Approximate Inference

PAI Tutorial

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Statistical Inference

What is statistical inference?

Statistical inference is the process of using data analysis to deduce properties of an underlying probability distribution. (Wikipedia)

- Use a model to relate data to a quantity of interest.

Examples:

- Maximum likelihood $x_{\text{ML}} = \arg\max_x P(Y = y|X = x)$
- **Bayesian inference** $P(X|Y) \propto P(Y|X)P(Y)$.
- Computing conditional/marginals in a Bayes Net

Bayesian Inference

The **Bayesian model** specifies:

- $P(Y|X)$, likelihood of Y given hypothesis/latent factors X.
- $P(X)$ prior probability of X ("belief").

→ Joint distribution $P(X, Y) = P(X)P(Y|X)$.

Bayesian inference asks to compute, e.g.

- *posterior distribution* $P(X|Y = y) = \frac{P(Y=y|X)P(X)}{P(Y=y)}$
- *maximum a posteriori* estimate $x_{\text{MAP}} = \arg\max_x P(X = x|Y = y)$
- *posterior sample* $x \sim P(X|Y = y)$

But: Evidence $P(Y = y) = \sum_x P(y, x)$ is often difficult to compute.

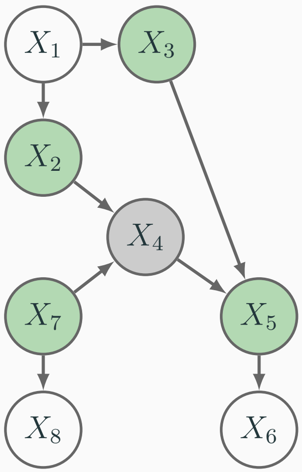
Bayesian Networks

Bayes Net:

- Defines a joint distribution $P(X_1, \ldots, X_m)$
- Inference: e.g. $P(X_1 | X_4 = T)$

Queries are difficult to compute in general:

- Need to marginalize.



Approximate Inference

Exact inference can be difficult:

- Bayesian inference requires to compute the marginal $P(Y)$.
- Computing conditional/marginals in Bayes Nets not always efficient.
- Factor distribution $P(X) = \frac{1}{Z} \prod_{i=1}^{m} \Phi_i(X_{A_i})$.

Goal: Approximate $P(X) = \frac{1}{Z}\Phi(X)$, where $\Phi(X) \geq 0$ and $Z = \sum_x \Phi(x)$.

Two popular approaches: Variational Inference and MCMC

Goal: Approximate $P(X) = \frac{1}{Z}\Phi(X)$, where $\Phi(X) \geq 0$, $Z = \sum_x \Phi(x)$.

Variational Inference

$$Q = \arg\min_{Q \in \mathcal{Q}} \mathrm{KL}(Q \| P)$$

- Choose a class of distributions $\mathcal{Q}$
- Solve optimization problem.
- Jordan et al. (1999)

Markov Chain Monte Carlo

- *Idea:* Set up a Markov chain
- Define transition kernel $T(X, X')$
- With stationary distribution $P(X)$
- Metropolis et al. (1953)

$\rightarrow$ *Sample P(X) from the Markov chain.*

Variational Inference:

$$Q = \arg\min_{Q \in \mathcal{Q}} \mathrm{KL}(Q \| P)$$

Variational Inference: Evidence Lower Bound

Goal: Approximate $P(X) = \frac{1}{Z}\Phi(X)$, where $\Phi(X) \geq 0$, $Z = \sum_x \Phi(x)$.

$$\begin{aligned}
\mathrm{KL}(Q\|P) &= \sum_x Q(x) \log \frac{Q(x)}{P(x)} \\
&= \sum_x Q(x) \log Q(x) - \sum_x Q(x) \log \Phi(x) + \log(Z)
\end{aligned}$$

$$\arg\min_{Q \in \mathcal{Q}} KL(Q\|P) = \arg\max_{Q \in \mathcal{Q}} \underbrace{\sum_x Q(x) \log \Phi(x) - \sum_x Q(x) \log Q(x)}_{:= \mathsf{ELBO}(Q)}$$

Evidence Lower Bound for Bayesian Inference

Goal: Approximate $P(X|Y=y) \propto \Phi(X) = P(Y=y|X)P(X)$

$$
\begin{aligned}
\text{ELBO}(Q) &= \sum_x Q(x)\log(P(Y|x)P(x)) - \sum_x Q(x)\log Q(x) \\
&= \sum_x Q(x)\log(P(Y|x)) - \text{KL}(Q(X)||P(X))
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_x Q(x)\log\left(\frac{P(Y,x)}{P(x)}\right) - \sum_x Q(x)\log\frac{Q(x)}{P(x)}. \\
&= \sum_x Q(x)\log(P(x|Y)P(Y)) - \sum_x Q(x)\log Q(x) \\
&= \sum_x Q(x)\log P(Y) - \sum_x Q(x)\log\frac{Q(x)}{P(x|Y)} \\
&= \log P(Y) - KL(Q(X)\,||\,P(X|Y)).
\end{aligned}
$$

→ *Trade-off between likelihood and prior.*

$$
\begin{aligned}
\text{ELBO}(Q) &= \log P(Y) - \text{KL}(Q(X)||P(X|Y)) \\
&\leq \log P(Y)
\end{aligned}
$$

→ *Maximize lower-bound on evidence.*

Mean Field Variational Inference

Need to choose class of distributions $\mathcal{Q}$.

Mean field approximation: $Q(x) = \prod_{i=1}^{m} Q_i(x_i)$.

$$\mathrm{ELBO}(Q) = \sum_x \prod_{i=1}^{m} Q_i(x_i) \log \Phi(x) - \sum_{i=1}^{m} \sum_{x_i} Q_i(x_i) \log Q_i(x_i)$$

Objective for Q_j:

$$\mathrm{ELBO}_j(Q) = \sum_{x_j} Q_j(x_j) \underbrace{\sum_{x_{j-}} \prod_{i \neq j} Q_i(x_i) \log \Phi(x)}_{\log \exp(\sum \prod \cdots)} - \sum_{x_j} Q_j(x_j) \log Q_j(x_j) + const$$

Exact update for Q_j:

$$Q_j^* = \arg\max_{Q_j} \mathrm{ELBO}_j(Q) \propto \exp\left(\sum_{x_{j-}} \prod_{i \neq j} Q_i(x_i) \log \Phi(x)\right)$$

Mean Field Coordinate Ascent

CAVI (Coordinate Ascent Variational Inference):

Choose ordering of $X_1, \ldots, X_m$
Initialize $Q_1, \ldots, Q_m$
repeat
  for $j = 1{:}m$ **do**
    $Q_j \leftarrow \arg\max_{Q_j} \mathsf{ELBO}_j(Q) \propto \exp\left(\sum_{x_{j-}} \prod_{i \neq j} Q_i(x_i) \log \Phi(x)\right)$
until converged

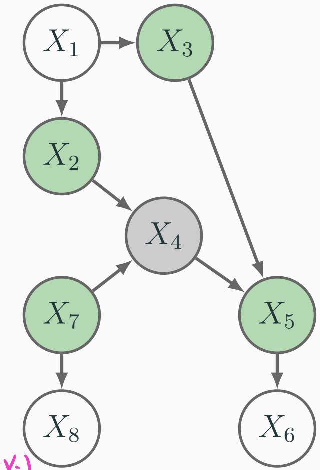
$$\mathsf{ELBO}_j(Q) = \sum_{x_j} Q_j(x_j) \sum_{x_{j-}} \prod_{i \neq j} Q_i(x_i) \log \Phi(x) - \sum_{x} Q_j(x_j) \log Q_j(x_j)$$

Mean Field Variational Inference: Bayes Nets

Markov Blanket:

$\text{mb}(X_j) = \text{parents}(X_j) \cup \text{children}(X_j) \cup \text{co-parents}(X_j)$

- ▷ $\text{co-parents}(X_j) = \text{parents}(\text{children}(X_j)) \setminus X_j$
- ▷ $\forall i \neq j \, , X_j \perp X_i | X_{\text{mb}(X_j)}$



CAVI update only depends on Markov Blanket:

$$Q_j \propto \exp\left(\sum_{x_{j-}} \prod_{i \neq j} Q_i(x_i) \log \Phi(x)\right)$$

$$\propto \exp\left(\sum_{x_{\text{mb}(X_j)}} \prod_{i \in \text{mb}(X_j)} Q_i(x_i) \log P(X_j | X_{\text{mb}(X_j)})\right)$$

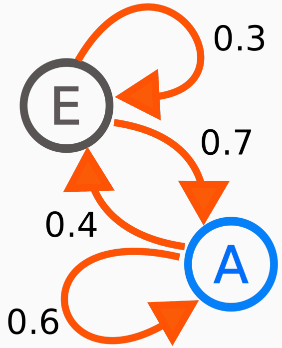
只需更新 M.B. 里面的元素. mb(Xj)

Markov Chain Monte Carlo

Markov Chains

Markov Chain:

- Sequence of random variables $X^{(1)}, X^{(2)}, X^{(3)}, \ldots$ on $\mathcal{S}$
- States space $\mathcal{S} = \{S_1, \ldots, S_k\}$
- Initial distribution: $P(X^{(1)} = S)$
- Transition kernel: $T(S, S') = P(X^{(t)} = S' | X^{(t-1)} = S)$
- Can be written as $k \times k$ matrix T.



$T = \begin{pmatrix} 0.3 & 0.7 \\ 0.4 & 0.6 \end{pmatrix}$

Stationary distribution: $\pi(S) = \lim_{t\to\infty} P(X^{(t)} = S)$

- Satisfies $\pi(S)T(S, S') = \pi(S)$
- Matrix notation: $\pi^\top T = \pi^\top$ (left eigenvector)
- Independent of initial distribution (mild conditions)

MCMC: General Idea

Goal: Approximate $P(X) = \frac{1}{Z}\Phi(X)$, where $\Phi(X) \geq 0$, $Z = \sum_x \Phi(x)$.

Markov Chain Monte Carlo (MCMC)

Idea: Construct Markov chain with stationary distribution $P(X)$.

- Simulating the Markov chain to draw samples $\sim P(X)$

Detailed balance condition:

$$\pi(S)T(S, S') = \pi(S')T(S', S)$$

- Implies that $\pi(S)$ is the stationary distribution.
- Define $T(X, X')$ that satisfies detailed balance for Φ:

$$\Phi(X)T(X, X') = \Phi(X')T(X', X)$$

MCMC: Gibbs Sampling

Gibbs Sampling:

Initialize $x_1, \ldots, x_m$

repeat

  for $j = 1{:}m$ **do**

    $x_j \leftarrow X_j \sim \frac{1}{Z_j}\Phi(X_1 = x_1, \ldots, X_j, \ldots, X_m = x_m)$

until converged

- ▷ Draw samples conditioned on all other variables.
- ▷ We'll show detailed balance for $j \sim \text{Uniform}(\{1, \ldots, m\})$

Gibbs Sampling: Detailed Balance

Gibbs sampling generates Markov chain $X^{(1)}, X^{(2)}, X^{(3)}, \ldots$

- $X^{(t)} = (X_1^{(t)}, \ldots, X_m^{(t)})$

$$T(X, X') = \begin{cases} 0 & \text{if } X_i \neq X_i' \text{ and } X_j \neq X_j' \text{ for } i \neq j \\ \propto P(X_1, \ldots, X_m) & X = X' \\ \propto \frac{1}{m} P(X_{1:j-1}, X_j', X_{j+1:m}) & \exists j,\ X_j \neq X_j' \text{ and } X_i = X_i' \,\forall\, i \neq j \end{cases}$$

Detailed Balance:

- Case 1) & 2) are easy
- Case 3) $j,\ X_j \neq X_j'$ and $X_i = X_i' \,\forall\, i \neq j$

$$\underline{P(X_{1:m})} \cdot \frac{1}{m} \underline{P(X_{1:j-1}, X_j', X_{j+1:m})} = \underline{P(X_{1:m}')} \cdot \frac{1}{m} \underline{P(X_{1:j-1}', X_j, X_{j+1:m}')}$$

Gibbs Sampling on Bayes Nets

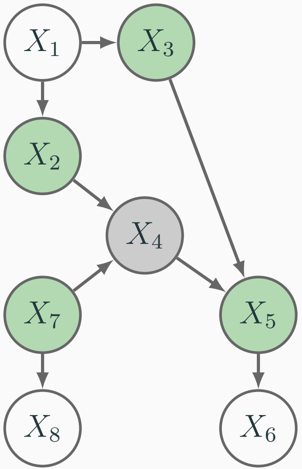
Markov Blanket:

$\text{mb}(X_j) = \text{parents}(X_j) \cup \text{children}(X_j) \cup \text{co-parents}(X_j)$

- co-parents(X_j) = parents(children(X_j)) $\setminus X_j$
- $\forall i \neq j \;, X_j \perp X_i | X_{\text{mb}(X_j)}$

Gibbs sample only depends on Markov Blanket:

$$X_j \sim P(X_{1:j-1} = x_{1:j-1}, X_j, X_{j+1:m} = x_{j+1:m})$$
$$\sim P(X_j, X_{\text{mb}(X_j)} = x_{\text{mb}(X_j)})$$



MCMC and Variational Inference

MCMC: 渐近.

- ▷ Asymptotically correct
- ▷ Computationally expensive, if it takes long to converge
- ▷ Difficult to detect convergence (burn-in)
- ▷ Does not generate iid samples

Variational Inference:

- ▷ Faster
- ▷ Easy to monitor optimization progress
- ▷ Class of distributions $\mathcal{Q}$ often misspecifed, i.e. $P \notin \mathcal{Q}$.
- ▷ Optimization can be difficult

Further Reading

- Bayesian Inference, MCMC and Variational Inference:

https://towardsdatascience.com/25a8aa9bce29

- Technical Review on Variational Inference:

https://arxiv.org/abs/1601.00670

- Forward & Reverse KL:

https://blog.evjang.com/2016/08/variational-bayes.html