Block coordinate descent algorithm for L1/L2 Regularized Logistic Regression

Abstract

The strucutre learning algorithm proposed for discrete graphical models described in Ravikumar et al. $^{(3)}$ involves solving an L1/L2 Regularized Logistic Regression problem. In this note, we describe the Block coordinate descent algorithm being used for solving this problem. This algorithm was proposed in Meier et al. $^{(1)}$.

1 Notation

Let us recall the notation used in Ravikumar et al. $^{(3)}$ and the dropbox note $^{(2)}$. Consider a discrete pairwise graphical model describing a probability distribution over p variables, each of which can take one of m discrete values. Let $D = \{1, \ldots, m-1\}$ denote the set of the first m-1 values.

$$Pr(x) \propto \exp(\sum_{s \in V} \phi_s(x_s) + \sum_{(s,t) \in E} \phi_{st}(x_s, x_t)).$$
 (1)

Using indicator variables, any set of potential functions can then be written as

$$\phi_s(x_s) = \sum_{j \in D} \theta_{s;j}^* \ I[x_s = j] \quad \text{for } s \in V, \text{ and}$$

$$\phi_{st}(x_s, x_t) = \sum_{(j,k) \in D^2} \theta_{st;jk}^* \ I[x_s = j, \ x_t = k] \quad \text{for } (s,t) \in E.$$

Thus, the Markov random field can be parameterized in terms of the vector $\theta_s^* \in \mathbf{R}^{m-1}$ for each $s \in V$, and the vector $\theta_{st}^* \in \mathbf{R}^{(m-1)^2}$ associated with each edge.

The conditional probability distribution of values taken by node r is given by:

$$\mathbb{P}_{\Theta}\left[X_r = m \mid X_{\backslash r} = x_{\backslash r}\right] = \frac{1}{1 + \sum_{\ell} \exp(\theta_{r;\ell}^* + \sum_{t \in V \backslash \{r\}} \sum_k \theta_{rt;\ell k}^* I[x_t = k])}$$
(2)

and, for $j \in \{1, ..m - 1\}$:

$$\mathbb{P}_{\Theta}[X_r = j \mid X_{\backslash r} = x_{\backslash r}] = \frac{\exp(\theta_{r;j}^* + \sum_{t \in V \backslash \{r\}} \sum_k \theta_{rt;jk}^* I[x_t = k])}{1 + \sum_{\ell} \exp(\theta_{r;\ell}^* + \sum_{t \in V \backslash \{r\}} \sum_k \theta_{rt;\ell k}^* I[x_t = k])}.$$
(3)

In the above expression, it is assumed that $\forall t \notin \Gamma(r), \ \theta_{rt}$ are zero vectors. Let Θ be the set of all parameters involved in Equation 3. Given a set $S = \left\{x^{(1)}..x^{(n)}\right\}$ of n sample-points, we can deduce the neighborhood N(r) of r by estimating the parameter vectors $\forall t \in V \setminus \{r\}: \theta_{rt}^*$. In particular, we solve the problem:

$$\min_{\Theta} -n^{-1} \sum_{i=1}^{n} \log P_{\Theta}(x_r^{(i)} | x_{\backslash r}^{(i)}) + \lambda \sum_{v \in V \setminus \{r\}} \|\theta_{rv}\|_2.$$

2 Solving the logistic regression problem

The algorithm we use for solving l1/l2 regularized logistic regression works best when the design matrix is group-orthogonalized. So, we find it convenient to describe this algorithm in general terms, rather than in terms of parameters Θ introduced earlier.

2.1 Problem setting

We now introduce the l1/l2 regularized logistic regression in general terms. Let Y be the response variable, and X be the predictor variables whose relationship is being modelled using a multi-class logistic model. Further, suppose that any predictor vector $x \in R^{p'+1}$ includes the intercept; that is $x_1 = 1$ always. Suppose that the Y takes values in the set $\{1..m\}$, and that each predictor X_i takes values in the set $\{1..m\}$. Then, the logistic model we deal with is described below:

$$\mathbb{P}_{\beta}^{*}[Y = m \mid X = x] = \frac{1}{1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_{\ell}^{*T} x)}$$

and, for $j \in \{1, ..m - 1\}$:

$$\mathbb{P}_{\beta}^{*}[Y = j \mid X = x] = \frac{\beta_{j}^{*T} x}{1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_{\ell}^{*T} x)}.$$
 (4)

Let $\{\beta_0^*, \beta_1^*, ...\beta_G^*\}$ be a partition of the parameters β^* , which need not coincide with the partitioning $\{\beta_\ell^*|\ell\in\{1..m-1\}\}$ used in Equation 4. We work with the prior belief that β^* is group-sparse: that is, we assume that most of the vectors in $\{\beta_1^*, ...\beta_G^*\}$ are actually zero vectors. So, given n observations $\{(x^{(i)}, y^{(i)})\}$, to estimate β^* , we will solve the problem:

$$\min_{\beta} n^{-1} \sum_{i=1}^{n} -\log P_{\beta}(y^{(i)}|x^{(i)}) + \lambda \sum_{g \in \{1...G\}} \|\beta_g\|_{2}.$$

2.2 Details of some computations

The algorithm to solve this problem will involve computation of the negative log likelihood function $nll(\beta|(x^{(i)},y^{(i)})) = -\log P_{\beta}(y^{(i)}|x^{(i)})$, its gradient, and the diagonal of its Hessian. The negative log likelihood given the observation (x,y) and its gradient are computed by evaluating the following expressions ¹:

$$\begin{aligned} nll(\beta|(x,y=m)) &= \log(1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_{\ell}^T x)) \\ \frac{\partial nll(\beta|(x,y=m))}{\partial \beta_{i,j}} &= (1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_{\ell}^T x))^{-1} \exp(\beta_{\ell}^T x) x_j. \end{aligned}$$

and for $q \in \{1, ..m' - 1\}$:

$$nll(\beta|(x, y = q)) = -\beta_q^T x + \log(1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_\ell^T x))$$
$$\frac{\partial nll(\beta|(x, y = m))}{\partial \beta_{i=q,j}} = -x_j + (1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_\ell^T x))^{-1} \exp(\beta_q^T x)$$
$$\frac{\partial nll(\beta|(x, y = m))}{\partial \beta_{i\neq q,j}} = (1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_\ell^T x))^{-1} \exp(\beta_i^T x) x_j.$$

The diagonal of the Hessian is computed by evaluating the following expression:

$$\begin{split} \frac{\partial^2 n l l(\beta|(x,y=m))}{\partial \beta_{i,j}^2} &= (1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_\ell^T x))^{-1} \exp(\beta_i^T x) x_j^2 \\ &- (1 + \sum_{\ell \in \{1..m-1\}} \exp(\beta_\ell^T x))^{-2} \exp(2\beta_i^T x) x_j^2. \end{split}$$

Given n observations $S = \left\{ (x^{(i)}, y^{(i)}) \right\}$, we define

$$nll(\beta|S) = n^{-1} \sum_{i=1:n} nll(\beta|(x^{(i)}, y^{(i)})).$$

2.3 The block coordinate descent algorithm

The algorithm is specified as Algorithm 1.

References

Lukas Meier, Sara van de Geer, and Peter Buhlmann. The group lasso for logistic regression. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 70(1):53-71, February 2008. ISSN 1369-7412. doi: 10.1111/j.1467-9868.2007.00627.x. URL http://dx.doi.org/10.1111/j.1467-9868.2007.00627.x.

¹Here we return to the partitioning $\{\beta_{\ell}^* | \ell \in \{1..m-1\}\}$ used in Equation 4.

Algorithm 1 Block coordinate descent algorithm

```
Input: \beta^{(0)}, Sample set S = \{(x^{(i)}, y^{(i)})\} of n points, \lambda, tol.
Output: \beta.
   \beta \leftarrow \beta^{(0)}
   loop
       for all g \in \{0, ..G\} do
          Compute nll(\beta|S), \nabla nll(\beta|S)_q, diag(\nabla^2 nll(\beta|S)_{qq}), where the subscripts
          indicate that we refer to the portions of the gradient and hessian corre-
          sponding to the vairables \beta_q.
          h_g \leftarrow -\max \{diag(\nabla^2 nll(\beta|S)_{gg}), 10^{-5}\}.
          d \leftarrow 0.
          if g = 0 then
             d_g \leftarrow \nabla nll(\beta|S)/h_g.
             z \leftarrow -\nabla nll(\beta|S)_g - h_g\beta_g.
             if ||z||_2 \le \lambda then d_g \leftarrow -\beta.
                d_g \leftarrow -h_g^{-1}[-\nabla nll(\beta|S)_g - \lambda \frac{z}{\|z\|_2}].
             end if
          end if
          if \max |d| \ge tol then
             Get \alpha from line search along d with \alpha_0 = 2, \delta = 0.75, \sigma = .01.
          \beta_g \leftarrow \beta_g + \alpha d_g. end if
       end for
       Return if decrease in objective value is less than tol.
   end loop
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- [2] Pradeep Ravikumar. Learning Discrete Graphical Models [Dropbox note], 2010.
- [3] Pradeep Ravikumar, M. J. Wainwright, and J. Lafferty. Highdimensional ising model selection using l1-regularized logistic regression. *Annals of Statistics*, 2009.