Machine Learning Notebook

Cong Bao

Contents

Chapter 1

Introduction

1.1 About this Notebook

1.2 Policy of Use

Chapter 2

Mathematics Basics

2.1 Probability

2.1.1 Basic Rules

Three Axioms of Probability Let Ω be a sample space. A probability assigns a real number $P(X)$ to each event $X \subseteq \Omega$ in such a way that

1. $P(X) \geq 0, \forall X$
2. If $X_1, X_2, \ldots$ are pairwise disjoint events ($X_1 \cap X_2 = \emptyset,\ i \neq j,\ i, j = 1, 2, \ldots$), then $P\left(\bigcup_{i=1}^{\infty} X_i\right) = \sum_{i=1}^{\infty} P(X_i)$. (This property is called countable additivity.)
3. $P(\Omega) = 1$

Joint Probability The probability both event A and B occur. $P(X, Y) = P(X \cap Y)$.

Marginalization The probability distribution of any variable in a joint distribution can be recovered by integrating (or summing) over the other variables.

1. For continuous r.v. $P(x) = \int P(x, y)\, dy$; $P(y) = \int P(x, y)\, dx$.
2. For discrete r.v. $P(x) = \sum_y P(x, y)$; $P(y) = \sum_x P(x, y)$.
3. For mixed r.v. $P(x, y) = \sum_w \int P(w, x, y, z)\, dz$, where w is discrete and z is continuous.

Conditional Probibility $P(X = x|Y = y)$ is the probability $X = x$ occurs given the knowledge $Y = y$ occurs. Conditional probability can be extracted from joint probability that

$$P(x|y = y^*) = \frac{P(x, y = y^*)}{\int P(x, y = y^*)\, dx} = \frac{P(x, y = y^*)}{P(y = y^*)}$$

Usually, the formula is written as $P(x|y) = \frac{P(x,y)}{P(y)}$.

Product Rule The formula can be rearranged as $P(x,y) = P(x|y)\,P(y) = P(y|x)\,P(x)$. In case of multiple variables

$$\begin{aligned} P(w,x,y,z) &= P(w,x,y|z)\,P(z) \\ &= P(w,x|y,z)\,P(y|z)\,P(z) \\ &= P(w|x,y,z)\,P(x|y,z)\,P(y|z)\,P(z) \end{aligned}$$

Independence If two variables x and y are independent, then r.v. x tells nothing about r.v. y (and vice-versa)

$$\begin{aligned} P(x|y) &= P(x) \\ P(y|x) &= P(y) \\ P(x,y) &= P(x)\,P(y) \end{aligned}$$

Baye's Rule By rearranging formula in Product Rule, we have

$$\begin{aligned} P(y|x) &= \frac{P(x|y)\,P(y)}{P(x)} \\ &= \frac{P(x|y)\,P(y)}{\int P(x,y)\,dy} \\ &= \frac{P(x|y)\,P(y)}{\int P(x|y)\,P(y)\,dy} \end{aligned}$$

Expectation Expectation tells us the excepted or average value of some function $f(x)$, taking into account the distribution of x.

$$\begin{aligned} \mathbf{E}[f(x)] &= \sum_x f(x)P(x) \\ \mathbf{E}[f(x)] &= \int f(x)P(x)\,dx \end{aligned}$$

Definition in two dimensions: $\mathbf{E}[f(x,y)] = \iint f(x,y)P(x,y)\,dx\;dy$

Function $f(\bullet)$	Expectation
x^k	k^{th} moment about zero
$(x-\mu_x)^k$	k^{th} moment about the mean

Function $f(\bullet)$	Expectation
x	mean, μ_x
$(x-\mu_x)^2$	variance
$(x-\mu_x)^3$	skew
$(x-\mu_x)^4$	kurtosis
$(x-\mu_x)(x-\mu_y)$	covariance of x and y

Besides, Expectation has the following four rules

1. Expected value of a constant is the constant $\mathbf{E}[\kappa] = \kappa$.
2. Expected value of constant times function is constant times excepted value of function $\mathbf{E}[kf(x)] = k\mathbf{E}[f(x)]$.
3. Expectation of sum of functions is sum of expectation of functions $\mathbf{E}[f(x) + g(y)] = \mathbf{E}[f(x)] + \mathbf{E}[g(x)]$.
4. Expectation of product of functions in variables x and y is product of expectations of functions if x and y are independent $\mathbf{E}[f(x)g(y)] = \mathbf{E}[f(x)]\mathbf{E}[g(y)], x \perp\!\!\!\perp y$.

2.1.2 Common Probability Distributions

Bernoulli Bernoulli distribution describes situation where only two possible outcomes $y = 0/y = 1$ or failure/success.

1. $P(x) = \mathbf{Bern}_x[\lambda] = \lambda^x(1-\lambda)^{1-x}$
2. univariate, discrete, binary
3. $x \in \{0, 1\}$; $\lambda \in [0, 1]$
4. $\mathbf{E}[x] = \lambda$, $\mathbf{Var}[x] = \lambda(1-\lambda)$

Beta Beta distribution is the conjugate distribution to Bernoulli distribution.

1. $P(\lambda) = \mathbf{Beta}_\lambda[\alpha, \beta] = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\lambda^{\alpha-1}(1-\lambda)^{\beta-1}$
2. univariate, continuous, unbounded
3. $\lambda \in \mathbb{R}$; $\alpha \in \mathbb{R}_+$, $\beta \in \mathbb{R}_+$
4. $\mathbf{E}[\lambda] = \frac{\alpha}{\alpha+\beta}$, $\mathbf{Var}[\lambda] = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$

Categorical Categorical distribution describes situation with K possible outcomes.

1. $P(x) = \mathbf{Cat}_x[\boldsymbol{\lambda}]$, $P(x = k) = \lambda_k$, $P(\boldsymbol{x} = \boldsymbol{e}_k) = \prod_{j=1}^K \lambda_j^{x_j} = \lambda_k$
2. univariate, discrete, multi-valued
3. $x \in \{1, 2, \ldots, K\}$; $\lambda_k \in [0, 1]$ where $\sum_k \lambda_k = 1$
4. $\mathbf{E}[x_i] = \lambda_i$, $\mathbf{Var}[x_i] = \lambda_i(1-\lambda_i)$, $\mathbf{Cov}[x_i, x_j] = -\lambda_i\lambda_j$ $(i \neq j)$

Dirichlet Dirichlet distribution is the conjugate distribution to categorical distribution.

1. $P(\boldsymbol{\lambda}) = \mathbf{Dir}_{\boldsymbol{\lambda}}[\boldsymbol{\alpha}] = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \lambda_k^{\alpha_k - 1}$
2. multivariate, continuous, bounded, sums to one
3. $\boldsymbol{\lambda} = [\lambda_1, \lambda_2, \ldots, \lambda_K]^\top$, $\lambda_k \in [0, 1]$, $\sum_{k=1}^K \lambda_k = 1$; $\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_K]$, $\alpha_k \in \mathbb{R}_+$
4. $\mathbf{E}[\lambda_i] = \frac{\alpha_i}{\sum_k \alpha_k}$, $\mathbf{Var}[\lambda_i] = \frac{\alpha_i(\sum_k \alpha_k - \alpha_i)}{(\sum_k \alpha_k)^2(\sum_k \alpha_k + 1)}$, $\mathbf{Cov}[\lambda_i, \lambda_j] = \frac{-\alpha_i\alpha_j}{(\sum_k \alpha_k)^2(\sum_k \alpha_k + 1)}$ $(i \neq j)$

Univariate Normal Univariate normal distribution describes single continuous variable.

1. $P(x) = \mathbf{Norm}_x[\mu, \sigma^2] = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
2. univariate, continuous, unbounded
3. $x \in \mathbb{R}$; $\mu \in \mathbb{R}$, $\sigma^2 \in \mathbb{R}_+$
4. $\mathbf{E}[x] = \mu$, $\mathbf{Var}[x] = \sigma^2$

Normal Inverse Gamma Normal inverse gamma distribution is a conjugate distribution to univariate normal distribution.

1. $P(\mu, \sigma^2) = \mathbf{NormInvGam}_{\mu,\sigma^2}[\alpha, \beta, \gamma, \delta] = \frac{\sqrt{\gamma}}{\sqrt{2\pi\sigma^2}} \frac{\beta^\alpha}{\Gamma(\alpha)} (\frac{1}{\sigma^2})^{\alpha+1} exp\left(-\frac{2\beta+\gamma(\delta-\mu)^2}{2\sigma^2}\right)$
2. bivariate, continuous, μ unbounded, σ^2 bounded below
3. $\mu \in \mathbb{R}$, $\sigma^2 \in \mathbb{R}_+$; $\alpha \in \mathbb{R}_+$, $\beta \in \mathbb{R}_+$, $\gamma \in \mathbb{R}_+$, $\delta \in \mathbb{R}$
4. $\mathbf{E}[\mu] = \delta$, $\mathbf{E}[\sigma^2] = \frac{\beta}{\alpha-1}$ $(\alpha > 1)$, $\mathbf{Var}[\mu] = \frac{\beta}{(\alpha-1)\gamma}$ $(\alpha > 1)$, $\mathbf{Var}[\sigma^2] = \frac{\beta^2}{(\alpha-1)^2(\alpha-2)}$ $(\alpha > 2)$, $\mathbf{Cov}[\mu, \sigma^2] = 0$ $(\alpha > 1)$

Multivariate Normal Multivariate normal distribution describes multiple continuous variables. It takes two parameters: a vector containing mean position $\boldsymbol{\mu}$, and a symmetric positive definite covariance matrix $\boldsymbol{\Sigma}$.

1. $P(\boldsymbol{x}) = \mathbf{Norm}_{\boldsymbol{x}}[\boldsymbol{\mu}, \boldsymbol{\Sigma}] = \frac{1}{\sqrt{det(2\pi\boldsymbol{\Sigma})}} exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$
2. multivariate, continuous, unbounded
3. $\boldsymbol{x} \in \mathbb{R}^K$; $\boldsymbol{\mu} \in \mathbb{R}^K$, $\boldsymbol{\Sigma} \in \mathbb{R}^{K\times K}$ (positive semi-definite matrix)
4. $\mathbf{E}[\boldsymbol{x}] = \boldsymbol{\mu}$, $\mathbf{Var}[\boldsymbol{x}] = \boldsymbol{\Sigma}$

Normal Inverse Wishart Normal inverse wishart distribution is a conjugate distribution to multivariate normal distribution.

1. $P(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathbf{NormInvWis}_{\boldsymbol{\mu},\boldsymbol{\Sigma}}[\alpha, \boldsymbol{\Psi}, \gamma, \boldsymbol{\delta}]$
   $= \frac{\gamma^{D/2}|\boldsymbol{\Psi}|^{\alpha/2}|\boldsymbol{\Sigma}|^{-\frac{\alpha+D+2}{2}}}{(2\pi)^{D/2}2^{(\alpha\boldsymbol{\Sigma})/2}\Gamma_D(\alpha/2)} exp\left(-\frac{1}{2}(\mathrm{Tr}(\boldsymbol{\Psi}\boldsymbol{\Sigma}^{-1}) + \gamma(\boldsymbol{\mu}-\boldsymbol{\delta})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}-\boldsymbol{\delta})\right)$
2. multivariate, $\boldsymbol{\mu}$ unbounded, $\boldsymbol{\Sigma}$ square, positive definite
3. $\boldsymbol{\mu} \in \mathbb{R}^K$, $\boldsymbol{\Sigma} \in \mathbb{R}^{K\times K}$; $\alpha \in \mathbb{R}_{>D-1}$, $\boldsymbol{\Psi} \in \mathbb{R}^{K\times K}$, $\gamma \in \mathbb{R}_+$, $\boldsymbol{\delta} \in \mathbb{R}^K$

2.2 Linear Algebra

2.3 Calculus

2.4 Informatics

2.5 Optimization

Chapter 3

Machine Learning Basics

3.1 Regularization

3.1.1 Under-fitting & Over-fitting

Under-fitting If $N > D$ (e.g. 30 data points, 2 dimensions) we have more equations than unknowns: over-determined system. Input-output relations can only hold approximately.

Over-fitting If $N < D$ (e.g. 30points, 15265 dimensions) we have more unknowns than equations: under-determined system. Input-output equations hold exactly, but we are simply memorizing data.

3.1.2 Bias & Variance

High Bias & Low Variance A rigid model's (low complexity) performance is more predictable in the test set but the model may not be good even on the training set.

Low Bias & High Variance A flexible model (high complexity) approximates the target function well in the training set but can "overtrain" and have poor performance on the test set.

3.1.3 Vector Norm

L1, ("Manhattan") norm $||\boldsymbol{w}||_1 = \sum_{d=1}^{D} |w_d|$

L2, ("Euclidean") norm $||\boldsymbol{w}||_2 = \sqrt{\sum_{d=1}^{D} w_d^2} = \sqrt{\langle \boldsymbol{w}, \boldsymbol{w} \rangle} = \sqrt{\boldsymbol{w}^\top \boldsymbol{w}}$

Lp norm, p>1 $||\boldsymbol{w}||_p = \left(\sum_{d=1}^{D} w_d^p \right)^{1/p}$

3.1.4 Penalize Complexity

In linear regression, the residual vector is $\boldsymbol{\epsilon} = \boldsymbol{y} - \boldsymbol{\Psi}\boldsymbol{w}$. The loss function is $L(\boldsymbol{w}) = \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}$. We add a complexity term $R(\boldsymbol{w}) = ||\boldsymbol{w}||_2 = \boldsymbol{w}^\top \boldsymbol{w}$ to the loss function. Hence, the original loss function becomes $L(\boldsymbol{w}) = \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon} + \lambda \boldsymbol{w}^\top \boldsymbol{w}$.

Without regularization, the loss function is $L(\boldsymbol{w}) = \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}$. Let $\nabla L(\boldsymbol{w}^*) = 0$, we have $\boldsymbol{w}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{y}$.

With L2-regularization, the loss function is $L(\boldsymbol{w}) = \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon} + \lambda \boldsymbol{w}^\top \boldsymbol{w}$. Let $\nabla L(\boldsymbol{w}^*) = 0$, we have $\boldsymbol{w}^* = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \boldsymbol{y}$. The additional $\lambda \mathbf{I}$ makes the data matrix more robust to calculate inversion.

3.2 Cross-Validation

We can select hyperparameters with (cross-)validation. Cross-validation excludes part of the training data from parameter estimation, and use them only to predict the test error.

K-fold cross validation: split data set into K folds and each time train on (K-1) folds and valid on the remaining fold until all folds have been used as validation fold. The cross-validation error is the average of K validation errors. We pick hyperparameters that minimize cross-validation error.

3.3 Bayesian Learning

3.3.1 Bayes' Rule Terminology

Bayes' Rule:

$$P(y|x) = \frac{P(x|y)\,P(y)}{\int P(x|y)\,P(y)\,dy}$$

Prior $P(y)$ what we know about y before seeing x. In parameters learning we choose prior that is conjugate to likelihood.

Likelihood $P(x|y)$ propensity for observing a certain value of x given a certain value of y.

Posterior $P(y|x)$ what we know about y after seeing x. Posterior must have same form as conjugate prior distribution.

Evidence $\int P(x|y)\,P(y)\,dy$ a constant to ensure that the LHS is a valid distribution. Posterior must be a distribution which implies that evidence equals to a constant κ from conjugate relation.

3.3.2 Maximum Likelihood

Fitting As the name suggests we find the parameters under which the data $\boldsymbol{x}_{1...I}$ are most likely. Here, we have assumed that data was independent.

$$\begin{aligned}\hat{\boldsymbol{\theta}} &= \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, P\left(\boldsymbol{x}_{1...I}|\boldsymbol{\theta}\right) \\ &= \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i=1}^{I} P\left(\boldsymbol{x}_i|\boldsymbol{\theta}\right)\end{aligned}$$

Predictive Density Evaluate new data point $\boldsymbol{x}^*$ under probability distribution $P\left(\boldsymbol{x}^*|\hat{\boldsymbol{\theta}}\right)$ with best parameters.

3.3.3 Maximum a Posterior (MAP)

Fitting As the name suggests we find the parameters which maximize the posterior probability $P\left(\boldsymbol{\theta}|\boldsymbol{x}_{1...I}\right)$. Again we have assumed that data was independent.

$$\begin{aligned}\hat{\boldsymbol{\theta}} &= \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, P\left(\boldsymbol{\theta}|\boldsymbol{x}_{1...I}\right) \\ &= \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \frac{P\left(\boldsymbol{x}_{1...I}|\boldsymbol{\theta}\right) P\left(\boldsymbol{\theta}\right)}{P\left(\boldsymbol{x}_{1...I}\right)} \\ &= \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \frac{\prod_{i=1}^{I} P\left(\boldsymbol{x}_i|\boldsymbol{\theta}\right)\ P\left(\boldsymbol{\theta}\right)}{P\left(\boldsymbol{x}_{1...I}\right)}\end{aligned}$$

Since the denominator does not depend on the parameters we can instead maximize

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i=1}^{I} P\left(\boldsymbol{x}_i|\boldsymbol{\theta}\right)\ P\left(\boldsymbol{\theta}\right)$$

Predictive Density Evaluate new data point $\boldsymbol{x}^*$ under probability distribution with MAP parameters $P\left(\boldsymbol{x}^*|\hat{\boldsymbol{\theta}}\right)$

3.3.4 Bayesian Approach

Fitting Compute the posterior distribution over possible parameter values using Bayes' rule. Principle: There are many values that could have explained the data. Instead of picking one set of parameters, try to capture all of the possibilities.

$$P\left(\boldsymbol{\theta}|\boldsymbol{x}_{1...I}\right) = \frac{\prod_{i=1}^{I} P\left(\boldsymbol{x}_i|\boldsymbol{\theta}\right)\ P\left(\boldsymbol{\theta}\right)}{P\left(\boldsymbol{x}_{1...I}\right)}$$

Predictive Density (a) Each possible parameter value makes a prediction. (b) Some parameters more probable than others.

$$P\left(\boldsymbol{x}^{*}|\boldsymbol{x}_{1\ldots I}\right)=\int P\left(\boldsymbol{x}^{*}|\boldsymbol{\theta}\right)P\left(\boldsymbol{\theta}|\boldsymbol{x}_{1\ldots I}\right)d\boldsymbol{\theta}$$

Make a prediction that is an infinite weighted sum (integral) of the predictions for each parameter value ($P\left(\boldsymbol{x}^{*}|\boldsymbol{\theta}\right)$), where weights are the probabilities ($P\left(\boldsymbol{\theta}|\boldsymbol{x}_{1\ldots I}\right)$).

3.3.5 Example: Normal Distribution

3.3.6 Example: Categorical Distribution

3.4 Machine Learning Models

Chapter 4

Regression

4.1 Linear Regression

4.2 Non-linear Regression

4.3 Logistic Regression

Chapter 5

Support Vector Machines

Bibliography

Appendix A

Test

test