1 Bayesian Regression

$w \sim N(0, \sigma_p^2 I)$, $\epsilon \sim N(0, \sigma_n^2 I)$, $y = Xw + \epsilon$

$y|w \sim N(Xw, \sigma_n^2 I)$

$w|y \sim N((X^T X + \lambda I)^{-1} X^T y, (X^T X + \lambda I)^{-1} \sigma_n^2)$

2 Kalman Filter

$\begin{cases} X_{t+1} = FX_t + \epsilon_t & \epsilon_t \sim N(0, \Sigma_x) \\ Y_t = HX_t + \eta_t & \eta_t \sim N(0, \Sigma_y) \end{cases} X_1 \sim N(\mu_p, \Sigma_p)$

Then if X_0 is Gaussian then $X_t|Y_{1:t} \sim N(\mu_t, \sigma_t)$:

$\mu_{t+1} = F\mu_t + K_{t+1}(y_{t+1} - HF\mu_t)$

$\Sigma_{t+1} = (I - K_{t+1}H)(F\Sigma_t F^T + \Sigma_x)$

$K_{t+1} = (F\Sigma_t F^T + \Sigma_x)H^T (H(F\Sigma_t F^T + \Sigma_x)H^T + \Sigma_y)^{-1}$

3 Gaussian Processes

$f \sim GP(\mu, k) \Rightarrow \forall \{x_1, \ldots, x_n\} \, \forall n < \infty$

$[f(x_1) \ldots f(x_n)] \sim N([\mu(x_1) \ldots \mu(x_n)], K)$

where $K_{ij} = k(x_i, x_j)$

3.1 Gaussian Process Regression

$f \sim GP(\mu, k)$ then: $f|y_{1:n}, x_{1:n} \sim GP(\tilde{\mu}, \tilde{k})$

$\tilde{\mu}(x) = \mu(x) + K_{A,x}^T (K_{AA} + \epsilon I_n)^{-1} (y_A - \mu_A)$

$\tilde{k}(x, x') = k(x, x') - K_{A,x}^T (K_{AA} + \epsilon I_n)^{-1} K_{A,x'}$

Where: $K_{A,x} = [k(x_1, x) \ldots k(x_n, x)]^T$

$[K_{AA}]_{ij} = k(x_i, x_j)$ and $\mu_A = [\mu(x_1 \ldots x_n)]^T$

3.2 Kernels

$k(x, y)$ is a kernel if it's symmetric semidefinite positive:

$\forall \{x_1, \ldots, x_n\}$ then for the Gram Matrix $[K]_{ij} = k(x_i, x_j)$ holds $c^T K c \geq 0 \forall c$

Some Kernels: (h is the bandwidth hyperp.)

Gaussian (rbf): $k(x, y) = \exp(-\frac{\|x-y\|^2}{h^2})$

Exponential: $k(x, y) = \exp(-\frac{\|x-y\|}{h})$

Linear kernel: $k(x, y) = x^T y$ (here $K_{AA} = XX^T$)

3.3 Optimization of Kernel Parameters

Given a dataset A, a kernel function $k(x, y; \theta)$.

$y \sim N(0, K_y(\theta))$ where $K_y(\theta) = K_{AA}(\theta) + \sigma_n^2 I$

$\hat{\theta} = \arg\max_\theta \log p(y|X; \theta)$

In GP: $\hat{\theta} = \arg\min_\theta y^T K_y^{-1}(\theta) y + \log |K_y(\theta)|$

We can from here $\nabla \downarrow$:

$\nabla_\theta \log p(y|X; \theta) = \frac{1}{2} tr\left(\left(\alpha\alpha^T - K^{-1}\right) \frac{\partial K}{\partial \theta}\right)$, $\alpha = K^{-1} y$

Or we could also be baysian about θ

3.4 Aproximation Techniques

Local method: $k(x_1, x_2) = 0$ if $\|x_1 - x_2\| \gg 1$

Random Fourier Features: if $k(x, y) = \kappa(x - y)$ $p(w) = \mathcal{F}\{\kappa(\cdot), w\}$. Then $p(w)$ can be normalized to be a density.

$\kappa(x - y) = \mathbb{E}_{p(w)}\left[\exp\left\{iw^T(x - y)\right\}\right]$ antitransform

$\kappa(x - y) = \mathbb{E}_{b \sim \mathcal{U}([0, 2\pi]), w \sim p(w)}\left[z_{w,b}(x) z_{w,b}(y)\right]$

where $z_{w,b}(x) = \sqrt{2} cos(w^T x + b)$. I can MC extract features z. If # features is $\ll$ n then this is faster ($X^T X$ vs XX^T)

Inducing points: We a vector of inducing variables u

$f_A|_u \sim N(K_{Au} K_u u^{-1} u, K_{AA} - K_{Au} K_u u^{-1} K_{uA})$

$f_*|_u \sim N(K_{*u} K_u u^{-1} u, K_{**} - K_{*u} K_u u^{-1} K_{u*})$

Subset of Regressors (SoR): $\blacksquare \to 0$

FITC: $\blacksquare \to$ its diagonal

4 Review of useful concepts and Introduction

4.1 Multivariate Gaussian

$f(x) = \frac{1}{2\pi\sqrt{|\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}$

Suppose we have a Gaussian random vector $X_V \sim N(\mu_V, \Sigma_{VV})$.

Suppose we take two disjoint subsets of V: $A = i_1, \ldots, i_k$ and $B = j_1, \ldots, j_m$.

Then, the conditional distribution:

$P(X_A|X_B = x_B) = N(\mu_{A|B}, \Sigma_{A|B})$ is Gaussian:

$\mu_{A|B} = \mu_A + \Sigma_{AB} \Sigma_{BB}^{-1} (x_B - \mu_B)$

$\Sigma_{A|B} = \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA}$

4.2 Convex / Jensen's inequality

g(x) is convex $\Leftrightarrow x_1, x_2 \in \mathbb{R}, \lambda \in [0, 1] : g''(x) > 0$

$g(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda g(x_1) + (1 - \lambda)g(x_2)$

$\varphi(\mathrm{E}[X]) \leq \mathrm{E}[\varphi(X)]$

4.3 Kullback-Leiber divergence

$KL(p\|q) = \mathbb{E}_p\left[\log \frac{p(x)}{q(x)}\right]$

if $p_0 \sim \mathcal{N}(\mu_0, \Sigma_0)$, $p_1 \sim \mathcal{N}(\mu_1, \Sigma_1) \Rightarrow KL(p_0\|p_1)$

$= \frac{1}{2}\left(tr\left(\Sigma_1^{-1}\Sigma_0\right) + (\mu_1 - \mu_0)^T \Sigma_1^{-1} (\mu_1 - \mu_0) - k + \log \frac{|\Sigma_1|}{|\Sigma_0|}\right)$

$\hat{q} = \arg\min_q KL(p\|q) \Rightarrow$ overconservative

$\hat{q} = \arg\min_q KL(q\|p) \Rightarrow$ overconfident

4.4 Review Probability

Probability space (Ω, F, P): Set of atomic events Ω. Set of all non-atomic events (σ-Algebra): $F \in 2^\Omega$. Probability measure: $P : F \to [0, 1]$

Bayes' rule: $P(B|A) = P(A, B)/P(A) = P(A|B)P(B)/P(A)$, where $P(A) = \sum_b P(A|B)P(A)$

Union: $P(A \cup B) = P(A) + P(B) - P(A \cap B)$

Rules for joint distributions:

Sum rule (Marginalization):

$P(X_{1:i-1}, X_{i+1:n}) = \sum_{x_i} P(X_{1:i-1}, X_i = x_i, X_{i+1:n})$

Product rule (Chain rule):

$P(X_{1:n}) = P(x_1)P(X_2|X_1)\ldots P(X_n|X_{1:n-1})$

Conditional Independence:

$X \perp Y|Z$ iff $P(X, Y|Z) = P(X|Z)P(Y|Z)$

If $P(Y|Z) > 0 \Rightarrow P(X|Z, Y) = P(X|Z)$

Properties of Conditional Independence:

Symmetry: $X \perp Y \mid Z \Rightarrow Y \perp X \mid Z$

Decomposition: $X \perp (Y, W) \mid Z \Rightarrow X \perp Y \mid Z$

Contraction: $(X \perp Y \mid Z) \wedge (X \perp W \mid Y, Z) \Rightarrow X \perp Y, W \mid Z$

Weak union: $X \perp Y, W \mid Z \Rightarrow X \perp Y \mid Z, W$

Intersection: $(X \perp Y \mid W, Z) \wedge (X \perp W \mid Y, Z) \Rightarrow X \perp Y, W \mid Z$

5 Bayesian Networks

5.1 Basic concepts

A Bayesian network (G, P) consists of:

- A BN structure G (directed, acyclic graph)
- A set of conditional probability distributions
- (G, P) defines the joint distribution: $P(X_1, \ldots, X_n) = \prod_i P(X_i|Pa_{X_i})$

BNs with 3 nodes:

5.2 Active trails and d-separation

An undirected path in a BN structure G is called active trail for observed variables $O \in X_1, \ldots, X_n$ of for every consecutive triple of variables X, Y, Z on the path:

- **indirect causal effect**: $X \to Y \to Z$ and Y unobserved
- **indirect evidential effect**: $X \leftarrow Y \leftarrow Z$ and Y unobserved
- **common cause**: $X \leftarrow Y \to Z$ and Y unobserved.
- **common effect**: $X \to Y \leftarrow Z$ and Y or any of Y's descendants is observed.

Any variables X_i and X_j for which there is no active trail for observations O are called d-separated by O.

Theorem: $d - sep(X_i; X_j|O)) \quad \Rightarrow X \perp Y|Z$

Converse does not hold in general!

6 Exact inference (tree-structured BN)

6.1 Variable elimination

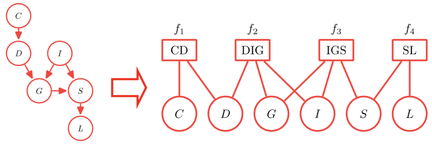
- Given a BN and query $P(X|E = e)$
- Choose an ordering of $X_1, \ldots, X_n$ **Eliminate variables from the outside in!**
- Set up initial factors: $f_i = P(X_i|Pa_i)$
- For $i = 1 : n, X_i \notin X, E$
  - Collect and multiply all factors f that include X_i
  - Generate new factor by marginalizing out X_i: $g_{X_i} = \sum_{x_i} \prod_j f_j$
  - Add g to set of factors
- Renormalize $P(x, e)$ to get $P(x|e)$

Variable elimination for polytrees:

- Pick a root, (avoiding X and E)
- Orient edges towards root
- Eliminate variables according to topological order

6.2 Avoiding recomputation: factor graphs

FG for a BN is a bipartite graph consisting of variables (circles) and factors (rectangles). **It is not a unique representation.**



6.2.1 Sum-product/Belief Propagation (BP) Algorithm:

- Initialize all messages as uniform distribution
- Until converged to:
  - Pick a root in the factor graph and reorient the edges towards this root.
  - Update messages according to this ordering. Do passes from leaves to root and from root to leaves.
- If a leaf node is a variable node: $\mu_{x \to f}(x) = 1$ - If a leaf node is a factor node: $\mu_{f \to x}(x) = f(x)$ - Messages from node v to factor u:

$\mu_{v \to u}(x_v) = \prod_{u' \in N(v) \setminus \{u\}} \mu_{u' \to v(x_v)}$

- Messages from factor u to node v:

$\mu_{u \to v}(x_v) = \sum_{x_u \sim x_v} f_u(x_u) \prod_{v' \in N(u) \setminus \{v\}} \mu_{v' \to u(x'_v)}$

  - Break once all messages change by $\leq \epsilon$

Hope: after convergence, we have:

$P(X_v = x_v) = \frac{1}{Z} \prod_{u \in N(v)} \mu_{u \to v}(x_v)$

$P(\overrightarrow{X_u} = \overrightarrow{x_u}) = \frac{1}{Z} f_u(\overrightarrow{x_u}) \prod_{v \in N(u)} \mu_{v \to u}(x_v)$

If we have a polytree Bayesian network:

- Choose one node as root
- Send messages from leaves to root and from root to leaves

7 Approximate inference

7.1 Laplace Approximation

$\hat{\theta} = \arg\max_\theta p(\theta|y)$

$\Lambda = -\nabla_\theta \nabla_\theta \log p(\theta|y)|_{\theta = \hat{\theta}}$

$p(\theta|y) \simeq q(\theta) = N(\hat{\theta}, \Lambda^{-1})$

7.2 Variationa Inverence

$\hat{q} = \arg\min_{q \in Q} KL(q\|p(\cdot|y))$

$\hat{q} = \arg\max_{q \in Q} \mathbb{E}_{\theta \sim q}[\log p(y|\theta)] - KL(q\|p(\cdot))$

$ELBO \doteq \mathbb{E}_{\theta \sim q}[\log p(y|\theta)] - KL(q\|p(\cdot)) \leq \log p(y)$

7.3 Variable elimination for MPE (most probable explanation):

With loopy graphs, BP is often **overconfident/oscillates**.

- Given BN and evidence E=e
- Choose an ordering of $X_1, \ldots x_n$
- Set up initial factors $f_i = P(X_i|Pa_i)$
- For $i = 1 : n, X_i \notin E$:
  - Collect and multiply all factors f_j that include X_i
  - Generate new factor by maximizing out X_i: $g_i = \max_{w = x_i} \prod_j f_j$
  - Add g to set of factors
- For $i = n-1 : 1, X_i \notin E$: $\hat{x}_i = \operatorname{argmax}_{x_i} g_i(x_i, \hat{x}_{i+1:n})$

Retrieving MAP from Max-Product (MAP = MPE for a subset of RVs):
- 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).

7.4 Sampling based inference: compute marginals as expectations

Hoeffding's inequality: Suppose f is bounded in $[0, C]$. Then: $P(|E_P[f(X)] - \frac{1}{N}\sum_{i=1}^N f(x_i)| \geq \epsilon) \leq 2exp\left(\frac{-2N\epsilon^2}{C^2}\right)$

Monte Carlo Sampling from a BN:
- Sort variables in topological ordering X_1, X_n
- For $i = 1$ to n, sample: $x_i \sim P(X_1 = x_1, ..., X_{i-1} = x_{i-1})$

Rejection Sampling:
- Collect samples over all variables: $\hat{P}(X_A = x + A | X_B = x_B) = \frac{Count(x_A, x_B)}{Count(x_B)}$
- Throw away samples that disagree with x_B
- Count fraction of x_a on remaining samples

7.4.1 Directly sampling from the posterior: MCMC

Markov Chain:: A (stationary) MC is a sequence of RVs $X_1, ..., X_N$, with prior $P(X_1)$ and transition probabilities $P(X_{t+1}|X_t)$ independent of t.

Markov assumpt.: $X_{1:t-1} \perp X_{t+1:T} | X_t, \forall t > 1$

Stationarity assumption: $P(X_{t+1} = x | X_t = x') = P(X_t = x | X_{t-1} = x'), \forall t > 1$

If ergodic (= there exists a finite t such that every state can be reached in exactly t steps), then: it has a unique and positive stationary distribution $\pi(X) > 0$, such for all x: $\lim_{N \to \infty} P(X_N = x) = \pi(x)$ and $\pi(X) \perp P(X_1)$.

If MC satisfies the **detailed balance equation** (for unnormalized distribution Q, for all x, x': $Q(x)P(x'|x) = Q(x')P(x|x')$), then the MC has stationarity distribution $\pi(X) = 1/Z Q(X)$.

Designing Markov Chains:
- Proposal distribution $R(X'|X)$: given $X_t = x$, sample "proposal"$x' \sim R(X'|X = x)$
- Acceptance distribution
  - Suppose $X_t = x$
  - With probability $\alpha = min\left\{1, \frac{Q(x')R(x|x')}{Q(x)R(x'|x)}\right\}$ set: $X_{t+1} = x'$
  - With probability $1 - \alpha$, set $X_{t+1} = x$

MCMC for graphical models: Gibbs sampling (Random Vs Practical variant):
- Start with initial assignment x to all variables
- Fix observed variables $X_B = x_B$
- For $t = 1$ to ∞, do:
  - Pick a variable i uniformly at random from $\{1, ..., n\} \setminus B$ / Set ordering, and then, for each X_i (except those in B)
  - Set v_i = values of all x except x_i
  - Sample x_i from $P(X_i|v_i)$

8 Dynamical models (include time)

8.1 Examples with one variable per time step

$X_1, ..., X_T$ (unobserved) hidden states
$Y_1, ..., Y_T$ (noisy) observations

HMMs (polytrees: can use belief propagation): X_i categorical, Y_i categorical (or arbitrary)

Kalman filters: X_i, Y_i Gaussian distributions
- $P(X_1)$: prior belief about location at time i
- $P(X_{t+1}|X_t)$: **'Motion model'** (how do I expect my target to move in the environment?): $X_{t+1} = FX + \epsilon_t$ where $\epsilon_t \sim N(0, \Sigma_x)$
- $P(Y_t|X_t)$: **'Sensor model'** (what do I observe if target is at location X_t?) $Y_t = HX_t + \eta_t$ where $\eta_t \sim N(0, \Sigma_y)$

8.2 Inference tasks

Filtering: $P(X_t|y_{1,...,t})$ Is it raining today?

Prediction: $P(X_{t+\tau}|Y_{1:t})$ Rain 5 days from now? Example for one step: $P(X_{t+1}|Y_{1:t}) = \sum_x P(X_{t+1}, X_t = x_t|Y_{1:t}) = \sum_x P(X_{t+1}|X_t = x_t)P(X_t|Y_{1:t})$ (with KFs, you need **integrals**!)

Smoothing: $P(X_\tau|y_{1:t})$ with $\tau < t$ Did it rain last week? [Can use sum-product (aka forward-backward).]

MPE: $\underset{x_{1:T}}{argmax} P(x_{1:T}|y_{1:T})$ Can use max product (aka Viterbi algorithm).

Bayesian filtering: Start with $P(X_1)$:
At time t, assume we have $P(X_t|y_{1:t-1})$
Conditioning: $P(X_t|y_{1:t}) = \frac{P(X_t|y_{1:t-1})P(y_t|X_t)}{\sum_{x_t} P(X_t|y_{1:t-1})P(y_t|X_t)}$
Prediction ($O(n^2)$ vs $O(n)$ in conditioning): $P(X_{t+1}|y_{1:t}) = \sum_x P(X_{t+1}|X_t)P(X_t|y_{1:t})$

Since HMM is a polytree, smoothing/MPE can be computed by VE/BP. Kalman filtering: Bayesian filtering for continuous problems. RV corrupted by Gaussian distributions with zero mean. **Bayesian filtering is basically the same, except that sums turn to integrals. General Kalman update**
- Transition model: $P(x_{t+1}|x_t) = N(x_{t+1}; Fx_t, \Sigma_x)$
- Sensor model: $P(y_t|x_t) = N(y_t; Hx_t, \Sigma_y)$
- Kalman update:
$\mu_{t+1} = F\mu_t + K_{t+1}(y_{t+1} - HF\mu_t)$
$\Sigma_{t+1} = (I - K_{t+1})(F\Sigma_t F^T + \Sigma_x)$
- Kalman gain: $K_{t+1} = (F\Sigma_t F^T + \Sigma_x)H^T(H(F\Sigma_t F^T + \Sigma_x)H^T + \Sigma_y)^{-1}$

8.3 Examples with > 1 variable per time step

Dynamic Bayesian Networks: a BN at every time step
These models typically have many loops. Exact inference is usually intractable.

8.4 Approx. infer. for filtering (DBNs and non-linear Kalman filters): Particle filtering

Suppose: $P(X_t|y_{1:t}) \approx \frac{1}{N}\sum_{i=1}^N \delta_{x_{i,t}}$, where δ is the indicator function. **Prediction**: Propagate each particle: $x_i' \sim P(X_{t+1}|x_{i,t})$

Conditioning:
- weight particles $w_i = \frac{1}{Z}P(y_{t+1}|x_i')$
- resample N particles $x_{i,t+1} \sim \frac{1}{Z}\sum_{i=1}^N w_i \delta_{x_i'}$

Conclusion we came to: $Z = \sum_{i=1}^N w_i \delta_{x_i}$

9 Probabilistic Planning

9.1 Markov Decision Processes

An MDP is specified by a quintuple: $(X, A, r, P(x'|x, a), \gamma)$, where X are states, A are actions, $r(x, a)$ is a reward function and transition probabilities:
$P(x'|x, a) = \text{Prob(Next state} = x'|\text{Action } a)$

Objective: find a stationary policy $\pi : S \to A$ that maximizes the sum of cumulative rewards.

Value of a state given a policy : sum of cumulative rewards, given that the initial state is this state $\to$ **Bellman equation:**

$V^\pi(s) = \mathbb{E}\left[\sum_{t=0}^\infty \gamma^t r(s_t, \pi(s_t), s_{t+1})|s_0 = s\right]$
$= \sum_{s' \in S} P(s'|s, \pi(s))\left[r(s, \pi(s), s') + \gamma V^\pi(s')\right]$
$= r(s, \pi(s)) + \gamma \sum_{s' \in S} P(s'|s, \pi(s))V^\pi(s')$

Theorem (Bellman): a policy is optimal iff it is greedy w.r.t. its induced value function!
$V^*(x) = max_a[r(x, a) + \gamma \sum_{x'} P(x'|x, a)V^*(x')]$
Bellman equation mais geral:
$V^*(x) = max_a[\sum_{x'} P(x'|x, a)(r(a, x, x') + \gamma V^*(x'))]$
Optimal policy:
$\pi^*(s) = \underset{a \in A}{argmax}[r(x, a) + \gamma \sum_{x'} P(x'|x, a)V^*(x')]$

9.2 Policy iteration (Cost $O(S^3 + SA\Delta)$)

Start with an arbitrary (e.g. random) policy π. Until converged, do:
- Compute value function $V^\pi(x)$
- Compute greedy policy π_G w.r.t. V^π
- Set $\pi \leftarrow \pi_G$

Guaranteed to monotonically improve and to converge to an **optimal** policy π^* in $O(n^2 m/(1 - \gamma))$ iterations (converges in polynomial number of iterations)!

9.3 Value iteration (Cost $O(SA\Delta)$)

Initialize $V_0(x) = max_a r(x, a)$
For $t = 1$ to ∞:
- For each (x, a), let: $Q_t(x, a) = r(x, a) + \gamma \sum_{x'} P(x'|x, a)V_{t-1}(x')$
- For each x, let $V_t(x) = \max_a Q_t(x, a)$
- Break if $\|V_t - V_{t-1}\|_\infty = \max_x |V_t(x) - V_{t-1}(x)| \leq \epsilon$

Then choose greedy policy w.r.t V_t.
Guaranteed to converge to ϵ-optimal policy (finds approximate solution in polynomial number of iterations)!

9.4 POMDP = Belief-state MDP

States = beliefs over states for original POMDP $B = \Delta(1, ..., n) = \{b : 1, ..., n \to [0, 1], \sum_x b(x) = 1\}$
Actions: same as original MDP

Transition model:
- Stochastic observation: $P(Y_t|b_t) = \sum_{x=1}^n P(Y_t|X_t = x)b_t(x)$
- State update (Bayesian filtering!), given b_t, y_t, a_t: $b_{t+1}(x') = \frac{1}{Z}\sum_x b_t(x)P(y_t|x)P(X_{t+1} = x'|X_t = x, a_t)$

Reward function: $r(b_t, a_t) = \sum_x b_t(x)r(x, a_t)$

9.5 Example of approx. solution to POMDPs: Policy gradients

- Assume parameterized policy: $\pi(b) = \pi(b; \theta)$
- For each parameter θ the policy induces a Markov chain
- Can compute expected reward $J(\theta)$ by sampling.
- Find optimal parameters through search (gradient ascent): $\theta^* = \underset{\theta}{argmax} \quad J(\theta)$

10 Learning models from training data

10.1 Learning from i.i.d data

Algorithm for Bayes Net MLE:
Given BN of structure G and dataset D of complete observations
For each X_i estimate: $\hat{\theta}_{X_i|Pa_i} = \frac{Count(X_i, Pa_i)}{Count(Pa_i)}$
Pseudo-counts for lime and cherry flavor: $\theta_{F=c} \frac{Count(F=c) + \alpha_c}{N + \alpha_c + \alpha_l}$

10.1.1 Score based structure learning

Define scoring function $S(G; D)$ and search over BN structure G: $G^* = \underset{G}{argmax} S(G; D)$

Examples of scores:
MLE Score:
$logP(D|\theta_G, G) = N\sum_{i=1}^n \hat{I}(X_i; Pa_i) + const.$
Where mutual information ($I(X_i, X_j) \geq 0$) is:
$I(X_i, X_j) = \sum_{x_i, x_j} P(x_i, x_j) log \frac{P(x_i, x_j)}{P(x_i)P(x_j)}$
Empirical mutual information:
$\hat{P}(x_i, x_j) = \frac{Count(x_i, x_j)}{N}$
$\hat{I}(X_i, X_j) = \sum_{x_i, x_j} \hat{P}(x_i, x_j) log \frac{\hat{P}(x_i, x_j)}{\hat{P}(x_i)\hat{P}(x_j)}$

Regularizing a Bayes Net:
$S_{BIC}(G) = \sum_{i=1}^n \hat{I}(X_i; Pa_i) - \frac{logN}{2N}|G|$
where G is the number of parameters, n the

number of variables and N the number of training examples.

Chow-Liu algorithm:

- For each pair X_i, X_j of variables, compute: $\hat{P}(x_i, x_j) = \frac{Count(x_i,x_j)}{N}$
- Compute mutual information
- Define complete graph with weight of edge (X_i, X_j) given by the mutual information
- Find max spanning tree $\rightarrow$ undirected tree
- Pick any variable as root and orient the edges away using breadth-first search.

11 Reinforcement Learning

11.1 Model-based RL

11.1.1 ϵ greedy

With probability ϵ, pick random action. With prob $(1-\epsilon)$, pick best action. If sequence ϵ satisfies Robbins Monro criteria $\rightarrow$ convergence to optimal policy with prob 1.

11.1.2 R_{max} algorithm

Input: starting x_0, discount factor γ.
Initially: add fairy tale state x^* to MDP
- Set $r(x,a) = R_{max}$ for all states x and actions a
- Set $P(x^*|x,a) = 1$ for all states x and actions a
- Choose the optimal policy for r and P

Repeat: 1. Execute policy π and, for each visited state/action pair, update $r(x,a)$
2. Estimate transition probabilities $P(x^{'}|x,a)$
3. If observed 'enough' transitions/rewards, recompute policy π, according to current model P and r.

Ënough"? See Hoeffding's inequality. To reduce error ϵ, need more samples N.

Theorem: With probability $1-\delta$, R_{max} will reach an ϵ-optimal policy in a number of steps that is polynomial in $|X|, |A|, T, 1/\epsilon$ and $log(1/\delta)$. Memory $O(|X^2||A|)$.

11.2 Model-free RL: estimate V*(x) directly

11.2.1 Q-learning

$Q(x,a) \leftarrow (1-\alpha_t)Q(x,a) + \alpha_t(r + \gamma \max_{a'} Q(x',a'))$

Theorem: If learning rate α_t satisfies: $\sum_t \alpha_t = \infty$ and $\sum_t \alpha_t^2 < \infty$ (Robbins-Monro), and actions are chosen at random, then Q learning converges to optimal Q^* with probability 1.

Optimistic Q learning:

Initialize: $Q(x,a) = \frac{R_{max}}{1-\gamma} \prod_{t=1}^{T_{init}} (1-\alpha_t)^{-1}$

Same convergence time as with R_{max}. Memory $O(|X||A|)$. Comp: $O(|A|)$.

Parametric Q-function approximation: $Q(x,a;\theta) = \theta^T \phi(x,a)$ to scale to large state spaces. (You can use Deep NN here!)

SGD for ANNs: initialize weights. For t = 1,2..., pick a data point (x,y) uniformly at random. Take step in negative gradient direction. (In practise, mini-batches).

Deep Q Networks: use CNN to approx Q function. $L(\theta) = \sum_{(x,a,r,x') \in D} (r + \gamma \underset{a'}{max} Q(x',a';\theta^{old}) - Q(x,a;\theta))^2$ **Double DQN:** current network for evaluating argmax (too optimistic, and you remove θ^{old} and put θ).

11.3 Gaussian processes

A GP is an (infinite) set of random variables (RV), indexed by some set X, i.e., for each x in X, there is a RV Y_x where there exists functions $\mu : X \rightarrow \mathbb{R}$ and $K : X \times X \rightarrow \mathbb{R}$ such that for all: $A \in X, \quad A = x_1, ... x_k$, it holds that $Y_A = [Y_{x_1}, ..., Y_{x_k}] \sim N(\mu_a, \Sigma_{AA})$, where: $\Sigma_{AA} =$ matrix with all combinations of $K(x_i, x_j)$.

K is called kernel (covariance) function (must be symmetric and pd) and μ is called mean function. **Making prediction with GPs:** Suppose $P(f) = GP(f;\mu,K)$ and we observe $y_i = f(\overrightarrow{x_i}) + \epsilon_i$, $A = \{\overrightarrow{x_1} : \overrightarrow{x_k}\}$ $P(f(x)|\overrightarrow{x_1} : \overrightarrow{x_k}, y_{1:k}) = GP(f;\mu',K')$. In particular, $P(f(x)|\overrightarrow{x_1} : \overrightarrow{x_k}, y_{1:k}) = N()f(x);\mu_{x|A},\sigma^2_{x|a}$, where $\mu_{x|a} = \mu(\overrightarrow{x}) + \Sigma_{x,A}(\Sigma_{AA} + \sigma^2 I)^{-1}\Sigma^T_{x,A}(\overrightarrow{y_A} - \mu_A)$ and $\sigma^2_{x|a} = K(\overrightarrow{x},\overrightarrow{x}) - \Sigma_{x,A}(\Sigma_{AA} + \sigma^2 I)^{-1}\Sigma^T_{x,A}$. **Closed form formulas for prediction!**