



Online Learning for Large Scale Mixture Models

Mohammad Pasande

School of Electrical and Computer Engineering
University of Tehran

Aug, 2022

Outline

- 1 Preliminaries
- 2 Optimization
- 3 Proposed Method
- 4 Experiments
- 5 Conclusion

Gaussian Mixture (GM)

'Many years ago I called the Laplace–Gaussian curve the normal curve, which name, while it avoids an international question of priority, has the disadvantage of leading people to believe that all other distributions of frequency are in one sense or another "abnormal".'

Karl Pearson

Gaussian Mixture (GM)

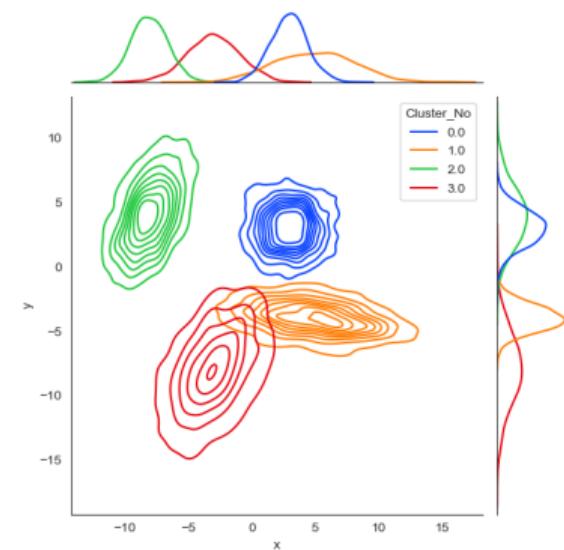
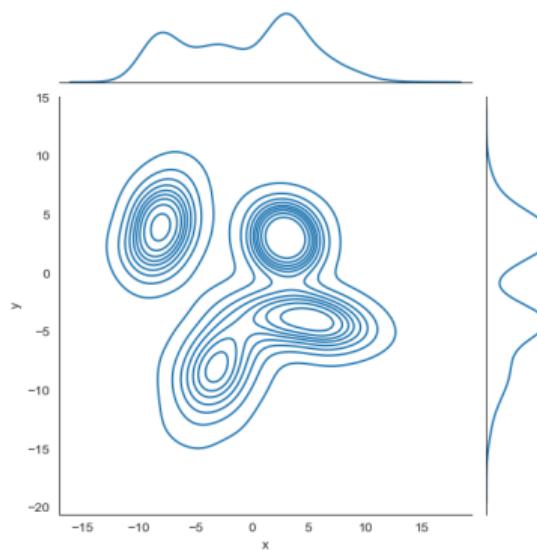
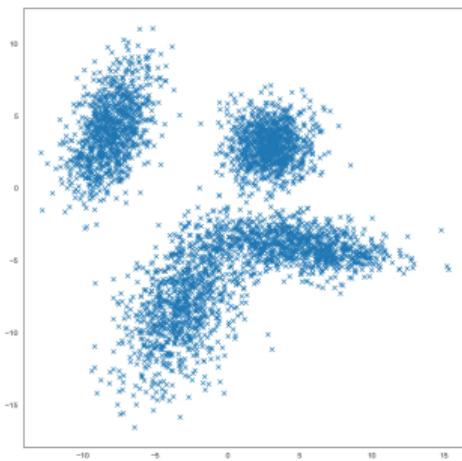
$$\mathcal{N}(x|\mu, \Sigma^{-1}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu)\right) \quad (1)$$

$$p(x) = \sum_{k=1}^K \pi_k \mathcal{N}(x|\mu_k, \Sigma_k^{-1})$$

s. t. $\pi_k \geq 0$ & $\sum_{k=1}^K \pi_k = 1.$

$$\zeta^T \Sigma^{-1} \zeta \geq 0 \quad (\forall \zeta \in \mathbb{R}^D).$$

Gaussian Mixture Model (GMM)

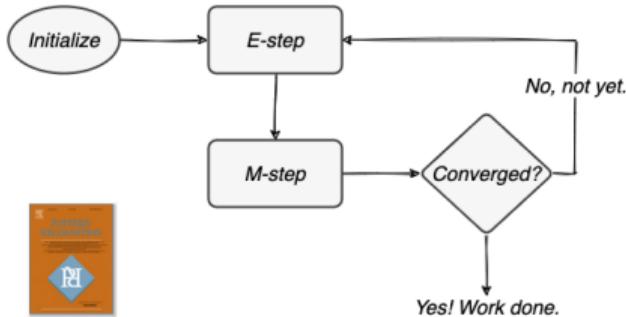


Parameter Estimation

- Expectation Maximization (EM, CEM, Incr-EM, ...)



Pattern Recognition
Volume 114, June 2021, 107836



A new EM algorithm for flexibly tied GMMs with large number of components

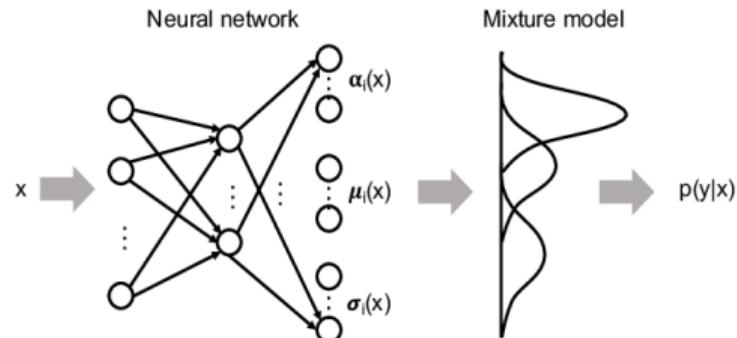
Hadi Asheri, Reshad Hosseini, Babak Nadjar Araabi

The Proposed Hybrid Algorithm outperforms others in both convergence and time performance.[Asheri et al., 2021]

GMM Type	Learning Algorithm	BSDS500 (64)	CIFAR10 (89)	CIFAR100 (98)	MAGIC (10)	MNIST (154)	STL (101)	SVHN (100)	USPS (65)	WAVE (21)	YEAR (90)
basic	EM	48.24	116.39	127.95	9.87	139.75	114.37	87.32	52.7	29.16	100.89
	CD-EM	15.95	113.93	125.38	9.71	130.36	95.59	70.06	49.82	29.06	95.28
flexibly tied	FNMR-EM	16.73	114.46	125.01	9.72	131.86	96.04	70.10	49.94	29.68	96.16
	FNMR-CD-EM	15.95	113.79	124.84	9.71	130.29	95.56	70.01	49.82	29.04	95.26

Parameter Estimation

- Expectation Maximization (EM, CEM, Incr-EM, ...)
- Neural Networks (Mixture Density Networks)



Parameter Estimation

- Expectation Maximization (EM, CEM, Incr-EM, ...)
- Neural Networks (Mixture Density Networks)
- **Numerical Optimization**

$$\text{loss} := \mathcal{L}(\pi_k, \mu_k, \Sigma_k^{-1}) = - \sum_{i=1}^N \log \left\{ \sum_{k=1}^K \pi_k \mathcal{N}(x_i | \mu_k, \Sigma_k) \right\} \quad NLL \quad (2)$$

$$\begin{aligned} & \underset{\theta}{\text{minimize}} \quad \mathcal{L}(\pi_k, \mu_k, \Sigma_k^{-1}) \\ & \text{subject to} \quad \pi_k \geq 0 \quad \& \quad \sum_{k=1}^K \pi_k = 1. \\ & \quad \Sigma_k^{-1} \succeq 0. \end{aligned} \quad (3)$$

The Passion Of Constraints!

- π_k Constraint:

$$\pi_j = \frac{\exp(\eta_j)}{\sum_{k=1}^K \exp(\eta_k)}$$

AKA: SoftMax. Dobby is FREE!

The Passion Of Constraints!

- π_k Constraint:

$$\pi_j = \frac{\exp(\eta_j)}{\sum_{k=1}^K \exp(\eta_k)}$$

AKA: SoftMax.

Dobby is FREE!

- Σ_k^{-1} Constraint:

- Cholesky Decomposition:

$$\Sigma^{-1} = LDL^T$$

The Passion Of Constraints!

- π_k Constraint:

$$\pi_j = \frac{\exp(\eta_j)}{\sum_{k=1}^K \exp(\eta_k)}$$

AKA: SoftMax.

Dobby is FREE!

- Σ_k^{-1} Constraint:

- Reformulation Trick [Hosseini and Sra, 2015] :

$$S_k = \begin{pmatrix} \Sigma_k^{-1} + \mu_k \mu_k^T & \mu_k \\ \mu_k^T & 1 \end{pmatrix}; y = (x \ 1)^T$$

The Passion Of Constraints!

- π_k Constraint:

$$\pi_j = \frac{\exp(\eta_j)}{\sum_{k=1}^K \exp(\eta_k)}$$

AKA: SoftMax.

Dobby is FREE!

- Σ_k^{-1} Constraint:

- Semi-Tied [Gales, 1999] :

$$\Sigma_k^{-1} = U D_k U^T$$

How About UDU^T ?

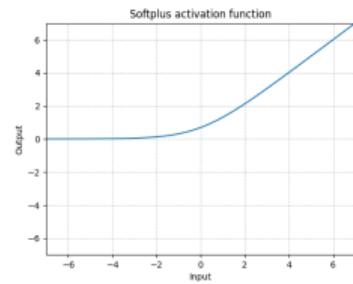
Simplify the Σ^{-1} as much as you can!

- put the orthogonal constraint on U :

$$UU^T = I_D \quad \Rightarrow \quad \det(\Sigma_k^{-1}) = \prod_{j=1}^D d_k^{(j)}$$

- consider each $d_k^{(j)}$ is a SoftPlus output:

$$d_k^{(j)} = \frac{1}{\beta} \log (1 + \exp(\beta \hat{d}_k^{(j)})) \quad \Rightarrow \quad D_k \succeq 0$$



- inject more flexibility using component-wise scalar:

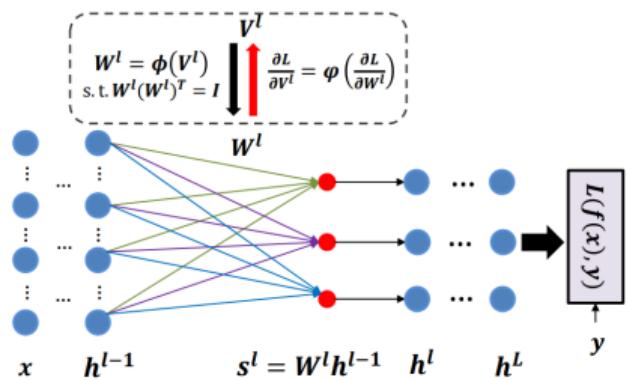
$$UD_k U^T \rightarrow \lambda_k UD_k U^T$$

Optimization

Orthonormality

$$O(n) = \{X \in \mathbb{R}^{n \times n} : X^T X = I_n\} \rightarrow SO(n) = \{X \in O(n) : \det(X) = +1\}$$

[Huang et al., 2018]



[Bansal et al., 2018]

Double Soft Orthogonality

$$\lambda(\|W^T W - I\|_F + \|WW^T - I\|_F)$$

Mutual Coherence

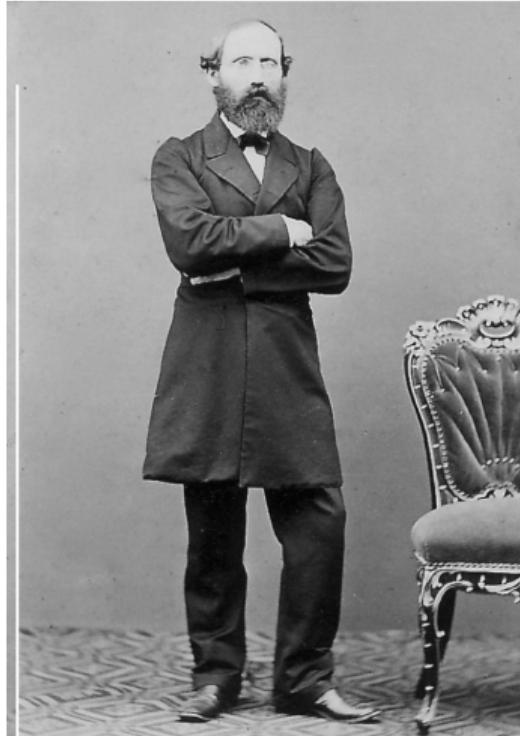
$$\lambda(\|W^T W - I\|_\infty)$$

Spectral Restricted Isometry Property

$$\lambda(Sup_{z \in \mathbb{R}^n, z \neq 0} |\frac{\|(Wz)\|}{\|z\|} - 1|)$$

Riemannian Manifold

You might want to sit down for this



Riemannian Manifold

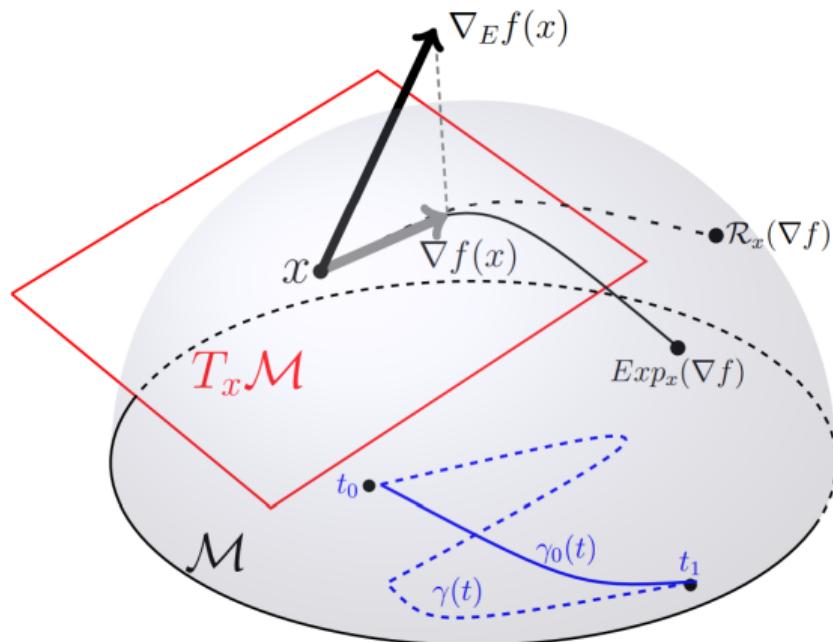
Better



Riemannian Metric := $\langle \cdot, \cdot \rangle_x$

- Bilinear
- Symmetric
- Positive Definite

Riemannian Manifold

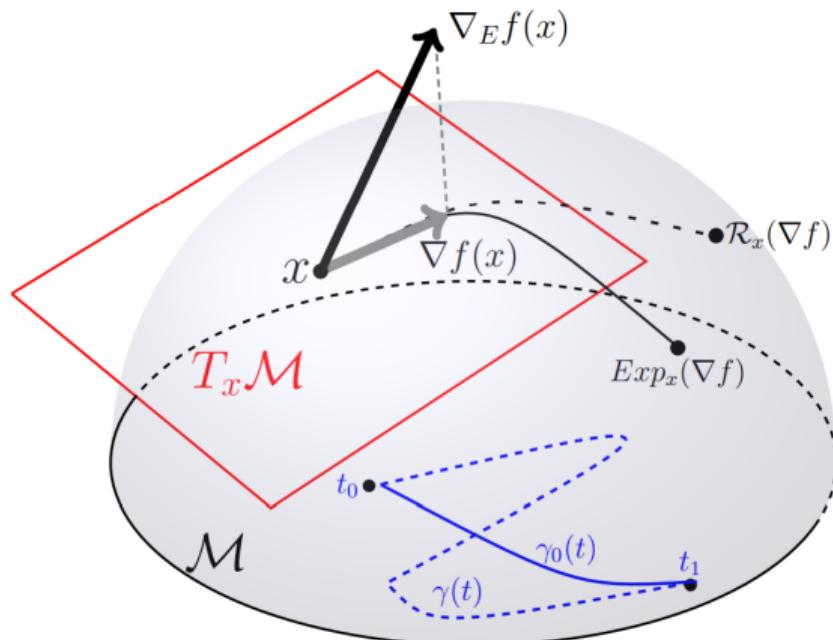


- $\{x \in \mathbb{R}^{n+1} \mid \|x\|_2 = 1\}$
- $g : T_x \mathcal{M} \times T_x \mathcal{M} \rightarrow \mathbb{R}$
- $\gamma_0(t) : \text{Geodesic}$
- $\nabla_E f$ and ∇f indicate the Euclidean gradient and Riemannian gradient
- $Exp_x(\cdot) : \text{Exponential Map}$
- $\mathcal{R}_x(\cdot) : \text{Retraction function}$

Riemannian Manifold (Let There be Light)

' To deal with hyper-planes in a 14-dimensional space, visualize a 3-D space and say "fourteen" to yourself very loudly. Everyone does it.'

Geoffrey E. Hinton



- $\{x \in \mathbb{R}^{n+1} \mid \|x\|_2 = 1\}$
- $g : T_x\mathcal{M} \times T_x\mathcal{M} \rightarrow \mathbb{R}$
- $\gamma_0(t) : \text{Geodesic}$
- $\nabla_E f$ and ∇f indicate the Euclidean gradient and Riemannian gradient
- $Exp_x(\cdot) : \text{Exponential Map}$
- $\mathcal{R}_x(\cdot) : \text{Retraction function}$

Stochastic Gradient Descent on GMM [Hosseini and Sra, 2020]

$$\begin{aligned}
 f_i(\eta_k, S_k) &:= \log \left\{ \sum_{k=1}^K \frac{\exp(\eta_k)}{\sum_{j=1}^K \exp(\eta_j)} \mathcal{N}(y_i; 0, S_k) \right\} + \frac{1}{n} \left(\sum_{k=1}^K \psi(S_k; \Psi) + \phi(\{\eta_k\}_{k=1}^{K-1}; \zeta) \right), \\
 \left\{ \{S_k \succ 0\}_{k=1}^K, \{\eta_k\}_{k=1}^{K-1} \right\} &\leftarrow Ret \left(\eta_t \nabla f_i \left(\{S_k \succ 0\}_{k=1}^K, \{\eta_k\}_{k=1}^{K-1} \right) \right). \tag{4}
 \end{aligned}$$

Note.

In case of S_k , $(\nabla f_i(\cdot))$ refers to the Riemannian gradient which can be achieved by mapping the Euclidean gradient $(\nabla_E f_i(\cdot))$ on the manifold of Symmetric Positive Definite (SPD) matrices.

Proposed Method

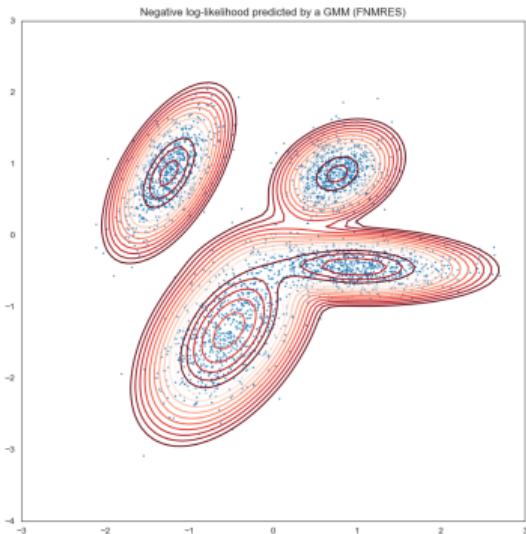
General SGD for GMM

Algorithm 1 SGD GMM using UD_kU^T

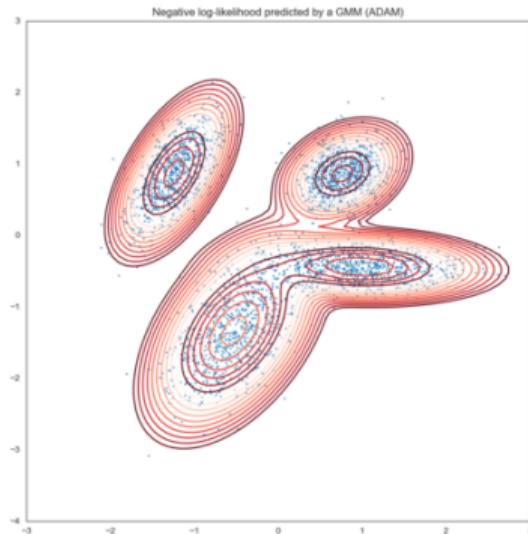
```
1: Initial values of  $U$ ,  $\hat{D}_k$ ,  $\eta_k$  and  $\mu_k$ ;  
2: while epoch < MaxNo.EPOCHs do  
3:   for each Train iteration do  
4:      $\nabla_E \mathcal{L}_i$  : Compute Stochastic Euclidean Gradient;  
5:     Take a Stochastic Gradient step;  
6:     Compute the negative log-likelihood;  
7:   end for  
8: end while
```

Is it working?

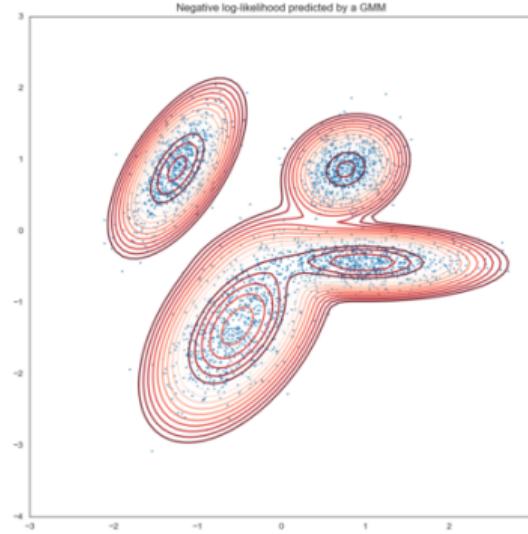
Using CD-FNMRES EM



Using ADAM



Using vanilla EM (Kmeans initialization)



Adaptive Coordinate-wise CLIPping SGD with Orthogonality Constraint

Algorithm 2 ACClipping Gradient Descent with orthogonality constraint (using Retraction)

```
1:  $M_t, \tau_t \leftarrow 0, 0$ ; {Initialize}
2: for  $t = 1, \dots, T$  do
3:    $M_{t+1} \leftarrow \beta_1 M_t + (1 - \beta_1) \mathcal{G}_t$  ; { $\mathcal{G}$  as euclidean gradient}
4:    $\tau_{t+1}^\alpha \leftarrow \beta_2 \tau_t^\alpha + (1 - \beta_2) |\mathcal{G}_t|^\alpha$ 
5:    $\hat{\mathcal{G}} = \min\left(\frac{\tau_{t+1}}{|M_{t+1}| + \epsilon}, 1\right) M_{t+1}$  ; {Adaptive Coordinate-wise CLIPping}
6:    $M_{t+1} \leftarrow \text{Proj}(\hat{\mathcal{G}})$  {Project onto the tangent space}
7:    $X_{t+1} \leftarrow \mathcal{R}_{X_t}(-\alpha M_{t+1})$  {Retraction,  $\alpha$  is the learning rate}
8: end for
```

Controlled Datasets

- Separation:

$$\forall i \neq j \|\mu_i - \mu_j\| \geq c \max_{i,j}\{tr(\Sigma_i), tr(\Sigma_j)\}$$

High Sep. : $c = 10$, Mid Sep. : $c = 1$, Low Sep. : $c = 0.1$

Smallest Eigenvalue : $e = 10$

No. of Clusters : $K = 5$ No. of Dimensions : $d = 5$

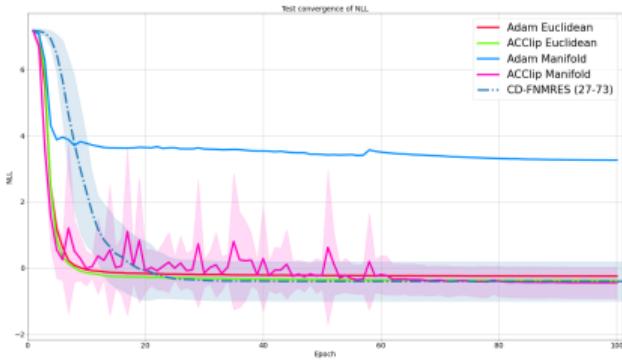
No. of Data Points : $10d^2, 100d^2, 1000d^2$

No. of Tests : $N = 10$

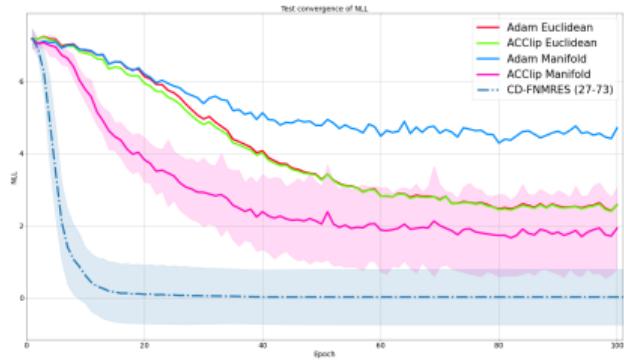
- Errors:

- Averaged NLL over N Tests
- Frobenius norm of differences for Covariance matrices
- Cosine similarity distance of differences for Mean Vectors
- difference of L2 Norms for weight Vectors

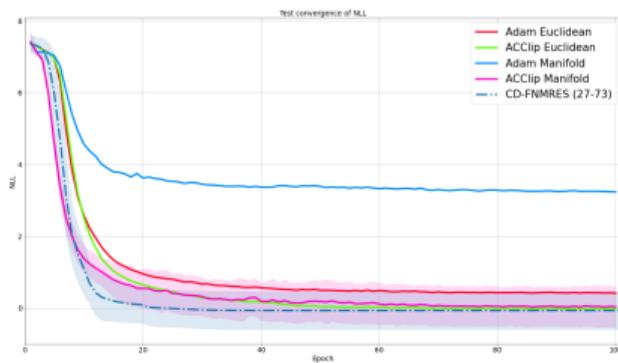
High Sep. NLL



2500 datapoints

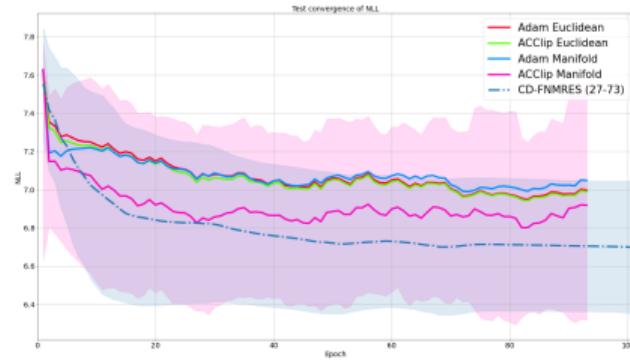
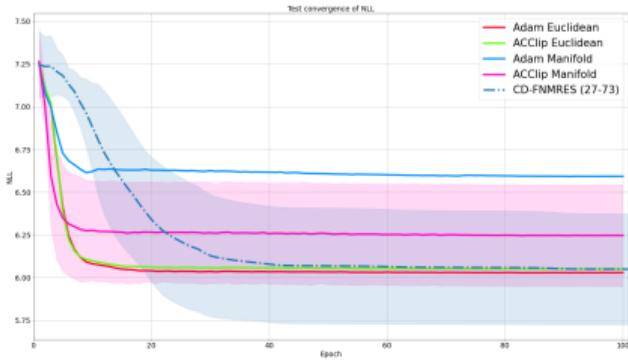


25000 datapoints



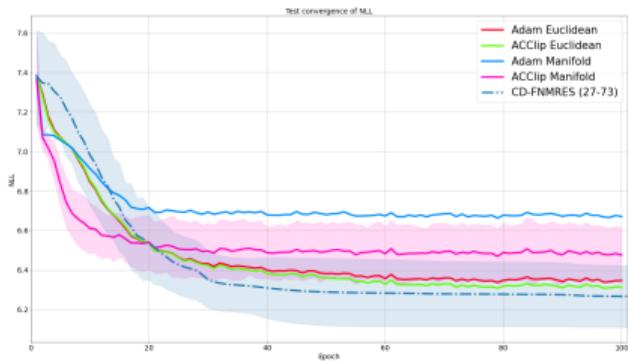
250 datapoints

Mid Sep. NLL



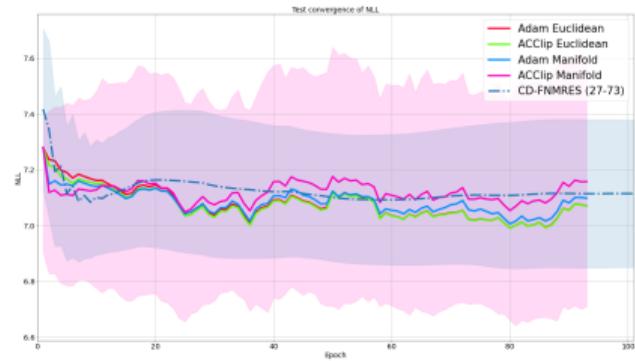
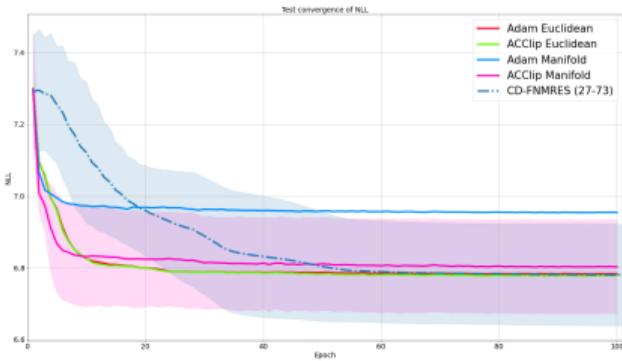
2500 datapoints

25000 datapoints



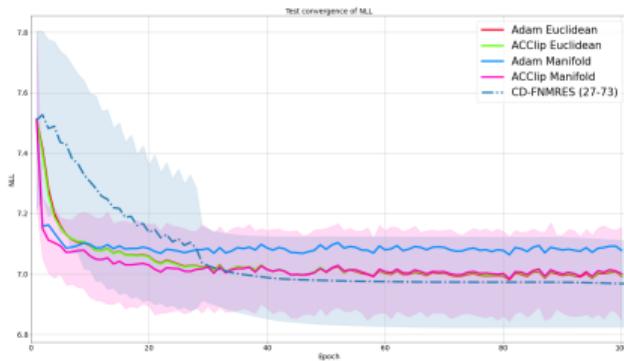
250 datapoints

Low Sep. NLL



2500 datapoints

25000 datapoints



250 datapoints

Experiments

Experiment Setup

DataSet	No. Sample	Dimension	Description
WAVE	5000	21	Waveform Database Generator Generator generating 3 classes of waves. Each class is generated from a combination of 2 of 3 "base" waves.
SVHN	99289	32 × 32	The dataset is obtained from house numbers in Google Street View images. There are 531,131 additional samples that we do not use.
USPS	7291	16 × 16	The dataset contains normalized handwritten digits, automatically scanned from envelopes by the U.S. Postal Service.
YEAR	515345*	90	The dataset are audio features from different songs. It has been gathered to be utilized to predict the release year of a song.

Table: DataSet Description

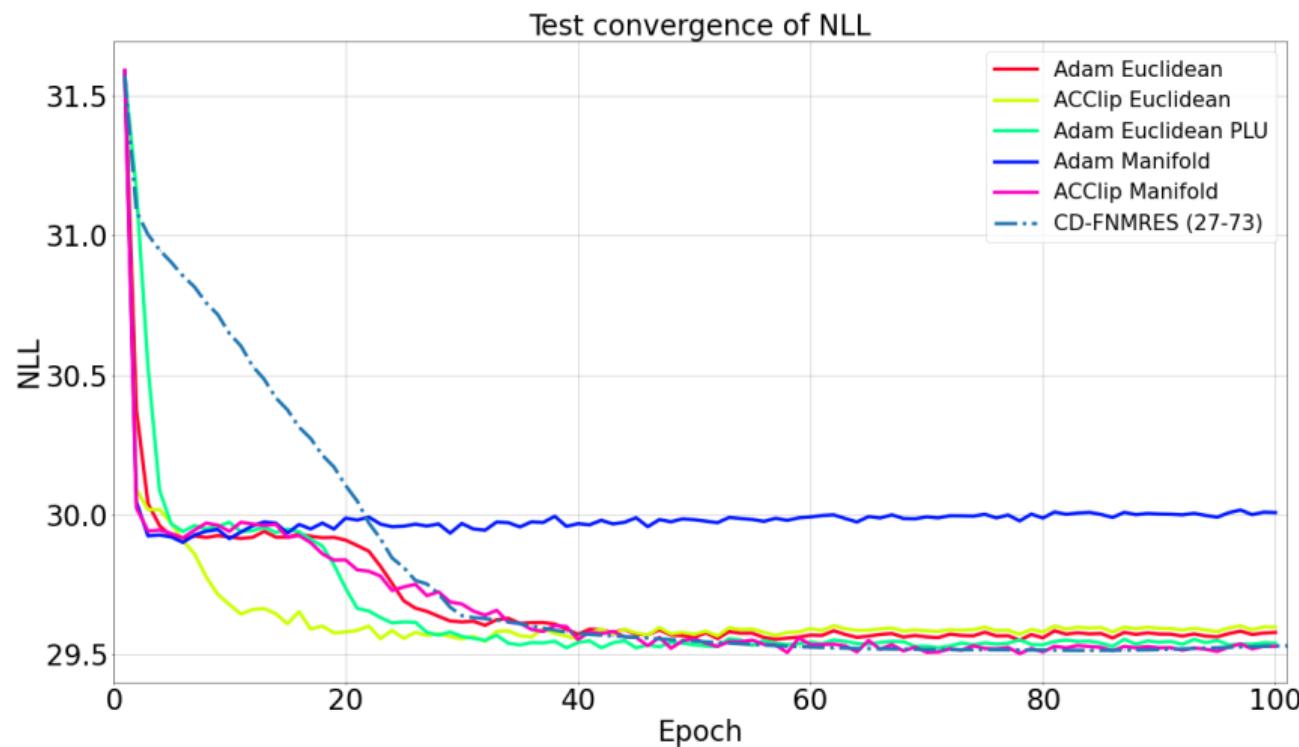
* 125000 of that had been used in tests

Experiment Setup

- The proportion is 80% Train set and 20% Test set in all Datasets.
- Dimension reduction with explained variance consideration is applied to data in some cases.
- Data had been whitened before entering the procedure.
- Number of components is fixed to dimension of dataset.
- Batch Size is always 128
- Single CPU Core was used
- Cosine Annealing was used for step-size decay

* 125000 of that had been used in tests

Experiment Results (WAVE[21])

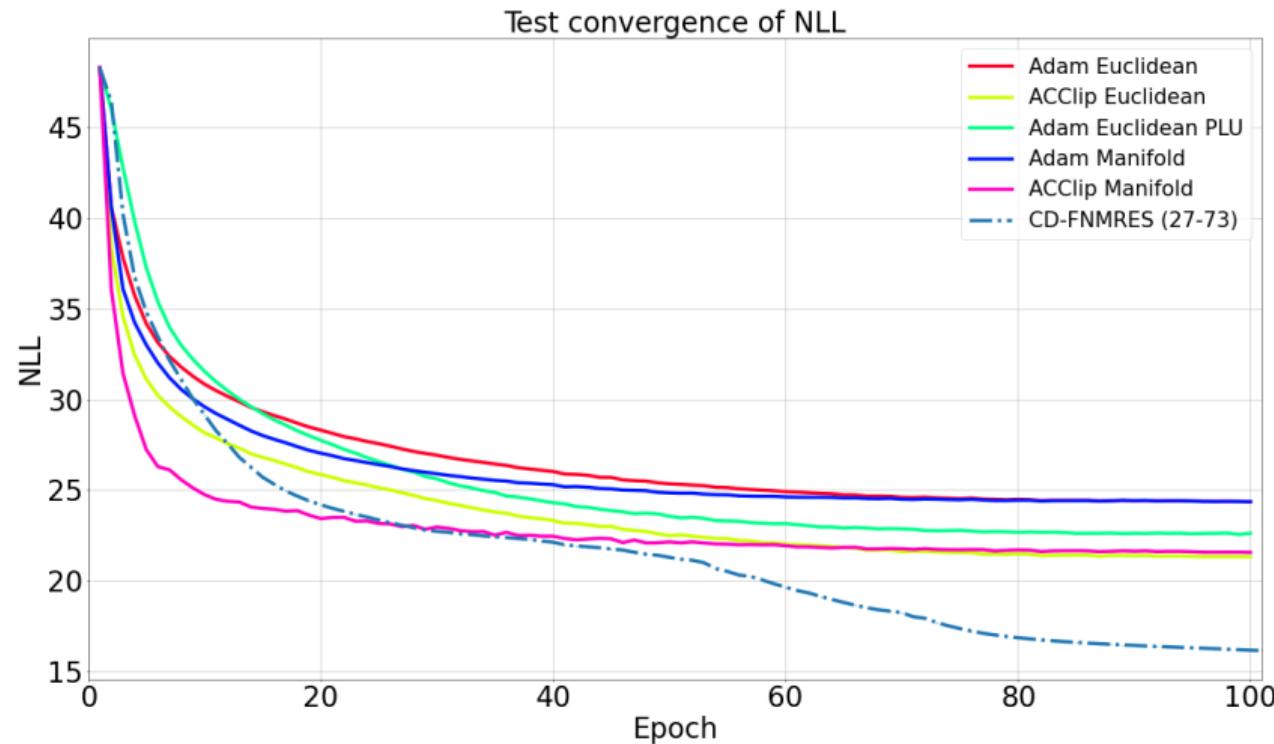


Experiment Results (WAVE[21])

Method	NLL	Time per epoch	Comments
Adam Euclidean	29.57	$0.49 \pm 0.01s$	
ACClip Euclidean	29.58	$0.57 \pm 0.01s$	
Adam Euclidean PLU	29.54	$0.72 \pm 0.04s$	
Adam Manifold	29.99	$0.43 \pm 0.01s$	qr Ret
ACClip Manifold	29.51	$0.65 \pm 0.02s$	qr Ret
CD-FNMRES	29.53	$0.23 \pm 0.03s$	27-73

Table: Time performance

Experiment Results (SVHN[30])

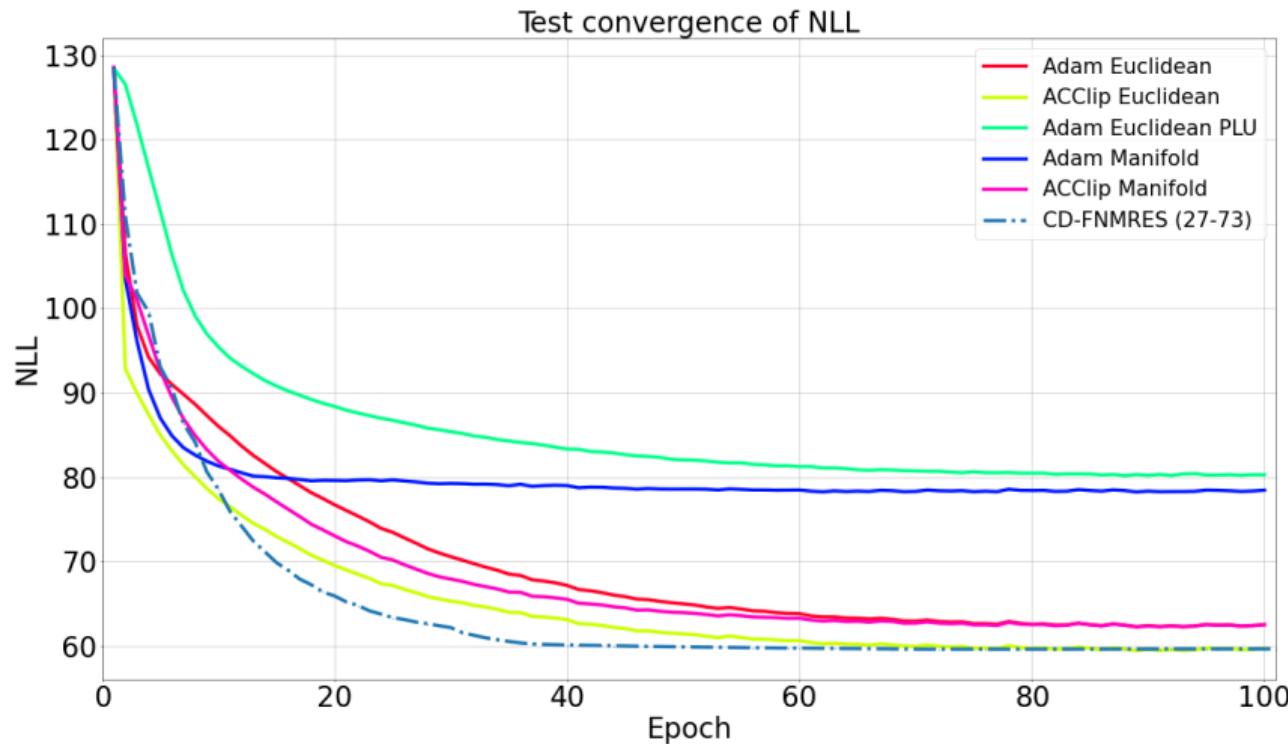


Experiment Results (SVHN[30])

Method	NLL	Time per epoch	Comments
Adam Euclidean	24.37	$15.45 \pm 0.45s$	
ACClip Euclidean	21.33	$16.33 \pm 0.57s$	
Adam Euclidean PLU	25.31	$24.18 \pm 1.51s$	
Adam Manifold	24.36	$12.72 \pm 0.39s$	qr Ret
ACClip Manifold	21.57	$14.71 \pm 0.37s$	qr Ret
CD-FNMRES	29.53	$4.55 \pm 0.57s$	27-73

Table: Time performance

Experiment Results (USPS[65])

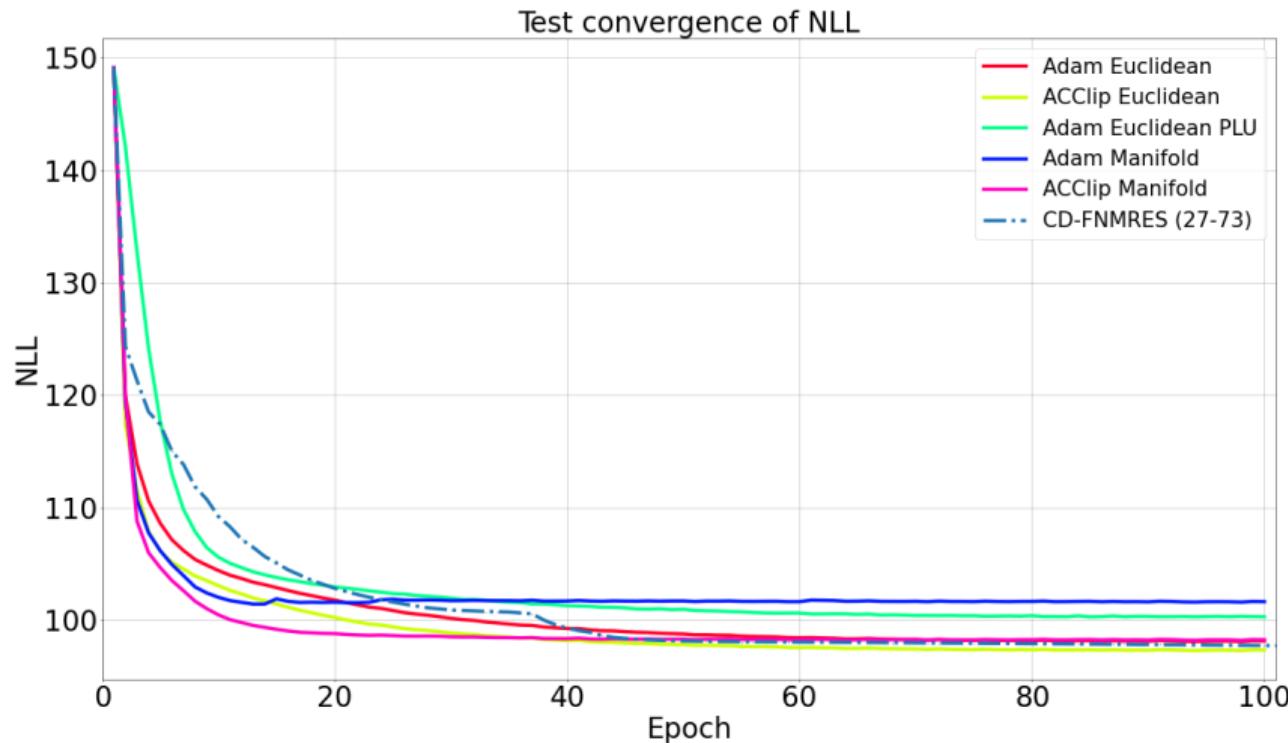


Experiment Results (USPS[65])

Method	NLL	Time per epoch	Comments
Adam Euclidean	62.51	$4.43 \pm 0.44s$	
ACClip Euclidean	59.73	$4.75 \pm 0.37s$	
Adam Euclidean PLU	80.24	$8.95 \pm 0.94s$	
Adam Manifold	78.47	$3.77 \pm 0.40s$	qr Ret
ACClip Manifold	62.52	$5.25 \pm 0.37s$	qr Ret
CD-FNMRES	59.66	$15.75 \pm 8.37s$	27-73

Table: Time performance

Experiment Results (YEAR[90])

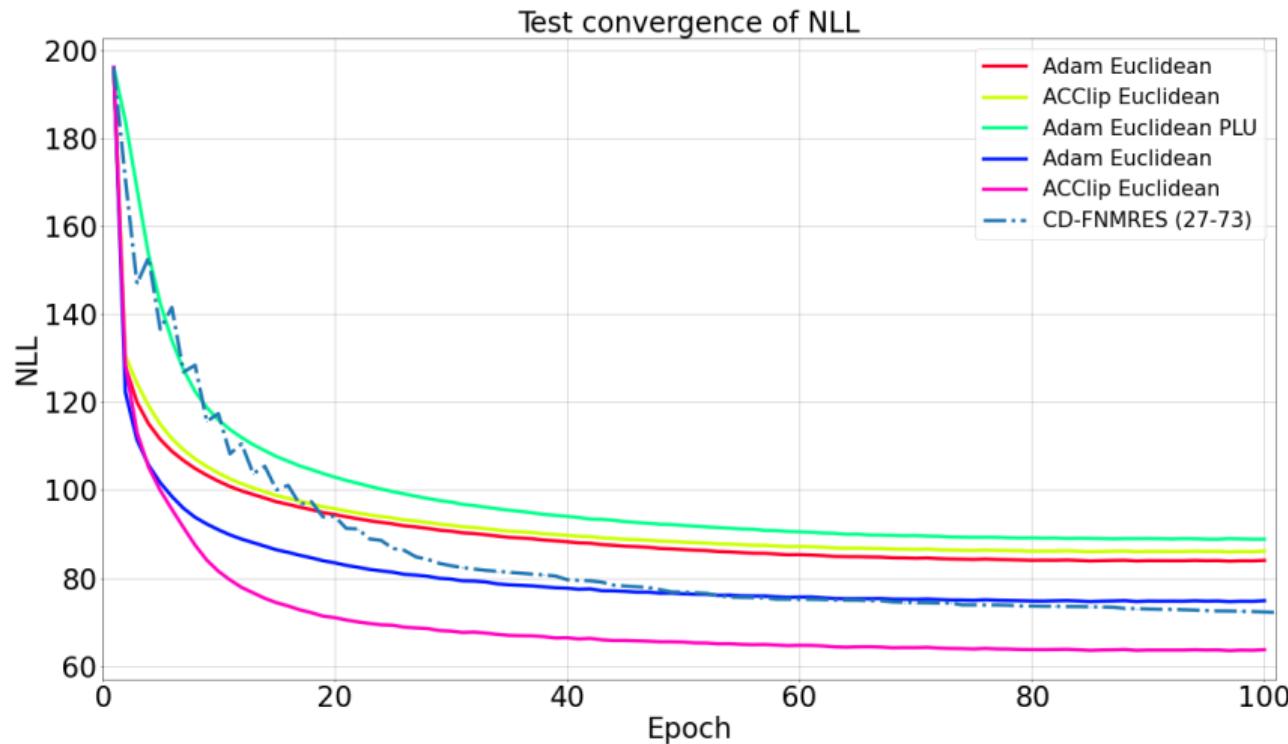


Experiment Results (YEAR[90])

Method	NLL	Time per epoch	Comments
Adam Euclidean	98.16	$94.63 \pm 5.53s$	
ACClip Euclidean	97.31	$103.34 \pm 5.87s$	
Adam Euclidean PLU	100.31	$195.47 \pm 16.31s$	
Adam Manifold	101.61	$78.13 \pm 4.07s$	qr Ret
ACClip Manifold	98.22	$97.37 \pm 3.72s$	qr Ret
CD-FNMRES	97.74	$141.06 \pm 60.20s$	27-73

Table: Time performance

Experiment Results (SVHN[100])



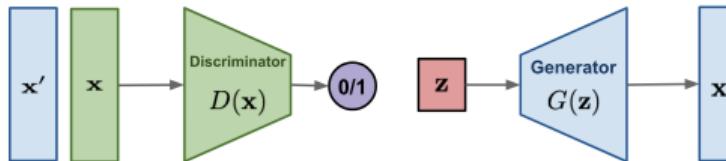
Experiment Results (SVHN[100])

Method	NLL	Time per epoch	Comments
Adam Euclidean	83.90	$83.37 \pm 6.49s$	
ACClip Euclidean	85.95	$90.41 \pm 6.54s$	
Adam Euclidean PLU	88.82	$185.96 \pm 19.33s$	
Adam Manifold	85.54	$86.04 \pm 3.19s$	qr Ret
ACClip Manifold	63.57	$85.01 \pm 13.34s$	qr Ret
CD-FNMRES	72.17	$216.30 \pm 107.42s$	27-73

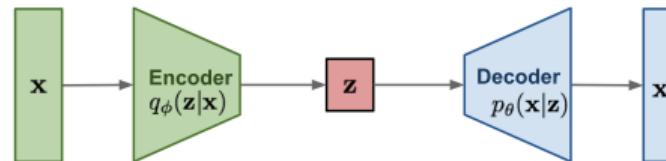
Table: Time performance

Flow-based Deep Generative Models

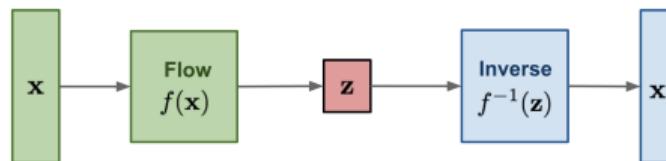
GAN: minimize the classification error loss.



VAE: maximize ELBO.

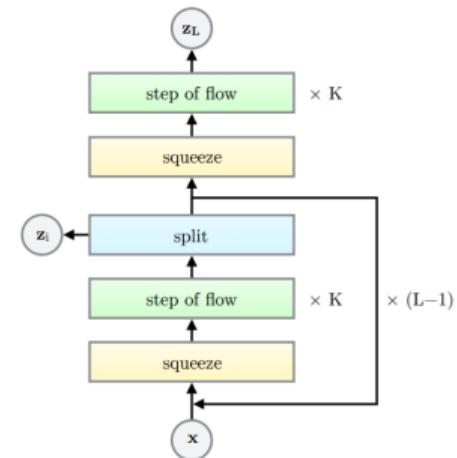
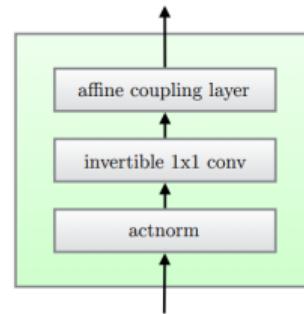
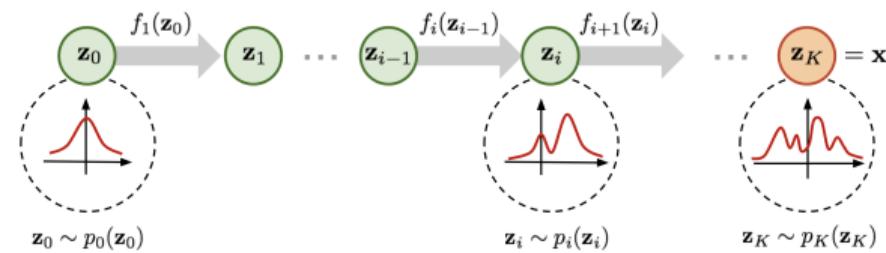


Flow-based generative models:
minimize the negative log-likelihood

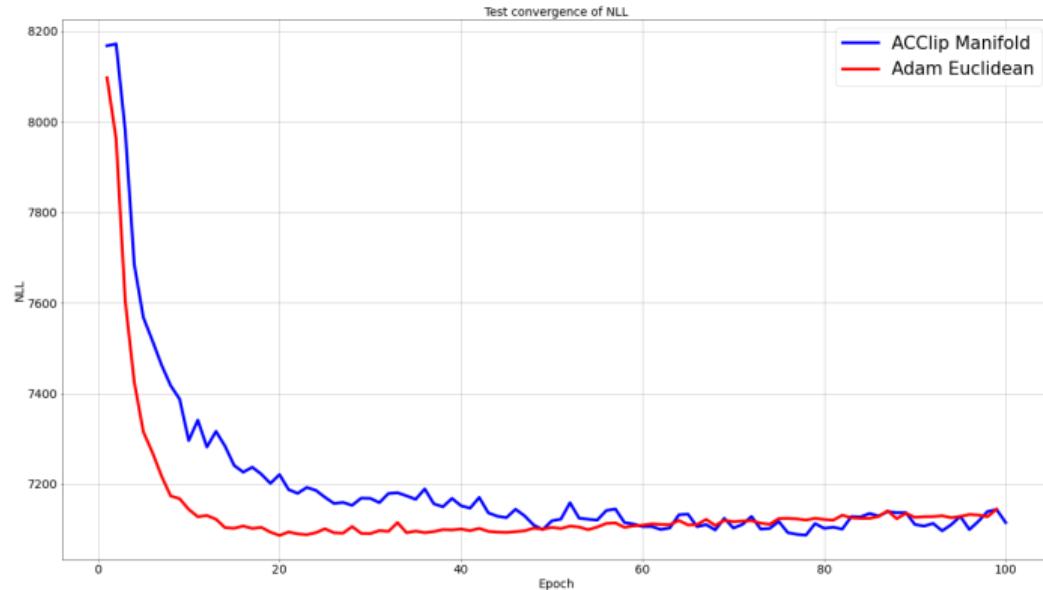


Flow-based Deep Generative Models

[Kingma and Dhariwal, 2018]



GLOW Results



GLOW Results

Last 3 Epochs of
ADAM



GLOW Results

Last 3 Epochs of
ADAM



Last 3 Epochs of
Ours



GLOW Results

Last 3 Epochs of
ADAM



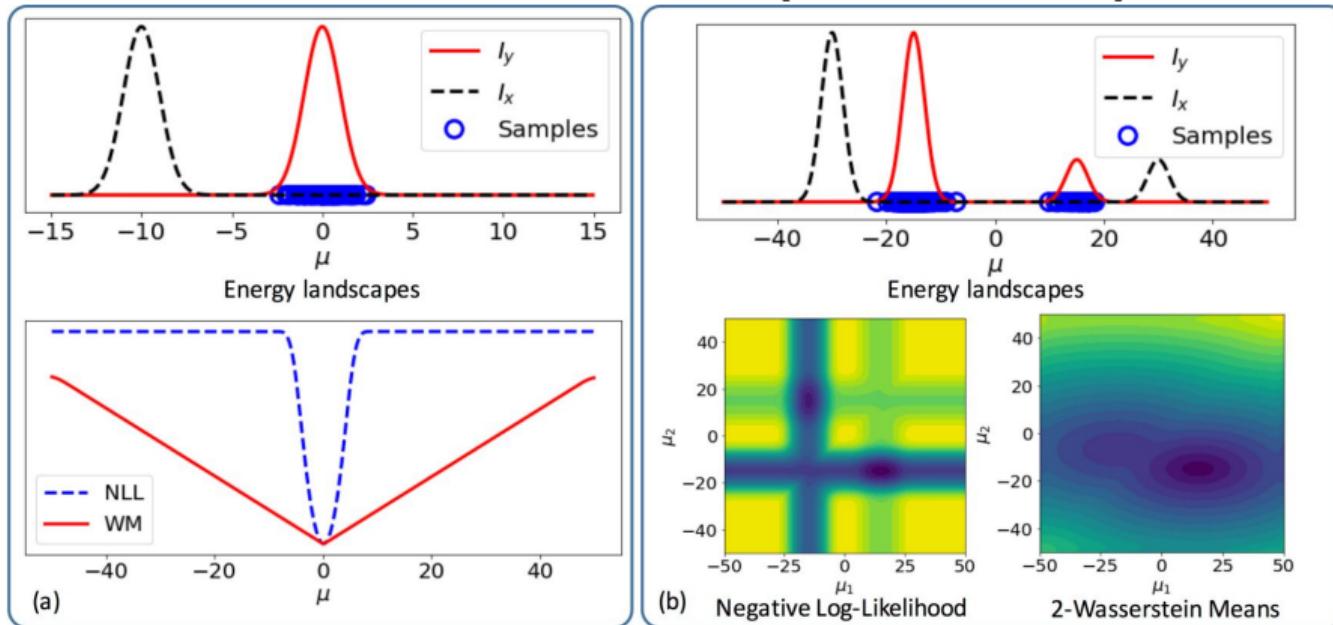
Last 3 Epochs of
Ours



Conclusion

Discussion

Parameter Estimation is HARD! [Kolouri et al., 2018]



Discussion

- We have investigated the online numerical solution for parameter estimation off GMM in sharing parameter scheme.
- An online optimization algorithm on $SO(n)$ is proposed which has been tested on both GMM and GLOW.
- The PLU factorization was shown to be not suitable for GMM parameter estimation.

References I

-  Asheri, H., Hosseini, R., and Araabi, B. N. (2021).
A new em algorithm for flexibly tied gmms with large number of components.
Pattern Recognition, 114:107836.
-  Bansal, N., Chen, X., and Wang, Z. (2018).
Can we gain more from orthogonality regularizations in training deep networks?
Advances in Neural Information Processing Systems, 31.
-  Gales, M. J. (1999).
Semi-tied covariance matrices for hidden markov models.
IEEE transactions on speech and audio processing, 7(3):272–281.
-  Hosseini, R. and Sra, S. (2015).
Matrix manifold optimization for gaussian mixtures.
Advances in Neural Information Processing Systems, 28:910–918.

References II

-  Hosseini, R. and Sra, S. (2020).
An alternative to em for gaussian mixture models: batch and stochastic riemannian optimization.
Mathematical Programming, 181(1):187–223.
-  Huang, L., Liu, X., Lang, B., Yu, A., Wang, Y., and Li, B. (2018).
Orthogonal weight normalization: Solution to optimization over multiple dependent stiefel manifolds in deep neural networks.
In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32.
-  Kingma, D. P. and Dhariwal, P. (2018).
Glow: Generative flow with invertible 1x1 convolutions.
Advances in neural information processing systems, 31.

References III



- Kolouri, S., Rohde, G. K., and Hoffmann, H. (2018).
Sliced wasserstein distance for learning gaussian mixture models.
In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*,
pages 3427–3436.

Thanks for Your Attention

Please feel free to share comments or ask questions!

mohammad.pasande@ut.ac.ir

