Graphical Models and Variational Inference

Demian Wassermann, Inria
Graphical Models: Discrete Inference and Learning
Introduction to DAG and their relationship with Probability Functions (Pearl)

[Pearl 1987]

[2019 Kong et al]
Introduction to DAG and their relationship with Probability Functions (Pearl)

Latent Dirichlet Allocation

U: is a Dirichlet or “clustering variable”
Z: is a “Topic”
W: is an observed “Word”

[Blei et al 2003]

Each “box” or template represents a set of i.i.d. random variables with the same distribution
Introduction to DAG and their relationship with Probability Functions (Pearl)

Latent Dirichlet Allocation

U: is a Dirichlet or “clustering variable”
Z: is a “Topic”
W: is an observed “Word”

[Blei et al 2003]

Each “box” or template represents a set of i.i.d. random variables with the same distribution

The greyed nodes, represent observations

The William Randolph Hearst Foundation will give $1.25 million to Lincoln Center, Metropolitan Opera Co., New York Philharmonic and Juilliard School. “Our board felt that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit as important as our traditional areas of support in health, medical research, education and the social services,” Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center's share will be $200,000 for its new building, which will house young artists and provide new public facilities. The Metropolitan Opera Co. and New York Philharmonic will receive $400,000 each. The Juilliard School, where music and the performing arts are taught, will get $250,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual $100,000 donation, too.
Introduction to DAG and their relationship with Probability Functions (Pearl)

\[ U_j \sim \text{Dirichlet}(\alpha), \alpha < 1 \]
\[ Z_{i,j} \sim \text{Multinomial}(U_j) \]
\[ W_{i,j} \sim \text{Multinomial}(\gamma_{Z_{i,j}}) \]

Then, we are looking for the posterior

\[ P(U, Z \mid W, \alpha, \gamma) = \frac{P(U, Z, W \mid \alpha, \gamma)}{P(W \mid \alpha, \gamma)} \]

\[ P(U, Z, W \mid \alpha, \gamma) = \prod_j \int P(U_j \mid \alpha) \left( \prod_i \sum_{Z_{i,j}} P(Z_{i,j} \mid U_j) P(W_{i,j} \mid Z_{i,j}, \gamma) \right) dU_j \]
Introduction to DAG and their relationship with Probability Functions (Pearl)

\[ U_j \sim \text{Dirichlet}(\alpha), \alpha < 1 \]
\[ Z_{i,j} \sim \text{Multinomial}(U_j) \]
\[ W_{i,j} \sim \text{Multinomial}(\gamma Z_{i,j}) \]

Then, we are looking for the posterior

\[ P(U, Z | W, \alpha, \gamma) = \frac{P(U, Z, W | \alpha, \gamma)}{P(W | \alpha, \gamma)} \]

\[ P(U, Z, W | \alpha, \gamma) = \prod_j P(U_j | \alpha) \left( \prod_i \sum_{Z_{i,j}} P(Z_{i,j} | U_j) P(W_{i,j} | Z_{i,j}, \gamma) \right) dU_j \]
Introduction to DAG and their relationship with Probability Functions (Pearl)

\[ U_j \sim \text{Dirichlet}(\alpha), \alpha < 1 \]
\[ Z_{i,j} \sim \text{Multinomial}(U_j) \]
\[ W_{i,j} \sim \text{Multinomial}\left(\gamma_{Z_{i,j}}\right) \]

Then, we are looking for the posterior

\[
P(U, Z | W, \alpha, \gamma) = \frac{P(U, Z, W | \alpha, \gamma)}{P(W | \alpha, \gamma)}
\]

\[
P(U, Z, W | \alpha, \gamma) = \prod_j \int P(U_j | \alpha) \left( \prod_i \sum_{Z_{i,j}} P(Z_{i,j} | U_j) P(W_{i,j} | Z_{i,j}, \gamma) \right) dU_j
\]
Relationship between a Directed Graphical Model and its Probability Law (Pearl and Paz 1985)

\[ P(W_1, \ldots, W_I, Z_1, \ldots, Z_I, U_1, \ldots, U_J, \alpha, \gamma) = \prod_j \prod_i P(W_i | Z_i, \gamma) P(Z_i | U_j) P(U_j | \alpha) \]

In general, for a graphical model Graphical Model with vertices V and edges E

\[ GM = (V, E), P(V) = \prod_{v \in V} P(v | Pa(v)), Pa(v) = \{v' : v' \to v \in E\} \]
Relationship between a Directed Graphical Model and its Probability Law (Pearl and Paz 1985)

Here, the report and the sound are independent, given that we know if there was an earthquake: They are **conditionally** independent.

\[ P(R, S \mid E) = P(R \mid E)P(S \mid E) \text{ iif } I(R, S, E) \]
Relationship between a Directed Graphical Model and its Probability Law (Pearl and Paz 1985)

\[ P(W_1, \ldots, W_I, Z_1, \ldots, Z_I, U_1, \ldots, U_J, \alpha, \gamma) = \Pi_j \Pi_i P(W_i | Z_i, \gamma) P(Z_i | U_j) P(U_j | \alpha) \]

However, our usual problem is: given observed variables \( O \) and latent variables \( L \), to compute the posterior \( P(L | O) \)

\[ P(L | O) = \frac{\Pi_{v \in V} P(v | Pa(v))}{\Pi_o P(o | Pa(o))}, \quad GM = (V = L \cup O, E), \quad \forall l \in L : o \rightarrow l \in E \]
Relationship between a Directed Graphical Model and its Probability Law (Pearl and Paz 1985)

\[ P(L \mid O) = \frac{\prod_{v \in V} P(v \mid Pa(v))}{\prod_{o} P(o \mid Pa(o))} \]

\[ GM = (V = L \cup O, E), \quad \forall l \in L : o \rightarrow l \in E \]

In the case of continuous variables this is

\[ P(L \mid O) = \frac{\int_{L \cup O} P(L, O) dO}{P(L)} \]
No analytical solution, for the general case
Relationship between a Directed Graphical Model and its Probability Law (Pearl and Paz 1985)

\[
P(L \mid O) = \frac{\prod_{v \in V} P(v \mid Pa(v))}{\prod_{o} P(o \mid Pa(o))}, \quad GM = (V = L \cup O, E), \quad \forall l \in L : o \rightarrow l \in E
\]

Can we approximate \(P(L \mid O)\)?

\[
Q(L) \approx P(L \mid O) = \frac{P(L, O)}{\int P(L, O) dO}
\]
Approximations to Density Laws

Can we approximate $P(L \mid O)$? 

$Q(L) \simeq P(L \mid O) = \frac{P(L, O)}{\int P(L, O)dO}$

- First try: MacLaurin

  $Q(L) = \sum P(L = l \mid O) + P'(L = l \mid O)(l - L) + \ldots$

  problem: how to guarantee that $Q(L)$ is a probability law?

- Second try: cumulant approximations (changing the random $L$ by $X$)

  $\phi(t) = \log \mathbb{E}_{X \sim Q(X)}[\exp(tX)] = \sum \kappa_n \frac{t^n}{n!} = \kappa_1 t + \kappa_2 \frac{t^2}{2!} + \ldots = \mu t + \sigma^2 \frac{t^2}{2!} + \ldots$

$Q(L) \simeq P(L \mid O) \simeq P(L, O, O) = P(L, O) \int P(L, O)dO$
Approximations to Density Laws

Can we approximate \( P(L \mid O) \)?

\[
Q(L) \simeq P(L \mid O) = \frac{P(L, O)}{\int P(L, O) dO}
\]

- First try: MacLaurin

\[
Q(L) = \sum P(L = l \mid O) + P'(L = l \mid O)(l - L) + \ldots
\]

problem: how to guarantee that \( Q(L) \) is a probability law?

- Second try: cumulant approximations (changing the random \( L \) by \( X \))

\[
\phi(t) = \log \mathbb{E}_{X \sim Q(X)}[\exp(tX)] = \sum_{n} \frac{\kappa_{n}}{n!} t^n = \kappa_1 t + \frac{\kappa_2}{2} t^2 + \ldots = \mu t + \sigma^2 \frac{t^2}{2} + \ldots
\]

- However, a probability law has either up to two moments, or an infinite number (Cramèr 1938)
Approximations to Density Laws

Can we approximate $P(L \mid O)$? $Q(L) \approx P(L \mid O) = \frac{P(L, O)}{\int P(L, O) dO}$

- Other options: Edgesworth, approximations which come from this identity

$$\phi(t) = \log \mathbb{E}_X[\exp(itX)] = \sum_n \kappa_n \frac{(it)^n}{n!},$$

$$\psi(t) = \log \mathbb{E}_X[\exp(itX)] = \sum_n \gamma_n \frac{(it)^n}{n!},$$

$$\hat{\phi}(t) = \sum_n (\kappa_n - \gamma_n) \frac{(it)^n}{n!} + \log \psi(t)$$

However, they are not guaranteed to be probability laws for finite samples.
Approximations to Density Laws

Can we approximate $P(L \mid O)$? 

$$Q(L) \simeq P(L \mid O) = \frac{P(L, O)}{\int P(L, O) \, dO}$$

• So? What do we do?

• We choose an approximate distribution $Q_\theta(X)$ — replacing $L$ by $X$ and $O$ by $Z$ for notation — from a given family, with parameters $\theta$. Then 

$$Q^* = Q_{\theta^*} : \theta^* = \arg \min_{\theta} D(Q_\theta(X), P(X \mid Z))$$

so we need to define the right similarity measurement $D$ to compare distributions. And in standard Variational Inference (VI), $Z$ is notation for $O$
Approximations to Density Laws

Can we approximate \( P(L | O) \)? \( Q(L) \approx P(L | O) \)

- So? What do we do?

- We choose an approximate distribution \( Q_\theta(X) \) — replacing \( L \) by \( X \) and \( O \) by \( Z \) for notation — from a given family, with parameters \( \theta \). Then

\[
Q^* = Q_{\theta^*} : \theta^* = \arg \min_{\theta} D(Q_\theta(X), P(X | Z))
\]

so we need to define the right similarity measurement \( D \) to compare distributions. And in standard Variational Inference (VI), \( Z \) is notation for \( O \)

This is what we call Variational Inference
So Which $D$ and $Q$ Should We Choose?

\[ Q^* = Q_{\theta^*} : \theta^* = \arg \min_{\theta} D(Q_\theta(X), P(X | Z)) \]

$X$ the latent variables and $Z$ the observations

Let’s start with “analytical” ideas:

\[ D(Q_\theta(X), P(X | Z)) = \int (Q_\theta(x) - P(x | Z))^2 dx \]

• What does it mean for two distributions to be close in the $L_2$ sense?
  • How easy is it to obtain bounds and closed form solutions?

• $Q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma)$: This is called the Laplace approximation
  • Even simpler $\Sigma = \sigma^2 \text{Id}$, which boils down to $Q_\mu(X) = \prod_i Q_{\mu_i}(X_i)$
So Which $D$ and $Q$ Should We Choose?

$$Q^* = Q_{\theta^*} : \theta^* = \arg \min_{\theta} D(Q_{\theta}(X), P(X|Z))$$

$X$ the latent variables and $Z$ the observations

More Information theoretic

$$D_{KL}(Q_{\theta}(X), P(X|Z)) = \mathbb{E}_{X \sim Q_{\theta}} \left[ -\log \frac{P(X|Z)}{Q_{\theta}(X)} \right] = - \int dQ_{\theta}(x) \log \frac{P(x|Z)}{Q_{\theta}(x)}$$

- The Kullback-Leibler divergence is based on information theory
- Known formulations for common cases

- Mean field $Q_{\theta=\mu}(X) = \prod_i Q_{\mu_i}(X_i)$

[Blei et al 2017]
A Case for Mean Field KL-based VI

Mean Field Theory for Sigmoid Belief Networks

Lawrence K. Saul
Tommi Jaakkola
Michael I. Jordan
Center for Biological and Computational Learning
Massachusetts Institute of Technology
79 Amherst Street, E10-243
Cambridge, MA 02139

Abstract

We develop a mean field theory for sigmoid belief networks based on ideas from statistical mechanics. Our mean field theory provides a tractable approximation to the true probability distribution in these networks; it also yields a lower bound on the likelihood of evidence. We demonstrate the utility of this framework on a benchmark problem in statistical pattern recognition—the classification of handwritten digits.

Figure 7: Binary images of handwritten digits: two and five.
So Which $D$ and $Q$ Should We Choose?

$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$

$X$ the latent variables and $Z$ the observations

A second order information-theoretic model

$D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X \sim Q_\theta} \left[-\log \frac{P(X|Z)}{Q_\theta(X)}\right] = -\int dQ_\theta(x) \log \frac{P(x|Z)}{Q_\theta(x)}$

$Q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma)$: This is called the Laplace approximation
But Laplace is Better

Variational Inference in Nonconjugate Models

1. Draw coefficients $\theta \sim \mathcal{N}(\mu_0, \Sigma_0)$.
2. For each data point $n$ and its covariates $t_n$, draw its class label from

$$z_n | \theta, t_n \sim \text{Bernoulli} \left( \sigma(\theta^\top t_n) z_{n,1}, \sigma(-\theta^\top t_n) z_{n,2} \right),$$

<table>
<thead>
<tr>
<th>Yeast</th>
<th>Accuracy</th>
<th>Log Likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jaakkola and Jordan (1996)</td>
<td>79.7%</td>
<td>-0.678</td>
</tr>
<tr>
<td>Laplace inference</td>
<td>80.1%</td>
<td>-0.449</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Scene</th>
<th>Accuracy</th>
<th>Log Likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>87.4%</td>
<td>-0.670</td>
</tr>
<tr>
<td></td>
<td>89.4%</td>
<td>-0.259</td>
</tr>
</tbody>
</table>
So Which $D$ and $Q$ Should We Choose?

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$$

$X$ the latent variables and $Z$ the observations

A second order information-theoretic model

$$D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X \sim Q_\theta} \left[ -\log \frac{P(X|Z)}{Q_\theta(X)} \right] = -\int dQ_\theta(x) \log \frac{P(x|Z)}{Q_\theta(x)}$$

$Q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma)$ : This is called the Laplace approximation
So Which $D$ Should We Choose? Finding Bounds

$$D_{KL}(Q_\theta(X), P(X \mid Z)) = \mathbb{E}_{X \sim Q_\theta} \left[ -\log \frac{P(X \mid Z)}{Q_\theta(X)} \right] = - \int dQ_\theta(x) \log \frac{P(x \mid Z)}{Q_\theta(x)}$$

But our graphical model is more adapted to sample from $P(X, Z)$ than from $P(X \mid Z)$.

Then, can we find a way to efficiently minimise $D_{KL} \left( Q_\theta(X), \frac{P(X, Z)}{P(Z)} \right)$ when, in general, we don’t know the probability of “evidence” $P(Z)$?

Let’s see in the next slide....
So Which \( D \) Should We Choose? Finding Bounds

\[
D_{KL}(Q_\theta(X), P(X \mid Z)) = \mathbb{E}_{X \sim Q_\theta} \left[ -\log \frac{P(X \mid Z)}{Q_\theta(X)} \right] = - \int dQ_\theta(x) \log \frac{P(x \mid Z)}{Q_\theta(x)}
\]

And we know that

\[
\log P(Z) = \log \int dx P(x, Z) = \log \int \frac{dQ_\theta(x)P(x, Z)}{Q_\theta(x)} = \log \mathbb{E}_{X \sim Q_\theta} \left[ \frac{P(X, Z)}{Q_\theta(X)} \right]
\]

with \( Z \) being the observed data (\( O \) before) and \( X \) our latent variables (\( L \))

then, \( P(Z) = \log \mathbb{E}_{X \sim Q_\theta} \left[ \frac{P(X, Z)}{Q_\theta(X)} \right] \geq E_{X \sim Q_\theta} \left[ \frac{P(X, Z)}{Q_\theta(X)} \right] \triangleq \mathcal{L}(\theta) \)

\[
\min_\theta D_{KL}(Q_\theta(X), P(X \mid Z)) = \log P(Z) - \max_\theta \mathcal{L}(\theta)
\]

Hence, it is enough to maximise the Evidence Lower Bound (ELBO): \( \mathcal{L}(\theta) \)
So Which $D$ and $Q$ Should We Choose?

$q^* = q_{\theta^*} : \theta^* = \arg\min_{\theta} D(q_\theta(X), P(X|Z))$

$X$ the latent variables and $Z$ the observations

A simplified second order information-theoretic model

$\theta = \arg\max_{\theta} \mathcal{L}(\theta) = \mathbb{E}_{X \sim q_\theta} \left[ \log \frac{P(X, Z)}{q_\theta(X)} \right]$

$q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma) : This$ is called the Laplace approximation
But Laplace is Better (they use ELBO)

Variational Inference in Nonconjugate Models

1. Draw coefficients \( \theta \sim \mathcal{N}(\mu_0, \Sigma_0) \).
2. For each data point \( n \) and its covariates \( t_n \), draw its class label from

\[
    z_n \mid \theta, t_n \sim \text{Bernoulli} \left( \sigma(\theta^\top t_n)^{z_{n,1}} \sigma(-\theta^\top t_n)^{z_{n,2}} \right),
\]

<table>
<thead>
<tr>
<th>Yeast</th>
<th>Accuracy</th>
<th>Log Likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jaakkola and Jordan (1996)</td>
<td>79.7%</td>
<td>-0.678</td>
</tr>
<tr>
<td>Laplace inference</td>
<td>80.1%</td>
<td>-0.449</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Scene</th>
<th>Accuracy</th>
<th>Log Likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>87.4%</td>
<td>-0.670</td>
</tr>
<tr>
<td></td>
<td>89.4%</td>
<td>-0.259</td>
</tr>
</tbody>
</table>

Chong Wang
Machine Learning Department
Carnegie Mellon University
Pittsburgh, PA, 15213, USA

David M. Blei
Department of Computer Science
Princeton University
Princeton, NJ, 08540, USA

CHONGW@CS.CMU.EDU
BLEI@CS.PRINCETON.EDU
More General $Q_\theta$

$Q^* = Q_{\theta^*} : \theta^* = \arg\min_\theta D(Q_\theta(X), P(X|Z))$

$X$ the latent variables and $Z$ the observations

• Gaussian Processes: A measure over continuous functions where any discrete sample of the domain follows a Gaussian law.

$P(f(x)) : (f(x_1), \ldots, f(x_N)) \sim N(\mu_{x_1, \ldots, x_N}, \Sigma_{x_1, \ldots, x_N})$

• Support Transformations: $Q_\theta(X) \triangleq \phi_\theta(X)$

$X \sim \mathcal{N}(\mu, \Sigma), \phi_\theta$ a parametric mass-preserving diffeomorphism
More General $Q_\theta$

$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$

$X$ the latent variables and $Z$ the observations

- Support Transformations: $Q_\theta(X) \triangleq N_{\mu, \Sigma}(\phi_\theta(X)) \left| J_{\phi_\theta}(X) \right|$

$X \sim \mathcal{N}(\mu, \Sigma)$, $\phi_\theta$ a parametric mass-preserving diffeomorphism

[Kucukelbir et al. 17]
More General $Q_\theta$

$Q^* = Q_{\theta^*} : \theta^* = \operatorname{arg\ min}_\theta D(Q_\theta(X), P(X \mid Z))$

$X$ the latent variables and $Z$ the observations

- Support Transformations: $Q_\theta(X) \triangleq N_{\mu, \Sigma}(\phi_\theta(X)) \quad J_{\phi_\theta}(X)$

$\phi_\theta(X) \sim \mathcal{N}(\mu, \Sigma)$, $\phi_\theta$ a stochastic flow or learnable diffeomorphism

[Papamakarios et al. 21]
Current Problems in VI

- Scalability
- Amortization [Gershman et al 2014]
- Preservation of dependencies
- Auto-regressive models

Query 1: $P(B|C) = P(C|B)P(B)/P(C)$
Query 2: $P(A|C) = \sum_B P(A|B)P(B|C)$

Amortisation, reused probability in blue

Figure 1: A Bayesian network modeling brightness constancy in visual perception, a possible inverse factorization, and two of the local joint distributions that determine the inverse conditionals.

[Stuhlmüller et al 14]
Other Modern Bayesian Techniques

• Variational AutoEncoders

• Likelihood-free Inference

\[ \theta = \arg \max_\theta \mathcal{L}(\theta) = \mathbb{E}_{X \sim Q_\theta} \left[ \log \frac{P(X, Z)}{Q_\theta(X)} \right] \]

P(Z|X) = \frac{P(X|Z)P(Z)}{P(X)}

Likelihood \quad Prior \quad Evidence

VAE: Z \sim N(\mu(X), \Sigma(X))