

Bayesian Models in Machine Learning

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Frequentist vs. Bayesian

- Frequentist point of view:
 - Probability is the frequency of an event occurring in a large (infinite) number of trials
 - E.g. When flipping a coin many times, what is the proportion of heads?
- Bayesian
 - Inferring probabilities for events that have never occurred or believes which are not directly observed
 - Prior believes are specified in terms of prior probabilities
 - Taking into account uncertainty (posterior distribution) of the estimated parameters or hidden variables in our probabilistic model.

Coin flipping example

$$P(\text{head}|\mu) = \mu \quad P(\text{tail}|\mu) = 1 - \mu$$

$$\mathbf{x} = [x_1, x_2, x_3, \dots, x_N] = [\text{tail}, \text{head}, \text{head}, \dots, \text{tail}]$$

- Lets flip the coin $N = 1000$ times getting $H = 750$ heads and $T = 250$ tails.
- What is μ ? Intuitive (and also ML) estimate is $750 / 1000 = 0.75$.
- Given some μ , we can calculate probability (likelihood) of X

$$P(\mathbf{x}|\mu) = \prod_i P(x_i|\mu) = \mu^H (1 - \mu)^T$$

- Now lets express our *ignorant* prior belief about μ as:

$$p(\mu) = \mathcal{U}(0,1)$$

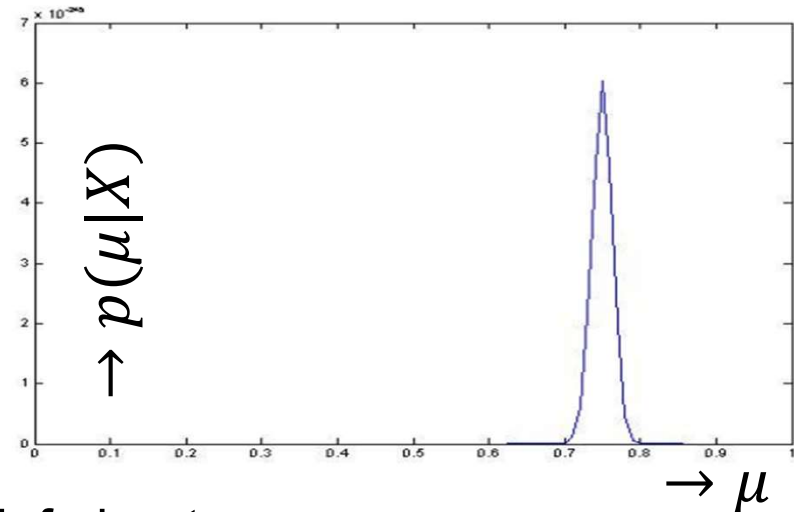
Then using Bayes rule, we obtain probability density function for μ :

$$p(\mu|\mathbf{x}) = \frac{P(\mathbf{x}|\mu)p(\mu)}{P(\mathbf{x})} = \frac{\prod_i P(x_i|\mu) \cdot 1}{P(\mathbf{x})} \propto \mu^H (1 - \mu)^T$$

Coin flipping example (cont.)

$$N = 1000, H = 750, T = 250$$

$$p(\mu|\mathbf{x}) \propto \mu^H (1 - \mu)^T$$



- Posterior distribution is our *new* belief about μ
- Flipping the coin once more, what is the probability of head?

$$\begin{aligned} p(head|\mathbf{x}) &= \int p(head, \mu|\mathbf{x}) d\mu = \int P(head|\mu, \mathbf{x}) p(\mu|\mathbf{x}) d\mu \\ &= (H + 1)/(N + 2) = 751/1002 = 0.7495 \end{aligned}$$

- Note that we never computed value of μ
- Rule of succession used by Pierre-Simon Laplace to estimate that the probability of sun rising tomorrow is $(5000 \cdot 365.25 + 1)/(5000 \cdot 365.25 + 2)$

Distributions from our example

- Likelihood of observed data $P(X|\mu)$ given a parametric model of probability distribution
 - Bernoulli distribution with parameter μ
- Prior on the parameters of the model $p(\mu)$
 - Uniform prior as a special case of Beta distribution
- Posterior distribution of model parameters given an observed data

$$p(\mu|X) = \frac{P(X|\mu)p(\mu)}{P(X)}$$

- Posterior predictive distribution of a new observation give prior (training) observations

$$p(head|X) = \int P(head|\mu)p(\mu|X)d\mu$$

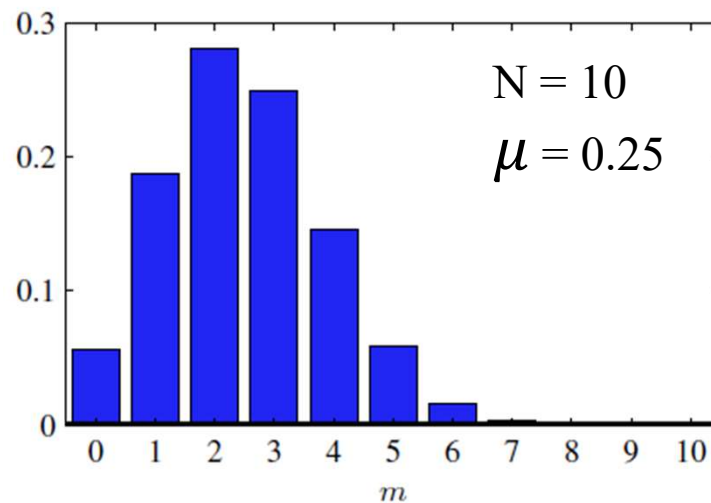
Bernoulli and Binomial distributions

$$\text{Bern}(x|\mu) = \mu^x(1 - \mu)^{1-x}$$

- The “coin flipping” distribution is **Bernoulli distribution**
- Flipping the coin once, what is the probability of $x = 1$ (head) or $x = 0$ (tail)

$$\text{Bin}(m|N, \mu) = \binom{N}{m} \mu^m (1 - \mu)^{N-m}$$

- Related **binomial distribution** is also described by single probability μ
- How many heads do I get if I flip the coin N times?

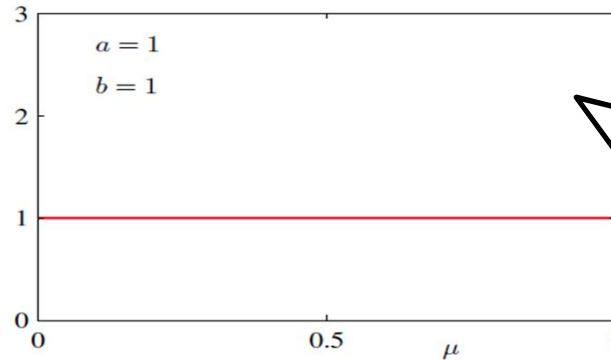
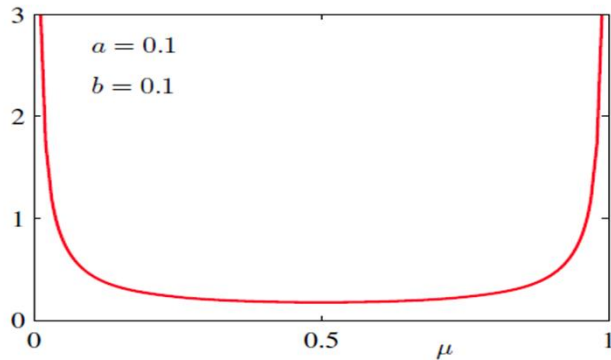


Beta distribution

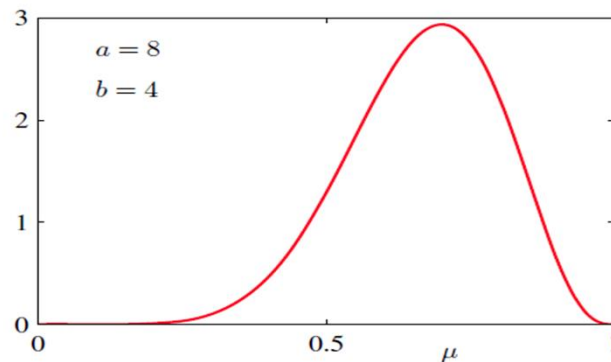
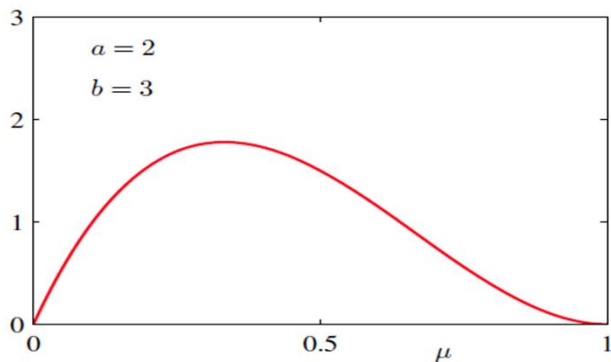
$$\text{Beta}(\mu|a, b) = \frac{\Gamma(a + b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1 - \mu)^{b-1}$$

Normalizing constant

- **Beta distribution** has “similar” form as Bern or Bin, but it is now function of μ
- Continuous distribution for μ over the interval (0,1)
- Can be used to express our prior beliefs about the Bernoulli dist. parameter μ



Uniform distribution over μ as was the prior in our coin flipping example



Beta as a conjugate prior

$$\mathbf{x} = [x_1, x_2, x_3, \dots, x_N] = [1, 0, 0, 1, \dots, 0]$$

$$P(\mathbf{x}|\mu) = \prod_i \text{Bern}(x_i|\mu) = \prod_i \mu^{x_i} (1 - \mu)^{1-x_i} = \mu^H (1 - \mu)^T$$

$$\text{Beta}(\mu|a, b) = \frac{\Gamma(a + b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1 - \mu)^{b-1}$$

$$\begin{aligned} p(\mu|\mathbf{x}) &= \frac{P(\mathbf{x}|\mu)p(\mu)}{P(\mathbf{x})} \propto \mu^H (1 - \mu)^T \mu^{a-1} (1 - \mu)^{b-1} \\ &= \mu^{H+a-1} (1 - \mu)^{T+b-1} \propto \text{Beta}(\mu|H+a, T+b) \end{aligned}$$

Sufficient statistics

- Using **Beta as a prior for Bernoulli parameter μ** results in **Beta posterior distribution** → **Beta is conjugate prior to Bernoulli**
- $a - 1$ and $b - 1$ can be seen as a prior counts of heads and tails.
- Continuous distribution of μ over the interval $(0,1)$
- Beta distribution can be used to express our prior beliefs about the Bernoulli distributions parameter μ

Categorical and Multinomial distribution

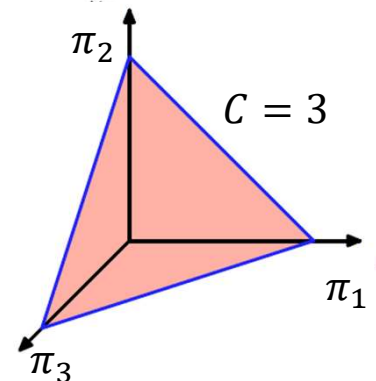
$$\mathbf{x} = [0, 0, 1, 0, 0, 0]$$

One-hot encoding of a discrete event ( on a dice)

$$\boldsymbol{\pi} = [\pi_1, \pi_2, \dots, \pi_C]$$

Probabilities of the events
(eg. $[\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}]$ for fair dice)

$$\text{Cat}(\mathbf{x}|\boldsymbol{\pi}) = \prod_c \pi_c^{x_c} \quad \sum_c \pi_c = 1 \rightarrow \boldsymbol{\pi} \text{ is a point on a simplex}$$



- **Categorical distribution** simply “returns” the probability of a given event \mathbf{x}
- Sample from the distribution is the event (or its one-hot encoding)

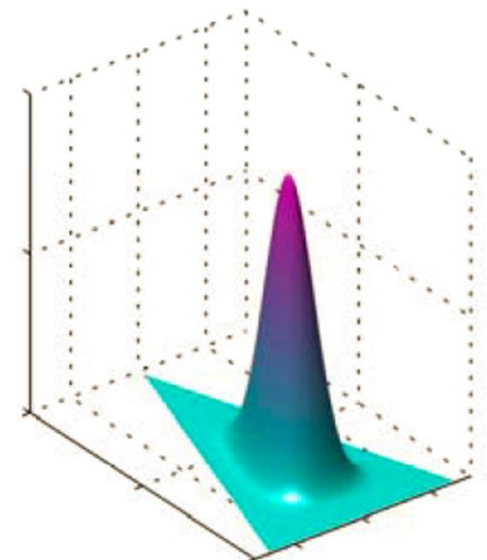
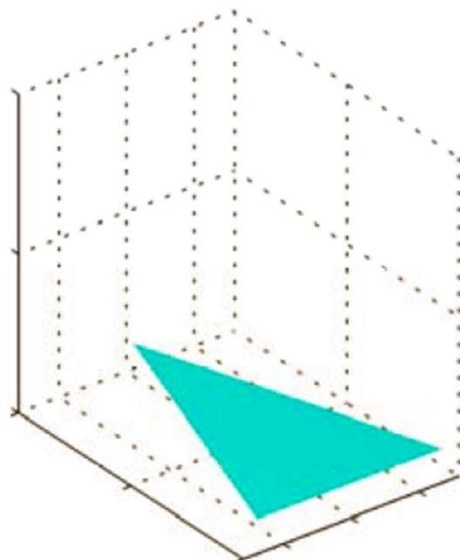
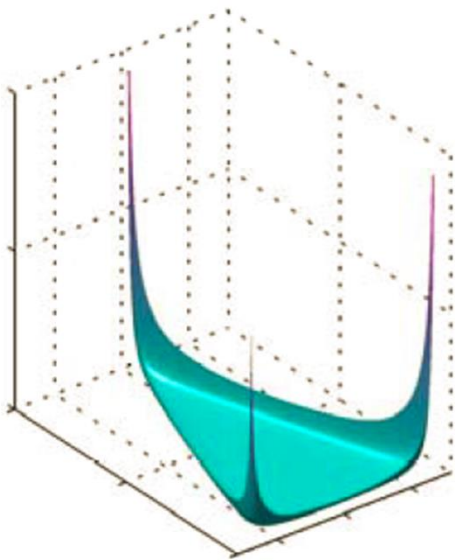
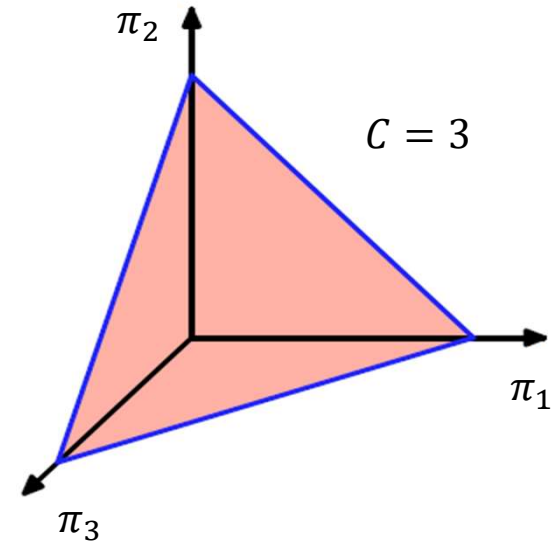
$$\text{Mult}(m_1, m_2, \dots, m_C | \boldsymbol{\pi}, N) = \binom{N}{m_1 m_2 \dots m_C} \prod_c \pi_c^{m_c}$$

- **Multinomial distribution** is also described by single probability vector $\boldsymbol{\pi}$
- How many ones, twos, threes, ... do I get if I throw the dice N times?
- Sample from the distribution is vector of numbers (e.g. 11x one, 8x two, ...)

Dirichlet distribution

$$\text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}) = \frac{\Gamma(\sum_c \alpha_c)}{\Gamma(\alpha_1) \dots \Gamma(\alpha_C)} \prod_{c=1}^C \pi_c^{\alpha_c-1}$$

- **Dirichlet distribution** is continuous distribution over the points $\boldsymbol{\pi}$ on a K dimensional simplex.
- Can be used to express our prior beliefs about the categorical distribution parameter $\boldsymbol{\pi}$



Dirichlet as a conjugate prior

$$P(\mathbf{X}|\boldsymbol{\pi}) = \prod_n \text{Cat}(\mathbf{x}_n|\boldsymbol{\pi}) = \prod_n \prod_c \pi_c^{x_{cn}} = \prod_c \pi_c^{m_c}$$

$$\text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}) = \frac{\Gamma(\sum_c \alpha_c)}{\Gamma(\alpha_1) \dots \Gamma(\alpha_C)} \prod_{c=1} \pi_c^{\alpha_c-1}$$

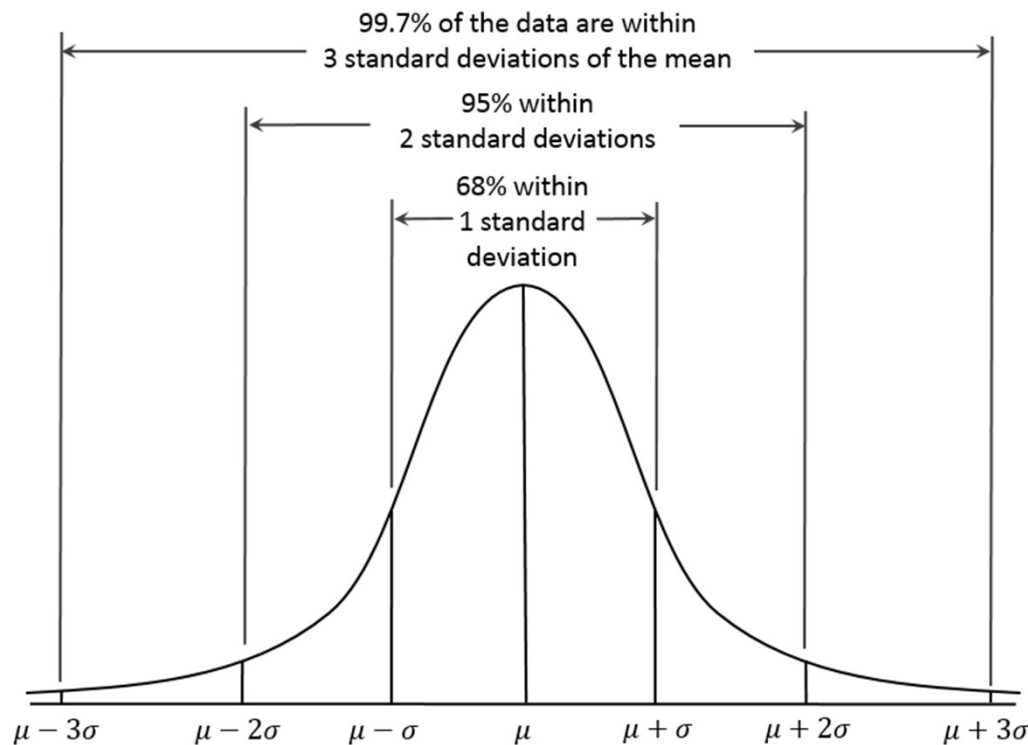
$$\begin{aligned} p(\boldsymbol{\pi}|\mathbf{X}) &= \frac{P(\mathbf{X}|\boldsymbol{\pi})p(\boldsymbol{\pi})}{P(\mathbf{X})} \propto \prod_c \pi_c^{m_c} \prod_c \pi_c^{\alpha_c-1} \\ &= \prod_{c=1} \pi_c^{m_c+\alpha_c-1} \propto \text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha} + \mathbf{m}) \end{aligned}$$

Sufficient statistics

- Using **Dirichlet as a prior for Categorical parameter π** results in **Dirichlet posterior** distribution \rightarrow **Dirichlet is conjugate prior to Categorical dist.**
- $\alpha_c - 1$ can be seen as a prior count for the individual events.

Gaussian distribution (univariate)

$$p(x) = \mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



ML estimates of parameters

$$\mu = \frac{1}{N} \sum_n x_n$$

$$\sigma^2 = \frac{1}{N} \sum_n (x_n - \mu)^2$$

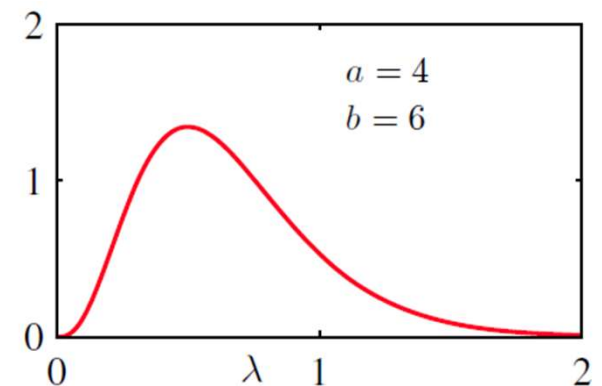
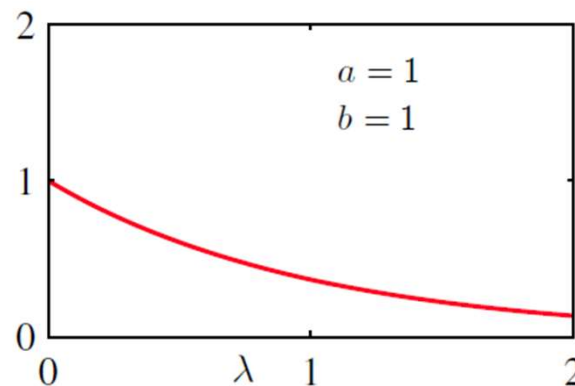
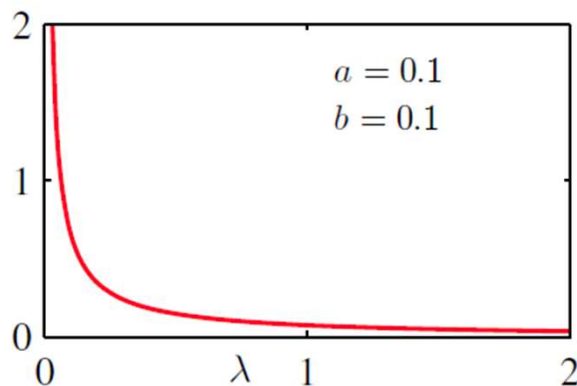
Gamma distribution

Normal distribution can be expressed in terms of precision $\lambda = \frac{1}{\sigma^2}$

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \sqrt{\frac{\lambda}{2\pi}} e^{-\frac{\lambda}{2}(x-\mu)^2}$$

$$\text{Gam}(\lambda|a, b) = \frac{1}{\Gamma(a)} b^a \lambda^{a-1} e^{-b\lambda}$$

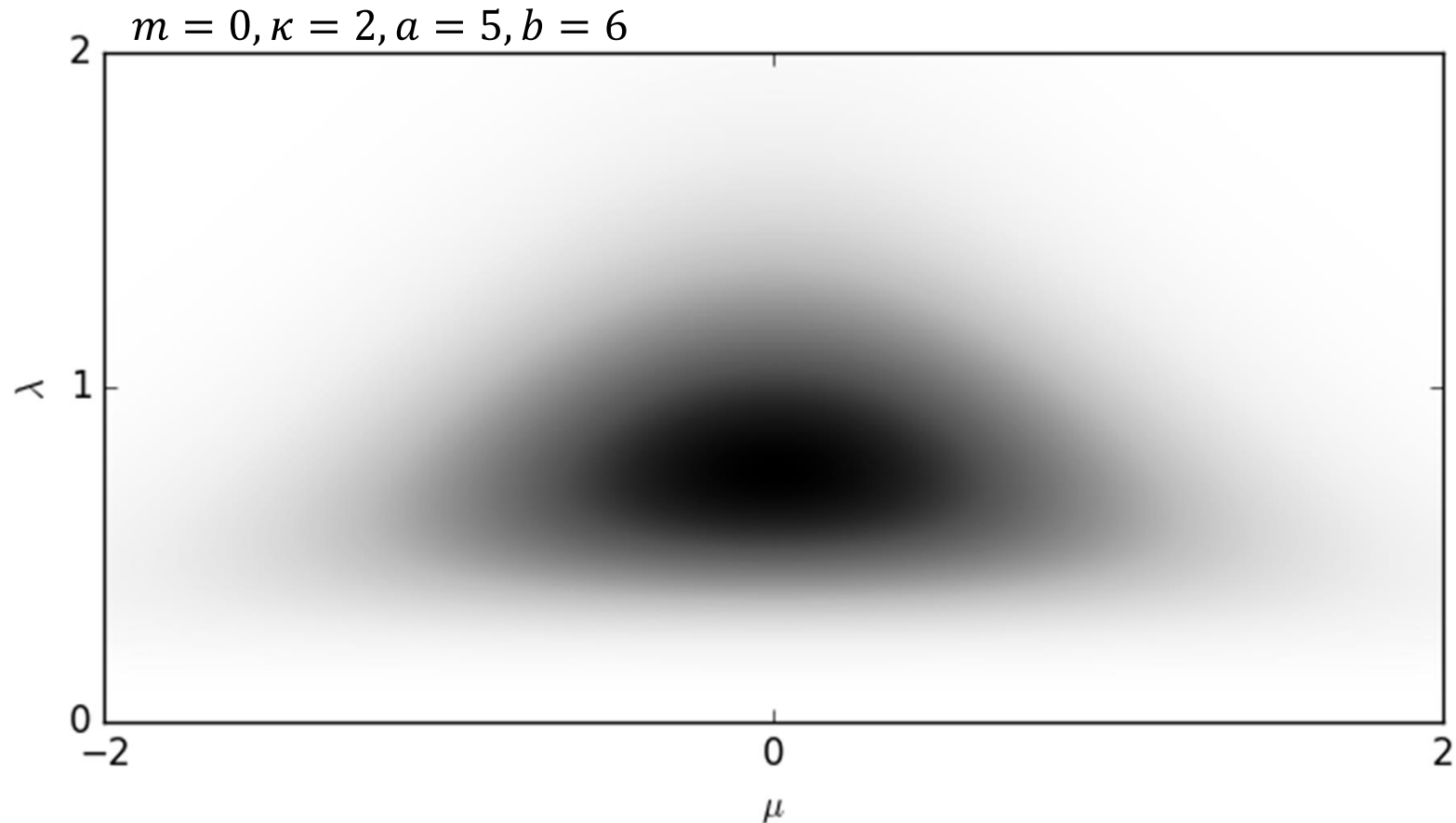
Gamma distribution defined for $\lambda > 0$ can be used as a prior over the precision



NormalGamma distribution

$$\text{NormalGamma}(\mu, \lambda | m, \kappa, a, b) = \mathcal{N}(\mu | m, (\kappa\lambda)^{-1}) \text{Gam}(\lambda | a, b)$$

Joint distribution over μ and λ . Note that μ and λ are not independent.



NormalGamma distribution

- **NormalGamma distribution** is the conjugate prior for Gaussian dist.
- Given observations $\mathbf{x} = [x_1, x_2, x_3, \dots, x_N]$, the posterior distribution

$$p(\mu, \lambda | \mathbf{x}) = \frac{p(\mathbf{x} | \mu, \lambda) p(\mu, \lambda)}{p(\mathbf{x})}$$

$$\propto \prod_i \mathcal{N}(x_i; \mu, \sigma^2) \text{NormalGamma}(\mu, \lambda | m, \kappa, a, b)$$

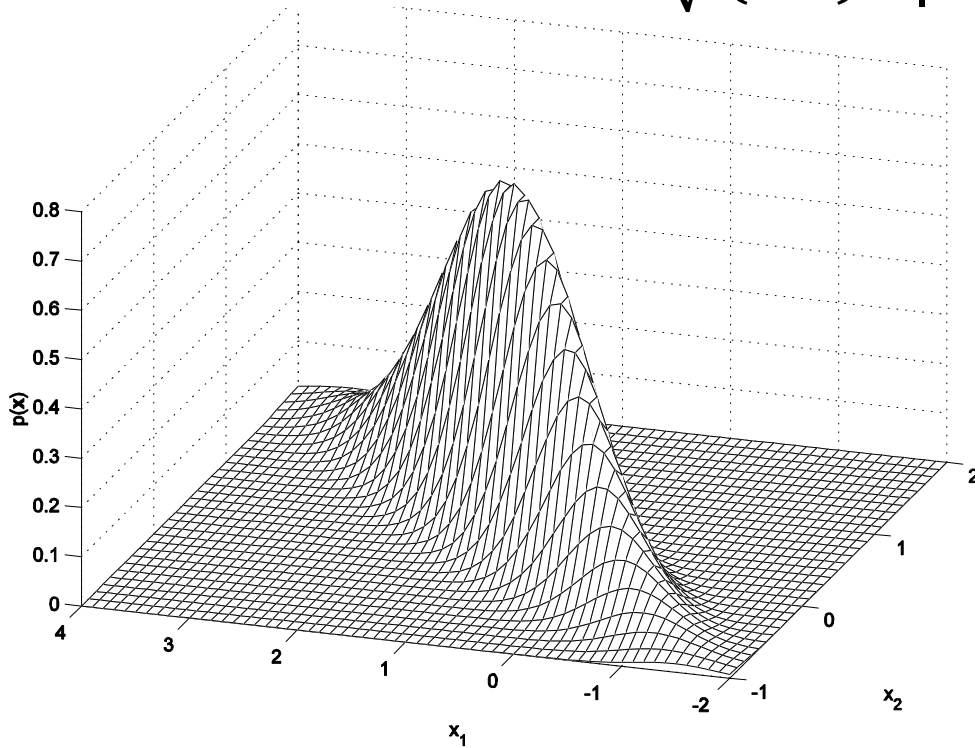
$$\propto \text{NormalGamma} \left(\mu, \lambda \left| \frac{\kappa m + N \bar{x}}{\kappa + N}, \kappa + N, a + \frac{N}{2}, b + \frac{N}{2} \left(s + \frac{\kappa (\bar{x} - m)^2}{\kappa + N} \right) \right. \right)$$

Defined in terms of sufficient statistics N and

$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n \quad s = \frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})^2$$

Gaussian distribution (multivariate)

$$p(x_1, \dots, x_D) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$



ML estimates of parameters

$$\boldsymbol{\mu} = \frac{1}{N} \sum_n \mathbf{x}_n$$

$$\boldsymbol{\Sigma} = \frac{1}{N} \sum_n (\mathbf{x}_n - \boldsymbol{\mu})(\mathbf{x}_n - \boldsymbol{\mu})^T$$

Gaussian distribution (multivariate)

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$

Conjugate prior is **Normal-Wishart**

$$p(\boldsymbol{\mu}, \boldsymbol{\Lambda} | \boldsymbol{\mu}_0, \beta, \mathbf{W}, \nu) = \mathcal{N}(\boldsymbol{\mu} | \boldsymbol{\mu}_0, (\beta \boldsymbol{\Lambda})^{-1}) \mathcal{W}(\boldsymbol{\Lambda} | \mathbf{W}, \nu)$$

where

$$\mathcal{W}(\boldsymbol{\Lambda} | \mathbf{W}, \nu) = B |\boldsymbol{\Lambda}|^{(\nu-D-1)/2} \exp\left(-\frac{1}{2} \text{Tr}(\mathbf{W}^{-1} \boldsymbol{\Lambda})\right)$$

is **Wishart distribution** and

$$\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$$

Exponential family

- All the distributions described so far are distributions from the **exponential family**, which can be expressed in the following form

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x}) g(\boldsymbol{\eta}) \exp\{\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})\}$$

- For example for Gaussian distribution:

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x - \frac{\mu^2}{2\sigma^2}\right\}$$

$$\boldsymbol{\eta} = \begin{pmatrix} \mu/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix} \quad \mathbf{u}(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix} \quad g(\boldsymbol{\eta}) = \sqrt{-\frac{2\eta_2}{2\pi}} \exp\left(\frac{\eta_1^2}{4\eta_2}\right) \quad h(x) = 1$$

- To evaluate likelihood of set of observations:

$$\begin{aligned} \prod_n \mathcal{N}(x_n; \mu, \sigma^2) &= \exp\left\{-\frac{1}{2\sigma^2} \sum_n x_n^2 + \frac{\mu}{\sigma^2} \sum_n x_n - N \left(\frac{\mu^2}{2\sigma^2} + \frac{\log(2\pi\sigma^2)}{2}\right)\right\} \\ &= g(\boldsymbol{\eta})^N \exp\left\{\boldsymbol{\eta}^T \sum_{n=1}^N \mathbf{u}(x_n)\right\} \prod_n h(x_n) \end{aligned}$$

Exponential family

For any distributions from exponential family

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x}) g(\boldsymbol{\eta}) \exp\{\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})\}$$

- Likelihood $p(\mathbf{X}|\boldsymbol{\eta})$ of observed data $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N]$ can be evaluated using the sufficient statistics N and $\sum_{n=1}^N \mathbf{u}(\mathbf{x}_n)$:

$$p(\mathbf{X}|\boldsymbol{\eta}) = g(\boldsymbol{\eta})^N \exp\left\{\boldsymbol{\eta}^T \sum_{n=1}^N \mathbf{u}(x_n)\right\} \prod_n h(x_n)$$

- Conjugate prior distribution over parameter $\boldsymbol{\eta}$ exists in form:

$$p(\boldsymbol{\eta}|\boldsymbol{\theta}, \nu) = f(\boldsymbol{\theta}, \nu) g(\boldsymbol{\eta})^\nu \exp\{\boldsymbol{\eta}^T \boldsymbol{\theta}\}$$

- Posterior distribution takes the same form as the conjugate prior and we need only the prior parameters and the sufficient stats to evaluate it:

$$p(\boldsymbol{\eta}|\mathbf{X}) = p\left(\boldsymbol{\eta} \mid \boldsymbol{\theta} + \sum_{n=1}^N \mathbf{u}(x_n), \nu + N\right) \propto g(\boldsymbol{\eta})^{N+\nu} \exp\left\{\boldsymbol{\eta}^T \left(\boldsymbol{\theta} + \sum_{n=1}^N \mathbf{u}(x_n)\right)\right\}$$

- $\frac{\boldsymbol{\theta}}{\nu}$ can be seen as prior observation and ν as prior count of observation

Parameter estimation revisited

- Lets estimate again parameters $\boldsymbol{\eta}$ of a chosen $p(\mathbf{x}|\boldsymbol{\eta})$ distribution given some of observed data $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N]$
- Using the Bayes rule, we get the posterior distribution

$$p(\boldsymbol{\eta}|\mathbf{X}) = \frac{P(\mathbf{X}|\boldsymbol{\eta})p(\boldsymbol{\eta})}{P(\mathbf{X})}$$

- We can choose the most likelihood parameters: **Maximum a-posteriori (MAP)** estimate

$$\hat{\boldsymbol{\eta}}^{MAP} = \arg \max_{\boldsymbol{\eta}} p(\boldsymbol{\eta}|\mathbf{X}) = \arg \max_{\boldsymbol{\eta}} p(\mathbf{X}|\boldsymbol{\eta})p(\boldsymbol{\eta})$$

- Assuming flat (constant) prior $p(\boldsymbol{\eta}) = \text{const}$, we obtain **Maximum likelihood (ML)** estimate as a special case:

$$\hat{\boldsymbol{\eta}}^{ML} = \arg \max_{\boldsymbol{\eta}} P(\mathbf{X}|\boldsymbol{\eta})$$

Posterior predictive distribution

- We do not need to obtain a point estimate of the parameters $\hat{\eta}$
- It is always good to postpone making hard decisions
- Instead, we can take into account the uncertainty encoded in the posterior distribution $p(\eta|\mathbf{X})$ when evaluating **posterior predictive probability** for a new data point x' (as we did in our coin flipping example)

$$p(x'|\mathbf{X}) = \int p(x', \eta|\mathbf{X})d\eta = \int p(x'|\eta)p(\eta|\mathbf{X})d\eta$$

- Rather than using one most likely setting of parameters $\hat{\eta}$, we average over their different setting, which could possibly generate the observed data \mathbf{X}
 - ➔ this approach is robust to overfitting

Posterior predictive for Bernoulli

- Beta prior on parameters of Bernoulli distribution leads to Beta posterior

$$\begin{aligned} p(\mu|\mathbf{x}) &\propto \prod_n \text{Bern}(x_n|\mu) \text{Beta}(\mu|a_0, b_0) \propto \text{Bern}(\mu|a_0 + H, b_0 + T) \\ &= \text{Bern}(\mu|a_N, b_N) \end{aligned}$$

- The posterior predictive distribution is again Bernoulli

$$\begin{aligned} p(x'|\mathbf{x}) &= \int p(x'|\mu)p(\mu|\mathbf{x}) d\mu = \int \text{Bern}(x'|\mu)\text{Beta}(\mu|a_N, b_N) d\mu \\ &= \text{Bern}\left(x' \left| \frac{a_N}{a_N + b_N} \right.\right) = \text{Bern}\left(x' \left| \frac{a_0 + H}{a_0 + b_0 + N} \right.\right) \end{aligned}$$

- In our coin flipping example:

$$p(\mu) = \mathcal{U}(0,1) = \text{Beta}(\mu|a_0, b_0) = \text{Beta}(\mu|1,1)$$

$$p(\mu|\mathbf{x}) = \text{Beta}(\mu|a_N, b_N) = \text{Beta}(\mu|a_0 + H, b_0 + T) = \text{Beta}(\mu|1 + 750, 1 + 250)$$

$$p(x'|\mathbf{x}) = \text{Bern}\left(x' \left| \frac{a_N}{a_N + b_N} \right.\right) = 751/1002 = 0.7495$$

Posterior predictive for Categorical

- Dirichlet prior on parameters of Categorical distribution leads to Dirichlet posterior

$$p(\boldsymbol{\pi}|\mathbf{X}) \propto \prod_n \text{Cat}(\mathbf{x}_n|\boldsymbol{\pi}) \text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}_0) \propto \text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}_0 + \mathbf{m}) = \text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}_N)$$

- The posterior predictive distribution is again Categorical

$$\begin{aligned} p(\mathbf{x}'|\mathbf{X}) &= \int p(\mathbf{x}'|\boldsymbol{\pi})p(\boldsymbol{\pi}|\mathbf{X}) d\boldsymbol{\pi} = \int \text{Cat}(\mathbf{x}'|\boldsymbol{\pi})\text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}_N) d\boldsymbol{\pi} \\ &= \text{Cat}\left(\mathbf{x}' \left| \frac{\boldsymbol{\alpha}_N}{\sum_c \alpha_{Nc}} \right.\right) = \text{Cat}\left(\mathbf{x}' \left| \frac{\boldsymbol{\alpha}_0 + \mathbf{m}}{\sum_c \alpha_{0c} + m_c} \right.\right) \end{aligned}$$

Student's t-distribution

- NormalGamma prior on parameters of Gaussian distribution leads to NormalGamma posterior

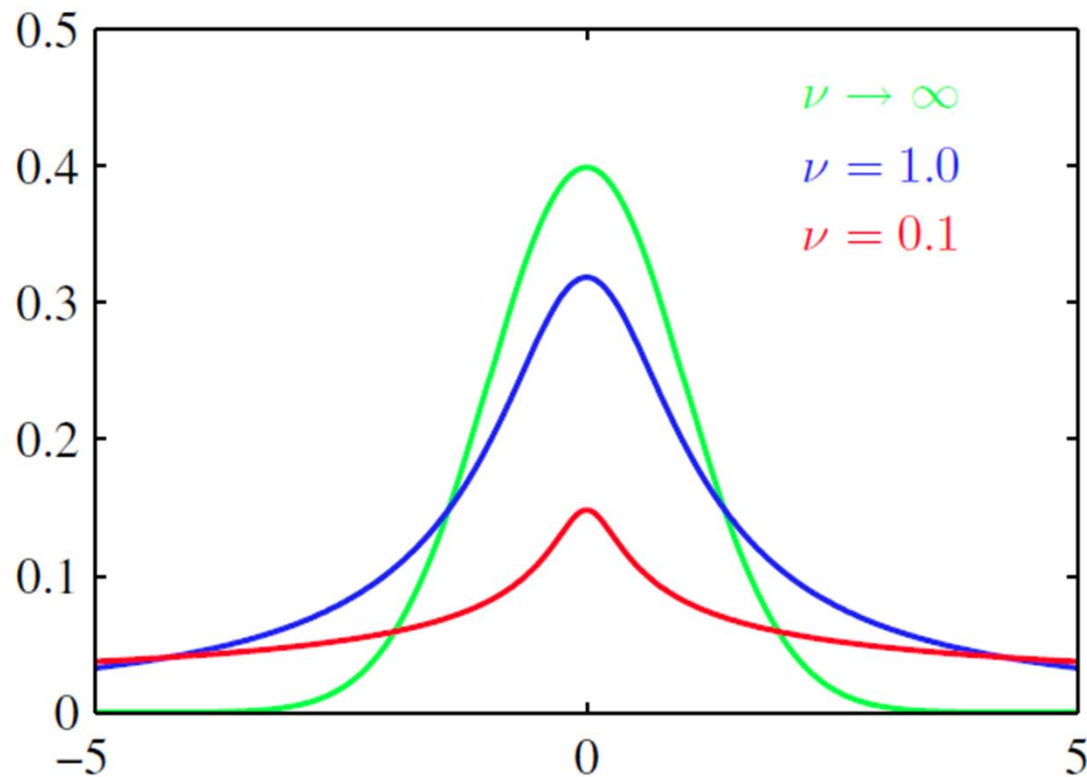
$$\begin{aligned} p(\mu, \lambda | \mathbf{x}) &\propto \prod_i \mathcal{N}(x_i; \mu, \sigma^2) \text{NormalGamma}(\mu, \lambda | m_0, \kappa_0, a_0, b_0) \\ &\propto \text{NormalGamma}\left(\mu, \lambda \left| \frac{\kappa_0 m_0 + N \bar{x}}{\kappa_0 + N}, \kappa_0 + N, a_0 + \frac{N}{2}, b_0 + \frac{N}{2} \left(s + \frac{\kappa_0 (\bar{x} - m_0)^2}{\kappa_0 + N} \right) \right.\right) \\ &= \text{NormalGamma}(\mu, \lambda | m_N, \kappa_N, a_N, b_N) \end{aligned}$$

- The posterior predictive distribution is Student's t-distribution

$$\begin{aligned} p(x' | \mathbf{x}) &= \iint p(x' | \mu, \lambda) p(\mu, \lambda | \mathbf{x}) \, d\mu \, d\lambda \\ &= \iint \mathcal{N}(x' | \mu, \lambda) \text{NormalGamma}(\mu, \lambda | m_N, \kappa_N, a_N, b_N) \, d\mu \, d\lambda \\ &= \text{St}(x' | m_N, 2a_N, \frac{a_N \kappa_N}{b_N (\kappa_N + 1)}) \end{aligned}$$

Student's t-distribution

$$\text{St}(x | \mu, \nu, \gamma) = \frac{\Gamma\left(\frac{\nu}{2} + \frac{1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} \left(\frac{\gamma}{\pi\nu}\right)^{\frac{1}{2}} \left[1 + \frac{\gamma(x - \mu)^2}{\nu}\right]^{-\frac{\nu}{2} - \frac{1}{2}}$$



- Gaussian distribution is a special case of Student's with degree of freedom $\nu \rightarrow \infty$
- For the posterior $p(\mu, \lambda | \mathbf{x})$, $\nu = 2a_N = 2a_0 + N$