Probability Distributions 1

수학과 오서영

1. Binary Variables

Single binary random variable $x \in \{0,1\}$ **example)** x : outcome of flipping a coin (x=1 : head, x=0 : tail) Damaged coin? -> probability of landing heads is not same

The probability of x=1 :
$$p(x=1|\mu) = \mu$$
 where $0 \le \mu \le 1$ $p(x=0|\mu) = 1 - \mu$.

Bernoulli distribution:

Bern
$$(x|\mu) = \mu^x (1-\mu)^{1-x}$$
 $\mathbb{E}[x] = \mu$ $var[x] = \mu(1-\mu)$

1. Binary Variables

Dataset $\mathcal{D} = \{x_1, \dots, x_N\}$ (observed values) **Likelihood function** (function of μ)

- Assumption : observations are independent from $p(x|\mu)$

$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \prod_{n=1}^{N} \mu^{x_n} (1-\mu)^{1-x_n}$$

We can estimate μ by **maximizing** the likelihood function

$$\ln p(\mathcal{D}|\mu) = \sum_{n=1}^{N} \ln p(x_n|\mu) = \sum_{n=1}^{N} \{x_n \ln \mu + (1 - x_n) \ln(1 - \mu)\}$$

->
$$\mu_{\rm ML} = \frac{1}{N} \sum_{n=1}^{N} x_n$$
 (sample mean)

$$\frac{\partial}{\partial \mu} \ln p(\mathcal{D}|\mu) = 0 \Leftrightarrow$$

$$\frac{\partial}{\partial \mu} \sum_{n=1}^{N} \left(x_n \ln \mu + (1 - x_n) \ln(1 - \mu) \right) = 0 \Leftrightarrow$$

$$\sum_{n=1}^{N} \frac{\partial}{\partial \mu} \left(x_n \ln \mu + (1 - x_n) \ln(1 - \mu) \right) = 0 \Leftrightarrow$$

$$\sum_{n=1}^{N} \left(\frac{1}{\mu} x_n - \frac{1}{1 - \mu} (1 - x_n) \right) = 0 \Leftrightarrow$$

$$\sum_{n=1}^{N} \left(\frac{1}{\mu} x_n - \frac{1}{1 - \mu} + \frac{1}{1 - \mu} x_n \right) = 0 \Leftrightarrow$$

$$\sum_{n=1}^{N} \left(\frac{1}{\mu} x_n + \frac{1}{1 - \mu} x_n \right) = \frac{N}{1 - \mu} \Leftrightarrow$$

$$\sum_{n=1}^{N} \left(\frac{1 - \mu}{\mu} x_n + x_n \right) = N \Leftrightarrow$$

$$\sum_{n=1}^{N} \frac{1}{\mu} x_n = N \Leftrightarrow$$

1. Binary Variables

m: The number of observations of x=1

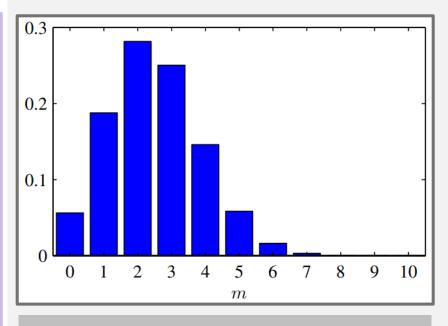
$$\mu_{\rm ML} = \frac{1}{N} \sum_{n=1}^{N} x_n = \frac{m}{N}$$

Overfitting by observed dataset -> prior distribution? **Binomial distribution**:

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

$$\mathbb{E}[m] \equiv \sum_{m=0}^{N} m \operatorname{Bin}(m|N,\mu) = N\mu$$

$$\operatorname{var}[m] \equiv \sum_{m=0}^{N} (m - \mathbb{E}[m])^{2} \operatorname{Bin}(m|N,\mu) = N\mu(1-\mu).$$



Binomial distribution with N=10, mu=0.25

Binomial distribution : overfitting for small dataset -> prior : proportional to powers of μ and 1- μ

Beta distribution:

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

$$\longrightarrow \operatorname{normalization} \longrightarrow \int_0^1 \operatorname{Beta}(\mu|a,b) \, \mathrm{d}\mu = 1.$$

where $\Gamma(x)$ is the gamma function

$$\mathbb{E}[\mu] = \frac{a}{a+b}$$

$$\operatorname{var}[\mu] = \frac{ab}{(a+b)^2(a+b+1)}.$$

Posterior distribution over μ

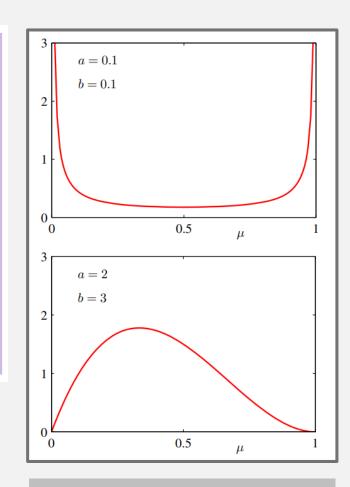
: multiplying beta prior by the binomial likelihood function and normalizing

$$p(\mu|m, l, a, b) = \frac{\Gamma(m+a+l+b)}{\Gamma(m+a)\Gamma(l+b)} \mu^{m+a-1} (1-\mu)^{l+b-1}.$$

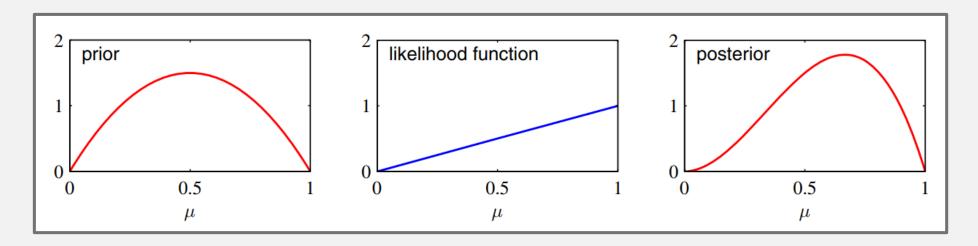
where l = N - m (tail)

-> The posterior distribution also follows the beta distribution.

a, b : effective number of observation



a, b: hyperparameters



Sequential Bayesian inference

Prior: beta with a=2, b=2

Likelihood : N = 1

Posterior: beta with a=3, b=2

Sequential approach to learning

Maximum likelihood methods can also be cast into a sequential framework

- the posterior distribution can act as the prior if subsequent observations arrive
- -> taking one observation at a time and after each observation **updating** the current posterior distribution by multiplying by the likelihood of the incoming observation
- It is **independent** of the choice of prior and of the likelihood function and **depends only** on the assumption of data

$$p(x=1|\mathcal{D}) = \int_0^1 p(x=1|\mu)p(\mu|\mathcal{D}) \,d\mu = \int_0^1 \mu p(\mu|\mathcal{D}) \,d\mu = \mathbb{E}[\mu|\mathcal{D}].$$
$$p(x=1|\mathcal{D}) = \frac{m+a}{m+a+l+b}$$

If m, I are large, MLE!

2.2. Multinomial Variables

Discrete random variables $\mathbf{x}=(0,0,1,0,0,0)^{\mathrm{T}}$ where k is represented k-th element being 1 and all others being 0. -> $x_k=1$ by the parameter μ_k

Generalization of Bernoulli distribution -> Categorical distribution :

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^K \mu_k^{x_k}$$
 where $\mu_k \geqslant 0$ and $\sum_k \mu_k = 1$

Since parameter $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)^{\mathrm{T}}$ (vector),

$$\sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu}) = \sum_{k=1}^{K} \mu_k = 1$$
 proof

$$\mathbb{E}[\mathbf{x}|\boldsymbol{\mu}] = \sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu})\mathbf{x} = (\mu_1, \dots, \mu_M)^{\mathrm{T}} = \boldsymbol{\mu}.$$

$$egin{aligned} \sum_{\mathbf{x}} p(\mathbf{x}|oldsymbol{\mu}) &= \sum_{\mathbf{x}} \prod_{k=1}^K \mu_k^{x_k} \ &= \prod_{k=1}^K \mu_k^{x_k^1} + \dots + \prod_{k=1}^K \mu_k^{x_k^K} \ &= \sum_{k=1}^K \mu_k = 1 \end{aligned}$$

$$\begin{split} \mathbb{E}[\mathbf{x}] &= \mathbb{E}[\mathbf{x}|\boldsymbol{\mu}] \\ &= \sum_{\mathbf{x}} \mathbf{x} p(\mathbf{x}|\boldsymbol{\mu}) \\ &= \sum_{\mathbf{x}} \mathbf{x} \prod_{k=1}^{K} \mu_k^{x_k} \\ &= \mathbf{x}^1 \prod_{k=1}^{K} \mu_k^{x_k^1} + \dots + \mathbf{x}^K \prod_{k=1}^{K} \mu_k^{x_k^K} \\ &= (\mu_1, \dots, \mu_K)^{\mathrm{T}} \end{split}$$

2.2. Multinomial Variables

dataset D of N independent observations $\mathbf{x}_1, \dots, \mathbf{x}_N$ likelihood function :

$$p(\mathcal{D}|\boldsymbol{\mu}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \mu_k^{x_{nk}} = \prod_{k=1}^{K} \mu_k^{(\sum_n x_{nk})} = \prod_{k=1}^{K} \mu_k^{m_k}$$

-> likelihood function depends on N data only through the K quantities :

$$m_k = \sum_n x_{nk}$$

-> Sufficient statistics

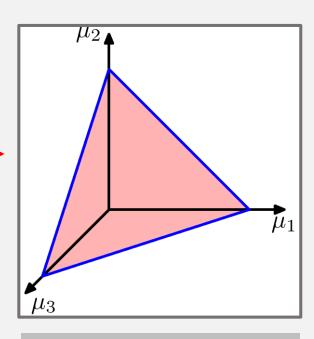
2.2.1 The Dirichlet distribution

Family of prior distributions for parameters $\{\mu_k\}$ of multinomial

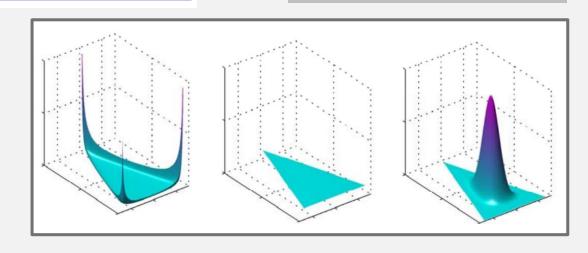
distributions. Conjugate prior : $p(\pmb{\mu}|\pmb{\alpha}) \propto \prod_{k=1}^K \mu_k^{\alpha_k-1}$ where $0 \leqslant \mu_k \leqslant 1$ $\sum_k \mu_k = 1$

$$Dir(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_K)} \prod_{k=1}^K \mu_k^{\alpha_k - 1}$$

where $\Gamma(x)$: gamma function and $\alpha_0 = \sum_{k=1}^{K} \alpha_k$.



K-1 dimensions



Simplex?

Continuous random variable x

Gaussian = normal distribution:

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

Multi-dimension

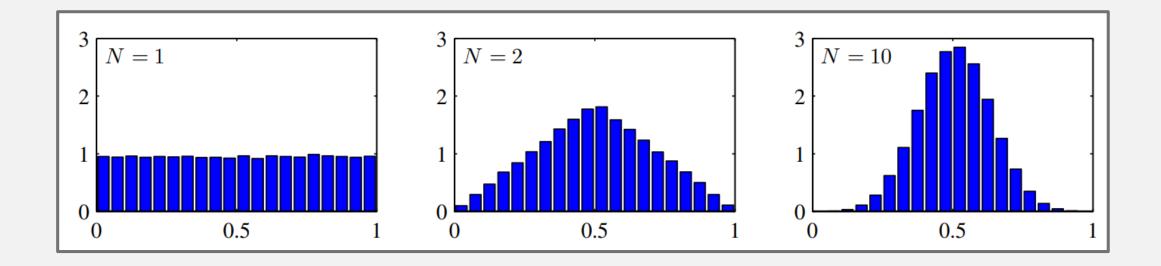
$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\}$$

where D by D covariance matrix

-> the distribution maximizing the entropy is a Gaussian distribution.

Central limit theorem

The sum of a set of random variables has a distribution that becomes increasingly Gaussian as the number of terms increase.



Important analytical properties of Gaussian Distribution

functional dependence of the Gaussian on x is through the quadratic form

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$
 where Δ is Mahalanobis distance

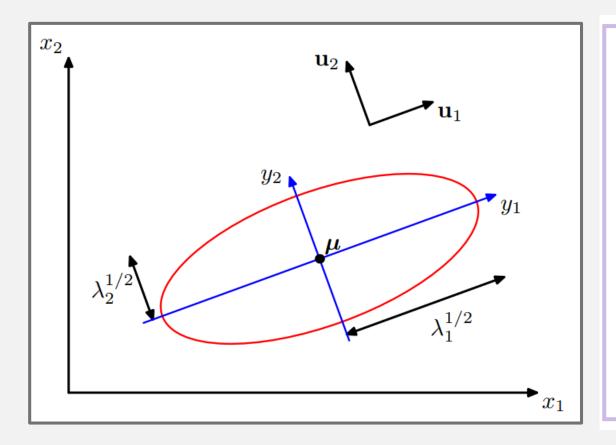
- Eigenvector equation for covariance matrix : $\Sigma \mathbf{u}_i = \lambda_i \mathbf{u}_i$ symmetric orthonormal

$$\mathbf{u}_i^{\mathrm{T}}\mathbf{u}_j = I_{ij}$$

$$I_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise.} \end{cases} \quad \Rightarrow \quad \mathbf{\Sigma} = \sum_{i=1}^D \lambda_i \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}} \quad \Rightarrow \quad \Delta^2 = \sum_{i=1}^D \frac{y_i^2}{\lambda_i}$$

$$\mathbf{\Sigma}^{-1} = \sum_{i=1}^D \frac{1}{\lambda_i} \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}}. \qquad \mathbf{y} = \mathbf{U}(\mathbf{x} - \boldsymbol{\mu})$$

-> y : new coordinate system defined by the orthonormal vecter U



Red

: elliptical surface of constant probability density of Gaussian

The major axes of the ellipse are defined by the eigenvectors U of covariance matrix

 $\lambda_2^{1/2}$ scale ellipse, centroid : mu -> i.e all eigenvalues > 0

Gaussian distribution in the new coordinate system defined by y

$$J_{ij} = \frac{\partial x_i}{\partial y_j} = U_{ji}$$
 where J: jacobian matrix, U: orthonormal -> $|\mathbf{J}|^2 = |\mathbf{U}^{\mathrm{T}}|^2 = |\mathbf{U}^{\mathrm{T}}| |\mathbf{U}| = |\mathbf{U}^{\mathrm{T}}\mathbf{U}| = |\mathbf{I}| = 1$ -> $|\mathbf{J}| = 1$

$$-> |\mathbf{J}|^2 = |\mathbf{U}^{\mathrm{T}}|^2 = |\mathbf{U}^{\mathrm{T}}| |\mathbf{U}| = |\mathbf{U}^{\mathrm{T}}\mathbf{U}| = |\mathbf{I}| = 1$$
 $-> |\mathbf{J}| = 1$

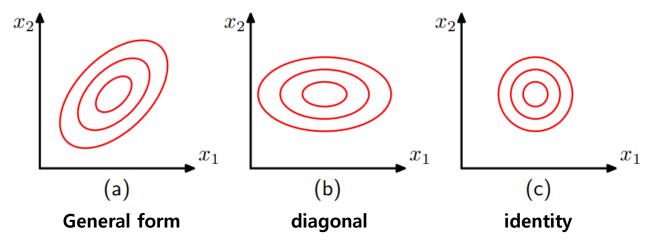
$$|\mathbf{\Sigma}|^{1/2} = \prod_{j=1}^D \lambda_j^{1/2}.$$

$$p(\mathbf{y}) = p(\mathbf{x})|\mathbf{J}| = \prod_{j=1}^{D} \frac{1}{(2\pi\lambda_j)^{1/2}} \exp\left\{-\frac{y_j^2}{2\lambda_j}\right\}$$

-> Product of independent normal distributions

Significant limitations

- **1.** General symmetric covariance matrix has D(D+1)/2 independent parameters and There are another independent parameters in mu -> total : D(D+3)/2 (many..)
- -> restrict the covariance matrix to diagonal matrix or identity matrix



- **2.** Gaussian distribution is intrinsically unimodal (i.e., has a single maximum)
- -> unable to approximate multimodal distributions.

2.3.1 Conditional Gaussian distributions

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$$-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) =$$

$$-\frac{1}{2}(\mathbf{x}_{a} - \boldsymbol{\mu}_{a})^{\mathrm{T}} \boldsymbol{\Lambda}_{aa}(\mathbf{x}_{a} - \boldsymbol{\mu}_{a}) - \frac{1}{2}(\mathbf{x}_{a} - \boldsymbol{\mu}_{a})^{\mathrm{T}} \boldsymbol{\Lambda}_{ab}(\mathbf{x}_{b} - \boldsymbol{\mu}_{b})$$

$$-\frac{1}{2}(\mathbf{x}_{b} - \boldsymbol{\mu}_{b})^{\mathrm{T}} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_{a} - \boldsymbol{\mu}_{a}) - \frac{1}{2}(\mathbf{x}_{b} - \boldsymbol{\mu}_{b})^{\mathrm{T}} \boldsymbol{\Lambda}_{bb}(\mathbf{x}_{b} - \boldsymbol{\mu}_{b}).$$

Quadratic form of \mathbf{x}_a i.e $p(\mathbf{x}_a|\mathbf{x}_b)$: Gaussian (Covariance?)

Diff twice
$$-\frac{1}{2}\mathbf{x}_a^{\mathrm{T}}\mathbf{\Lambda}_{aa}\mathbf{x}_a \rightarrow \mathbf{\Sigma}_{a|b} = \mathbf{\Lambda}_{aa}^{-1}.$$

- Summary) $p(\mathbf{x}_a, \mathbf{x}_b)$: Gaussian -> $p(\mathbf{x}_a | \mathbf{x}_b)$: Gaussian