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2. Probability Distribution

2.0. Introduction

1) Chapter Scope
   A. Examples of probability distributions
   B. Their properties
2) Purpose of Introducing Distributions
   A. a building blocks for more complex models
   B. a recipe to discuss some essential statistical concept, e.g., Bayesian inference
   C. to model the probability distribution p(**x**), i.e., density estimation

      * Model Selection becomes an issue since density estimation is fundamentally ill-posed problem in that infinitely many distributions can fit the observed data set.
3) Parametric distribution vs. Non-Parametric distribution
   A. Parametric distribution
      i. binomial distribution, multinomial distribution, Gaussian distribution (continuous R.V.)
      ii. For density estimation, the parameters shall be determined with an observed data set.
         1. Frequentist: specific values for parameters (earned by optimizing some criterion, e.g., likelihood function)
         2. Bayesian: estimate posterior distribution with introduced prior distributions over the parameters as well as the observed data
      iii. Conjugate Priors: To simplify the Bayesian analysis, use conjugate prior which let posterior distribution be in the same form of prior distribution.
         1. Exponential family of distributions is presented as it possesses a number of important properties.
   B. Non-Parametric distribution
      i. Distribution form is not forced by a user but typically depends on the size of the data set
      ii. Still has the parameters but they do not determine the distribution form but the complexity
      iii. Histogram, nearest-neighbors, kernels

Table. 1 Conjugate prior with posterior distribution in exponential family

Conjugate Prior	**Posterior Distribution**
Dirichlet distribution	Multinomial distribution
Gaussian distribution	Gaussian distribution

2.1. Binary Variables

2.1.1. Bernoulli distribution

2.1.1.1. Definition

$$\mathrm{Bern}(\mathrm{x}|\mu) = \ \mu^{x}(1-\mu)^{1-x}, where \ \ 0 \le \mu < 1 \ \ and \ \ x \in \{0,1\} \tag{2.1}$$

2.1.1.2. Properties

$$\mathbb{E}[\mathrm{x}] = \mu \tag{2.2}$$

$$var[x] = \ \mu(1-\mu) \tag{2.3}$$

2.1.2. Density estimation

$$\mathcal{D} = \{x_1, \dots, x_N\}$$

2.1.2.1. Frequentist

1) Estimate μ by maximizing the likelihood function, i.e., maximize the log of likelihood

$$\ln\big(p(\boldsymbol{\mathcal{D}}|\mu)\big) = \sum_{\mathrm{n}=1}^{\mathrm{N}} \ln p(x_n|\mu) = \ \sum_{\mathrm{n}=1}^{\mathrm{N}} \{\, x_n \ln\mu + (1-\mu)\ln(1-\mu)\} \tag{2.4}$$

2) The above log likelihood function depends on the N observations only through their sum, i.e., *sufficient statistics*: $\sum_n x_n$.

3) $\mu_{ML} = \ \frac{m}{N}$ = *sample mean*

2.1.2.2. Bayesian

Flip a coin 3 times resulting all heads → what is the reasonable prediction? (overfitting)

2.1.2.2.1. Binomial distribution

1) Definition

$$\mathrm{Bin}(\mathrm{m}|\mathrm{N},\mu) = \ \binom{N}{m}\mu^{x}(1-\mu)^{1-x} \tag{2.5}$$

2) Properties

For independent events, 1) the means of the sum is the sum of the mean and 2) the variance of the sum is the sum of the variance

$$\mathbb{E}[\mathrm{m}] = N\mu \tag{2.6}$$

$$\mathrm{var}[\mathrm{m}] = N\mu(1-\mu) \tag{2.7}$$

2.1.2.2.2. The beta distribution (conjugate prior for the binomial distribution)

1) Motivation for the conjugate prior distribution

A. Prior distribution is required in order to develop a Bayesian treatment.

B. Make posterior distribution have the same functional form as the prior (conjugacy).

2) Definition

$$\mathrm{Beta}(\mu|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}, \text{gamma coefficient for the normalization purpose}$$

$$\mathbb{E}[\mu] = \frac{a}{a+b} \tag{2.8}$$

$$\mathrm{var}[\mu] = \frac{ab}{(a+b)^2(a+b+1)} \tag{2.9}$$

3) Gamma function

$$\Gamma(x) \equiv \int_0^\infty u^{x-1}e^{-u}\,du \tag{2.10}$$

$$\Gamma(x+1) = x\Gamma(x), \Gamma(1) = 1, \Gamma(x+1) = x! \tag{2.11}$$

a and b controls the distribution of the parameter μ, and thus called *hyperparameters*

4) Posterior distribution

The posterior distribution of μ: prior distribution(beta) × likelihood function(binomial)

→ Normalization

$$\mathrm{p}(\mu|m,l,a,b) = \mathrm{Beta}(\mu|a,b) \times \mathrm{Bin}(\mathrm{m}|\mathrm{N},\mu) = \frac{\Gamma(m+a+l+b)}{\Gamma(m+a)\Gamma(l+b)}\mu^{m+a-1}(1-\mu)^{l+b-1} \tag{2.12}$$

$$l = N - m = \#\ of\ \ tails$$

$$\mathrm{m} = \#\ \text{of heads}$$

A. Sequential nature

i. a and b (in the prior): *effective number of observations* of x = 1 and x = 0, respectively

ii. The posterior can act as the prior if subsequent observation is followed. If following observation is x=1(x=0), a(b) will increase by 1.

iii. Bayesian viewpoint raises such sequential approach of learning

B. Prediction of the future outcome

$$p(x=1|\boldsymbol{\mathcal{D}}) = \int_0^1 p(x=1|\,\mu)p(\mu|\boldsymbol{\mathcal{D}})d\mu = \int_0^1 \mu p(\mu|\boldsymbol{\mathcal{D}})d\mu = \mathbb{E}[\mu|\boldsymbol{\mathcal{D}}] \tag{2.13}$$

$$p(x=1|\boldsymbol{\mathcal{D}}) = \frac{m+a}{m+a+l+b} \tag{2.14}$$

$\rightarrow Total\ \ fraction\ \ of\ \ an\ \ effective\ \ number\ \ for\ \ x=1\ \ (including\ \ both\ \ real\&fictituous)$

C. Big Data

i. Bayesian result converges to ML (general phenomenon):

$$p(x=1|\boldsymbol{\mathcal{D}}) = \mathbb{E}[\mu|\boldsymbol{\mathcal{D}}] = \mu_{ML} = sample\ \ mean = \frac{m}{N} \tag{2.15}$$

ii. $\mathrm{var}[\mu|\boldsymbol{\mathcal{D}}]$ is approaching zero (Eq 2.9):

In general, the posterior variance is smaller than the prior variance on average (not for every observation)

$$\mathbb{E}_{\mathcal{D}}\big[var_\theta[\theta|\mathcal{D}]\big] = \ var_\theta[\theta] - var_{\mathcal{D}}\big[\mathbb{E}_\theta[\theta|\mathcal{D}]\big] \tag{2.16}$$

2.2. Multinomial Variables

2.2.1. Multinomial Distribution

2.2.1.1. Definition

$$\mathrm{Mult}(m_1, m_2, \dots, m_K|\boldsymbol{\mu}, N) = \ \binom{N}{m_1, m_2, \dots, m_K}\prod_{k=1}^{K}{\mu_k}^{m_k} \tag{2.17}$$

$$m_k = \ \sum\nolimits_n x_{nk}$$

It is the generalization of the Bernoulli distribution to more than two outcomes(states).

2.2.1.2. Properties

$$\mathbb{E}[\boldsymbol{x}|\boldsymbol{\mu}] = \ \sum\nolimits_{\boldsymbol{x}} p(\boldsymbol{x}|\boldsymbol{\mu})\boldsymbol{x} = (\mu_1, \dots, \mu_K)^T = \ \ \boldsymbol{\mu}$$

2.2.2. Density estimation

2.2.2.1. Frequentist

$$\mathcal{D} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$$

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

Sufficient statistic for this distribution = $m_k = \sum_n x_{nk}$

$${\mu_k}^{ML} = \frac{m_k}{N}$$

2.2.2.2. Bayesian (Dirichlet distribution)

$$Dir(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\dots\cdots\Gamma(\alpha_K)}\prod_{k=1}^{K}{\mu_k}^{\alpha_k-1} \tag{2.18}$$

$$\alpha_0 = \sum_{k=1}^{K}\alpha_k$$

$$\mathrm{p}(\mu|\mathcal{D},\alpha) \propto \text{likelihood} \times \text{prior} = \mathrm{p}(\mathcal{D}|\mu)\mathrm{p}(\mu|\alpha) = Dir(\boldsymbol{\mu}|\boldsymbol{\alpha}+\boldsymbol{m})$$

$$= \frac{\Gamma(\alpha_0+N)}{\Gamma(\alpha_1+m_1)\dots\cdots\Gamma(\alpha_K+m_K)}\prod_{k=1}^{K}{\mu_k}^{\alpha_k+m_k-1}$$

$$* \alpha_k = \ effective\ number\ of\ observations\ of\ x_k = 1$$

2.3. Gaussian Distribution

Gaussian is a widely used model for continuous variable whereas Bernoulli, Binomial, Multinomial are for discrete.

2.3.1. Definition

2.3.1.1. Single variable

$$\mathcal{N}(\mathrm{x}|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}}e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{2.19}$$

2.3.1.2. Multivariate

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{D}{2}}}\frac{1}{|\boldsymbol{\Sigma}|^{\frac{1}{2}}}e^{-\frac{(\mathbf{x}-\boldsymbol{\mu})^{\mathbf{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}{2}} \tag{2.20}$$

2.3.2. Motivation

1) Gaussian maximizes the entropy for the single, continuous, and real variable.
2) Central Limit Theorem: the sum of a set of random variables becomes more Gaussian as the # of

variable increases (under certain mild condition), e.g., binomial becomes Gaussian as N→∞.

2.3.3. Geometrical form (Transformation)

1) Mahalanobis distance:

$$\Delta^2 = (\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) \tag{2.21}$$

2) $\boldsymbol{\Sigma}$ can be symmetric = its eigenvalue is real & eigenvectors can be an orthonormal set

2.3.3.1. Transform

$$\boldsymbol{\Sigma} = \sum_{i=1}^{D} \lambda_i \boldsymbol{u_i}\boldsymbol{u_i}^T \tag{2.22}$$

$$\boldsymbol{\Sigma}^{-1} = \sum_{i=1}^{D} {\lambda_i}^{-1} \boldsymbol{u_i}\boldsymbol{u_i}^T \tag{2.23}$$

Therefore, equation 2.21 becomes,

$$\Delta^2 = \sum_{i=1}^{D} \frac{{y_i}^2}{\lambda_i} \tag{2.24}$$

$$y_i = {\boldsymbol{u}_i}^{\mathrm{T}}(\mathbf{x}-\boldsymbol{\mu}) \tag{2.25}$$

$$\mathbf{y} = \mathbf{U}(\mathbf{x}-\boldsymbol{\mu}) \tag{2.26}$$

2.3.3.2. Requirements for normalization

1) Positive definite: Properly normalized with elliptical shape
   A. Center: @ $\boldsymbol{\mu}$
   B. Axes: along $\mathbf{u}$
   C. Scaling factor: ${\lambda_i}^{1/2}$
2) Positive semi-definite: subspace of lower dimensionality (singular)
3) Negative eigenvalue: Probability cannot be defined

2.3.3.3. Normalization

$$|\mathbf{J}|^2 = 1$$

By transforming (shift, rotate) and using a new coordinate system, Multivariate Gaussian becomes the product of D independent univariate Gaussian distribution: $\prod_{j=1}^{D} 1 = 1 \therefore \text{Normalized}$

2.3.3.4. Properties

2.3.3.4.1. First moment

$$\mathbb{E}[\boldsymbol{x}] = \boldsymbol{\mu}$$

2.3.3.4.2. Second moment (Covariance)

$$\mathrm{cov}[\mathbf{x}] = \mathbb{E}[(\boldsymbol{x} - \mathbb{E}[\boldsymbol{x}])(\boldsymbol{x} - \mathbb{E}[\boldsymbol{x}])^{\mathrm{T}}] = \boldsymbol{\Sigma}$$

$$\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}] = \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}} + \boldsymbol{\Sigma}$$

2.3.4.Limitation and Alternatives

2.3.4.1. Too many parameters

Total of D(D+3)/2 parameters determining Gaussian distribution (grows quadratically with D)

1) Just use Gaussian: D(D+3)/2
2) $\boldsymbol{\Sigma} = \mathrm{diag}(\boldsymbol{\sigma_i}^2)$: 2D (axis-aligned ellipsoid)
3) $\boldsymbol{\Sigma} = \sigma^2\boldsymbol{I}$: D+1 (isotropic covariance)

2.3.4.2. Unimodal

Introduce latent variable as a solution

1) Discrete latent variable
   A. Mixture of Gaussian
2) Continuous latent variable
   A. Markov random field: to model pixel intensities of an image considering spatial organization
   B. Linear dynamical system: to model time series data for applications such tracking
   C. Probabilistic graphical model

2.3.5.Conditional Gaussian distribution