1 Probabilities

$$\mathrm{P}(A\,|\,B) = \frac{\mathrm{P}(B|A)\cdot \mathrm{P}(A)}{\mathrm{P}(B)} = \frac{\mathrm{P}(A\cap B)}{\mathrm{P}(B)}$$

$$\mathrm{P}(A,B) = \mathrm{P}(A\cap B) = \mathrm{P}(A|B)\mathrm{P}(B) = \mathrm{P}(B|A)\mathrm{P}(A)$$

$$\mathrm{P}(A\cup B) = \mathrm{P}(A) + \mathrm{P}(B) - \mathrm{P}(A\cap B)$$

$$\mathrm{P}(X_1,\dots,X_n) = \mathrm{P}(X_1)\mathrm{P}(X_2|X_1)\mathrm{P}(X_3|X_1,X_2)\cdots \mathrm{P}(X_n|X_1,\dots,X_{n-1})$$

$$\mathrm{P}(X,Y|Z) = \mathrm{P}(X|Y,Z)\mathrm{P}(Y|Z)$$

$$\mathrm{P}(X=x) = \sum_y \mathrm{P}(X=x,Y=y) = \sum_y \mathrm{P}(X=x\,|\,Y=y)\mathrm{P}(Y=y)$$

Conditional independence: $X\perp Y|Z$ iff $\mathrm{P}(X,Y|Z) = \mathrm{P}(X|Z)\mathrm{P}(Y|Z)$.
If $\mathrm{P}(Y|Z) > 0$ equivalent to $\mathrm{P}(X|Z,Y) = \mathrm{P}(X|Z)$

2 Bayes Network

Naive Bayes Effects are conditionally independent given a cause.
Bayesian network (G,P)**:** DAG with cond. prob. dist. $\mathrm{P}(X_s|Pa_{X_s})$. (G,P) defines joint distribution $\mathrm{P}(X_{1:n}) = \prod_i \mathrm{P}(X_i|Pa_{X_i})$.
Specifying a BN Variables $X_1,\cdots,X_n$. Pick order. For all $i\in[n]$ find 1. min. subset $A\subseteq\{X_1,\dots,X_{i-1}\}$ s.t. $X_i\perp X_{\bar{A}}|X_A$. 2. Specify/learn $\mathrm{P}(X_i|A)$. BN defined this way are sound. Ordering matters a lot for compactness of representation!
Active Trails If for all consecutive triplets X,Y,Z.

- $X\rightarrow Y\rightarrow Z$ & Y is unobserved
- $X\leftarrow Y\leftarrow Z$ & Y is unobserved
- $X\leftarrow Y\rightarrow Z$ & Y is unobserved
- $X\rightarrow Y\leftarrow Z$ & Y or any of $Y's$ descendants is oberserved

A and *B d-seperated by O* iff no active trail exists with observations O. Implies c.i.: d-sep$(A;B|O)\Rightarrow A\perp B|O$. Algo for d-sep.: BFS

3 Inference

Typical Queries Conditional Distribution, MPE ($\mathrm{argmax}_{e,b,a}\mathrm{P}(e,b,a|J=t,M=f)$), MAP ($\mathrm{argmax}_e\mathrm{P}(e|J=t,M=f)$)

3.1 Exact Inference

Variable Elimination

- Given BN and Query $\mathrm{P}(Q|E=e)$ (E = evidence variables)
- Choose an ordering of $X_1,\dots,X_n$
- Set up initial factors: $fi = \mathrm{P}(X_i|P_{ai})$
- For $i=1:n$, $X_i\in X\setminus\{Q,E\}$

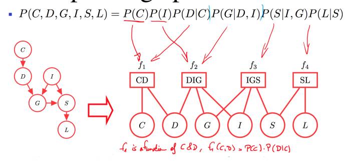
1. Collect and multiply all factors f that include X_i
2. Generate new factor by marginalizing out X_i
3. Add g to set of factors, $g = \sum_{x_i}\prod_j f_j$

- Renormalize $\mathrm{P}(q,e)$ to get $\mathrm{P}(q|e) = \frac{1}{\sum_q \mathrm{P}(q,e)}\mathrm{P}(q,e)$

Variable Elimination for Polytrees
Polytree: A DAG is a polytree iff dropping edge directions results in a tree

- Pick root
- Orient edges towards the root (only in this algo, not in actual BN)
- Eliminate in topological ordering (descendants before parents)

Factor Graph of BN is bipartite graph with variables on one side and factors on the other.


$P(C,D,G,I,S,L) = P(C)P(I)P(D|C)P(G|D,I)P(S|I,G)P(L|S)$
C
D
I
G
S
L
f_1
f_2
f_3
f_4
CD
DIG
IGS
SL
C
D
G
I
S
L
f_1 is a function of C&D, $f_1(C,D) = P(C)\cdot P(D|C)$

Sum-Product / Belief Propagation Algorithm

- Initialize all messages as uniform distribution
- Until converged do

1. Pick some ordering on the factor graph edges (+directions)
2. Update messages according to this ordering

Messages from variable v to factor u:
$\mu^{(t+1)}_{v\to u}(x_v) = \prod_{u'\in N(v)\setminus\{u\}}\mu^{(t)}_{u'\to v}(x_v)$
Messages from factor u to variable v:
$\mu^{(t+1)}_{u\to v}(x_v) = \sum_{x_u\sim x_v} f_u(x_u)\prod_{v'\in N(u)\setminus\{v\}}\mu^{(t)}_{v'\to u}(x_{v'})$
3. Break once all messages change by at most ε
Intention: $\hat{\mathrm{P}}(X_v = x_v)\propto\prod_{u\in N(v)}\mu_{u\to v}(x_v)$
$\hat{\mathrm{P}}(X_u = x_u)\propto f_u(x_u)\prod_{v\in N(u)}\mu_{v\to u}(x_u)$

Belief Propagation on Trees (converges in two rounds)

- Factor graph of polytree is a tree!
- Choose one node as root
- Send messages from leaves to root, and from root to leaves

Variable Elimination for MPE

- Given BN and evidence $E=e$
- Choose an ordering of $X_1,\dots,X_n$
- Set up initial factors: $f_i = \mathrm{P}(X_i|Pa_i)$
- For $i=1:n, X_i\notin E$

1. Collect and multiply all factors f_j that include X_i
2. Generate new factor by maximizing out $X_i, g_i = \max_{x_i}\prod_j f_j$
3. Add g to set of factors

- For $i=n:-1:1, X_i\notin E$: $\hat{x}_i = \mathrm{argmax}_{x_i} g_i(x_i,\hat{x}_{i+1:n})$

Example

$$\mathrm{argmax}_{e,b,a}\mathrm{P}(e,b,a|J,M) = \mathrm{argmax}_{e,b,a}\cancel{\tfrac{1}{Z}}\mathrm{P}(e,b,a,J,M)$$
$$= \mathrm{argmax}_{e,b,a}\mathrm{P}(e)\mathrm{P}(b)\mathrm{P}(a|e,b)\mathrm{P}(J|a)\mathrm{P}(M|a)$$
$$= \mathrm{argmax}_a\mathrm{P}(J|a)\mathrm{P}(M|a)\mathrm{argmax}_e\mathrm{P}(e)\mathrm{argmax}_b\mathrm{P}(b)\mathrm{P}(a|e,b)$$
$$a^* = \mathrm{argmax}_a P(J|a)P(M|a)g_e(a)$$
$$e^* = \mathrm{argmax}_e P(J|a^*)P(M|a^*)P(e)g_b(a^*,e)$$

Max-product Message Passing on Factor Graphs Messages from variable v to factor u:
$\mu^{(t+1)}_{v\to u}(x_v) = \prod_{u'\in N(v)\setminus\{u\}}\mu^{(t)}_{u'\to v}(x_v)$
Messages from factor u to variable v:
$\mu^{(t+1)}_{u\to v}(x_v) = \max_{x_u\sim x_v} f_u(x_u)\prod_{v'\in N(u)\setminus\{v\}}\mu^{(t)}_{v'\to u}(x_{v'})$

Retrieving MAP From Max-Product

- Define max-marginals: $P_{max}(X_v = x_v) = \max_{x\sim x_v}P(x)$
- For tree factor graphs, max-product computes max-marginals: $P_{max}(X_v = x_v)\propto\prod_{u\in N(v)}\mu_{u\to v}(x_v)$
- Can retrieve MAP solution from these (must be careful when ties need to be broken)

3.2 Approximate Inference

Problem: if BN contains loops. Loopy belief propagation will in general not converge $\rightarrow$ Sampling Based Inference

Monte Carlo Sampling from a BN (forward Sampling)

- Sort variables in topological ordering $X_1,\dots,X_n$
- For $i=1$ to n do: Sample $xi\sim P(X_i|X_1 = x_1,\dots,X_{i-1} = x_{i-1})$

Computing Probabilities Through Sampling
Marginals: $P(w=t)\approx\frac{1}{N}\sum_{i=1}^N[w=t]x^{(i)} = \frac{Count(w=t)}{N}$
Conditionals: $P(C=t|W=t) = \frac{P(C=t,W=t)}{P(w=t)}\approx\frac{Count(W=t,C=t)}{Count(W=t)}$
Rejection Sampling “Normalen Würfel nehmen um Verteilung von 1..5 zu samplen, 6 wird jeweils ignoriert”
$\hat{P}(X_A = x_A|X_B = x_B)\approx\frac{Count(x_a,x_B)}{Count(x_B)}$
Throw away samples that disagree with x_B problematic if x_B is a rare event.
Markov Chain A Markov chain is sequence of RVs, $X_1,\dots,X_N$ with *Prior* $\mathrm{P}(X_1)$ & *transition probabilities* $\mathrm{P}(X_{t+1}|X_t)$ independent of t.
Ergodic: $\exists t\in\mathbb{N}$ s.t. every state is reachable from every state in exactly t steps. Then it has unique, positive, stationary distribution.
$\exists$ unique stat. $\pi(x) > 0$ *s.t.* $\forall x\lim_{N\to\infty}\mathrm{P}(X_N = x) = \pi(x)$ indep. of $\mathrm{P}(X_1)$.
Ergodic Theorem: $\lim_{N\to\infty}\frac{1}{N}\sum_i f(x_i) = \sum_{x\in D}\pi(x)f(x)$, where D finite state space.
Sampling from MC Sample $x_1\sim\mathrm{P}(X_1), x_2\sim\mathrm{P}(X_2|X_1 = x_1),\dots,x_N\sim\mathrm{P}(X_N|X_{N-1} = x_{N-1})$. If simulated “sufficiently long”, sample X_N is drawn “very close” to the stationary dist. π.

Gibbs Sampling: Random Order

- Start with initial assignment x to all variables
- Fix observed variables X_B to their observed value x_B
- For $t=1$ to ∞ do

1. Pick a variable i uniformly at random from $\{1,..,n\}\setminus B$
2. Set v_i =values of all x except x_i
3. Update x_i by sampling from $\mathrm{P}(X_i|v_i)$

Satisfies detailed balance equation! For unnormalized Q $\forall x,x'$: $\frac{1}{Z}Q(x)P(x'|x) = \frac{1}{Z}Q(x')P(x|x')$

Gibbs Sampling: Practical Variant

- Start with initial assignment $x^{(0)}$ to all variables
- Fix observed variables X_B to their observed value x_B
- For $t=1$ to ∞ do

1. Set $x^{(t)} = x^{(t-1)}$
2. For each variable X_i (except those in B)
3. Set $v_i =$ values of all $x^{(t)}$ except x_i
4. Sample $x_i^{(t)}$ from $\mathrm{P}(X_i|v_i)$

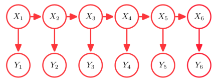
No detailed balance, but also has correct stationary distribution.
Ex. for Michi $\mathrm{P}(C|S,R,W=1) = \frac{\mathrm{P}(C,S,R,W=1)}{\sum_{c'}\mathrm{P}(C=c',S,R,W=1)}$.

3.3 Temporal models

Markov Chains
Markov assumption: $x_{t+1}\perp x_{1:t-1}|x_t\forall t$
Stationary asm.: $P(x_{t+1} = x|x_t = x') = P(x_{t'+1}|\;x_{t'} = x')\forall t,t'$
k-order: Next state depend on last k states.

Prediction in Markov Chains

$$\mathrm{P}(X_i|X_1 = x) = \sum_{x'}\mathrm{P}(X_i,X_{i-1} = x'|X_1 = x)$$
$$= \sum_{x'}\mathrm{P}(X_i|X_{i-1} = x',X_1 = x)\mathrm{P}(X_{i-1} = x'|X_1 = x)$$
$$= \sum_{x'}\mathrm{P}(X_i|X_{i-1} = x')\mathrm{P}(X_{i-1} = x'|X_1 = x)$$
$$= f(\mathrm{P}(X_{i-1}|X_1 = x)) = f^{i-1}(\mathrm{P}(X_1 = x))$$



Hidden Markov Model/ Kalman Filters
$X_1,...,X_T$: Unobserved (hidden) variables (called states)
$Y_1,...,Y_T$: Observations
HMMs: X_i categorical, Y_i categorical (or arbitrary)
Kalman Filters: X_i,Y_i Gaussian distributions

Inference Tasks Filtering: $P(X_t|y_{1:t})$; Prediction: $P(X_{t+T}|y_{1:t})$; Smoothing: $P(X_t|y_{1:T})$ for $1 \leq t < T$; MPE: $\text{argmax}_{X_{1:T}} P(X_{1:T}|\, y_{1:T})$
In principle, can use variable elimination / belief propagation with new variables Xt, Yt at each time step. Problem need to rerun every time, complexity grows with time!

Bayesian Filtering Suppose we already have computed $P(X_t|y_{1,...,t})$ now want to efficiently compute $P(X_{t+1}|y_{1,...,t+1})$
- Start with $P(X_1)$
- At time t (Assume we have: $P(X_t|y_{1,...,t-1})$
- Conditioning: $P(X_t|y_{y1:t}) = \frac{1}{Z} P(X_t|y_{1:t-1})P(y_t|X_t)$
- $Z = \sum P(x,y_t|\, y_{1:t-1})$
- Prediction: $P(X_{t+1}|y_{y1:t}) = \sum_{x_t} P(X_t|y_{1:t})P(X_{t+1}|x_t)$

Computation is recursive (cost independent of t)!

Dynamic Bayesian Networks If we have more than one variable at each time step
- At every timestep have a replicated BN
- Variables at each time step t called a slice S_t
- "Temporal" edges connecting S_{t+1} with S_t (usually sharing parameters – stationarity)
- Can use standard approximate inference techniques (many loops) but high complexity over timesteps

Particle filtering Approximate the posterior at each time by samples (particles), which are propagated and reweighted over time. True distribution (possibly continuous): $P(x)$, N i.i.d. samples: $x_1,..x_N$; Represent: $P(x) \approx \frac{1}{N}\sum_{i=1}^N \delta_{x_i}(x)$. E.g. $\delta_{x_i}(x) := x_i = x$
- Suppose $P(X_t|\, y_{1:t}) \approx \frac{1}{N}\sum_{i=1}^N \delta_{x_{i,t}}$ (measurement)
- Prediction: Propagate each particle: $x_i' \sim P(X_{t+1}|x_{i,t})$ (movement)
- Conditioning: Weigh particles: $w_i = \frac{1}{Z}P(y_{t+1}|\, x_i')$
- Conditioning: Resample N particles: $x_{i,t+1} \sim \frac{1}{N}\sum_{i=1}^N w_i \delta_{x_i'}$

3.4 Probabilistic planning

How should we control the robot to maximize reward?

Markov Decision Process (MDP) – "controlled Markov chain": States $X = \{1,...,n\}$, actions $A = \{1,...,m\}$, transition probabilities $\mathrm{P}(x'|x,a) = \Pr[\text{next state } = x'|\text{Action } a \text{ in state } x)]$ and reward function $r(x,a,x')$.
Modes Finite horizon (T timesteps) or discounted rewards (∞ timesteps but discount factor $\gamma \in [0,1)$).

Value of policy deterministic (fixed) policy $\pi : X \to A$.

$$\begin{aligned} V_\pi(x) &= J(\pi|X_0 = x) = \mathbb{E}[\textstyle\sum_{t=0}^\infty \gamma^t r(X_t,\pi(X_t))|X_0 = x] \\ &= \textstyle\sum_{x'} \mathrm{P}(x'|x,\pi(x))[r(x,\pi(x),x') + \gamma V_\pi(x')]. \\ &= r(x,\pi(x)) + \gamma \textstyle\sum_{x'} \mathrm{P}(x'|x,\pi(x))V_\pi(x') \end{aligned}$$

Given π, compute V_π exactly by solving linear system!

Greedy policy

$$\begin{aligned} \pi_g(x) &= \text{argmax}_a \textstyle\sum_{x'} \mathrm{P}(x'|x,a)(r(x,a,x') + \gamma V_\pi(x')) \\ &= \text{argmax}_a r(x,a) + \gamma \textstyle\sum_{x'} \mathrm{P}(x'|x,\pi(x))V_\pi(x')). \end{aligned}$$

Bellmann Eq. Policy opt. $\iff$ greedy w.r.t. its induced value function.
$V^*(x) = \max_a[r(x,a) + \gamma \sum_{x'} \mathrm{P}(x'|x,a)V^*(x')]$.

Policy iteration Start with random (or smartly chosen) policy π. Until convergence: State value function $V_\pi(x) \forall x$, solve linear system. New policy is greedy policy $\pi \leftarrow \pi_G$ w.r.t. V_π.
Converged when $\pi = \pi_G$. Guaranteed to monotonically improve, thus converging to an optimal policy in poly. steps. Iteration: $O(n^3)$-time.

Value iteration Initialize $V_0(x) = \max_a r(x,a)$. In time step t until convergence:

$$Q^t(x,a) = r(x,a) + \gamma \sum_{x'} \mathrm{P}(x'|x,a)V_{t-1}(x'), \forall x,a$$

$$V_t(x) = \max_a Q^t(x,a), \forall x$$

Stop if $\max_x |V_t(x) - V_{t-1}(x)| < \varepsilon$ else loop with greedy policy w.r.t. V_t.
Converges to ε-optimal policy in polynomial steps. Iteration: $O(n \cdot m \cdot a)$-time. Not monotonically increasing.

Partially Observable MDP (POMDP) "controlled HMM"
Key idea: Interpret POMDP as an MDP with enlarged state space: New states correspond to beliefs $P(X_t|y_{1:t})$ in the original POMDP

4 Learning BN

Learn from i.i.d. data: 1.) Learning structure (conditional independencies) 2.) Learning parameters (CPDs)

4.1 Parameter learning

$P(X_1,...,X_N) = \prod_{i=1}^n P(X_i|Pa_i,\theta_{i|\ Pa_i})$
Given: BN structure G & Data set D of complete observations For each variable X_i estimate: $\hat{\theta}_{X_i|\ Pa_i} = \frac{Count(X_i,Pa_i)}{Count(Pa_i)}$ (MLE)
We can also use a Beta prior (A priori knowledge) or simple regularization.

4.2 Structure learning

Score based structure learning: scoring function S(G;D). Quantifies, for each structure G the fit to the data D.
$G^* = \text{argmax}_G S(G;D)$; MLE: $S(G;D) = \max_\theta \log P(D|\theta,G)$
$\log P(D|\theta_{G,\text{ MLE for G}},G) = N\sum_{i=1}^n \hat{I}(X_i;Pa_i) + c$.
Problem: Optimal solution for MLE is always the fully connected graph.

Mutual Information (MI) $I(X_i;X_j) = \sum_{X_i,X_j} \mathrm{P}(X_i,X_j)\log\frac{\mathrm{P}(x_i,x_j)}{\mathrm{P}(x_i)\mathrm{P}(x_j)} \geq 0$

Empirical MI $\hat{\mathrm{P}}(X_i,X_j) = \frac{\#(X_i,X_j)}{N}$, $\hat{I}(X_i;X_j) = \sum_{x_i,x_j} \hat{\mathrm{P}}(x_i,x_j)\log\frac{\hat{\mathrm{P}}(x_i,x_j)}{\hat{\mathrm{P}}(x_i)\hat{\mathrm{P}}(x_j)}$

Entropy $H(X_i) = -\sum_{x_i} \mathrm{P}(x_i)\log\mathrm{P}(x_i) = \mathbb{E}_{x_i}[-\log\mathrm{P}(x_i)]$.

Properties of MI $I(X_i;X_j) = 0$ iff X_i,X_j independent. Symmetric. $I(X_A;X_B) = H(X_A) - H(X_A|X_B)$. $B \subseteq C \implies I(X_A;X_B) \leq I(X_A;X_C)$.

Bayesian Information Criterion (BIC) (Regularizing) $S_{BIC}(G) = \sum_{i=1}^n \hat{I}(X_i;Pa_i) - \frac{\log N}{2N}|G|$ where $|G|$ is # of parameters of G, n is # of variables, N is # of training examples.
"Haha this is now NP hard but finding optimal tree-shaped BN is possible"

Chow-Liu algorithm Given samples of $X_1,...,X_n$. Find BN with exactly one parent per variable. Gives opt. tree w.r.t. BIC.
- For each pair X_i,X_j of variables compute $\hat{P}(x_i,x_j)$
- Compute Mutual Information $\hat{I}(X_i,X_j)$
- Take graph K_n, weight edge $(X_i,X_j) = \hat{I}(X_i,X_j)$
- Find maximum spanning tree of graph $\to$ undirected tree
- Pick any variable as root and orient the edges away using BFS

5 Reinforcement Learning

"Learn mapping from (seq. of) actions to rewards"

5.1 Passive Reinforcement

Execute a set of trials in the environment using (fixed) policy π Reduction to a supervised problem. But does not exploit that values of states are not independent! (Bellman)

5.2 Active Reinforcement Learning

Not interested in fixed policy; need to decide action in every state. Fundamental Dilemma: Exploration-Exploitation.
- Always pick a random action - will eventually estimate all prob and rewards. May do extremely poorly.
- Always pick the best action according to current knowledge - quickly get some rewards but can get stuck in suboptimal action.

5.2.1 Model-based RL

Learn the MDP - optimize policy based on MDP.

Learning the MDP

Estimate transitions: $\hat{P}(X_{t+1}|X_t,A_t) = \frac{Count(X_{t+1},X_t,A_t)}{Count(X_t,A_t)}$

Estimate rewards: $\hat{r}(X = x,A = a) = \frac{\sum_{t:x_t=x,a_t=a} r_t}{Count(X=x,A=a)}$

ε_t **greedy** With probability ε_t: Pick random action; With probability $(1-\varepsilon_t)$: Pick best action

R_{max} **Algorithm** Init: $r(x,a) = R_{max}$. $P(x^*|x,a) = 1$ where x^* is a "fairy tale" state: $r(x^*,a) = r_{max} \forall a$ Choose optimal π according to r,P
Repeat: Execute Pi. $\forall (x,a) \in visited$. update $r(x,a)$. Estimate $P(x'|x,a)$.
After "enough" rewards, recompute π according to r,P.
Depends heavily on state space $O(|x|^3)$

5.2.2 Model-free RL

Estimate the value function directly.

Q-Learning $Q^*(x,a) = r(x,a) + \gamma \cdot \max_{a'}(Q^*(x',a'))$; γ is discount factor.
Algorithm Init Q matrix to zero (or R if *optimistic*).
- Select/Observe init state x
- Repeat until end state (restart after epoch):
- Select a according to policy (i.e. ε-greedy, or $\pi(x) = \text{argmax}_a Q(x,a)$).
- Observe new state x' and reward $r(x,a,x')$.
- $Q^{(t+1)}(x,a) \leftarrow (1-\alpha_t)Q^{(t)}(x,a) + \alpha_t(r(x,a,x') + \gamma \max_{a'} Q^{(t)}(x',a'))$
- $Q^{(t+1)}(x,a') \leftarrow Q^{(t)}(x,a') \forall a \neq a'$, remaining actions stay same.
- $Q^{(t+1)}(x'',a') \leftarrow Q^{(t)}(x'',a') \forall x'' \neq x$, remaining states stay same.
- $x \leftarrow x'$

Depends on action space $O(|a|)$ (matrix size), i.e. iteration time is in $O(|a|)$.

Monte Carlo Tree Search (MCTS) Action selection planning Simulate to terminal state observe reward and then propagate back result. Tree policies: epsilon greedy, random. Stop after sufficient runs or time budget.

Gradient Based Optimzation Objective Function: Mean Squared Value Error Parameterize V_π & use SDG: $\theta_{t+1} = \theta_t - \frac{1}{2} \cdot \alpha \nabla (V_\pi(s_t) - \hat{V}(s_t;\theta))^2$ Can use Monte Carlo Estimate as surrogate for $V_\pi(s_t)$

Policy Gradient Method Learning a parameterized policy without the detour of learning a value function: $\pi(b) = \pi(b;\theta)$ & again GD