## Composing graphical models with neural networks for structured representations and fast inference

Matthew J Johnson (<u>mattjj@google.com</u>) Deep Learning Summer School Montreal 2017

















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[1] Lee and Glass. A Nonparametric Bayesian Approach to Acoustic Model Discovery. ACL 2012.[2] Lee. Discovering Linguistic Structures in Speech: Models and Applications. MIT Ph.D. Thesis 2014.





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## Frame 0





Alexander Wiltschko, Matthew Johnson, et al., Neuron 2015.

## Frame 0





Alexander Wiltschko, Matthew Johnson, et al., Neuron 2015.



### image manifold















## Recurrent neural networks? [1,2,3]







Figure 2. LSTM Autoencoder Model

[1] Srivastava, Mansimov, Salakhutdinov. Unsupervised learning of video representations using LSTMs. ICML 2015.

[2] Ranzato, MarcAurelio, et al. Video (language) modeling: a baseline for generative models of natural videos. Preprint 2015.

[3] Sutskever, Hinton, and Taylor. The Recurrent Temporal Restricted Boltzmann Machine. NIPS 2008.

## Recurrent neural networks? [1,2,3]





Figure 2. LSTM Autoencoder Model

Figure 1. LSTM unit

## Probabilistic graphical models? [4,5,6]



[1] Srivastava, Mansimov, Salakhutdinov. Unsupervised learning of video representations using LSTMs. ICML 2015.

[2] Ranzato, MarcAurelio, et al. Video (language) modeling: a baseline for generative models of natural videos. Preprint 2015.

[3] Sutskever, Hinton, and Taylor. The Recurrent Temporal Restricted Boltzmann Machine. NIPS 2008.

[4] Fox, Sudderth, Jordan, Willsky. Bayesian nonparametric inference of switching dynamic linear models. IEEE TSP 2011.

[5] Johnson and Willsky. Bayesian nonparametric hidden semi-Markov models. JMLR 2013.

[6] Murphy. Machine learning: a probabilistic perspective. MIT Press 2012.







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supervised learning



supervised learning



unsupervised learning

Deep learning

Deep learning

+ structured representations

+ structured representations

+ priors and uncertainty

#### Deep learning

#### + structured representations

- + priors and uncertainty
- rigid assumptions may not fit

#### Deep learning
- + structured representations
- + priors and uncertainty
- rigid assumptions may not fit
- feature engineering

- + structured representations
- + priors and uncertainty
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+ arbitrary inference queries

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- neural net "goo"
- difficult parameterization
- + flexible, high capacity
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- neural net "goo"
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- limited inference queries
- data- and compute-hungry
- recognition networks learn how to do inference









**Inference:** recognition networks output conjugate potentials, then apply fast graphical model inference







**Inference:** recognition networks output conjugate potentials, then apply fast graphical model inference

**Application:** learn syllable representation of behavior from video

































































 $p(\theta)$  conjugate prior on global variables  $p(x \mid \theta)$  exponential family on local variables



 $\theta$ 

 $x_n$ 

 $y_n$ 

 $p(\theta)$ conjugate prior on global variables $p(x \mid \theta)$ exponential family on local variables $p(\gamma)$ any prior on observation parameters $p(y \mid x, \gamma)$ neural network observation model









Gaussian mixture model

Linear dynamical system

Hidden Markov model

[1] Palmer, Wipf, Kreutz-Delgado, and Rao. Variational EM algorithms for non-Gaussian latent variable models. NIPS 2005.

[2] Ghahramani and Beal. Propagation algorithms for variational Bayesian learning. NIPS 2001.

[3] Beal. Variational algorithms for approximate Bayesian inference, Ch. 3. U of London Ph.D. Thesis 2003.

[4] Ghahramani and Hinton. Variational learning for switching state-space models. Neural Computation 2000.



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Hidden Markov model



Switching LDS

[4]



Mixture of Experts

[2]

**Driven LDS** 



**IO-HMM** 



Factorial HMM

[1] Palmer, Wipf, Kreutz-Delgado, and Rao. Variational EM algorithms for non-Gaussian latent variable models. NIPS 2005.

[2] Ghahramani and Beal. Propagation algorithms for variational Bayesian learning. NIPS 2001.

[3] Beal. Variational algorithms for approximate Bayesian inference, Ch. 3. U of London Ph.D. Thesis 2003.

[4] Ghahramani and Hinton. Variational learning for switching state-space models. Neural Computation 2000.

[5] Jordan and Jacobs. Hierarchical Mixtures of Experts and the EM algorithm. Neural Computation 1994.

[6] Bengio and Frasconi. An Input Output HMM Architecture. NIPS 1995.

[7] Ghahramani and Jordan. Factorial Hidden Markov Models. Machine Learning 1997.







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Linear dynamical system





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[4]



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000

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admixture / LDA / NMF

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- [2] Ghahramani and Beal. Propagation algorithms for variational Bayesian learning. NIPS 2001.
- [3] Beal. Variational algorithms for approximate Bayesian inference, Ch. 3. U of London Ph.D. Thesis 2003.

[2]

- [4] Ghahramani and Hinton. Variational learning for switching state-space models. Neural Computation 2000.
- [5] Jordan and Jacobs. Hierarchical Mixtures of Experts and the EM algorithm. Neural Computation 1994.
- [6] Bengio and Frasconi. An Input Output HMM Architecture. NIPS 1995.

Canonical correlations analysis

- [7] Ghahramani and Jordan. Factorial Hidden Markov Models. Machine Learning 1997.
- [8] Bach and Jordan. A probabilistic interpretation of Canonical Correlation Analysis. Tech. Report 2005.
- [9] Archambeau and Bach. Sparse probabilistic projections. NIPS 2008.
- [10] Hoffman, Bach, Blei. Online learning for Latent Dirichlet Allocation. NIPS 2010.



## Inference?



$$\frac{q^*(x)}{q(x)} \stackrel{\Delta}{=} \arg \max_{q(x)} \mathcal{L}[q(\theta)q(x)]$$

## Natural gradient SVI for nice exp. fam. PGMs

[1] Hoffman, Bach, Blei. Online learning for Latent Dirichlet Allocation. NIPS 2010.[2] Hoffman, Blei, Wang, and Paisley. Stochastic variational inference. JMLR 2013.



 $p(x \mid \theta)$  is a linear dynamical system  $p(y \mid x, \theta)$  is a linear-Gaussian observation  $p(\theta)$  is a conjugate prior





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 $q(\theta)q(x) \approx p(\theta, x \mid y)$ 





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 $\eta_x^*(\eta_\theta) \stackrel{\Delta}{=} \arg\max_{\eta_x} \mathcal{L}(\eta_\theta, \eta_x) \qquad \mathcal{L}_{SVI}(\eta_\theta) \stackrel{\Delta}{=} \mathcal{L}(\eta_\theta, \eta_x^*(\eta_\theta))$ 





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Proposition (natural gradient SVI of Hoffman et al. 2013)

$$\widetilde{\nabla}\mathcal{L}_{SVI}(\eta_{\theta}) = \eta_{\theta}^{0} + \mathbb{E}_{q^{*}(x)}(t_{xy}(x,y),1) - \eta_{\theta}$$





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Proposition (natural gradient SVI of Hoffman et al. 2013)

$$\widetilde{\nabla}\mathcal{L}_{SVI}(\eta_{\theta}) = \eta_{\theta}^{0} + \sum_{n=1}^{N} \mathbb{E}_{q^{*}(x_{n})}(t_{xy}(x_{n}, y_{n}), 1) - \eta_{\theta}$$















Step 3: compute natural gradient



arbitrary inference queries





 $p(x \mid \theta)$  is a linear dynamical system  $p(y \mid x, \gamma)$  is a neural network decoder  $p(\theta)$  is a conjugate prior,  $p(\gamma)$  is generic





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$$\mathcal{L}(\eta_{\theta}, \eta_{\gamma}, \eta_{x}) \triangleq \mathbb{E}_{q(\theta)q(\theta)q(x)} \left[ \log \frac{p(\theta, \gamma, x)p(y \mid x, \gamma)}{q(\theta)q(\gamma)q(x)} \right]$$





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$$\eta_{\boldsymbol{x}}^{\star}(\eta_{\theta},\eta_{\gamma}) \triangleq \underset{\eta_{\boldsymbol{x}}}{\arg \max} \mathcal{L}(\eta_{\theta},\eta_{\gamma},\eta_{\boldsymbol{x}})$$

$$\mathcal{L}_{SVI}(\eta_{\theta},\eta_{\gamma}) \triangleq \mathcal{L}(\eta_{\theta},\eta_{\gamma},\boldsymbol{\eta_{x}^{\star}}(\eta_{\theta},\eta_{\gamma}))$$



# $\boldsymbol{q^*}(\boldsymbol{x}) \triangleq \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}(\boldsymbol{y}; \boldsymbol{\phi}), \boldsymbol{\Sigma}(\boldsymbol{y}; \boldsymbol{\phi}))$

### Variational autoencoders and amortized inference

[1] Kingma and Welling. Auto-encoding variational Bayes. ICLR 2014.

[2] Rezende, Mohamed, and Wierstra. Stochastic backpropagation and approximate inference in deep generative models. ICML 2014







## $q^{\star}(x_n) \triangleq \mathcal{N}(x_n \mid \mu(y_n; \phi), \, \Sigma(y_n; \phi))$





 $\mathcal{L}_{\text{VAE}}(\eta_{\gamma}, \phi) \triangleq \mathcal{L}(\eta_{\gamma}, \eta_{x}^{\star}(\phi))$ 

$$\begin{array}{c} \mu_{t}(y_{t};\phi_{\mu}) & \mathsf{O} \\ J_{t,t}(y_{t};\phi_{D}) & \mathsf{O} \\ J_{t,t+1}(y_{t},y_{t+1};\phi_{B}) & \mathsf{O} \end{array}$$

[1] Archer, Park, Buesing, Cunningham, Paninski. Black box variational inference for state space models. ICLR 2016 Workshops.
[2] Gao\*, Archer\*, Paninski, Cunningham. Linear dynamical neural population models through nonlinear embeddings. NIPS 2016.

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Archer, Park, Buesing, Cunningham, Paninski. Black box variational inference for state space models. ICLR 2016 Workshops.
Gao\*, Archer\*, Paninski, Cunningham. Linear dynamical neural population models through nonlinear embeddings. NIPS 2016.
Krishnan, Shalit, Sontag. Structured inference networks for nonlinear state space models. AISTATS 2017.





Natural gradient SVI

- expensive for general obs.



Natural gradient SVI

- expensive for general obs.

+ optimal local factor



- expensive for general obs.
- + optimal local factor
- + exploits conj. graph structure



- expensive for general obs.
- + optimal local factor
- + exploits conj. graph structure
- + arbitrary inference queries



- expensive for general obs.
- + optimal local factor
- + exploits conj. graph structure
- + arbitrary inference queries
- + natural gradients



 $q^{*}(x) \triangleq \underset{q(x)}{\arg \max} \mathcal{L}[q(\theta)q(x)] \qquad q^{*}(x) \triangleq \mathcal{N}(x \mid \mu(y;\phi), \Sigma(y;\phi))$ 

Natural gradient SVI

Variational autoencoders

- expensive for general obs.
- + optimal local factor
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q(x)

 $q^{*}(x) \triangleq \arg \max \mathcal{L}[q(\theta)q(x)] \qquad q^{*}(x) \triangleq \mathcal{N}(x \mid \mu(y;\phi), \Sigma(y;\phi))$ 

Natural gradient SVI

- expensive for general obs.

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Variational autoencoders

- + fast for general obs.
- suboptimal local inference
- $-\phi$  does all local inference
- limited inference queries
- no cheap natural gradients







q(x)

 $q^{*}(x) \triangleq \arg \max \mathcal{L}[q(\theta)q(x)] \qquad q^{*}(x) \triangleq \mathcal{N}(x \mid \mu(y; \phi), \Sigma(y; \phi))$ 



Natural gradient SVI

Variational autoencoders

Structured VAEs [1]

- expensive for general obs.
- + optimal local factor
- + exploits conj. graph structure
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- + natural gradients

- suboptimal local inference

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[1] Johnson, Duvenaud, Wiltschko, Datta, and Adams. Composing graphical models and neural networks. NIPS 2016.





 $q^{*}(x) \triangleq \arg \max \mathcal{L}[q(\theta)q(x)] \qquad q^{*}(x) \triangleq \mathcal{N}(x \mid \mu(y; \phi), \Sigma(y; \phi))$ 

p

q



 $q^*(x) \triangleq ?$ 

Natural gradient SVI

- expensive for general obs.
- + optimal local factor
- + exploits conj. graph structure
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Structured VAEs [1]

- + fast for general obs.
- ± optimal given conj. evidence
- + exploits conj. graph structure
- + arbitrary inference queries
- + natural gradients on  $\eta_{\theta}$

[1] Johnson, Duvenaud, Wiltschko, Datta, and Adams. Composing graphical models and neural networks. NIPS 2016.

**Inference:** recognition networks output conjugate potentials, then apply fast graphical model inference










$$\mathcal{L}[q(\theta)q(\gamma)q(x)] \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)}\left[\log \frac{p(\theta,\gamma,x)p(y \mid x,\gamma)}{q(\theta)q(\gamma)q(x)}\right]$$



$$\mathcal{L}[q(\theta)q(\gamma)q(x)] \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[\log \frac{p(\theta,\gamma,x)p(y \mid x,\gamma)}{q(\theta)q(\gamma)q(x)} \right]$$
$$q(\theta) \leftrightarrow \eta_{\theta} \qquad q(\gamma) \leftrightarrow \eta_{\gamma} \qquad q(x) \leftrightarrow \eta_{x}$$





$$\mathcal{L}(\eta_{\theta}, \eta_{\gamma}, \eta_{x}) \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[ \log \frac{p(\theta, \gamma, x)p(y \mid x, \gamma)}{q(\theta)q(\gamma)q(x)} \right]$$





$$\mathbb{E}_{q(\gamma)}\log p(y_t \,|\, x_t, \gamma)$$



$$\mathcal{L}(\eta_{\theta}, \eta_{\gamma}, \eta_{x}) \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[ \log \frac{p(\theta, \gamma, x)p(y \mid x, \gamma)}{q(\theta)q(\gamma)q(x)} \right]$$





$$\mathbb{E}_{q(\gamma)}\log p(y_t \,|\, x_t, \gamma)$$



$$\mathcal{L}(\eta_{\theta}, \eta_{\gamma}, \eta_{x}) \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[ \log \frac{p(\theta, \gamma, x)p(y \mid x, \gamma)}{q(\theta)q(\gamma)q(x)} \right]$$

$$\widehat{\mathcal{L}}(\eta_{\theta}, \eta_{x}, \phi) \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[ \log \frac{p(\theta, \gamma, x) \exp\{\psi(x; y, \phi)\}}{q(\theta)q(\gamma)q(x)} \right]$$

where  $\psi(x; y, \phi)$  is a conjugate potential for  $p(x \mid \theta)$ 





$$\mathbb{E}_{q(\gamma)}\log p(y_t \,|\, x_t, \gamma)$$



 $\psi(x_t; y_t, \phi)$ 

$$\mathcal{L}(\eta_{\theta}, \eta_{\gamma}, \eta_{x}) \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[ \log \frac{p(\theta, \gamma, x)p(y \mid x, \gamma)}{q(\theta)q(\gamma)q(x)} \right]$$

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$$\mathbb{E}_{q(\gamma)}\log p(y_t \,|\, x_t, \gamma)$$



$$\eta_x^*(\eta_\theta, \phi) \triangleq \underset{\eta_x}{\operatorname{arg\,max}} \widehat{\mathcal{L}}(\eta_\theta, \eta_x, \phi) \qquad \mathcal{L}_{\mathrm{SVAE}}(\eta_\theta, \eta_\gamma, \phi) \triangleq \mathcal{L}(\eta_\theta, \eta_\gamma, \eta_x^*(\eta_\theta, \phi))$$

$$\mathcal{L}(\eta_{\theta}, \eta_{\gamma}, \eta_{x}) \triangleq \mathbb{E}_{q(\theta)q(\gamma)q(x)} \left[ \log \frac{p(\theta, \gamma, x)p(y \mid x, \gamma)}{q(\theta)q(\gamma)q(x)} \right]$$

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where  $\psi(x; y, \phi)$  is a conjugate potential for  $p(x \mid \theta)$ 















Step 3: sample, compute flat grads



Step 2: run fast PGM algorithms



Step 3: sample, compute flat grads



Step 2: run fast PGM algorithms





Step 3: sample, compute flat grads



Step 2: run fast PGM algorithms



#### Step 4: compute natural gradient





Step 3: sample, compute flat grads



Step 2: run fast PGM algorithms



#### Step 4: compute natural gradient





 $\left( \right)$ 



latent space

data space



 $\left( \right)$ 



latent space

data space







arbitrary inference queries\*



\*see next slide

## SVAEs can use any inference network architectures



Archer, Park, Buesing, Cunningham, Paninski. Black box variational inference for state space models. ICLR 2016 Workshops.
Gao\*, Archer\*, Paninski, Cunningham. Linear dynamical neural population models through nonlinear embeddings. NIPS 2016.



**SVAEs** 

### **Application:** learn syllable representation of behavior from video







![](_page_136_Figure_0.jpeg)

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![](_page_138_Picture_0.jpeg)

start rear

![](_page_139_Picture_0.jpeg)

start rear

![](_page_140_Picture_0.jpeg)

fall from rear

![](_page_141_Picture_0.jpeg)

fall from rear

# grooming

![](_page_142_Picture_1.jpeg)

# grooming

![](_page_143_Picture_1.jpeg)
**Modeling idea:** graphical models on latent variables, neural network models for observations



**Inference:** recognition networks output conjugate potentials, then apply fast graphical model inference

**Application:** learn syllable representation of behavior from video



## Thanks!







