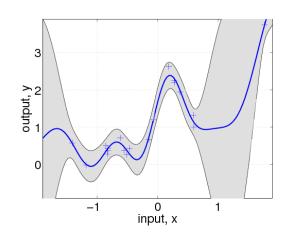
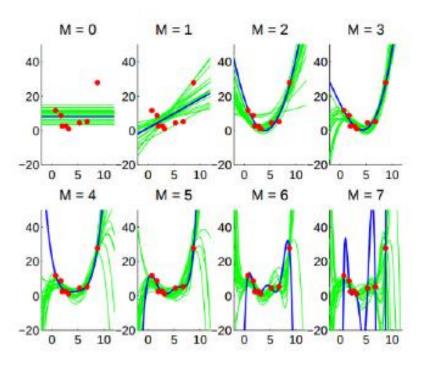
# Probabilistic Bayesian Modelling

#### Probabilistic Model

- x an observation (random variable/vector)
- $X = \{x_1, x_2, ..., x_n\}$ , set of observations, evidence, data
- Probabilistic model a mathematical form which provides stochastic information about the random variable x
- $\theta$  parameters of a model
- M hyperparameters of a model





# Modelling Goals

- Estimation (of the underlying model parameters)  $p(\theta, m/X)$ 
  - Understand
  - Generate new data

- Prediction  $p(x^* | \theta)$  or  $p(x^* | X)$ ,  $x^*$  is a new observation
- Model comparison  $p(X/\theta_1) > p(X/\theta_2)$
- Solving the first goal helps solve the second and third goals

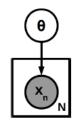
## Some probabilities of interest

- Likelihood function  $p(x|\theta)$  or the "observation model" specifies how data is generated
  - Measures data fit (or "loss") w.r.t. the given parameter  $\theta$
- Prior distribution  $p(\theta)$  specifies how likely different parameter values are a priori
  - Also corresponds to imposing a "regularizer" over  $\theta$
- Domain knowledge can help in the specification of the likelihood and the prior

NB: We are talking about probability distributions and not single (point) probabilities

#### Maximum Likelihood Estimation

 $\bullet$  Perhaps the simplest way is to find  $\theta$  that makes the observed data most likely or most probable



 $\bullet$  Formally, find  $\theta$  that maximizes the probability of the observed data

$$\hat{\theta} = \arg \max_{\theta} \log p(\mathbf{X}|\theta)$$

• However, this gives a single "point" estimate of  $\theta$ . Doesn't tell us about the uncertainty in  $\theta$ 

# Rules of Probability

Keep in mind these two simple rules of probability: sum rule and product rule

$$P(a) = \sum_{b} P(a, b)$$
 (Sum Rule)  
 $P(a, b) = P(a)P(b|a) = P(b)P(a|b)$  (Product Rule)

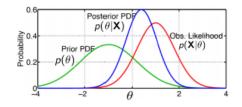
- Note: For continuous random variables, sum is replaced by integral:  $P(a) = \int P(a, b) db$
- Another rule is the Bayes rule (can be easily obtained from the above two rules)

$$P(b|a) = \frac{P(b)P(a|b)}{P(a)} = \frac{P(b)P(a|b)}{\int P(a,b)db} = \frac{P(b)P(a|b)}{\int P(b)P(a|b)db}$$

## Bayesian Estimation

Can infer the parameters by computing the posterior distribution (Bayesian inference)

$$p(\theta|\mathbf{X},m) = \frac{p(\mathbf{X},\theta|m)}{p(\mathbf{X}|m)} = \frac{p(\mathbf{X}|\theta,m)p(\theta|m)}{\int p(\mathbf{X}|\theta,m)p(\theta|m)d\theta} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Marginal likelihood}}$$

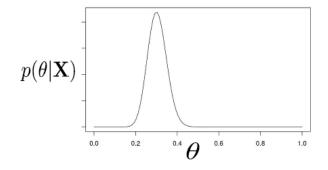


- Cheaper alternative: Point Estimation of the parameters. E.g.,
  - Maximum likelihood estimation (MLE): Find  $\theta$  that makes the observed data most probable  $\hat{\theta}_{ML} = \arg\max_{\theta} \log p(\mathbf{X}|\theta)$
  - Maximum-a-Posteriori (MAP) estimation: Find  $\theta$  that has the largest posterior probability

$$\hat{\theta}_{MAP} = \arg\max_{\theta} \log p(\theta|\mathbf{X}) = \arg\max_{\theta} [\log p(\mathbf{X}|\theta) + \log p(\theta)]$$

#### Posterior Distribution

- ullet Posterior provides us a holistic view about heta given observed data
- ullet A simple unimodal posterior distribution for a scalar parameter  $\theta$  might look something like



- ullet Various types of estimates regarding heta can be obtained from the posterior, e.g.,
  - Mode of the posterior (same as the MAP estimate)
  - Mean and median of the posterior
  - Variance/spread of the posterior (uncertainty in our estimate of the parameters)

#### Predictions

- Posterior can be used to compute the posterior predictive distribution (PPD) of new observation
- The PPD of a new observation  $x_*$  given previous observations

$$p(\mathbf{x}_*|\mathbf{X},m) = \int p(\mathbf{x}_*,\theta|\mathbf{X},m)d\theta = \int p(\mathbf{x}_*|\theta,\mathbf{X},m)p(\theta|\mathbf{X},m)d\theta$$
$$= \int p(\mathbf{x}_*|\theta,m)p(\theta|\mathbf{X},m)d\theta$$

- ullet Note: In the above, we assume that the observations are i.i.d. given heta
- ullet Computing PPD requires doing a posterior-weighted averaging over all values of heta
- If the integral in PPD is intractable, we can approximate the PPD by plug-in predictive

$$p(\mathbf{x}_*|\mathbf{X},m)\approx p(\mathbf{x}_*|\hat{\theta},m)$$

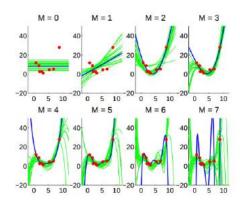
.. where  $\hat{\theta}$  is a point estimate of  $\theta$  (e.g., MLE/MAP)

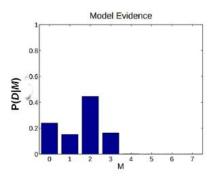
# Marginal Likelihood

• Recall the Bayes rule for computing the posterior

$$p(\theta|\mathbf{X},m) = \frac{p(\mathbf{X},\theta|m)}{p(\mathbf{X}|m)} = \frac{p(\mathbf{X}|\theta,m)p(\theta|m)}{\int p(\mathbf{X}|\theta,m)p(\theta|m)d\theta} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Marginal likelihood}}$$

- The denominator in the Bayes rule is the marginal likelihood (a.k.a. "model evidence")
- Note that  $p(\mathbf{X}|m) = \mathbb{E}_{p(\theta|m)}[p(\mathbf{X}|\theta,m)]$  is the average/expected likelihood under model m
- For a good model, we would expect this "averaged" quantity to be large (most  $\theta$ 's will be good)





# Model Comparison/Averaging

- Marginal likelihood is hard-to-compute (due to integral) but a very useful quantity
- It can be used for doing model selection
  - Choose model m that has largest posterior probability

$$\hat{m} = \arg \max_{m} p(m|\mathbf{X}) = \arg \max_{m} \frac{p(\mathbf{X}|m)p(m)}{p(\mathbf{X})} = \arg \max_{m} p(\mathbf{X}|m)p(m)$$

- If all models are equally likely a priori then  $\hat{m} = \arg \max_{m} p(\mathbf{X}|m)$
- If m is a hyperparam, then  $\arg \max_m p(\mathbf{X}|m)$  is MLE-II based hyperparameter estimation
- Marginal likelihood can be used to compute  $p(m|\mathbf{X})$  and then perform Bayesian Model Averaging

$$p(\mathbf{x}_*|\mathbf{X}) = \sum_{m=1}^{M} p(\mathbf{x}_*|\mathbf{X}, m) p(m|\mathbf{X})$$

# Simple Example (MLE)

- Consider a sequence of N coin tosses (call head = 0, tail = 1)
- The  $n^{th}$  outcome  $\boldsymbol{x}_n$  is a binary random variable  $\in \{0,1\}$
- Assume  $\theta$  to be probability of a head (parameter we wish to estimate)
- Each likelihood term  $p(\boldsymbol{x}_n \mid \theta)$  is Bernoulli:  $p(\boldsymbol{x}_n \mid \theta) = \theta^{\boldsymbol{x}_n} (1 \theta)^{1 \boldsymbol{x}_n}$
- Log-likelihood:  $\sum_{n=1}^{N} \log p(\mathbf{x}_n \mid \theta) = \sum_{n=1}^{N} \mathbf{x}_n \log \theta + (1 \mathbf{x}_n) \log(1 \theta)$
- Taking derivative of the log-likelihood w.r.t.  $\theta$ , and setting it to zero gives

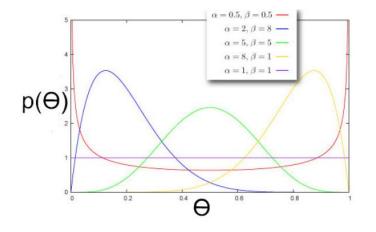
$$\hat{\theta}_{MLE} = \frac{\sum_{n=1}^{N} \mathbf{x}_n}{N}$$

•  $\hat{\theta}_{MLE}$  in this example is simply the fraction of heads!

#### MAP Estimate

- MAP estimation can incorporate a prior  $p(\theta)$  on  $\theta$
- Since  $\theta \in (0,1)$ , one possibility can be to assume a Beta prior

$$p(\theta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha - 1} (1 - \theta)^{\beta - 1}$$



- $\alpha, \beta$  are called hyperparameters of the prior (these can have intuitive meaning; we'll see shortly)
  - Note that each likelihood term is still a Bernoulli:  $p(\mathbf{x}_n|\theta) = \theta^{\mathbf{x}_n}(1-\theta)^{1-\mathbf{x}_n}$
  - The log posterior probability =  $\sum_{n=1}^{N} \log p(\mathbf{x}_n | \theta) + \log p(\theta)$
  - Ignoring the constants w.r.t.  $\theta$ , the log posterior probability:

$$\sum_{n=1}^{N} \{ \boldsymbol{x}_{n} \log \theta + (1 - \boldsymbol{x}_{n}) \log (1 - \theta) \} + (\alpha - 1) \log \theta + (\beta - 1) \log (1 - \theta)$$

ullet Taking derivative w.r.t. heta and setting to zero gives

$$\hat{\theta}_{MAP} = \frac{\sum_{n=1}^{N} \mathbf{x}_n + \alpha - 1}{N + \alpha + \beta - 2}$$

• Note: For  $\alpha=1, \beta=1$ , i.e.,  $p(\theta)=\mathsf{Beta}(1,1)$  (equivalent to a uniform prior),  $\hat{\theta}_{MAP}=\hat{\theta}_{MLE}$ 

## Bayesian Estimate

- Recall that each likelihood term was Bernoulli:  $p(\mathbf{x}_n|\theta) = \theta^{\mathbf{x}_n}(1-\theta)^{1-\mathbf{x}_n}$
- Let's again choose the prior  $p(\theta)$  as Beta:  $p(\theta) = \text{Beta}(\alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$
- The posterior distribution will be proportional to the product of likelihood and prior

$$p(\theta|\mathbf{X}) \propto \prod_{n=1}^{N} p(\mathbf{x}_n|\theta) p(\theta)$$

$$\propto \theta^{\alpha + \sum_{n=1}^{N} \mathbf{x}_n - 1} (1 - \theta)^{\beta + N - \sum_{n=1}^{N} \mathbf{x}_n - 1}$$

• From simple inspection, note that the posterior  $p(\theta|\mathbf{X}) = \text{Beta}(\alpha + \sum_{n=1}^{N} \mathbf{x}_n, \beta + N - \sum_{n=1}^{N} \mathbf{x}_n)$ 

Posterior has the same form as prior – conjugate prior

#### Predictions

- ullet Let's say we want to compute the probability that the next outcome  $oldsymbol{x}_{N+1} \in \{0,1\}$  will be a head
- The plug-in predictive distribution using a point estimate  $\hat{\theta}$  (e.g., using MLE/MAP)

$$p(\mathbf{x}_{N+1} = 1 | \mathbf{X}) \approx p(\mathbf{x}_{N+1} = 1 | \hat{\theta}) = \hat{\theta}$$
 or equivalently  $p(\mathbf{x}_{N+1} | \mathbf{X}) \approx \text{Bernoulli}(\mathbf{x}_{N+1} | \hat{\theta})$ 

• The posterior predictive distribution (averaging over all  $\theta$  weighted by their posterior probabilities):

$$p(\mathbf{x}_{N+1} = 1|\mathbf{X}) = \int_0^1 P(\mathbf{x}_{N+1} = 1|\theta) p(\theta|\mathbf{X}) d\theta$$

$$= \int_0^1 \theta \times \text{Beta}(\theta|\alpha + N_1, \beta + N_0) d\theta$$

$$= \mathbb{E}[\theta|\mathbf{X}]$$

$$= \frac{\alpha + N_1}{\alpha + \beta + N}$$

• Therefore the posterior predictive distribution:  $p(\mathbf{x}_{N+1}|\mathbf{X}) = \text{Bernoulli}(\mathbf{x}_{N+1} \mid \mathbb{E}[\theta|\mathbf{X}])$ 

#### Multinomial Model

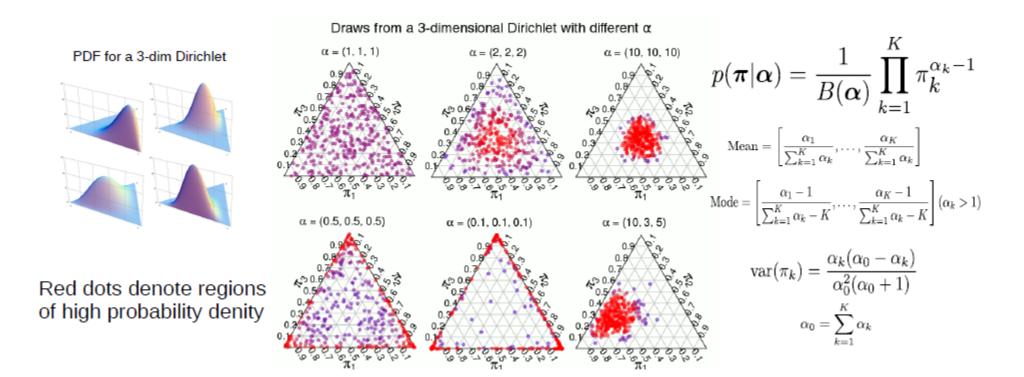
- Assume N discrete-valued observations  $\{x_1, \ldots, x_N\}$  with each  $x_n \in \{1, \ldots, K\}$ , e.g.,
  - $x_n$  represents the outcome of a dice roll with K faces
  - $x_n$  represents the class label of the *n*-th example (total K classes)
  - $x_n$  represents the identity of the n-th word in a sequence of words
- Assume likelihood to be multinoulli with unknown params  $\pi = [\pi_1, \dots, \pi_K]$  s.t.  $\sum_{k=1}^K \pi_k = 1$

$$p(x_n|\pi) = \text{multinoulli}(x_n|\pi) = \prod_{k=1}^{\mathbb{I}[x_n=k]} \pi_k^{\mathbb{I}[x_n=k]}$$

- $\bullet$   $\pi$  is a vector of probabilities ("probability vector"), e.g.,
  - Biases of the K sides of the dice
  - Prior class probabilities in multi-class classification
  - Probabilities of observing each words in the vocabulary
- Assume a conjugate Dirichlet prior on  $\pi$  with hyperparams  $\alpha = [\alpha_1, \dots, \alpha_K]$  (also,  $\alpha_k \geq 0, \forall k$ )

$$p(\boldsymbol{\pi}|\boldsymbol{\alpha}) = \mathsf{Dirichlet}(\boldsymbol{\pi}|\alpha_1, \dots, \alpha_K) = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \pi_k^{\alpha_k - 1} = \frac{1}{B(\boldsymbol{\alpha})} \prod_{k=1}^K \pi_k^{\alpha_k - 1}$$

#### Dirichlet Distribution



#### **Estimation**

• The posterior over  $\pi$  is easy to compute in this case due to conjugacy b/w multinoulli and Dirichlet

$$p(\boldsymbol{\pi}|\mathbf{X}, \boldsymbol{\alpha}) = \frac{p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\alpha})p(\boldsymbol{\pi}|\boldsymbol{\alpha})}{p(\mathbf{X}|\boldsymbol{\alpha})} = \frac{p(\mathbf{X}|\boldsymbol{\pi})p(\boldsymbol{\pi}|\boldsymbol{\alpha})}{p(\mathbf{X}|\boldsymbol{\alpha})}$$

• Assuming  $x_n$ 's are i.i.d. given  $\pi$ ,  $p(\mathbf{X}|\pi) = \prod_{n=1}^N p(x_n|\pi)$ , therefore

$$p(\boldsymbol{\pi}|\mathbf{X},\boldsymbol{\alpha}) \propto \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{\mathbb{I}[x_n=k]} \prod_{k=1}^{K} \pi_k^{\alpha_k-1} = \prod_{k=1}^{K} \pi_k^{\alpha_k + \sum_{n=1}^{N} \mathbb{I}[x_n=k]-1}$$

- ullet Even without computing the normalization constant  $p(\mathbf{X}|\alpha)$ , we can see that it's a Dirichlet! :-)
- Denoting  $N_k = \sum_{n=1}^N \mathbb{I}[x_n = k]$ , i.e., number of observations with value k, the posterior will be

$$p(\boldsymbol{\pi}|\mathbf{X},\boldsymbol{\alpha}) = \mathsf{Dirichlet}(\boldsymbol{\pi}|\alpha_1 + N_1,\ldots,\alpha_K + N_K)$$

#### Gaussian Models

- Univariate with fixed variance
- Univariate with fixed mean
- Univariate with varying mean and variance
- Multivariate

#### Fixed Variance Gaussian Model

ullet Consider N i.i.d. observations  ${f X}=\{x_1,\ldots,x_N\}$  drawn from a one-dim Gaussian  ${\cal N}(x|\mu,\sigma^2)$ 

$$p(x_n|\mu,\sigma^2) = \mathcal{N}(x|\mu,\sigma^2) \propto \exp\left[-\frac{(x_n-\mu)^2}{2\sigma^2}\right]$$

$$p(\mathbf{X}|\mu,\sigma^2) = \prod_{n=1}^{N} p(x_n|\mu,\sigma^2)$$

- ullet Assume the mean  $\mu\in\mathbb{R}$  of the Gaussian is unknown and assume variance  $\sigma^2$  to be known/fixed
- ullet We wish to estimate the unknown  $\mu$  given the data  ${f X}$ 
  - Let's choose a Gaussian prior on  $\mu$ , i.e.,  $p(\mu) = \mathcal{N}(\mu|\mu_0, \sigma_0^2)$  with  $\mu_0, \sigma_0^2$  as fixed

## Bayesian Estimate of Mean

• The posterior distribution for the unknown mean parameter  $\mu$ 

$$p(\mu|\mathbf{X}) = \frac{p(\mathbf{X}|\mu)p(\mu)}{p(\mathbf{X})} \propto \prod_{n=1}^{N} \exp\left[-\frac{(x_n - \mu)^2}{2\sigma^2}\right] \times \exp\left[-\frac{(\mu - \mu_0)^2}{2\sigma_0^2}\right]$$

• Simplifying the above (using completing the squares trick) gives  $p(\mu|\mathbf{X}) \propto \exp\left[-\frac{(\mu-\mu_N)^2}{2\sigma_N^2}\right]$  with

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

$$\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2} \bar{x} \qquad \text{(where } \bar{x} = \frac{\sum_{n=1}^N x_n}{N}\text{)}$$

**Notion of Sufficient Statistics** 

#### Prediction

- What is the posterior predictive distribution  $p(x_*|\mathbf{X})$  of a new observation  $x_*$ ?
- Using the inferred posterior  $p(\mu|\mathbf{X})$ , we can find the posterior predictive distribution

$$p(x_*|\mathbf{X}) = \int p(x_*|\mu, \sigma^2) p(\mu|\mathbf{X}) d\mu = \int \mathcal{N}(x_*|\mu, \sigma^2) \mathcal{N}(\mu|\mu_N, \sigma_N^2) d\mu = \mathcal{N}(x_*|\mu_N, \sigma^2 + \sigma_N^2)$$

- Note; Can also get the above result by thinking of  $x_*$  as  $x_* = \mu + \epsilon$  where  $\mu \sim \mathcal{N}(\mu_N, \sigma_N^2)$ , and  $\epsilon \sim \mathcal{N}(0, \sigma^2)$  is independently added observation noise
- Note that, as per the above, the uncertainty in distribution of  $x_*$  now has two components
  - $\circ$   $\sigma^2$ : Due to the noisy observation model,  $\sigma^2_N$ : Due to the uncertainty in  $\mu$
- ullet In contrast, the plug-in predictive posterior, given a point estimate  $\hat{\mu}$  (e.g., MLE/MAP) would be

$$p(x_*|\mathbf{X}) = \int p(x_*|\mu, \sigma^2) p(\mu|\mathbf{X}) d\mu \approx p(x_*|\hat{\mu}, \sigma^2) = \mathcal{N}(x_*|\hat{\mu}, \sigma^2)$$

• Note that as  $N \to \infty$ , both approaches would give the same  $p(x_*|\mathbf{X})$  since  $\sigma_N^2 \to 0$ 

#### Fixed Mean Gaussian Model

ullet Again consider N i.i.d. observations  ${f X}=\{x_1,\ldots,x_N\}$  drawn from a one-dim Gaussian  ${\cal N}(x|\mu,\sigma^2)$ 

$$p(x_n|\mu,\sigma^2) = \mathcal{N}(x|\mu,\sigma^2)$$
 and  $p(\mathbf{X}|\mu,\sigma^2) = \prod_{n=1}^N p(x_n|\mu,\sigma^2)$ 

- ullet Assume the variance  $\sigma^2 \in \mathbb{R}_+$  of the Gaussian is unknown and assume mean  $\mu$  to be known/fixed
- Let's estimate  $\sigma^2$  given the data **X** using fully Bayesian inference (not MLE/MAP)
- We first need a prior distribution for  $\sigma^2$ . What prior  $p(\sigma^2)$  to choose in this case?
- If we want a conjugate prior, it should have the same form as the likelihood

$$p(x_n|\mu,\sigma^2) \propto (\sigma^2)^{-1/2} \exp\left[-\frac{(x_n-\mu)^2}{2\sigma^2}\right]$$

• An inverse-gamma prior  $IG(\alpha, \beta)$  has this form  $(\alpha, \beta)$  are shape and scale hyperparams, resp)

$$p(\sigma^2) \propto (\sigma^2)^{-(\alpha+1)} \exp\left[-\frac{\beta}{\sigma^2}\right]$$
 The posterior  $p(\sigma^2|\mathbf{X}) = IG(\alpha + \frac{N}{2}, \beta + \frac{\sum_{n=1}^{N}(x_n - \mu)^2}{2}).$ 

The posterior 
$$p(\sigma^2|\mathbf{X}) = IG(\alpha + \frac{N}{2}, \beta + \frac{\sum_{n=1}^{N}(x_n - \mu)^2}{2})$$
. Again IG due to conjugacy.

#### Gaussian Model: Mean and Variance

- Goal: Infer the mean and precision of a univariate Gaussian  $\mathcal{N}(x|\mu,\lambda^{-1})$
- ullet Given N i.i.d. observations  ${f X}=\{x_1,\ldots,x_N\}$ , the likelihood will be

$$p(\mathbf{X}|\mu,\lambda) = \prod_{n=1}^{N} \sqrt{\frac{\lambda}{2\pi}} \exp\left[-\frac{\lambda}{2}(x_n - \mu)^2\right] \propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^N \exp\left[\lambda\mu \sum_{n=1}^{N} x_n - \frac{\lambda}{2} \sum_{n=1}^{N} x_n^2\right]$$

• Let's choose the following joint distribution as the prior (compare its form with  $p(\mathbf{X}|\mu,\lambda)$ )

$$p(\mu, \lambda) \propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^{\kappa_0} \exp\left[\lambda\mu c - \lambda d\right] = \underbrace{\exp\left[-\frac{\kappa_0\lambda}{2}(\mu - c/\kappa_0)^2\right]}_{\text{prop. to a Gaussian}} \underbrace{\lambda^{\kappa_0/2} \exp\left[-\left(d - \frac{c^2}{2\kappa_0}\right)\lambda\right]}_{\text{prop. to a gamma}}$$

• The above is known as the Normal-gamma (NG) distribution (product of a Normal and a gamma)

$$p(\mu, \lambda) = \mathcal{N}(\mu | \mu_0, (\kappa_0 \lambda)^{-1})$$
Gamma $(\lambda | \alpha_0, \beta_0) = NG(\mu, \lambda | \mu_0, \kappa_0, \alpha_0, \beta_0)$  (note:  $\mu$  and  $\lambda$  are coupled in the Gaussian part)

where 
$$\mu_0 = c/\kappa_0$$
,  $\alpha_0 = 1 + \kappa_0/2$ ,  $\beta_0 = d - c^2/2\kappa_0$  are prior's hyperparameters

NG is conjugate to Gaussian when both mean & precision are unknown

#### Gaussian Model: Mean and Variance

• Due to conjugacy,  $p(\mu, \lambda | \mathbf{X})$  will also be NG:  $p(\mu, \lambda | \mathbf{X}) \propto p(\mathbf{X} | \mu, \lambda) p(\mu, \lambda)$ 

$$p(\mu, \lambda | \mathbf{X}) = \mathsf{NG}(\mu_N, \kappa_N, \alpha_N, \beta_N) = \mathcal{N}(\mu | \mu_N, (\kappa_N \lambda)^{-1}) \mathsf{Gamma}(\lambda | \alpha_N, \beta_N)$$

where the updated posterior hyperparameters are given by<sup>1</sup>

$$\mu_N = \frac{\kappa_0 \mu_0 + N \bar{x}}{\kappa_0 + N}, \quad \kappa_N = \kappa_0 + N$$

$$\frac{1}{\kappa_0 N} \sum_{k=0}^{N} \kappa_0 N(k)$$

$$\alpha_N = \alpha_0 + N/2, \quad \beta_N = \beta_0 + \frac{1}{2} \sum_{n=1}^N (x_n - \bar{x})^2 + \frac{\kappa_0 N(\bar{x} - \mu_0)^2}{2(\kappa_0 + N)}$$

Posterior Predictive Distribution:

$$p(x_*|\mathbf{X}) = \int \underbrace{p(x_*|\mu, \lambda)}_{\text{Courseign}} \underbrace{p(\mu, \lambda|\mathbf{X})}_{\text{Normal-Comma}} d\mu d\lambda = t_{2\alpha_N} \left( x_* |\mu_N, \frac{\beta_N(\kappa_N + 1)}{\alpha_N \kappa_N} \right)$$

#### Multivariate Gaussian

ullet The (multivariate) Gaussian with mean  $\mu$  and cov. matrix  $oldsymbol{\Sigma}$ 

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

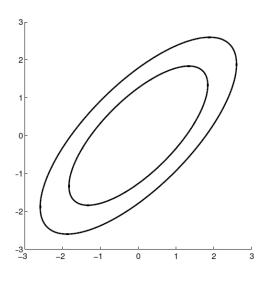
$$= \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} \exp \left\{ -\frac{1}{2} \operatorname{trace} \left[ \boldsymbol{\Sigma}^{-1} \mathbf{S} \right] \right\} \quad \text{where } \mathbf{S} = (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^\top$$

• An alternate representation: The "information form"

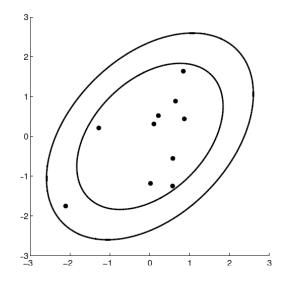
$$\mathcal{N}_c(\mathbf{x}|\boldsymbol{\xi},\boldsymbol{\Lambda}) = (2\pi)^{-D/2}|\boldsymbol{\Lambda}|^{1/2}\exp\left\{-\frac{1}{2}\left(\mathbf{x}^{\top}\boldsymbol{\Lambda}\mathbf{x} + \boldsymbol{\xi}^{\top}\boldsymbol{\Lambda}^{-1}\boldsymbol{\xi} - 2\mathbf{x}^{\top}\boldsymbol{\xi}\right)\right\}$$

where  $\mathbf{\Lambda} = \mathbf{\Sigma}^{-1}$  and  $\mathbf{\xi} = \mathbf{\Sigma}^{-1} \mu$  are the "natural parameters" (more when we discuss exp. family).

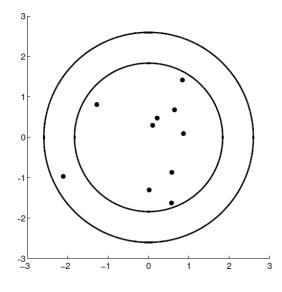
#### Multivariate Gaussians



$$\Sigma = \left[ egin{array}{cc} 1 & .7 \\ .7 & 1 \end{array} 
ight] \qquad \qquad \Sigma = \left[ egin{array}{cc} 1 \\ .4 \end{array} 
ight]$$

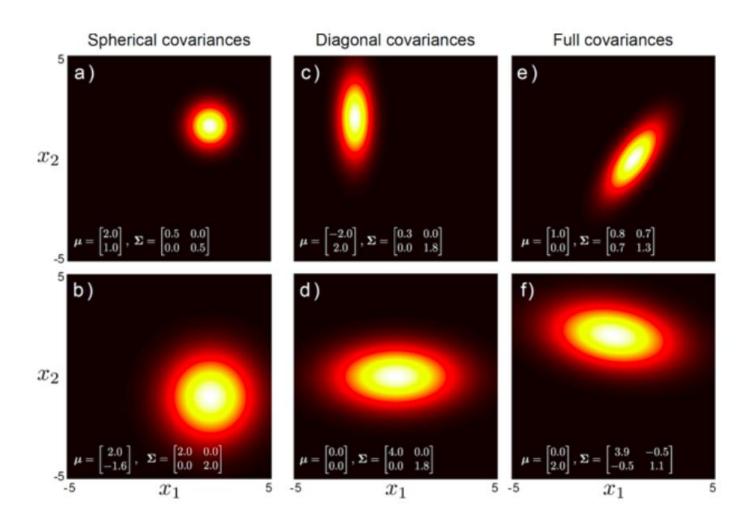


$$\Sigma = \left[ egin{array}{cc} 1 & .4 \ .4 & 1 \end{array} 
ight]$$



$$\Sigma = \left[ egin{array}{cc} 1 & \mathbf{0} \ \mathbf{0} & 1 \end{array} 
ight]$$

#### Covariance Matrix



# Multivariate Gaussians: Grouped Variables

• Given  ${\pmb x}$  having multivariate Gaussian distribution  ${\mathcal N}({\pmb x}|{\pmb \mu},{\pmb \Sigma})$  with  ${\pmb \Lambda}={\pmb \Sigma}^{-1}$ . Suppose

$$egin{array}{lll} oldsymbol{x} &=& egin{bmatrix} oldsymbol{x}_a \ oldsymbol{x}_b \end{bmatrix} & oldsymbol{\mu} &=& egin{bmatrix} oldsymbol{\mu}_a \ oldsymbol{\Sigma}_{ba} & oldsymbol{\Sigma}_{bb} \end{bmatrix} & oldsymbol{\Lambda} &=& egin{bmatrix} oldsymbol{\Lambda}_{aa} & oldsymbol{\Lambda}_{ab} \ oldsymbol{\Lambda}_{ba} & oldsymbol{\Lambda}_{bb} \end{bmatrix} \end{array}$$

• The marginal distribution of one block, say  $\mathbf{x}_a$ , is a Gaussian

$$p(\mathbf{x}_a) = \int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b = \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$$

• The conditional distribution of  $\mathbf{x}_a$  given  $\mathbf{x}_b$ , is Gaussian, i.e.,  $p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b})$  where

$$\mathbf{\Sigma}_{a|b} = \mathbf{\Lambda}_{aa}^{-1} = \mathbf{\Sigma}_{aa} - \mathbf{\Sigma}_{ab} \mathbf{\Sigma}_{bb}^{-1} \mathbf{\Sigma}_{ba}$$
 ("smaller" than  $\mathbf{\Sigma}_{aa}$ ; makes sense intuitively)

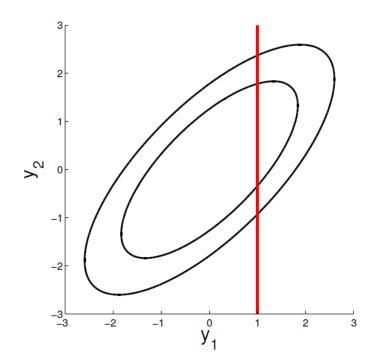
$$\mu_{a|b} = \sum_{a|b} \{ \Lambda_{aa} \mu_a - \Lambda_{ab} (x_b - \mu_b) \}$$

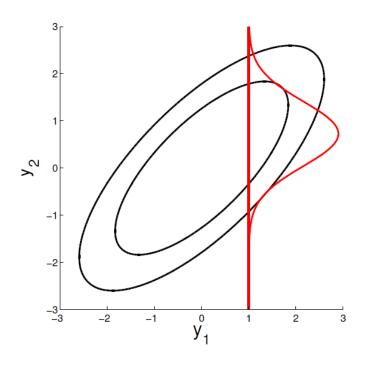
$$= \mu_a - \Lambda_{aa}^{-1} \Lambda_{ab} (x_b - \mu_b)$$

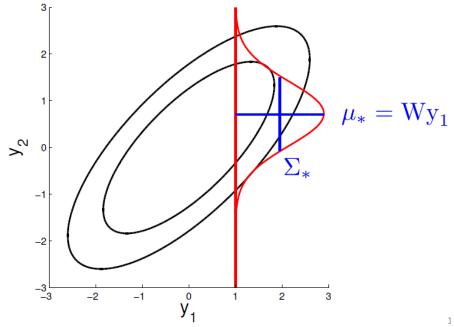
$$= \mu_a + \sum_{ab} \sum_{bb}^{-1} (x_b - \mu_b)$$

### Conditional Distributions

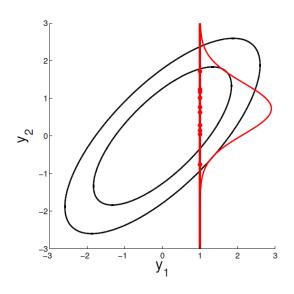
$$p(\mathsf{y}_2|\mathsf{y}_1,\Sigma) \propto \exp\left(-\frac{1}{2}(\mathsf{y}_2 - \mu_*){\Sigma_*}^{-1}(\mathsf{y}_2 - \mu_*)\right)$$

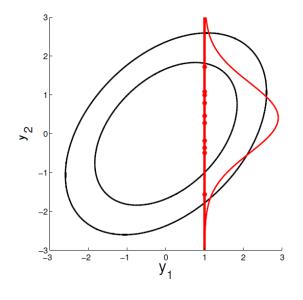






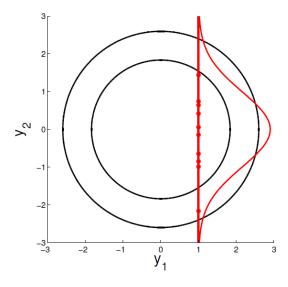
#### Conditional Distributions





$$\Sigma = \left[ egin{array}{cc} 1 & .7 \\ .7 & 1 \end{array} 
ight]$$

$$\Sigma = \left[ egin{array}{cc} 1 & .4 \ .4 & 1 \end{array} 
ight]$$



$$\Sigma = \left[ \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right]$$

#### Multivariate Gaussian

- The parameters are now the mean vector and the covariance/precision matrix
- Posterior updates for these have forms similar to that in the univariate case
- For the mean, commonly a multivariate Gaussian prior is used
  - Posterior is also Gaussian due to conjugacy
- For the covariance matrix (with mean fixed), commonly an inverse-Wishart prior is used
  - Posterior is also inverse-Wishart due to conjugacy
- For the precision matrix (with mean fixed), commonly a Wishart prior is used
  - Posterior is also Wishart due to conjugacy
- When both parameters are unknown, there still exist conjugate joint priors
  - $\bullet$  Normal-Inverse Wishart for mean + cov matrix, Normal-Wishart for mean + precision matrix

Wishart Distribution: Multidimensional extension of Gamma distribution

#### Linear Transformation of Random Variables

- Suppose  $\mathbf{x} = f(\mathbf{z}) = \mathbf{A}\mathbf{z} + \mathbf{b}$  be a linear function of an r.v.  $\mathbf{z}$  (not necessarily Gaussian)
- ullet Suppose  $\mathbb{E}[oldsymbol{z}] = oldsymbol{\mu}$  and  $\mathsf{cov}[oldsymbol{z}] = oldsymbol{\Sigma}$ 
  - Expectation of x

$$\mathbb{E}[x] = \mathbb{E}[\mathsf{A}z + \mathsf{b}] = \mathsf{A}\mu + \mathsf{b}$$

Covariance of x

$$cov[x] = cov[Az + b] = A\Sigma A^T$$

- Likewise if  $x = f(z) = a^T z + b$  is a scalar-valued linear function of an r.v. z:
  - $\bullet \ \mathbb{E}[x] = \mathbb{E}[\mathbf{a}^T \mathbf{z} + b] = \mathbf{a}^T \boldsymbol{\mu} + b$
  - $\operatorname{var}[x] = \operatorname{var}[\mathbf{a}^T \mathbf{z} + b] = \mathbf{a}^T \mathbf{\Sigma} \mathbf{a}$
- These properties are often helpful in obtaining the marginal distribution p(x) from p(z)

#### Linear Gaussian Model

• Consider linear transformation of a Gaussian r.v. z with  $p(z) = \mathcal{N}(z|\mu, \Lambda^{-1})$ , plus Gaussian noise

$$|\mathbf{x} = \mathbf{A}\mathbf{z} + \mathbf{b} + \boldsymbol{\epsilon}|$$
 where  $p(\epsilon) = \mathcal{N}(\epsilon|\mathbf{0}, \mathbf{L}^{-1})$ 

• Easy to see that, conditioned on z, x too has a Gaussian distribution

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{A}\mathbf{z}+\mathbf{b},\mathbf{L}^{-1})$$

- This is called a Linear Gaussian Model. Very commonly encountered in probabilistic modeling
- The following two distributions are of particular interest. Defining  $\Sigma = (\Lambda + A^{\top}LA)^{-1}$ , we have

$$p(\boldsymbol{z}|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{p(\boldsymbol{z})} = \mathcal{N}(\boldsymbol{z}|\boldsymbol{\Sigma}\left\{\boldsymbol{A}^{\top}\boldsymbol{L}(\boldsymbol{x}-\boldsymbol{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\right\}, \boldsymbol{\Sigma})$$

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} = \mathcal{N}(\mathbf{x}|\mathbf{A}\boldsymbol{\mu}+\mathbf{b},\mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\top}+\mathbf{L}^{-1})$$

## Exponential Family Distributions

Defines a class of distributions. An Exponential Family distribution is of the form

$$\rho(\mathbf{x}|\theta) = \frac{1}{Z(\theta)}h(\mathbf{x})\exp[\theta^{\top}\phi(\mathbf{x})] = h(\mathbf{x})\exp[\theta^{\top}\phi(\mathbf{x}) - A(\theta)]$$

- $\mathbf{x} \in \mathcal{X}^m$  is the random variable being modeled (where  $\mathcal{X}$  denotes some space, e.g.,  $\mathbb{R}$  or  $\{0,1\}$ )
- $\theta \in \mathbb{R}^d$ : Natural parameters or canonical parameters defining the distribution
- $\phi(\mathbf{x}) \in \mathbb{R}^d$ : Sufficient statistics (another random variable)
  - Why "sufficient":  $p(x|\theta)$  as a function of  $\theta$  depends on x only via  $\phi(x)$
- $Z(\theta) = \int h(\mathbf{x}) \exp[\theta^{\top} \phi(\mathbf{x})] d\mathbf{x}$ : Partition function
- $A(\theta) = \log Z(\theta)$ : Log-partition function (also called the <u>cumulant function</u>)
- h(x): A constant (doesn't depend on  $\theta$ )

# Expressing a Distribution in Exp-family form

- Recall the form of exp-fam distribution:  $h(\mathbf{x}) \exp[\theta^{\top} \phi(\mathbf{x}) A(\theta)]$
- To write any exp-fam dist p() in the above form, write it as  $exp(\log p())$ , e.g., for Binomial

$$\exp\left(\log \operatorname{Binomial}(x|N,\mu)\right) = \exp\left(\log \binom{N}{x} \mu^{x} (1-\mu)^{N-x}\right)$$

$$= \exp\left(\log \binom{N}{x} + x \log \mu + (N-x) \log(1-\mu)\right)$$

$$= \binom{N}{x} \exp\left(x \log \frac{\mu}{1-\mu} - N \log(1-\mu)\right)$$

Now compare the resulting expression with the exponential family form

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp(\theta^{\top} \phi(\mathbf{x}) - A(\theta))$$

## Gaussian as Exponential Form

• Let's try to write a univariate Gaussian in the exponential family form

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp[\theta^{\top} \phi(\mathbf{x}) - A(\theta)]$$

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] = \frac{1}{\sqrt{2\pi}} \exp\left[\frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}x^2 - \frac{\mu^2}{2\sigma^2} - \log\sigma\right]$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left[\left[\frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}\right]^{\top} \begin{bmatrix} x \\ x^2 \end{bmatrix} - \left(\frac{\mu^2}{2\sigma^2} + \log\sigma\right)\right]$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left[\left[\frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}\right]^{\top} \begin{bmatrix} x \\ x^2 \end{bmatrix} - \left(\frac{\mu^2}{2\sigma^2} + \log\sigma\right)\right]$$

$$\bullet \ \theta = \begin{bmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}, \text{ and } \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix} = \begin{bmatrix} -\frac{\theta_1}{2\theta_2} \\ -\frac{1}{2\theta_2} \end{bmatrix}$$

• 
$$A(\theta) = \frac{\mu^2}{2\sigma^2} + \log \sigma = \frac{-\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) - \frac{1}{2}\log(2\pi)$$

- Many other distribution belong to the exponential family
  - Bernoulli
  - Beta
  - Gamma
  - Multinoulli/Multinomial
  - Dirichlet
  - Multivariate Gaussian
  - .. and many more (https://en.wikipedia.org/wiki/Exponential\_family)
- Note: Not all distributions belong to the exponential family, e.g.,
  - Uniform distribution  $(x \sim \text{Unif}(a, b))$

## MLE on Exponential Families

ullet Suppose we have data  $\mathcal{D} = \{ m{x}_1, \dots, m{x}_N \}$  drawn i.i.d. from an exponential family distribution

$$p(\boldsymbol{x}|\theta) = h(\boldsymbol{x}) \exp \left[\theta^{\top} \phi(\boldsymbol{x}) - A(\theta)\right]$$

To do MLE, we need the overall likelihood. This is simply a product of the individual likelihoods

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{N} p(\mathbf{x}_i|\theta) = \left[\prod_{i=1}^{N} h(\mathbf{x}_i)\right] \exp\left[\theta^{\top} \sum_{i=1}^{N} \phi(\mathbf{x}_i) - NA(\theta)\right] = \left[\prod_{i=1}^{N} h(\mathbf{x}_i)\right] \exp\left[\theta^{\top} \phi(\mathcal{D}) - NA(\theta)\right]$$

- To estimate  $\theta$  (as we'll see shortly), we only need  $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(\mathbf{x}_i)$  and N
- Size of  $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(\mathbf{x}_i)$  does not grow with N (same as the size of each  $\phi(\mathbf{x}_i)$ )
- Only exponential family distributions have finite-sized sufficient statistics
  - No need to store all the data; can simply store and recursively update the sufficient statistics

- The likelihood is of the form  $p(\mathcal{D}|\theta) = \left[\prod_{i=1}^{N} h(\mathbf{x}_i)\right] \exp\left[\theta^{\top} \phi(\mathcal{D}) NA(\theta)\right]$
- The log-likelihood is (ignoring constant w.r.t.  $\theta$ ):  $\log p(\mathcal{D}|\theta) = \theta^{\top}\phi(\mathcal{D}) NA(\theta)$
- Note: This is concave in  $\theta$  (since  $-A(\theta)$  is concave). Maximization will yield a global maxima of  $\theta$
- MLE for exp-fam distributions can <u>also</u> be seen as doing moment-matching. To see this, note that

$$\nabla_{\theta} \left[ \theta^{\top} \phi(\mathcal{D}) - NA(\theta) \right] = \phi(\mathcal{D}) - N \nabla_{\theta} [A(\theta)] = \phi(\mathcal{D}) - N \mathbb{E}_{p(\mathbf{x}|\theta)} [\phi(\mathbf{x})] = \sum_{i=1}^{N} \phi(\mathbf{x}_i) - N \mathbb{E}_{p(\mathbf{x}|\theta)} [\phi(\mathbf{x})]$$

• Therefore, at the "optimal" (i.e., MLE)  $\hat{\theta}$ , where the derivative is 0, the following must hold

$$\mathbb{E}_{p(\boldsymbol{x}|\theta)}[\phi(\boldsymbol{x})] = \frac{1}{N} \sum_{i=1}^{N} \phi(\boldsymbol{x}_i)$$

matching the expected moments of the distribution with empirical moments

## Bayesian Estimate in Exponential Families

• We saw that the total likelihood given N i.i.d. observations  $\mathcal{D}\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N\}$ 

$$p(\mathcal{D}|\theta) \propto \exp\left[\theta^{\top}\phi(\mathcal{D}) - NA(\theta)\right]$$
 where  $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(\mathbf{x}_i)$ 

• Let's choose the following prior (note: it looks similar in terms of  $\theta$  within the exponent)

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) = h(\theta) \exp \left[\theta^{\top} \boldsymbol{\tau}_0 - \nu_0 A(\theta) - A_c(\nu_0, \boldsymbol{\tau}_0)\right]$$

• Ignoring the prior's log-partition function  $A_c(\nu_0, \tau_0) = \log \int_{\theta} h(\theta) \exp \left[\theta^{\top} \tau_0 - \nu_0 A(\theta)\right] d\theta$ 

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) \propto h(\theta) \exp\left[\theta^{\top} \boldsymbol{\tau}_0 - \boldsymbol{\nu}_0 A(\theta)\right]$$

- Comparing the prior's form with the likelihood, we notice that

  - $\tau_0$  is the <u>total sufficient statistics</u> of these  $\nu_0$  pseudo-observations

#### Posterior Distribution

As we saw, the likelihood is

$$p(\mathcal{D}|\theta) \propto \exp\left[\theta^{\top}\phi(\mathcal{D}) - NA(\theta)\right]$$
 where  $\phi(\mathcal{D}) = \sum_{i=1}^{N} \phi(\mathbf{x}_i)$ 

And the prior we chose is

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) \propto h(\theta) \exp\left[\theta^{\top} \boldsymbol{\tau}_0 - \boldsymbol{\nu}_0 A(\theta)\right]$$

• For this form of the prior, the posterior  $p(\theta|\mathcal{D}) \propto p(\theta)p(\mathcal{D}|\theta)$  will be

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp\left[\theta^{\top}(\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta)\right]$$

- Note that the posterior has the same form as the prior; such a prior is called a conjugate prior (note: all exponential family distributions have a conjugate prior having a form shown as above)
- Thus posterior hyperparams  $\nu_0{}', \tau_0{}'$  are obtained

$$\nu_0' \leftarrow \nu_0 + N$$
 $\tau_0' \leftarrow \tau_0 + \phi(\mathcal{D})$ 

#### Contd..

• Assuming the prior  $p(\theta|\nu_0, \tau_0) \propto h(\theta) \exp \left[\theta^{\top} \tau_0 - \nu_0 A(\theta)\right]$ , the posterior was

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp \left[\theta^{\top} (\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta)\right]$$

- Assuming  $\tau_0 = \nu_0 \bar{\tau}_0$ , we can also write the prior as  $p(\theta|\nu_0, \bar{\tau}_0) \propto \exp\left[\theta^\top \nu_0 \bar{\tau}_0 \nu_0 A(\theta)\right]$
- Can think of  $\bar{\tau}_0 = au_0/
  u_0$  as the average sufficient statistics per pseudo-observation
- The posterior can be written as

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp \left[\theta^{\top} (\nu_0 + N) \frac{\nu_0 \bar{\tau}_0 + \phi(\mathcal{D})}{\nu_0 + N} - (\nu_0 + N) A(\theta)\right]$$

• Denoting  $\bar{\phi} = \frac{\phi(D)}{N}$  as the average suff-stats per real observation, the posterior updates are

$$\nu_0' \leftarrow \nu_0 + N$$

$$\bar{\tau}_0' \leftarrow \frac{\nu_0 \bar{\tau}_0 + N \bar{\phi}}{\nu_0 + N}$$

#### Posterior Predictive Distribution

- ullet Assume some past (training) data  $\mathcal{D} = \{ oldsymbol{x}_1, \dots, oldsymbol{x}_N \}$  generated from an exp. family distribution
- ullet Assme some test data  $\mathcal{D}'=\{ ilde{\pmb{x}}_1,\ldots, ilde{\pmb{x}}_{N'}\}$  from the same distribution  $(N'\geq 1)$
- The posterior predictive distribution of  $\mathcal{D}'$  (probability distribution of new data given old data)

$$p(\mathcal{D}'|\mathcal{D}) = \int p(\mathcal{D}'|\theta)p(\theta|\mathcal{D})d\theta$$

$$\begin{split} p(\mathcal{D}'|\mathcal{D}) &= \int p(\mathcal{D}'|\theta)p(\theta|\mathcal{D})d\theta \\ &= \int \underbrace{\left[\prod_{i=1}^{N'}h(\tilde{\mathbf{x}}_i)\right]}_{\text{constant w.r.t. }\theta} \exp\left[\theta^{\top}\phi(\mathcal{D}') - N'A(\theta)\right]h(\theta) \exp\left[\theta^{\top}(\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta) - \underbrace{A_c(\nu_0 + N, \boldsymbol{\tau}_0 + \phi(\mathcal{D}))}_{\text{constant w.r.t. }\theta}\right]d\theta \end{split}$$

## Summary of Single Node Models

- Likelihood, Prior, Posterior, Predictive, Model averaging
- Hyperparameters (Parametric/Non-parametric models)
- Conjugate priors and closed form expression
- Point estimates (MLE, MAP), Distribution Estimates (Bayesian)
- Generative models
- Bernoulli (coin)
- Multinomial (dice)
- Gaussians (continuous variables)
- Exponential families

# Questions