

**Multivariate Gaussian**

$$\frac{1}{(2\pi)^{n/2} \sqrt{|\Sigma|}} \exp(-\frac{1}{2}(y - \mu)^T \Sigma^{-1} (y - \mu))$$

$$p(X_A|X_B = x_B) = \mathbb{N}(\mu_{A|B}, \Sigma_{A|B})$$

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

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

$$f^* = w^T x^*, y = w^T x + \varepsilon$$

$$P(f^* | X, y, x^*) = \mathbb{N}(mu^T x^*, x^{*T} \Sigma x^*)$$

$$P(y | X, y, x^*) = \mathbb{N}(mu^T x^*, x^{*T} \Sigma x^* + \sigma_n^2)$$

**MAP,MLE**

$$w_{MLE} = (X^T X)^{-1} X^T y$$

$$P(w|X, y) = P(w|\mu_w, \Sigma_w)$$

$$\Sigma_w = (\sigma_w^{-2} \mathbb{I} + \sigma_y^{-2} X^T X)^{-1}$$

$$\mu = \sigma_y^{-2} \Sigma_w X^T y$$

$$w_{MAP} = \sigma_y^{-2} \Sigma_w X^T y$$

$$\lambda = \sigma_y^2 / \sigma_w^2, \sigma_y^2 = \frac{1}{n} \sum_{i \leq n} (y_i - w^T x_i)^2, \sigma_w^2 = \frac{\sigma_y^2}{\lambda}$$

**Bayesian Filtering**

Conditioning

$$P(X_t | y_{1:t}) = \frac{1}{Z} P(X_t | y_{1:t+1}) P(y_t | X_t)$$

Prediction

$$P(X_{t+1} | y_{1:t}) = \int P(X_{t+1} | x_t) P(x_t | t_{1:t})$$

$$\mu_{t+1} = \frac{\sigma_y^2 \mu_t + (\sigma_t^2 + \sigma_x^2) y_{t+1}}{\sigma_t^2 + \sigma_x^2 + \sigma_y^2}$$

$$\sigma_{t+1}^2 = \frac{(\sigma_t^2 + \sigma_x^2) \sigma_y^2}{\sigma_t^2 + \sigma_x^2 + \sigma_y^2}$$

**Kalman Filters**

$$X_{t+1} = F X_t + \varepsilon_t, Y_t = H X_t + \eta_t$$

TM:  $P(x_{t+1} | x_t) = N(x_{t+1}; F x_t, \Sigma_x)$

SM:  $P(y_t | x_t) = N(y_t; H x_t, \Sigma_y)$

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

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

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

**Gaussian Processes**

Optimizing Kernel Params: Max Marginal Likelihood:  $\log(p(y|X, \theta)) = -\frac{1}{2} y^T K_y^{-1} y - \frac{1}{2} \log |K_y| - \frac{n}{2} \log(2\pi)$

**Kernels**

A valid kernel function must be:

- positive semi-definite
- symmetric

$$\text{linear } k(x, x') = x x'^T$$

Squared Exponential:

$$k(x, x') = \exp(-||x - x'||_2^2 / h^2)$$

Exponential:

$$k(x, x') = \exp(-||x - x'||_2 / h^2)$$

Matern:

$$k(x, x') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu} ||x - x'||_2}{\rho} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu} ||x - x'||_2}{\rho} \right)$$

Stationary Kernel:

$$k(x, x') = k(x - x')$$

**Isotropic Kernel**

$$k(x, x') = k(||x - x'||_2)$$

**Fast GP Methods**

Shift Invariant K:  $k(x, y) = k(x - y)$

A SI Kernel is positive semi-definite only if  $p(w)$  is nonnegative

$$k(x - y) = \int_{\mathbb{R}^d} p(w) e^{j w^T (x - y)} dw = \mathbb{E}_{w,b} [z_{w,b}(x) z_{w,b}(y)] = \frac{1}{m} \sum_{i \leq n} z_{w^i, b^i}(x) z_{w^i, b^i}(y) = \phi(x)^T \phi(y)$$

Inducing points:  $p(f^*, f) \sim q(f^*, f) = \int q(f^* | u) q(f | u) p(u) du$

$$p(f, f) = N(K_{f,u} K_{u,u}^{-1} u, K_{f,f} - Q_{f,f})$$

$$p(f^*, f) = N(K_{f^*,u} K_{u,u}^{-1} u, K_{f^*,f^*} - Q_{f^*,f^*}) \text{ where } Q_{A,B} = K_{A,u} K_{u,u}^{-1} K_{u,A}$$

SoR Approx:

$$p(f, f) = N(K_{f,u} K_{u,u}^{-1} u, 0)$$

FITC Approx:

$$p(f, f) = N(K_{f,u} K_{u,u}^{-1} u, \text{diag}(K_{f,f} - Q_{f,f}))$$

**Approximate Inference**

Laplace Approximation

$$q(\theta) = N(\theta; \hat{\theta}, \Lambda^{-1})$$

$$\hat{\theta} = \text{argmax}_\theta p(\theta | y)$$

$$\text{GD} = w \leftarrow w(1 - 2\lambda \eta_t) + \eta_t y x^T (Y - y | w, x)$$

$$\Lambda = -\nabla \nabla \log(p(\hat{\theta} | y)) = \sum_{i \leq n} x_i x_i^T \pi_i (1 - \pi_i), \pi = \sigma(\hat{w}^T x_i)$$

Var. Inf.=KL Divergence

$$q^* \in \text{argmax}_{q \in \mathcal{Q}} KL(q || p) = \int q(\theta) \log \frac{q(\theta)}{p(\theta)} d\theta$$

$$p = N(\mu_0, \Sigma_0, q = N(\mu_1, \Sigma_1))$$

$$KL(p || q) = \frac{1}{2} (tr(\Sigma_1^{-1} \Sigma_0) + (\mu_1 - \mu_0)^T \Sigma_1^{-1} (\mu_1 - \mu_0) - d + \ln(\frac{|\Sigma_1|}{|\Sigma_0|}))$$

Entropy

$$H(q) = -\int q(\theta) \log(q(\theta)) d\theta$$

Minimizing KL

$$\text{argmin}_q KL(q || p) = \text{argmax}_q \mathbb{E}_{\theta \sim q(\theta)} [\log p(y | \theta)] - KL(q || p(\cdot)) = \text{argmax}_q \mathbb{E}_{\theta \sim q(\theta)} [\log p(y, \theta)] + H(q)$$

Maximizing ELBO

$$\log(p(y)) \geq \mathbb{E}[\log p(y | \theta)] - KL(q || p(\cdot))$$

Gradient ELBO

$$\nabla_{C,\mu} \mathbb{E}_{\varepsilon \sim N(0, I)} [\log p(y | C\varepsilon + \mu)] - \nabla_{C,\mu} KL(q_{C,\mu} || p(\cdot))$$

**Markov Chain Monte Carlo**

Law of Large Numbers

$$E_P[f(X)] = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i \leq N} f(x_i)$$

Hoeffding's Inequality:

**fbounded in [0,C]**

$$P(|\mathbb{E}P[f(x)] - \frac{1}{N} \sum_{i \leq N} f(x_i)| > \varepsilon) \leq 2 \exp(-2N\varepsilon^2/C)$$

Stationary Distribution

$$\lim_{N \rightarrow \infty} P(X_N = x) = \pi(x)$$

Detailed Balance Equation

$$Q(x)P(x'|x) = Q(x')P(x|x')$$

Designing Markov Chain

Proposal Distribution= $R(X'|X)$

$$X_t = x, x' \sim R(X'|X = x)$$

$$\alpha = \min \frac{Q(x')R(x|x')}{Q(x)R(x'|x)} \rightarrow X_{t+1} = x'$$

Metropolis, Hastings: The stationary distribution is  $Z^{-1} Q(x)$

Gibbs Sampling

$$x_0 \leftarrow x_0$$

for  $t = 1 \rightarrow \infty$

$$i \sim (1..n)/B$$

$$x_i \sim P(X_{i+1} | x_{-i})$$

Variance of Gibbs

$$x_0 \leftarrow x_0$$

for  $t = 1 \rightarrow \infty$

$$x^{(t)} = x^{(t-1)}$$

for  $i = 1 \rightarrow \infty$

$$x_i \sim P(X_{i+1} | x_{-i})$$

Ergodic Thm (Special Case): suppose  $X_2, \dots, X_n$  is an ergodic Markov chain over a finite state space  $D$  with stationary distribution  $\pi$  and let  $f$  be a function in  $D$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N f(x_i) = \sum_{x \in D} \pi(x) f(x)$$

Markov Processes continuous case

$$p(x) = \frac{1}{Z} \exp(-f(x))$$

$$\alpha = \min \frac{R(x'|x)}{R(x|x')} \exp(f(x) - f(x')) \rightarrow X_{t+1}$$

Metropolis Adjusted Langevin Algorithm

$$R(x'|x) = \mathbb{N}(x'; x + \tau \nabla f(x); 2\tau I)$$

Stochastic Gradient Langevin Dynamics

$$\theta_0 = \theta_0$$

$$Fort = 0, 1, \dots$$

$$\varepsilon_t \sim \mathbb{N}(0, 2\eta_t I)$$

$$\theta_{t+1} = \theta_t - \eta_t (\nabla \log p(\theta_t) + \frac{n}{m} \sum_{j \leq m} \nabla \log p(y_{i,j} | \theta_t, x_{i,j})) + \varepsilon_t$$

**Bayesian Neural Networks**

Heteroscedastic noise

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

Log Likelihood

$$\text{argmin}_\theta \lambda ||\theta||_2^2 + \sum_{i \leq n} ||y_i - \mu(x_i, \theta)||^2 + \frac{1}{2} \log \sigma(x_i; \theta)^2$$

Gradient

$$\nabla_\lambda L(\lambda) = \nabla_{C,\mu} \frac{n}{m} \sum_{j \leq m} \log p(y_{i,j} | C\varepsilon^{(j)} + \mu, x_{i,j}) - \nabla_{C,\mu} KL(q_{C,\mu} || p(\cdot))$$

Prediction Mean and Variance

$$P(y^* | X, y, x^*) \simeq \frac{1}{m} \sum_{j \leq m} \mathbb{N}(y^*; \mu(x^*, \theta^{(j)}), \sigma^2(x^*, \theta^{(j)}))$$

Mean= $\frac{1}{m} \sum_{j \leq m} \mu(x^*, \theta^{(j)})$

Var= $\mathbb{E}[Var[y^* | x^*, \theta]] +$

$Var[y^* | x^*, \theta] +$

$$\simeq \frac{1}{m} \sum_{j \leq m} \sigma^2(x^*, \theta^{(j)}) + \frac{1}{m} \sum_{j \leq m} (\mu(x^*, \theta^{(j)}) - \bar{\mu}(x^*))^2$$

DropOuts VI

$$q(\theta | \lambda) = \prod_j (q_j(\theta_j | \lambda_j))$$

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

Probabilistic Ensembles

$$p(y^* | X, y, x^*) = \frac{1}{m} \sum_{j \leq m} p(y^* | x^*, \theta^{(j)})$$

**Active Learning**

Mutual Information: Given random samples  $X$  and  $y$   $I(X;Y)$  quantifies how much observing  $Y$  reduces the uncertainty of  $X$

$$I(X;Y) = \sum_{y \in Y} \sum_{x \in X} P(x, y) \log \left( \frac{P(x,y)}{P(x)P(y)} \right)$$

$$I(X;Y) = H(Y) - H(\varepsilon) = \frac{1}{2} \ln((2\pi e)^d |\Sigma - \sigma^2 \mathbb{I}|) - \frac{1}{2} \ln((2\pi e)^d |\sigma^2 \mathbb{I}|) = \frac{1}{2} \ln(\sigma^{-2} \Sigma - \mathbb{I})$$

$$F(S) = H(f) - H(f|y_S) = I(f; y_S) = \frac{1}{2} \ln |\mathbb{I} + \sigma^{-2} \Sigma|$$

Optimizing MI

$$x_{t+1} = \text{argmax}_x F(S_t U x) = \text{argmax}_{x \in D} \sigma_{S_t}^2$$

Submodularity of MI

$$\forall x \in D \forall A \subseteq B \subseteq D : F(A \cup x) - F(A) \geq F(B \cup x) - F(B)$$

Greedy Constant Factor

$$F(S_t) = (1 - \frac{1}{e}) \max_{S \subseteq D, |S| \leq T} F(S)$$

Natural Generalization MI optimization

$$= x'$$

$$x_{t+1} \in \text{argmax}_x \frac{\sigma_x^2}{\sigma_0^2}$$

Learning to Optimize

$$f \in F : D \rightarrow \mathbb{R}, y_t = f(x_t) + \varepsilon_t$$

$$CR : R_T = \sum_{i \leq T} (\max_x f(x) - f(x_t))$$

Sublinearity:  $R_T / T \rightarrow 0$

implies  $\max_t f(x_t) \rightarrow f(x^*)$

Upper Confidence Sampling

$$x_t = \text{argmax}_{x \in D} \mu_{t-1}(x) + \beta_t \sigma_t - 1(x)$$

Regret of GP-UCB: assuming  $\beta_t$  correct

$$\frac{1}{T} \sum_{t \leq T} [f(x^*) - f(x_t)] = O^*(\sqrt{\frac{\gamma T}{T}}) \text{ where } \gamma T = \max_{|S| \leq T} I(f; y_S)$$

Frequentist approach:

$$\frac{1}{T} \sum_{t \leq T} [f(x^*) - f(x_t)] = O^*(\sqrt{\frac{\beta_T \gamma T}{T}})$$

Expected Improvement

$$x_t = \text{argmax}_{x \in D} EI(x)$$

$$EI = E[(t - y)_+] = \int_{-\infty}^{\infty} (t - y)_+ p(y|x) dy$$

$$y_t = f(x_t) + \varepsilon_t$$

Bayesian update for  $\mu_y, \sigma_t$  Thompson Sampling

$$\tilde{f} \sim P(f | x_{1:t}, y_{1:t})$$

$$x_{t+1} = \text{argmax}_{x \in D} \tilde{f}(x)$$

**Markov Decision Processes**

A set of States  $1, \dots, n$

A set of actions  $1, \dots, m$

Transition Probabilities

$$P(X_{t+1} = x' | X_t = x) = P(x' | x, \pi(x))$$

$$P(X_{t+1} | x' | X_t = x) = \sum_a \pi(a | x) P(x' | x, a)$$

Reward Function

$$EV: J(\pi) = E[r(X_0, \pi(X_0)) + \gamma r(X_1, \pi(X_1)) + \gamma^2 r(X_2, \pi(X_2)) + \dots]$$

$$V^\pi(x) = J(\pi | X_0 = x) = \mathbb{E}_{x=1:\infty} [\sum_{t \leq \infty} \gamma^t r(X_t, \pi(X_t)) | X_0 = x] = r(x, \pi(x)) + \gamma \sum_{x'} P(x' | x, \pi(x)) V^\pi(x')$$

Solving for a policy

$$V^\pi = (I - \gamma T^\pi)^{-1} r^\pi$$

Fixed point iteration

$$V_t^\pi = r^\pi + \gamma T^\pi V_{t-1}^\pi$$

$$t \geq \frac{\ln \frac{\|V_0^\pi - V^\pi\|_\infty}{\frac{\varepsilon}{\gamma}}}{\ln \frac{1}{\gamma}}$$

Greedy Policy

$$\pi(x) \nu = \text{argmax}_a r(x, a) + \gamma \sum_{x'} P(x' | x, a) V(x')$$

Theorem (Bellman): A policy acts greedily w.r.t its induced value function

$$V^*(x) = \max_a [r(x, a) + \gamma \sum_{x'} P(x' | x, a) V^*(x')]$$

MDP

observation:  $P(Y_t | X_t)$

state update:  $P(X_{t+1} | X_t, A_t)$

typically extremely intractable  $\rightarrow$

PODPS= $\mathbb{B} = \nabla(1, \dots, N) = b : 1, \dots, n \rightarrow [0, 1], \sum_x b(x) = 1$

observation:  $P(Y_{t+1} = Y | b_t(x), A_t) = \sum_{x,x'} b_t(x) P(x' | x, A_t) P(y | x')$

state update:  $b_{t+1} = \frac{1}{Z} \sum_x b_t(x) P(X_{t+1} = x' | X_t = x, A_t) P(y_{t+1} | x')$

reward:  $r(b_t, A_t) = \sum_x b_t(x) r(x, A_t)$

**Reinforcement Learning**

**Model Based**

$$P(X_{t+1} | X_t, A) \simeq \frac{\text{Count}(X_{t+1}, X_t, A)}{\text{Count}(X_t, A)}$$

$$r(x, a) \simeq \frac{1}{N_{x,a}} \sum_{t: X_t=x, A_t=a} R_t$$

$\varepsilon$  greedy

$\varepsilon_t \sim$  pick random action

$1 - \varepsilon_t \sim$  pick best action

Converges if  $\varepsilon_t$  satisfies Monroe's Conditions:  $\sum_t \varepsilon_t = \infty, \sum_t \varepsilon_t \leq \infty$

The  $R_{max}$  Algorithm

$r(s, a) = R_{max}$  for unknown states

$P(x^* | x, a) = 1$  add a fairy tale state

- For each visited action pair  $x, a$  update  $(x, a)$

- Estimate Transition Probabilities  $P(x' | x, a)$

- If observed enough" compute policy  $\pi$

ENOUGH? Hoeffding's Bound

$$P(|\mu - \frac{1}{n} \sum_{i \leq n} Z_i| \geq \varepsilon) \leq 2 \exp(-2n\varepsilon^2/C^2), n \in O(\frac{R_{max}^2}{\varepsilon^2} \log(\frac{1}{\delta}))$$

