

Logistic regression with a latent binary variable and noisy labels

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1 Model

Following [1], consider a set of N training data points $D = \{(\mathbf{x}_1, c_1) \dots (\mathbf{x}_N, c_N)\}$ where $\mathbf{x}_n \in \mathbb{R}^M$ denote M -dimensional real-valued explanatory data (e.g. gene expression levels) and $c_n \in \{0, 1 \dots K-1\}$ denotes a categorical label with K possible values (e.g. clinician-assigned label incorporating some degree of uncertainty).

We aim to fit this with a two-stage model, first regressing the explanatory data \mathbf{x}_n to a latent binary variable representing ground truth $b_n \in \{0, 1\}$ (e.g. disease state), then modeling clinical labeling as a categorical variable $c_n|b_n$ that is conditionally-independent of the explanatory data given the ground truth

$$\begin{aligned} P(b = 1|\mathbf{x}, \mathbf{w}) &= \sigma(\mathbf{w}^T \mathbf{x}) \\ P(c = k|b = j, \mathbf{z}) &= z_{j,k} \end{aligned}$$

where $\sigma(x) = \frac{1}{1+e^{-x}}$ is the logistic function, $\mathbf{w} \in \mathbb{R}^M$ are weight parameters for the logistic regression model, and \mathbf{z} are probability parameters for the label observation model.

We put a Laplace double-exponential (Lasso) prior on \mathbf{w} , and a uniform¹ Dirichlet prior on each row of \mathbf{z}

$$\begin{aligned} P(\mathbf{w}) &\propto \prod_{m=1}^M \exp(-|w^{(m)}|) \\ P(\mathbf{z}) &\propto \prod_{j \in \{0,1\}} \delta \left(1 - \sum_{k=0}^{K-1} z_{j,k} \right) \end{aligned}$$

This is equivalent to Section 2.2 of [1], with the sum over j in equation (8) of that paper constrained to $j \in \{0, 1\}$ instead of $j \in \{0, 1 \dots K-1\}$. The paper derives a conjugate gradient optimization algorithm, and proves its convergence.

¹For identifiability of b , we need to break the symmetry of the Dirichlet prior slightly; e.g. by adding a pseudocount of 1 for all $b \rightarrow c$ mappings that “agree”.

1.1 Quartile approach

An alternate model is to use the interpretation of logistic regression where a latent *continuous-valued* random variable (obtained by adding logistically-distributed noise to $\mathbf{w}^T \mathbf{x}$) is used to obtain the labels (b, c) , e.g. with c corresponding to the quartiles.

I haven't pursued this model, as the assumption that c corresponds to quartiles of the latent variable underlying logistic regression seems like a possible misfit to the situation of arbitrarily designated clinical labels (although, conceivably, my assumption that c is independent of \mathbf{x} given b is just as bad, or worse).

2 EM algorithm

How to use the training data D to fit the weights \mathbf{w} and probabilities \mathbf{z} ? One approach is to use the EM (Expectation Maximization) algorithm [2], treating the binary-valued latent variables $B = \{b_n\}$ as *missing data*, the dataset $D = (X, C)$ as *observed data* (with inputs $X = \{\mathbf{x}_n\}$ and observed labels $C = \{c_n\}$), and the weights and probabilities $\theta = (\mathbf{w}, \mathbf{z})$ as the *parameters* to be fit by the algorithm.

The conjugate gradient parameter optimization approach derived by [1] may well be superior to the EM method. However I've outlined the EM approach here for reference.

The likelihood to be maximized is $P(C, \theta|X) = \sum_B P(B, C, \theta|X)$ where

$$\begin{aligned} P(B, C, \theta|X) &= P(\theta)P(B, C|\theta, X) \\ &= P(\mathbf{w})P(\mathbf{z})P(B|\mathbf{w}, X)P(C|\mathbf{z}, B) \end{aligned}$$

At the $(i+1)$ 'th iteration, the parameters found by the EM algorithm are

given by maximizing the expected log-likelihood

$$\begin{aligned}
\theta^{(i+1)} &= \operatorname{argmax}_{\theta} \mathcal{E}(\theta || \theta^{(i)}) \\
\mathcal{E}(\theta || \theta^{(i)}) &= \sum_B P(B | \theta^{(i)}, X, C) \log P(B, C, \theta | X) \\
&= \log P(\mathbf{w}) + \log P(\mathbf{z}) + \sum_B P(B | \theta^{(i)}, X, C) [\log P(B | \mathbf{w}, X) + \log P(C | \mathbf{z}, B)] \\
&= \log P(\mathbf{w}) + \log P(\mathbf{z}) \\
&\quad + \sum_n \sum_{j \in \{0,1\}} P(b_n = j | \theta^{(i)}, \mathbf{x}_n, c_n) [\log P(b_n = j | \mathbf{w}, \mathbf{x}_n) + \log P(c_n | \mathbf{z}, b_n = j)] \\
&= \mathcal{E}_{\mathbf{w}} + \mathcal{E}_{\mathbf{z}} \\
\mathcal{E}_{\mathbf{w}} &= \log P(\mathbf{w}) + \sum_n \left[(1 - \beta_n^{(i)}) \log(1 - \sigma(\mathbf{w}^T \mathbf{x}_n)) + \beta_n^{(i)} \log \sigma(\mathbf{w}^T \mathbf{x}_n) \right] \\
\mathcal{E}_{\mathbf{z}} &= \log P(\mathbf{z}) + \sum_n \left[(1 - \beta_n^{(i)}) \log z_{0,c_n} + \beta_n^{(i)} \log z_{1,c_n} \right] \\
\beta_n^{(i)} &= P(b_n = 1 | \theta^{(i)}, \mathbf{x}_n, c_n) \\
P(b_n = 1 | \theta, \mathbf{x}_n, c_n) &= \frac{1}{1 + \frac{P(c_n, b_n=0 | \theta, \mathbf{x}_n)}{P(c_n, b_n=1 | \theta, \mathbf{x}_n)}} \\
&= \frac{1}{1 + \frac{(1 - \sigma(\mathbf{w}^T \mathbf{x}_n)) z_{0,c_n}}{\sigma(\mathbf{w}^T \mathbf{x}_n) z_{1,c_n}}}
\end{aligned}$$

The maximization of $\mathcal{E}_{\mathbf{w}}$ w.r.t. \mathbf{w} is a weighted, Lasso-penalized logistic regression (the weights being the $\beta_n^{(i)}$).

The maximization of $\mathcal{E}_{\mathbf{z}}$ w.r.t. \mathbf{z} should be solvable exactly.

2.1 Implementation of weighted logistic regression in R

The maximization of $\mathcal{E}_{\mathbf{w}}$ w.r.t. \mathbf{w} can be performed using R's `glm()` function (generalized linear model regression) with `family = binomial(link = "logit")` (logistic regression is equivalent to binomial-family GLM regression with the “logit” link function) and using the `weights` argument to specify the weights ($\beta_1^{(i)} \dots \beta_N^{(i)}$) (weights correspond implicitly to frequency of observations of each case, which intuitively is how posterior probabilities of missing data are interpreted in EM).

This can then be worked into an R program that implements EM.

References

- [1] Jakramate Bootkrajang and Ata Kabán. Label-noise robust logistic regression and its applications. In *Proceedings of the 2012 European Conference on Machine Learning and Knowledge Discovery in Databases - Volume Part I, ECML PKDD'12*, pages 143–158, Berlin, Heidelberg, 2012. Springer-Verlag.

- [2] A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the em algorithm. *JOURNAL OF THE ROYAL STATISTICAL SOCIETY, SERIES B*, 39(1):1–38, 1977.