Mixture Model Auto-Encoders: Deep Clustering through Dictionary Learning **IEEE ICASSP 2022 Paper #4887**





Harvard University School of Engineering



Andrew H. Song

Harvard Medical School Brigham and Women's Hospital



Demba Ba

Harvard University School of Engineering













• Unsupervised: No labels







- Unsupervised: No labels \bullet
 - Cannot rely on labeled patterns in training set (like in classification)







- Unsupervised: No labels \bullet
 - Cannot rely on labeled patterns in training set (like in classification)





- Unsupervised: No labels
 - Cannot rely on labeled patterns in training set (like in classification)
- High-dimensional: Simple metrics (e.g. Euclidean distance) are no longer informative





- Unsupervised: No labels
 - Cannot rely on labeled patterns in training set (like in classification)
- High-dimensional: Simple metrics (e.g. Euclidean distance) are no longer informative
 - Classical clustering algorithms (e.g. *K*-means) do not work well





- Unsupervised: No labels
 - Cannot rely on labeled patterns in training set (like in classification)
- High-dimensional: Simple metrics (e.g. Euclidean distance) are no longer informative
 - Classical clustering algorithms (e.g. *K*-means) do not work well









Model-Based Signal Processing



Model-Based Signal Processing

- Simple models with principled effects (e.g. sparsity, low rank, dictionary learning)
- Incorporate prior knowledge and learns few parameters
- Theoretically understood & interpretable design



Model-Based Signal Processing

- Simple models with principled effects (e.g. sparsity, low rank, dictionary learning)
- Incorporate prior knowledge and learns few parameters
- Theoretically understood & interpretable design



Deep Learning

Model-Based Signal Processing

- Simple models with principled effects (e.g. sparsity, low rank, dictionary learning)
- Incorporate prior knowledge and learns few parameters
- Theoretically understood & interpretable design

Deep Learning

- Black-box architectures (e.g. CNN, RNN, Transformer)
- Heavily over-parameterized
- Scalable training on large datasets (e.g. batch processing, GPUs)





Model-Based Signal Processing

Model-Based Deep Learning [1]

- Simple models with principled effects (e.g. sparsity, low rank, dictionary learning)
- Incorporate prior knowledge and learns few parameters
- Theoretically understood & interpretable design

Deep Learning

- Black-box architectures (e.g. CNN, RNN, Transformer)
- Heavily over-parameterized
- Scalable training on large datasets (e.g. batch processing, GPUs)

[1] Shlezinger, N., Whang, J., Eldar, Y. C., & Dimakis, A. G. (2020). Model-based deep learning. arXiv preprint arXiv:2012.08405.





Model-Based Signal Processing

- Simple models with principled effects (e.g. sparsity, low rank, dictionary learning)
- Incorporate prior knowledge and learns few parameters
- Theoretically understood & interpretable design

Model-Based Deep Learning [1]

- Multi-layer architecture derived from interpretable signal processing model
- Can use model to inject prior knowledge into deep architecture (fewer params)
- Can leverage deep learning technology for scalable training

Deep Learning

- Black-box architectures (e.g. CNN, RNN, Transformer)
- Heavily over-parameterized
- Scalable training on large datasets (e.g. batch processing, GPUs)

[1] Shlezinger, N., Whang, J., Eldar, Y. C., & Dimakis, A. G. (2020). Model-based deep learning. arXiv preprint arXiv:2012.08405.





 Propose Mixture Model Auto-Encoders (MixMate) — a novel deep architecture for clustering signals/images

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - *modeling*)

• Derived from statistical signal processing models (i.e. dictionary learning and mixture

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - modeling)
 - Trained as a neural network on large datasets

• Derived from statistical signal processing models (i.e. *dictionary learning* and *mixture*

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - modeling)
 - Trained as a neural network on large datasets
- clustering problem, while also providing...

• Derived from statistical signal processing models (i.e. dictionary learning and mixture

• Achieve superior performance over other state-of-the-art deep learning architectures for the

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - modeling)
 - Trained as a neural network on large datasets
- clustering problem, while also providing...
 - Order-of-magnitude fewer parameters (i.e. 50x smaller)

• Derived from statistical signal processing models (i.e. dictionary learning and mixture

• Achieve superior performance over other state-of-the-art deep learning architectures for the

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - Derived from statistical signal processing models (i.e. *dictionary learning* and *mixture* modeling)
 - Trained as a neural network on large datasets
- Achieve superior performance over other state-of-the-art deep learning architectures for the clustering problem, while also providing...
 - Order-of-magnitude fewer parameters (i.e. 50x smaller)
 - Simpler parameter initialization scheme

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - Derived from statistical signal processing models (i.e. *dictionary learning* and *mixture* modeling)
 - Trained as a neural network on large datasets
- Achieve superior performance over other state-of-the-art deep learning architectures for the clustering problem, while also providing...
 - Order-of-magnitude fewer parameters (i.e. 50x smaller)
 - Simpler parameter initialization scheme
 - Ability to cluster incomplete/missing data

- Propose Mixture Model Auto-Encoders (MixMate) a novel deep architecture for clustering signals/images
 - modeling)
 - Trained as a neural network on large datasets
- clustering problem, while also providing...
 - Order-of-magnitude fewer parameters (i.e. 50x smaller)
 - Simpler parameter initialization scheme
 - Ability to cluster incomplete/missing data

Derived from statistical signal processing models (i.e. dictionary learning and mixture

• Achieve superior performance over other state-of-the-art deep learning architectures for the

signal processing model!

MixMate Model Intro to Dictionary Learning



Dataset of Natural Signals (e.g. images of handwritten digits)

Dictionary (e.g. collection of strokes)





Sparse Codes (e.g. how much of each stroke)

MixMate Model Mixture of Dictionary Learning Models



handwritten 1's)

(e.g. collection of strokes for 1's)





Cluster #2 (e.g. images of handwritten 2's)

Dictionary #2 (e.g. collection of strokes for 2's)

 $x^{(4)}$

 $x^{(3)}$

MixMate Model Mixture of Dictionary Learning Models



<u>Key Insight: Each cluster of images is generated by a *different* dictionary.</u>





Cluster #2 (e.g. images of handwritten 2's)

Dictionary #2 (e.g. collection of strokes for 2's)

 $x^{(4)}$

MixMate Model **Mixture of Dictionary Learning Models**

Assume *K* total clusters.

 $z \sim Cate$ (Latent) cluster identity: (Latent) sparse code: (Observed) data:

<u>Goal:</u> Learn parameters/dictionaries: $A_1, A_2, ..., A_K$ Infer latent variables (for each y):

<u>Key Insight: Each cluster of images is generated by a *different* dictionary.</u>

$$\operatorname{egorical}(\pi_1, \pi_2, \ldots, \pi_K)$$

$$\sum_{k=1}^{K} \pi_k = 1$$

- $x \sim \text{Laplace}(\lambda) \propto \exp(-\lambda ||x||_1)$
- $y | x, z = k \sim \mathcal{N}(A_k x, I) \propto \exp(-||y A_k x||_2^2)$
 - Z, X

 A_1 (F)ISTA Encoder 1

A

(F)ISTA Encoder 1

Sparse Coding Problem with A_1

 $\hat{x}_1 = \arg\min_{x} ||y - A_1x||_2^2 + \lambda ||x||_1$

 \hat{x}_1

Sparse Coding Problem with A_1

 $\hat{x}_1 = \arg\min_{x} ||y - A_1x||_2^2 + \lambda ||x||_1$

$$\hat{y}_1 = A\hat{x}_1$$

$$\hat{E}_1 = ||y - \hat{y}_1||_2^2 + \lambda ||\hat{x}_1||_1$$

Compute probability of z = 1

$$p(z = 1 | y) \propto \exp(-E_1)$$

Compute probability of z = K $p(z = K | y) \propto \exp(-E_K)$

 $p(z = 1 | y) \propto \exp(-E_1)$

	DEC*	DCN*	DAMIC*	K-DAE*]	MixMate
					INIT	TRAIN
MNIST						
NMI	0.80	0.81	0.86	0.86	0.75	$\textbf{0.86} \pm 0.03$
ARI	0.75	0.75	0.82	0.82	0.72	$\textbf{0.85}\pm0.04$
ACC	0.84	0.83	0.88	0.88	0.84	$\textbf{0.92}\pm0.04$
Params	2.1 M	2.1 M	22.1 M	21.4 M		0.4 M
Fashion						
NMI	0.54	0.55	0.65	0.65	0.60	$\textbf{0.68} \pm 0.02$
ARI	0.40	0.42	0.48	0.48	0.44	0.52 ± 0.01
ACC	0.51	0.50	0.60	0.60	0.57	$\textbf{0.63} \pm 0.01$
Params	N/A	N/A	N/A	N/A		0.4 M
USPS						
NMI	0.77	0.68	0.78	0.80	0.79	0.82 ± 0.01
ARI	N/A	N/A	0.70	0.71	0.73	$\textbf{0.76} \pm 0.02$
ACC	0.76	0.69	0.75	0.77	0.79	$\textbf{0.81} \pm 0.03$
Params	N/A	N/A	N/A	N/A		0.08 M

		DEC*	DCN*	DAMIC*	K-DAE*	MixMate	
						INIT	TRAIN
	MNIST						
	NMI	0.80	0.81	0.86	0.86	0.75	$\textbf{0.86} \pm 0.03$
Clustering metrics	ARI	0.75	0.75	0.82	0.82	0.72	$\textbf{0.85}\pm0.04$
(higher=better,	ACC	0.84	0.83	0.88	0.88	0.84	0.92 ± 0.04
1.0 is best)	Params	2.1 M	2.1 M	22.1 M	21.4 M		0.4 M
	Fashion						
	NMI	0.54	0.55	0.65	0.65	0.60	$\textbf{0.68} \pm 0.02$
	ARI	0.40	0.42	0.48	0.48	0.44	$\textbf{0.52}\pm0.01$
	ACC	0.51	0.50	0.60	0.60	0.57	$\textbf{0.63} \pm 0.01$
	Params	N/A	N/A	N/A	N/A		0.4 M
	USPS						
	NMI	0.77	0.68	0.78	0.80	0.79	$\textbf{0.82} \pm 0.01$
	ARI	N/A	N/A	0.70	0.71	0.73	$\textbf{0.76} \pm 0.02$
	ACC	0.76	0.69	0.75	0.77	0.79	$\textbf{0.81} \pm 0.03$
	Params	N/A	N/A	N/A	N/A		0.08 M

Other state-of-the-art deep clustering networks [1]

	DEC*	DCN*	DAMIC*	K-DAE*	N	MixMate
					INIT	TRAIN
MNIST						
NMI	0.80	0.81	0.86	0.86	0.75	$\textbf{0.86} \pm 0.03$
ARI	0.75	0.75	0.82	0.82	0.72	$\textbf{0.85}\pm0.04$
ACC	0.84	0.83	0.88	0.88	0.84	$\textbf{0.92}\pm0.04$
Params	2.1 M	2.1 M	22.1 M	21.4 M		0.4 M
Fashion						
NMI	0.54	0.55	0.65	0.65	0.60	$\textbf{0.68} \pm 0.02$
ARI	0.40	0.42	0.48	0.48	0.44	0.52 ± 0.01
ACC	0.51	0.50	0.60	0.60	0.57	0.63 ± 0.01
Params	N/A	N/A	N/A	N/A		0.4 M
USPS						
NMI	0.77	0.68	0.78	0.80	0.79	0.82 ± 0.01
ARI	N/A	N/A	0.70	0.71	0.73	$\textbf{0.76} \pm 0.02$
ACC	0.76	0.69	0.75	0.77	0.79	$\textbf{0.81}\pm0.03$
Params	N/A	N/A	N/A	N/A		0.08 M
	MNIST NMI ARI ACC Params Fashion NMI ARI ACC Params NMI ARI ACC Params	DEC*DEC*MNISTNMI0.80ARI0.75ACC0.84Params2.1 MFashion0.54NMI0.54ARI0.40ACC0.51ParamsN/AUSPSN/ANMI0.77ARIN/AACC0.76ParamsN/A	DEC*DCN*MNISTNMI0.800.81ARI0.750.75ACC0.840.83Params2.1 M2.1 MFashionNMI0.540.55ARI0.400.42ACC0.510.50ParamsN/AN/AUSPSNMI0.770.68ARIN/AN/AACC0.760.69ParamsN/AN/A	DEC* DCN* DAMIC* MNIST	DEC* DCN* DAMIC* K-DAE* MNIST	DEC* DCN* DAMIC* K-DAE* M MNIST Init Init Init MMI 0.80 0.81 0.86 0.86 0.75 ARI 0.75 0.75 0.82 0.82 0.72 ACC 0.84 0.83 0.88 0.88 0.84 Params 2.1 M 2.1 M 21.4 M Init Fashion Init 0.55 0.65 0.65 0.60 ARI 0.54 0.55 0.65 0.65 0.60 ARI 0.40 0.42 0.48 0.44 0.44 ACC 0.51 0.50 0.60 0.57 0.57 Params N/A N/A N/A 0.44 0.44 ACC 0.51 0.50 0.60 0.57 0.57 Params N/A N/A N/A 0.57 0.57 Params N/A N/A N/A 0.57 0.57

Other state-of-the-art deep clustering networks [1]

-		DEC*	DCN*	DAMIC*	K-DAE*	N	/lixMate
						INIT	TRAIN
	MNIST						
	NMI	0.80	0.81	0.86	0.86	0.75	$\textbf{0.86} \pm 0.03$
Clustering metrics	ARI	0.75	0.75	0.82	0.82	0.72	$\textbf{0.85}\pm0.04$
(higher=better,	ACC	0.84	0.83	0.88	0.88	0.84	0.92 ± 0.04
1.0 is best)	Params	2.1 M	2.1 M	22.1 M	21.4 M		0.4 M
	Fashion						
	NMI	0.54	0.55	0.65	0.65	0.60	$\textbf{0.68} \pm 0.02$
	ARI	0.40	0.42	0.48	0.48	0.44	0.52 ± 0.01
	ACC	0.51	0.50	0.60	0.60	0.57	$\textbf{0.63} \pm 0.01$
	Params	N/A	N/A	N/A	N/A		0.4 M
[1] Opochinsky Y. Chazan, S.	USPS						
E., Gannot, S., & Goldberger, J. (2020 May) K-autoencoders	NMI	0.77	0.68	0.78	0.80	0.79	0.82 ± 0.01
deep clustering. In <i>ICASSP</i>	ARI	N/A	N/A	0.70	0.71	0.73	$\textbf{0.76} \pm 0.02$
Conference on Acoustics,	ACC	0.76	0.69	0.75	0.77	0.79	$\textbf{0.81} \pm 0.03$
<i>(ICASSP)</i> (pp. 4037-4041).	Params	N/A	N/A	N/A	N/A		0.08 M

MixMate obtains best performance on all metrics for all datasets...

Other state-of-the-art deep clustering networks [1]

		DEC*	DCN*	DAMIC*	K-DAE*	N	AixMate
						INIT	TRAIN
	MNIST						
	NMI	0.80	0.81	0.86	0.86	0.75	$\textbf{0.86} \pm 0.03$
Clustering metrics	ARI	0.75	0.75	0.82	0.82	0.72	0.85 ± 0.04
(higher=better,	ACC	0.84	0.83	0.88	0.88	0.84	0.92 ± 0.04
1.0 is best)	Params	2.1 M	2.1 M	22.1 M	21.4 M		0.4 M
	Fashion						
	NMI	0.54	0.55	0.65	0.65	0.60	$\textbf{0.68} \pm 0.02$
	ARI	0.40	0.42	0.48	0.48	0.44	0.52 ± 0.01
	ACC	0.51	0.50	0.60	0.60	0.57	$\textbf{0.63}\pm0.01$
	Params	N/A	N/A	N/A	N/A		0.4 M
[1] Opochinsky, Y., Chazan, S.	USPS						
E., Gannot, S., & Goldberger, J. (2020, May), K-autoencoders	NMI	0.77	0.68	0.78	0.80	0.79	0.82 ± 0.01
deep clustering. In <i>ICASSP</i>	ARI	N/A	N/A	0.70	0.71	0.73	$\textbf{0.76} \pm 0.02$
Conference on Acoustics,	ACC	0.76	0.69	0.75	0.77	0.79	$\textbf{0.81} \pm 0.03$
<i>(ICASSP)</i> (pp. 4037-4041). IEEE.	Params	N/A	N/A	N/A	N/A		0.08 M

MixMate obtains best performance on all metrics for all datasets...

...with the fewest number of parameters (up to 50x fewer)!

Other state-of-the-art deep clustering networks [1]

		DEC*	DCN*	DAMIC*	K-DAE*	N	AixMate	MixMate obtains	
						INIT	TRAIN	hest nerformance	
	MNIST							on all metrics for	
	NMI	0.80	0.81	0.86	0.86	0.75	0.86 ± 0.03	oll detecto	
Clustering metrics	ARI	0.75	0.75	0.82	0.82	0.72	0.85 ± 0.04	all Ualasels	
(higher=better,	ACC	0.84	0.83	0.88	0.88	0.84	0.92 ± 0.04		
1.0 is best)	Params	2.1 M	2.1 M	22.1 M	21.4 M		0.4 M	with the fewest	
	Fashion							number of	
	NMI	0.54	0.55	0.65	0.65	0.60	0.68 ± 0.02	parameters (up to	
	ARI	0.40	0.42	0.48	0.48	0.44	0.52 ± 0.01	50x fewer)!	
	ACC	0.51	0.50	0.60	0.60	0.57	$\textbf{0.63} \pm 0.01$		
	Params	N/A	N/A	N/A	N/A		0.4 M	These numbers	
[1] Onochinsky Y. Chazan, S.	USPS							change even if 9	
E., Gannot, S., & Goldberger, J.	NMI	0.77	0.68	0.78	0.80	0.79	$\textbf{0.82} \pm 0.01$	images have 25	
deep clustering. In <i>ICASSP</i>	ARI	N/A	N/A	0.70	0.71	0.73	$\textbf{0.76} \pm 0.02$	nivole miecino	
Conference on Acoustics,	ACC	0.76	0.69	0.75	0.77	0.79	$\textbf{0.81} \pm 0.03$		
<i>Speech and Signal Processing</i> <i>(ICASSP)</i> (pp. 4037-4041).	Params	N/A	N/A	N/A	N/A		0.08 M		
IEEE.								incomplete da	

Why does MixMate work so well? Latent sparsity really helps!

Each of the 10 auto-encoder's output is labeled with (recon error, L0 norm of code)

Clustering depends on *both* reconstruction error and latent sparsity.

input

(0.032, 15)

(0.033, 17) (0.025, 18) (0.025, 15)

Why does MixMate work so well? Latent sparsity really helps!

Each of the 10 auto-encoder's output is labeled with (recon error, L0 norm of code)

Clustering depends on *both* reconstruction error and latent sparsity.

input

(0.032, 15)

(0.033, 17)

Why does MixMate work so well? Latent sparsity really helps!

Each of the 10 auto-encoder's output is labeled with (recon error, L0 norm of code)

Clustering depends on *both* reconstruction error and latent sparsity.

input

(0.033, 17)

For more information...

- Paper: <u>https://ieeexplore.ieee.org/document/9747848</u>
 - Lin, A., Song, A. H., & Ba, D. (2022, May). Mixture Model Auto-Encoders: **Deep Clustering through Dictionary Learning.** In *ICASSP 2022-2022* IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP) (pp. 3368-3372). IEEE.
 - More information on theory behind our MixMate architecture, initialization scheme, tuning the sparsity level, etc.
- Code: <u>https://github.com/al5250/mixmate</u>

11