Perspectives on Probabilistic Graphical Models

Dong Liu

Information Science and Engineering

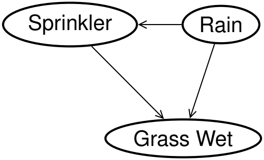
KTH - Royal Institute of Technology

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

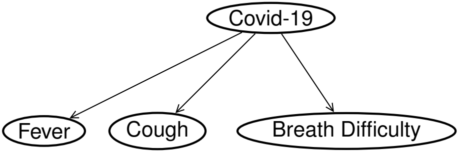
Slide is available at: https://github.com/FirstHandScientist/phdthesis

Why are Probabilistic Graphical Models interested?

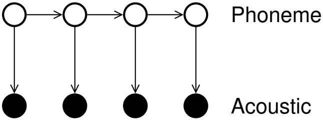
DIRECTED GRAPH REPRESENTATION



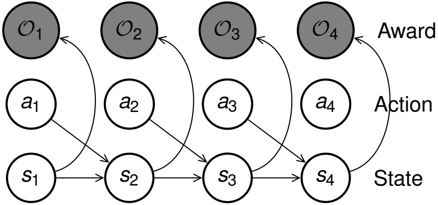
Is the sprinkler working?



Is the person get contiguous by COVID?

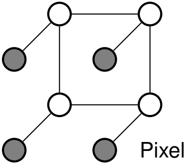


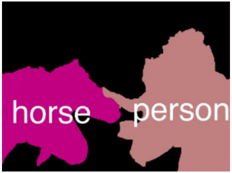
Speech Recognition



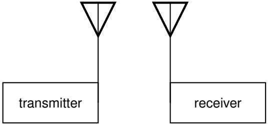
Control, reinforcement learning

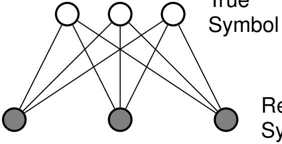
UNDIRECTED GRAPH REPRESENTATIONS



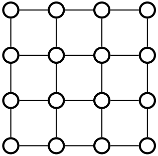


Vision Perception



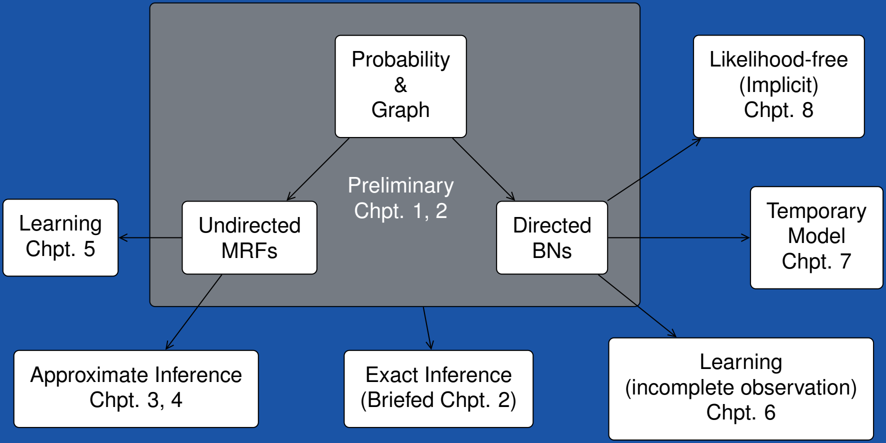


Digital communication



- 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 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 $\mathcal{I} = \{\psi_A,\psi_B,\cdots,\psi_M\}$
  - $Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}}\prod_a \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$.

USAGE OF GRAPHICAL MODELS

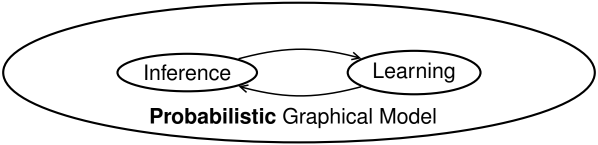
- The common inference problems:
  - Computing the likelihood of observed data.
  - Computing the marginals distribution $p(\boldsymbol{x}_A)$ over particular subset $A \subset \mathcal{V}$ of nodes
  - Computing the conditional distribution $p(\boldsymbol{x}_A|\boldsymbol{x}_B)$,
  - Computing the partition 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:

USAGE OF 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:



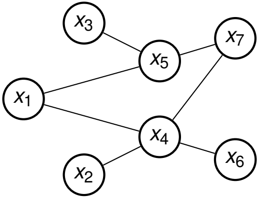
WHAT IS THE STATE OF x?

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 $\{x_i^n\}_{n=1}^N$

It is similar for the case when $\boldsymbol{x}$ is of interests, instead of x_i.

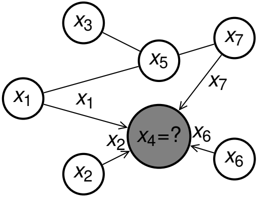


what is the state of x_4

WHAT IS THE STATE OF x?

Gibbs sampling: let us guess by sampling

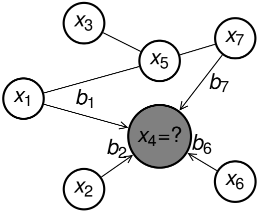
Sample iteratively: $x_i \sim p(x_i|\boldsymbol{x}_{-i}) \sim p(x_i, \boldsymbol{x}_{-i})$



Queries by collected samples $\{\boldsymbol{x}^n\}_1^N$.

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

Propagating beliefs iteratively

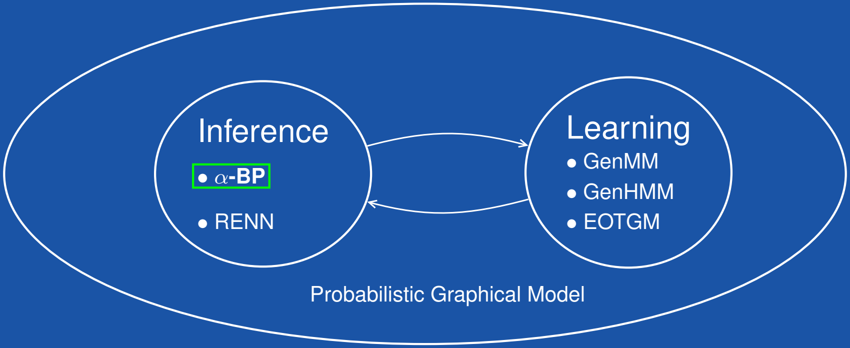


Queries by collected samples $\{b_i\}$.

Intuition from *Gibbs (variational) free energy*

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

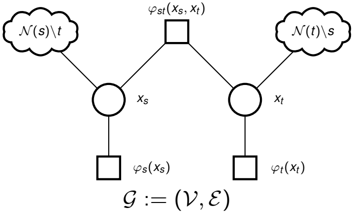
with trial $b(\boldsymbol{x})$. Instance: Bethe free energy.


Inference
• α-BP
• RENN
Learning
• GenMM
• GenHMM
• EOTGM
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

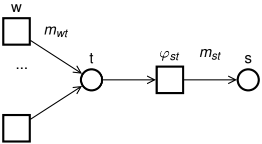


Approximate local minimization:

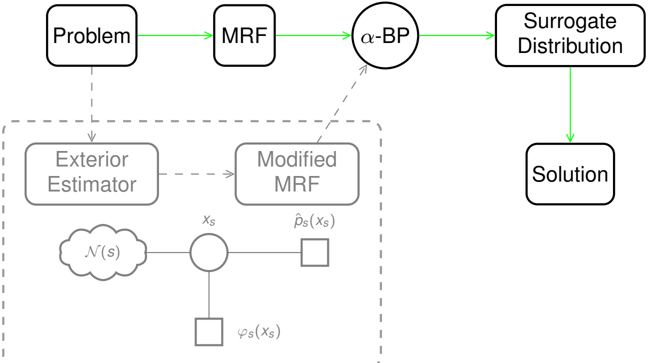
- Direct minimization: $\underset{\tilde{\varphi}_{ts}^{\text{new}}(x_t,x_s)}{\text{argmin}}\, \mathcal{D}_{\alpha_{ts}}(p^{\backslash(t,s)}(\boldsymbol{x})\varphi_{ts}(x_t, x_s) \| q^{\backslash(t,s)}(\boldsymbol{x})\tilde{\varphi}_{ts}^{\text{new}}(x_t, x_s))$
- Local minimization: $\underset{\tilde{\varphi}_{ts}^{\text{new}}(x_t,x_s)}{\text{argmin}}\,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

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

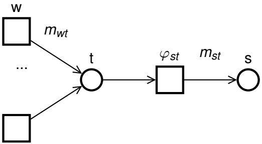
Updating message via α-BP:



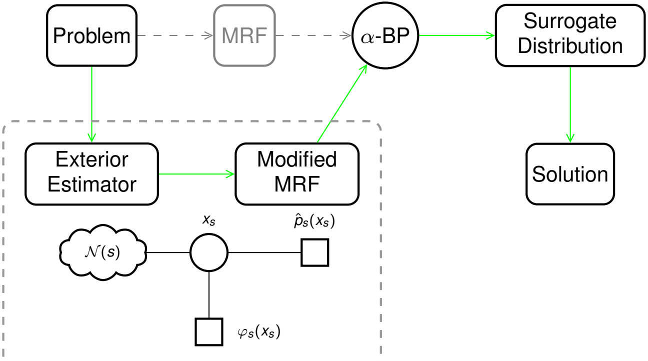
$$\underbrace{m_{ts}^{\text{new}}(x_s)}_{\text{new msg. to s}} \propto \underbrace{m_{ts}(x_s)^{1-\alpha_{ts}}}_{\text{old msg. to s}} \left[\sum_{x_t} \varphi_{ts}(x_t, x_s)^{\alpha_{ts}} \underbrace{m_{st}(x_t)^{1-\alpha_{ts}}}_{\text{old msg. to t}} \underbrace{\varphi_t(x_t) \prod_{w \in \mathcal{N}(t)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



Updating message via α-BP:



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



Insights of α-BP

Connection to standard BP

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

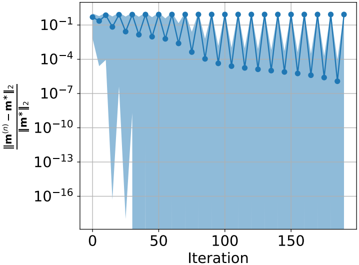
For binary, symmetric log-potentials

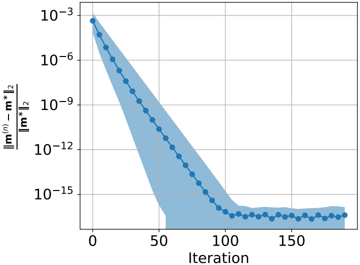
$$
\begin{aligned}
\varphi_{st}(x_s, x_t) &= \exp\left\{\theta_{st}(x_s, x_t)\right\}, \\
\varphi_s(x_s) &= \exp\left\{\theta_s(x_s)\right\}.
\end{aligned}
$$

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

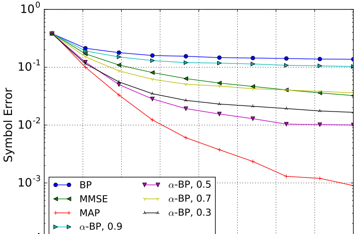
$$
M_{(t\to s),(u\to v)} = \begin{cases}
|1-\alpha_{ts}|, & u = t, v = s, \\
|1-\alpha_{ts}| \tanh|\alpha_{ts}\theta_{ts}|, & u = s, v = t, \\
\tanh|\alpha_{ts}\theta_{ts}|, & u \in \mathcal{N}(t)\setminus s, v = t, \\
0, & \text{otherwise}.
\end{cases}
$$

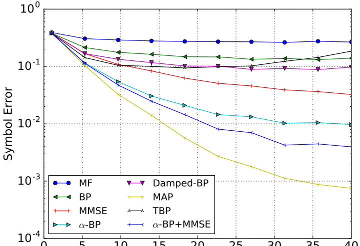
Some Numerical Results

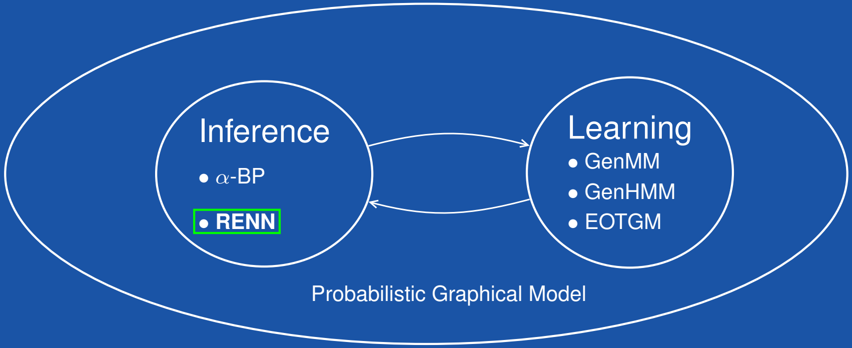




Numerical illustration of convergence, with normalized error $\|\boldsymbol{m}^{(n)} - \boldsymbol{m}^*\|_2 / \|\boldsymbol{m}^*\|_2$ versus the number of iterations. Number of nodes $N = 16$. Blue region denotes the range from minimum to maximum of the normalized error of 100 graph realizations, whereas the curve stands for mean error of the 100 realized graphs.



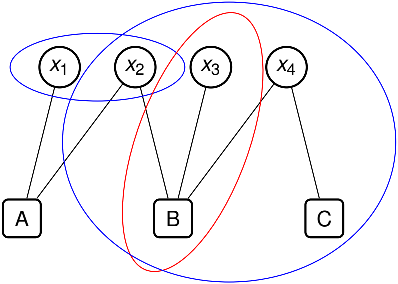



Inference
• α-BP
• **RENN**
Learning
• GenMM
• GenHMM
• EOTGM
Probabilistic Graphical Model

CONTINUING: WHAT IS THE STATE OF x?

YEDIDIA, FREEMAN, WEISS: A STEP TO GENERALIZATION

Message among variables & factors $\rightarrow$ message among regions Maybe I should combine this slide to the next one



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

Generalized belief propagation (GBP) generalizes loopy BP

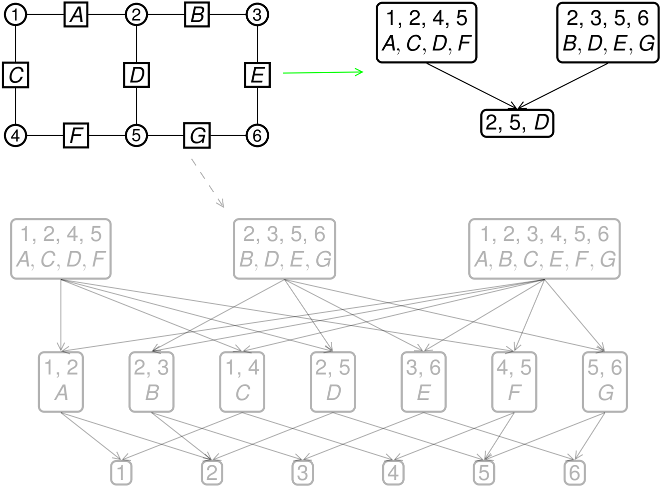
- usual better approximation than LBP
- higher complexity
- sensitive to scheduling of region messages

Corresponding to minimization of approximated **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.

An Toy Example of Region Graphs

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



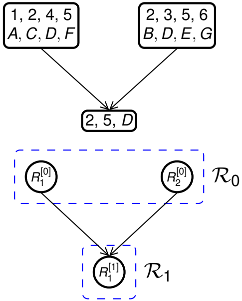
- Clustering nodes
- Valid regions
- Energy Calculated per region
- Msg. Scheduling
- ...
- See Section 4.1

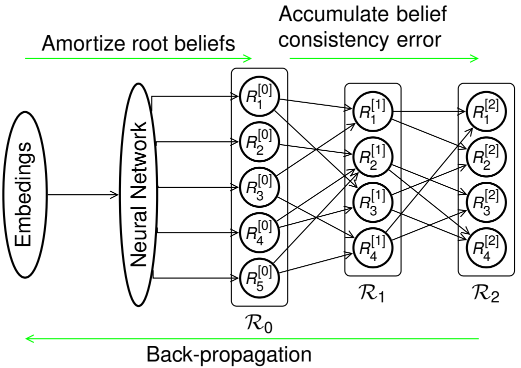
RENN: Region-based Energy Neural Network

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

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

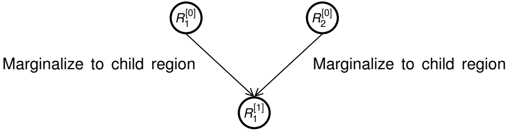
- counting number: balance the contribution of each region
- region average energy: $-\sum_{a\in A_R} \ln \varphi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$





RENN

Non-root belief:



Average incoming marginalization from parents

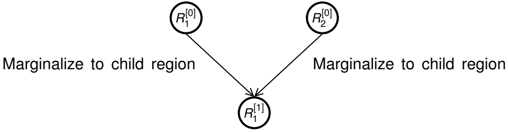
Objective of RENN:

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

RENN Inference:

RENN

Non-root belief:

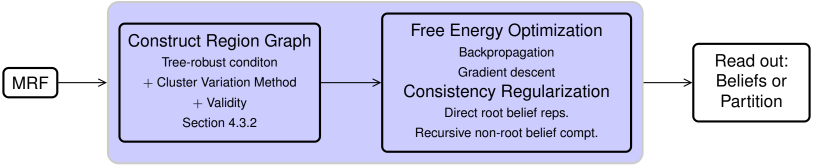


Average incoming marginalization from parents

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 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	**0.049** ± 0.078
	100	0.283 ± 0.024	0.085 ± 0.041	0.062 ± 0.024	0.064 ± 0.019	0.074 ± 0.034	**0.025** ± 0.011
	225	0.284 ± 0.019	0.100 ± 0.025	0.076 ± 0.025	0.073 ± 0.013	0.073 ± 0.012	**0.046** ± 0.011
	400	0.279 ± 0.014	0.110 ± 0.016	0.090 ± 0.016	0.079 ± 0.009	0.083 ± 0.009	**0.061** ± 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	**0.951** ± 0.112
	100	0.582 ± 0.112	0.827 ± 0.134	0.902 ± 0.059	0.899 ± 0.043	0.903 ± 0.049	**0.983** ± 0.012
	225	0.580 ± 0.080	0.801 ± 0.078	0.863 ± 0.088	0.869 ± 0.037	0.873 ± 0.037	**0.949** ± 0.022
	400	0.596 ± 0.054	0.779 ± 0.059	0.822 ± 0.047	0.852 ± 0.024	0.841 ± 0.028	**0.912** ± 0.025
$\log Z$ error	25	2.512 ± 1.060	0.549 ± 0.373	0.557 ± 0.369	**0.169** ± 0.142	0.762 ± 0.439	0.240 ± 0.140
	100	13.09 ± 2.156	1.650 ± 1.414	1.457 ± 1.365	**0.524** ± 0.313	2.836 ± 2.158	1.899 ± 0.495
	225	29.93 ± 4.679	3.348 ± 1.954	3.423 ± 2.157	**1.008** ± 0.653	3.249 ± 2.058	4.344 ± 0.813
	400	51.81 ± 4.706	5.738 ± 2.107	5.873 ± 2.211	**1.750** ± 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

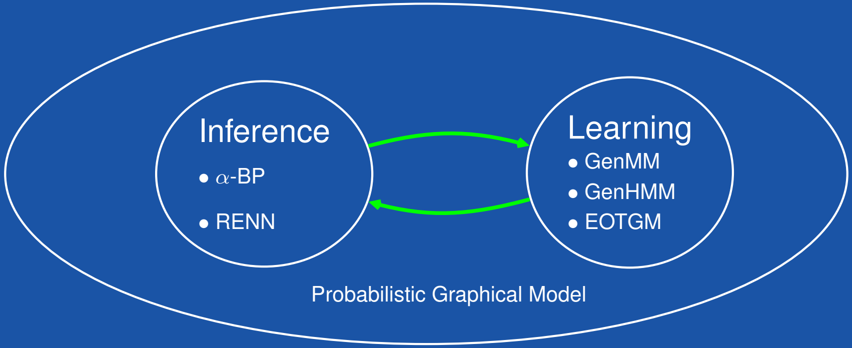
Richer Comparisons

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)

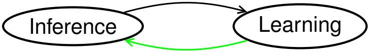
	Mean Field	Loopy BP	Damped BP	GBP	Inference Net	RENN
Grid $\mathcal{G}$, $N=400$, $J_{ij} \sim \mathcal{N}(0,1)$, $h_i \sim \mathcal{N}(0,0.1^2)$	9.897	425.0	328.3	286.3	74.41	101.0
Complete $\mathcal{G}$, $N=16$, $J_{ij} \sim \mathcal{N}(0,1)$, $h_i \sim \mathcal{N}(0,1)$	0.457	0.777	1.285	14.29	12.45	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

Two Direction Impact

Why impact in two direction?

- Learning to Inference:



Stuff we have been taken as default, a given $p(\boldsymbol{x}; \boldsymbol{\theta})$

- built by expert knowledge, or
- built by extracting information from evidence (empirical data).

- Inference to Learning:

Model learning: an error trial process that compares inferred 'fact' and actual fact (evidence).
Model learning usually needs inference as a subroutine, which sometimes are replaced by sampling in particle based methods.

Two Direction Impact

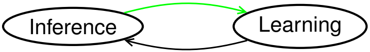
Why impact in two direction?

- Learning to Inference:

Stuff we have been taken as default, a given $p(\boldsymbol{x};\boldsymbol{\theta})$

  - built by expert knowledge, or
  - built by extracting information from evidence (empirical data).

- Inference to Learning:



Model learning: an error trial process that compares inferred 'fact' and actual fact (evidence).
Model learning usually needs inference as a subroutine, which sometimes are replaced by sampling in particle based methods.

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:

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

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 Helmholtz free energy or marginal probabilities.
- Stationary points translate into moment matching.

Inference Routine in Learning

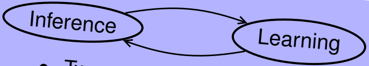
What is $\boldsymbol{\theta}$ in $p(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})}\prod_a \psi_a(\boldsymbol{x}_a;\boldsymbol{\theta}_a)$?

A direct view:

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

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... al probabilities.
- Stationary...

LEARNING MRFS

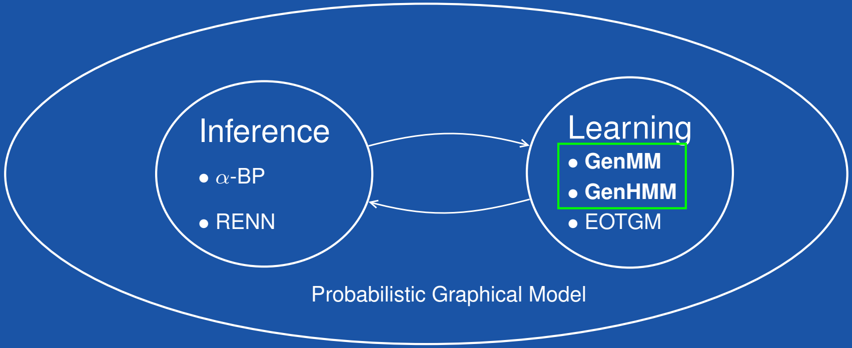
WHAT IS $\boldsymbol{\theta}$ IN $p(\boldsymbol{x};\boldsymbol{\theta})$?

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

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

Connect Free Energy to Evidence Lower Bounder:

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

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

- Maximizing (incomplete) likelihood
- Minimizing free energy

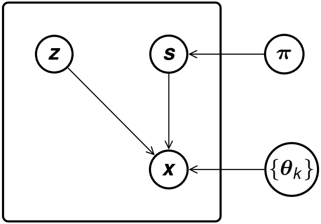
This gives the EM as a coordinate ascent method:

$$\text{E step}: \quad q^{(t+1)} = \underset{q}{\text{argmax}}\ F(q, \boldsymbol{\theta}^{(t)}),$$

$$\text{M step}: \quad \boldsymbol{\theta}^{(t+1)} = \underset{\boldsymbol{\theta}}{\text{argmax}}\ F(q^{(t+1)}, \boldsymbol{\theta}).$$

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 $p^*(\boldsymbol{x}) \overset{?}{\in} \mathcal{H}$
- A general desire:

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

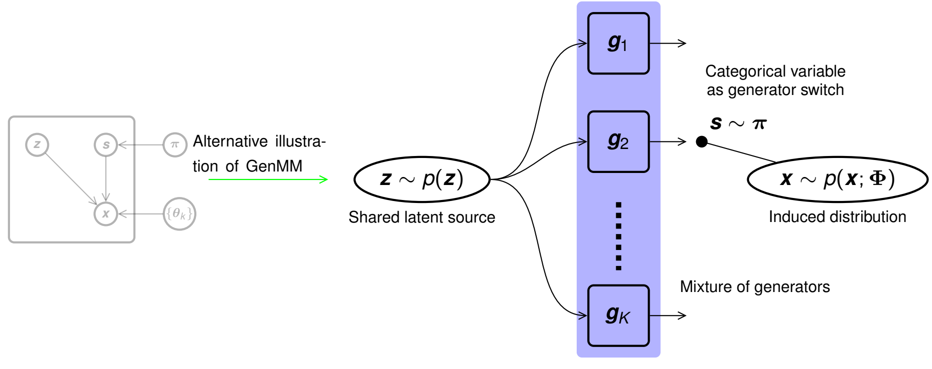
This brings up the finite **mixture** models.

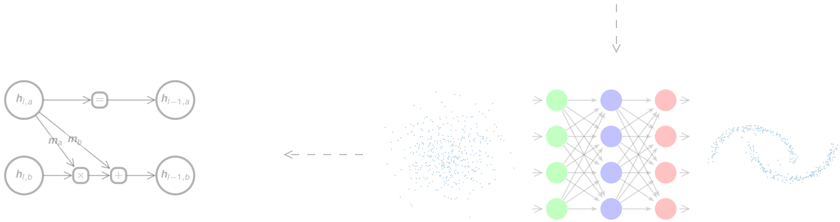
$$p(\boldsymbol{x};\boldsymbol{\Theta}) = \sum_{k=1}^{K} \pi_k p_k(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k p(\underbrace{\boldsymbol{g}(\boldsymbol{z};\boldsymbol{\theta}_k)}_{\text{Variable change via generator } \boldsymbol{g}})$$

What to expect from GenMM:

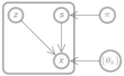
- Flexible and expressive model, enlarging hyperspace $\mathcal{H}$
- Tractable likelihood
- Compatible with typical statistical models
- Compatible with NN tools/frameworks
- Scale to high-dimensional structured data
- Efficient in sampling (data generation)
- ...

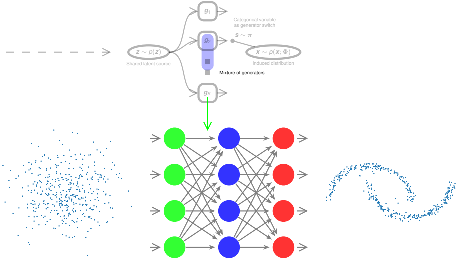
A High-level View of GenMM: finite mixture



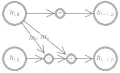


A High-level View of GenMM: flow gears





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

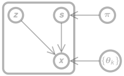


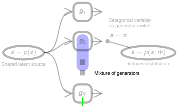
$$\underbrace{p(\tilde{\boldsymbol{x}})|_{\tilde{\boldsymbol{x}}=\tilde{\boldsymbol{g}}(\boldsymbol{z})}}_{\text{Induced distribution}} = \underbrace{p(\boldsymbol{z})}_{\substack{\text{Assumed known distribution} \\ \text{easy to sample}}} \cdot \underbrace{\left|\det\left(\frac{\partial \boldsymbol{z}}{\partial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

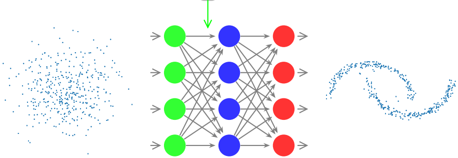
A toy example:

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

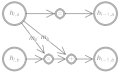
A High-level View of GenMM: flow gears







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

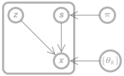


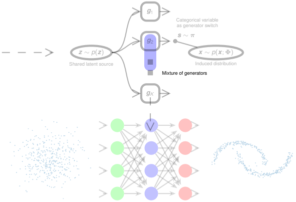
$$\underbrace{p(\tilde{\boldsymbol{x}})|_{\tilde{\boldsymbol{x}}=\tilde{\boldsymbol{g}}(\boldsymbol{z})}}_{\text{Induced distribution}} = \underbrace{p(\boldsymbol{z})}_{\substack{\text{Assumed known distribution} \\ \text{easy to sample}}} \cdot \underbrace{\left|\det\left(\frac{\partial \boldsymbol{z}}{\partial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

Powering it with a L-layer neural network implementation:

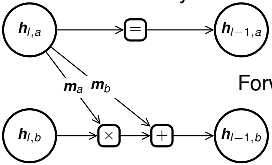
$$\boldsymbol{z} = \boldsymbol{h}_0 \underset{\tilde{\boldsymbol{f}}_1}{\overset{\tilde{\boldsymbol{g}}_1}{\rightleftarrows}} \boldsymbol{h}_1 \underset{\tilde{\boldsymbol{f}}_2}{\overset{\tilde{\boldsymbol{g}}_2}{\rightleftarrows}} \cdots\cdots\cdots \underset{\tilde{\boldsymbol{f}}_L}{\overset{\tilde{\boldsymbol{g}}_L}{\rightleftarrows}}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

A HIGH-LEVEL VIEW OF GENMM: ZOOM INTO LAYER





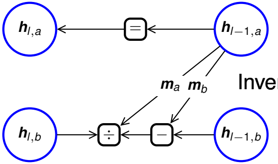
RealNVP structure by Dinh et al



Forward

Pick up one layer to zoom in

$$\boldsymbol{h}_{l-1} = \begin{bmatrix} \boldsymbol{h}_{l-1,a} \\ \boldsymbol{h}_{l-1,b} \end{bmatrix} = \begin{bmatrix} \boldsymbol{h}_{l,a} \\ \boldsymbol{m}_a(\boldsymbol{h}_{l,a}) \odot \boldsymbol{h}_{l,b} + \boldsymbol{m}_b(\boldsymbol{h}_{l,a}) \end{bmatrix}$$



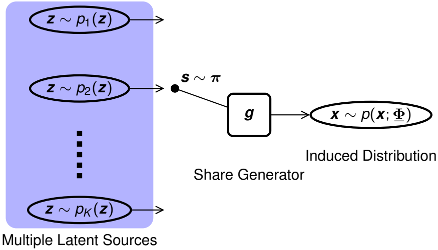
Inverse

$$\boldsymbol{h}_{l} = \begin{bmatrix} \boldsymbol{h}_{l,a} \\ \boldsymbol{h}_{l,b} \end{bmatrix} = \begin{bmatrix} \boldsymbol{h}_{l-1,a} \\ \left(\boldsymbol{h}_{l-1,b} - \boldsymbol{m}_b(\boldsymbol{h}_{l-1,a})\right) \oslash \boldsymbol{m}_a(\boldsymbol{h}_{l-1,a}) \end{bmatrix}$$

- $\odot$ denotes element-wise product, $\oslash$ denotes element-wise division
- Mapping $\boldsymbol{m}_a$, $\boldsymbol{m}_b$ 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.

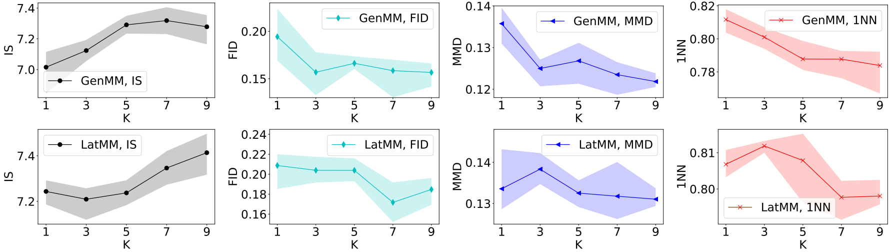
Alternative Mixture and Remark



Remark On GenMM/GenHMM

- Free dimension for flexibility: number of mixture + complexity of functional form of neural networks
- Compatible with 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

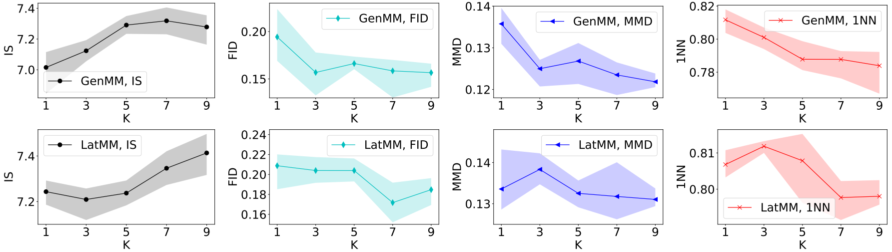
Semantic Scores and Examples

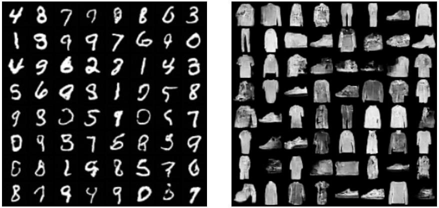


IS, FID, MMD and 1NN of GenMM and LatMM for MNIST dataset.

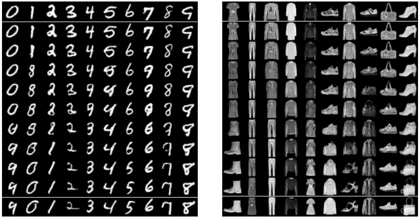
- IS: Inseption Score
- FID: Frechet Inception Distance
- MMD: Maximum Mean Discrepancy
- 1NN: 1-Nearest Neighbor

Semantic Scores and Examples





Generated samples by GenMM and LatMM.



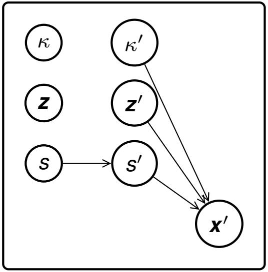
Interpolation in latent space

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

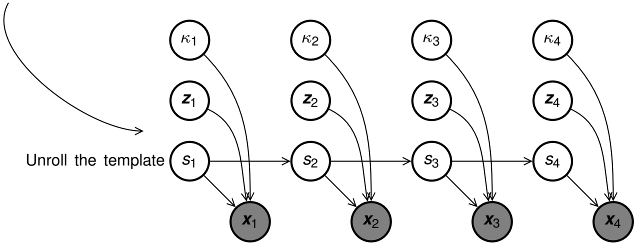


At time t, the probabilistic model of a state $s \in \mathcal{S}$ is then given by

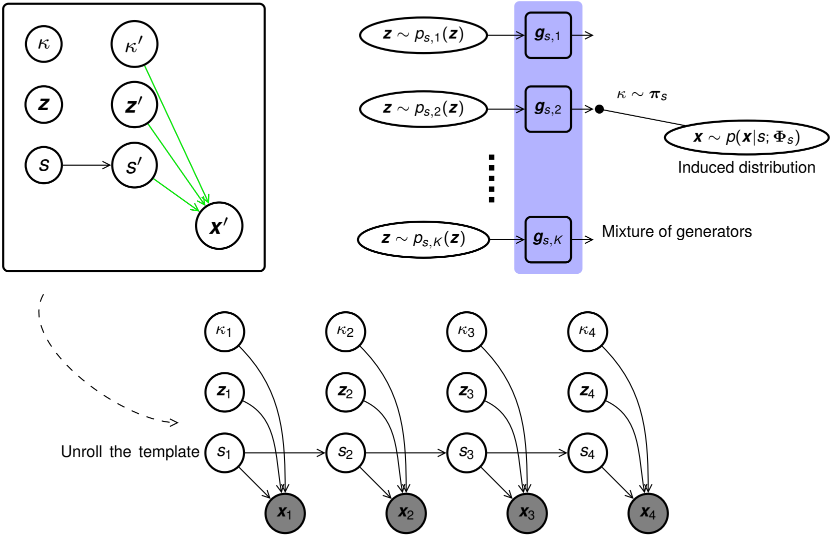
$$p(\boldsymbol{x}|s;\boldsymbol{\Phi}_s) = \sum_{\kappa=1}^{K} \pi_{s,\kappa} p(\boldsymbol{x}|s,\kappa;\boldsymbol{\theta}_{s,\kappa}),$$

where

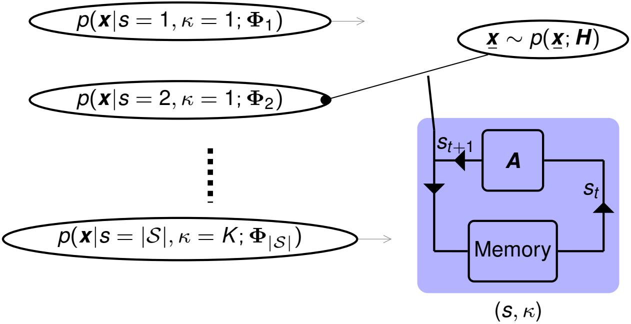
- $\pi_{s,\kappa} = p(\kappa|s;\boldsymbol{H})$, naturally $\sum_{\kappa=1}^{K} \pi_{s,\kappa} = 1$
- $p_k(\boldsymbol{x})$ is induced by the kth generator $\boldsymbol{g}_k(\boldsymbol{z}) = \boldsymbol{g}(\boldsymbol{z};\boldsymbol{\theta}_k)$



GenHMM: Bring the concept into HMM



ALTERNATIVE VIEW OF GENHMM



We define the hypothesis set of HMM as $\mathcal{H} := \{\boldsymbol{H}|\boldsymbol{H} = \{\mathcal{S}, \boldsymbol{q}, \boldsymbol{A}, p(\boldsymbol{x}|s;\boldsymbol{\Phi}_s)\}\}$, where

- $\mathcal{S}$ is the set of hidden states of $\boldsymbol{H}$.
- $\boldsymbol{q} = \left[q_1, q_2, \cdots, q_{|\mathcal{S}|}\right]^\intercal$ is the initial state distribution of $\boldsymbol{H}$ with $|\mathcal{S}|$ as cardinality of $\mathcal{S}$. For $i \in \mathcal{S}$, $q_i = p(s_1 = i;\boldsymbol{H})$. We use s_t to denote the state s at time t.
- $\boldsymbol{A}$ matrix of size $|\mathcal{S}| \times |\mathcal{S}|$ is the transition matrix of states in $\boldsymbol{H}$. That is, $\forall i,j \in \mathcal{S}$, $\boldsymbol{A}_{i,j} = p(s_{t+1} = j|s_t = i;\boldsymbol{H})$.
- For a given hidden state s, the density function of the observable signal is $p(\boldsymbol{x}|s;\boldsymbol{\Phi}_s)$, where $\boldsymbol{\Phi}_s$ is the parameter set that defines this probabilistic model. Denote $\boldsymbol{\Phi} = \{\boldsymbol{\Phi}_s | s \in \mathcal{S}\}$.

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

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

Use EM to solve:

E-step: the expected likelihood function

$$\mathcal{Q}(\boldsymbol{H};\boldsymbol{H}^{\mathrm{old}}) = \mathbb{E}_{\hat{p}(\underline{\boldsymbol{x}}),p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\boldsymbol{H}^{\mathrm{old}})}\left[\log\, p(\underline{\boldsymbol{x}},\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}};\boldsymbol{H})\right],$$

where $\mathbb{E}_{\hat{p}(\underline{\boldsymbol{x}}),p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\boldsymbol{H}^{\mathrm{old}})}[\cdot]$ denotes the expectation operator by distribution $\hat{p}(\underline{\boldsymbol{x}})$ and $p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\boldsymbol{H}^{\mathrm{old}})$.

M-step: the maximization step

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

The problem (**??**) can be reformulated as

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

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

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

Use EM to solve: ...

E-step: the ...

where $\mathbb{E}_{\hat{p}(\underline{\boldsymbol{x}}),p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\ldots)}$ ... ...ution $\hat{p}(\underline{\boldsymbol{x}})$ and $p(\underline{\boldsymbol{s}},\underline{\boldsymbol{\kappa}}|\underline{\boldsymbol{x}};\boldsymbol{H}^{\mathrm{old}})$.

- $F = \mathcal{Q}$ + Entropy
- E-step require inference (message-passing)
- No optimality in M-step (NN generators).
- 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 problem (**??**) can be reformulated as

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

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

Application to Speech Recognition

Configuration of generators of 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

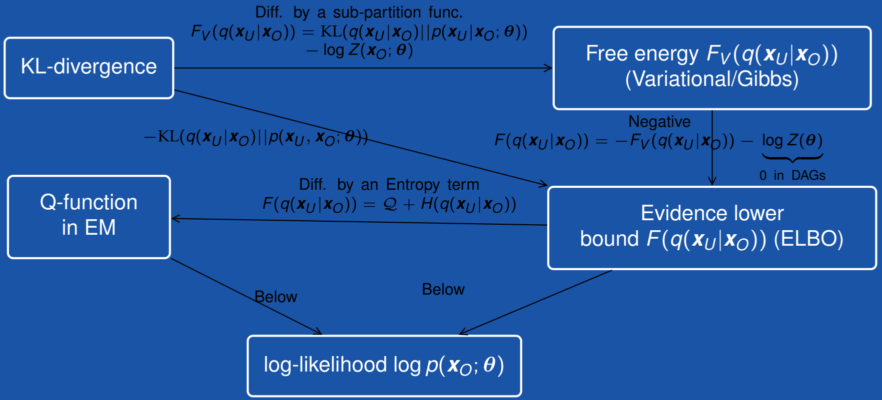
Model	Criterion	K=1	K=3	K=5
GMM-HMM	Accuracy	62.3	68.0	68.7
	Precision	67.9	72.6	73.0
	F1	63.7	69.1	69.7
GenHMM	Accuracy	76.7	**77.7**	77.7
	Precision	76.9	**78.1**	78.0
	F1	76.1	**77.1**	77.0

Robustness to perturbation of noise.

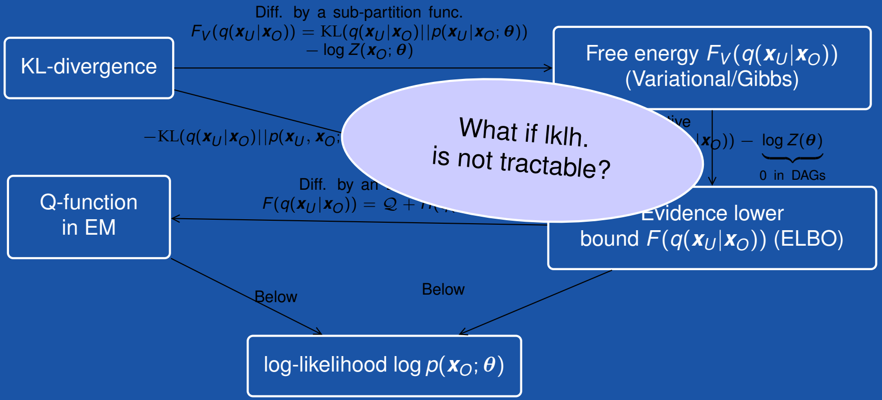
Model	Criterion	White Noise SNR 15dB	20dB	25dB	30dB
GMM-HMM	Accuracy	36.6	44.2	50.8	57.1
	Precision	59.2	64.2	68.4	70.6
	F1	39.9	47.7	53.9	59.9
GenHMM	Accuracy	52.4	62.0	69.7	**74.3**
	Precision	60.0	65.9	71.7	**74.8**
	F1	52.5	62.0	69.3	**73.5**

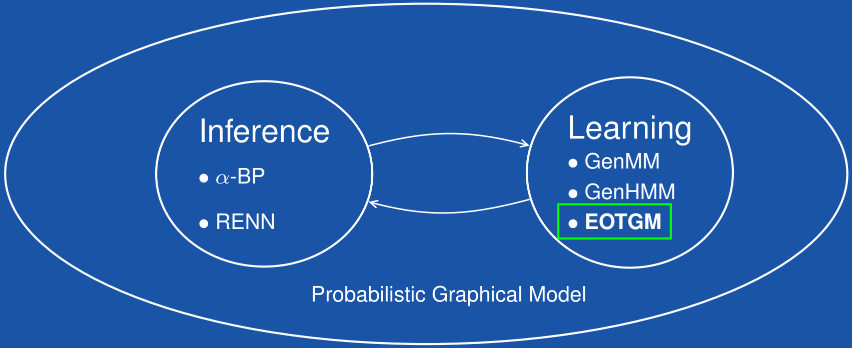
For our conducted experiments of applying GenHMM to sepsis detection for infants, see Section 7.5.

What Have We been Talking About?



What Have We been Talking About?




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

SUMMARY

- Brief on probabilistic graphic models
- Overview of inference methods
- A focus on the message-passing
- Transition to inference methods with NN

Thank you for your attention.
Q&A.