

机器学习的数学笔记

X

目录

Notation	ii
1 逻辑回归	1
1.1 二项逻辑回归模型	1
1.2 Softmax回归模型	3
2 附录：信息熵	6
2.1 相关概念	6
参考文献	8
索引	9

Notation

This section provides a concise reference describing notation used throughout this document. If you are unfamiliar with any of the corresponding mathematical concepts, Goodfellow *et al.* (2016) describe most of these ideas in chapters 2–4.

Numbers and Arrays

a	A scalar (integer or real)
\mathbf{a}	A vector
\mathbf{A}	A matrix
\mathbf{A}	A tensor
\mathbf{I}_n	Identity matrix with n rows and n columns
\mathbf{I}	Identity matrix with dimensionality implied by context
$\mathbf{e}^{(i)}$	Standard basis vector $[0, \dots, 0, 1, 0, \dots, 0]$ with a 1 at position i
$\text{diag}(\mathbf{a})$	A square, diagonal matrix with diagonal entries given by \mathbf{a}
a	A scalar random variable
\mathbf{a}	A vector-valued random variable
\mathbf{A}	A matrix-valued random variable

Sets and Graphs

\mathbb{A}	A set
\mathbb{R}	The set of real numbers
$\{0, 1\}$	The set containing 0 and 1
$\{0, 1, \dots, n\}$	The set of all integers between 0 and n
$[a, b]$	The real interval including a and b
$(a, b]$	The real interval excluding a but including b
$\mathbb{A} \setminus \mathbb{B}$	Set subtraction, i.e., the set containing the elements of \mathbb{A} that are not in \mathbb{B}
\mathcal{G}	A graph
$Pa_{\mathcal{G}}(\mathbf{x}_i)$	The parents of \mathbf{x}_i in \mathcal{G}

Indexing

a_i	Element i of vector \mathbf{a} , with indexing starting at 1
a_{-i}	All elements of vector \mathbf{a} except for element i
$A_{i,j}$	Element i, j of matrix \mathbf{A}
$\mathbf{A}_{i,:}$	Row i of matrix \mathbf{A}
$\mathbf{A}_{:,i}$	Column i of matrix \mathbf{A}
$A_{i,j,k}$	Element (i, j, k) of a 3-D tensor \mathbf{A}
$\mathbf{A}_{::,i}$	2-D slice of a 3-D tensor
\mathbf{a}_i	Element i of the random vector \mathbf{a}

Linear Algebra Operations

\mathbf{A}^\top	Transpose of matrix \mathbf{A}
\mathbf{A}^+	Moore-Penrose pseudoinverse of \mathbf{A}
$\mathbf{A} \odot \mathbf{B}$	Element-wise (Hadamard) product of \mathbf{A} and \mathbf{B}
$\det(\mathbf{A})$	Determinant of \mathbf{A}

Calculus

$\frac{dy}{dx}$	Derivative of y with respect to x
$\frac{\partial y}{\partial x}$	Partial derivative of y with respect to x
$\nabla_{\mathbf{x}} y$	Gradient of y with respect to \mathbf{x}
$\nabla_{\mathbf{X}} y$	Matrix derivatives of y with respect to \mathbf{X}
$\nabla_{\mathbf{X}} y$	Tensor containing derivatives of y with respect to \mathbf{X}
$\frac{\partial f}{\partial \mathbf{x}}$	Jacobian matrix $\mathbf{J} \in \mathbb{R}^{m \times n}$ of $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$
$\nabla_{\mathbf{x}}^2 f(\mathbf{x})$ or $\mathbf{H}(f)(\mathbf{x})$	The Hessian matrix of f at input point \mathbf{x}
$\int f(\mathbf{x}) d\mathbf{x}$	Definite integral over the entire domain of \mathbf{x}
$\int_{\mathbb{S}} f(\mathbf{x}) d\mathbf{x}$	Definite integral with respect to \mathbf{x} over the set \mathbb{S}

Probability and Information Theory

$a \perp b$	The random variables a and b are independent
$a \perp b \mid c$	They are conditionally independent given c
$P(a)$	A probability distribution over a discrete variable
$p(a)$	A probability distribution over a continuous variable, or over a variable whose type has not been specified
$a \sim P$	Random variable a has distribution P
$\mathbb{E}_{\mathbf{x} \sim P}[f(\mathbf{x})]$ or $\mathbb{E}f(\mathbf{x})$	Expectation of $f(\mathbf{x})$ with respect to $P(\mathbf{x})$
$\text{Var}(f(\mathbf{x}))$	Variance of $f(\mathbf{x})$ under $P(\mathbf{x})$
$\text{Cov}(f(\mathbf{x}), g(\mathbf{x}))$	Covariance of $f(\mathbf{x})$ and $g(\mathbf{x})$ under $P(\mathbf{x})$
$H(\mathbf{x})$	Shannon entropy of the random variable \mathbf{x}
$D_{\text{KL}}(P \parallel Q)$	Kullback-Leibler divergence of P and Q
$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$	Gaussian distribution over \mathbf{x} with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$

Functions

$f : \mathbb{A} \rightarrow \mathbb{B}$	The function f with domain \mathbb{A} and range \mathbb{B}
$f \circ g$	Composition of the functions f and g
$f(\mathbf{x}; \boldsymbol{\theta})$	A function of \mathbf{x} parametrized by $\boldsymbol{\theta}$. (Sometimes we write $f(\mathbf{x})$ and omit the argument $\boldsymbol{\theta}$ to lighten notation)
$\log x$	Natural logarithm of x
$\sigma(x)$	Logistic sigmoid, $\frac{1}{1 + \exp(-x)}$
$\zeta(x)$	Softplus, $\log(1 + \exp(x))$
$\ \mathbf{x}\ _p$	L^p norm of \mathbf{x}
$\ \mathbf{x}\ $	L^2 norm of \mathbf{x}
x^+	Positive part of x , i.e., $\max(0, x)$
$\mathbf{1}_{\text{condition}}$	is 1 if the condition is true, 0 otherwise

Sometimes we use a function f whose argument is a scalar but apply it to a vector, matrix, or tensor: $f(\mathbf{x})$, $f(\mathbf{X})$, or $f(\mathbf{X})$. This denotes the application of f to the array element-wise. For example, if $\mathbf{C} = \sigma(\mathbf{X})$, then $C_{i,j,k} = \sigma(X_{i,j,k})$ for all valid values of i , j and k .

Datasets and Distributions

p_{data}	The data generating distribution
\hat{p}_{data}	The empirical distribution defined by the training set
\mathbb{X}	A set of training examples
$\mathbf{x}^{(i)}$	The i -th example (input) from a dataset
$\mathbf{y}^{(i)}$ or $\mathbf{y}^{(i)}$	The target associated with $\mathbf{x}^{(i)}$ for supervised learning
\mathbf{X}	The $m \times n$ matrix with input example $\mathbf{x}^{(i)}$ in row $\mathbf{X}_{i,:}$

Chapter 1

逻辑回归

1.1 二项逻辑回归模型

二项逻辑回归模型是如下的条件概率分布

$$P(Y = 1|\mathbf{x}) = \frac{\exp(\boldsymbol{\theta}^T \mathbf{x} + b)}{1 + \exp(\boldsymbol{\theta}^T \mathbf{x} + b)}$$
$$P(Y = 0|\mathbf{x}) = \frac{1}{1 + \exp(\boldsymbol{\theta}^T \mathbf{x} + b)}$$

其中 $\mathbf{x} \in \mathbb{R}^n$ 是输入变量， $Y \in \{0, 1\}$ 是输出变量， $\boldsymbol{\theta} \in \mathbb{R}^n$ 和 $b \in \mathbb{R}$ 是参数。 \mathbf{x} 和 $\boldsymbol{\theta}$ 为 n 维列向量。

若令 $\boldsymbol{\theta} = (\theta^{(1)}, \dots, \theta^{(n)}, b)^T$ ， $\mathbf{x} = (x^{(1)}, \dots, x^{(n)}, 1)^T$ ，那么条件概率可以表示为

$$P(Y = 1|\mathbf{x}) = \frac{\exp(\boldsymbol{\theta}^T \mathbf{x})}{1 + \exp(\boldsymbol{\theta}^T \mathbf{x})}$$
$$P(Y = 0|\mathbf{x}) = \frac{1}{1 + \exp(\boldsymbol{\theta}^T \mathbf{x})} \quad (1.1)$$

1.1.1 模型的参数估计

对于给定的训练集 $\mathbb{X} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$ ，可应用极大似然估计法估计模型参数。

为表示方便，令 $P(Y = 1|\mathbf{x}) = \pi(\mathbf{x})$ ， $P(Y = 0|\mathbf{x}) = 1 - \pi(\mathbf{x})$ ，似然函数为

$$L(\boldsymbol{\theta}) = \prod_{i=1}^N (\pi(\mathbf{x}_i))^{y_i} (1 - \pi(\mathbf{x}_i))^{1-y_i}$$

那么对数似然函数为

$$\begin{aligned}
 \log L(\boldsymbol{\theta}) &= \sum_{i=1}^N (y_i \log \pi(\mathbf{x}_i) + (1 - y_i) \log(1 - \pi(\mathbf{x}_i))) \\
 &= \sum_{i=1}^N \left(y_i \log \frac{\pi(\mathbf{x}_i)}{1 - \pi(\mathbf{x}_i)} + \log(1 - \pi(\mathbf{x}_i)) \right) \\
 &= \sum_{i=1}^N (y_i (\boldsymbol{\theta}^T \mathbf{x}_i) - \log(1 + \exp(\boldsymbol{\theta}^T \mathbf{x}_i)))
 \end{aligned} \tag{1.2}$$

1.1.1.1 参数估计：梯度下降法

根据公式 (1.2)，对数似然函数对 $\boldsymbol{\theta}$ 的偏导为

$$\begin{aligned}
 \nabla_{\boldsymbol{\theta}} \log L(\boldsymbol{\theta}) &= \sum_{i=1}^N \left(y_i \mathbf{x}_i - \frac{\exp(\boldsymbol{\theta}^T \mathbf{x}_i) \mathbf{x}_i}{1 + \exp(\boldsymbol{\theta}^T \mathbf{x}_i)} \right) \\
 &= \sum_{i=1}^N (y_i - \pi(\mathbf{x}_i)) \mathbf{x}_i
 \end{aligned}$$

由此处求对数似然函数的最大值，故需要沿着梯度上升的方向进行迭代，迭代公式为

$$\begin{aligned}
 \boldsymbol{\theta} &:= \boldsymbol{\theta} + \alpha \frac{\partial}{\partial \boldsymbol{\theta}} \log L(\boldsymbol{\theta}) \\
 &= \boldsymbol{\theta} + \alpha \sum_{i=1}^N (y_i - \pi(\mathbf{x}_i)) \mathbf{x}_i
 \end{aligned} \tag{1.3}$$

其中 α 称为学习率，是一个正常数。

公式 (1.3) 可以用矩阵表示

$$\boldsymbol{\theta} := \boldsymbol{\theta} + \alpha X^T \boldsymbol{\Lambda} \tag{1.4}$$

其中 $\boldsymbol{\Lambda} = \begin{pmatrix} y_1 - \pi(\mathbf{x}_1) \\ y_2 - \pi(\mathbf{x}_2) \\ \dots \\ y_N - \pi(\mathbf{x}_N) \end{pmatrix}_{N \times 1}$ ， X 是由训练数据构成的 $N \times (n+1)$ 矩阵(每一行对应一个样本，每一列对应样本的一个维度，其中还包括一维常数项)。

1.1.1.2 参数估计：随机梯度下降法

梯度下降算法在每次更新回归系数时需要遍历整个数据集，当数据集数量庞大或者

特征过多时，该方法的计算复杂度太高。改进方法是每次迭代仅用一个样本来更新回归系数，称为随机梯度下降法。

具体而言，对于训练集中的每一个样本 (x_i, y_i) ，计算该样本梯度，并依据迭代公式：

$$\boldsymbol{\theta} := \boldsymbol{\theta} + \alpha (y_i - \pi(\mathbf{x}_i)) \mathbf{x}_i \quad (1.5)$$

与公式 (1.3) 相比，随机梯度下降的迭代公式 (1.5) 中

- 误差变量是数值，而不是向量
- 不再有矩阵变换的过程

所以随机梯度下降算法的计算效率较高，缺点是存在解的不稳定性(如解存在周期性波动)的问题。为了解决这一问题，并进一步加快收敛速度，可以通过随机选取样本来更新回归系数。

1.2 Softmax回归模型

Softmax模型是二项回归模型在多分类问题上的推广，在多分类问题中，类标签 Y 可以取两个以上的值。

假设 Y 的取值集合是 $\{1, 2, \dots, K\}$ ，Softmax模型是如下的条件概率分布

$$P(Y = k | \mathbf{x}) = \frac{\exp(\boldsymbol{\theta}_k^T \mathbf{x})}{\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x})} \quad (1.6)$$

其中 $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K \in \mathbb{R}^{n+1}$ 是模型的参数。

为方便起见，下文用矩阵 $\boldsymbol{\Theta}_{K \times (n+1)}$ 表示全部的模型参数

$$\boldsymbol{\Theta} = \begin{bmatrix} \boldsymbol{\theta}_1^T \\ \vdots \\ \boldsymbol{\theta}_K^T \end{bmatrix}$$

1.2.1 模型的参数估计

令 $P(Y = k | \mathbf{x}) = \pi_k(\mathbf{x})$ ，与二项逻辑回归类似，Softmax的似然函数可以表示为

$$L(\boldsymbol{\Theta}) = \prod_{i=1}^N \prod_{k=1}^K (\pi_k(\mathbf{x}_i))^{\mathbb{1}_{y_i=k}}$$

对数似然函数为

$$\log L(\Theta) = \sum_{i=1}^N \sum_{k=1}^K \mathbb{1}_{y_i=k} \log \pi_k(\mathbf{x}_i) \quad (1.7)$$

1.2.1.1 参数估计：梯度下降法

首先求

$$\frac{\partial \pi_k(\mathbf{x}_i)}{\partial \boldsymbol{\theta}_k} = \frac{\mathbf{x}_i \exp(\boldsymbol{\theta}_k^T \mathbf{x}_i) \left(\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x}) - \exp(\boldsymbol{\theta}_k^T \mathbf{x}_i) \right)}{\left(\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x}) \right)^2} \quad (1.8)$$

故根据公式 (1.7)，得到Softmax模型的对数似然函数的梯度

$$\begin{aligned} \nabla_{\boldsymbol{\theta}_k} \log L(\Theta) &= \sum_{i=1}^N \mathbb{1}_{y_i=k} \frac{1}{\pi_k(\mathbf{x}_i)} \frac{\partial \pi_k(\mathbf{x}_i)}{\partial \boldsymbol{\theta}_k} \\ &= \sum_{i=1}^N \mathbb{1}_{y_i=k} \frac{1}{\pi_k(\mathbf{x}_i)} \frac{\mathbf{x}_i \exp(\boldsymbol{\theta}_k^T \mathbf{x}_i) \left(\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x}_i) - \exp(\boldsymbol{\theta}_k^T \mathbf{x}_i) \right)}{\left(\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x}_i) \right)^2} \\ &= \sum_{i=1}^N \mathbb{1}_{y_i=k} \frac{\mathbf{x}_i \left(\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x}_i) - \exp(\boldsymbol{\theta}_k^T \mathbf{x}_i) \right)}{\sum_{j=1}^K \exp(\boldsymbol{\theta}_j^T \mathbf{x}_i)} \\ &= \sum_{i=1}^N \mathbb{1}_{y_i=k} \mathbf{x}_i (1 - \pi_k(\mathbf{x}_i)) \end{aligned} \quad (1.9)$$

对于任意第 k 个分类的参数 $\boldsymbol{\theta}_k$ ，可沿着梯度上升的方向进行迭代

$$\boldsymbol{\theta}_k := \boldsymbol{\theta}_k + \alpha \sum_{i=1}^N \mathbb{1}_{y_i=k} \mathbf{x}_i (1 - \pi_k(\mathbf{x}_i)) \quad (1.10)$$

公式 (1.10)的迭代关系用矩阵可以表示为

$$\boldsymbol{\theta}_k := \boldsymbol{\theta}_k + \alpha X^T \mathbf{\Lambda} \quad (1.11)$$

其中 $\mathbf{\Lambda} = \begin{pmatrix} \mathbb{1}_{y_1=k} (1 - \pi_k(\mathbf{x}_1)) \\ \mathbb{1}_{y_2=k} (1 - \pi_k(\mathbf{x}_2)) \\ \dots \\ \mathbb{1}_{y_N=k} (1 - \pi_k(\mathbf{x}_N)) \end{pmatrix}_{N \times 1}$, X 是由训练数据构成的 $N \times (n+1)$ 矩阵(每一行对应一个样本, 每一列对应样本的一个维度, 其中还包括一维常数项)。

Chapter 2

附录：信息熵

假设¹ X 是一个取有限值的离散随机变量(本文只考虑离散情况)，概率分布为 $P(X = x_i) = p_i, i = 1 \dots n$ 。

那么 $I(x_i) = -\log p(x_i)$ 称为事件 x_i 的自信息量，随机变量 X 的熵定义为 X 的自信息量的数学期望，即

$$H(X) = \mathbb{E}(I(x_i)) = -\sum_{i=1}^n p_i \log p_i$$

熵反映的是随机变量不确定程度的大小：熵的值越大，不确定程度越高。

2.1 相关概念

2.1.1 条件熵和相对熵

条件熵是指在联合概率空间上熵的条件自信息的数学期望。在已知 X 时， Y 的条件熵为

$$H(Y|X) = \mathbb{E}_{x,y} I(y_j|x_i) = -\sum_x \sum_y P(x,y) \log P(y|x) \quad (2.1)$$

Lemma 2.1.1. 与公式 (2.1)等价的定义为给定 X 条件下 Y 的条件分布概率的熵的数学期望

$$H(Y|X) = \mathbb{E}_x H(Y|X = x) = \sum_x P(x) H(Y|X = x)$$

¹本章参考了信息论与编码(<http://www.docin.com/p-957983839-f6.html>)和信息论基础(<https://wenku.baidu.com/view/5319fed3b9f3f90f76c61b1a.html>)

证明.

$$\begin{aligned}
H(Y|X) &= - \sum_x \sum_y P(x, y) \log P(y|x) \\
&= - \sum_x \sum_y P(x) P(y|x) \log P(y|x) \\
&= - \sum_x P(x) \sum_y P(y|x) \log P(y|x) \quad (P(x) \text{ 与 } y \text{ 无关}) \\
&= \sum_x P(x) \left[- \sum_y P(y|x) \log P(y|x) \right] \\
&= \sum_x P(x) H(Y|X = x)
\end{aligned}$$

□

$H(Y|X)$ 的含义是已知在 X 发生的前提下， Y 发生**新带来的熵**。

相对熵(也称KL散度，交叉熵等)定义为两个随机变量的概率分布之比的数学期望。

设 $Q(x), P(x)$ 是随机变量 X 中取值的两个概率分布，则 P 对 Q 的相对熵是

$$D_{\text{KL}}(P||Q) = \sum_x P(x) \log \frac{P(x)}{Q(x)} = \mathbb{E}_x \log \frac{P(x)}{Q(x)} \quad (2.2)$$

参考文献

Goodfellow, I., Bengio, Y., and Courville, A. (2016). *Deep Learning*. MIT Press. ii

索引

Conditional independence, iv
Covariance, iv

Derivative, iv
Determinant, iii

Element-wise product, *see* Hadamard product
Graph, iii

Hadamard product, iii
Hessian matrix, iv

Independence, iv
Integral, iv

Jacobian matrix, iv

Kullback-Leibler divergence, iv

Matrix, ii, iii

Norm, v

Scalar, ii, iii
Set, iii
Shannon entropy, iv
Sigmoid, v
Softplus, v

Tensor, ii, iii
Transpose, iii

Variance, iv
Vector, ii, iii