Perspectives on Probabilistic Graphical Models

Dong Liu

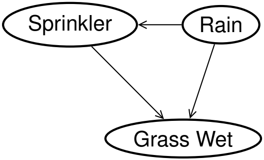
Information Science and Engineering
Department of Intelligent Systems
KTH - Royal Institute of Technology

Profile page: https://firsthandscientist.github.io/

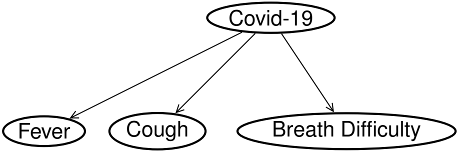
Slide is available at: https://github.com/FirstHandScientist/phdthesis

Why are probabilistic graphical models interesting?

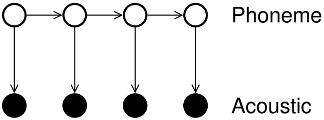
Directed Graph Representation



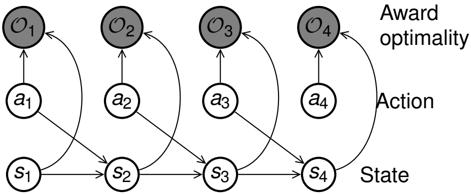
Is the sprinkler working?



Is the person infected by COVID?



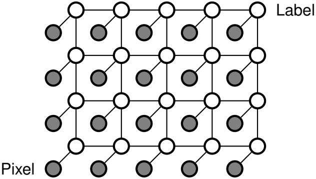
Speech Recognition

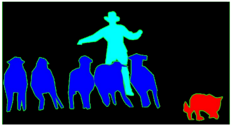


Decision-making (reinforcement learning)

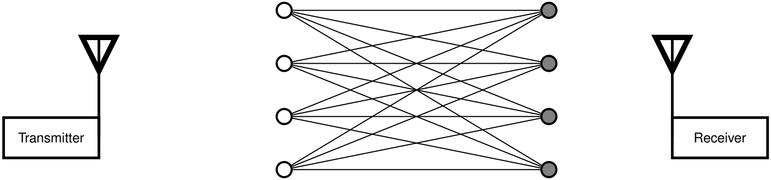
Undirected Graph Representations

Coco

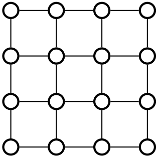




Vision Perception



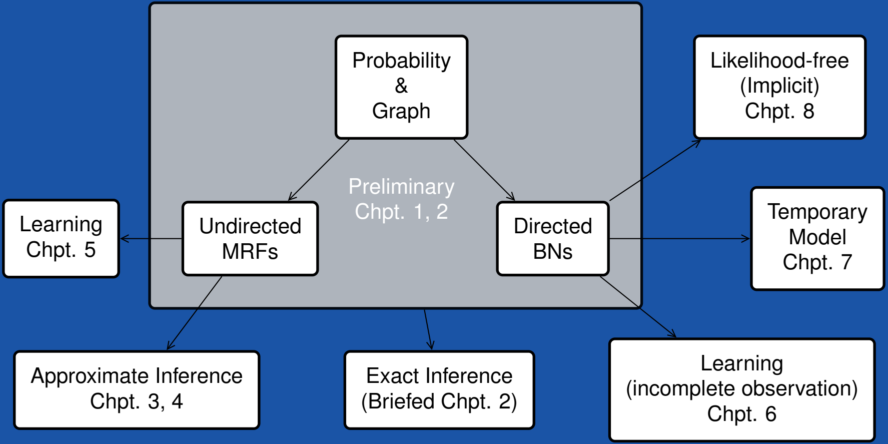
Digital communication



Physics
Ising or Potts

- Error-control codes
- Computational biology
- Natural language processing
- etc.

A Guide to This Dissertation



WHAT ARE PROBABILISTIC GRAPHICAL MODELS

Informally...

- attributes of our interests in a system $\rightarrow$ variable nodes
- relationship of these factors $\rightarrow$ structures of a graph

Intrinsic property: **reasoning with uncertainty**

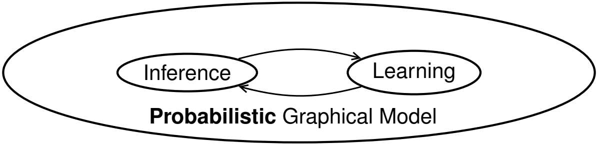
A directed/undirected graph encoding dependencies/indepedencies of distribution $p(\boldsymbol{x};\boldsymbol{\theta})$:

- A BN/Generative model is a directed graph
  - $p(\boldsymbol{x};\boldsymbol{\theta}) = \prod_{n=1}^{N} p(x_n|\mathcal{P}(x_n))$
  - $\mathcal{P}(\cdot)$ are parent nodes
  - the local functions are proper distributions
- An MRF denoted by an undirected graph $\mathcal{G}(\mathcal{V},\mathcal{E})$
  - The probability distribution (Gibbs distribution) is $p(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{a\in\mathcal{I}} \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$
  - a indexes potential functions $\mathcal{I} = \{\psi_A, \psi_B, \cdots, \psi_M\}$
  - $Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \prod_a \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$.

What to do with Graphical Models

- The common inference problems:
  - Computing the likelihood of observed data.
  - Computing the marginals distribution $p(\boldsymbol{x}_A)$ over particular subset $A \subset \mathcal{V}$ of nodes
  - Computing the conditional distribution $p(\boldsymbol{x}_A | \boldsymbol{x}_B)$,
  - Computing the partition function or the Helmholtz free energy (for MRFs)
- Learning:
  - To model or determine $p(\boldsymbol{x}; \boldsymbol{\theta})$.

Two key components interacting with each other:

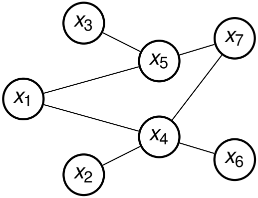


WHAT IS THE STATE OF x?

A TOY EXAMPLE

Assume that we are interested into the state of node i in an MRF, it can be answered by

- the probability $p(x_i)$, or
- an empirical version, a collection of samples $\{x_i^n\}_{n=1}^N$



What is the state of x_4

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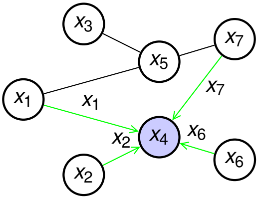

Gibbs sampling: let us guess by sampling

- Sample iteratively:
  $x_i \sim p(x_i|\boldsymbol{x}_{-i}) \sim p(x_i, \boldsymbol{x}_{-i})$
- Queries answered by collecting samples $\{\boldsymbol{x}^n\}_1^N$.

WHAT IS THE STATE OF x?

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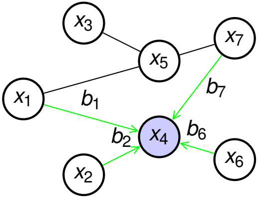


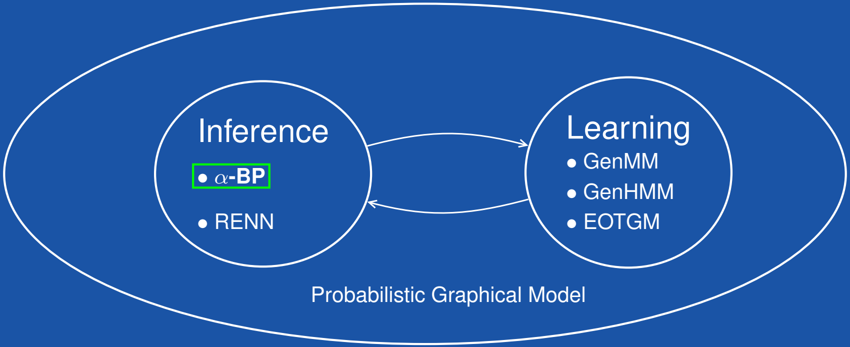
Mean Field and BP: *message in form of sample values* $\rightarrow$ *message in form of belief*

- Propagating beliefs iteratively
- Queries by collected beliefs $\{b_i\}$.

Intuition from *Gibbs (variational) free energy*

$$F_V(b) = \mathrm{KL}(b(\boldsymbol{x})||p(\boldsymbol{x};\boldsymbol{\theta})) - \log Z(\boldsymbol{\theta})$$

with trial $b(\boldsymbol{x})$. Instance: Bethe free energy.


Inference
• α-BP
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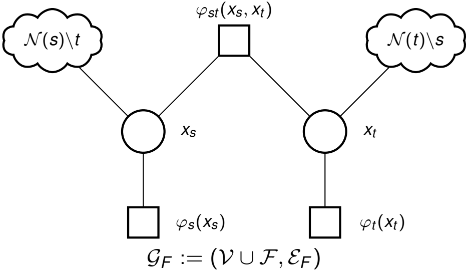
Probabilistic Graphical Model

ALTERNATIVE VEIW OF BP: α-BP

Input:

- A pairwise Markov random field: $p(\boldsymbol{x}) \propto \prod_{s\in\mathcal{V}} \varphi_s(x_s) \prod_{(s,t)\in\mathcal{E}} \varphi_{st}(x_s, x_t)$
- A trial distribution: $q(\boldsymbol{x}) \propto \prod_{s\in\mathcal{V}} \tilde{\varphi}_s(x_s) \prod_{(s,t)\in\mathcal{E}} \tilde{\varphi}_{st}(x_s, x_t)$ with factorization $\tilde{\varphi}_{s,t}(x_s, x_t) := m_{st}(x_t) m_{ts}(x_s)$
- A metric: α-Divergence

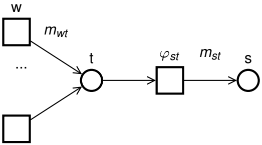


Definition of α-divergence $\mathcal{D}_\alpha(p\|q) = \frac{\sum_{\boldsymbol{x}} \alpha p(\boldsymbol{x}) + (1-\alpha) q(\boldsymbol{x}) - p(\boldsymbol{x})^\alpha q(\boldsymbol{x})^{1-\alpha}}{\alpha(1-\alpha)}$

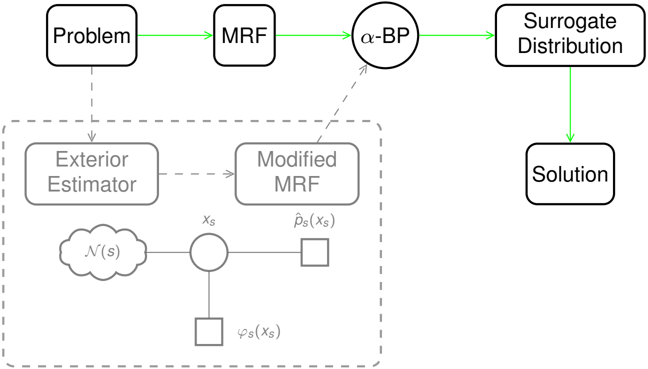
Approximate local minimization:

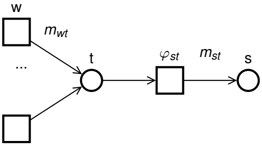
- Direct minimization: $\underset{\tilde{\varphi}_{ts}^{\text{new}}(x_t, x_s)}{\operatorname{argmin}} \mathcal{D}_{\alpha_{ts}}\left(p^{\backslash(t,s)}(\boldsymbol{x})\varphi_{ts}(x_t, x_s) \| q^{\backslash(t,s)}(\boldsymbol{x})\tilde{\varphi}_{ts}^{\text{new}}(x_t, x_s)\right)$
- Local minimization: $\underset{\tilde{\varphi}_{ts}^{\text{new}}(x_t, x_s)}{\operatorname{argmin}} \mathcal{D}_{\alpha_{ts}}\left(q^{\backslash(t,s)}(\boldsymbol{x})\varphi_{ts}(x_t, x_s) \| q^{\backslash(t,s)}(\boldsymbol{x})\tilde{\varphi}_{ts}^{\text{new}}(x_t, x_s)\right)$, say you are updating $\tilde{\varphi}_{ts}^{\text{new}}(x_t, x_s) = m_{ts}^{\text{new}}(x_s) m_{st}(x_t)$

Updating message via α-BP:



$$\underbrace{m_{ts}^{\text{new}}(x_s)}_{\text{new msg. to s}} \propto \underbrace{m_{ts}(x_s)^{1-\alpha_{ts}}}_{\text{old msg. to s}} \left[\sum_{x_t} \varphi_{ts}(x_t, x_s)^{\alpha_{ts}} \underbrace{m_{st}(x_t)^{1-\alpha_{ts}}}_{\text{old msg. to t}} \underbrace{\varphi_t(x_t) \prod_{w \in \mathcal{N}(t) \setminus s} m_{wt}(x_t)}_{\text{msg. from variable node } t \text{ to factor } \varphi_{st}}\right].$$





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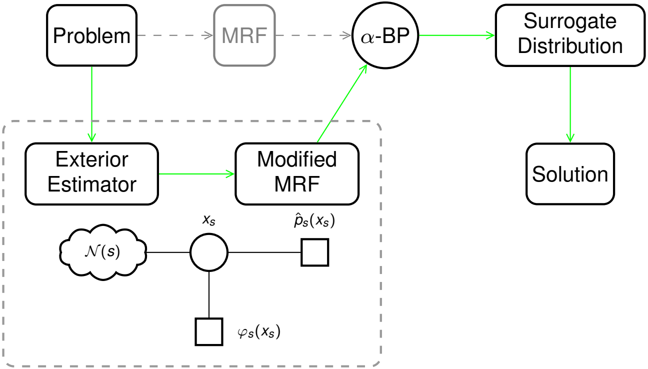


Insights of α-BP

Connection to standard BP

- $\alpha \to 0$
- α-divergence reduces to KL-divergence
- Update rule of α-BP reduces to $m_{ts}^{\text{new}}(x_s) \propto \sum_{x_t} \varphi_{st}(x_s, x_t)\varphi_t(x_t) \prod_{w \in \mathcal{N}(t)\backslash s} m_{wt}(x_t)$, which is standard BP update rule

Convergence

For an arbitrary pairwise Markov random field over binary variables, if the largest singular value of matrix $\boldsymbol{M}(\boldsymbol{\alpha}, \boldsymbol{\theta})$ is less than one, α-BP converges to a fixed point. The associated fixed point is unique.

See Corollary 3.1 for relaxed condition where singular value computation is avoided.

What does that mean

- You can safely use α-BP as an alternative to (loopy) BP
- You can use matrix $\boldsymbol{M}$ to check if you are guaranteed to get stable solution from α-BP

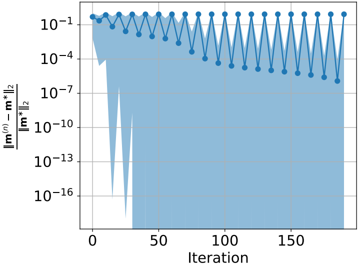
For binary, symmetric log-potentials

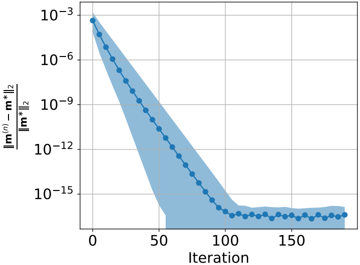
$$\varphi_{st}(x_s, x_t) = \exp\{\theta_{st}(x_s, x_t)\},$$
$$\varphi_s(x_s) = \exp\{\theta_s(x_s)\}.$$

Matrix $\boldsymbol{M}(\boldsymbol{\alpha}, \boldsymbol{\theta})$, size $|\vec{\mathcal{E}}| \times |\vec{\mathcal{E}}|$, indexed by directed edges $(t \to s)$, as

$$M_{(t\to s),(u\to v)} = \begin{cases} |1-\alpha_{ts}|, & u = t, v = s, \\ |1-\alpha_{ts}| \tanh|\alpha_{ts}\theta_{ts}|, & u = s, v = t, \\ \tanh|\alpha_{ts}\theta_{ts}|, & u \in \mathcal{N}(t)\backslash s, v = t, \\ 0, & \text{otherwise}. \end{cases}$$

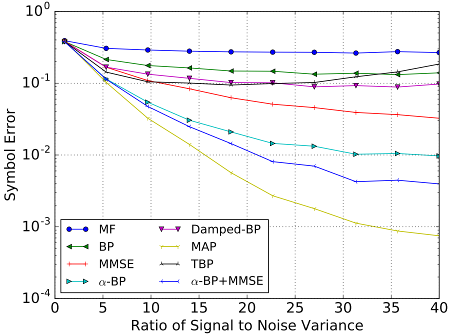
Some Numerical Results: Convergence



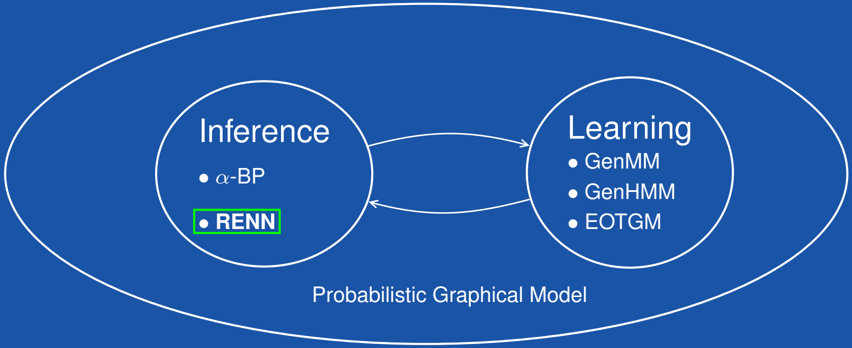


Numerical illustration of convergence, with normalized error $\|\boldsymbol{m}^{(n)} - \boldsymbol{m}^*\|_2/\|\boldsymbol{m}^*\|_2$ versus the number of iterations. Blue region: range of the normalized error of 100 graph realizations. Curve: mean error of the 100 realized graphs.

Some Numerical Results: Application Case



Numerical results of α-BP: symbol error of MIMO detection.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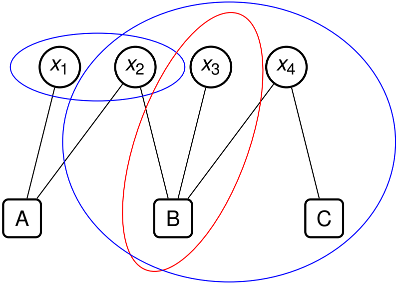
CONTINUING: WHAT IS THE STATE OF x?

YEDIDIA, FREEMAN, WEISS: A STEP TO GENERALIZATION

Message among variables & factors → message among regions



- Blue region: valid region
- Red region: invalid region

Generalized belief propagation (GBP) generalizes loopy BP

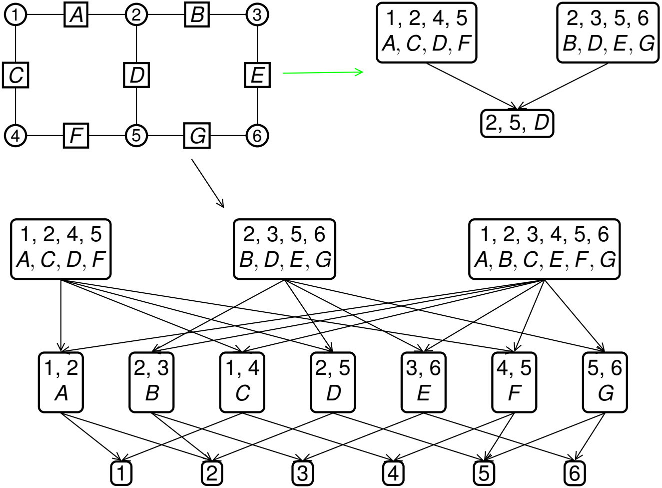
- usual better approximation than LBP
- higher complexity
- sensitive to scheduling of region messages

Approximating **variational free energy** $F_v(b)$ **with trial** b **including** $\{b_R\}$.

A *region R* is a set V_R of variables nodes and a set A_R of factor nodes, such that if a factor node 'a' belongs to A_R, all the variables nodes neighboring a are in V_R.

A Toy Example of Region Graphs

Factor graph representation of MRF (2-by-3 grid) with factor nodes.
MRF $\rightarrow$ region graph:



- Clustering nodes
- level/layer-wise
- Hierarchical
- Msg. Scheduling
- ...
- See Section 4.1

RENN: Region-based Energy Neural Network

The **region-based free energy** of a region graph is

$$F_{\mathcal{R}}(\mathcal{B};\boldsymbol{\theta}) = \sum_{R\in\mathcal{R}} \underbrace{c_R}_{\text{Counting number}} \sum_{\boldsymbol{x}_R} \underbrace{b_R(\boldsymbol{x}_R)}_{\text{Belief on region R}} \Big(\underbrace{E_R(\boldsymbol{x}_R;\boldsymbol{\theta}_R)}_{\text{Region average energy}} + \ln b_R(\boldsymbol{x}_R)\Big),$$

- counting number: balance the contribution of each region
- region average energy: $-\sum_{a\in A_R} \ln \varphi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$

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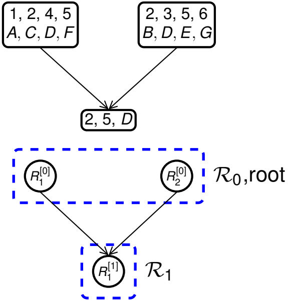
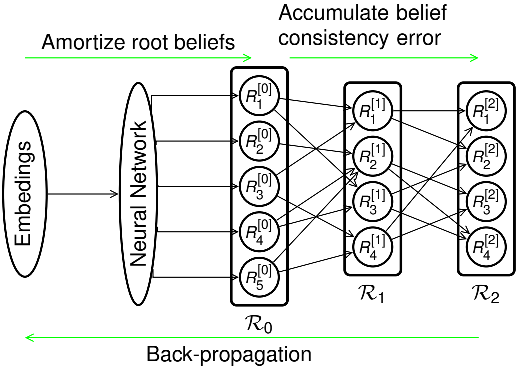
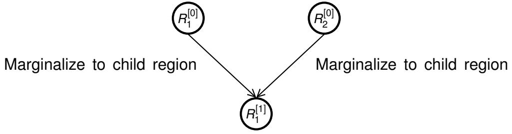




RENN

Non-root belief:



Average incoming marginalization from parents

Objective of RENN:

$$\min_{\substack{\text{parameter}\\ \text{of NN}}} \underbrace{\textbf{region-based free energy}(F_R)}_{\text{Assumulated average of all regions}} + \underbrace{\textbf{panelty on belief consistency}}_{\text{Recursively computed via levels of region graph}}$$

RENN

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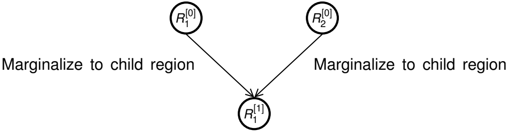

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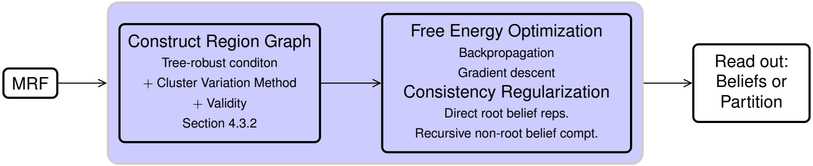
RENN Inference:



RENN

Insights of RENN

Generalization

Bethe free energy can be recovered from region-based free energy:

- two-level region graph representation
- constraint that each region can contain at most one factor node

Section 4.2.1

Attributes of RENN

- RENN requires neither sampling technique nor training data (ground-truth marginal probabilities) in performing inference tasks;
- RENN does gradient descent w.r.t. its neural network parameter instead of iterative message-passing, and returns approximation of marginal probabilities and partition estimation in one-shot
- No message propagation, thus no need of message scheduling
- Competitive performance and efficiency

Some Numerical Comparisons

Ising model: $p(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})}\exp\left(\sum_{(i,j)\in\mathcal{E}_F} J_{ij}x_ix_j + \sum_{i\in\mathcal{V}} h_ix_i\right)$, $\boldsymbol{x}\in\{-1,1\}^N$,

- J_{ij} is the pairwise log-potential between node i and j, $J_{ij}\sim\mathcal{N}(0,1)$
- h_i is the node log-potential for node i, $h_i\sim\mathcal{N}(0,\gamma^2)$

Inference on grid graph ($\gamma = 0.1$).

Metric	n	Mean Field	Loopy BP	Damped BP	GBP	Inference Net	RENN
ℓ_1 error	25	0.271 ± 0.051	0.086 ± 0.078	0.084 ± 0.076	0.057 ± 0.024	0.111 ± 0.072	$\mathbf{0.049} \pm 0.078$
	100	0.283 ± 0.024	0.085 ± 0.041	0.062 ± 0.024	0.064 ± 0.019	0.074 ± 0.034	$\mathbf{0.025} \pm 0.011$
	225	0.284 ± 0.019	0.100 ± 0.025	0.076 ± 0.025	0.073 ± 0.013	0.073 ± 0.012	$\mathbf{0.046} \pm 0.011$
	400	0.279 ± 0.014	0.110 ± 0.016	0.090 ± 0.016	0.079 ± 0.009	0.083 ± 0.009	$\mathbf{0.061} \pm 0.009$
Correlation ρ	25	0.633 ± 0.197	0.903 ± 0.114	0.905 ± 0.113	0.923 ± 0.045	0.866 ± 0.117	$\mathbf{0.951} \pm 0.112$
	100	0.582 ± 0.112	0.827 ± 0.134	0.902 ± 0.059	0.899 ± 0.043	0.903 ± 0.049	$\mathbf{0.983} \pm 0.012$
	225	0.580 ± 0.080	0.801 ± 0.078	0.863 ± 0.088	0.869 ± 0.037	0.873 ± 0.037	$\mathbf{0.949} \pm 0.022$
	400	0.596 ± 0.054	0.779 ± 0.059	0.822 ± 0.047	0.852 ± 0.024	0.841 ± 0.028	$\mathbf{0.912} \pm 0.025$
$\log Z$ error	25	2.512 ± 1.060	0.549 ± 0.373	0.557 ± 0.369	$\mathbf{0.169} \pm 0.142$	0.762 ± 0.439	0.240 ± 0.140
	100	13.09 ± 2.156	1.650 ± 1.414	1.457 ± 1.365	$\mathbf{0.524} \pm 0.313$	2.836 ± 2.158	1.899 ± 0.495
	225	29.93 ± 4.679	3.348 ± 1.954	3.423 ± 2.157	$\mathbf{1.008} \pm 0.653$	3.249 ± 2.058	4.344 ± 0.813
	400	51.81 ± 4.706	5.738 ± 2.107	5.873 ± 2.211	$\mathbf{1.750} \pm 0.869$	3.953 ± 2.558	7.598 ± 1.146

- ℓ_1 error of beliefs v.s. true
- correlation ρ between true and approximate marginals,
- $\log Z$ error, true v.s. free energy approximation.

Some Numerical Comparisons

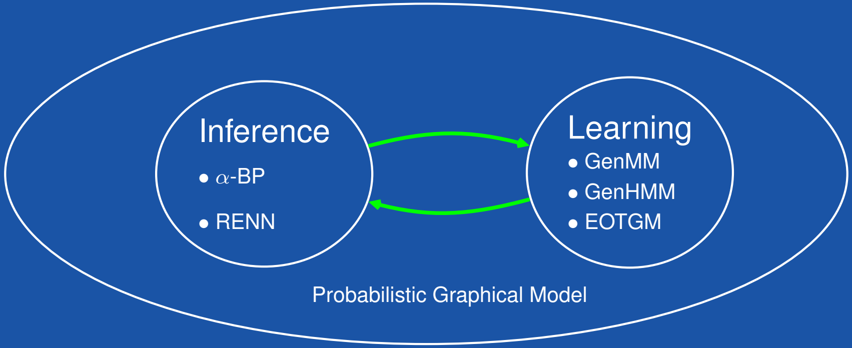
Richer Comparisons

Inference on grid and complete graphs.

		Metric		Mean Field	Loopy BP	Damped BP	GBP	Inference Net	RENN
High Temp -erature	Complete graph N=16 $J_{ij} \sim \mathcal{N}(0,1)$ $h_i \sim \mathcal{N}(0,\gamma^2)$	ℓ_1-error	$\gamma=1$	0.273 ± 0.086	0.239 ± 0.059	0.239 ± 0.059	0.260 ± 0.086	0.249 ± 0.067	**0.181** ± 0.092
			$\gamma=4$	0.197 ± 0.049	0.181 ± 0.035	0.180 ± 0.034	0.210 ± 0.070	0.174 ± 0.030	**0.125** ± 0.050
		$\log Z$ error	$\gamma=1$	20.66 ± 5.451	178.7 ± 22.18	178.9 ± 21.88	153.3 ± 25.29	213.6 ± 12.75	**14.41** ± 4.135
			$\gamma=4$	**10.74** ± 7.385	565.7 ± 73.33	566.1 ± 73.13	106.0 ± 54.43	588.3 ± 62.58	14.72 ± 4.155
Low Temp -erature	Grid graph N=100 $J_{ij} \sim \mathcal{U}(-u,u)$ $h_i \sim \mathcal{U}(-1,1)$	ℓ_1 error	5	0.257 ± 0.065	0.115 ± 0.071	0.120 ± 0.073	0.250 ± 0.024	0.164 ± 0.036	**0.100** ± 0.046
			15	0.328 ± 0.068	0.228 ± 0.088	0.267 ± 0.147	0.303 ± 0.026	0.279 ± 0.024	**0.207** ± 0.054
		$\log Z$ error	5	42.65 ± 17.86	7.346 ± 7.744	**5.444** ± 4.811	8.369 ± 7.401	65.60 ± 8.786	11.34 ± 4.724
			15	164.9 ± 56.07	58.40 ± 41.36	101.9 ± 54.31	**23.10** ± 15.06	224.3 ± 25.52	78.85 ± 15.08

Average consumed time per inference instance (unit: second)

	Mean Field	Loopy BP	Damped BP	GBP	Inference Net	RENN
Grid $\mathcal{G}$, $N=400$, $J_{ij} \sim \mathcal{N}(0,1)$, $h_i \sim \mathcal{N}(0,0.1^2)$	9.897	425.0	328.3	286.3	74.41	101.0
Complete $\mathcal{G}$, $N=16$, $J_{ij} \sim \mathcal{N}(0,1)$, $h_i \sim \mathcal{N}(0,1)$	0.457	0.777	1.285	14.29	12.45	16.16
Grid $\mathcal{G}$, $N=100$, $J_{ij} \sim \mathcal{U}(-15,15)$, $h_i \sim \mathcal{U}(-1,1)$	2.314	253.3	229.3	53.72	103.4	79.38
Complete $\mathcal{G}$, $N=9$, $J_{ij} \sim \mathcal{U}(-15,15)$, $h_i \sim \mathcal{U}(-1,1)$	0.502	15.86	18.23	3.213	17.21	7.857


Inference
• α-BP
• RENN
Learning
• GenMM
• GenHMM
• EOTGM
Probabilistic Graphical Model

Inference Routine in Learning

What is $\boldsymbol{\theta}$ in $p(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})}\prod_a \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$?

A direct view:

$$\max_{\boldsymbol{\theta}} \log p(\boldsymbol{x};\boldsymbol{\theta}) = \max_{\boldsymbol{\theta}} \sum_a \log \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a) \underbrace{-\log Z(\boldsymbol{\theta})}_{\text{can be est. by min } F_V},$$

An alternative view:

$$\frac{\partial \log p(\boldsymbol{x};\boldsymbol{\theta})}{\partial \boldsymbol{\theta}_a} = \frac{\partial \log \varphi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)}{\partial \boldsymbol{\theta}_a} - \underbrace{\mathbb{E}_{p(\boldsymbol{x}_a;\boldsymbol{\theta})}\left[\frac{\partial \log \varphi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)}{\partial \boldsymbol{\theta}_a}\right]}_{\text{can be est. by beliefs}}.$$

Remark:

- This essentially requires estimation of partition function or marginal probabilities.
- Stationary points translate into moment matching.

Inference Routine in Learning

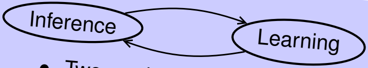
What is $\boldsymbol{\theta}$ in $p(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})}\prod_a \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$?

A direct view:

$$\max_{\boldsymbol{\theta}} \log p(\boldsymbol{x};\boldsymbol{\theta}) = \max_{\boldsymbol{\theta}} \sum_a \log \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a) \quad \underbrace{-\log Z(\boldsymbol{\theta})}_{\text{can be est. by min } F_V} \quad ,$$

An alternative view:

$$\frac{\partial \log p(\boldsymbol{x};\boldsymbol{\theta})}{\partial \boldsymbol{\theta}_a} = \frac{\partial \log \varphi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)}{\partial \boldsymbol{\theta}_a} - \underbrace{\mathbb{E}_{p(\boldsymbol{x}_a;\boldsymbol{\theta})}\left[\frac{\partial \log \varphi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)}{\partial \boldsymbol{\theta}_a}\right]}_{\text{be est. by beliefs}} .$$



- Two modules are not necessarily coupled
- Each module may be replaced by another algorithm while the other one remains.

Remark:

- This essen ... babilities.
- Stationary

LEARNING MRFS

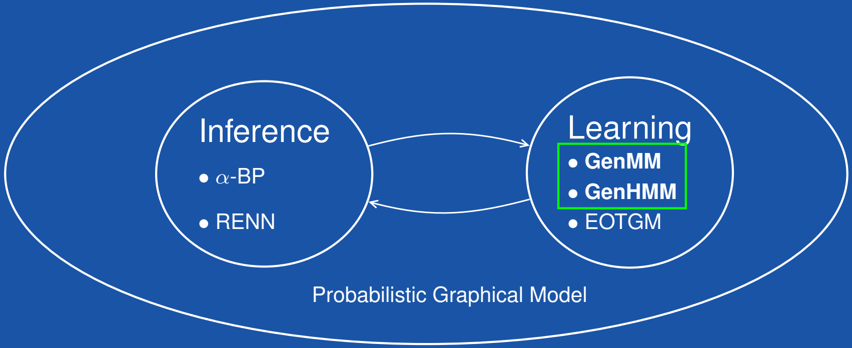
WHAT IS $\boldsymbol{\theta}$ IN $p(\boldsymbol{x};\boldsymbol{\theta})$?

Table of negative log-likelihood of learned MRFs

N	True	Exact	Mean Field	Loopy BP	Damped BP	GBP	Inference Net	RENN
Grid Graph								
25	9.000	9.004	9.811	9.139	9.196	10.56	9.252	**9.048**
100	19.34	19.38	23.48	19.92	20.02	28.61	20. 29	**19.76**
225	63.90	63.97	69.01	66.44	66.25	92.62	68.15	**64.79**
Complete Graph								
9	3.276	3.286	9.558	5.201	5.880	10.06	5.262	**3.414**
16	4.883	4.934	28.74	13.64	18.95	24.45	13.77	**5.178**

Average consumed time per epoch (unit: second) for two MRF learning cases.

	Mean Field	Loopy BP	Damped BP	GBP	Inference Net	RENN
Grid $\mathcal{G}, N=225$	40.09	335.1	525.1	12.37	19.49	16.03
Complete $\mathcal{G}, N=16$	2.499	12.40	5.431	1.387	0.882	2.262


Inference
• α-BP
• RENN
Learning
• GenMM
• GenHMM
• EOTGM
Probabilistic Graphical Model

Incomplete Observation

Partial observation: $\boldsymbol{x} = [\underbrace{\boldsymbol{x}_U}_{\textit{Unobserved}}, \underbrace{\boldsymbol{x}_O}_{\textit{Observed}}]$

$$l(\boldsymbol{x}_O;\boldsymbol{\theta}) = \log \sum_{\boldsymbol{x}_U} p(\boldsymbol{x}_U, \boldsymbol{x}_O;\boldsymbol{\theta}) = \log \underbrace{Z(\boldsymbol{x}_O;\boldsymbol{\theta})}_{\sum_{\boldsymbol{x}_U}\tilde{p}(\boldsymbol{x};\boldsymbol{\theta})} - \log Z(\boldsymbol{\theta}),$$

Connect Free Energy to Evidence Lower Bounder:

$$\begin{aligned} l(\boldsymbol{x}_O;\boldsymbol{\theta}) &\geqslant -\underbrace{F_v(q(\boldsymbol{x}_U|\boldsymbol{x}_O))}_{\text{Variational Free Energy}} - \log Z(\boldsymbol{\theta}) \\ &= \mathbb{E}_{q(\boldsymbol{x}_U|\boldsymbol{x}_O)}\left[\log \frac{p(\boldsymbol{x}_U, \boldsymbol{x}_O;\boldsymbol{\theta})}{q(\boldsymbol{x}_U|\boldsymbol{x}_O)}\right] \\ &= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_U|\boldsymbol{x}_O)}[\log p(\boldsymbol{x}_U, \boldsymbol{x}_O;\boldsymbol{\theta})] + H(q(\boldsymbol{x}_U|\boldsymbol{x}_O))}_{\text{Evidence Lower Bound } F(q,\boldsymbol{\theta})} \end{aligned}$$

Intuition of maximizing $F(q,\boldsymbol{\theta})$

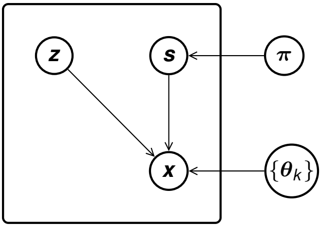
- Maximizing (incomplete) likelihood
- Minimizing free energy

This gives the EM as a coordinate ascent method:

$$\begin{aligned} \text{E step}: \quad & q^{(t+1)} = \operatorname*{argmax}_q F(q, \boldsymbol{\theta}^{(t)}), \\ \text{M step}: \quad & \boldsymbol{\theta}^{(t+1)} = \operatorname*{argmax}_{\boldsymbol{\theta}} F(q^{(t+1)}, \boldsymbol{\theta}). \end{aligned}$$

Generator Mixed Model

Equipping EM with Normalizing Flows



- Ideal case: The underline true $p^*(\boldsymbol{x})$ is in hypothesis space $\mathcal{H}$, i.e. $p^*(\boldsymbol{x}) \in \mathcal{H}$.
- Out of reach: Test $p^*(\boldsymbol{x}) \overset{?}{\in} \mathcal{H}$
- Luckily, what is at our hands is:

$$\mathcal{H} \text{ is large} \rightarrow \text{condidate } p(\boldsymbol{x}; \boldsymbol{\theta}) \text{ is flexible}$$

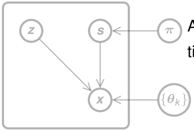
This brings up the finite **mixture** models.

$$p(\boldsymbol{x}; \boldsymbol{\Theta}) = \sum_{k=1}^{K} \pi_k p_k(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k p(\underbrace{\boldsymbol{g}(\boldsymbol{z}; \boldsymbol{\theta}_k)}_{\text{Variable change via generator } \boldsymbol{g}})$$

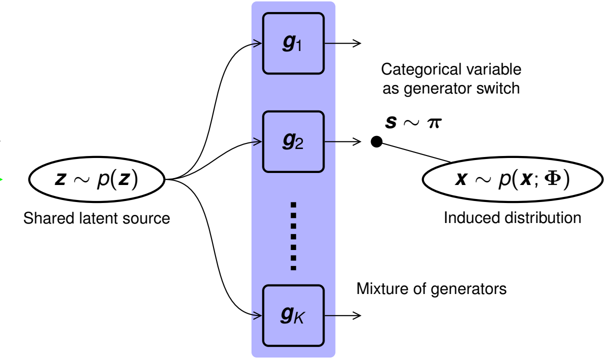
What to expect from GenMM:

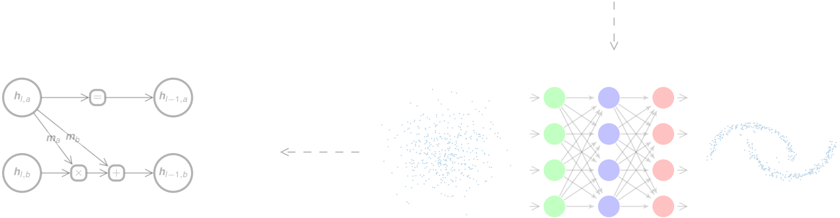
- Flexible and expressive model, enlarging hyperspace $\mathcal{H}$
- Tractable likelihood
- Compatible with typical statistical models
- Compatible with NN tools/frameworks
- Scale to high-dimensional structured data
- Efficient in sampling (data generation)
- ...

A High-level View of GenMM: finite mixture

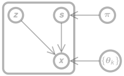


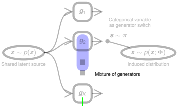
Alternative illustration of GenMM

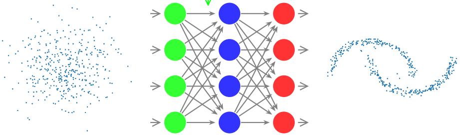




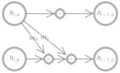
A HIGH-LEVEL VIEW OF GENMM: FLOW GEARS







When the k-th generator is selected, i.e., $s_k = 1$ and $s_{k'} = 0$ for $k' \neq k$, say $\tilde{\boldsymbol{x}} = \boldsymbol{x}|_{s_k=1}$. By following the change of variable rule

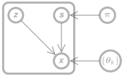


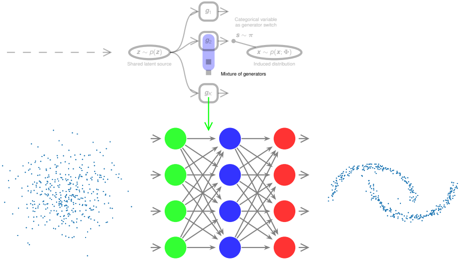
$$\underbrace{p(\tilde{\boldsymbol{x}})|_{\tilde{\boldsymbol{x}}=\tilde{\boldsymbol{g}}(\boldsymbol{z})}}_{\text{Induced distribution}} = \underbrace{p(\boldsymbol{z})}_{\substack{\text{Assumed known distribution}\\ \text{easy to sample}}} \cdot \underbrace{\left|\det\left(\frac{\partial \boldsymbol{z}}{\partial \tilde{\boldsymbol{x}}}\right)\right|}_{\substack{\text{Computational load}\\ \text{depends on the mapping}}}.$$

A toy example:

Gaussian linear transform: $Z \sim \mathrm{N}(0,1) \xrightarrow{X=\sigma\cdot Z+\mu} X \sim \mathrm{N}(\mu,\sigma)$

A HIGH-LEVEL VIEW OF GENMM: FLOW GEARS





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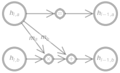
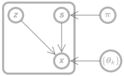


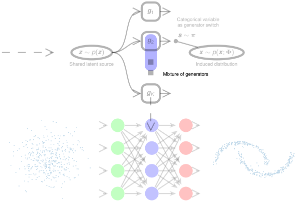
$$\underbrace{p(\tilde{\boldsymbol{x}})|_{\tilde{\boldsymbol{x}}=\tilde{\boldsymbol{g}}(\boldsymbol{z})}}_{\text{Induced distribution}} = \underbrace{p(\boldsymbol{z})}_{\substack{\text{Assumed known distribution}\\ \text{easy to sample}}} \cdot \underbrace{\left|\det\left(\frac{\partial \boldsymbol{z}}{\partial \tilde{\boldsymbol{x}}}\right)\right|}_{\substack{\text{Computational load}\\ \text{depends on the mapping}}}.$$

Powering it with a L-layer neural network implementation:

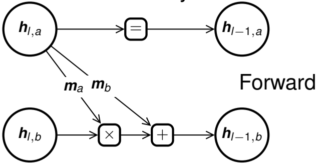
$$\boldsymbol{z} = \boldsymbol{h}_0 \underset{\tilde{\boldsymbol{f}}_1}{\overset{\tilde{\boldsymbol{g}}_1}{\rightleftarrows}} \boldsymbol{h}_1 \underset{\tilde{\boldsymbol{f}}_2}{\overset{\tilde{\boldsymbol{g}}_2}{\rightleftarrows}} \cdots\cdots\cdots \underset{\tilde{\boldsymbol{f}}_L}{\overset{\tilde{\boldsymbol{g}}_L}{\rightleftarrows}} \boldsymbol{x} = \boldsymbol{h}_L$$

A HIGH-LEVEL VIEW OF GENMM: ZOOM INTO LAYER



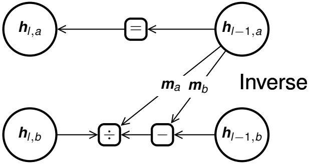


RealNVP structure by Dinh et al



Pick up one layer to zoom in

$$h_{l-1} = \begin{bmatrix} h_{l-1,a} \\ h_{l-1,b} \end{bmatrix} = \begin{bmatrix} h_{l,a} \\ m_a(h_{l,a}) \odot h_{l,b} + m_b(h_{l,a}) \end{bmatrix}$$

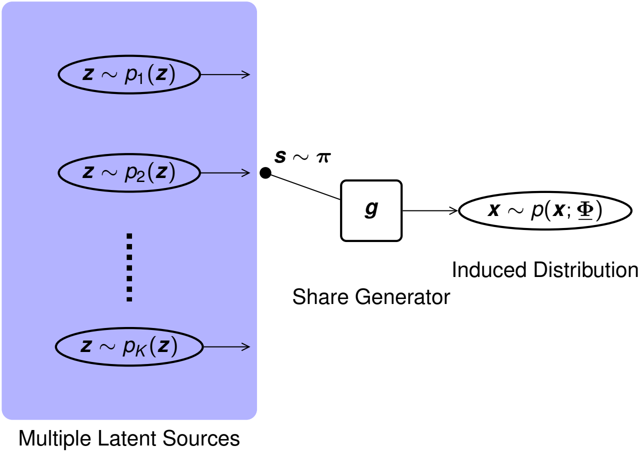


$$h_l = \begin{bmatrix} h_{l,a} \\ h_{l,b} \end{bmatrix} = \begin{bmatrix} h_{l-1,a} \\ \left(h_{l-1,b} - m_b(h_{l-1,a})\right) \oslash m_a(h_{l-1,a}) \end{bmatrix}$$

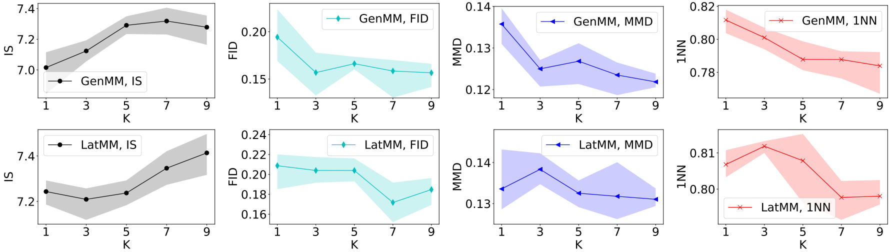
- $\odot$ denotes element-wise product, $\oslash$ denotes element-wise division
- Mapping m_a, m_b can be as complex as possible and not necessary invertible
- Same computation complexity of forward and inverse mapping
- Triangular matix of Jacobian

Alternative arch. on market: Auto-regressive flow, Glow, ODE, etc.

LatMM: Alternative Mixture



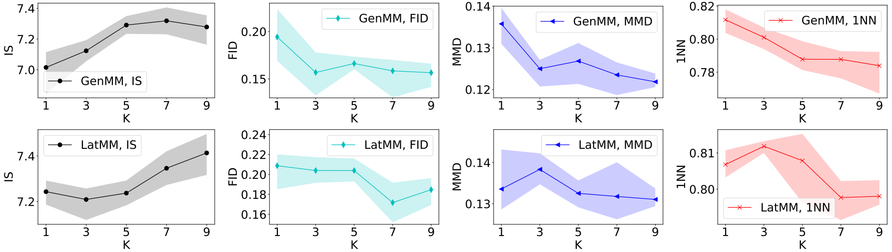
Semantic Scores and Examples

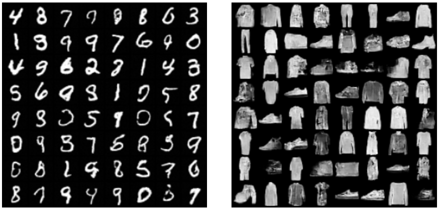


IS, FID, MMD and 1NN of GenMM and LatMM for MNIST dataset.

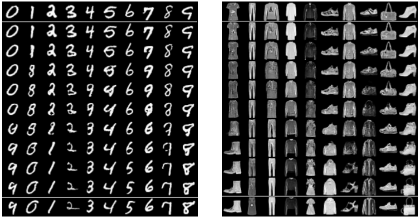
- IS: Inseption Score (large is good)
- FID: Frechet Inception Distance (small is good)
- MMD: Maximum Mean Discrepancy (small is good)
- 1NN: 1-Nearest Neighbor (the closer to 0.5 the better)

Semantic Scores and Examples





Generated samples by GenMM and LatMM.



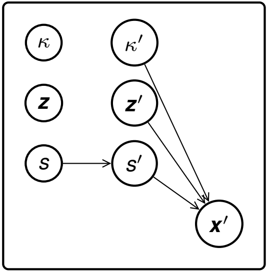
Interpolation in latent space

Application to Classification Tasks

Application to classification with maximum likelihood. Test Accuracy Table of GenMM for Classification Task

Dataset	K=1	K=2	K=3	K=4	K=10	K=20	State Of Art
Letter	0.9459	0.9513	0.9578	0.9581	0.9657	**0.9674**	0.9582
Satimage	0.8900	0.8975	0.9045	0.9085	0.9105	**0.9160**	0.9090
Norb	0.9184	0.9257	0.9406	0.9459	0.9538	**0.9542**	0.8920

GenHMM: Bring the concept into HMM



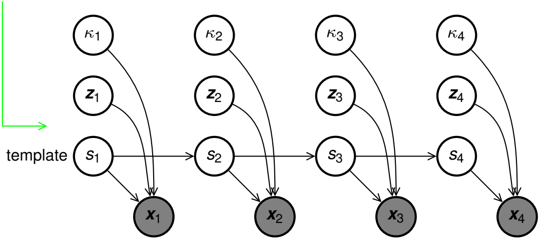
At time t, the probabilistic model of a state $s \in \mathcal{S}$ is then given by

$$p(\boldsymbol{x}|s; \boldsymbol{\Phi}_s) = \sum_{\kappa=1}^{K} \pi_{s,\kappa} p(\boldsymbol{x}|s, \kappa; \boldsymbol{\theta}_{s,\kappa}),$$

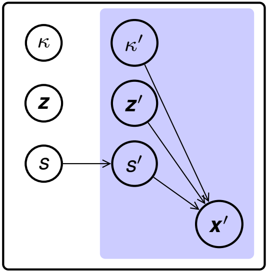
where

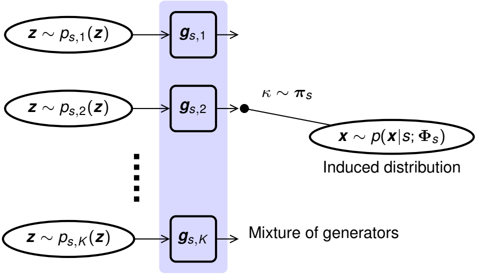
- $\pi_{s,\kappa} = p(\kappa|s; \boldsymbol{H})$, naturally $\sum_{\kappa=1}^{K} \pi_{s,\kappa} = 1$
- $p(\boldsymbol{x}|s, \kappa; \boldsymbol{\theta}_{s,\kappa})$ is induced by the kth generator $\boldsymbol{g}_k(\boldsymbol{z}) = \boldsymbol{g}(\boldsymbol{z}; \boldsymbol{\theta}_k)$

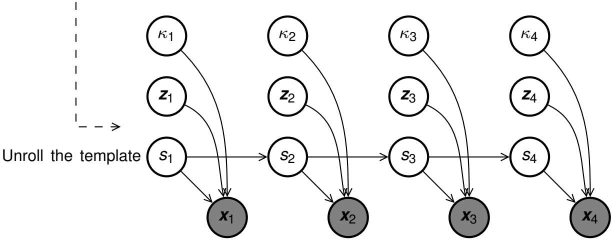
Unroll the template



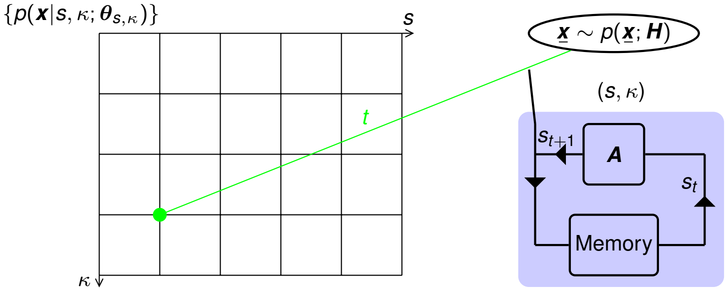
GenHMM: Bring the concept into HMM







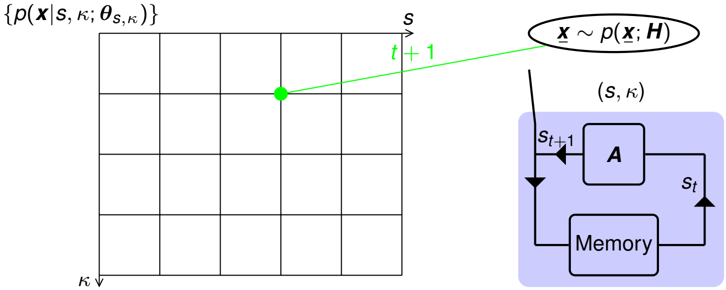
Alternative View of GenHMM



Hypothesis set of GenHMM as $\mathcal{H} := \{\boldsymbol{H}|\boldsymbol{H} = \{\mathcal{S}, \boldsymbol{q}, \boldsymbol{A}, p(\boldsymbol{x}|s;\boldsymbol{\Phi}_s)\}\}$

- $\mathcal{S}$: the set of hidden states of $\boldsymbol{H}$.
- $\boldsymbol{q} = \left[q_1, \cdots, q_{|\mathcal{S}|}\right]^\mathsf{T}$: the initial state distributions of $\boldsymbol{H}$. $q_i = p(s_1 = i; \boldsymbol{H})$.
- $\boldsymbol{A}$: the transition matrix of states in $\boldsymbol{H}$.
- $\boldsymbol{\Phi} = \{\boldsymbol{\Phi}_s | s \in \mathcal{S}\}$.

Alternative View of GenHMM



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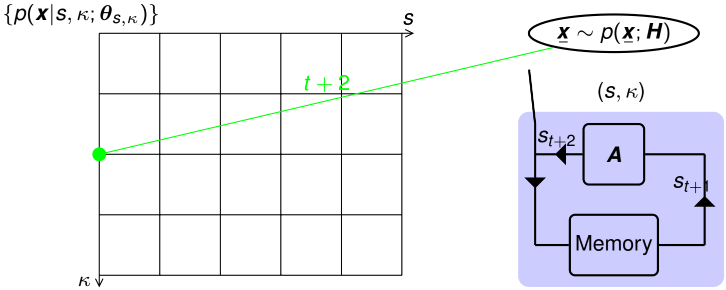
- $\boldsymbol{A}$: the transition matrix of states in $\boldsymbol{H}$.
- $\boldsymbol{\Phi} = \{\boldsymbol{\Phi}_s | s \in \mathcal{S}\}$.

ALTERNATIVE VIEW OF GENHMM



Hypothesis set of GenHMM as $\mathcal{H} := \{\boldsymbol{H}|\boldsymbol{H} = \{\mathcal{S}, \boldsymbol{q}, \boldsymbol{A}, p(\boldsymbol{x}|s;\boldsymbol{\Phi}_s)\}\}$

- $\mathcal{S}$: the set of hidden states of $\boldsymbol{H}$.
- $\boldsymbol{q} = \left[q_1, \cdots, q_{|\mathcal{S}|}\right]^{\intercal}$: the initial state distributions of $\boldsymbol{H}$. $q_i = p(s_1 = i; \boldsymbol{H})$.
- $\boldsymbol{A}$: the transition matrix of states in $\boldsymbol{H}$.
- $\boldsymbol{\Phi} = \{\boldsymbol{\Phi}_s | s \in \mathcal{S}\}$.

Learning Intuition

With empirical distribution $\hat{p}(\underline{\boldsymbol{x}}) = \frac{1}{N}\sum_n \delta_{\underline{\boldsymbol{x}}^{(n)}}(\underline{\boldsymbol{x}})$, learning of GenHMM boils down to

$$\min_{\boldsymbol{H}\in\mathcal{H}} \mathrm{KL}(\hat{p}(\underline{\boldsymbol{x}})\|p(\underline{\boldsymbol{x}};\boldsymbol{H}))$$

Then problem becomes maximum likelihood estimation

$$\hat{\boldsymbol{H}} = \arg\max_{\boldsymbol{H}\in\mathcal{H}} \log \prod_i p(\underline{\boldsymbol{x}}^i;\boldsymbol{H}),$$

E-step: the $\mathcal{Q}$ function

$$\mathcal{Q}(\boldsymbol{H};\boldsymbol{H}^{\mathrm{old}}) = \underbrace{\mathbb{E}_{\hat{p}(\underline{\boldsymbol{x}}),p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\boldsymbol{H}^{\mathrm{old}})}}_{\substack{\text{w.r.t. distribution } \hat{p}(\underline{\boldsymbol{x}})\\ \text{and } p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\boldsymbol{H}^{\mathrm{old}})}} \underbrace{[\log p(\underline{\boldsymbol{x}},\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}};\boldsymbol{H})]}_{\substack{\text{complete lklh.}\\ \text{factorize over time}}},$$

M-step: the maximization step

$$\max_{\boldsymbol{H}} \mathcal{Q}(\boldsymbol{H};\boldsymbol{H}^{\mathrm{old}}).$$

The M-step can be reformulated as

$$\max_{\boldsymbol{H}} \mathcal{Q}(\boldsymbol{H};\boldsymbol{H}^{\mathrm{old}}) = \underbrace{\max_{\boldsymbol{q}} \mathcal{Q}(\boldsymbol{q};\boldsymbol{H}^{\mathrm{old}})}_{\text{Initial State}} + \underbrace{\max_{\boldsymbol{A}} \mathcal{Q}(\boldsymbol{A};\boldsymbol{H}^{\mathrm{old}})}_{\text{Transition}} + \underbrace{\max_{\boldsymbol{\Phi}} \mathcal{Q}(\boldsymbol{\Phi};\boldsymbol{H}^{\mathrm{old}})}_{\text{Generators}}, \quad (1)$$

Maximizing a lower bound of $\log \prod_i p(\underline{\boldsymbol{x}}^{(i)};\boldsymbol{H})$.

LEARNING INTUITION

With empirical distribution $\hat{p}(\underline{\boldsymbol{x}}) = \frac{1}{N}\sum_n \delta_{\underline{\boldsymbol{x}}^{(n)}}(\underline{\boldsymbol{x}})$, learning of GenHMM boils down to

$$\min_{\boldsymbol{H}\in\mathcal{H}} \mathrm{KL}(\hat{p}(\underline{\boldsymbol{x}})\|p(\underline{\boldsymbol{x}};\boldsymbol{H}))$$

Then problem becomes maximum likelihood estimation

$$\hat{\boldsymbol{H}} = \arg\max \log \prod_i p(\underline{\boldsymbol{x}}^i;\boldsymbol{H}),$$

E-step: the

- $F = \mathcal{Q}$ + Entropy
- E-step require inference (message-passing)
- No optimality in M-step (NN generators, bash-size gradient descent).
- Still, guaranteed non-decreasing lklh. (c.f. Proposition 7.1)

M-step: the maximization step

$$\max_{\boldsymbol{H}} \mathcal{Q}(\boldsymbol{H};\boldsymbol{H}^{\mathrm{old}}).$$

The M-step can be reformulated as

$$\max_{\boldsymbol{H}} \mathcal{Q}(\boldsymbol{H};\boldsymbol{H}^{\mathrm{old}}) = \underbrace{\max_{\boldsymbol{q}} \mathcal{Q}(\boldsymbol{q};\boldsymbol{H}^{\mathrm{old}})}_{\text{Initial State}} + \underbrace{\max_{\boldsymbol{A}} \mathcal{Q}(\boldsymbol{A};\boldsymbol{H}^{\mathrm{old}})}_{\text{Transition}} + \underbrace{\max_{\boldsymbol{\Phi}} \mathcal{Q}(\boldsymbol{\Phi};\boldsymbol{H}^{\mathrm{old}})}_{\text{Generators}}, \quad (1)$$

Maximizing a lower bound of $\log \prod_i p(\underline{\boldsymbol{x}}^{(i)};\boldsymbol{H})$.

Application of GenHMM

Speech Recognition:

Configuration GenHMM in experiments on TIMIT

Latent distribution $p_{s,\kappa}(\boldsymbol{z})$ $s \in \mathcal{S}, \kappa = 1, 2, \cdots, K$	Standard Gaussian
Number of flow blocks	4
Non-linear mapping $\boldsymbol{m}_a$, $\boldsymbol{m}_b$	Multiple layer perception 3 layers and with hidden dimension 24

Phoneme classification / recognition

Model	Criterion	K=1	K=3	K=5
GMM-HMM linear variable change	Accuracy Precision F1	62.3 67.9 63.7	68.0 72.6 69.1	68.7 73.0 69.7
GenHMM non-linear variable change	Accuracy Precision F1	76.7 76.9 76.1	**77.7** **78.1** **77.1**	77.7 78.0 77.0

Robustness to perturbation of noise.

Model	Criterion	White Noise SNR 15dB	20dB	25dB	30dB
GMM-HMM	Accuracy	36.6	44.2	50.8	57.1
	Precision	59.2	64.2	68.4	70.6
	F1	39.9	47.7	53.9	59.9
GenHMM	Accuracy	52.4	62.0	69.7	**74.3**
	Precision	60.0	65.9	71.7	**74.8**
	F1	52.5	62.0	69.3	**73.5**

Application to sepsis detection for infants, c.f. see Section 7.5.

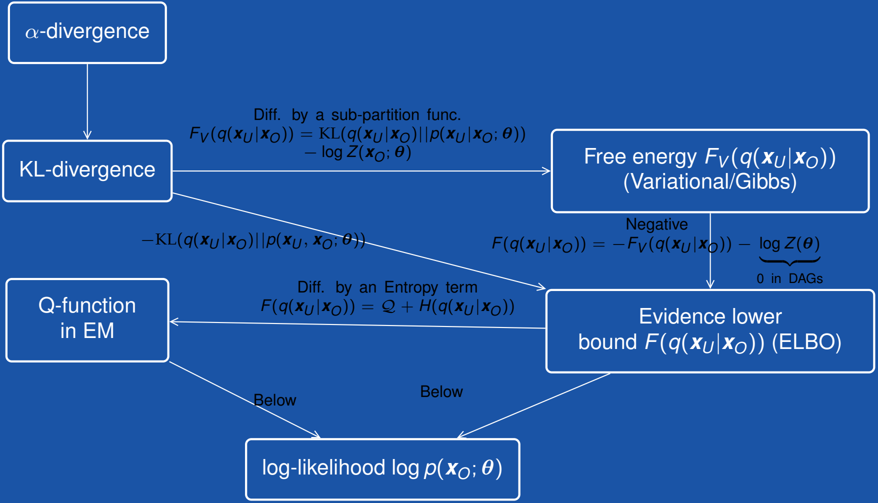
- generative training + discriminative training
- innovative feature inspired from acoustic signal feature

REMARK ON GENMM/GENHMM

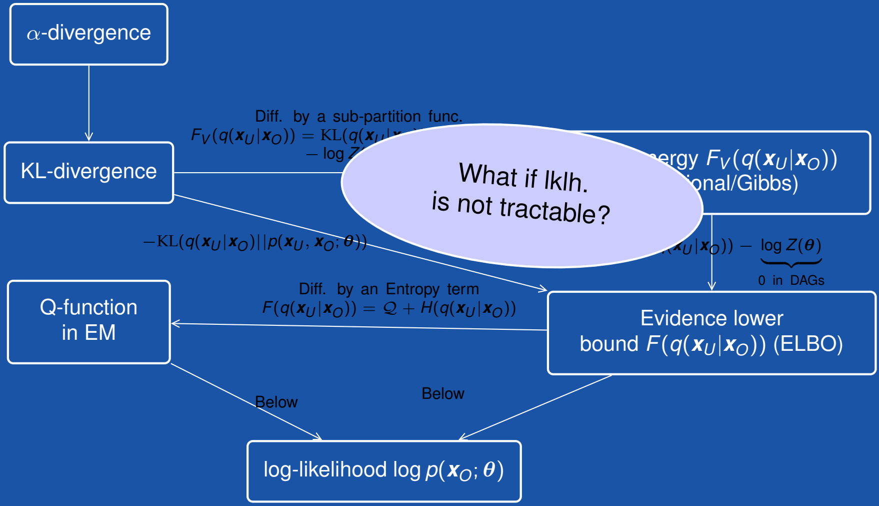
Attributes

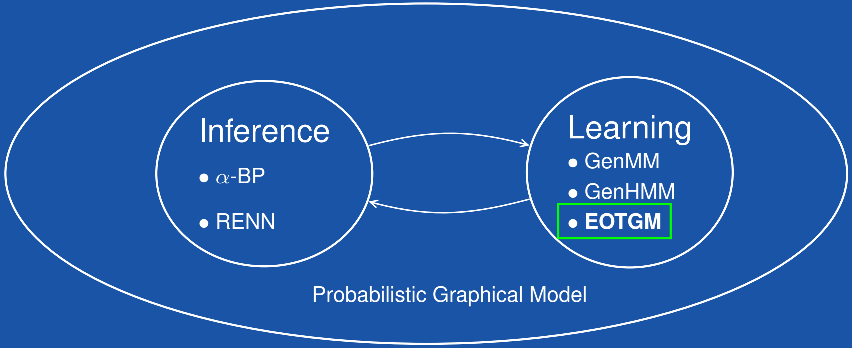
- Free dimension for flexibility: number of mixture + complexity of functional form of neural networks
- Compatible with classic statistic methods and neural network techniques (error back-propagation, optimizer)
- Embed batch-gradient descent into M-step
- Lack of closed-form update rule and generator changes at each gradient step. We tackle by maintaining old and new generators in EM steps

What Have We been Talking About?



What Have We been Talking About?




Inference
• α-BP
• RENN
Learning
• GenMM
• GenHMM
• EOTGM
Probabilistic Graphical Model

WHERE IS THE LEARNING INFO. FROM?

$$\boldsymbol{Z} \longrightarrow \boxed{\boldsymbol{g}} \longrightarrow \boldsymbol{X}$$

~~How different they are~~

- ~~likelihood~~
- ~~Evidence lower bound, free energy~~
- ~~KL-divergence, α-divergence~~

Empirical samples

add-on

Optimal transport (OT): moving mass from a dist. to another

$$T(p^*, p) = \min_{\pi \in \Pi(p^*, p)} \langle \underbrace{\pi}_{\text{marginalize to } p^*,\, p}, \underbrace{\boldsymbol{M}}_{\substack{\text{cost matrix} \\ \text{pair-wise sample difference}}} \rangle,$$

Key attributes:

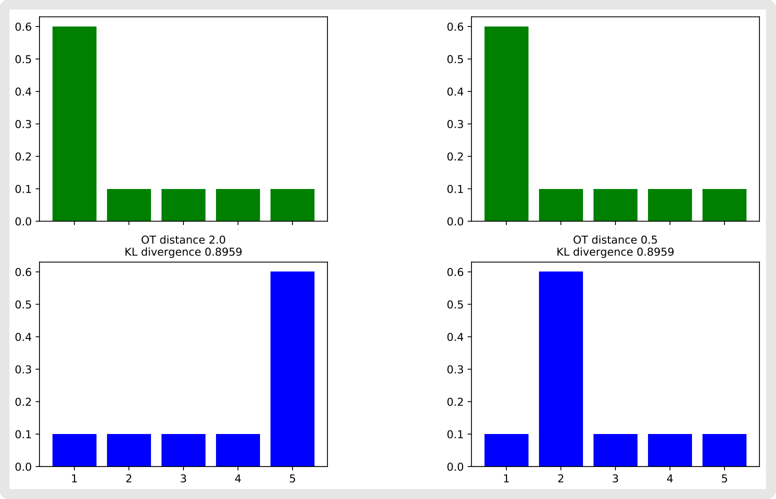
- Doesnot require tractible lklh.
- Learning gradient info. from sample comparison
- High complexity, each evaluation is sovling an optimization problem

WHERE IS THE LEARNING INFO. FROM?

How different they are

- likelihood

Empirical



A toy example

EOTGM: EOT BASED GENERATIVE MODEL

OT min $T(p^*, p)$ $\xrightarrow{\text{Kantorovich duality}}$ **WGAN, Arjovsky, et al**
Wasserstein Generative Adversarial Network
An adversarial game
1-Lipschitz function family

OT min $T(p^*, p)$ $\xrightarrow{\text{Entropy regularization}}$ **EOTGM**
NN generator + Sinkhorn solver
Applicable to implicit & explicit models

$$\underbrace{\min_{p}}_{\textit{induced by } \boldsymbol{g}} \underbrace{\min_{\pi\in\Pi(p^*,p)} \langle \pi, \boldsymbol{M} \rangle - \lambda H(\pi)}_{W(p^*,p)}$$

Alternatively scale the rows & columns of matrix $e^{-\boldsymbol{M}/\lambda}$ (Sinkhorn & Knopp) gives 'soft' solution

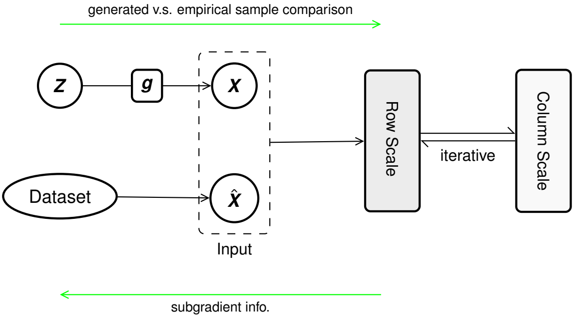
- joint distribution π^*
- subgradient β^*

which provides the gradient information for adjusting $\boldsymbol{g}$.

Marco Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport

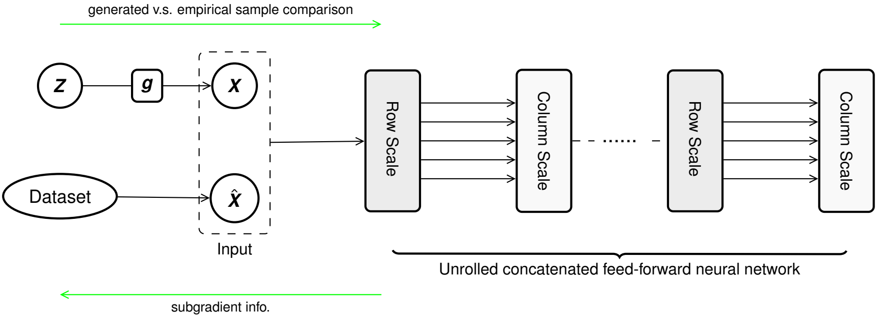
EOTGM AND EOTGAN

EOTGM



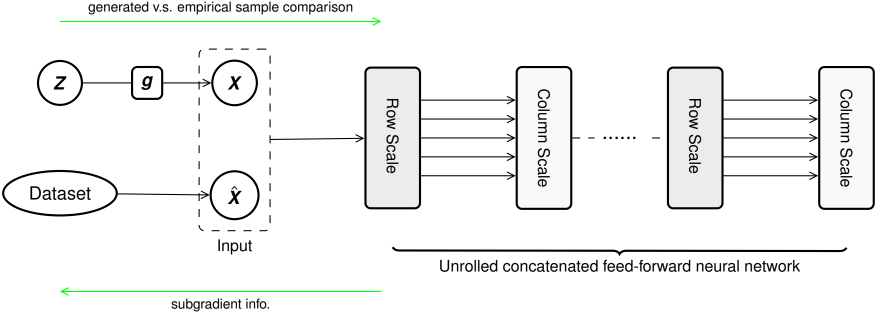
EOTGM AND EOTGAN

EOTGM

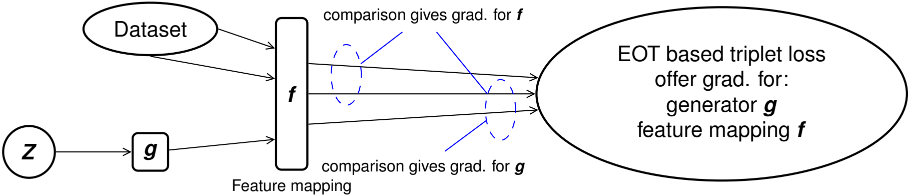


EOTGM AND EOTGAN

EOTGM



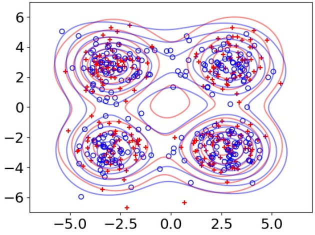
EOTGAN: learn implicit distribution with feature mapping, c.f. Section 8.2.2

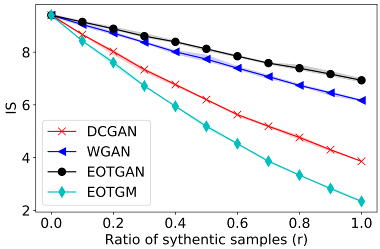


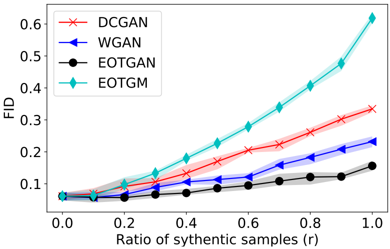
NUMERICAL

→ Toy distribution learning (target at 4-mixture Gaussians) using EOTGM. Real samples (red '+') and contour (red curve), versus generated samples (blue 'o') and contour (blue curve) by ***g***.

↓ Comparison of IS and FID (on MNIST) versus mixing ratio r.







SUMMARY

Wrap-up

- Inference with message-passing and analysis
- Inference with free energy minimization by neural networks
- Inference .. Learning: their interactions
- Neural network generators in EM for more flexible modeling; A Further step into temporal models
- A bonus modeling method for likelihood-free learning

Thank you for your attention.
Q&A.