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

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

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

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

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

3.2 Kernels

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

$\forall \{x_1, \dots, x_n\}$ 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 $\nabla \downarrow$:

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

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): ■ $\to 0$

FITC: ■ $\to$ 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 $\begin{bmatrix} X_A \\ X_B \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix}, \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}\right) \Rightarrow X_A|X_B = x_B \sim \mathcal{N}\left(\mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(x_B - \mu_B), \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}\right)$

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 Information Theory elements:

Entropy: $H(X) \doteq -\mathbb{E}_{x \sim p_X}[\log p_X(x)]$

$H(X|Y) \doteq -\mathbb{E}_{(x,y) \sim p_{(X,Y)}}\left[\log p_{Y|X}(y|x)\right]$

if $X \sim \mathcal{N}(\mu, \Sigma) \Rightarrow H(X) = \frac{1}{2} \log\left[(2\pi e)^d \det(\Sigma)\right]$

Chain Rule: $H(X, Y) = H(Y|X) + H(X)$

Mutual Info: $I(X, Y) \doteq KL(p_{(X,Y)} \| p_X p_Y)$

$I(X, Y) = H(X) - H(X|Y)$

if $X \sim \mathcal{N}(\mu, \Sigma)$, $Y = X + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$:

then $I(X, Y) = \frac{1}{2} \log\left[\det(I + \frac{1}{\sigma^2}\Sigma)\right]$

4.4 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

5 Approximate inference

5.1 Laplace Approximation

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

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

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

5.2 Variationa Inverence

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

$\hat{q} = ELBO$ Evidence Lower Bound

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

5.3 Markov Chain Monte Carlo

Idea: All we need is sampling from postirior

Ergodic Markov Chain:

$\exists t$ s.t. $\mathbb{P}(i \to j$ in t steps$) > 0 \ \forall i, j \Rightarrow$

$\exists! \pi = \lim_{N \to \infty} \mathbb{P}(X_n = x)$ Limit distribution

Ergodic Theorem: if $(X_i)_{i \in \mathbb{N}}$ is ergodic:

$\lim_{N \to \infty} \frac{1}{n} \sum_{i=1}^N f(X_i) = \mathbb{E}_{x \sim \pi}[f(x)]$

Detailed Blanced Equation:

$P(x|x')$ is the transition model of a MC:

if $R(x)P(x'|x) = R(x')P(x|x')$ then R is the limit distribution of the MC

Metropolis Hastings Algo: Sample from a MC which has $P(x) = \frac{Q(x)}{Z}$ as limit dist.

Result: $\{X_i\}_{i \in \mathbb{N}}$ sampled from the MC
init: $R(x|x')$
/* Good R choice → fast convergence */
init: $X_0 = x_0$
for $t \leftarrow 1, 2, \dots$ **do**
  $x' \sim R(\cdot, x_{t-1})$
  $\alpha = \min\left\{1; \frac{Q(x')R(x_{t-1}|x')}{Q(x_{t-1})R(x'|x_{t-1})}\right\}$
  with *probability* α **do**
    $X_t = x'$;
  otherwise $X_t = x_{t-1}$;

Metropolis Adj. Langevin Algo (MALA):

Energy function: $P(x) = \frac{Q(x)}{Z} = \frac{1}{Z}\exp(-f(x))$

We chose: $R(x|x') = \mathcal{N}(x' - \tau\nabla f(x), 2\tau I)$

Stoch. Grad. Langevin Dynamics (SGLD):

We use SGD to Approximate ∇f. Converges also without acceptance step

Hamilton MC: SGD performance improoved by adding momentum (consider last step ∇f)

Gibbs sampling: Practical when $X \in \mathbb{R}^n$

Used when $P(X_{1:n})$ is hard but $P(X_i|X_{-i})$ is easy.

init: $x_0 \in \mathbb{R}^n$; $(x_0^{(B)} = x^{(B)})$ B is our data
for $t = 1, 2, \dots$ **do**
  $x_t = x_{t-1}$
  with $i \sim \mathcal{U}(\{1 : n\} \setminus B)*$ **do**
    $x_{t-1}^{(i)} \sim P(x^{(i)}|x^{(-i)})$

$*$ if we do it $\forall i \notin B$ no DBE but more practical

5.4 Variable elimination for MPE (most probable explanation):

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

6 Bayesian Neural Nets

Likelihood: $p(y|x; \theta) = \mathcal{N}(f_1(x, \theta), \exp(f_2(x, \theta)))$

Prior: $p(\theta) = \mathcal{N}(0, \sigma_p^2)$

$\theta_{MAP} = \arg\max \log(p(y, \theta))$

6.1 Variation inference:

Usually we use $Q =$ Set of Gaussians

$\hat{q} = \arg\max ELBO$ Reparameterization trick

q approx. the posterior but how to predict?

$p(y^*|x^*, \mathcal{D}) \simeq \frac{1}{m}\sum_{j=1}^m p(y^*|x^*, \theta^{(i)})$, $\theta \sim \hat{q}(\theta)$

Gaussian Mixture distribution: $\mathbb{V}(y^*|x^*, \mathcal{D}) \simeq$

$\simeq \frac{1}{m}\sum_{j=1}^m \sigma^2(x^*, \theta^{(i)}) + \frac{1}{m}\sum_{j=1}^m \left(\mu(x^*, \theta^{(j)} - \overline{\mu}(x^*))\right)$

■ $\to$Aletoric, ■ $\to$Epistemic

Dropouts Regularization: Random ignore nodes in SGD iteration: Equavalent to VI with

$Q = \left\{q(\cdot|\lambda) = \prod_j q_j(\theta_j|\lambda),\ \lambda \in \mathbb{R}^d\right\}$

where $q_j(\theta_j|\lambda) = p\delta_0(\theta_j) + (1 - p)\delta_{\lambda_j}(\theta_j)$

This allows to do Dropouts also in prediction

6.2 MCMC:

MCMC but cannot store all the $\theta^{(i)}$:

1) Subsampling: Only store a subset of the $\theta^{(i)}$

2) Gaussian Aproximation: We only keep:

$\mu_i = \frac{1}{T}\sum_{j=1}^T \theta_i^{(j)}$ and $\sigma_i = \frac{1}{T}\sum_{j=1}^T (\theta_i^{(j)} - \mu_i)^2$

And updete them online.

Predictive Esnable NNs:

Let $\mathcal{D} = \{(x_i, y_i)\}_{i=1:n}$ be our dataset.

Train θ_i^{MAP} on $\mathcal{D}_i$ with $i = 1, \dots, m$

$\mathcal{D}_i$ is a Bootstrap of $\mathcal{D}$ of same size

and $p(y^*|x^*, \mathcal{D}) \simeq \frac{1}{m}\sum_{j=1}^m p(y^*|x^*, \theta_i^{MAP})$

6.3 Model calibration

Train $\hat{q}$ on $\mathcal{D}_{train}$

Evaluate $\hat{q}$ on $\mathcal{D}_{val} = \{(y', x')\}_{i=1:m}$

Held-Out-Likelihood $\doteq \log p(y'_{1:m}|x'_{1:m}, \mathcal{D}_{train})$

$\geq \mathbb{E}_{\theta \sim \hat{q}}\left[\sum_{i=1}^m \log p(y'_i|x'_i, \theta)\right]$ (Jensen)

$\simeq \frac{1}{k}\sum_{j=1}^k \sum_{i=1}^m \log p(y'_i|x'_i, \theta^{(j)})$, $\theta^{(j)} \sim \hat{q}$

Evaluate predicted accuracy: We divide $\mathcal{D}_{val}$ into bins according to predicted confidence values. In each bin we compare accuracy with confidence

7 Active Learning

Let $\mathcal{D}$ be the set of observable points.

We can observe $\mathcal{S} \subseteq \mathcal{D}, |\mathcal{S}| \leq R$

Information Gain: $\hat{\mathcal{S}} = \arg\max_{\mathcal{S}} F(\mathcal{S}) = I(f, y_{\mathcal{S}})$

For GPs: $F(\mathcal{S}) = \frac{1}{2}\log\left|I + \frac{1}{\sigma^2}K_{\mathcal{S}\mathcal{S}}\right|$

This is NP Hard, $\Rightarrow$ Greedy Algo:

init: $\mathcal{S}^* = \emptyset$
for $t = 1 : R$ **do**
  $x_t = \arg\max_{x \in \mathcal{D}} F(\mathcal{S}^* \cup \{x\})$
  $\left(x_t = \arg\max_{x \in \mathcal{D}} \sigma_x^2 | \mathcal{S}$ for GPs$\right)$
  $\left(x_t = \arg\max_{x \in \mathcal{D}} \frac{\sigma^2_{f|\mathcal{S}}(x)}{\sigma_n^2(x)}$ for heter. GPs$\right)$
  $\mathcal{S}^* = \mathcal{S} \cup \{x_t\}$

F is **Submodular** if: $\forall x \in \mathcal{D}$,$\forall A \subseteq B \subseteq D$ holds that: $F(A \cup \{x\}) - F(A) \geq F(B \cup \{x\}) - F(B)$

F is Submodular $\Rightarrow F(\mathcal{S}^*) \geq \left(1 - \frac{1}{e}\right) F(\hat{\mathcal{S}})$

8 Bayesian Optimization

Like Active Learning but we only want to find the optima. We pick $x_1, x_2, \ldots$ from $\mathcal{D}$ and observe $y_i = f(x_t) + \epsilon_t$.

Comulative regret: $R_T = \sum_{t=1}^{T} \left(\max_{x \in \mathcal{D}} f(x) - f(x_t)\right)$

Oss: $\frac{R_T}{T} \to 0 \Rightarrow \max_t f(x_t) \to \max_{x \in \mathcal{D}} f(x)$

8.1 Upper Confidence Sampling

With GP $x_t = \arg\max_{x \in \mathcal{D}} \mu_{t-1}(x) + \beta_t \sigma_{t-1}(x)$

Chosing the correct β_t we get: $\frac{R_T}{T} = \mathcal{O}\left(\sqrt{\frac{\gamma_T}{T}}\right)$.

Where $\gamma_t = \max_{|\mathcal{S}|<T} I(f; y_{\mathcal{S}})$. On d dims:

Linear: $\gamma_T = \mathcal{O}(d \log T)$ RBF: $\gamma_T = \mathcal{O}((logT)^{d+1})$

Optimal $\beta_t = \mathcal{O}(\|f\|_K^2 + \gamma_t \log^3 T)$

Oss: $\beta \uparrow$=more exploration

8.2 Thompson Samling

$x_t = \arg\max_{x \in \mathcal{D}} \tilde{f}(x), \quad \tilde{f} \sim p(f | x_{1:n}, y_{1:n})$

8.3 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 $P(A) = \sum_b P(A|B)P(B)$

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):

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

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

9 Bayesian Networks

9.1 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: $P(X_1,...,X_n) = \prod_i P(X_i|Pa_{X_i})$

BNs with 3 nodes:

9.2 Active trails and d-separation

An undirected path in a BN structure G is called active trail for observed variables $O \in X_1,...,X_n$ 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!

10 Exact inference (tree-structured BN)

10.1 Variable elimination

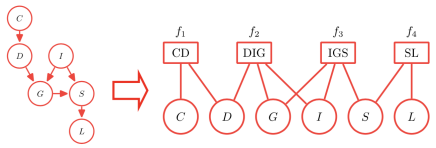
- Given a BN and query $P(X|E=e)$
- Choose an ordering of $X_1,...,X_n$ **Eliminate variables from the outside in!**
- Set up initial factors: $f_i = P(X_i|Pa_i)$
- For $i = 1:n, X_i \notin X,E$
  - Collect and multiply all factors f that include X_i
  - Generate new factor by marginalizing out X_i: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

10.2 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.**



10.2.1 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

11 Dynamical models (include time)

11.1 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 $\eta_t \sim N(0, \Sigma_y)$

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

11.3 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.

11.4 Approx. infer. for filtering (DBNs and nonlinear 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: $Z = \sum_{i=1}^{N} w_i \delta_{x_i}$

12 Probabilistic Planning

12.1 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:

$P(x'|x,a) = \text{Prob}(\text{Next state} = x' | \text{Action } a)$

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:

$\pi^*(s) = \underset{a \in A}{argmax}[r(x,a) + \gamma \sum_{x'} P(x'|x,a)V^*(x')]$

12.2 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 $O(n^2m/(1-\gamma))$ iterations (converges in polynomial number of iterations)!

12.3 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)!

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

12.5 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): $\theta^* = \arg\max_\theta J(\theta)$

13 Learning models from training data

13.1 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: $\theta_{F=c} \frac{Count(F=c)+\alpha_c}{N+\alpha_c+\alpha_l}$

13.1.1 Score based structure learning

Define scoring function $S(G;D)$ and search over BN structure G: $G^* = \arg\max_G S(G;D)$

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 → undirected tree
- Pick any variable as root and orient the edges away using breadth-first search.

14 Reinforcement Learning

14.1 Model-based RL

14.1.1 ϵ greedy

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

14.1.2 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.
Enough"? 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 $O(|X^2||A|)$.

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

14.2.1 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. $L(\theta) = \sum_{(x,a,r,x')\in D}(r + \gamma \max_{a'} Q(x',a';\theta^{old}) - Q(x,a;\theta))^2$ **Double DQN:** current network for evaluating argmax (too optimistic, and you remove θ^{old} and put θ).

14.3 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 $\mu : X \to \mathbb{R}$ and $K : X \times X \to \mathbb{R}$ 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: Σ_{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 $y_i = f(\vec{x_i}) + \epsilon_i$, $A = \{\vec{x_1} : \vec{x_k}\}$ $P(f(x)|\vec{x_1} : \vec{x_k}, y_{1:k}) = GP(f;\mu',K')$. In particular, $P(f(x)|\vec{x_1} : \vec{x_k}, y_{1:k}) = N()f(x);\mu_{x|A}, \sigma^2_{x|a}$, where $\mu_{x|a} = \mu(\vec{x}) + \Sigma_{x,A}(\Sigma_{AA} + \sigma^2 I)^{-1}\Sigma_{x,A}^T(\vec{y_A} - \mu_A)$ and $\sigma^2_{x|a} = K(\vec{x},\vec{x}) - \Sigma_{x,A}(\Sigma_{AA} + \sigma^2 I)^{-1}\Sigma_{x,A}^T$.
Closed form formulas for prediction!