Identifiable deep generative models via sparse decoding

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Collaborators

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University of Montreal and Mila

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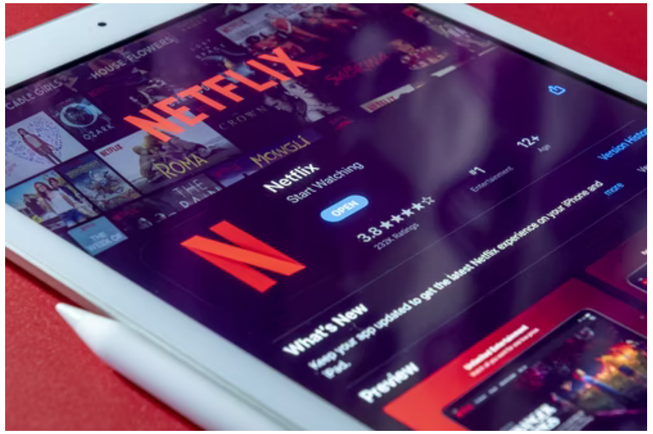
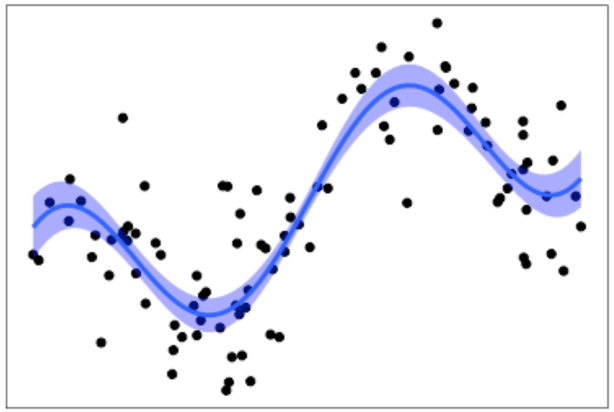
University of Michigan

Dave Blei
Columbia University



We have large, complicated data; we want **meaningful representations** of it.

What is a **meaningful representation**?



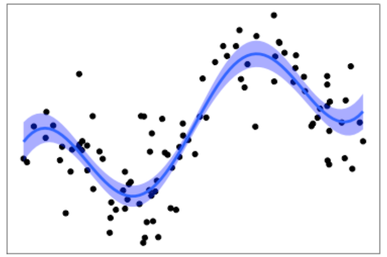
Flexible: capture nonlinear associations

Interpretable: what features are associated?

Identifiable: one optimal representation

Past work (non-exhaustive)

Interpretable



Flexible

Linear methods

- Nonnegative matrix factorization
  Donoho and Stodden, 2003
- Anchored topic models *Arora et al. 2013*
- Anchored linear factor analysis *Bing et al. 2020*
- PCA+Varimax *Rohe and Zeng, 2020*

Identifiable

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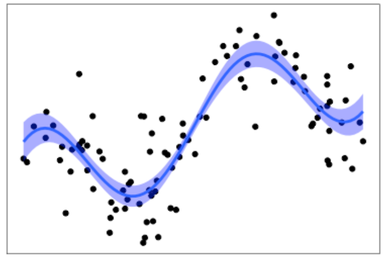

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Identifiable

Weakly supervised methods

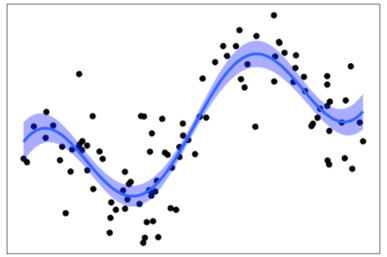
- Auxiliary data *Khemakhem et al. 2020*
- Data augmentation *von Kügelgen et al. 2021*
- Temporal information *Locatello et al. 2020, Hälvä et al. 2021, Lippe et al. 2022*

Constraints on function classes

- Independent mechanisms *Gresele et al. 2022*
- Sparse structure *Zheng et al. 2022*

Past work (non-exhaustive)

- Output-Interpretable VAE
  Ainsworth et al. 2018



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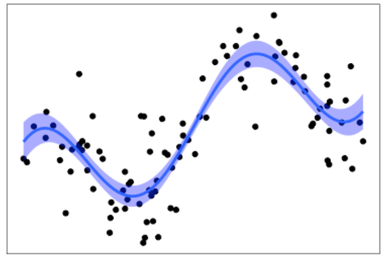

Interpretable

Identifiable deep generative models via sparse decoding *Moran et al. 2022*

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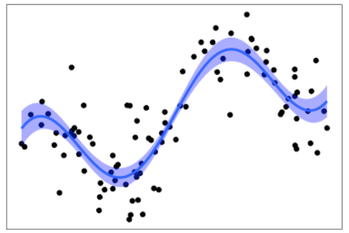
This work

The Sparse VAE: introduce sparsity into a flexible factor-to-feature mapping

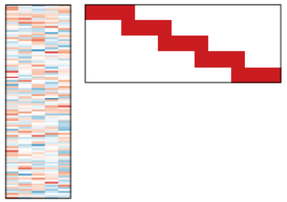


- **Flexible:** fits a neural network model with a variational autoencoder (VAE)

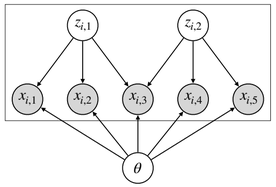
- **Interpretable:** can inspect which features are important for the representation

- **Identifiable:** a single optimal representation (under certain assumptions)

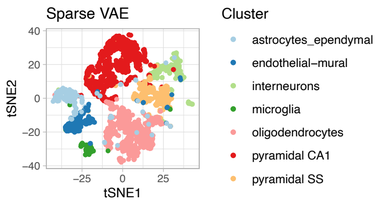
Roadmap



Identifiability and the role of sparsity



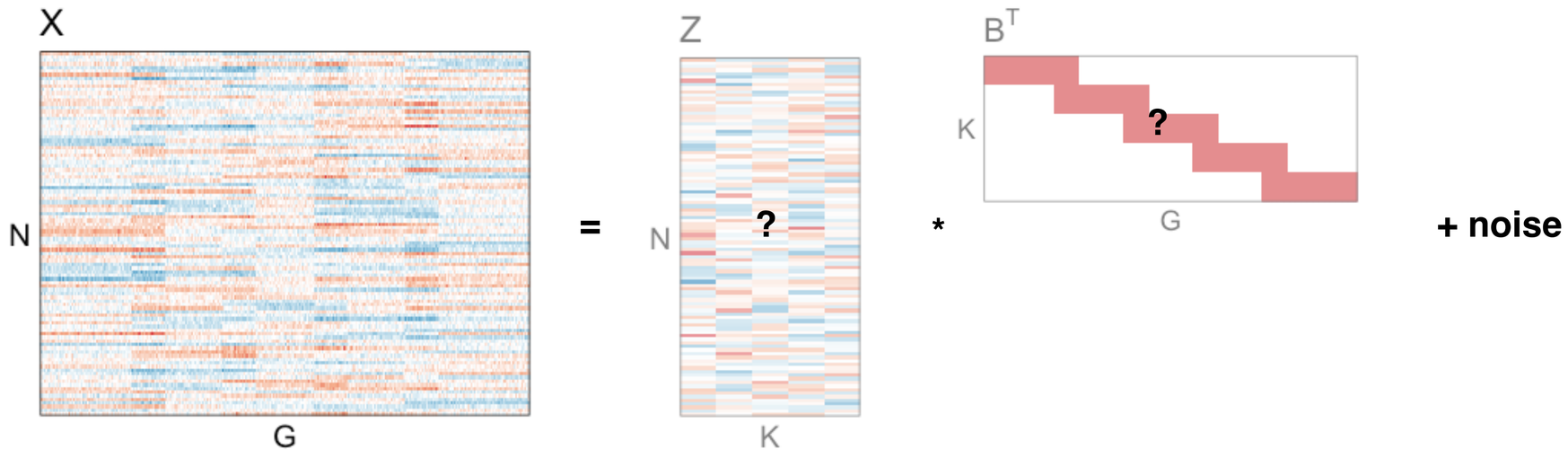
The Sparse VAE



Experimental results

The linear case

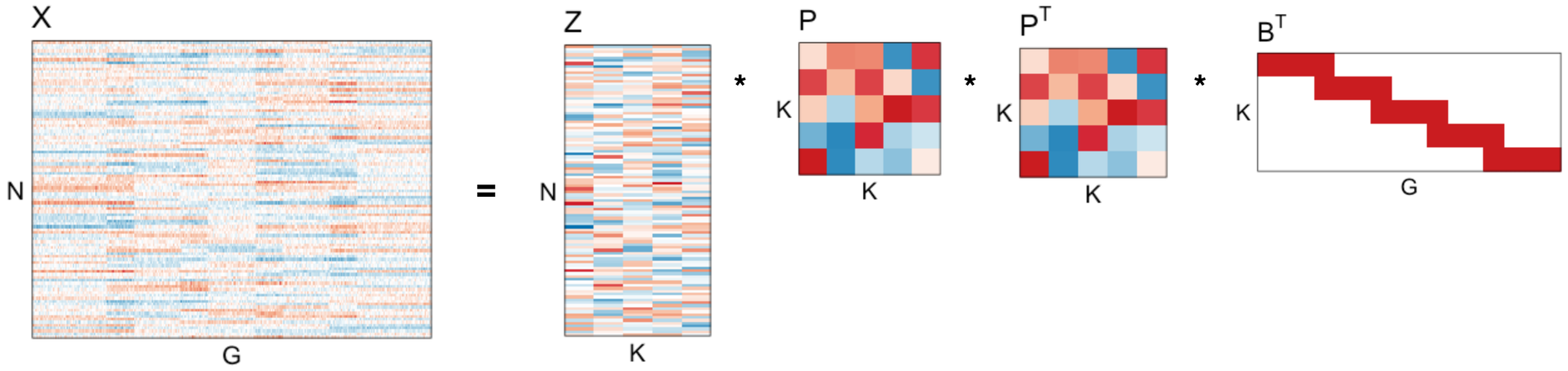
Linear factor analysis model: $\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{B}^T + \boldsymbol{E}$



- Data: $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N]^T \in \mathbb{R}^{N \times G}$
- Latent factors: $\boldsymbol{Z} = [\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N]^T \in \mathbb{R}^{N \times K}$
- Latent loadings: $\boldsymbol{B} = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_K] \in \mathbb{R}^{G \times K}$
- Noise: $\boldsymbol{E} = [\boldsymbol{e}_1, \ldots, \boldsymbol{e}_N] \in \mathbb{R}^{N \times G}$

Lack of identifiability

Linear factor analysis model: $\boldsymbol{X} = (\boldsymbol{ZP})(\boldsymbol{BP})^T + \boldsymbol{E}, \quad \boldsymbol{PP}^T = \boldsymbol{I}$



+ noise

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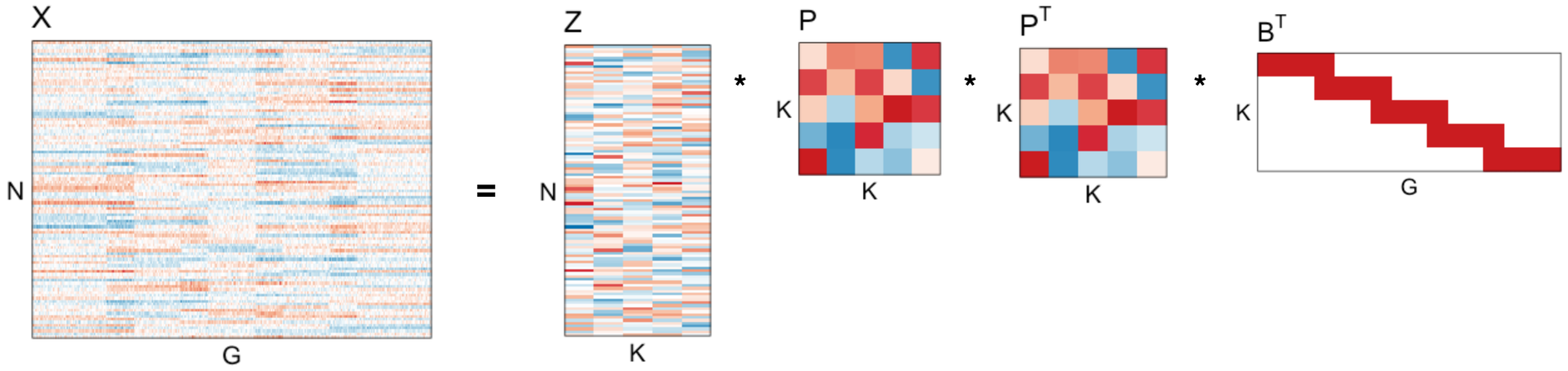

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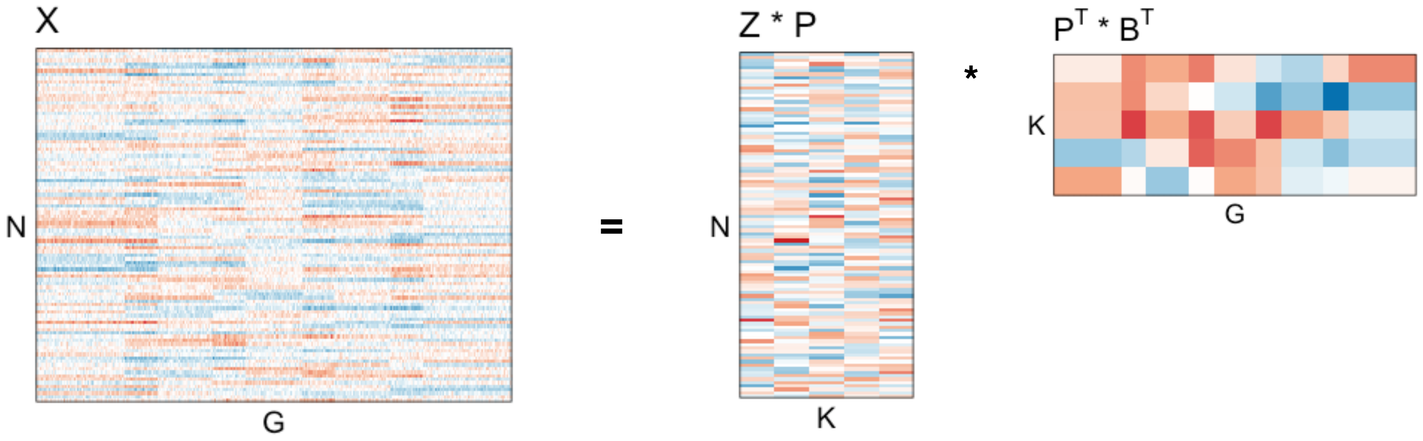

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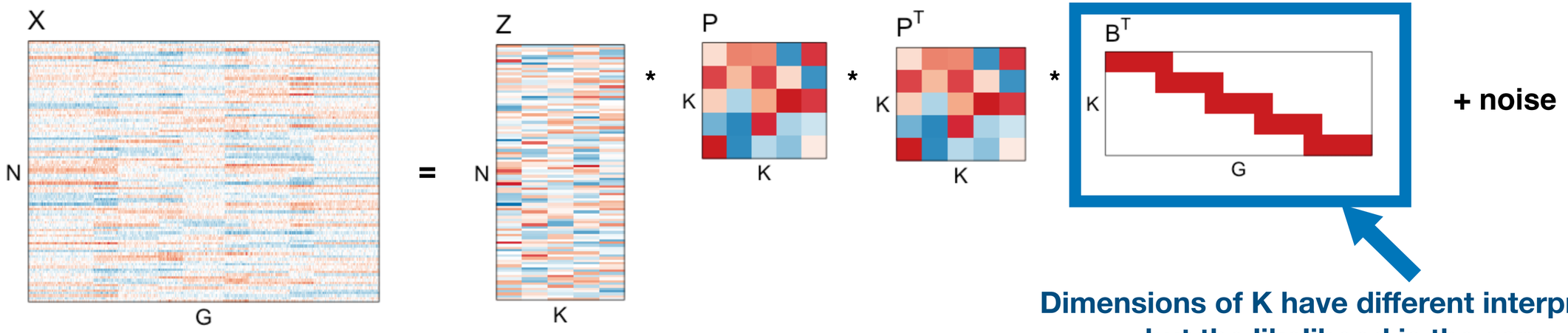
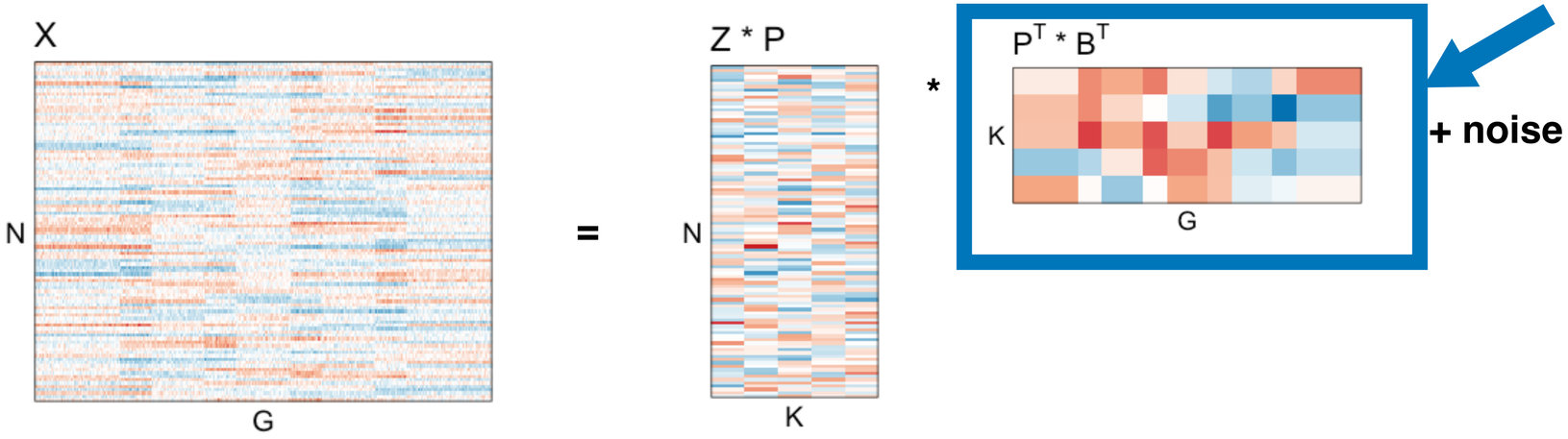


Dimensions of K have different interpretations but the likelihood is the same... which to choose?

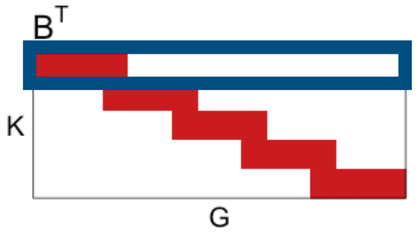


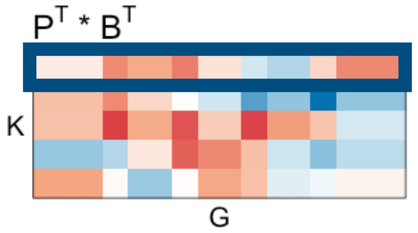
Lack of identifiability

Some problems:

- **Exploratory data analysis:** may select wrong features for further hypothesis testing

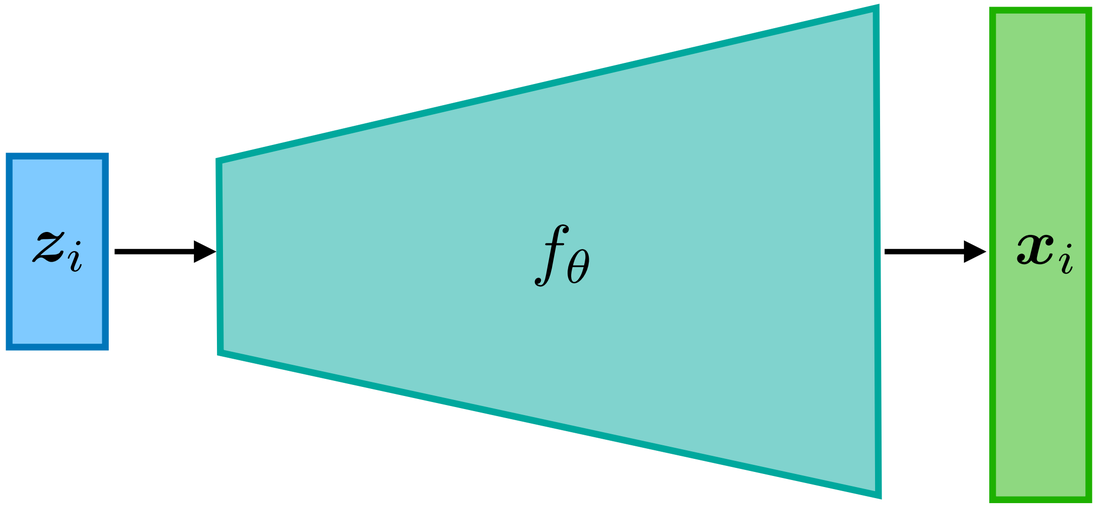
- **Generalization:** if factor-to-feature mapping mixes dimensions, may not generalize well to differently distributed factors





The nonlinear case

- Deep generative model: $\boldsymbol{x}_i = f_\theta(\boldsymbol{z}_i) + \boldsymbol{\varepsilon}_i, \quad \boldsymbol{\varepsilon}_i \sim \mathcal{N}_G(0, \Sigma)$



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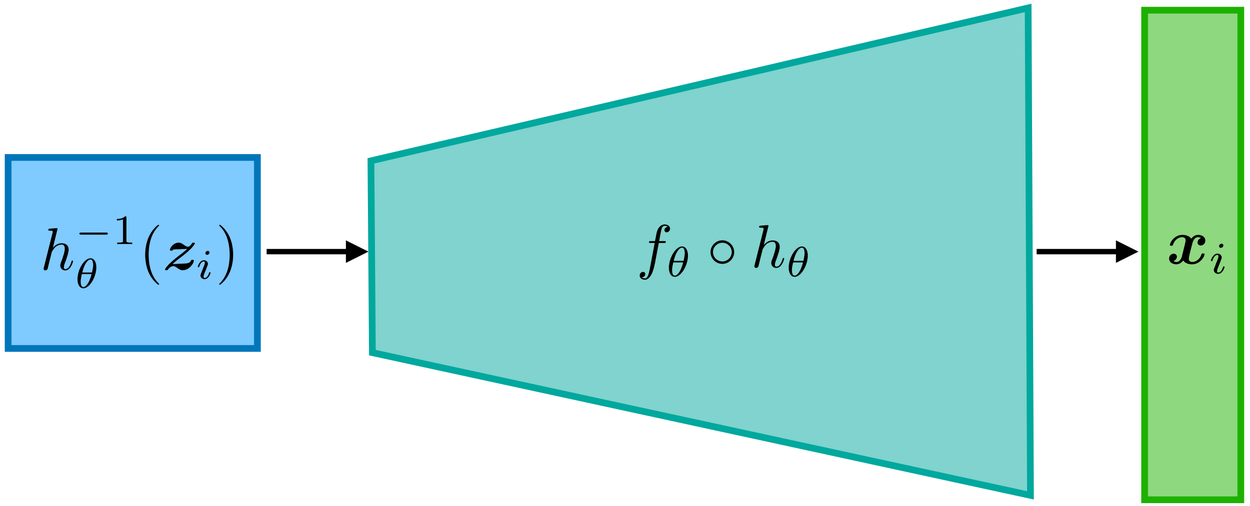

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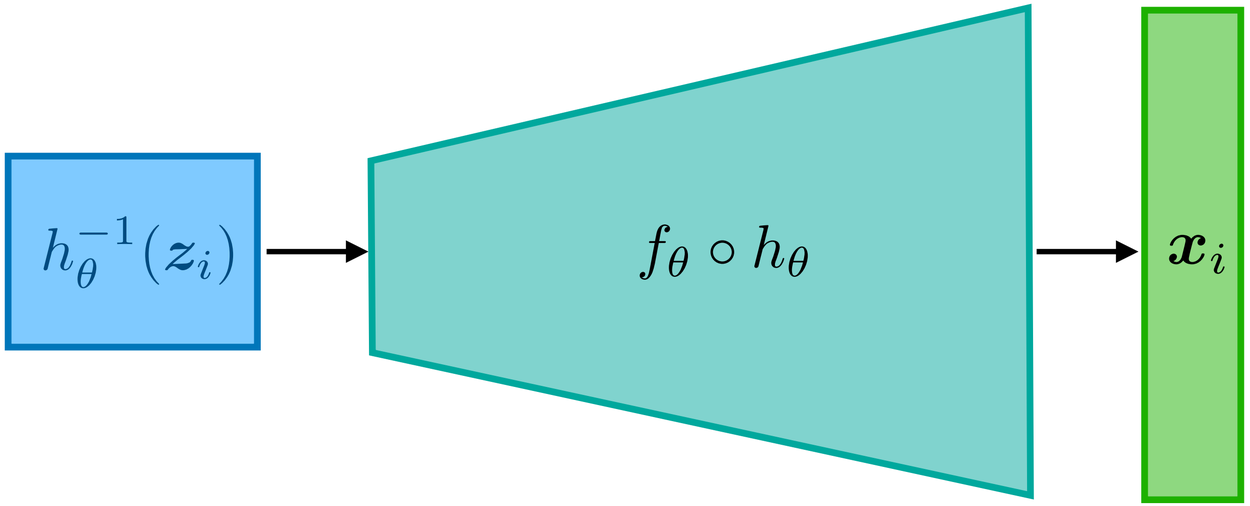

z_i and $h_\theta^{-1}(z_i)$ can have very different interpretations... which to choose?

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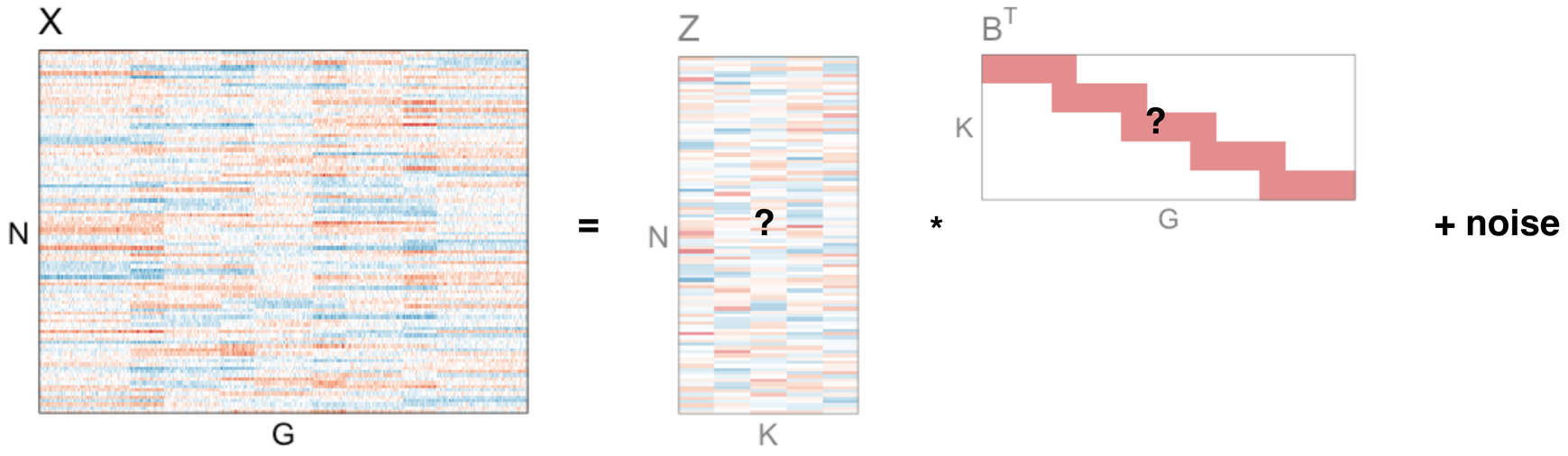
How can sparsity help?

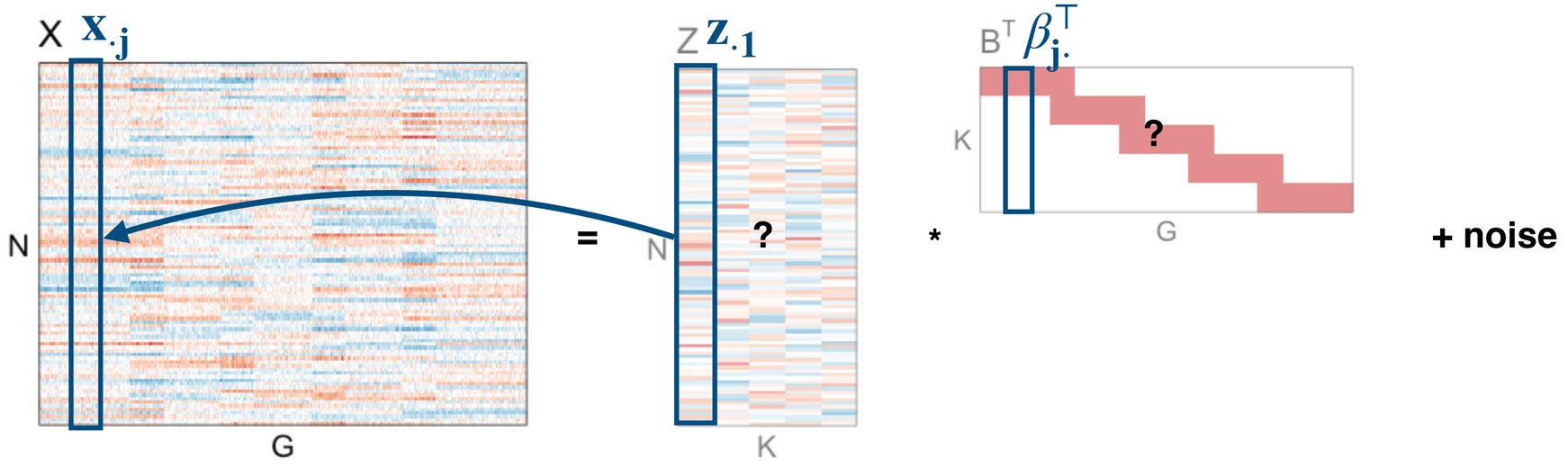


Linear factor analysis

<u>Theorem</u> [*Bing et al. 2020*] Factors z are identifiable if, for every $k = 1, \ldots, K$, there are at least two **anchor features** (+ other assumptions)

How can sparsity help?

$$\mathbf{x}_{\cdot \mathbf{j}} = \mathbf{z}_{\cdot \mathbf{1}} \times \beta_{j1} + \varepsilon_{\cdot j}$$



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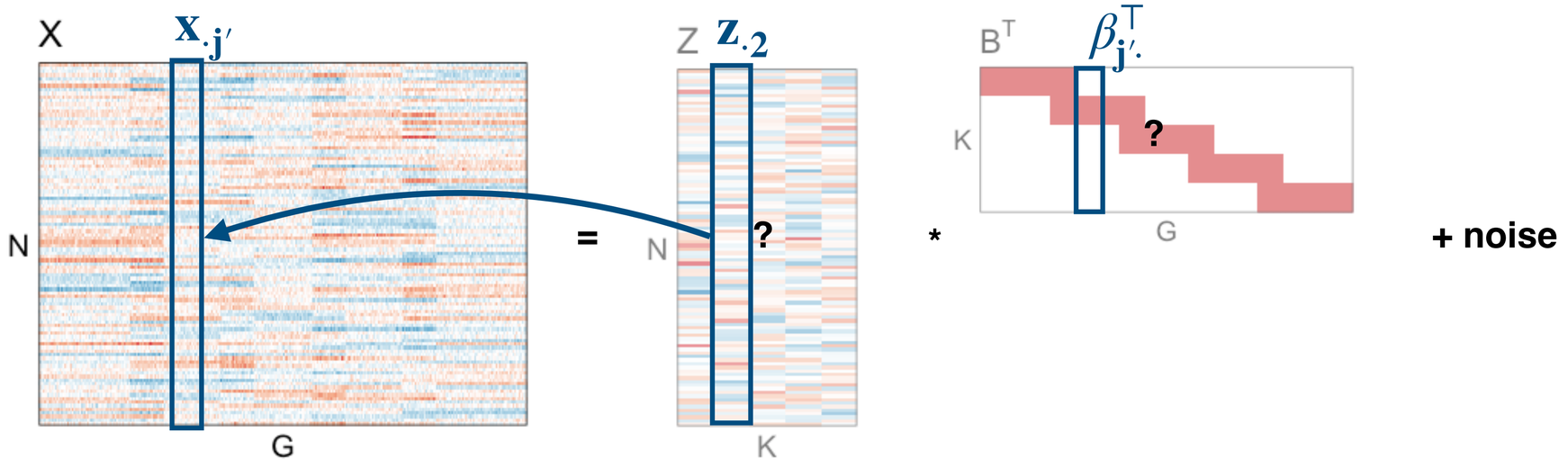
How can sparsity help?

$$\mathbf{x}_{\cdot \mathbf{j}'} = \mathbf{z}_{\cdot \mathbf{2}} \times \beta_{j'2} + \varepsilon_{\cdot j'}$$



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Our work: how do we generalize this to the nonlinear case?

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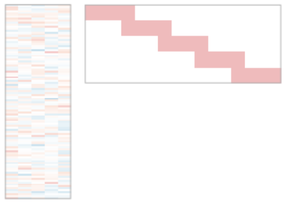
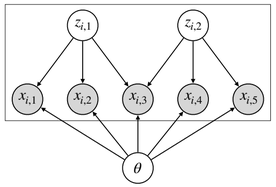
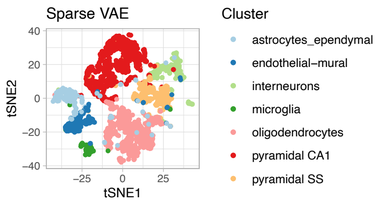
Roadmap



Identifiability and the role of sparsity



The Sparse VAE

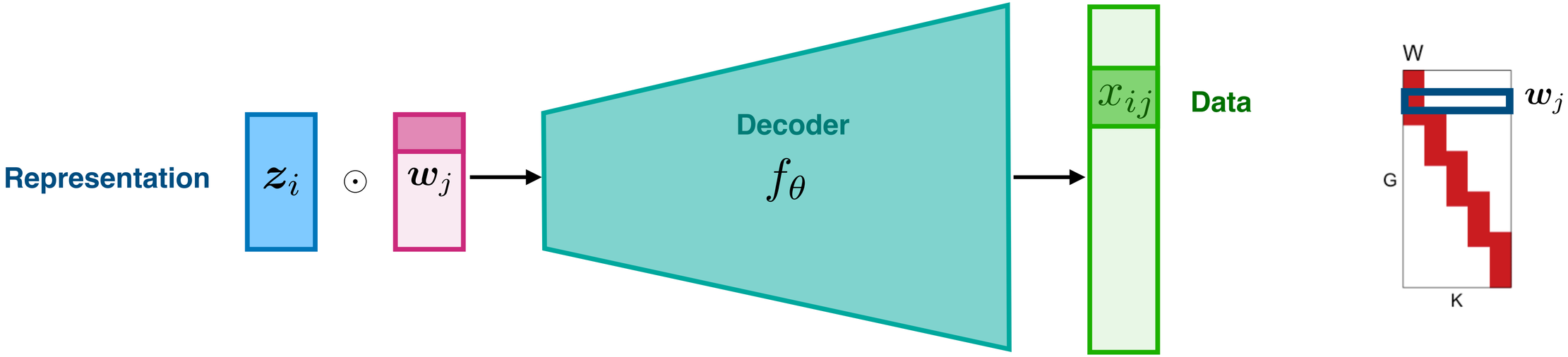


Experimental results

Setup

- Sparse deep generative model: $x_{ij} = f_\theta(\boldsymbol{w}_j \odot \boldsymbol{z}_i)_j + \varepsilon_{ij}, \quad \varepsilon_{ij} \sim \mathcal{N}(0, \sigma_j^2)$

- Introduces masking matrix: $\boldsymbol{W} = [\boldsymbol{w}_1, \ldots, \boldsymbol{w}_G]^T \in \mathbb{R}^{G \times K}$



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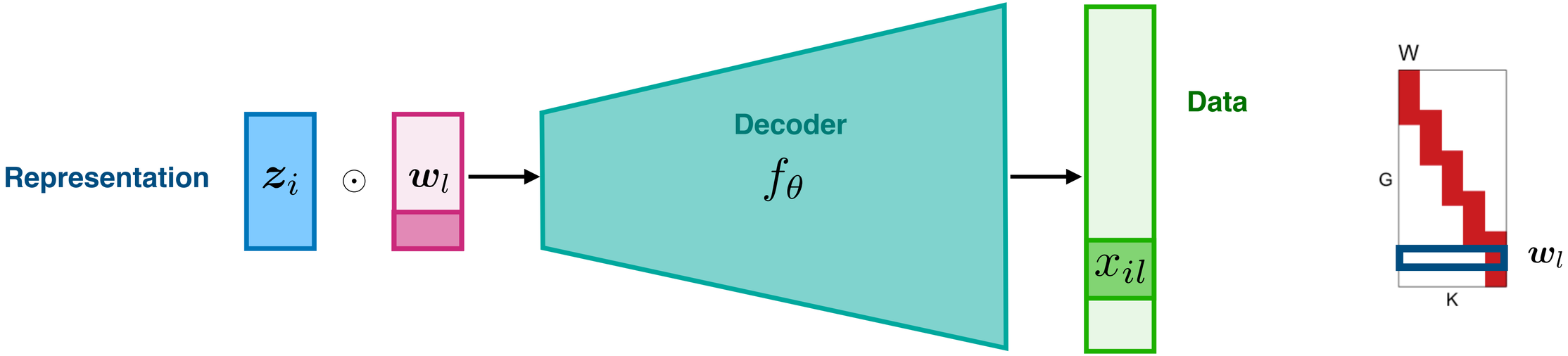

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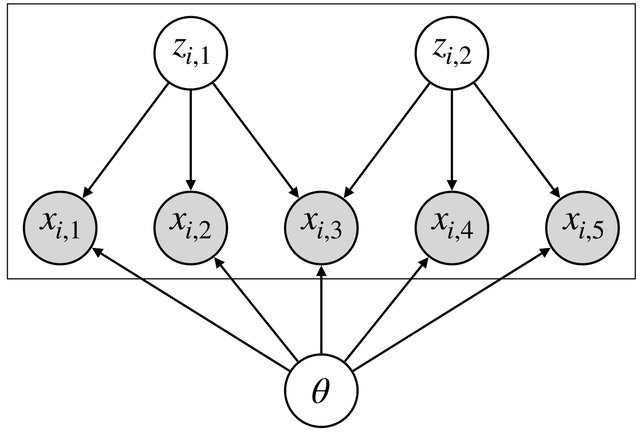
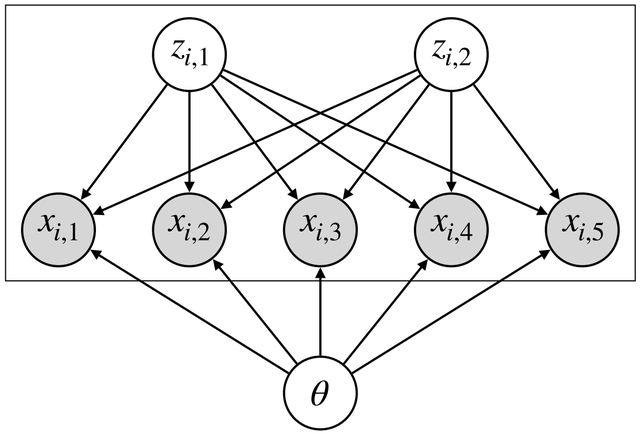


Deep generative model



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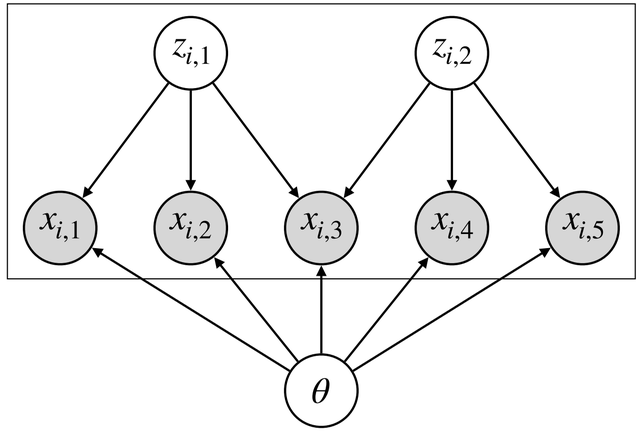
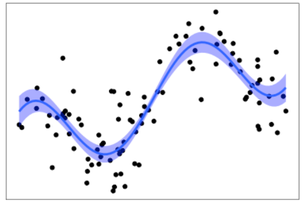
Sparse deep generative model





Flexible: uses neural networks for encoder and decoder

Interpretable: can inspect which features depend on which factors

Identifiability

Identifiable: a single optimal representation

Formal definition:

- if two solutions $\{\theta, Z\}$ and $\{\widetilde{\theta}, \widetilde{Z}\}$ have equal likelihood $p_\theta(\boldsymbol{X}|\boldsymbol{Z}) = p_{\widetilde{\theta}}(\boldsymbol{X}|\widetilde{\boldsymbol{Z}})$, then we must have $\{\theta, Z\} = \{\widetilde{\theta}, \widetilde{Z}\}$.

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Our goal:

- each dimension of $Z = (z_{\cdot 1}, \ldots, z_{\cdot K})$ is identified up to coordinate-wise transform
- i.e. if two solutions $\boldsymbol{Z}, \widetilde{\boldsymbol{Z}}$ have equal likelihood, then $z_{\cdot k} = g_k(\widetilde{z}_{\cdot k})$

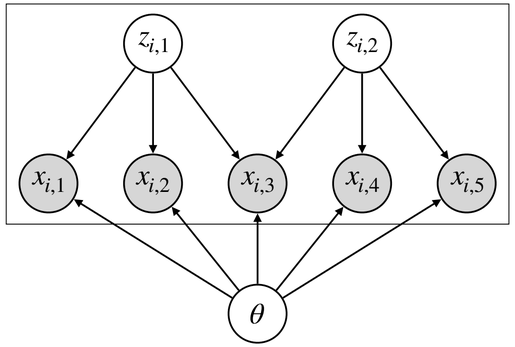
Identifiability

- <u>Theorem</u> *[Moran et al. 2021]* Factors Z are identifiable (up to coordinate-wise transform) under the following assumptions:

For each factor k, there are two features with

$$\mathbb{E}[x_{ij}|\boldsymbol{z}_i] = \mathbb{E}[x_{ij'}|\boldsymbol{z}_i] = f(z_{ik})$$

1. Anchor features



Suppose j is an anchor feature for factor k. For a non anchor feature l, we have

$$|w_{jk}| \sum_{i=1}^{N} |B_{ijk}|^2 \geq \sum_{i=1}^{N} \sum_{k'=1}^{K} |w_{lk'}||B_{ijk}||B_{ilk'}|$$

where $B_{ijk} = \dfrac{\partial f_\theta(\boldsymbol{w}_j \odot \boldsymbol{z}_i))_j}{\partial z_{ik}}$.

2. Scale of neural network

$$\min\{\mathrm{Var}(z_{ik}), \mathrm{Var}(z_{ik'})\} > |\mathrm{Cov}(z_{ik}, z_{ik'})|$$

3. Factor covariance

Identifiability

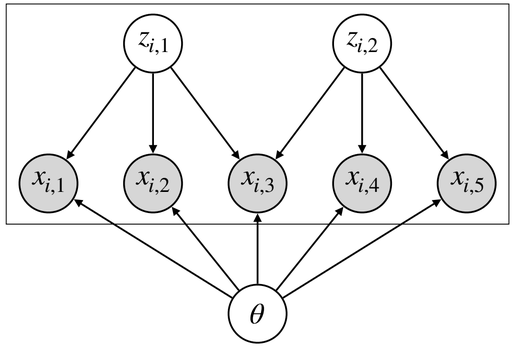
- <u>Theorem</u> *[Moran et al. 2021]* Factors Z are identifiable (up to coordinate-wise transform) under the following assumptions:

For each factor k, there are two features with

$$\mathbb{E}[x_{ij}|\boldsymbol{z}_i] = \mathbb{E}[x_{ij'}|\boldsymbol{z}_i] = f(z_{ik})$$

don't need to be known in advance

1. Anchor features



Suppose j is an anchor feature for factor k. For a non anchor feature l, we have

$$|w_{jk}| \sum_{i=1}^{N} |B_{ijk}|^2 \geq \sum_{i=1}^{N} \sum_{k'=1}^{K} |w_{lk'}||B_{ijk}||B_{ilk'}|$$

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2. Scale of neural network

$$\min\{\mathrm{Var}(z_{ik}), \mathrm{Var}(z_{ik'})\} > |\mathrm{Cov}(z_{ik}, z_{ik'})|$$

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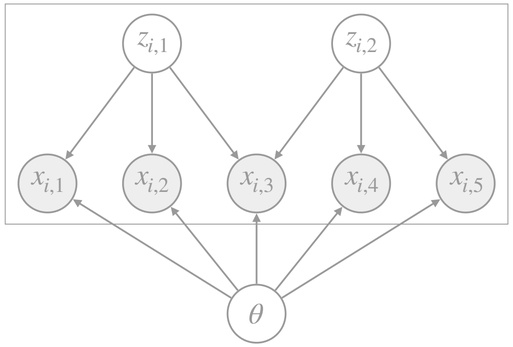

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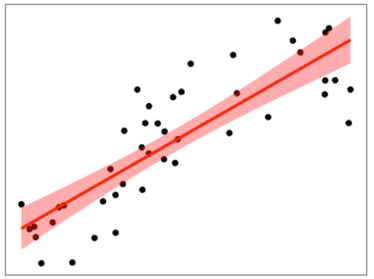

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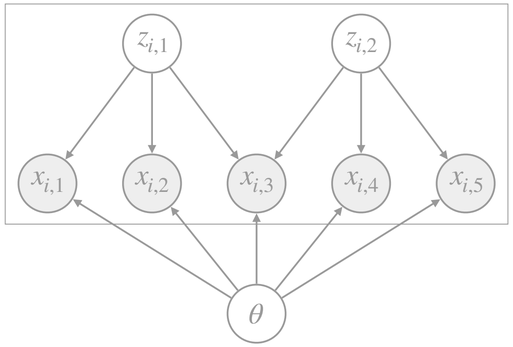

Suppose j is an anchor

Satisfied by neural networks with ReLU activations and independent weights

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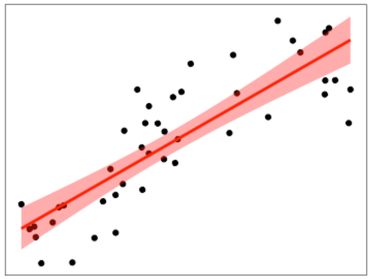

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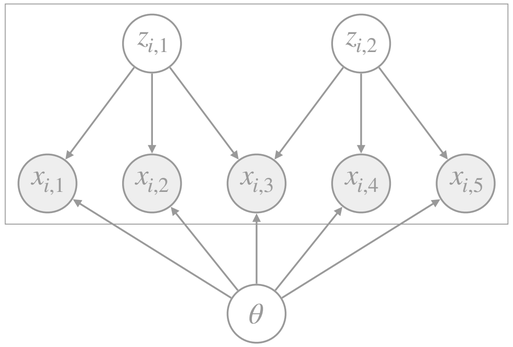

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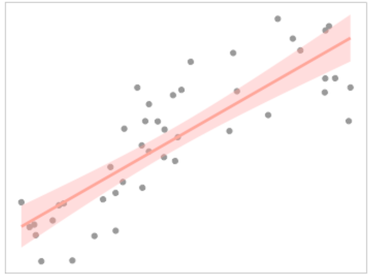

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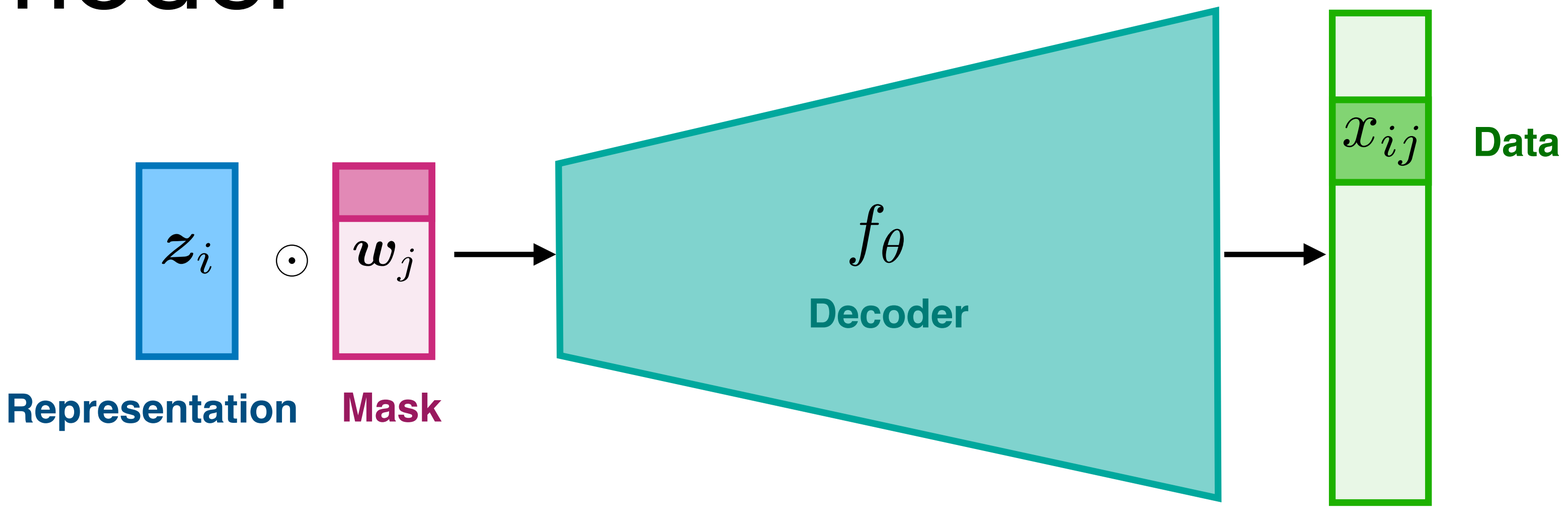
3. Factor covariance

The Sparse VAE model

Generative model:

$$\theta \sim \mathcal{N}(0, \tau)$$
$$w_{jk} \sim \text{Spike-and-Slab Lasso}(\lambda_0, \lambda_1, a, b)$$
$$\boldsymbol{z}_i \sim \mathcal{N}_K(0, \boldsymbol{C})$$
$$x_{ij} \sim \mathcal{N}((f_\theta(\boldsymbol{w}_j \odot \boldsymbol{z}_i)_j, \sigma_j^2)$$



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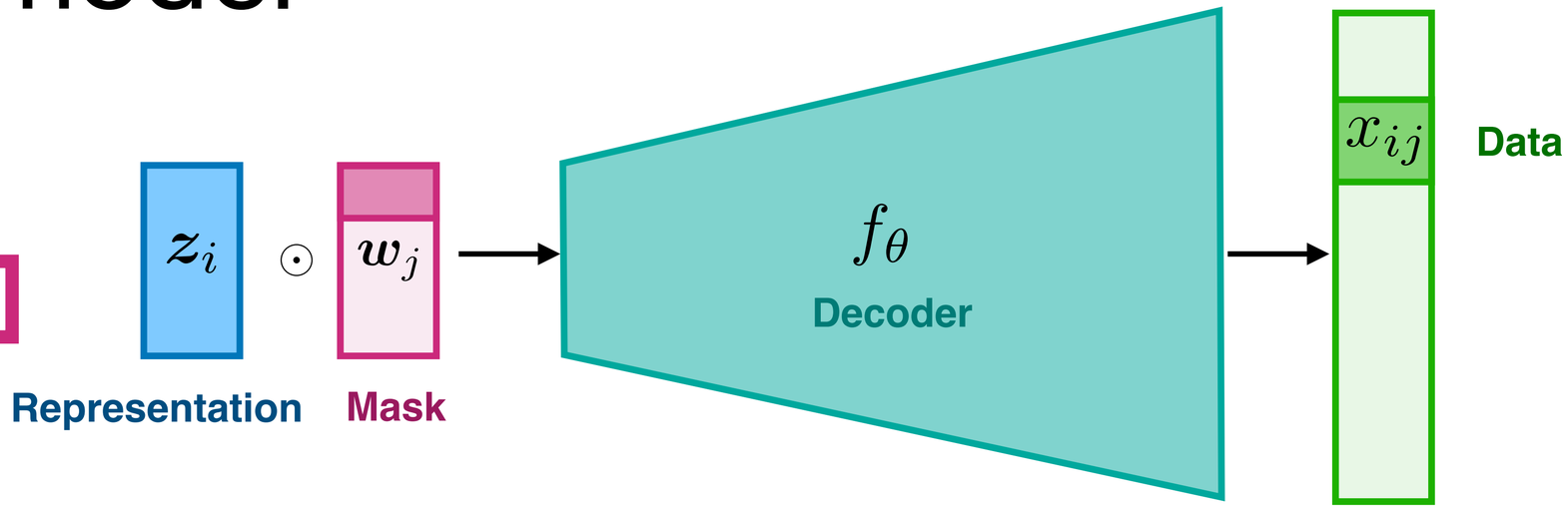
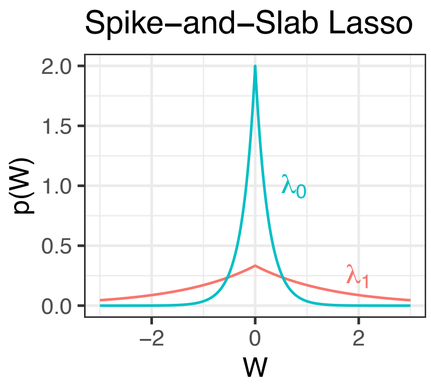


Induce sparsity in W via Spike-and-Slab Lasso prior
[Rockova and George, 2018]

$$\eta_k \sim \text{Beta}(a, b)$$

$$\gamma_{jk} \sim \text{Bernoulli}(\eta_k)$$

$$w_{jk} = \gamma_{jk} \frac{\lambda_1}{2} e^{-\lambda_1 |w_{jk}|} + (1 - \gamma_{jk}) \frac{\lambda_0}{2} e^{-\lambda_0 |w_{jk}|}$$



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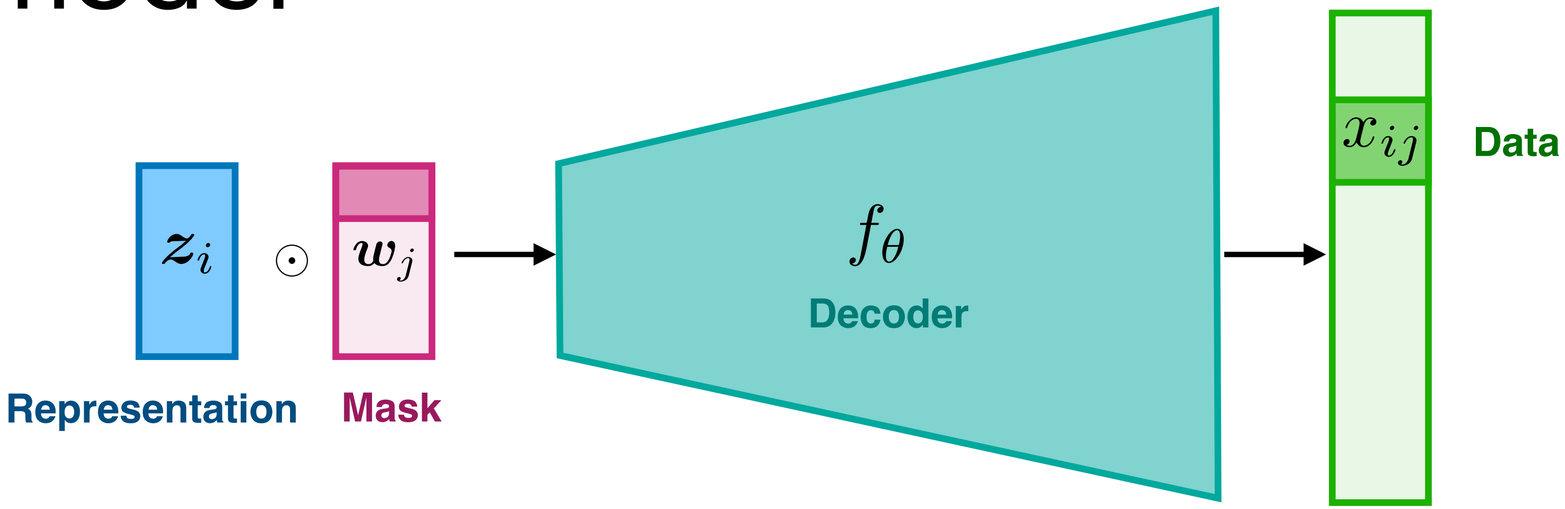
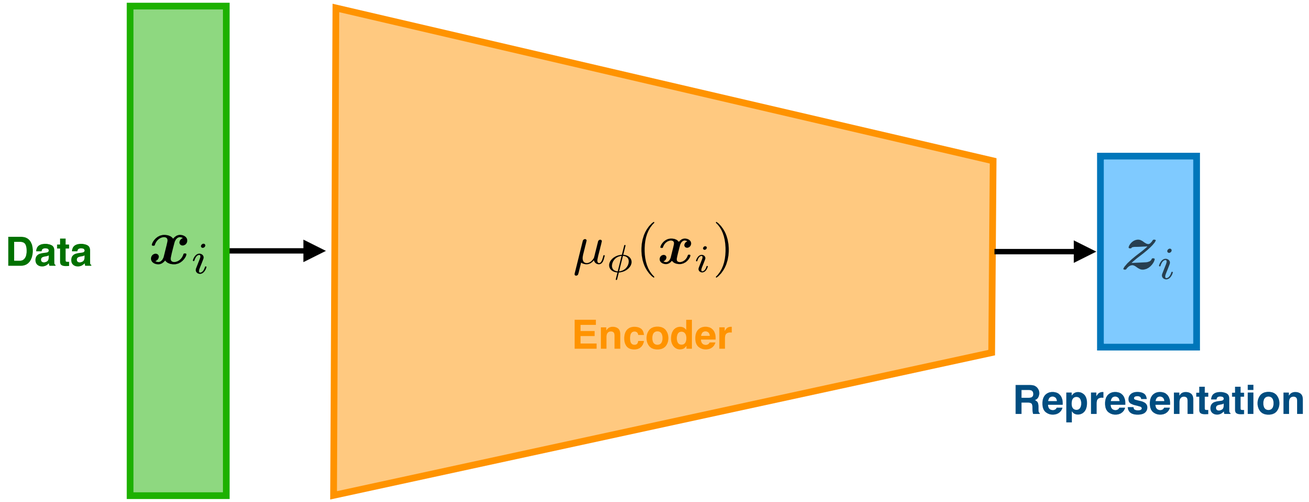


Inference:

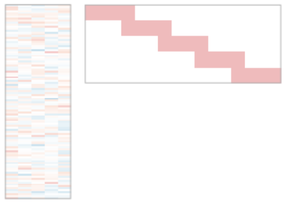
- Fit with a variational EM algorithm
- Variational approximation for z_i:

$$q_\phi(\boldsymbol{z}_i|\boldsymbol{x}_i) \sim \mathcal{N}_K(\mu_\phi(\boldsymbol{x}_i), \sigma_\phi^2(\boldsymbol{x}_i))$$

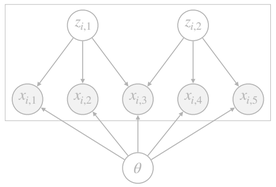
- Stochastic gradient ascent for W, θ, ϕ
- EM steps for Spike-and-Slab Lasso parameters



Roadmap



Identifiability and the role of sparsity



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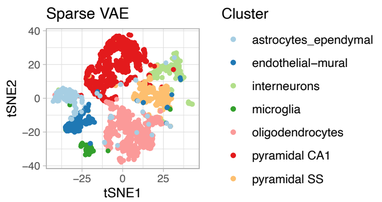
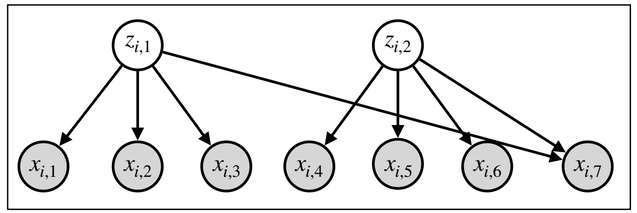


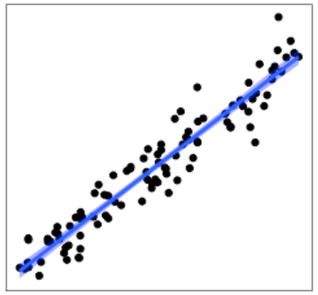
Experimental results

Experiments

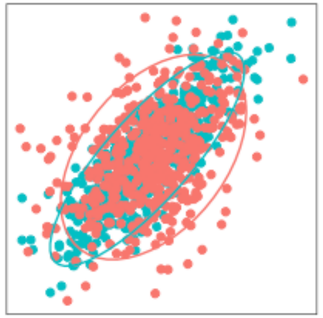
1. Recovering true factors



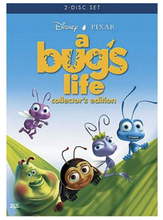
2. Prediction



3. Domain adaptation (train/test data have different distributions)



4. Interpretability



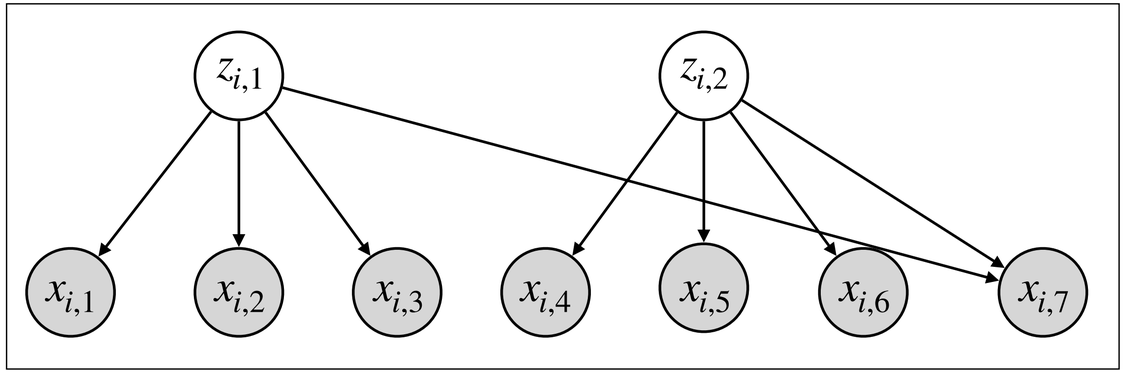
Experiments

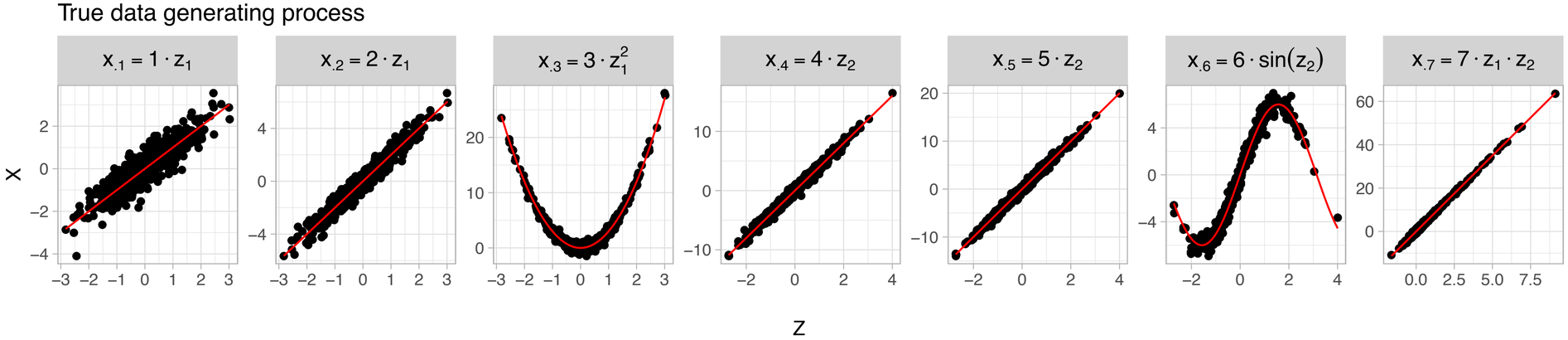
Methods compared	Identifiable?	Sparse?
Sparse VAE *[Moran et al. 2021]*	✓	✓ Decoder
VAE [*Kingma and Welling, 2014; Rezende et al. 2014]*	✗	✗
beta-VAE *[Higgins et al. 2017]*	✗	✗
Variational Sparse Coding *[Tonolini et al. 2020]*	✗	✓ Factors z_i

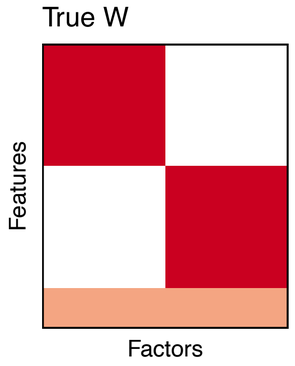
Recovering true factors

Synthetic Gaussian data

$N = 1000$ samples, $G = 7$ features, $K = 2$ factors







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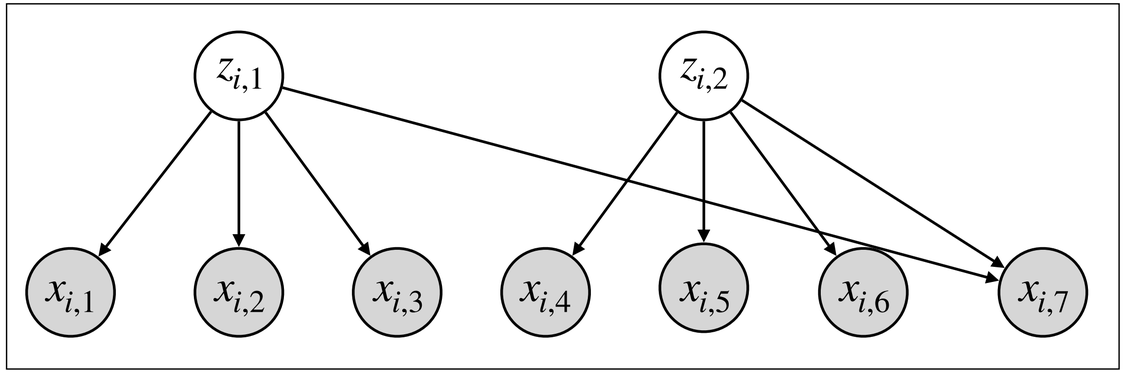
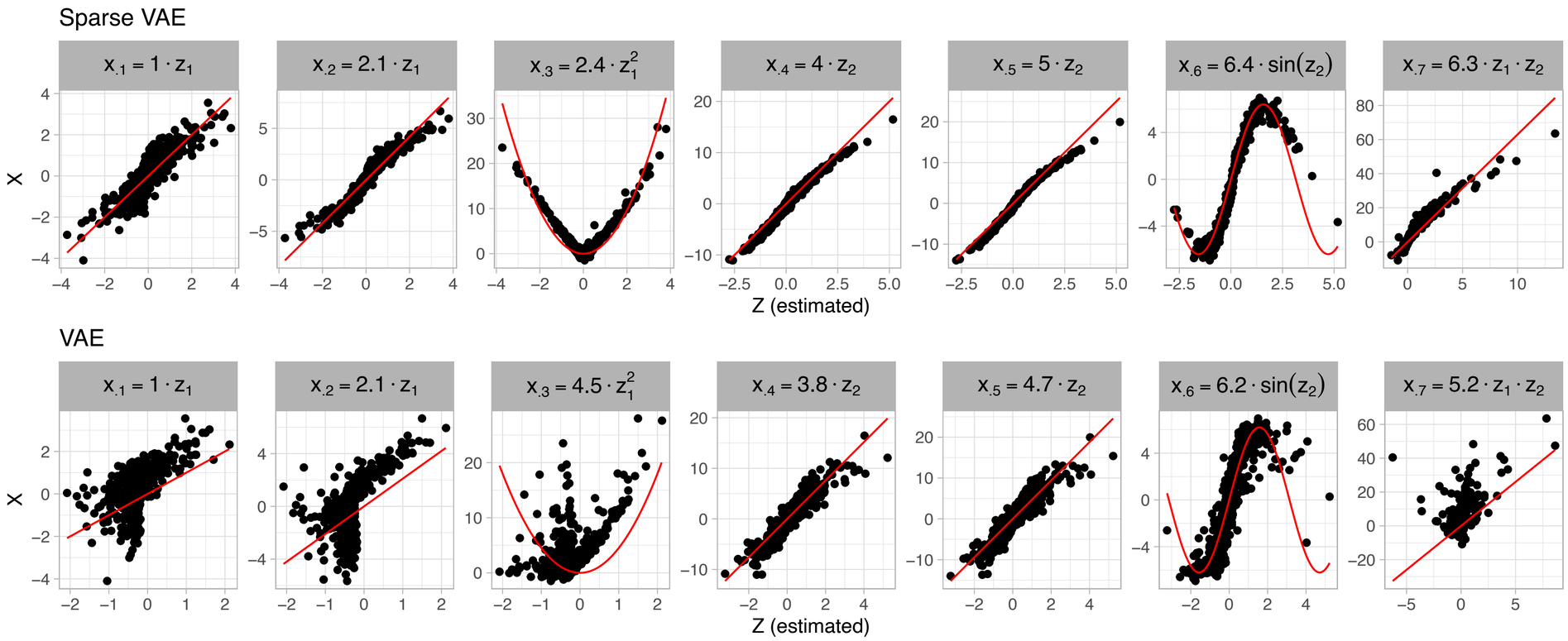
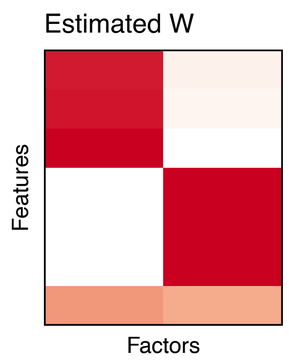
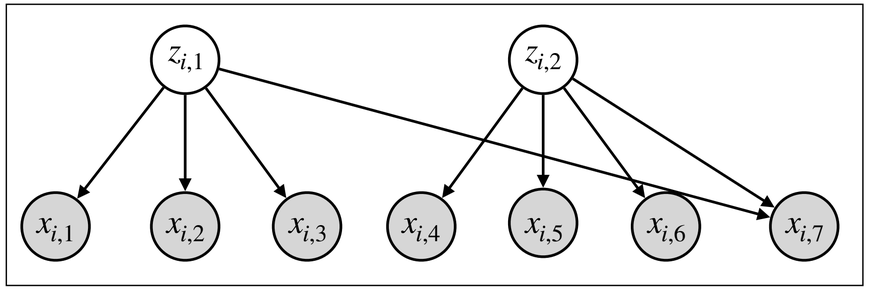






Sparse VAE successfully recovers true factors, VAE does not

Recovering true factors



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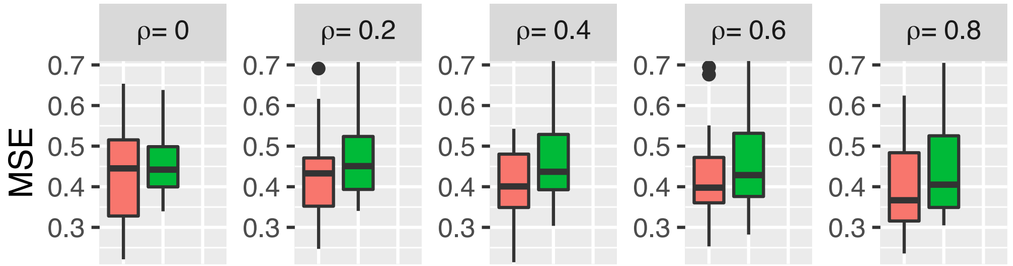
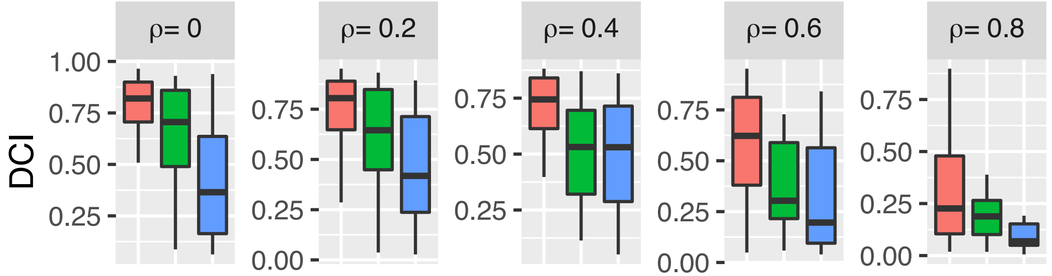
Increasing correlation of true factors



Heldout Mean Square Error (MSE) (lower is better)

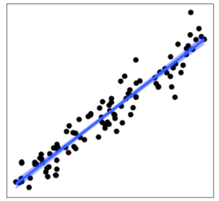


Method

- SparseVAE
- VAE
- VSC

Ground truth factor recovery (DCI disentanglement score) (higher is better)

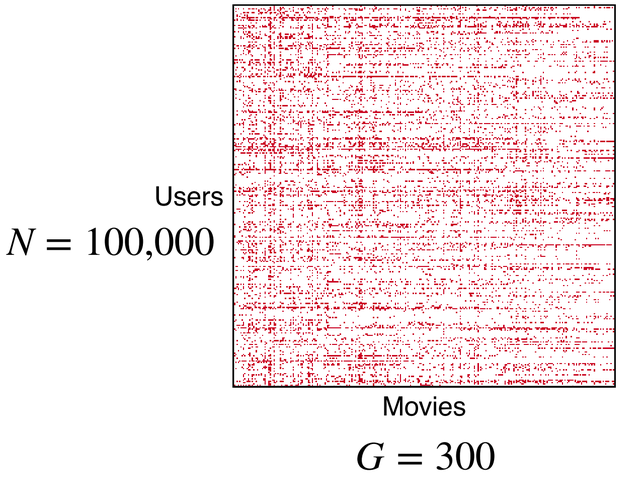
Prediction



MovieLens: ratings of movies by different users *[Harper and Konstan, 2015]*

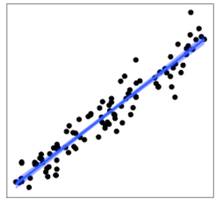
MovieLens

Method	Log loss	Recall@5	NDCG@10
Sparse VAE	**170.9 (2.1)**	**0.98 (0.002)**	**0.98 (0.003)**
VAE	175.9 (2.4)	0.97 (0.001)	0.96 (0.001)
β-VAE ($\beta = 2$)	178.2 (2.4)	0.95 (0.002)	0.93 (0.002)
VSC	192.2 (2.3)	0.79 (0.008)	0.77 (0.009)



NDCG: normalized discounted cumulative gain

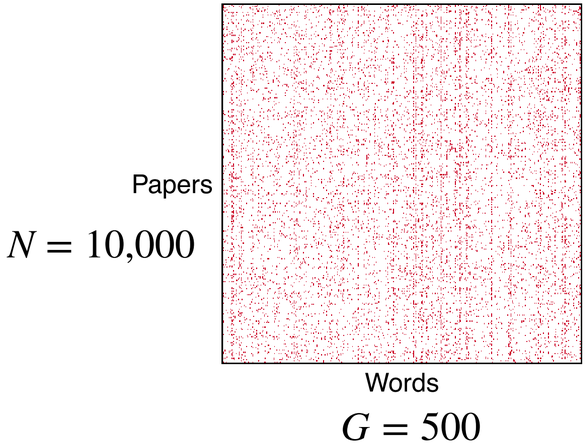
Prediction



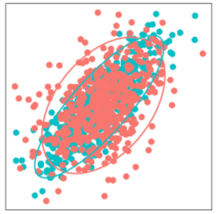
- **PeerRead:** word counts in paper abstracts *[Kang et al. 2018]*

PeerRead

Method	Log Loss
Sparse VAE	**245.0 (2.0)**
VAE	252.6 (1.4)
β-VAE ($\beta = 2$)	254.5 (3.0)
VSC	252.9 (2.0)



Domain adaptation

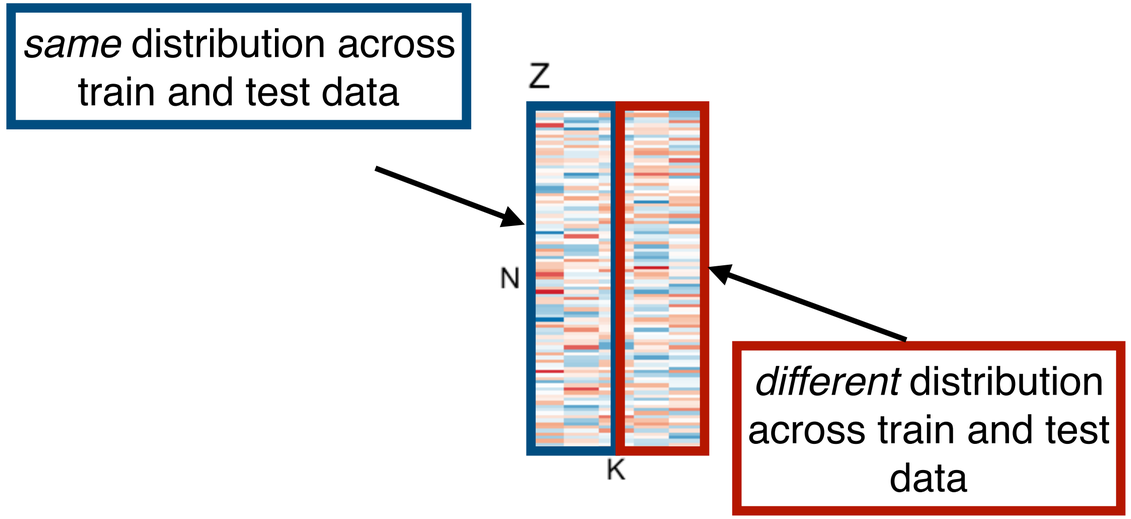


Data: semi-synthetic PeerRead ($N = 10{,}000,\ G = 500$)

- Generate factors with different distributions across train and test data
- Difficulty: correlation level of factors in training data

Average log loss on test data

	Difficulty		
Method	High	Medium	Low
Sparse VAE	**52.4 (0.4)**	**49.2 (0.3)**	**48.6 (0.1)**
VAE	54.6 (0.5)	52.3 (0.2)	50.8 (0.2)
β-VAE ($\beta = 2$)	54.7 (0.3)	52.1 (0.2)	51 (0.4)
VSC	58.7 (0.6)	56.1 (0.3)	55.4 (0.2)



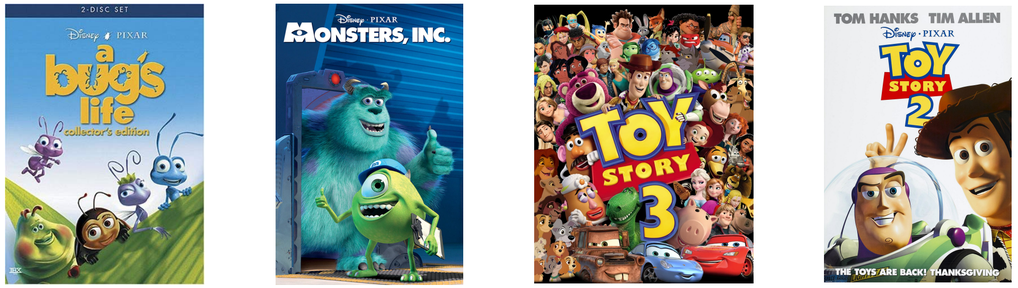
Interpretability

MovieLens: Sparse VAE finds meaningful factors via the matrix W

Sci-Fi Factor

The Fifth Element; Alien; Gattaca; Aliens

Pixar Factor



A Bug's Life; Monsters, Inc.; Toy Story 3 & 2

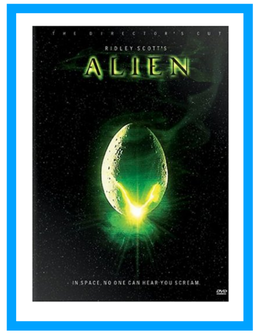
Action/Adventure Factor

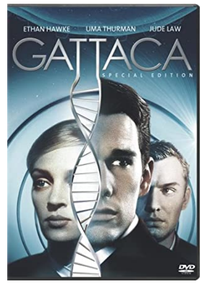
Star Wars V, IV & VI; Indiana Jones I

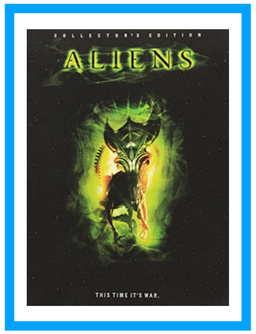
Interpretability

MovieLens: Sparse VAE finds meaningful factors via the matrix W

Sci-Fi Factor

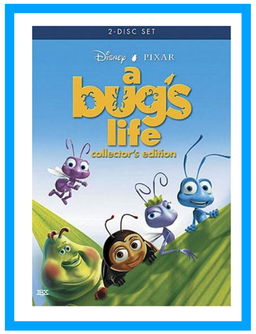






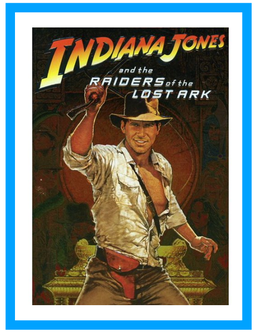
The Fifth Element; Alien; Gattaca; Aliens

Pixar Factor



A Bug's Life; Monsters, Inc.; Toy Story 3 & 2

Action/Adventure Factor



Star Wars V, IV & VI; Indiana Jones I

Anchor features

Downstream tasks

Single-cell RNA molecule counts in mouse cortex cells *[Zeisel et al. 2015]*

- $N = 3005$ cells, $G = 558$ genes
- Cells are from different regions of mouse cortex

Downstream tasks

Single-cell RNA molecule counts in mouse cortex cells *[Zeisel et al. 2015]*

- $N = 3005$ cells, $G = 558$ genes
- Cells are from different regions of mouse cortex

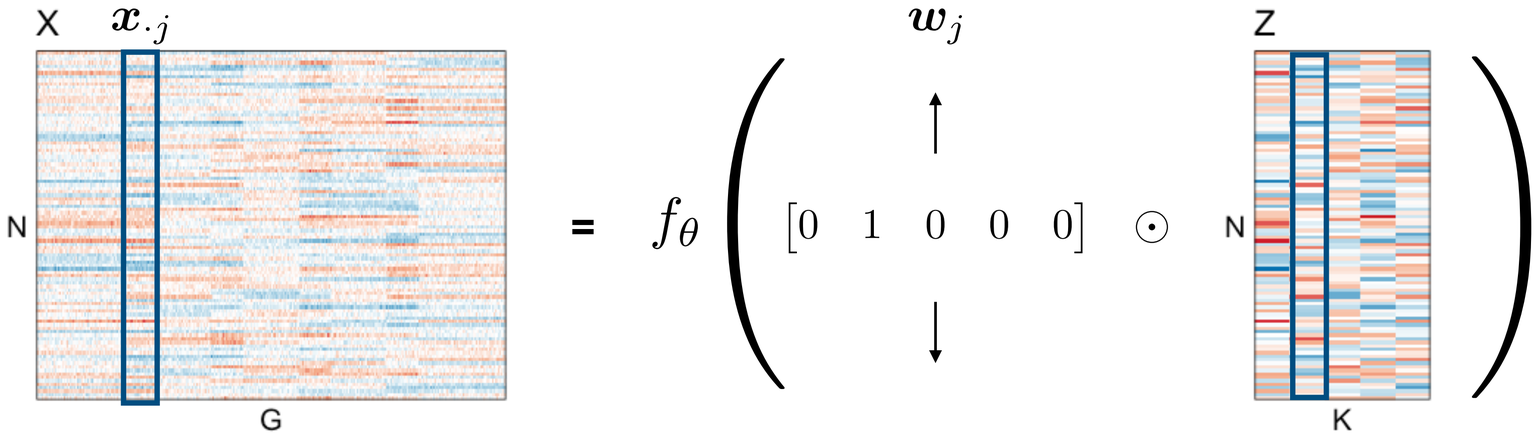
- Sparse VAE factors better predict cell label compared to other methods

Method	Sparse VAE	VAE	NMF	VSC
Accuracy	**0.95 (0.003)**	0.94 (0.016)	0.91 (0.007)	0.89 (0.062)

- Genes found by Sparse VAE were enriched for 39 biological processes

Future work

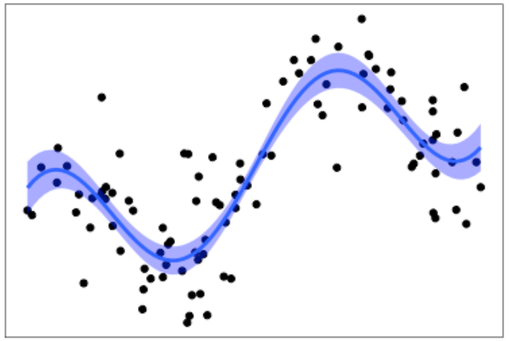
- Extend to image data
  - Sparse VAE requires each feature have a consistent meaning (pixels do not)



  - How to learn image "features" and retain identifiability?

Conclusion

We developed the **Sparse VAE** for representation learning:



Flexible

Interpretable

Identifiable

Moran, Sridhar, Wang and Blei

Identifiable Deep Generative Models via Sparse Decoding

[arXiv:2110.10804]

GitHub

gemoran/sparse-vae-code

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Sparse VAE algorithm

- MAP objective function:

$$\mathcal{L}(\theta, \phi, \boldsymbol{W}, \boldsymbol{\eta}) = \sum_{i=1}^{N} \left\{ \mathbb{E}_{q_\phi(\boldsymbol{z}_i|\boldsymbol{x}_i)} [\log p_\theta(\boldsymbol{x}_i|\boldsymbol{z}_i, \boldsymbol{W})] - D_{KL}(q_\phi(\boldsymbol{z}_i|\boldsymbol{x}_i)||p(\boldsymbol{z}_i)) \right\} \tag{9}$$
$$+ \mathbb{E}_{\boldsymbol{\Gamma}|\boldsymbol{W}^{(t)}, \boldsymbol{\eta}^{(t)}} \left[\log[p(\boldsymbol{W}|\boldsymbol{\Gamma}) p(\boldsymbol{\Gamma}|\boldsymbol{\eta}) p(\boldsymbol{\eta})] \right],$$

Algorithm 1: The Sparse VAE

input: data $\boldsymbol{X}$, hyperparameters $\lambda_0, \lambda_1, a, b, \boldsymbol{C}$
output: factor distributions $q_\phi(\boldsymbol{z}|\boldsymbol{x})$, selector matrix $\boldsymbol{W}$, parameters θ
while *not converged* **do**
For $j = 1, \ldots, G;\ k = 1, \ldots, K$, update:

$$\mathbb{E}\left[\gamma_{jk}|w_{jk}, \eta_k\right] = [1 + (1 - \eta_k)/\eta_k \psi_0(w_{jk})/\psi_1(w_{jk})]^{-1}.$$

For $k = 1, \ldots, K$, update:

$$\eta_k = \left(\sum_{j=1}^{G} \mathbb{E}\left[\gamma_{jk}|w_{jk}, \eta_k\right] + a - 1 \right) \Big/ (a + b + G - 2).$$

Update $\theta, \phi, \boldsymbol{W}$ with stochastic gradient ascent according to Eq. 9.
end