1 Maximum Likelihood Estimator

- Consitent,asymptotic unbiased. $\hat{\theta}_n^{\text{MLE}} \xrightarrow{\mathbb{P}} \theta_0$.
- Asymptotic normal. $\sqrt{n}(\hat{\theta}_n^{\text{MLE}} - \theta_0) \xrightarrow{\mathcal{D}} \mathcal{N}(0, I_n)$, $I_n(\theta_0) = \mathbb{E}[-\dot{s}_\theta] = \mathbb{E}[s_\theta s_\theta^\top]$ 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 $n \to \infty$. $\hat{\theta}^{\text{MLE}}$ not efficient if n finite. Stein estimator always better.
- Equivariance, if $\hat{\theta}_n$ is MLE, $\hat{\gamma} = g(\hat{\theta}^{\text{MLE}})$ is MLE of $\mathcal{L}(g^{-1}(\gamma))$. Proof by optimally 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

Let D be the training dataset and $\hat{f}$ be the predictive function. $\mathbb{E}_D \mathbb{E}_{Y|X}(\hat{f}(X) - Y)^2 = \mathbb{E}_D \mathbb{E}_{Y|X}[(\hat{f}(X) - \mathbb{E}_{Y|X} Y)^2 + (\mathbb{E}_{Y|X} Y - Y)^2] = \mathbb{E}_D(\hat{f}(X) - \mathbb{E}(Y \mid X))^2 + \mathbb{E}_D(\mathbb{E}(Y \mid X) - Y)^2 = \mathbb{E}_D(\hat{f}(x) - \mathbb{E}_D \hat{f}(x))^2 + \left(\mathbb{E}_D \hat{f}(x) - \mathbb{E}(Y \mid X)\right)^2 + \mathbb{E}_D(\mathbb{E}(Y \mid X) - Y)^2$. It means that expected square error (training) = variance of prediction + squared bias + variance of 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 (maximum a posterior) estimation. A Gaussian prior on β is equivalent to Ridge and a Laplacian prior is equivalent to Lasso. Using SVD, we get Ridge has built-in model selection: $X\beta^{\text{Ridge}} = \sum_{j=1}^d [d_j^2/(d_j^2 + \lambda)] u_j u_j^T Y$ (each $u_j u_j^T Y$ can be viewed as a model). Lasso has more sparse estimations because the gradient of regularization does not shrink as in the case of 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 $\beta | X, Y \sim \mathcal{N}(\mu_\beta, \Sigma_\beta)$, $\Sigma_\beta = (\sigma^{-2} X^T X + \Lambda)^{-1}$, $\mu_\beta = \sigma^2 \Sigma_\beta X^T Y$.

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) $k(x, x') = \phi(x)^T \phi(x')$ 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: let $V \sim \mathcal{N}(0, K_1)$, $W \sim \mathcal{N}(0, k_2)$ and is independent to V, then $\textbf{Cov}(V_i W_i, V_j W_j) = \textbf{Cov}(V_i, V_j)\textbf{Cov}(W_i, W_j) = k_1 \cdot k_2(x_i, x_j)$. (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 $k(x, y) = e^{-\|x-y\|^2/2\sigma^2} = e^{-\|x\|^2/2\sigma^2} \times e^{x^T y/2\sigma^2} \times e^{-\|y\|^2/2\sigma^2}$ is valid. (1) $x^T y$ linear kernel is valid (2) then $\exp(\frac{1}{\sigma^2} x^T y)$ 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

1. 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.
2. Probabilistic Discriminative, modeling $p(y \mid x)$: (1) probability for prediction, (2) medium computational cost and (3) medium bias.
3. 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 $p(x, y) = p(y) p(x \mid y)$. Since y has finite states, model $p(y)$ and $p(x \mid y)$ for different y. The modeling requires to (1) guess a distribution family and (2) infer parameters by MLE.

Compute $p(y \mid x)$ by discriminant analysis (DA)

Linear DA

Goal: classify a sample into two Gaussian distribution with $\Sigma_0 = \Sigma_1$. After calculation, $p(y = 1 \mid x) = 1/(1 + \exp(-\log \frac{p(x|y=1)p(y=1)}{p(x|y=0)p(y=0)})) = 1/(1 + \exp(w_1^T x + w_0))$ since the quadratic term is eliminated due to $\Sigma_0 = \Sigma_1$.

Quadratic DA

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

Optimization Methods

Optimal Learning Rate for Gradient Descent

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

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

However, naive gradient descent has two weaknesses: (1) it often has a zig-zag behavior, especially in a very narrow, long and slightly downward valley; (2) the gradient update is small near the stationary point. This can be mitigated by adding a momentum term in the update: $w^{k+1} = w^k - \eta \nabla L(w^k) + \mu^k (w^k - w^{k-1})$ which speeds the update towards the "common" direction.

Newton's Method

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

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. $p(w \mid X, Y) \propto p(w, X, Y) \propto \exp(-R(w))$, where $R(w) = -\log p(w, X, Y)$. Let $w^* = \textbf{argmin} R(w)$ be the MAP estimation and Taylor-expand $R(w)$ at w^*: $R(w) \approx R(w^*) + \frac{1}{2}(w - w^*)^T H_R(w^*)(w - w^*)$. Therefore, $p(w \mid X, Y) \propto \exp(-R(w^*) - \frac{1}{2}(w - w^*)^T H_R(w^*)(w - w^*))$ and thus $(w \mid X, Y) \sim \mathcal{N}(w^*, H_R^{-1}(w^*))$.

AIC & BIC

- Define $\text{BIC} = k \log N - 2 \log \hat{L}$, where k is #parameters and $\hat{L}$ is the likelihood $p(x \mid w^*)$. 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

Goal: for $y_i \in \{0, 1\}$, find w, s.t. $y_i w^T x_i > 0$ for any i. The classification function is $c(x) = \textbf{sgn}(w^T x)$.

$L(y, c(x)) = 0$ if $y w^T x > 0$ and $L(y, c(x)) = -y w^T x$ o.w. By gradient descent, the Perceptron is guaranteed to converge if (1) the data is linearly separable, (2) learning rate $\eta(k) > 0$, (3) $\sum_k \eta(k) \to +\infty$ and (4) $(\sum_k \eta(k)^2)/(\sum_k \eta(k))^2 \to 0$. However, there exists multiple solutions if the data is linearly separable.

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., $\max(w^T u_1 - w^T u_0)^2/(w^T S w)$, 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 Constrain

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) $\exists \overline{x}$ s.t. $g_i(\overline{\mathbf{x}}) < 0$ and $h_j(\overline{\mathbf{x}}) = 0$, 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: $\max_{w,b}\left\{\frac{1}{\|w\|}\min_i y_i(w^\top x_i+b)\right\} \Leftrightarrow \max_{w,b,t} t$ 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 $(w_{y_i}^\top x + b_{y_i}) - (w_y^\top x + b_y) \geq 1-\xi_i, \forall y \neq y_i$

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 $\sigma^2 = \mathrm{Var} b(x)$ covariance $\rho^2 = \mathrm{Cov}(b(x), b'(x))/\sigma^2$. 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 $f_t(x) = \mathrm{argmin}_{b(x)} \sum w_i^{(t)} \mathbb{I}_{\{y_i \neq b(\mathbf{x}_i)\}}$ (2) error $\epsilon_t = (\sum w_i^{(t)}\mathbb{I}_{\{y_i\neq f_t(x_i)\}})/\sum w_i^{(t)}$ (3) estimator weight $\alpha_t = \log(\frac{1-\epsilon_t}{\epsilon_t})$ (4) data weight $w_i^{(t+1)} = w_i^{(t)} e^{\alpha_t \mathbb{I}_{\{y_i\neq f_t(\mathbf{x}_i)\}}}$

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

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** $\hat{c}(x) = \mathrm{sgn}(f_M(x))$. Adaboost is GB with $L(y,\hat{y}) = e^{-y\hat{y}}$.

8 Generative Models

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

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 $l = \sum\log(p_\theta(x_i))$

$$\log(p_\theta(x_i)) = \mathbb{E}_{Z\sim q_\phi(z|x_i)}[\log p_\theta(x_i)] = \mathbb{E}_Z\left[\log\frac{p_\theta(x_i\mid z)p_\theta(z)}{p_\theta(z\mid x_i)}\right]$$
$$= \mathbb{E}_Z\left[\log\frac{p_\theta(x_i\mid z)p_\theta(z)}{p_\theta(z\mid x_i)}\frac{q_\phi(z\mid x_i)}{q_\phi(z\mid x_i)}\right]$$
$$= \mathbb{E}_Z[\log p_\theta(x_i\mid z)] - \mathbb{E}_Z\left[\log\frac{q_\phi(z\mid x_i)}{p_\theta(z)}\right] + \mathbb{E}_Z\left[\log\frac{q_\phi(z\mid x_i)}{p_\theta(z\mid x_i)}\right] =$$
$$\underbrace{\mathbb{E}_Z[\log p_\theta(x_i\mid z)] - D_{KL}(q_\phi(z\mid x_i)\|p_\theta(z))}_{\mathcal{L}(x_i,\theta,\phi)} + \underbrace{D_{KL}(q_\phi(z\mid x_i)\|p_\theta(z\mid x_i))}_{\geq 0}$$

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

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 $\theta^\infty \to \arg_{\theta^*}\mathbb{E}[\ell(\theta^*)] \triangleq 0$?
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) $\eta^{(t)} \to 0$ (2) $\sum\limits_{t<\infty}\eta(t) = \infty$ (3) $\sum\limits_{t<\infty}\eta^2(t) < \infty$, then $\mathbb{P}\left(\theta^* = \theta^{(t)}\right) \xrightarrow[t\to\infty]{} 1$.

Proof: $\mathbb{E}[(\theta^{(t+1)}-\theta^*)^2] = \mathbb{E}[((\theta^{(t)}-\theta^*) - \eta(t)l(\theta^{(t)}) - \eta(t)\gamma^{(t)})^2]$. $\gamma^{(t)}$ independent with $\theta^{(t)}$, $\ell(\theta^{(t)})$, so LHS $= \mathbb{E}[(\theta^*-\theta^{(t)})^2] - 2\eta(t)\mathbb{E}[\ell(\theta^{(t)})(\theta^*-\theta^{(t)})] + \eta^2(t)(\mathbb{E}[\ell^2(\theta^{(t)})] + \mathbb{E}[\gamma^2(t)]) \leq \mathbb{E}[(\theta^*-\theta^{(0)})^2] - 2\sum_{i\leq t}\eta(i)\mathbb{E}[\ell(\theta^{(i)})(\theta^*-\theta^{(i)})] + \sum_{i\leq t}\eta^2(i)\left(b^2+\sigma^2\right)$ Since $0 \leq \mathbb{E}[(\theta^*-\theta^{(t+1)})^2] \not< -\infty$, $0 = \lim\limits_{i\to\infty}\mathbb{E}[\ell(\theta^{(i)})(\theta^*-\theta^{(i)})] = \lim\limits_{i\to\infty}\mathbb{P}(\theta^*=\theta^{(i)})\mathbb{E}[\ell(\theta^{(i)})(\theta^*-\theta^{(i)})|\theta^*=\theta^{(i)}] + \mathbb{P}(\theta^*\neq\theta^{(i)})\mathbb{E}[\ell(\theta^{(i)})(\theta^*-\theta^{(i)})|\theta^*\neq\theta^{(i)}]$, $\lim\limits_{i\to\infty}\mathbb{P}\left(\theta^*\neq\theta^{(i)}\right) = 0$

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: $\Sigma \sim \mathcal{W}^{-1}(S,v) \propto |\Sigma|^{(v+p+1)/2}\exp(-\mathrm{Tr}(\Sigma^{-1}S)/2)$.
Normal Inverse Wishart as conjugate prior: $p(\mu,\Sigma|m_0,k_0,v_0,S_0) = \mathcal{N}(\mu|m,\Sigma/k_0)\mathcal{W}^{-1}(\Sigma|S_0,v_0)$
Update rule: $m_p = (k_0m_0 + N\overline{x})/(k_0+N)$, $k_p = k_0+N$, $v_p = v_0+N$, $S_p = S_0 + k_0m_0m_0^\top - k_pm_pm_p^\top + \sum(x_i-\overline{x})(x_i-\overline{x})^\top$.

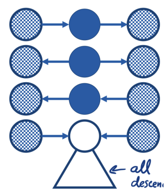
BI with Semi-Conjugate Prior

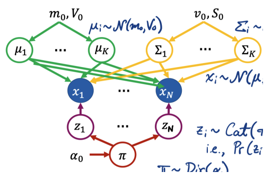
New prior: $\mu\sim\mathcal{N}(m_0,V_0)$, $\Sigma\sim\mathcal{W}^{-1}(S_0,v_0)$, then posterior $p(\mu,\Sigma|X)$ is intractable, but condition posterior is exact, $p(\mu|\Sigma,X) = \mathcal{N}(m_p,V_p)$, $V_p^{-1} = V_0^{-1} + N\Sigma^{-1}$, $V_p^{-1}m_p = V_0^{-1}m_0 + N\Sigma^{-1}\overline{x}$; $p(\Sigma|\mu,X) = \mathcal{W}^{-1}(S_p,v_p)$, $v_p = v_0+N$, $S_p = S_0 + \sum x_ix_i^\top + N\mu\mu^\top - 2N\overline{x}\mu^\top$.

Gibbs sampling: random variable $p(z_1,\cdots,z_p)$ intractable, cyclically resample z_i according to tractable conditional distribution $p(z_i|z_{/i})$ n times, when $n\to\infty$, $(z_1,\cdots,z_p)\sim p(z_1,\cdots,z_p)$
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 $z_i\sim\mathrm{Cat}(\pi)$, observed $x_i\sim\mathcal{N}(\mu_{z_i},\Sigma_{z_i})$. Prior: $\mu_k\sim\mathcal{N}(m_0,V_0)$, $\Sigma_k\sim\mathcal{W}^{-1}(S_0,v_0)$, $\pi\sim\mathrm{Dir}(\alpha) \propto \prod_k^K p_k^{\alpha_k-1}$. 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) $z^{(t)} \leftarrow p\left(\cdot|x,\mu^{(t-1)},\Sigma^{(t-1)}\right)$, (2) $\mu^{(t)} \leftarrow p\left(\cdot|x,\Sigma^{(t-1)},z^{(t)}\right)$, (3) $\Sigma^{(t)} \leftarrow p\left(\cdot|x,\mu^{(t)},z^{(t)}\right)$, (4) $\pi^{(t)} \leftarrow p\left(\cdot|x,z^{(t)}\right)$

BI for Non-Parametric GMM

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

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

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

Three Methods of Sampling from DP

In $K\to\infty$ 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 $\sum_{i=1}^n\frac{\alpha}{\alpha+i-1}\sim eq\alpha\log\left(1+\frac{n}{\alpha}\right)$

(2) Stick-breaking Construction samples π: $\beta_k\sim\mathrm{Beta}(1,\alpha)$, $\theta_k^*\sim H$, $\pi_k = \beta_k\prod_{l=1}^{k-1}(1-\beta_l)$

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

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(.,.), 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 poly($\frac{1}{\epsilon}$, $\frac{1}{\delta}$, size(c)) such that $P(\mathcal{R}(\hat{c}) - \inf_{c\in C}\mathcal{R}(c) \leq \epsilon) \geq 1-\delta$.
- $\mathcal{A}$ 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 $\mathcal{H}$.
- Finite $\mathcal{C}$, $\mathbf{P}(\mathcal{R}(\hat{c}_n^*) - \inf_{c\in\mathcal{C}}\mathcal{R}(c) > \epsilon) \leq 2|\mathcal{C}|\exp\left(-\frac{n\epsilon^2}{2}\right)$ is PAC-learnable.
- $\mathcal{C}$ with $\dim_{VC} = d < \infty$ is PAC-learnable, $\mathbf{P}(\mathcal{R}(\hat{c}_n^*) - \inf_{c\in\mathcal{C}}\mathcal{R}(c) > \epsilon) \leq 9n^d\exp\left(-\frac{n\epsilon^2}{32}\right)$

A Appendix

(1) $\partial_x(AB) = A\partial_xB + (\partial_xA)B$, (2) $\partial_xA^{-1} = -A^{-1}(\partial_xA)A^{-1}$, (3) $\partial_x\ln\det A = \mathrm{Tr}\left(A^{-1}\partial_xA\right)$,

Define $(\partial_Af)_{ij} := \partial_{a_{ji}}f$, then (4) $\partial_A\mathrm{Tr}(BA) = \partial_A\mathrm{Tr}(AB) = B$, (5) $\partial_A\ln\det A = A^{-1}$, (6) $\partial_A\mathrm{Tr}(ABA^\top) = (B+B^\top)A^\top$,

$\mathcal{N}(\mu,\Sigma) = (2\pi)^{-d/2}|\Sigma|^{-1/2}e^{-(x-\mu)^T\Sigma^{-1}(x-\mu)/2}$, Conditional $\mathbb{E}[y_2|y_1] = \mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(y_1-\mu_1)$, $\mathrm{Cov}[y_2\mid y_1] = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}$. Marginal $\mathbb{E}(y_2) = \mu_2$, $\mathrm{Cov}[y_2] = \Sigma_{22}$

$(A+UC^{-1}V)^{-1} = A^{-1} - A^{-1}U(C+VA^{-1}U)^{-1}VA^{-1}$.