

Fused LASSO using alternative direction method of multipliers (ADMM)

In many biological applications, we are interested in the association of a response variable $Y \in \mathbb{R}^{N \times 1}$, with respect to some predictor variables $X \in \mathbb{R}^{N \times p}$, across varying conditions. In the simple 2-condition scenario, we have the following model:

$$Y = X\beta + \epsilon$$

$$\epsilon \sim N(0, \sigma^2)$$

$$Y = [Y_1, Y_0]^T$$

$$X = \text{BlockDiag}(X_1, X_0)$$

In order to choose relevant predictor variables, we can impose an L1 penalty on the beta coefficient vector, β . Additionally, when we expect the relationship between the predictors and response to be mostly the same across groups, it is useful to impose a penalty on the beta coefficients of paired coefficients, β_j and β_{j+p} , between treatment and control groups.

$$\text{argmin}_{\beta} \frac{1}{2N} \|Y - X\beta\|_2^2 + \lambda_1 \|\beta\|_1 + \lambda_2 \|D\beta\|_1$$

However, because there are multiple nondifferentiable L1 penalty factors, the objective function cannot be optimized using standard gradient based methods. To efficiently solve this, we introduce two auxiliary variables, z and d , in place of β and $D\beta$.

$$z = \beta$$

$$d = D\beta$$

Our new objective function becomes:

$$\text{argmin}_{\beta} \frac{1}{2N} \|Y - X\beta\|_2^2 + \lambda_1 \|z\|_1 + \lambda_2 \|d\|_1$$

$$\text{s.t. } \beta - z = 0; \quad D\beta - d = 0$$

As this is a constrained optimization problem, we use the augmented Lagrangian as our objective function (See appendix for details on the derivation):

$$\begin{aligned}\mathcal{L}(\beta, z, d, u, w) = & \frac{1}{2N} \|Y - X\beta\|_2^2 + \lambda_1 \|z\|_1 + \lambda_2 \|d\|_1 \\ & + \frac{\rho_1}{2} \|\beta - z + \mu\| + \frac{\rho_2}{2} \|D\beta - d + w\|\end{aligned}$$

We can now differentiate with respect to β and then update z and d at each step. This procedure resembles a block coordinate descent algorithm, where we alternate between optimizing over β , (z, d) , and updating the dual variables (u, w) . The key is that we have removed the non-differentiable terms with respect to β and exchanged them for auxiliary variables so that the function is differentiable over β .

Step 1 – Update β

To update β , we differentiate the augmented Lagrangian with respect to β and set it equal to zero. This results in the following linear system:

$$\begin{aligned}\left(\frac{1}{N}X^T X + \rho_1 I + \rho_2 D^T D\right)\beta^{(k+1)} = & \frac{1}{N}X^T Y + \rho_1(z^{(k)} - \mu^{(k)}) + \rho_2(z^{(k)} - \mu^{(k)}) \\ & + \rho_2 D^T(d^{(k)} - w^{(k)})\end{aligned}$$

Which we solve by Cholesky factorization of the LHS and backsubstitution.

Step 2 – Update z and d

At the current step k , $z^{(k+1)}$ and $d^{(k+1)}$ can be updated as:

$$\begin{aligned}z^{(k+1)} &= S\left(\beta^{(k+1)} + \mu^{(k)}, \frac{\lambda_1}{\rho_1}\right) \\ d^{(k+1)} &= S\left(D\beta^{(k+1)} + w^{(k)}, \frac{\lambda_2}{\rho_2}\right)\end{aligned}$$

Where $S(x, t)$ is the soft threshold operator:

$$S(x, t) = \text{sign}(x) \cdot \max(|x| - t, 0)$$

The threshold $t_j = \frac{\lambda_j}{\rho_j}$ is based on the Karush Kuhn Tucker conditions of the augmented Lagrangian (see appendix for details).

Step 3 – Update u , w ,

$$u^{(k+1)} = \mu^{(k)} + \beta^{(k+1)} - z^{(k+1)}$$

$$w^{(k+1)} = w^{(k)} + D\beta^{(k+1)} - d^{(k+1)}$$

We iterate through steps 1-3 until the augmented Lagrangian decreases by less than 10^{-5} for ten consecutive iterations.

Appendix