## 1 Maximum Likelihood Estimator

Three properties of maximum likelihood esti-

- 1.  $\theta_{ML}$  is consistent.  $\theta_{ML} \to \theta_0$  when  $n \to \infty$ .
- 2.  $\theta_{ML}$  is asymptotically normal.  $\sqrt{n}(\theta_{ML} \theta_0$ ) ~  $\mathcal{N}(0, I_n(\theta_0))$  when  $n \to \infty$  and  $I_n(\theta_0)$ is the fisher information.
- 3.  $\theta_{ML}$  is asymptotically efficient.  $\theta_{ML}$  mi- **3** BLR and GP nimizes  $\mathbb{E}(\theta - \theta_0)^2$  when  $n \to \infty$  because the asymptotic variance equals the Rao-Cramer bound (MLE is asymptotically unbiased). Note: when *n* is finite,  $\theta_{ML}$  is not necessarily efficient, e.g., Stein estimator is

Rao-Cramer bound: for any unbiased estimator  $\hat{\theta}$  of  $\theta_0$ ,  $\mathbb{E}(\hat{\theta} - \theta_0)^2 \geq 1/I_n(\theta_0)$ , where  $I_n(\theta) = -\mathbb{E}(\frac{\partial^2}{\partial \theta^2} \log f(X; \theta) \mid \theta) =$  $\mathbb{E}(\frac{\partial}{\partial \theta} \log f(X; \theta) \mid \theta)^2$  is the fisher informati-

Sketch of Proof: define  $\Lambda = \frac{\partial \log P(X;\theta)}{\partial \theta}$ . Cauchy-Schwarz says  $Cov^2(\Lambda, \hat{\theta}) \leq Var(\Lambda)Var(\hat{\theta}) =$  $\mathbb{E}(\Lambda^2)$ **Var** $(\hat{\theta})$  because  $\mathbb{E}\Lambda = 0$ . Note that  $\mathbf{Cov}(\Lambda, \hat{\theta}) = \mathbb{E}(\Lambda \hat{\theta}) = \int_{X} \hat{\theta}(x) \frac{\partial}{\partial \theta} f(x; \theta) dx =$  $\frac{\partial}{\partial \theta} \int_X \hat{\theta}(x) f(x;\theta) dx = \frac{\partial}{\partial \theta} \mathbb{E} \hat{\theta} = 1$ . Therefore, A function is a kernel iff k(x,x') = k(x',x) (sym- $\operatorname{Var}(\hat{\theta}) \geq 1/\mathbb{E}(\Lambda^2)$ .

However, when the dimension of problem goes to infinity while keeping the data-dim ratio 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  $\beta$  is equivalent to Ridge and a Laplacian prior is equivalent to Lasso. Using

tion:  $X\beta^{\text{Ridge}} = \sum_{i=1}^{d} [d_i^2/(d_i^2 + \lambda)] u_i u_i^T Y$  (each  $u_i u_i^T Y$  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.

## **Bayesian Linear Regression**

 $Y = X\beta + \epsilon$ ,  $\epsilon \sim \mathcal{N}(0, \sigma^2)$  and a prior  $\beta \sim$  $\mathcal{N}(0,\Lambda^{-1})$ . By Bayesian,  $\beta \mid X,Y \sim \mathcal{N}(\mu_{\beta},\Sigma_{\beta})$ , where  $\mu_{\beta} = (X^T X + \sigma^2 \Lambda)^{-1} X^T Y$  and  $\Sigma_{\beta} =$ universally more efficient for single sam-  $\sigma^2(X^TX + \sigma^2\Lambda)^{-1}$ . MAP estimation of this prior (i.e.,  $\mu_{\beta}$ ) is equivalent to Ridge regression given  $\Lambda = \lambda I$  and  $\sigma = 1$ .

When  $\Lambda = \lambda I$ , under the prior,  $Y \sim$  $\mathcal{N}(0, \frac{1}{1}X^TX + \sigma^2I)$ . Therefore,  $\mathbf{Cov}(y_i, y_i) =$  $\frac{1}{\lambda}x_i^Tx_i$ . It means a prior that closer samples is more similar, i.e.,  $Cov(y_i, y_i)$  is large when  $x_i^T x_i$  is large. The kernel  $X^T \Lambda^{-1} X$  is thus called linear kernel. When a general kernel is used, Gaussian Process appears.

### **Gaussian Process**

Kernel Function

metry) and  $\int_{\Omega} k(x,x')f(x)f(x')dxdx' \ge 0$  for any  $f \in L_2$  and  $\Omega \in \mathbb{R}^d$  (semi-positiveness in continuous case) or K(X) is a valid covariance matrix for any X (semi-positiveness in discrete case). The latter is equivalent to either (1)  $\sum_{i,j} a_i a_j K(x_i, x_j) \ge 0$  for any  $a_{i,j}$  and  $k_{i,j}$ , or (2)  $k(x,x') = \phi(x)^T \phi(x')$  for some  $\phi$ .

Assume  $k_{1,2}$  are valid kernels, then the following are valid kernels:

- 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  $Cov(V_iW_i, V_iW_i) =$  $Cov(V_i, V_i) Cov(W_i, W_i) = k_1 \cdot k_2(x_i, x_i).$
- 3.  $k(x, x') = ck_1(x, x')$  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 poly-
- 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  $\phi$ . Example: RBF kernel  $k(x,y) = \exp(-\frac{1}{2\sigma^2}||x - y||^2)$  $|y|^2 = \exp(-\frac{1}{2\sigma^2}||x||^2)\exp(\frac{1}{\sigma^2}x^Ty)\exp(-\frac{1}{2\sigma^2}||y||^2)$  However, naive gradient descent has two separable.

SVD, we get Ridge has built-in model selec- is valid. Since  $x^Ty$  is the linear kernel and thus  $\exp(\frac{1}{\sigma^2}x^Ty)$  is a valid kernel, let  $f(x) = \exp(-\frac{1}{2\sigma^2}||x||^2)$ , we get the RBF function equals f(x)k(x,y)f(y), which is a valid kernel.

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.  $k(x, x') = \sum_{i} \lambda_{i} e_{i}(x) e_{i}(x').$ 

## **Conditional Gaussian**

 $\mathbb{E}(y_2 \mid y_1) = \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (y_1 - \mu_1), \mathbf{Var}(y_2 \mid y_1) =$  $\Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$ .

## 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  $\eta^* = \operatorname{argmin}_n L(w^k - \eta \cdot \nabla L(w^k))$ . By Taylor expansion of  $L(w^{k+1})$  at  $w^k$  and solve for the optimal  $\eta$ , we get  $\eta^* =$  $||\nabla L(w^k)||^2$  $\overline{\nabla L(w^k)^T H_L(w^k) \nabla L(w^k)}$ .

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  $w^{k+1}$ :  $L(w) \approx L(w) + (w - w^k)^T \nabla L(w^k) +$  $\frac{1}{2}(w-w^k)^T H_L(w^k)(w-w^k) \implies w^{k+1} = w^k - w^k$  $H_{\tau}^{-1}(w^k)\nabla L(w^k)$ .

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  $w^* = \operatorname{argmin} R(w)$  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,  $p(w \mid X, Y) \propto \exp(-R(w^*) - \frac{1}{2}(w - w^*))$  $(w^*)^T H_R(w^*)(w-w^*)$  and thus  $(w \mid X,Y) \sim$  $\mathcal{N}(w^*, H_R^{-1}(w^*)).$ 

AIC & BIC

- Define 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 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) = $sgn(w^Tx)$ .

L(y,c(x)) = 0 if  $yw^Tx > 0$  and L(y,c(x)) = $-yw^Tx$  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)  $\sum_{k} \eta(k) \rightarrow +\infty$  and (4)  $(\sum_{k} \eta(k)^2)/(\sum_{k} \eta(k))^2 \rightarrow 0$ . However, there exists multiple solutions if the data is linearly

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 Convex Optimization

Definition: the objective is convex and the feasible set is convex. The standard form is to minimize a convex function (f(w)) for convex f) under affine equality constraint  $(g_i(w) = 0)$ for affine  $g_i$ ) and convex non-positive constraint  $(h_i(w) \leq 0 \text{ for convex } h_i)$ .

#### **How to Solve**

- (1) Define Lagrangian:  $L(w, \lambda, \alpha) = f(w) +$  $\sum_{i} \lambda_{i} g_{i}(w) + \sum_{i} \alpha_{i} h_{i}(w)$  and  $\alpha_{i} \geq 0$ .
- (2) Check whether strong duality holds using Slater's condition (sufficient but not necessary): there is a strictly feasible point, i.e.,  $\exists w_0$ , s.t.  $g_i(w_0) = 0$  and  $h_i(w_0) < 0$ .
- (3) Solve for dL(w) = 0,  $g_i(w) = 0$ ,  $\alpha \ge 0$ ,  $h_i(w) \leq 0$  and  $\alpha_i h_i(w) = 0$  (complementary slackness).
- (4) Weak duality always holds and when Slater's condition holds it equals  $\min_{w} f(w)$ : solve  $\max_{\lambda,\alpha} \Theta(\lambda,\alpha)$  s.t.  $\alpha \geq 0$ , where  $\Theta(\lambda,\alpha) = 0$  $\min_{w} L(w, \lambda, \alpha)$ . The optimal in the weak duality is a lower bound for  $\min_{w} f(w)$  since  $\Theta(\lambda, \alpha) \leq \min_{w} f(w)$  for any  $\lambda$  and  $\alpha$ .

## 6 Support Vector Machine **Hard-Margin SVM**

The optimization form is to minimize  $\frac{1}{2}||w||^2$ s.t.  $y_i(w^Tx_i + w_0) \ge 1$   $(y_i \in \{-1, 1\})$ . It is convex and the Slater's condition holds under the assumption of linear separability.

By solving  $\min_{w,w_0} L(w, w_0, \alpha)$ , the duality form is  $\max_{\alpha} -\frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_i \alpha_i$ , s.t.  $\alpha_i \ge 0$ ,  $\sum_i \alpha_i y_i = 0$ .  $\dot{w}^* = \sum_{i \in \text{support vec}} \alpha_i^* y_i x_i$ .

## **Soft-Margin SVM & Kernel SVM**

When the data is not linearly separable, 8 Generative Models one solution is to add slack variables:  $\min_{\xi, w, w_0} \frac{1}{2} ||w||^2 + C \sum_i \xi_i$ , s.t.  $y_i(w^T x_i + w_0) \ge$  $1 - \xi_i$  and  $\xi_i \ge 0$ . Note: when the data is linearly separable, soft-margin does not necessarily produce the same cut-plane as the hard-margin SVM, especially when the margin is small due to few support vectors. When  $C \to \infty$ , it becomes hard-margin SVM.

The only difference in the dual form is that we need an extra condition  $0 \le \alpha \le C$ .  $\xi_i^* =$  $\max(0, 1 - v_i(w^{*T}x_i + w_0)).$ 

Another solution, Kernel SVM, is to use  $K(x_i, x_i) = \phi(x_i)^T \phi(x_i)$  to replace  $x_i^T x_i$ .

#### **Multi-class SVM**

Idea: use M := #class hyperplanes and maximize the generalized margin: min  $\sum_{i=1}^{M} w_i^T w_i$ s.t.  $w_{v_i}^T x_i + w_{v_i,0} - \max_{v \neq v_i} w_v^T x_i + w_{v,0} \ge 1$ .

## Structural SVM

Goal: predict a structured output label, e.g.,

Difficulty of predicting structures:

- 1. Compact representation of output space. Sol: use a score function and feature map  $\hat{y} = \operatorname{argmax}_{x} w^{T} \Psi(x, y).$
- 2. Efficient prediction (cannot use bruteforce search to find argmax). Sol: assume structures such as decomposable output spaces.
- 3. Define prediction error (cannot use 0/1 errors). Sol: use a loss function  $\Delta(y, \hat{y})$ .
- 4. Efficient training (cannot evaluate all constraints). Sol: iteratively add new constraints to the training.

 $\min_{\mathbf{w}, \boldsymbol{\xi} > 0} \frac{1}{2} \mathbf{w}^{\top} \mathbf{w} + C \sum_{i=1}^{n} \xi_{i}, \text{ s.t. } \mathbf{w}^{\top} \Psi (z_{i}, \mathbf{y}_{i}) \max_{z \neq z_i} [\Delta(z, z_i) + \mathbf{w}^\top \Psi(z, \mathbf{y}_i)] \ge -\xi_i, \forall \mathbf{y}_i \in \mathcal{Y}.$ 

## 7 Ensemble

#### **Random Forest**

Random feature selection induces regulation. Adaboost

Classifier weight  $\alpha_t = \frac{1}{\text{weighted err}_t} - 1$ . Sample weight  $w_{t+1} = \alpha_t w_t$  for mislabeled samples, o.w. unchanged.

Adaboost has following properties:

- 1. It minimizes exponential loss forwardly.
- 2. It trains max-margin classifiers.
- 3. It, as well as Random Forest, is spiky selfaveraging interpolators, which localize the effect of noise.
- 4. It falls into the double descent regime: over-parameterized models can have better generalization.

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

**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  $l = \sum \log(p_{\theta}(x_i))$ 

$$\begin{split} &\log\left(p_{\theta}\left(x_{i}\right)\right) = \mathbb{E}_{Z \sim q_{\phi}\left(z|x_{i}\right)}\left[\log p_{\theta}\left(x_{i}\right)\right] = \mathbb{E}_{Z}\left[\log\frac{p_{\theta}\left(x_{i}\mid z\right)p_{\theta}(z)}{p_{\theta}\left(z\mid x_{i}\right)}\right] \\ &= \mathbb{E}_{Z}\left[\log\frac{p_{\theta}\left(x_{i}\mid z\right)p_{\theta}(z)}{p_{\theta}\left(z\mid x_{i}\right)}\frac{q_{\phi}\left(z\mid x_{i}\right)}{q_{\phi}\left(z\mid x_{i}\right)}\right] \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - \mathbb{E}_{Z}\left[\log\frac{q_{\phi}\left(z\mid x_{i}\right)}{p_{\theta}(z)}\right] + \mathbb{E}_{Z}\left[\log\frac{q_{\phi}\left(z\mid x_{i}\right)}{p_{\theta}\left(z\mid x_{i}\right)}\right] = \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}(z)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)||p_{\theta}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x_{i}\mid z\right)\right] - D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)\right) + D_{KL}\left(q_{\phi}\left(z\mid x_{i}\right)\right) \\ &= \mathbb{E}_{Z}\left[\log p_{\theta}\left(x\mid x_{i}\right)\right] + D_{KL}\left[q_{\phi}\left(z\mid x_{i}\right)\right] + D_{KL}$$

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

# 9 Convergence of SGD, Robbins-Monro 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: $\Sigma \sim$ $\mathcal{W}^{-1}(S, v) \propto |\Sigma|^{(v+p+1)/2} \exp(-\operatorname{Tr}(\Sigma^{-1}S)/2).$

**Normal Inverse Wishart** as conjugate prior:  $p(\mu, \Sigma | m_0, k_0, v_0, S_0) = \mathcal{N}(\mu | m, \Sigma / k_0) \mathcal{W}^{-1}(\Sigma | S_0, v_0) \mathbf{Posterior}: G | \{\theta_i\}_{i=1}^n \sim \mathrm{DP}\left(\alpha + n, \frac{\alpha H + \sum_{i=1}^n \delta_{\theta_i}}{\alpha + n}\right)$ Update rule:  $m_p = (k_0 m_0 + N \bar{x})/(k_0 + N), k_p =$  $k_0 + N$ ,  $v_p = v_0 + N$ ,  $S_p = S_0 + k_0 m_0 m_0^{\top}$  $k_n m_n m_n^{\top} + \sum (x_i - \overline{x})(x_i - \overline{x})^{\top}$ .

## **BI with Semi-Conjugate Prior**

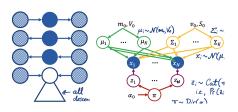
New prior:  $\mu \sim \mathcal{N}(m_0, V_0)$ ,  $\Sigma \sim \mathcal{W}^{-1}(S_0, v_0)$ , then posterior  $p(\mu, \Sigma | X)$  is intractable, but condition posterior is exact,  $p(\mu|\Sigma,X) =$  $\mathcal{N}(m_p, V_p), V_p^{-1} = V_0^{-1} + N\Sigma^{-1}, V_p^{-1}m_p =$  $V_0^{-1} m_0 + N \Sigma^{-1}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

**Gibbs sampling:** random variable  $p(z_1, \dots, z_n)$ intractable, cyclically resample  $z_i$  according to tractable conditional distribution  $p(z_i|z_{/i})$  n times, when  $n \to \infty$ ,  $(z_1, \dots, z_n) \sim p(z_1, \dots, z_n)$ 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  $z_i \sim$  $Cat(\pi)$ , observed  $x_i \sim \mathcal{N}(\mu_{z_i}, \Sigma_{z_i})$ . Prior:  $\mu_k \sim$  $\mathcal{N}(m_0, V_0), \ \Sigma_k \sim \mathcal{W}^{-1}(S_0, v_0), \ \pi \sim \operatorname{Dir}(\alpha) \propto$  $\prod_{k}^{K} p_{k}^{\alpha_{k}-1}$ . 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)  $z_i$ ,  $z_i$  (2)  $\mu$ ,  $\pi$  (3)  $\Sigma$ ,  $\pi$  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):  $\Theta$  parameter space, H prior distri on  $\Theta$ ,  $A_1, \dots, A_r$  arbitrary partition of  $\Theta$ . G a categorical distribution over  $\{A_i\}$  is  $G \sim \mathrm{DP}(\alpha, H)$  if  $(G(A_1), \ldots, G(A_r)) \sim$  $Dir(\alpha H(A_1),...,\alpha H(A_r)).$ 

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

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

## Three Methods of Sampling from DP

In  $K \to \infty$  GMM,  $\theta$  in DP is z, G is  $\pi$ .

(1) Chinese Restaurant Process (CRP), sample z, marginalize over  $\pi$ :

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

**Expect # of Class**  $\sum_{i=1}^{n} \frac{\alpha}{\alpha+i-1} \simeq \alpha \log \left(1 + \frac{n}{\alpha}\right)$ 

- (2) Stick-breaking Construction samples  $\pi$ :  $\beta_k \sim \text{Beta}(1,\alpha), \, \theta_k^* \sim H, \, \pi_k = \beta_k \prod_{l=1}^{k-1} (1-\beta_l)$
- (3) Marginalize over  $\mu$ ,  $\Sigma$  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  $P(\{\theta_i\}) = \prod_{i=1}^n G(\theta_i) dP(G)$ 

# 11 PAC Learning

• A learning algorithm A can learn  $c \in C$  if there is a poly(...), s.t. for (1) any distribution  $\mathcal{D}$  on  $\mathcal{X}$  and (2)  $\forall \epsilon \in [0, 1/2], \delta \in [0, 1/2],$ A outputs  $\hat{c} \in \mathcal{H}$  given a sample of size at

least poly $(\frac{1}{\epsilon}, \frac{1}{\delta}, \operatorname{size}(c))$  such that  $P(\mathcal{R}(\hat{c}) - \inf_{c \in C} \mathcal{R}(c) \le \epsilon) \ge 1 - \delta$ .

•  $\mathcal{A}$  is called an efficient PAC algorithm if it

- runs in polynomial of  $\frac{1}{\epsilon}$  and  $\frac{1}{\delta}$ .  $\mathcal{C}$  is (efficiently) PAC-learnable from  $\mathcal{H}$  if there is an algorithm A that (efficiently) learns
- C from  $\mathcal{H}$ .
   Finite  $\mathcal{C}$ ,  $\mathbf{P}(\mathcal{R}(\hat{c}_n^*) \inf_{c \in \mathcal{C}} \mathcal{R}(c) > \epsilon) \leq$  $2|\mathcal{C}| \exp\left(-\frac{n\epsilon^2}{2}\right) \text{ is PAC-learnable.}$ •  $\mathcal{C}$  with  $\dim_{VC} = d < \infty$  is PAC-learnable,
- $\mathbf{P}\left(\mathcal{R}\left(\hat{c}_{n}^{*}\right)-\inf_{c\in\mathcal{C}}\mathcal{R}(c)>\epsilon\right)\leq 9n^{d}\exp\left(-\frac{n\epsilon^{2}}{32}\right)$

## A Appendix

$$\frac{\partial \overrightarrow{u}^T \overrightarrow{v}}{\partial x} = \frac{\partial \overrightarrow{u}}{\partial x} \overrightarrow{v} + \frac{\partial \overrightarrow{v}}{\partial x} \overrightarrow{u}.$$

$$\frac{\partial A\overrightarrow{u}}{\partial x} = \frac{\partial \overrightarrow{u}}{\partial x} A^T.$$

$$\mathcal{N}(\mu, \Sigma)$$
:  $\frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu))$ .