; \mu_{a^{(m)}_{n,:}}, \Sigma_{A^{(m)}} \right) \right)$ | $\mu_{a^{(m)}_{n,:}} = (\tau^{(m)})_K (Z) \Sigma_{A^{(m)}}$ |
| $\Sigma^{-1}_{A^{(m)}} = (\text{diag}((\alpha^{(m)}))) + (\tau^{(m)}) (Z^T Z)$ |
| $\alpha^{(m)}_k$ | $\Gamma(\alpha^{(m)}_k | a^{(m)}_k, b^{(m)}_k)$ | $a^{(m)}_k = \frac{D_m}{2} + a^{\alpha^{(m)}}$ |
| $b^{(m)}_k = b^{\alpha^{(m)}} + \frac{1}{2} (A^{(m)})^T A^{(m)})_{k,k}$ |
| $\tau^{(m)}$ | $\Gamma(\tau^{(m)} | a^{\tau^{(m)}}, b^{\tau^{(m)})}$ | $a^{\tau^{(m)}} = \frac{D_m N}{2} + a^{\tau^{(m)}$ |
| $b^{\tau^{(m)}} = b^{\tau^{(m)}} + \frac{1}{2} \left( \sum_{n=1}^{N} \sum_{\tilde{n}=1}^{\tilde{N}} k^{(m)}_{n,\tilde{n}} \right)^2$ |
| $-2 \text{Tr} \left( (A^{(m)})^T K^{(m)} \right)$ |
| $+ \text{Tr} \left( (A^{(m)})^T A^{(m)} | Z^T Z \right) \right)$ |

Table 3: Updated rules, obtained by a mean field approximation, of $q$ distribution for the different variables of KSSHIBA model.
Table 4 shows the KSSHIBA mean-field factor update rules for the double ARD case. This formulation is used for the automatic inducing point selection.

Table 4: Updated $q$ distribution for the automatic support vector selection.

| Variable | $q^*$ distribution | Parameters |
|----------|--------------------|------------|
| $A^{(m)}$ | $\prod_{n=1}^{N} \mathcal{N}(a_{\alpha(n)}^{(m)} | \mu_{a_{\alpha(n)}^{(m)}}, \Sigma_{a_{\alpha(n)}^{(m)}})$ | $\mu_{A^{(m)}} = \langle \tau^{(m)} \rangle X^{(m)^T}(Z) \Sigma_{W^{(m)}}$ |
| $\gamma^{(m)}$ | $\prod_{n=1}^{N} \Gamma(\gamma_{\alpha(n)}^{(m)} | a_{\gamma_{\alpha(n)}^{(m)}}, b_{\gamma_{\alpha(n)}^{(m)}})$ | $a_{\gamma_{\alpha(n)}^{(m)}} = \frac{K_{c}}{2} + a_{\gamma(n)}^{(m)}$ |

B Databases

One of the main advantages of KSSHIBA is that it is able to simultaneously work with heterogeneous data (multi-label, categorical and regression). For this reason, we used databases for different scenarios to test the functionalities of the proposed model. The databases will be separated in different subsections based on the context in which they are used.

B.1 Multi-target regression databases

To prove the performance of KSSHIBA we have used different multi-dimensional regression databases. In particular, we used databases from the Mulan repository \cite{22,23,24}, presented in Table 5.

Table 5: Characteristic of the multi-task databases used in this work.

| Database | Samples | Features | Tasks |
|----------|---------|----------|-------|
| at1pd    | 337     | 411      | 6     |
| at7pd    | 296     | 411      | 6     |
| oes97    | 334     | 263      | 16    |
| oes10    | 403     | 298      | 16    |
| edm      | 154     | 16       | 2     |
| jura     | 359     | 15       | 3     |
| wq       | 1,060   | 16       | 14    |
| enb      | 768     | 8        | 2     |
| slump    | 103     | 7        | 3     |

B.2 Images databases

To test the proposed feature selection extension, we decided to use images databases due to providing more illustrative learnt relevance. We also used the Labeled Faces in the Wild (LFW) dataset \cite{26}. We used an aligned version of the dataset obtained by \cite{29} in order to work with images that are comparable. At the same time, the images were cropped to eliminate undesirable information and resized to reduce the computational cost of training the models, having images of $60 \times 40$ pixels. To limit the size of the database we only used the images of the 7 people with most images in the database. We also used the warpAR10P ($60 \times 40$ pixels), Yale ($32 \times 32$ pixels) and Olivetti ($32 \times 32$ pixels) databases, which can be found from the Feature Selection Repository already preprocessed. The characteristics of these databases are described in Table 6.

\footnote{http://featureselection.asu.edu/datasets.php}
Table 6: Characteristic of the faces databases used in this work.

| Database    | Samples | Features | Classes |
|-------------|---------|----------|---------|
| LFW         | 1,277   | 2,400    | 7       |
| warpAR10P   | 130     | 2,400    | 10      |
| Yale        | 165     | 1,024    | 15      |
| Olivetti    | 400     | 1,024    | 40      |

B.3 Classification databases

Finally, we used two different databases to analyse the extracted features and to assess the multi-view formulation of the model. We decided to used the widely available Oil [27] and MNIST [28] databases respectively. Due to the large amount of samples in the MNIST database and to be able to test the kernelized observations, we decided to only use 1,000 samples for the experiment. The description of the databases is available in Table 7.

Table 7: Characteristic of the faces databases used in this work.

| Database | Samples | Features | Classes |
|----------|---------|----------|---------|
| Oil      | 2,000   | 12       | 3       |
| MNIST    | 1,000   | 784      | 10      |

C Implementation details

We calculated the reported results with a nested 10-folds cross-validation. The outer CV is used to divide the dataset into training and test partitions, while the inner CV is in charge of validation and, therefore, it divides the training partition into a second training set and a validation set. This way we were able to estimate the performance of the whole framework and, additionally, validate the model parameters.

We used the coefficient of determination, R², to compare the performance of the different variations of the methods and to adjust the method hyperparameters, which were cross-validated.

To determine the number of iterations of the inference process of KSSHIBA, we used a convergence criteria based on the evolution of the lower bound. In particular, we stop the algorithm either when $\text{mean}(LB[-101 : -2]) > LB[-1](1 - 10^{-4})$, where $LB[-1]$ is the lower bound at the last iteration and $\text{mean}(LB[-101 : -2])$ the mean value of the previous values of the lower bound, or when it reaches $10^4$ iterations. The KSSHIBA models were randomly initialized 10 times, keeping the one with the best lower bound.

The implementation of this project was done using Python 3.7 and the cross validation was carried out using the package StratifiedKFold from Scikit-learn [30].

D Baselines

In order to truthfully compare the performance of the proposed algorithm, we decided to compare it with some state-of-the-art comparable to ours. In particular we wanted to focus on some of the most relevant algorithms for factor analysis. As we proposed a kernel version of a model we decided to compare to KPCA and KCCA with a gaussian (rbf) kernel to include non-linearity in the data. For each of these models we explored 20 values of $\gamma$ in logarithmic scale from $10^{-8}$ to $10^{10.5}$ divided by the number of tasks ($C$). In order to carry out predictions KPCA was combined with linear regression (LR), as KCCA can work in a supervised manner, we decided to use it with and without the LR for comparative purposes. Equivalently to KSSHIBA, which automatically selects the number of latent factors ($K_c$), we decided to use a criteria to determine the number of latents for KPCA and KCCA, in
particular we set them to the factors that explain 95% of the variance and number of tasks minus one $(C - 1)$ respectively. To compare the performance with different numbers of SVs, KPCA and KCCA followed Nyström [25] subsampling technique and cross-validated the optimum percentage of SVs from $[1, 2, 3, 4, 5, 10, \ldots, 100]$%.

Due to the equivalency to some of our functionalities, we compared our model with Manifold Relevance Determination (MRD), a shared GPLVMs approach that provides a non-linear latent representation for multi-view learning problems, extended in [18], including an Automatic Relevance Determination (ARD). We used the available library in Matlab setting the number of inducing points to the number of samples and the number of latents to twice the number of tasks $(2 + C)$. We used the rbf kernel with ard and set the number of model optimisation iterations to 100 due to the long computational time required to trained them.

Another kernel model used to compare with ours is SVR, where we also used a rbf kernel, exploring the same values of $\gamma$. The regularization parameter, $C$, has also been validated, exploring $11$ values in a logarithmic scale from $[10^{-4} \text{ to } 10^4]$.

Finally, we wanted to compare our model with a MLP neural network in two different scenarios: A different approach is also proven to compare the KSSHIBA. Now a MLP neural network where the dimensionality reduction comes by forcing it as a bottleneck in a hidden layers. The optimizer has been chosen to be Adam and the structure has been validated among two approaches:

- **MLP $(C - 1)$**: in this case we wanted to force a bottleneck in the hidden layers to have the same dimensionality reduction KCCA has. For this scenario, we validated two different configurations:
  - One hidden layer with $C - 1$ neurons.
  - Two hidden layer with $C - 1$ neurons and number of features $(D_m)$ neurons respectively.

- **MLP**: for this scenario we didn’t include a bottleneck, validating between these configurations:
  - One hidden layer with 100 neurons.
  - Two hidden layers with 100 and 50 neurons respectively.
  - Three hidden layers with 100, 50 and 100 neurons respectively.

### E Extended experiments

In this section we present a more extensive version of the results presented in the article. These results include some databases and baselines that we did not include due to the space limitations or the lack of relevance of the results. In particular, Table 8 includes KCCA and a MLP where the second hidden layer works as a feature extractor, including a bottleneck of $C - 1$.

Furthermore, Figure 8 depicts a comparison between the computational time needed to train KSSHIBA in Python and the MRD implementation available for Matlab. For this experiment we trained both models with different number of samples and measured the time needed to train each model.

Finally, Figure 9 presents the analysis of the effect of the number of SVs or inducing points (MRD) analysed in the Evaluation of the solution in terms of SVs. In particular, we include here the results obtained for the databases not included in the main article. The results on MRD are not included for the wg database because the model iterations have not ended at the moment this material is done due to the high computational time required by the library.

### Broader Impact

This article proposes a multi-view semi-supervised sparse model with kernelized observations that combine dimensionality reduction with estimation and classification problems functionalities. As such, it may impact potential solutions for problems characterized by multiple view data. Open source-code with exemplary Python notebooks will be released to ensure maximal dissemination.
Table 8: Results on the multitask databases of the KSSHIBA and the different methods under study. In this case the data is normalised and the kernel, if applied, is centred. Each subrow represents the mean and standard deviation of the R2 score (white) and latent factor (light gray) used, respectively.

|          | KSSHIBA | KSSHIBA $K_c = C - 1$ | MRD | KPCA + LR | KCCA | KCCA + LR | SVR rbf | MLP $K_c = C - 1$ | MLP |
|----------|---------|------------------------|-----|-----------|------|-----------|---------|-----------------|-----|
| oes97    | 0.63 ± 0.16 | 0.63 ± 0.17 | 0.34 ± 0.07 | 0.45 ± 0.20 | 0.33 ± 0.07 | 0.42 ± 0.22 | 0.39 ± 0.10 | 0.54 ± 0.24 | 15  |
| oes10    | 0.79 ± 0.08 | 0.76 ± 0.10 | 0.38 ± 0.07 | 0.50 ± 0.15 | 0.28 ± 0.06 | 0.60 ± 0.14 | 0.47 ± 0.12 | 0.75 ± 0.07 | 15  |
| edm      | 0.37 ± 0.19 | 0.16 ± 0.08 | -0.17 ± 0.45 | 0.38 ± 0.19 | 0.06 ± 0.08 | 0.15 ± 0.33 | 0.35 ± 0.19 | 0.69 ± 0.30 | 15  |
| jura     | 0.61 ± 0.10 | 0.22 ± 0.14 | 0.57 ± 0.06 | 0.38 ± 0.11 | -0.07 ± 0.09 | -0.56 ± 0.44 | 0.60 ± 0.05 | 0.23 ± 0.45 | 0.61 ± 0.06 |

Figure 8: Computational cost comparative between KSSHIBA and MRD.
Figure 9: R2 results with different percentages of SVs in the KSSHIBA, KCCA+LR and KPCA+LR or inducing points in MRD.

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