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Robust Generative Restricted Kernel Machines using Weighted Conjugate Feature Duality*

Introduction

Training performance can be highly affected by contamination, where outliers are encoded in the representation of the model. This results in the generation of noisy data. Here we introduce a weighted conjugate feature duality in the framework of Restricted Kernel Machines (RKMs). This formulation is used to fine-tune the latent space of generative RKMs using a weighting function based on the *Minimum Covariance Determinant* (MCD), which is a highly robust estimator of multivariate location and scatter. Experiments demonstrate the merit of the proposed work.

Contributions

- Introduced Robust Gen-RKM using *weighted conjugate-feature duality*.
- *Weighting function* based on MCD to identify & penalize the outliers in the latent space.
- Experiments demonstrate the *regularization* of latent-space thereby preserving the properties of Gen-RKM model.

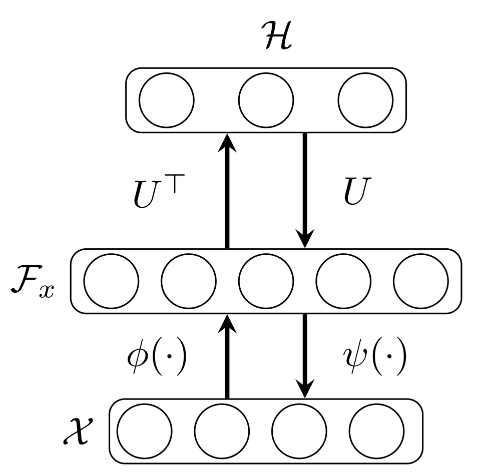


Figure: Schematic representation of Gen-RKM. The feature map and pre-image map correspond to ϕ and ψ respectively. The interconnection matrix U models dependencies between latent variables and the input data.

Weighted Conjugate Feature Duality

Let $D \succ 0$, then for any $e, h \in \mathbb{R}^n$, $\lambda > 0$:

$$\frac{1}{2\lambda} e^\top D e + \frac{\lambda}{2} h^\top D^{-1} h \geq e^\top h.$$

Substituting in KPCA objective:

$$\min_{U,e} \ \frac{\eta}{2}\mathrm{Tr}(U^\top U) - \frac{1}{2\lambda} e^\top D e$$
$$\text{s.t. } e_i = U^\top \phi(x_i), \quad \forall i = 1, \ldots, N,$$

yields the RKM training objective.

Explainability Aspect

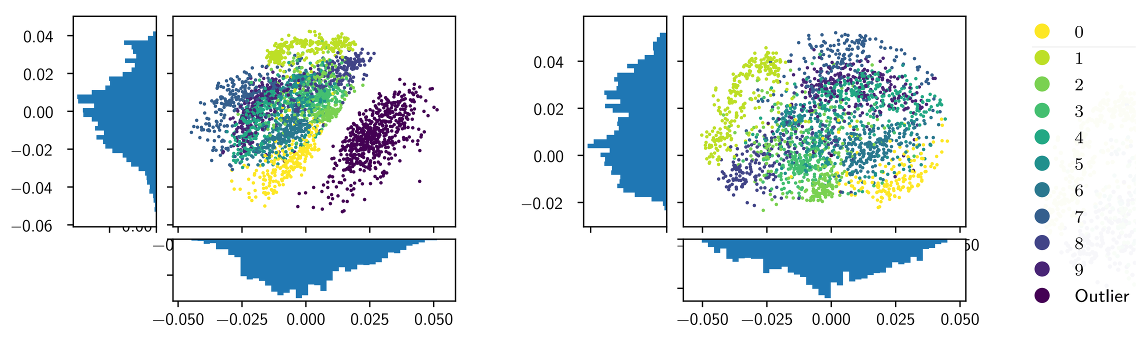
- Direct links with Restricted Boltzmann Machines
- Latent variables in RKMs corresponds to hidden variables in RBMs that are modelled by individual neurons.
- Latent space exploration (and uncorrelated feature learning) enhances the interpretability of the model.

RKM Training Objective

$$\mathcal{J} = \frac{\eta}{2}\mathrm{Tr}(U^\top U) + \sum_{i=1}^{N} -\phi(x_i)^\top U h_i + \frac{\lambda}{2} D_{ii}^{-1} h_i^\top h_i$$

Incase of explicit feature-map, joint training objective, for $c, \gamma > 0$ and reconstruction loss $\mathcal{L}(\cdot)$:

$$\min_{\theta,\zeta} \ \mathcal{J}^D = \mathcal{J} + \frac{c}{2}(\mathcal{J})^2 + \frac{\gamma}{N}\sum_{i=1}^{N} D_{ii}\mathcal{L}(x_i, \psi_\zeta(\phi_\theta(x_i)))$$



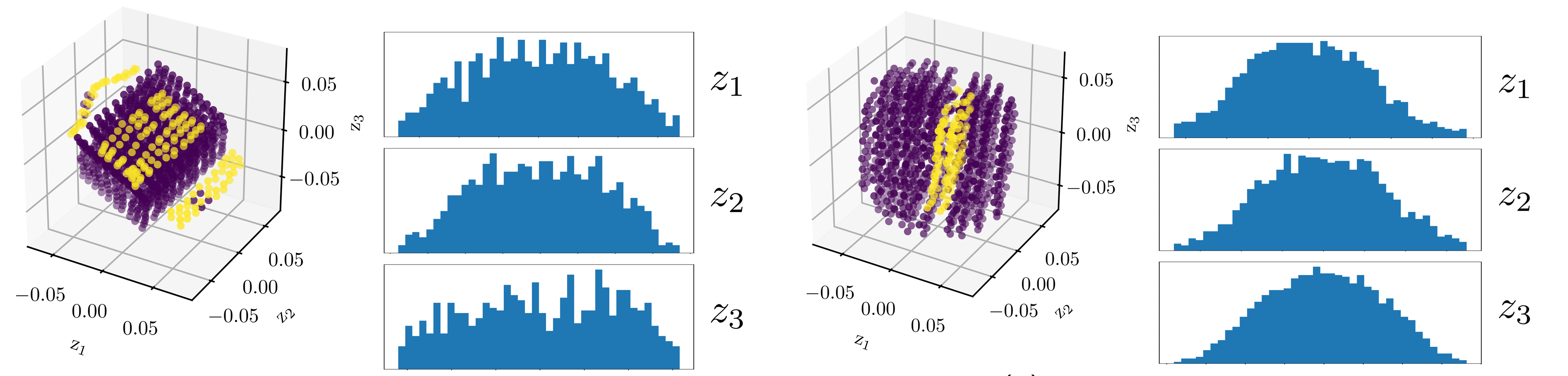
(a) Gen-RKM (b) Robust Gen-RKM

Figure: MNIST: Scatter-plot of latent variables, showing robustness against the outliers with 20% contamination in training set. Left figure shows the latent space of Gen-RKM, the right figure shows the robust version. Presence of outliers distorts the distribution of latent variables and by penalizing the outliers, histogram resembles a Gaussian distribution.

Outlier Detection in latent space

$$D_{ii} = \begin{cases} 1 & \text{if } d_i^2 \leq \chi^2_{s,\alpha} \\ 10^{-4} & \text{otherwise,} \end{cases}$$

where $d_i^2 = (h_i - \hat{\mu})^\top \hat{S}^{-1}(h_i - \hat{\mu})$ is squared Mahalanobis distance. Here $\hat{\mu}$ and $\hat{S}$ are the robustly estimated mean and covariance matrix respectively using the MCD estimator.



(a) Gen-RKM (b) Robust Gen-RKM

Figure: 3DShapes dataset: Scatter-plot of latent variables. Clean data is shown in purple, outliers in yellow. The training subset is contaminated with a fourth generating factor (20% of the data is considered as outliers). The outliers are penalized in the robust Gen-RKM, which moves them towards the origin.

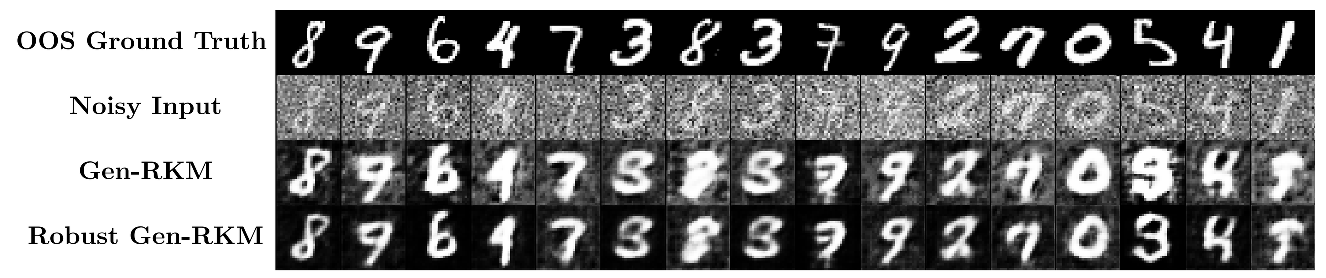


Figure: Robust denoising on the MNIST dataset. 20 % of the training data is contaminated with noise. The first and second row show the clean and noisy test images respectively. The third and fourth row show the denoised image using the Gen-RKM and robust Gen-RKM.

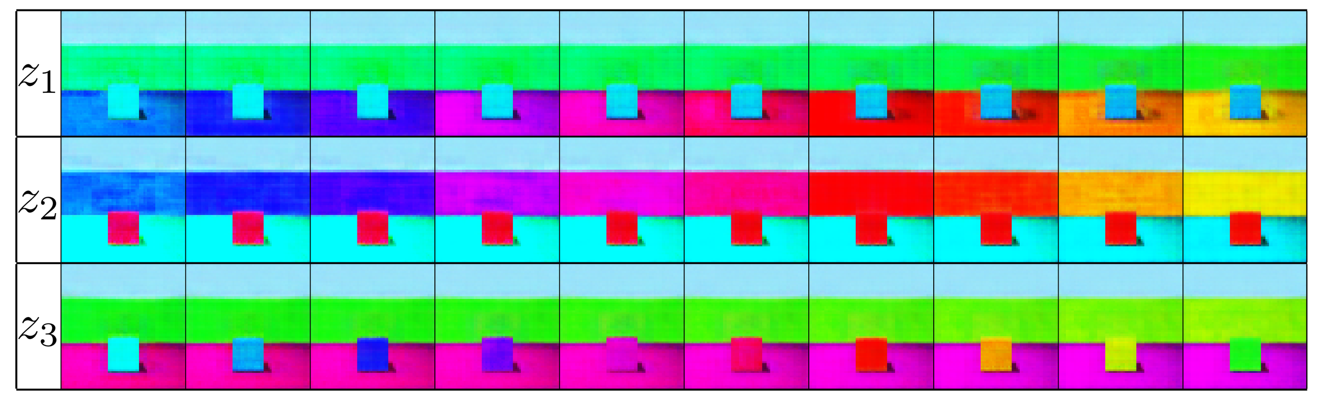
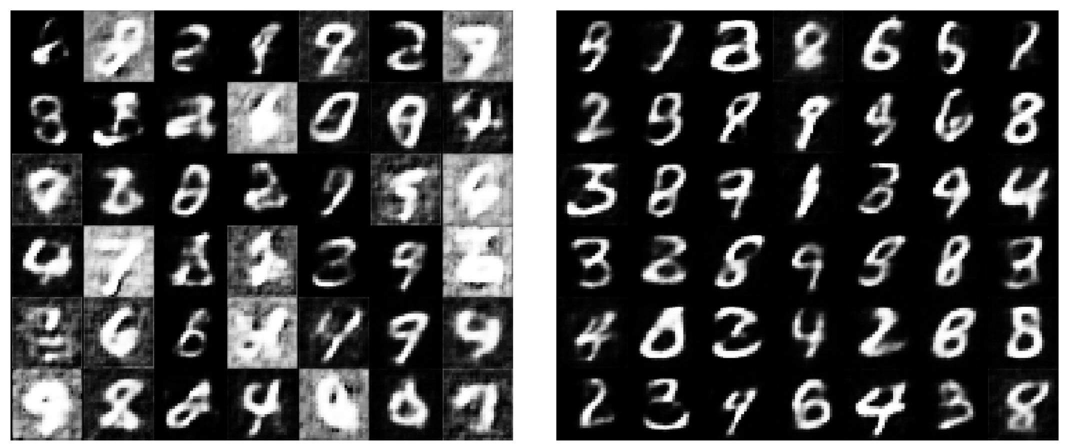


Figure: Illustration of latent traversals along the 3 latent dimensions for 3DShapes dataset using the robust Gen-RKM model. The first, second and third row distinctly captures the floor-hue, wall-hue and object-hue respectively while keeping other generative factors constant.



(a) Gen-RKM (b) Robust Gen-RKM

Figure: MNIST: Randomly generated images. When using robust procedure, the model does not encode the noisy images. As a consequence, no noisy images are generated.

Dataset	Fréchet Inception Distance	
MNIST	Gen-RKM	Robust Gen-RKM
	135.95	**87.03**
Fashion-MNIST	Gen-RKM	Robust Gen-RKM
	163.70	**155.32**

Table: FID Scores for 3000 randomly generated samples.

Conclusion

- Using weighted conjugate feature duality, RKM formulation for weighted kernel PCA is proposed.
- Highly robust estimator based on MCD is proposed to detect outliers in latent space.
- Consequently, a weighting scheme is proposed to penalize the outliers.
- Experiments demonstrate that the model is capable of generating denoised images.
- Furthermore, being a latent variable model, Robust Gen-RKM preserves the disentangled representation.

*https://arxiv.org/abs/2002.01180