Generative Modeling of Sequential Data

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What is Generative Modeling?

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- Short answer to why question: Extracting structure out of data, understanding data

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 - Document Analysis (LDA)
 - Audio Source Separation (NMF)
 - Image in-painting
 - Generating random images (my favorite)

Generative Modeling in Action

Weight and Heights of the members of an African tribe



$$egin{aligned} &h_n \ \sim \mathsf{Discrete}([\pi,1-\pi]) \ &x_n | h_n \ \sim \mathcal{N}(\mu_{h_n},\Sigma_{h_n}) \end{aligned}$$

Learning:

$$\max_{\theta} \sum_{n} \log p(x_n | \theta)$$

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A sequence example



Hugely popular NMF model: X = WH (figure stolen from Paris)

Learning distributions over sequences



Original Data

Generated with the method in Chapter 4 of this thesis.

Modeling/Representation

How we represent the data (what model/distribution we use)

Learning Paradigm

 The cost function used to measure between model distribution and underlying data distribution (e.g. maximum likelihood, adversarial training, method of moments)

Optimization

 Given the model and the learning paradigm, the procedure with which we obtain the model parameters.

Contributions in this thesis

- A Learning with multi-modal latent representations in implicit generative models (UAI 2018 submission (New)
- B Method of Moments Framework for HMMs with special structure (NIPS 2014, WASPAA 2015)
- C Convolutional neural nets for source separation (MLSP 2017 best paper award)
- D Diagonal RNNs in symbolic music modeling (WASPAA 2017)
- E Identifiable Factorial HMMs (NIPS 2015, ICASSP 2017 submissions)
- F GANs for source separation (ICASSP 2018) (New)



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Method of Moments framework for structured HMMs Method of Moments Introduction Two Step Estimation Framework

Factorial HMM

Factorial HMM introduction Shared Component Factorial Model Revealing Factorial Model

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Learning the base Distribution in Implicit Generative Models Methodology

Conclusions

Summary and thoughts

Learning in Latent Variable Models

Typical objective is Maximum Likelihood:

$$\begin{split} \max_{\theta} \mathbb{E}_{x} \log p(x|\theta) \\ = \max_{\theta} \mathbb{E}_{x} \log \sum_{h} p(x, h|\theta) \end{split}$$

- Observations: x.
- **Hidden Variables:** *h*.
- Parameters (to be optimized): θ .

Learning in Latent Variable Models

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- **Observations:** *x*.
- **Hidden Variables:** h.
- Parameters (to be optimized): θ .
- In general not convex.
- This poses a challenge in terms of optimization. In general, it is difficult to train latent variable models. Can we devise methods to more easily reach solutions around the global optimum?

Method of Moments

The idea is to estimate the models parameters θ by solving a system of non-linear equations formed with moments E[g_k(x)], k ∈ {1,...K}:

```
\mathbb{E}[g_1(x)] = f_1(\theta)
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 $\mathbb{E}[g_{\mathcal{K}}(x)] = f_{\mathcal{K}}(\theta)$

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$$\mathbb{E}[g_{\mathcal{K}}(x)] = f_{\mathcal{K}}(\theta)$$

► Canonical Example: x ~ G(a, b):

$$\mathbb{E}[x] = ab \qquad \longrightarrow \qquad b = (\mathbb{E}[x^2] - \mathbb{E}[x]^2) / \mathbb{E}[x]$$
$$\mathbb{E}[x^2] = ab^2 + a^2b^2 \qquad \qquad \widehat{a} = \mathbb{E}[x]^2 / (\mathbb{E}[x^2] - \mathbb{E}[x]^2)$$

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Can we do this for latent variable models?

Spectral Learning of Mixture of HMMs

[MHMM, Smyth 97]



 $egin{aligned} h_n &\sim \textit{Categorical}(\pi_n)\ \mathbf{x}_n &\sim \textit{HMM}(A_n,O_n) \end{aligned}$

Spectral Learning of Mixture of HMMs

[MHMM, Smyth 97]



$$h_n \sim Categorical(\pi_n)$$

 $\mathbf{x}_n \sim HMM(A_n, O_n)$

• Learning Goal: Estimate π_n, A_n, O_n , given $\mathbf{x}_{1:N}$

$$\bar{O} = \begin{bmatrix} O_1 & \dots & O_K \end{bmatrix}, \quad \bar{A} = \begin{bmatrix} A_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & A_2 & \dots & \mathbf{0} \\ & & \ddots & \\ \mathbf{0} & \mathbf{0} & \dots & A_K \end{bmatrix}, \quad \bar{\nu} = \begin{bmatrix} \pi_1 \nu_1 \\ \pi_2 \nu_2 \\ \vdots \\ \pi_K \nu_K \end{bmatrix}$$

An MHMM with *local* parameters θ_{1:K} = (O_{1:K}, A_{1:K}, ν_{1:K}, π) is an HMM with *global* parameters θ
= (O
, A
, ν
), where:

$$\bar{O} = \begin{bmatrix} O_1 & \dots & O_K \end{bmatrix}, \quad \bar{A} = \begin{bmatrix} A_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & A_2 & \dots & \mathbf{0} \\ & & \ddots & \\ \mathbf{0} & \mathbf{0} & \dots & A_K \end{bmatrix}, \quad \bar{\nu} = \begin{bmatrix} \pi_1 \nu_1 \\ \pi_2 \nu_2 \\ \vdots \\ \pi_K \nu_K \end{bmatrix}$$

- Estimating the global parameters $\bar{\theta}$ with a moment algorithm would introduce permutation \mathcal{P} and noise to the estimates.
- How to impose this structural constraint on the estimator?

An HMM with state marginals $p(h_t)$ is equivalent to a mixture model with mixing weights $\pi := \frac{1}{T} \sum_{t=1}^{T} p(h_t)$, and the same emission parameters.

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- First compute (estimate) \hat{O} , and $\hat{\pi}$.
- Then solve the convex problem:

$$egin{aligned} \widehat{A} &= rg\min_{A} \|M_2 - \widehat{O}A ext{diag}(\widehat{\pi}) \widehat{O}\|_F \ s.t. \ \mathbf{1}^{ op} A &= \mathbf{1}^{ op}, \ A &\geq 0. \ (\mathbf{1} - \mathcal{M}) \odot A &= 0, \end{aligned}$$

where \mathcal{M} encodes the block diagonal structure.

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Problem: \hat{O} is still permuted.

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s.t. $1^{\top}A = 1^{\top},$
 $A \ge 0.$
 $(1 - \mathcal{M}) \odot A = 0,$

where \mathcal{M} encodes the block diagonal structure.

- **Problem:** \hat{O} is still permuted.
- But \widehat{A} is de-permutable! (if we remove the block diagonal constraint)

Two stage estimation framework

- Get rough/permuted estimates for the parameters $\widehat{O}, \widehat{A}, \widehat{\pi}$.
- ▶ De-permute A. (Solve the graph problem dictated by model)
- Solve:

$$\begin{split} \min_{A} & \|M_2 - \widehat{O}A \operatorname{diag}(\widehat{\pi}) \widehat{O}\|_{F} \\ s.t. & \mathbf{1}^{\top} A = \mathbf{1}^{\top}, \\ & A \geq 0. \\ & f(\mathcal{M}, A) = \mathbf{0} \end{split}$$

• f, and \mathcal{M} depend on the model.

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• f, and \mathcal{M} depend on the model.

For MHMM \mathcal{M} is the complement of a binary block diagonal matrix.

Mixture of HMMs: De-permutation

• $\lim_{e\to\infty} \bar{A}^e = [\bar{v}_1 1_M^\top, \bar{v}_2 1_M^\top, \ldots, \bar{v}_K 1_M^\top]$, where \bar{v}_k is the k'th eigenvector of \bar{A} .



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• What happens for $\mathcal{P}(\bar{A})$:


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• What happens for $\mathcal{P}(\bar{A})$:



What happens in practice:



MHMM De-permutation Continued





• Then form rank- \widehat{K} reconstruction A^r :

$$A^{r} = V_{1:\widehat{K}} \Lambda_{1:\widehat{K}} V^{-1}$$

Then Cluster. (A La Spectral Clustering)

- Experiment: Clustering handwritten digit trajectories by learning MHMMs.
- ▶ We form datasets composed of digits 1-2, 1-3, 2-3, and so on.

Algorithm	1v2	1v3	1v4	1v5	2v3	2v4	2v5
Spectral	100	70	54	55	83	99	99
EM init. at Random	96	99	98	54	83	100	100
EM init. w/ Spectral	100	99	100	100	96	100	100

Numbers show percent clustering accuracies.

Initializing EM with the spectral algorithm boosts the results.

Generalization



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Generalization



Generalization



Bakis-HMM

▶ Is an HMM that can only move one state at a time.



- Every state is visited exactly once.
- Depermutation: Find a maximum weight Hamiltonian circuit on Â. (Traveling Salesman problem)



Experimental Results on Speech Onset Detection



- Triangles denote randomly initialized EM performance on run-time vs f-measure. (EM is implemented in C)
- Numbers show spectral + number of EM iterations.
- Spectral Algorithm accelerates EM learning.

Contribution and summary

 Contribution: A method of moments based framework for HMMs with special transition structure. (learning paradigm)

Helps in initializing EM. (optimization)

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Thoughts on method of moments:

► Good:

- Global
- Initialization: No need to worry about initialization (Great initializer for EM (optimization)).
- Scalable: Computationally cheap: Gather the moments, factorize a small matrix.
- Interesting/Theoretical: Bounds.

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- Interesting/Theoretical: Bounds.
- ► Bad:
 - Model Mismatch: Horrible in regards to model mismatch. (Hard assumption on model Unlike ML, which minimizes KL(p||q).
- ► Ugly:
 - You can get complex numbers for parameter estimates/likelihoods.

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Factorial HMM

Factorial HMM introduction Shared Component Factorial Model Revealing Factorial Model

Generative Models for Supervised Source Separation

Source Separation Introduction Convolutional Neural Network Models for Audio Generative Adversarial Source Separation

Learning the base Distribution in Implicit Generative Models Methodology Results

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Factorial HMM

[Ghahramani, Jordan; 97]



Factorial HMM

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The dictionary Activations noise

Some Dictionary Learning Perspective..

General Dictionary Learning



- PCA: Both O and R are orthogonal.
- ▶ ICA: Solvable if *R* has independent coordinates.
- Mixture Model: *R* is one sparse. Solvable is *O* has full column rank.
- ▶ Sparse Dictionary Learning: Solvable if *O* is square and *R* is sparse Bernouilli-Gaussian. [Spielman et al. 12]

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Factorial Models:

$$O = \begin{bmatrix} O^1 & \dots & O^K \end{bmatrix}, \ R = \begin{bmatrix} R^1 \\ \vdots \\ R^K \end{bmatrix}$$

- ▶ No constraint on *O*, columns of *R* are block-*K* sparse.
- No Unique Solution!!!

Rank Deficiency

 $\operatorname{rank}(R) \leq MK - (K - 1)$

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Proof Sketch:

 $\dim(\operatorname{null}(R^{\top})) \geq K - 1.$

Therefore from rank-nullity theorem $rank(R) \leq MK - (K - 1)$.

FHMM is unidentifiable

For a given assignment matrix $R \in \mathbb{R}^{KM \times T}$ There exists $O_1 \neq O_2$ such that $\prod_t \mathcal{N}(x_t | O_1 R, \sigma^2 I) = \prod_t \mathcal{N}(x_t | O_2 R, \sigma^2 I)$.

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Proof: Since dim(null(R^{\top})) $\geq K - 1$, $(O_1 - O_2)R = 0$, for $O_1 \neq O_2$.

Shared Component FM

$$\forall k, \ O^{k} = \begin{bmatrix} | & | & | & | & | \\ \mu_{k}^{1} & \mu_{2}^{k} & \dots & \mu_{M-1}^{k} & s \\ | & | & | & | & | \end{bmatrix}$$

SC-FM is identifiable

Given an assignment matrix \tilde{R} which is rank MK - (K - 1), the emission matrix of an SC-FM is identifiable.

Proof Sketch:

 $\dim(\operatorname{null}(R^{\top})) = 0.$

Therefore $(O_1 - O_2)R \neq 0$, $\forall O_1 \neq O_2$.

Learning Example for Shared Component Factorial Model

• **Gist:** If the shared component *s* is incoherent, then we can identify it, and reveal the other components.

Example Observations



Obtained Components with SC-FM

5201 6341

Components with regular model-EM



Learning Example for Shared Component Factorial Model

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Example Observations



Obtained Components with SC-FM

5201 6341

Components with regular model-EM



The shared component + incoherence assumption a bit too restrictive. Can we think of another model?

FHMM Identifiable Alternative 2



Identifiability follows similarly from the activation matrix R.

Revealing FHMM Practical Algorithm

Practical Algorithm for Revealing FHMM

- Cluster the data matrix $X \in \mathbb{R}^{L \times T}$ into clusters $X^c \in \mathbb{R}^{L \times C}$.
- Solve:

$$\begin{split} \min_{H} & \|X^{c} - X^{c}H\|_{F}^{2} + \beta \|H\|_{1}, \\ s.t. \ H_{i,i} &= 0, \text{ for } 1 \leq i \leq C, \\ & H \geq 0, \end{split}$$

where $H \in \mathbb{R}^{C \times C}$.

• Construct a bi-partite graph by reading the solution for *H*.

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where $H \in \mathbb{R}^{C \times C}$.

- Construct a bi-partite graph by reading the solution for H.
- Condition for learnability: Let O₁ = [x₀, x₁], O₂ = [y₀, y₁]. Observed combinations needs to form a connected graph (Connectivity), and we need to observe all nodes and edges (Observability).



Unsupervised audio source separation example

- ▶ We mixed recording of double bass and flute (at 0dB).
- The observed mixtures satisfy the connectivity constraint.

Original Mixture



Reconstruction

We obtain almost perfect source separation.



▶ The algorithm is robust to the choice of number of clusters *C*.

- Contribution 1: We have shown that the standard Factorial Model is not statistically identifiable. (modeling)
- Contribution 2: We have proposed two identifiable alternatives, along with practical parameter estimation algorithms. (modeling and optimization)
- Future work:
 - Can we relax the observability assumption so that we only require to observe less nodes in the connectivity graph?
 - Potential application in semi-supervised source separation.

Plan

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Source Separation





Generative Supervised Source Separation

Assumes the following generative model:

$$egin{aligned} s_1 &\sim p_{ ext{out}}(s_1|f_{ heta^1}(h_1)) \ s_2 &\sim p_{ ext{out}}(s_2|f_{ heta^2}^2(h_2)) \ x &\sim p_{ ext{out}}(x|s_1+s_2) \end{aligned}$$

Generative Supervised Source Separation

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First train the generative models for each source (with Maximum Likelihood):

$$\max_{\theta^k} \mathbb{E}_{s_k} p(s_k | f_{\theta^k}(h_k)),$$

where $h_k = f_{\theta_k}^{enc}(s_k)$, is some encoding.



Generative Supervised Source Separation

In test time, the source estimates are obtained via:



Separation Example

Separation is usually done on spectrograms.



• Because of non-negativity, we usually use $p(X|f_{\theta}(H)) = \mathcal{PO}(X; f_{\theta}(H))$
Non-Negative Matrix Factorization (NMF) [Smaragdis 2003]

$$f_{ heta}(H) = WH, \ W \geq 0, H \geq 0$$

Only, the forward model $f_{\theta}(H)$ is specified, H is obtained with an algorithm.

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Convolutive NMF [Smaragdis 2004]

$$f_{\theta}(H) = \sum_{k=0}^{K} W_k * H_k, \ W \ge 0, H \ge 0$$

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- Linear mappings allow adaptive step-size optimization algorithms such as EM, multiplicative update rules (even globally optimal methods such as method of moments). However representation wise, they are limited.
- Rest of the thesis will utilize generative models which employ more general non-linear mappings. (neural networks)

Neural Network Alternative for NMF [Smaragdis, Venkataramani, 2016]

$$egin{aligned} &f_{ heta}(X) = \sigma(WH(X)) \ &= \sigma(Wf_{ heta}^{ extsf{enc}}(X)) \ &= \sigma(W\sigma(W^{ extsf{enc}}X)) \end{aligned}$$

where $f_{\theta}^{\text{enc}}(X)$ is the encoder, and it is learned.

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Convolutive neural-net alternative?

Convolutive Neural Network Alternative

 Neural Network Alternatives for Convolutive NMF [Best student paper award, MLSP 2017]

$$f_{\theta}(H(X)) = \sigma\left(\sum_{k=0}^{K} W_k * H_k(X)\right),$$

where $H_k(X) = \sigma\left(\sum_j (W_k^{inv} * X)_j\right)$



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We can also try RNNs to model arbitrarily long dependencies.

RNNs in the encoder:

$$H_k(X) = \sigma\left(\sum_j (RNN_k(X))_j\right)$$



- **Dataset:** Male-female speaker mixtures from TIMIT dataset.
 - Training set: 9 utterances for each speaker.
 - Test set: Single sentence mixture at 0dB.
 - Evaluated for 25 pairs of speakers.
- Evaluation: BSS eval metrics. (SIR, SAR, SDR)
- We compare Feedforward-Feedforward, Convolutive-Convolutive, Recurrent-Convolutive Autoencoders.



- ► Conv-Conv, Conv-RNN, FF-FF autoencoders.
- Variance is over the speaker pairs.
- Significant SIR improvement with Convolutive Models.
- Recursive encoder model is better than the baseline, but not as good as the convolutive model.

Generative Adversarial Source Separation

- ▶ Maximum likelihood training requires specifying p_{out}(.)/loss function.
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• Define the likelihood via a classifier D(.).

In testing we can use the classifier:

$$\max_{h_1,h_2} p_{\text{out}}(x|f_{\theta^1}(h_1) + f_{\theta^2}(h_2)) + \lambda \left(\sum_{k=1}^2 D_{\xi_k}(f_{\theta^k}(h_k))\right)$$

Generative Adversarial Source Separation



Results

- Dataset: Male-female speaker mixtures from TIMIT dataset.
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 - Test set: Single sentence mixture at 0dB.
 - Evaluated for 25 pairs of speakers.
- Evaluation: BSS eval metrics. (SIR, SAR, SDR)
- We compare NMF, Variational Autoencoders, Denoising Autoencoder, GAN, and Wasserstein GAN, all with a multilayer perceptron architecture.



- Contribution 1: We developed a neural network model which is an analog of convolutive NMF, both with convolutional and recurrent neural network architectures. (representation)
- ► **Contribution 2:** We showed that GANs worked better than maximum likelihood based methods on a speech source separation task.
 - This is potentially because GANs are more agnostic to output noise. (learning paradigm)

Plan

Method of Moments framework for structured HMMs Method of Moments Introduction Two Step Estimation Framework

Factorial HMM

Factorial HMM introduction Shared Component Factorial Model Revealing Factorial Model

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Conclusions

Summary and thoughts



VAEs and GANs are very popular methods for generative model learning.



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- ▶ VAEs and GANs are very popular methods for generative model learning.
- ▶ VAE is learned by gradient descent optimizing a lower bound to likelihood.
- GAN model is an implicit generative model. It is learned by using an auxiliary "discriminator" network. Optimization is very very tricky.
- A big problem for both: They try to map a simplistic distribution such as isotropic Gaussian to the whole set of observations.

Get the base



VAEs:GANs: $h \sim \mathcal{N}(0, I)$ $h \sim \mathcal{N}(0, I)$ $x|h \sim \mathcal{N}(f_{\theta}(h), \sigma^2 I)$ $x|h = f_{\theta}(h)$







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Maximum Likelihood for Implicit Generative Model

Implicit Generative Models:

$$h \sim p_{\phi}^{0}(h), \ x = f_{\theta}(h)$$

where, p⁰_φ(h) is the base distribution and f_θ(h) is some forward mapping.
The likelihood is given by,

$$p_{\text{model}}(x| heta,\phi) = p_{\phi}^{0}(f_{ heta}^{-1}(x))V_{ heta}(x)$$

where $V_{\theta}(x) := \left| \det \frac{\partial f_{\theta}^{-1}(x)}{\partial x} \right| = \left| \det \frac{\partial f_{\theta}(h)}{\partial h} \right|^{-1}$, which measures the volume change due to the transformation.

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- Main problem: This requires a square transformation. No good for high dimensional structured data.
- Also joint optimization is difficult. (Joint in θ and ϕ)

Consider an autoencoder such that $f_{\theta}(f_{\psi}^{enc}(x)) \approx x$.

-Train the auto-encoder parameters θ , ψ such that:

$$\min_{\theta,\psi}\sum_{n}\|f_{\theta}(f_{\psi}^{enc}(x_{n}))-x_{n}\|$$

-Fit the base distribution on the latent space such that:

$$\max_{\phi} \sum_{n} \log p_{\phi}^{0}(f_{\psi}^{enc}(x_{n}))$$

This is approximately maximum likelihood:

$$= \max_{\phi} \sum_{n} \log p_{\phi}^{0}(f_{\psi}^{enc}(x_{n})) + \log V(x_{n})$$

Base distribution parameters are independent from the volume term.



▶ The likelihood for a sequence is given as:

$$p_{\text{model}}(x_{1:T}|\psi,\phi) = \prod_{t=1}^{T} p_{\phi}^{0}(f_{\psi}^{\text{enc}}(x_{t})|f_{\psi}^{\text{enc}}(x_{1:t-1}))V(x_{t}),$$

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- The algorithm: Fit an autoencoder. Then fit a sequential base distribution $p^{0}(.)$, such as an HMM or RNN.
- ▶ This is a bonus that comes with this method. Not straightforward to do sequence learn with GANs and VAEs.
MNIST

(top) Nearest neighbor samples to test instances (bottom) Random samples

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(top) Nearest neighbor samples to test instances (bottom) Random samples











VAE



GAN



Wasserstein GAN



IML



Algorithm	MNIST	CELEB-A	
IML	143	-8318	
VAE	132	-11003	
GAN	-5	-11970	
WGAN	64	-12986	

$$\begin{split} \mathsf{KDE} \ \mathsf{score} = & \frac{1}{N_{\mathsf{test}} N_{\mathsf{samples}}} \sum_{n=1}^{N_{\mathsf{test}}} \sum_{m=1}^{N_{\mathsf{samples}}} \mathcal{N}(x_n^{\mathsf{test}}; x_m^{\mathsf{sample}}, 0.1 I).\\ \approx & \mathsf{KL}(p_{\mathsf{data}}(x) \| p_{\mathsf{model}}(x | \theta)) \end{split}$$

Audio

We learn a distribution over overlapping windows in the time domain.



Original Data

 Contribution 1: We have developed a method which enables using multi-modal latent representations. (representation)

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- Contribution 2: The method does maximum likelihood for an approximate implicit model likelihood. (learning paradigm)
- Contribution 3: We have proposed an efficient algorithm for two step optimization. The algorithm is much less sensitive to hyper-parameter fine tuning, unlike GANs. (optimization)
- Overall, we get closer to \mathcal{M} :



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Conclusions Summary and thoughts The first half my PhD was focused more on optimization. My aim was to develop methods for "global" optimization.

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Summary

- The first half my PhD was focused more on optimization. My aim was to develop methods for "global" optimization.
- However, I do admit these methods require simple models. I think for success in real data applications one needs *realistic* models. Neural networks at the moment seem to be good models for this.

	Representation	Learning Paradigm	Optimization
Chapter 2	N.A.	MoM learning framework for HMMs	EM initialization with the MoM framwork
Chapter 3	Identifiable FHMM alternatives	N.A.	Proposed algorithms for FHMM
Chapter 4	Multi modal latent representation with IMLs	Maximum Likelihood Learning for Implicit Models	Two-Step optimization procedure
Chapter 5	Convolutive Architectures for Audio, Diagonal RNNs*	GANs in Audio	N.A.

*Not presented today for the interest of time.

Contributions in this thesis

- A Learning with multi-modal latent representations in implicit generative models (UAI 2018 submission (New)
- B Method of Moments Framework for HMMs with special structure (NIPS 2014, WASPAA 2015)
- C Convolutional neural nets for source separation (MLSP 2017 best paper award)
- D Diagonal RNNs in symbolic music modeling (WASPAA 2017)
- E Identifiable Factorial HMMs (NIPS 2015, ICASSP 2017 submissions)
- F GANs for source separation (ICASSP 2018) (New)



Some models are difficult to learn, and can use help in optimization: e.g. HMMs. Method of Moments is a good initialization scheme.

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- More agnostic models can help in generalization. (Source separation with GANs)
- Some models are not learnable (identifiable). In cases where we care about inference, this matters. (FHMM)
- My main belief after all this:
 - An approximate learning algorithm for an exact model is better than an exact algorithm for an approximate model. (IML, convolutive NMF are good examples for this)