

1 Maximum Likelihood Estimator

- Consistent, asymptotic unbiased. $\hat{\theta}_n^{\text{MLE}} \xrightarrow{P} \theta_0$.
- Asymptotic normal. $\sqrt{n}(\hat{\theta}_n^{\text{MLE}} - \theta_0) \xrightarrow{D} \mathcal{N}(0, I_n)$, $I_n(\theta_0) = \mathbb{E}[-s_\theta] = \mathbb{E}[s_\theta s_\theta^\top]$ Fisher info, $s_\theta(x) = \partial_\theta \ln p_\theta(x)$ score func, $\mathbb{E}_\theta s_\theta = 0$.
- Asymptotic efficient. $\hat{\theta}_n^{\text{MLE}}$ reaches CRLB when $n \rightarrow \infty$. $\hat{\theta}_n^{\text{MLE}}$ not efficient if n finite. Stein estimator always better.
- Equivariance, if $\hat{\theta}_n$ is MLE, $\hat{y} = g(\hat{\theta}_n^{\text{MLE}})$ is MLE of $\mathcal{L}(g^{-1}(y))$. Proof by optimality of MLE. Cramer-Rao lower bound (CRLB): for any unbiased $\hat{\theta}$ of θ_0 , $\mathbb{E}(\hat{\theta} - \theta_0)^2 \geq 1/I_n(\theta_0)$
Proof: $\text{Cov}[s_\theta, \hat{\theta}] = \mathbb{E}[s_\theta, \hat{\theta}] = \partial_\theta \mathbb{E}[\hat{\theta}] = \partial_\theta \theta = 1$. Cauchy-Schwarz $\text{Cov}^2[s_\theta, \hat{\theta}] \leq \text{Var}[s_\theta] \text{Var}[\hat{\theta}] = I_n(\theta) \mathbb{E}(\hat{\theta} - \theta_0)^2$ QED.
However, when dimension of problem goes to infinity while data-dim ratio is fixed, MLE is biased and the p -values are unreliable.

2 Regression

Bias-Variance trade-off

Training dataset, \hat{f} be the predictive function. $\mathbb{E}_D \mathbb{E}_{Y|X} (\hat{f}(X) - Y)^2 = \mathbb{E}_D (\hat{f}(x) - \mathbb{E}_D \hat{f}(x))^2 + (\mathbb{E}_D \hat{f}(x) - \mathbb{E}(Y|X))^2 + \mathbb{E}_D (\mathbb{E}(Y|X) - Y)^2 = \text{Model Variance} + \text{Bias}^2 + \text{Intrinsic Noise}$. The optimal trade-off is achieved by avoiding under-fitting (large bias) and over-fitting (large variance). Note that here the variance of output is computed by refitting the regressor on a new dataset.

Regularization

Ridge and Lasso can be viewed as MAP estimation with a prior on β . Ridge has a Gaussian Prior and LASSO a Laplacian prior. Using SVD, we get Ridge has built-in model selection: $X\beta^{\text{Ridge}} = \sum_{j=1}^d [d_j^2/(d_j^2 + \lambda)] u_j u_j^\top Y$ (each $u_j u_j^\top Y$ can be viewed as a model). Lasso has more sparse estimations because the gradient of regularization does not shrink as Ridge.

3 BLR and GP

Bayesian Linear Regression

$Y = X\beta + \epsilon \sim \mathcal{N}(0, \sigma^2)$. Prior $\beta \sim \mathcal{N}(0, \Lambda^{-1})$. Posterior $\beta|X, Y \sim \mathcal{N}(\mu_\beta, \Sigma_\beta)$, $\Sigma_\beta = (\sigma^{-2} X^\top X + \Lambda)^{-1}$, $\mu_\beta = \sigma^2 \Sigma_\beta X^\top Y$.

Gaussian Process

$Y = \begin{pmatrix} Y_0 \\ Y_1 \end{pmatrix}$ is the combination of observed and prediction value. Assume a Gaussian prior of $\mathcal{N}(0, K + \sigma^2 I)$, where $K_{ij} = k(x_i, x_j)$ is kernel. GP regression is the conditional/Posterior distribution on Y_0 , $\mathbb{E}[Y_1|Y_0] = K_{10}(\sigma^2 I_0 +$

$K_{00})^{-1} Y_0$, $\text{Cov}[Y_1] = \sigma^2 I_1 + K_{11} - K_{10}(\sigma^2 I_0 + K_{00})^{-1} K_{01}$. Bayesian LR is a special case of GP with linear kernel $k(x, y) = x^\top \Lambda^{-1} y$.

Kernel Function

A function is a kernel iff (1) symmetry $k(x, x') = k(x', x)$ and (2) semi-positive definite $\int_{\Omega} k(x, x') f(x) f(x') dx dx' \geq 0$ for any $f \in L_2$ and $\Omega \in \mathcal{R}^d$ (continuous) or $K(X) \geq 0$ (discrete). The latter is equivalent to (1) $a^\top K a \geq 0, \forall a$ or (2) $k(x, x') = \phi(x)^\top \phi(x')$ for some ϕ .

Kernel Construction

If $k_{1,2}$ are valid kernels, then followings are valid: (1) $k(x, x') = k_1(x, x') + k_2(x, x')$. (2) $k(x, x') = k_1(x, x') \cdot k_2(x, x')$. Proof: expand by Mercer's thm. (3) $k(x, x') = c k_1(x, x')$ for constant $c > 0$. (4) $k(x, x') = f(k_1(x, x'))$ if f is a polynomial with positive coefficients or the exp. Proof: polynomial can be proved by applying the product, positive scaling and addition. Exp can be proved by taking limit on the polynomial. (5) $k(x, x') = f(x) k_1(x, x') f(x')$. (6) $k(x, x') = k_1(\phi(x), \phi(x'))$ for any function ϕ .

Example: RBF kernel $k(x, y) = e^{-\|x-y\|^2/2\sigma^2} = e^{-\|x\|^2/2\sigma^2} \times e^{x^\top y/2\sigma^2} \times e^{-\|y\|^2/2\sigma^2}$ is valid. (1) $x^\top y$ linear kernel is valid (2) then $\exp(\frac{1}{\sigma^2} x^\top y)$ is valid, (3) let $f(x) = \exp(-\frac{1}{2\sigma^2} \|x\|^2)$, by rules $f(x)k(x, y)f(y)$ RBF is valid.

Mercer's Theorem: Assume $k(x, x')$ is a valid kernel. Then there exists an orthogonal basis e_i and $\lambda_i \geq 0$, s.t. $k(x, x') = \sum_i \lambda_i e_i(x) e_i(x')$.

4 Linear Methods for Classification

Concept Comparison

- Probabilistic Generative, modeling $p(x, y)$: (1) can create new samples, (2) outlier detection, (3) probability for prediction, (4) high computational cost and (5) high bias.
- Probabilistic Discriminative, modeling $p(y|x)$: (1) probability for prediction, (2) medium computational cost and (3) medium bias.
- Discriminative, modeling $y = f(x)$: (1) no probability for prediction, (2) low computational cost and (3) low bias.

Infer $p(x, y)$ for classification problems

Use $p(x, y) = p(y)p(x|y)$. Since y has finite states, model $p(y)$ and $p(x|y)$ for different y . The modeling requires to (1) guess a distribution family and (2) infer param by MLE.

Compute $p(y|x)$ by discriminant analysis (DA)

Linear DA Assumption: classify a sample into two Gaussian distribution with $\Sigma_0 =$

Σ_1 . After calculation, $p(y = 1|x) = 1/(1 + \exp(-\log \frac{p(x|y=1)p(y=1)}{p(x|y=0)p(y=0)})) = 1/(1 + \exp(w_1^\top x + w_0))$ since the quadratic term is eliminated due to $\Sigma_0 = \Sigma_1$.

Quadratic DA Assumption: classify a sample into two Gaussian distribution with $\Sigma_0 \neq \Sigma_1$. After calculation, $p(y = 1|x) = 1/(1 + \exp(x^\top W x + w_1^\top x + w_0))$.

Optimization Methods

Optimal Learning Rate for Gradient Descent

Goal: find $\eta^* = \argmin_{\eta} L(w^k - \eta \cdot \nabla L(w^k))$.

By Taylor expansion of $L(w^{k+1})$ at w^k and solve for the optimal η , we get $\eta^* = \|\nabla L(w^k)\|^2 / (\nabla L(w^k)^\top H_L(w^k) \nabla L(w^k))$.

Cons of naive gradient descent: (1) zig-zag behavior, especially in a very narrow, long and slightly downward valley; (2) gradient update is small near the stationary point. Mitigated by adding momentum into update, $w^{k+1} = w^k - \eta \nabla L(w^k) + \mu^k (w^k - w^{k-1})$, this speeds update towards "common" direction.

Newton's Method

Taylor-expand $L(w)$ at w_k to derive the optimal w^{k+1} : $L(w) \approx L(w^k) + (w - w^k)^\top \nabla L(w^k) + \frac{1}{2} (w - w^k)^\top H_L(w^k) (w - w^k) \Rightarrow w^{k+1} = w^k - H_L^{-1}(w^k) \nabla L(w^k)$.

Pros: (1) better updates compared to GD since it uses the second Taylor term and (2) does not require learning rate.

Cons: requires H_L^{-1} which is expensive.

Bayesian Method

In most cases, the posterior is intractable. Use approximation of posterior instead.

Laplacian Method

Idea: approximate posterior near the MAP estimation with a Gaussian distribution. $p(w|X, Y) \propto p(w, X, Y) \propto \exp(-R(w))$, where $R(w) = -\log p(w, X, Y)$. Let $w^* = \argmin R(w)$ be the MAP estimation and Taylor-expand $R(w)$ at w^* : $R(w) \approx R(w^*) + \frac{1}{2} (w - w^*)^\top H_R(w^*) (w - w^*)$. Therefore, $p(w|X, Y) \propto \exp(-R(w^*) - \frac{1}{2} (w - w^*)^\top H_R(w^*) (w - w^*))$ and thus $(w|X, Y) \sim \mathcal{N}(w^*, H_R^{-1}(w^*))$.

AIC & BIC

- Define $\text{BIC} = k \log N - 2 \log \hat{L}$, where k is #parameters and \hat{L} is the likelihood $p(x|w^*)$. A lower BIC means a better model.
- Define $\text{AIC} = 2k - 2 \log \hat{L}$. A lower AIC means a better model.

LDA by loss minimization

Perceptron for $y_i \in \{0, 1\}$, find w , s.t. $y_i w^\top x_i > 0$ for any i . Prediction is $c(x) = \text{sgn}(w^\top x)$.

$\text{Loss} L(y, c(x)) = \min\{0, -y w^\top x\}$. By GD $w^{(k+1)} \leftarrow w^{(k)} + \eta(k) \sum_i \text{wrong } y_i x_i$, Perceptron will converge if (1) data linearly separable, (2) learning rate $\eta(k) > 0$, (3) $\sum_k \eta(k) \rightarrow +\infty$ and (4) $(\sum_k \eta(k)^2) / (\sum_k \eta(k))^2 \rightarrow 0$. However, multiple solutions permitted if data linearly separable, solution unstable.

Fisher's LDA

Idea: project the two distribution into one dimension and maximize the ratio of the variance between the classes and the variance within the classes, i.e., $\max(w^\top u_1 - w^\top u_0)^2 / (w^\top S w)$, where $S = \Sigma_0 + \Sigma_1$. Let gradient be zero and solve for w^* , we get $w^* \propto S^{-1}(u_1 - u_0)$.

We first compute w^* and fit distributions of the two-class projection. Then apply Bayesian decision theory to make classification.

5 Optimization with Constraint

Problem $\min_x f(x)$ s.t. $g_i \in [I](x) \leq 0$ and $h_j \in [J](x) = 0$. Solve it with **KKT Cond**: (1) Stationary $\nabla f + \sum_i \lambda_i \nabla g_i + \sum_j \mu_j \nabla h_j = 0$, (2) $h_j(x) = 0$, (3) primal feasibility $g_i(x) \leq 0$, (4) dual feasibility $\lambda_i \geq 0$, (5) complementary slackness $\lambda_i g_i(x) = 0$.

Weak Duality: Lagrangian $L(x, \lambda, \mu) = f(x) + \lambda^\top g(x) + \mu^\top h(x)$, $\lambda > 0$. Dual function $F(\lambda, \mu) := \min_x L(x, \lambda, \mu)$. Denote \tilde{x} optima of original problem, then $\lambda^\top g(\tilde{x}) + \mu^\top h(\tilde{x}) \leq 0, \forall \lambda, \mu$, $F(\lambda, \mu) = \min_x L(x, \lambda, \mu) \leq L(\tilde{x}, \lambda, \mu) \leq f(\tilde{x}) = \min_{x, h(x)=0, g(x) \leq 0} f(x)$

Strong Duality in Convex Optimization

If **Slater's cond** (1) f convex (2) g convex (3) h linear (4) $\exists \bar{x}$ s.t. $g_i(\bar{x}) < 0$ and $h_j(\bar{x}) = 0$, then Strong Duality $\max_{\lambda, \mu} F(\lambda, \mu) = \min_{x, h(x)=0, g(x) \leq 0} f(x)$ holds.

6 Support Vector Machine

Linear Separable Case

Primal: $\max_{w, b, t} t$ s.t. $\forall i, t \leq y_i (w^\top x_i + b)$ and $\|w\| = 1 \Leftrightarrow \min_{w, b} \frac{1}{2} w^2$ s.t. $\forall i, 1 \leq y_i (w^\top x_i + b)$
(1) **KKT cond:** $\forall i, \alpha_i \geq 0, (1 - y_i (w^\top x_i + b)) \leq 0, \alpha_i (1 - y_i (w^\top x_i + b)) = 0$
(2) **Dual:** $\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$ s.t. $(\alpha_i \geq 0) \wedge (\sum_i \alpha_i y_i = 0)$

Non-separable Case

Introduce slack variables $\xi_i := \max\{1 - y_i(w^\top x_i + b), 0\} = [1 - y_i(w^\top x_i + b)]_+$ into loss.

Primal: $\min_{w,b} \frac{1}{2}w^2 + C \sum_i \xi_i = \min_{w,b} \frac{1}{2}w^2 + C[1 - y_i(w^\top x_i + b)]_+$. Hinge loss $[1 - x]_+$.

Equivalent form: $\min_{w,b} \frac{1}{2}w^2 + C \sum_i \xi_i$ s.t. $y_i(w^\top x_i + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$

Dual: $\max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$ s.t. $\sum_i \alpha_i y_i = 0$ and $0 \leq \alpha_i \leq C$

Multi-class SVM

$\min_{w=[w_{0:K-1}], b=[b_{0:K-1}]} \frac{1}{2}\|w\|^2 + \sum_i C \xi_i$ s.t. $\xi_i \geq 0$ and $(w_y^\top x + b_y) - (w_{y'}^\top x + b_{y'}) \geq 1 - \xi_i, \forall y \neq y_i$

Structural SVM

y is structured, e.g. trees, maximum margin between y_i, y_j depends on their similarity, so the condition changes to $w^\top \Psi(x_i, y_i) - w^\top \Psi(x_i, y) \geq \Delta(y_i, y) - \xi_i, \forall y \neq y_i$.

7 Ensemble

Bagging Each bagged estimator have bias $\beta = \mathbb{E}(y - b(x))^2$, variance $\sigma^2 = \text{Var}b(x)$ covariance $\rho^2 = \text{Cov}(b(x), b'(x))/\sigma^2$. Then $\mathbb{E}(y - \sum_m b^{(m)}(x)/M)^2 = \beta^2 + \sum_m \mathbb{E}(\beta - b^{(m)}(x))^2/M^2 = \beta^2 + \sigma^2/M + \sigma^2 \rho^2(1 - 1/M)$. In class we assume $\rho = 0$. Anyway Bagging reduces variance. Random Forest is a case of Bagging. Bagging induces implicit regularization.

Adaboost Initial $w_i^{(0)} = 1/n$. For $t \in [M]$, (1) train $f_t(x) = \arg\min_{b(x)} \sum_i w_i^{(t)} \mathbb{I}_{y_i \neq b(x_i)}$ (2) error $\epsilon_t = (\sum_i w_i^{(t)} \mathbb{I}_{y_i \neq f_t(x_i)}) / \sum_i w_i^{(t)}$ (3) estimator weight $\alpha_t = \log(\frac{1-\epsilon_t}{\epsilon_t})$ (4) data weight $w_i^{(t+1)} = w_i^{(t)} e^{\alpha_t \mathbb{I}_{y_i \neq f_t(x_i)}}$

Prediction $\hat{c} = \text{sgn}(\sum_{t=1}^M \alpha_t f_t(x))$

Gradient Boosting Initial $f_0(x) = 0$. For $t \in [M]$, (1) train $(\alpha_t, b^{(t)}) \leftarrow \arg\min_{\alpha > 0, b \in \mathcal{H}} \sum_{i=1}^n L(y_i, \alpha b(x_i) + f_{t-1}(x_i))$ (2) update function $f_t(x) \leftarrow \alpha_t b^{(t)}(x) + f_{t-1}(x)$. **Prediction** $\hat{c}(x) = \text{sgn}(f_M(x))$. Adaboost is GB with $L(y, \hat{y}) = e^{-y\hat{y}}$.

8 Generative Models

ELBO $\ln p(y) = \ln \int p(y | \theta) p(\theta) d\theta = \ln \mathbb{E}_{\theta \sim q} \left[p(y | \theta) \frac{p(\theta)}{q(\theta)} \right] \geq \mathbb{E}_{\theta \sim q} \left[\ln \left(p(y | \theta) \frac{p(\theta)}{q(\theta)} \right) \right] = \mathbb{E}_{\theta \sim q} [\ln p(y | \theta)] - KL(q || p(\cdot))$

VAE Goal: Find a latent representation z of x with simple prior $p_\theta(z)$. Problem: $p_\theta(x) = \mathbb{E}_\theta p(x|z)$ intractable. Solution: use encoder net $q_e(x|z)$ and $q_d(z|x)$ to model conditional and posterior prob.

ELBO for VAE training loss $l = \sum \ln(p_\theta(x_i))$

$$\begin{aligned} \ln(p_\theta(x_i)) &= \mathbb{E}_{z \sim q_\phi(z|x_i)} [\ln p_\theta(x_i)] = \mathbb{E}_Z \left[\ln \frac{p_\theta(x_i | z) p_\theta(z)}{p_\theta(z | x_i)} \right] \\ &= \mathbb{E}_Z \left[\ln \frac{p_\theta(x_i | z) p_\theta(z)}{p_\theta(z | x_i)} \frac{q_\phi(z | x_i)}{q_\phi(z | x_i)} \right] \\ &= \mathbb{E}_Z [\ln p_\theta(x_i | z)] - \mathbb{E}_Z \left[\ln \frac{q_\phi(z | x_i)}{p_\theta(z)} \right] + \mathbb{E}_Z \left[\ln \frac{q_\phi(z | x_i)}{p_\theta(z | x_i)} \right] \\ &= \underbrace{\mathbb{E}_Z [\ln p_\theta(x_i | z)] - \text{KL}(q_\phi(z | x_i) || p_\theta(z))}_{\text{ELBO } \mathcal{L}(x_i, \theta, \phi)} \end{aligned}$$

+ $\text{KL}(q_\phi(z | x_i) || p_\theta(z | x_i)) \geq \text{ELBO}$.

Generative Adversarial Network: Generator G and Discriminator D . Optimize $\min_G \max_D V(D, G)$ where $V(D, G) = \mathbb{E}_{x \sim p_{\text{data}}(x)} [\ln D(x)] + \mathbb{E}_{z \sim p_z(z)} [\ln(1 - D(G(z)))]$

9 Convergence of SGD, Robbins-Monro

Loss gradient $\ell(\cdot)$, SGD update $z^{(t)} \leftarrow \ell(\theta^{(t)} + \gamma^{(t)}, \theta^{(t+1)} \leftarrow \theta^{(t)} - \eta^{(t)} z^{(t)}$, $\gamma^{(t)}$ noise.

Problem: Whether $\theta^\infty \rightarrow \arg\theta^* \mathbb{E}[\ell(\theta^*)] \triangleq 0$?

Assume: (1) $\mathbb{E}[\gamma] = 0$, (2) $\mathbb{E}[\gamma^2] = \sigma$ (3) $(\theta - \theta^*)\ell(\theta) > 0, \forall \theta \neq \theta^*$ (4) $\exists b, \ell(\theta) < b, \forall \theta$. If (1) $\eta^{(t)} \rightarrow 0$ (2) $\sum \eta^{(t)} = \infty$ (3) $\sum \eta^{(t)^2} < \infty$,

then $\mathbb{P}(\theta^* = \theta^{(t)}) \xrightarrow[t \rightarrow \infty]{} 1$.

Proof: $\mathbb{E}[(\theta^{(t+1)} - \theta^*)^2] = \mathbb{E}[(\theta^{(t)} - \theta^*) - \eta^{(t)} \ell(\theta^{(t)}) - \eta^{(t)} \gamma^{(t)}]^2$. $\gamma^{(t)}$ independent with $\theta^{(t)}, \ell(\theta^{(t)})$, so LHS = $\mathbb{E}[(\theta^* - \theta^{(t)})^2] - 2\eta^{(t)} \mathbb{E}[\ell(\theta^{(t)})](\theta^* - \theta^{(t)}) + \eta^{(t)^2} \mathbb{E}[\ell^2(\theta^{(t)})] + \mathbb{E}[\gamma^2(t)] \leq \mathbb{E}[(\theta^* - \theta^{(0)})^2] - 2 \sum_{i \leq t} \eta^{(i)} \mathbb{E}[\ell(\theta^{(i)})](\theta^* - \theta^{(i)}) + \sum_{i \leq t} \eta^{(i)^2} (b^2 + \sigma^2)$ Since $0 \leq \mathbb{E}[(\theta^* - \theta^{(t+1)})^2] < \infty$, $0 = \lim_{i \rightarrow \infty} \mathbb{E}[\ell(\theta^{(i)})](\theta^* - \theta^{(i)}) = \lim_{i \rightarrow \infty} \mathbb{P}(\theta^* = \theta^{(i)}) \mathbb{E}[\ell(\theta^{(i)})](\theta^* - \theta^{(i)}) | \theta^* = \theta^{(i)} + \mathbb{P}(\theta^* \neq \theta^{(i)}) \mathbb{E}[\ell(\theta^{(i)})](\theta^* - \theta^{(i)}) | \theta^* \neq \theta^{(i)}$, $\lim_{i \rightarrow \infty} \mathbb{P}(\theta^* \neq \theta^{(i)}) = 0$

10 Non-parametric Bayesian Inference (BI) Exact Conjugate Prior of Multivariate Gaussian

Data: $x_i \sim \mathcal{N}(\mu, \Sigma)$ i.i.d.. Inverse Wishart: $\Sigma \sim \mathcal{W}^{-1}(S, \nu) \propto |\Sigma|^{(\nu+p+1)/2} \exp(-\text{Tr}(\Sigma^{-1}S)/2)$.

Normal Inverse Wishart as conjugate prior: $p(\mu, \Sigma | m_0, k_0, \nu_0, S_0) = \mathcal{N}(\mu | m, \Sigma/k_0) \mathcal{W}^{-1}(\Sigma | S_0, \nu_0)$ Update rule: $m_p = (k_0 m_0 + N \bar{x}) / (k_0 + N)$, $k_p = k_0 + N$, $\nu_p = \nu_0 + N$, $S_p = S_0 + k_0 m_0 m_0^\top - k_p m_p m_p^\top + \sum (x_i - \bar{x})(x_i - \bar{x})^\top$.

BI with Semi-Conjugate Prior

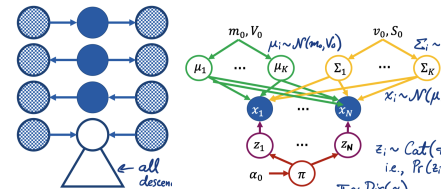
New prior: $\mu \sim \mathcal{N}(m_0, V_0)$, $\Sigma \sim \mathcal{W}^{-1}(S_0, \nu_0)$, then posterior $p(\mu, \Sigma | X)$ is intractable, but condition posterior is exact, $p(\mu | \Sigma, X) = \mathcal{N}(m_p, V_p)$, $V_p^{-1} = V_0^{-1} + N \Sigma^{-1}$, $V_p^{-1} m_p = V_0^{-1} m_0 + N \Sigma^{-1} \bar{x}$; $p(\Sigma | \mu, X) = \mathcal{W}^{-1}(S_p, \nu_p)$, $\nu_p = \nu_0 + N$, $S_p = S_0 + \sum x_i x_i^\top + N \mu \mu^\top - 2N \bar{x} \mu^\top$.

Gibbs sampling: random variable $p(z_1, \dots, z_p)$ intractable, cyclically resample z_i according to tractable conditional distribution $p(z_i | z_{\setminus i})$ n times, when $n \rightarrow \infty$, $(z_1, \dots, z_p) \sim p(z_1, \dots, z_p)$ Finally, replace posterior with MC sampling: $\mathbb{E}_{\theta|X} f(x|\theta) \approx \sum f(x|\theta_i)/N$

BI for Gaussian Mixture Model

Data model: latent K class variable $z_i \sim \text{Cat}(\pi)$, observed $x_i \sim \mathcal{N}(\mu_{z_i}, \Sigma_{z_i})$. Prior: $\mu_k \sim \mathcal{N}(m_0, V_0)$, $\Sigma_k \sim \mathcal{W}^{-1}(S_0, \nu_0)$, $\pi \sim \text{Dir}(\alpha) \propto \prod_k p_k^{\alpha_k - 1}$. Prior also intractable.

Goal Gibbs sampling for BI, but to simplify conditional distribution.



d-seperation: for verifying conditional independence. Given with observed variable set C , if every path from variable A to B is blocked on probability graph, then A and B are independent condition on C . By this thm: (1) z_i , z_j (2) μ , π (3) Σ , π all independent condition on other parameter. Sampling procedure: (1) $z^{(t)} \leftarrow p(\cdot | x, \mu^{(t-1)}, \Sigma^{(t-1)})$, (2) $\mu^{(t)} \leftarrow p(\cdot | x, \Sigma^{(t-1)}, z^{(t)})$, (3) $\Sigma^{(t)} \leftarrow p(\cdot | x, \mu^{(t)}, z^{(t)})$, (4) $\pi^{(t)} \leftarrow p(\cdot | x, z^{(t)})$

BI for Non-Parametric GMM

Goal: sample from infinite categorical distri. **Dirichlet Process (DP):** Θ parameter space, H prior distri on Θ , A_1, \dots, A_r arbitrary partition of Θ . G a categorical distribution over $\{A_i\}$ is $G \sim \text{DP}(\alpha, H)$ if $(G(A_1), \dots, G(A_r)) \sim \text{Dir}(\alpha H(A_1), \dots, \alpha H(A_r))$.

Posterior: $G | \{\theta_i\}_{i=1}^n \sim \text{DP}\left(\alpha + n, \frac{\alpha H + \sum_{i=1}^n \delta_{\theta_i}}{\alpha + n}\right)$

Condition on θ , Margin over G : $\theta_{n+1} | \theta_1, \dots, \theta_n \sim \frac{1}{\alpha + n} (\alpha H + \sum_{i=1}^n \delta_{\theta_i})$, Leads to CRP

Three Methods of Sampling from DP

In $K \rightarrow \infty$ GMM, θ in DP is z , G is π .

(1) Chinese Restaurant Process (CRP), sample z , marginalize over π :

$$p(z_n = k | \theta_{i < n}) = \begin{cases} n_k / (\alpha + n - 1), & \text{existing } k \\ \alpha / (\alpha + n - 1), & \text{new } k \end{cases}$$

Expect # of Class $\sum_{i=1}^n \frac{\alpha}{\alpha + i - 1} \approx e q \alpha \log(1 + \frac{n}{\alpha})$

(2) Stick-breaking Construction samples π :

$$\beta_k \sim \text{Beta}(1, \alpha), \theta_k^* \sim H, \pi_k = \beta_k \prod_{l=1}^{k-1} (1 - \beta_l)$$

(3) Marginalize over μ, Σ when sampling z (if intractable), less variance (Rao-Blackwell).

Exchangeability: $p(\{\theta_i\}) = \prod_{n=1}^N p(\theta_n | \{\theta_{i < n}\})$ unchanged after permuting sampling order.

DeFinetti's Thm any exchangeable distri is a mixture model $P(\{\theta_i\}) = \int \prod_{i=1}^n G(\theta_i) dP(G)$

11 PAC Learning

• A learning algorithm \mathcal{A} can learn $c \in C$ if there is a poly(\dots), s.t. for (1) any distribution \mathcal{D} on \mathcal{X} and (2) $\forall \epsilon \in [0, 1/2], \delta \in [0, 1/2]$, \mathcal{A} outputs $\hat{c} \in \mathcal{H}$ given a sample of size at least $\text{poly}(\frac{1}{\epsilon}, \frac{1}{\delta}, \text{size}(c))$ such that $\mathbb{P}(\mathcal{R}(\hat{c}) - \inf_{c \in C} \mathcal{R}(c) \leq \epsilon) \geq 1 - \delta$.

• \mathcal{A} is called an efficient PAC algorithm if it runs in polynomial of $\frac{1}{\epsilon}$ and $\frac{1}{\delta}$.

• C is (efficiently) PAC-learnable from \mathcal{H} if there is an algorithm \mathcal{A} that (efficiently) learns C from \mathcal{H} .

• VC inequality $\mathcal{R}(\hat{c}_n^*) - \mathcal{R}(c^*) \leq 2 \sup_{c \in C} |\hat{\mathcal{R}}_n(c) - \mathcal{R}(c)|$.

• $|C| < \infty$, feasible case $\min_{c \in C} \mathcal{R}(c) = 0$, $\mathbb{P}\{\mathcal{R}(\hat{c}_n^*) > \epsilon\} \leq |C| \exp(-n\epsilon)$. Proof $\mathbb{P}\{\mathcal{R}(\hat{c}_n^*) > \epsilon\} \leq \mathbb{P}\{\max_{c \in C: \hat{\mathcal{R}}_n(c)=0} \mathcal{R}(c) > \epsilon\} = \mathbb{E}\{\max_{c \in C} \mathbb{I}_{\{\hat{\mathcal{R}}_n(c)=0\}} \mathbb{I}_{\{\mathcal{R}(c) > \epsilon\}}\} \leq \sum_{c \in C: \mathcal{R}(c) > \epsilon} \mathbb{P}\{\hat{\mathcal{R}}_n(c) = 0\} \leq |C| \exp(-n\epsilon)$

• VC dim: max n s.t. $s(\mathcal{A}, n) = 2^n$. Growth function (shattering num) $s(\mathcal{A}, n)$ is the maximum number of concept class a hypothesis space can express. $s(\mathcal{A}, n) \leq \sum_{i=0}^V \binom{n}{i}$

• $|C| < \infty$, infeasible, $\mathbb{P}(\mathcal{R}(\hat{c}_n^*) - \inf_{c \in C} \mathcal{R}(c) > \epsilon) \leq 2|C| \exp(-2n\epsilon^2)$ is PAC-learnable. Proof $\mathcal{D}^m(\{S : \exists h \in \mathcal{H}, |L_S(h) - L_D(h)| > \epsilon\}) \leq \sum_{h \in \mathcal{H}} \mathcal{D}^m(\{S : |L_S(h) - L_D(h)| > \epsilon\})$, Hoeffding $\mathbb{P}[|L_S(h) - L_D(h)| > \epsilon] \leq 2 \exp(-2m\epsilon^2)$.

• C with $\dim_{VC} = d < \infty$ is PAC-learnable, $\mathbb{P}(\mathcal{R}(\hat{c}_n^*) - \inf_{c \in C} \mathcal{R}(c) > \epsilon) \leq 9n^d \exp(-\frac{n\epsilon^2}{32})$

A Appendix

(1) $\partial_x(AB) = A \partial_x B + (\partial_x A)B$, (2) $\partial_x A^{-1} = -A^{-1}(\partial_x A)A^{-1}$, (3) $\partial_x \ln \det A = \text{Tr}(A^{-1} \partial_x A)$.

Define $(\partial A)_{ij} := \partial_{a_{ji}} f$, then (4) $\partial_A \text{Tr}(BA) = \partial_A \text{Tr}(AB) = B$, (5) $\partial_A \ln \det A = A^{-1}$, (6) $\partial_A \text{Tr}(ABA^\top) = (B + B^\top)A^\top$, $\mathcal{N}(\mu, \Sigma) = (2\pi)^{-d/2} |\Sigma|^{-1/2} e^{-(x-\mu)^\top \Sigma^{-1} (x-\mu)/2}$, Conditional $\mathbb{E}[y_2 | y_1] = \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (y_1 - \mu_1)$, $\text{Cov}[y_2 | y_1] = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$. Marginal $\mathbb{E}(y_2) = \mu_2$, $\text{Cov}[y_2] = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$.

Markov $\mathbb{P}\{X \geq \epsilon\} \leq \mathbb{E}[X]/\epsilon$. Hoeffding (1) $\mathbb{E}[X] = 0, X \in [a, b], \mathbb{E}[\exp(sX)] \leq \exp(s^2(b-a)^2/8)$ (2) $X_i \in [a_i, b_i], S_n = \sum_{i=1}^n X_i, \mathbb{P}\{S_n - \mathbb{E} S_n \leq t\} \leq \exp(-2t^2 / \sum_{i=1}^n (b_i - a_i)^2)$