On the Equivalence of Likeihood & Cross Entropy

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Abstract

We demonstrate the duality of a general version of the Fisher's likelihood principle, especially maximum likelihood and Shannon's entropy, especially minimum cross entropy. We show that in a certain sense those two seemingly distinct concepts converge and are one of the same.

***K*eywords** Shannon's Entropy, Cross Entropy, Likelihood, Multinomial Classification,

1 Introduction

A casual view of statistics is that of frequencies and the basic rules of calculating probabilities are based on frequencies. However, this view is known to be fundamentally flawed. Consider a simple mental exercise demonstrating how this view fails is in the predictive realm when one wishes to estimate a tag (say -1 or $+1$) based on an observable pattern. Consider binary vectors (x_1, x_2) where x_1 and x_2 are either 0 or 1. There are four patters $(0,0),(0,1),(1,0),(1,1)$. Also assume that patterns are appended by a binary tag $y \in \{-1,+1\}$. Thus the data available to the statistician is $\mathscr{D} = \big\{(x_1,x_2,y) : x_j \in \{0,1\}, y \in \{-1,+1\}\big\}$. Put $\mathscr{D}_{+1} = \{(x_1,x_2,y) \in \mathscr{D} : y = +1\}$ and similarly, $\mathscr{D}_{-1}$. If, say, $|\mathscr{D}_{-1}|, |\mathscr{D}_{+1}| > 0.3|\mathscr{D}|$ and if, say, $|\mathscr{D}| > 10^3$, then one may estimate $\mathbb{P}(y = +1 \| x_1, x_2)$, call it $\widehat{p}$, as the fraction of points (x_1,x_2,y) with $y = +1$ and the complement $\mathbb{P}(y = -1 \| x_1,x_2) = 1 - \widehat{p}$. Now consider the binary vector $(x_1, x_2, \ldots, x_n)$ along with a tag $y \in \{-1,+1\}$. There are 2^n distinct binary vectors of length n. If $N = |\mathscr{D}| < 2^n$, then some pattern $(x_1^*, \ldots, x_n^*)$ has no corresponding element in $\mathscr{D}$. In other words, estimating $\mathbb{P}(y = +1 \| x_1^*, \ldots, x_n^*)$ using frequencies is impossible. Another approach is needed; one which uses frequencies only indirectly. One of those approaches makes use of the idea of likelihood.

1.1 Terminology

We use standard (classical) statistical notions & notation. A distribution F is a non-decreasing function on $\mathbb{R}$ with $\lim F(x) \to 0$ for $x \to -\infty$ and $\lim F(x) \to 1$ for $x \to \infty$. Use the 'hat' notation $\widehat{\theta}, \widehat{\mu}$, etc. for an estimate of θ, μ, etc.

2 Likelihood and Entropy

The likelihood framework assumes that data is sampled according to a distribution $p(\theta)$ which depends on an unknown parameter $\theta \in \Theta \subset \mathbb{R}^r$. Specifically, the distribution $p(\theta)$ is from a parametric family of distributions $\mathscr{P}(\theta)$. The sample $X_1, X_2, \ldots, X_n$ is *generated* from the family $\mathscr{P}(\theta)$. The underlying assumption is that the data $X_1, X_2, \ldots$ is sampled from some specific $p(\theta)$ where the functional form p is known, but the parameter θ isn't. With a sample $X_1, X_2, \ldots, X_n \sim p(t|\theta)$, assuming that the data $X_1, \ldots, X_n$ is conditionally independent of θ, the likelihood of the sample is

$$L_n(\theta) = L(X_1, \ldots, X_n|\theta) = p(X_1|\theta) \times p(X_2|\theta) \times \cdots \times p(X_n|\theta).$$

Ruminations. This significant assumption (about samples generated from a parametric family of distributions) may very well be, in many instances, quite fictitious but in many cases it's an assumption necessary to accomplish a goal such as to estimate the probability $\mathbb{P}(y=+1\|x_1,...,x_n)$. We won't get into the philosophy which underpins the assumption; we'll take it for granted, flawed as it is.

2.1 Maximum Likelihood Estimation

The MAXIMUM LIKELIHOOD ESTIMATE (MLE) is

$$\widehat{\theta}_n = \arg\max_{\theta\in\Theta} L(X_1,...,X_n|\theta).$$

We write $\widehat{\theta}_n$ to emphasize dependence of sample size n.

The properties of the MLE were studied extensively. A concise account is found in Ferguson's "Large Sample Theory", [1], and a more comprehensive in the two-volume treatise by Bickel and Doksum "Mathematical Statistics" [2]

2.2 Entropy

We use the term probability vector $\pi=(\pi_1,\pi_2,...,\pi_n)$ to indicate $\pi_j\geq 0, \sum\pi_j=1$. The [sic] SHANNON'S ENTROPY of π is

$$H(\pi) = -\sum \pi_j \log_2(\pi_j).$$

The reason for taking base-2 logarithm is rather historical. Claude Shannon, the founder of information theory was concerned with representing information and as a matter of convenience focused the study on binary strings to represent information. For details see Cover & Thomas [3], and MacKay [4]. Hence base-2 for logarithm was a natural choice but we'll omit the base because the analysis applies to any base >1, including, of course, the natural basis of logarithm.

For two probability vectors $\pi=(\pi_1,...,\pi_n)^T$ and $\nu=(\nu_1,...,\nu_n)^T$, the KULLBACK-LEIBLER (KL) DIVERGENCE is

$$KL(\pi;\nu) = \sum \pi_j \log\left(\frac{\pi_j}{\nu_j}\right) = \sum \pi_j \log(\pi_j) - \sum \pi_j \log(\nu_j).$$

Although the Kullback-Leibler divergence isn't a proper metric, it satisfies Gibb's inequality.

GIBB'S INEQUALITY: $KL(\pi;\nu)\geq 0$ and $KL(\pi;\nu)=0$ if and only if $\pi=\nu$.

The CROSS ENTROPY ρ of π and ν is the second part of the Kullback-Leibler divergence

$$\rho(\pi;\nu) = -\sum \pi_j \log \nu_j$$

We may extend the definition of Kullback-Leibler divergence to densities and define for any two densities f and g ($f,g\geq 0$ and $\int f=\int g=1$),

$$KL(f;g) = \int f(t)\log\frac{f(t)}{g(t)}dt.$$

Similarly, the cross entropy

$$\rho(f;g) = -\int f(t)\log(g(t))dt.$$

2.3 Likelihood, Kullback-Leibler and Cross Entropy

Consider the maximum likelihood estimate $\widehat{\theta}_n=\arg\max L(\theta;X_1,...,X_n)$. It's a consequence of the central limit theorem that for a large family of distributions the MLE is asymptotically Gaussian,

$$\frac{\widehat{\theta}_n-\theta}{var(\widehat{\theta}_n)} \sim N(0,1),$$

and consequently that $\widehat{\theta}_n\to\theta$, where θ is the 'true' parameter θ that the X_js are sampled from, [1], [2].

As we've mentioned earlier, KL is not metric; it's neither symmetric nor it satisfies the triangle inequality, yet it arises naturally in the analysis of likelihood ratios. Specifically consider a sample $X_1,X_2,...,X_n\sim f(x|\theta)$ with θ_0 the true value of θ, or alternatively, MLE $\theta_0=\arg\max_\theta L(\theta)$, and write

$$KL(\theta_0;\theta) = KL\big(f(x;\theta_0);f(x;\theta)\big).$$

From the strong law of large numbers

$$\frac{1}{n}\log\left(\frac{L_n(\theta_0)}{L_n(\theta)}\right) = \frac{1}{n}\sum_1^n \log\left(\frac{f(X_j|\theta_0)}{f(X_j|\theta)}\right) \xrightarrow{a.s.} \mathbb{E}_{\theta_0}\log\left(\frac{f(X|\theta_0)}{f(X|\theta)}\right) \tag{1}$$

The latter is $KL(\theta_0;\theta)$.

With data $X_1,\ldots,X_n \sim f(x|\theta)$ where $\theta\in\Theta\subset\mathbb{R}^r$ the LIKELIHOOD RATIO

$$\lambda_n = \frac{\sup_{\theta\in\Theta_0}\prod_1^n f(X_j|\theta)}{\sup_{\theta\in\Theta}\prod_1^n f(X_j|\theta)} = \frac{L_n(\theta_n^*)}{L_n(\widehat{\theta}_n)} \tag{2}$$

where $\theta_n^* = \arg\max_{\theta\in\Theta_0} L_n(\theta)$ and $\widehat{\theta}$ is the MLE of θ. We may treat λ_n in the same manner to derive formula (1).

3 Logistic Regression

Consider training pairs $(x^1,y^1),(x^2,y^2),\ldots,(x^N,y^N)$ where $x^j\in\mathbb{R}^p$ and $y^j\in\{0,1\}$. Arrange $x^1,x^2,\ldots,x^N$ as rows of a matrix $X=\left(x_{ij}\right)$, $i=1,2,\ldots,N$, $j=1,2,\ldots,p$. For $\beta\in\mathbb{R}^{p+1}$ and $x^T=(1,x_1,\ldots,x_p)$, and put $\beta^T x = \beta_0+\beta_1 x_1+\cdots+\beta_p x_p$ where $\beta=(\beta_0,\beta_1,\ldots,\beta_p)^T$.

Consider a model $\sigma:\mathbb{R}^p\to[0,1]$ which predicts a binary y for generic $x=(1,x_1,\ldots,x_p)$

$$\sigma(x;\beta) = \mathbb{P}(y=1\|x;\beta) = \frac{1}{1+\exp(-\beta^T x)} \tag{3}$$

In the parlance of neural networks, the function σ is called SIGMOID.

The value $\sigma(\beta^T x)$ represents $\mathbb{P}(y=+1\|x)$, the conditional probability $y=+1$ conditioned on x while the value $(1-\sigma(\beta^T x))$ represents the complementary probability, $\mathbb{P}(y=0\|x)$. One would conceive that a good estimate $\widehat{\beta}$ yields the correct value $\sigma(\widehat{\beta^T}x)\approx 1$ if the corresponding $y=+1$ and conversely $\sigma(\widehat{\beta}^T x)\approx 0$ if the corresponding $y=0$. In general, $0<\sigma(\beta^T x)<1$ and if $\beta^T x\to\infty$ then $\sigma(\beta^T x)\to 1$ while if $\beta^T x\to-\infty$ then $\sigma(\beta^T x)\to 0$.

THEOREM. The log likelihood

$$L(\beta) = \sum_j \left\{y^j\log(\sigma(\beta^T x^j) + (1-y^j)\log(1-\sigma(\beta^T x^j)\right\} \tag{4}$$

is a concave function of β and hence has a unique maximum.

Proof. Let L be the function on the right side of equation (4). Its derivative is:

$$\frac{\partial L(y|x,\beta)}{\partial\beta} = \sum_j (y^j - \sigma(\beta^T x^j))x^j$$

and hence its second derivative is:

$$\frac{\partial^2 L(y|x,\beta)}{\partial\beta^2} = -\sum \sigma(\beta^T x^j)\sigma(-\beta^T x^j)x^j(x^j)^T$$

which is a negative-definite function of β, proving the theorem.
□ It follows that the log likelihood has a maximum.

The view that minimizing sums of squares may be taken in lieu of likelihood generally falls on its face. For that we need to observe that the residual sum of squares, defined by

$$\phi(\beta) = \sum_1^N \left(y^j - \sigma(\beta^T x^j)\right)^2$$

is neither a convex nor a concave function of β, and hence may not have a unique minimum

$$\beta^* = \arg\min_{\beta\in\mathbb{R}^{p+1}} \sum_1^N \left(y^j - \sigma(\beta^T x^j)\right)^2$$

In fact, the second derivative of $\phi(\beta)$ takes the form:

$$\begin{aligned} \frac{\partial^2 \phi}{\partial \beta^2} &= 2 \sum_{j:y^j=1} \sigma_+ \sigma_- (\sigma_- - \sigma_+) x^j (x^j)^T \\ &- 2 \sum_{j:Y^j=0} \sigma_+ \sigma_- (\sigma_+ - \sigma_-) x^j (x^j)^T \end{aligned} \tag{5}$$

where

$$\sigma_+ = \sigma(\beta' X^j); \qquad \sigma_- = \sigma(-\beta' X^j)$$

But equation (5) is not necessarily positive or negative definite. On the other hand, by the law of large numbers, the minimizer of the residual sum of squares converges asymptotically (see e.g., Loeve: probability theory).

As an alternative, the Bayesian estimate of β, assuming e.g., a multivariate normal prior on β, has a unique posterior mean which can be approximately calculated in a number of ways (see Blei(2013,JMLR)).

3.1 Logit: Likelihood as Cross Entropy

Recall that the CROSS ENTROPY $\nu(\pi;\rho)$ of two probability vectors π and ρ is

$$\rho(\pi;\rho) = -\sum_j \pi_j \log(\rho_j).$$

The "weight-1" (0,1)-vector $y = (y_1, y_2, \ldots)$ satisfying $\sum y_j = 1$, is indeed a probability vector and the cross entropy of y and π is

$$\rho(y;\pi) = -\sum_j y_j \log(\pi_j).$$

Suppose $y_k = 1$ and all other components $y_j = 0$, $j \neq k$. Then

$$\rho(y;\pi) = -\log(\pi_k).$$

From equation (4), $l(\beta) = \log(L(\beta))$ is the sum of the two terms

$$\sum_j y^j \log\left(\sigma(\beta^T x^j)\right) + \sum_j (1-y^j) \log\left(\sigma(\beta^T x^i)\right).$$

MLE is the solution of logit.

$$\widehat{\beta} = \arg\max_\beta L(\beta) = \arg\max_\beta \prod_1^N \left[\frac{1}{1+\exp(-\beta^T x^j}\right]^{y^j} \left[1 - \frac{1}{1+\exp(-\beta^T x^j)}\right]^{1-y^j}. \tag{6}$$

Taking logarithms

$$\begin{aligned} l(\beta) &= \log(L(\beta))) \\ &= \sum_1^N y^j \log\left(\frac{1}{1+\exp(-\beta^T x^j)}\right) + \sum_1^N (1-y^j) \log\left(1 - \frac{1}{1+\exp(-\beta^T x)}\right. \\ &= \sum_1^N y^j \log\left(\frac{1}{1+\exp(-\beta^T x^j)}\right) + \sum_1^N (1-y^j) \log\left(\frac{\exp(-\beta^T x)}{1+\exp(-\beta^T x)}\right.. \end{aligned} \tag{7}$$

To simplify, we write $\phi(\beta) = \dfrac{\mathbf{1}}{\mathbf{1}+\exp(-\beta^{\mathbf{T}}\mathbf{x})} = \mathbb{P}(\mathbf{y} = +\mathbf{1} \| \mathbf{x}; \beta)$ and we get

$$= \sum_{\mathbf{1}}^{\mathbf{N}} \left[\mathbf{y^j} \phi(\beta) + (\mathbf{1} - \mathbf{y^j})(\mathbf{1} - \phi(\beta))\right] \tag{8}$$

Notice that each term $\mathbf{y^j}\phi(\beta) + (\mathbf{1}-\mathbf{y^j})(\mathbf{1}-\phi(\beta))$ is the negative of the cross entropy ρ of the probability vector $(\mathbf{y^j}, (\mathbf{1}-\mathbf{y^j}))$ and $(\phi(\beta;\mathbf{x^j}), \mathbf{1}-\phi(\beta;\mathbf{x^j}))$. **This demonstrates the relation between log-likelihood and cross entropy.**

4 Multinomial (m-nomial) Regression

In an analogy with logit, SOFTMAX is used to assign probability of class membership. The setup is similar to logit where class k is encoded as ONE-HOT vectors. Specifically, class k is represented by a the vector

$$y = (0 \quad 0 \quad . \quad . \quad 0 \quad 1 \quad 0 \quad . \quad . \quad 0)$$

with 1 in the kth spot and 0 elsewhere.

In the context of M-NOMIAL REGRESSION training pairs (x, y), $x \in \mathscr{X} \subset \mathbb{R}^p$ and tags y a K-HOT vector. It's customary to model an m-nomial regression as a neural network with p input nodes and m output nodes and optimize with respect to the hidden layers. Unfortunately, as of today (October of 2021) there isn't a prescription specifying an optimal architecture, however, rough guidelines do exist for specific problem instances.

To simplify, consider any network architecture with zero or more hidden layers. Consider output layer $v = (v_1, v_2, ..., v_m)$ where each node v_j receives r stimulii from a previous layer, $z = (z_{j1}, z_{j2}, ..., z_{jp})$, ($r = p$ if there is no hidden layer). With weights vector $\beta_j \in \mathbb{R}^r$ (plus bias β_{j0}) the node v assumes value $\beta_j^T z + \beta_{j0}$. Transformed the output layer by softmax:

$$\begin{aligned} \pi &= (\pi_1, \pi_2, ..., \pi_m) \\ &= \Big(\frac{\exp(\mathbf{t_1})}{\exp(\mathbf{t_1}) + ... + \exp(\mathbf{t_m})}, \frac{\exp(\mathbf{t_2})}{\exp(\mathbf{t_1}) + ... + \exp(\mathbf{t_m})}, ..., \frac{\exp(\mathbf{t_m})}{\exp(\mathbf{t_1}) + ... + \exp(\mathbf{t_m})}\Big) \end{aligned} \tag{9}$$

where $\mathbf{t_j} = \beta_{\mathbf{j}}^{\mathbf{T}} \mathbf{z} + \beta_{\mathbf{j0}}$ and of course $\pi_{\mathbf{j}} = \dfrac{\exp(\mathbf{t_j})}{\exp(\mathbf{t_1}) + \exp(\mathbf{t_2}) + \cdots + \exp(\mathbf{t_m})}$.
In fact, the last term is redundant because it's the 1-complement of the preceding terms.

A standard COST FUNCTION is the cross entropy

$$\rho(\mathbf{y}; \pi) = -\sum_{\mathbf{j}} \mathbf{y_j} \log(\pi_{\mathbf{j}}) \tag{10}$$

The weights (β_{ij}) are calculated by minimizing the cost function

$$\widehat{\beta} = \arg\min_{\beta} \rho(\mathbf{y}; \pi). \tag{11}$$

Take equation (10) and turn the cross entropy on its head and get what looks like likelihood of m-nonial

$$\rho(\mathbf{y}; \pi) = -\sum_{\mathbf{j}} \log(\pi_{\mathbf{j}}^{\mathbf{y_j}}) = -\log \Big[\prod_{\mathbf{j}} \pi_{\mathbf{j}}^{\mathbf{y_j}}\Big] \tag{12}$$

and minimizing $\rho(\mathbf{y}; \pi)$ is tantamount to maximizing the likelihood $\prod_{\mathbf{j}} \pi_{\mathbf{j}}^{\mathbf{y_j}}$.
OBSERVATIONS ON (5) Since y is one-hot, only a single $y_j \neq 0$, say $y_k = 1$, so (5) turns into the very simple expression $\rho(\mathbf{y}; \pi) = \log \pi_{\mathbf{k}}$ so in the aggregate, optimizing m-nomial model involves no more than the minimization problem

$$\widehat{\beta} = \arg\min_{\beta} \sum_{\mathbf{d}} \log(\pi_{\mathbf{j(d)}}^{\mathbf{d}}) \tag{13}$$

where $j(d)$ is the non-zero index corresponding to the one-hot y.

By (Cook(2007) and Taddy(2013)) we can extend the m-nomial regression to subject-specific m-nomial models which are used in Text analysis. First assume a matrix of output layers

$$\begin{aligned} v_1 &= (v_{1,1}, ..., v_{1,J}) \\ ... &= .... \\ v_I &= (v_{I,1}, ..., v_{I,J}) \end{aligned} \tag{14}$$

$i = 1, ..., I$ are the responses corresponding to subject $j = 1, ..., J$. Node $v_{i,j}$ assumes the value

$$\eta_{i,j} = \alpha_j + u_{ij} + w_i' \phi_j$$

Transformed by softmax, the output layer takes the form

$$\pi = \{\pi_{i,j}\}$$

$$\pi_{i,j} = \frac{\exp(\eta_{i,j})}{\sum_{i=1}^{I} \eta_{i,j}}$$

We can write the likelihood as:

$$L(\alpha, u, w_i, \phi_j) = \prod_{i,j} \pi^d_{(i,j)(d)}$$

$$\widehat{\beta} = \arg\min_{\beta} \sum_{\mathbf{d}} \log(\pi^{\mathbf{d}}_{(\mathbf{i},\mathbf{j})(\mathbf{d})}) \tag{15}$$

where $(i,j)(d)$ is the non-zero index corresponding to the one-hot y.

More generally, for a continuous response, y, if we model the values of y on an asymptotically large number of small (possibly multidimensional) intervals and regress the probabilities that y takes values in the respective intervals on the inputs associated with those intervals, we obtain an approximating multinomial with an asymptotically large number of parameters. Standard regression assumes that most of these parameters are the same. The assumption that the parameters are stochastically related to one another gives rise to the assumption that y is distributed according to a stochastic process.

5 Duality in Generalized Linear Models

Extention to Generalized Linear Models

The Generalized Linear Models deals with estimating the mean of a parametric family $f(x;\theta)$ where f belongs to the exponential family, having the form

$$f(x;\theta) = s(x)t(\theta)\exp(a(x)b(\theta)),$$

for some functions s, t, a and b, and the natural parameter $b(\theta)$. The mean $\mathbb{E}(X_j) = \mu_j$ is tied to covariate vector $x^j \in \mathbb{R}^{p+1}$ via a monotone and smooth link function g

$$g(\mu_j) = \beta_0 + \beta_1 x_1 + \ldots \beta_p x_p.$$

6 Concluding Remarks

6.1 Likelihood-Cross Entropy Duality

An apparent duality of likelihood and cross entropy, or just duality, is amply hinted throughout the literature. See MacKay [4], chapter 42 on the analysis of Hopefield Networks (page 516). Arguably, in the case of multinomial regression, duality may have been regarded as self-evident, unworthy of special attention. Yet, we believe that a careful analysis will lead to formalism.

7 Future work

In this short essay we've seen Formalize the likelihood-cross entropy duality.

Is the likelihood-cross entropy duality extends beyond the multinomial regression?

As an intermediate step, extend likelihood-cross entropy duality to a general regression setup where training pairs are (x, y) with $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$.

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8 Appendix

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