Bayesian Models in Machine Learning

Lukáš Burget

BRNO FACULTY UNIVERSITY OF INFORMATION OF TECHNOLOGY TECHNOLOGY

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Some images taken from: C. M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006.

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

 $P(head|\mu) = \mu$ $P(tail|\mu) = 1 - \mu$

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

- Let's 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?

$$
p(head|\mathbf{x}) = \int p(head, \mu|\mathbf{x}) d\mu = \int P(head|\mu, \mathbf{x}) p(\mu|\mathbf{x}) d\mu
$$

$$
= (H+1)/(N+2) = 751/1002 = 0.7495
$$

- 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 $(5000*365.25+1)/(5000*365.25+2)$

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)

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

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

Some images taken from :

C. M. Bishop. 2006.Pattern Recognition and Machine Learning. Springer.

Beta distribution Normalizing constant

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

- **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

Beta as a conjugate prior

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

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

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

$$
p(\mu|\mathbf{x}) = \frac{P(\mathbf{x}|\mu)p(\mu)}{P(\mathbf{x})} \propto \mu^H (1 - \mu)^T \mu^{a-1} (1 - \mu)^{b-1}
$$
 Statistics

$$
= \mu^{H+a-1} (1 - \mu)^{T+b-1} \propto \text{Beta}(\mu|H + a, T + b)
$$

- 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

 $\pi = [\pi_1, \pi_2, ..., \pi_C]$

 $C = 3$ π_2 $\mathbf{x} = [0, 0, 1, 0, 0, 0]$ One-hot encoding of a discrete event ($\begin{bmatrix} \bullet \\ \bullet \end{bmatrix}$ on a dice) Probabilities of the events (eg. $\left[\frac{1}{2}\right]$ $\frac{1}{6}, \frac{1}{6}$ $\frac{1}{6}, \frac{1}{6}$ $\frac{1}{6}, \frac{1}{6}$ $\frac{1}{6}, \frac{1}{6}$ $\frac{1}{6}, \frac{1}{6}$ 6 for fair dice)

 π_1

 π_{3}

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

- **Categorical distribution** simply "returns" the probability of a given event **x**
- Sample from the distribution is the event (or its one-hot encoding)

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

- **Multinomial distribution** is also described by single probability vector π
- 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

$$
\text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}) = \frac{\Gamma(\sum_{c} \alpha_{c})}{\Gamma(\alpha_{1}) \dots \Gamma(\alpha_{C})} \prod_{c=1} \pi_{c}^{\alpha_{c}-1}
$$

- **Dirichlet distribution** is continuous distribution over the points π on a K dimensional simplex.
- Can be used to express our prior beliefs about the categorical distribution parameter π

Dirichlet as a conjugate prior
\n
$$
P(X|\pi) = \prod_{n} \text{Cat}(x_n|\pi) = \prod_{n} \prod_{c} \pi_c^{x_{cn}} = \prod_{c} \pi_c^{m_c}
$$
\n
$$
\text{Dir}(\pi|\alpha) = \frac{\Gamma(\sum_{c} \alpha_c)}{\Gamma(\alpha_1) \dots \Gamma(\alpha_c)} \prod_{c=1} \pi_c^{\alpha_c - 1} \qquad \text{number of training observations of category } c
$$
\n
$$
p(\pi|X) = \frac{P(X|\pi)p(\pi)}{P(X)} \propto \prod_{c} \pi_c^{m_c} \prod_{c} \pi_c^{\alpha_c - 1} \underbrace{\text{Sufficient statistics}}_{m = [m_1, \dots, m_c],}
$$
\n
$$
= \prod_{c=1} \pi_c^{m_c + \alpha_c - 1} \propto \text{Dir}(\pi|\alpha + m)
$$

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

Gaussian distribution (univariate)

 $\sqrt{2}$

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

Gamma distribution

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

NormalGama(μ , $\lambda | m, \kappa, a, b) = \mathcal{N}(\mu | m, (\kappa \lambda)^{-1})$ 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 $\mathbf{x} = [x_1, x_2, x_3, ... x_N]$, the posterior distribution

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

$$
\propto \prod_{i} \mathcal{N}(x_i; \mu, \lambda^{-1}) \text{NormalGamma}(\mu, \lambda | m, \kappa, a, b)
$$

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

Defined in terms of sufficient statistics *N* and

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

Gaussian distribution (multivariate)

Gaussian distribution (multivariate) $\mathcal{N}\left(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}\right) =$ 1 $(2\pi)^D |\Sigma|$ e^{-} 1 2 $(\mathbf{x}-\boldsymbol{\mu})^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})$

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

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

is **Wishart distribution** and

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

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:

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

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

• To evaluate likelihood of set of observations:

$$
\prod_{n} \mathcal{N}(x_n; \mu, \sigma^2) = \exp\left\{-\frac{1}{2\sigma^2} \sum_{n} x_n^2 + \frac{\mu}{\sigma^2} \sum_{n} x_n - N\left(\frac{\mu^2}{2\sigma^2} + \frac{\log(2\pi\sigma^2)}{2}\right)\right\}
$$

$$
= g(\eta)^N \exp\left\{\eta^T \sum_{n=1}^N \mathbf{u}(x_n)\right\} \prod_{n} h(x_n)
$$

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 $p(X|\eta)$ of observed data $X = [x_1, x_2, ..., x_N]$ can be evaluated using the sufficient statistics N and $\sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)$:

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

- Conjugate prior distribution over parameter η exists in form: $p(\eta | \theta, v) = f(\theta, v) g(\eta)^v \exp{\{\eta^T \theta\}} = f(\theta, v) \exp{\{\widehat{\theta}^T v(\eta)\}}$
- Posterior distribution takes the same form as the conjugate prior and we need only the prior parameters and the sufficient stats to evaluate it:

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

• $\boldsymbol{\theta}$ $\mathcal V$ can be seen as prior observation and ν as prior count of observation

Parameter estimation revisited

- Let's estimate again parameters η of a chosen $p(\mathbf{x}|\boldsymbol{\eta})$ distribution given some of observed data $X = [x_1, x_2, ..., x_N]$
- 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

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

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

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

Posterior predictive distribution

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

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

• Rather than using one most likely setting of parameters $\hat{\eta}$, we average over their different setting, which could possibly generate the observed data X

 \rightarrow this approach is robust to overfitting

Posterior predictive for Bernoulli

- Beta prior on parameters of Bernoulli distribution leads to Beta posterior $p(\mu|\mathbf{x}) \propto |\mathbf{Bern}(x_n|\mu)$ Beta $(\mu|a_0, b_0) \propto \text{Beta}(\mu|a_0 + H, b_0 + T)$ \boldsymbol{n} $= \text{Beta}(\mu | a_N, b_N)$
- The posterior predictive distribution is again Bernoulli

$$
p(x'|\mathbf{x}) = \int p(x'|\mu)p(\mu|\mathbf{x}) d\mu = \int \text{Bern}(x'|\mu)\text{Beta}(\mu|a_N, b_N) d\mu
$$

$$
= \text{Bern}\left(x'\left|\frac{a_N}{a_N + b_N}\right.\right) = \text{Bern}\left(x'\left|\frac{a_0 + H}{a_0 + b_0 + N}\right.\right)
$$

• In our coin flipping example:

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

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

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

Posterior predictive for Categorical

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

$$
p(\pi|\mathbf{X}) \propto \prod_n \text{Cat}(\mathbf{x}_n|\pi) \, \text{Dir}(\pi|\alpha_0) \propto \text{Dir}(\pi|\alpha_0 + \mathbf{m}) = \text{Dir}(\pi|\alpha_N)
$$

• The posterior predictive distribution is again Categorical

$$
p(\mathbf{x}'|\mathbf{X}) = \int p(\mathbf{x}'|\boldsymbol{\pi})p(\boldsymbol{\pi}|\mathbf{X}) d\boldsymbol{\pi} = \int \text{Cat}(\mathbf{x}'|\boldsymbol{\pi})\text{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}_N) d\boldsymbol{\pi}
$$

$$
= \text{Cat}(\mathbf{x}'|\frac{\boldsymbol{\alpha}_N}{\sum_c \alpha_{Nc}}) = \text{Cat}(\mathbf{x}'|\frac{\boldsymbol{\alpha}_0 + \mathbf{m}}{\sum_c \alpha_{0c} + m_c})
$$

Student's t-distribution

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

$$
p(\mu, \lambda | \mathbf{x}) \propto \prod_{i} \mathcal{N}(x_i; \mu, \sigma^2) \text{NormalGamma}(\mu, \lambda | m_0, \kappa_0, a_0, b_0)
$$

$$
\propto \text{NormalGamma}(\mu, \lambda \left| \frac{\kappa_0 m_0 + N\bar{x}}{\kappa_0 + N}, \kappa_0 + N, a_0 + \frac{N}{2}, b_0 + \frac{N}{2} \left(s + \frac{\kappa_0 (\bar{x} - m_0)^2}{\kappa_0 + N} \right) \right)
$$

= NormalGamma(\mu, \lambda | m_N, \kappa_N, a_N, b_N)

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

$$
p(x'|\mathbf{x}) = \iint p(x'|\mu, \lambda) p(\mu, \lambda|\mathbf{x}) d\mu d\lambda
$$

=
$$
\iint \mathcal{N}(x'|\mu, \lambda^{-1}) \text{NormalGamma}(\mu, \lambda|m_N, \kappa_N, a_N, b_N) d\mu d\lambda
$$

=
$$
St\left(x'|m_N, 2a_N, \frac{a_N \kappa_N}{b_N(\kappa_N + 1)}\right)
$$

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