Feature Selection for Mixed-Effects Models

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Plan

Introduction

Linear Mixed-Effects Models Feature Selection for Mixed Models

Proposed Algorithm

Experiments

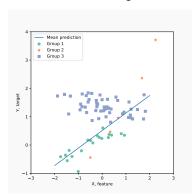
Application to Synthetic Problems Application to Real-World Problems

Future Work

Linear Mixed-Effect Models are a type of regression models for grouped data

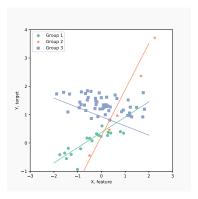
Dataset: m groups (X_i, y_i) , i = 1, ... m

Standard Linear Regression:



$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \Lambda)$$

Linear Mixed-Effect Model:



$$y_i = X_i(\beta + u_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \Lambda_i)$$

 $u_i \sim \mathcal{N}(0, \Gamma)$

$$\begin{aligned} y_i &= X_i(\beta + u_i) + \varepsilon_i \quad i = 1 \dots m \\ \varepsilon_i &\sim \mathcal{N}(0, \Lambda_i) \\ u_i &\sim \mathcal{N}(0, \Gamma) \end{aligned} \tag{1}$$

$$y_{i} = \frac{X_{i}}{(\beta + u_{i})} + \varepsilon_{i} \quad i = 1 \dots m$$

$$\varepsilon_{i} \sim \mathcal{N}(0, \Lambda_{i})$$

$$u_{i} \sim \mathcal{N}(0, \Gamma)$$
(1)

 $ightharpoonup X_i \in \mathbb{R}^{n_i \times p}$ – features, or covariates,

$$y_i = X_i \beta + Z_i u_i + \varepsilon_i \quad i = 1 \dots m$$

 $\varepsilon_i \sim \mathcal{N}(0, \Lambda_i)$
 $u_i \sim \mathcal{N}(0, \Gamma)$ (1)

- ▶ $X_i \in \mathbb{R}^{n_i \times p}$ fixed features, or covariates, $Z_i \in \mathbb{R}^{n_i \times q}$ random features
- \triangleright p number of fixed features, q number of random effects.

$$y_{i} = X_{i} \frac{\beta}{\beta} + Z_{i} u_{i} + \varepsilon_{i} \quad i = 1 \dots m$$

$$\varepsilon_{i} \sim \mathcal{N}(0, \Lambda_{i})$$

$$u_{i} \sim \mathcal{N}(0, \Gamma)$$
(1)

- ▶ $X_i \in \mathbb{R}^{n_i \times p}$ fixed features, or covariates, $Z_i \in R^{n_i \times q}$ random features
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- $lacktriangleright eta \in \mathbb{R}^p$ fixed effects, or mean effects

$$y_{i} = X_{i}\beta + Z_{i} \mathbf{u}_{i} + \varepsilon_{i} \quad i = 1 \dots m$$

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- $\beta \in \mathbb{R}^p$ fixed effects, or mean effects
- $\mathbf{v}_i \in \mathbb{R}^q$ random effects

$$y_{i} = X_{i}\beta + Z_{i}u_{i} + \varepsilon_{i} \quad i = 1 \dots m$$

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- $\mathbf{v}_i \in \mathbb{R}^q$ random effects
- $\Gamma \in \mathbb{R}^{q \times q}$ covariance matrix of random effects

$$y_{i} = X_{i}\beta + Z_{i}u_{i} + \varepsilon_{i} \quad i = 1 \dots m$$

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- lacksquare $arepsilon_i \in \mathbb{R}^{n_i}$ observation noise

$$y_{i} = X_{i}\beta + Z_{i}u_{i} + \varepsilon_{i} \quad i = 1 \dots m$$

$$\varepsilon_{i} \sim \mathcal{N}(0, \Lambda_{i})$$

$$u_{i} \sim \mathcal{N}(0, \Gamma)$$
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- $\mathbf{v}_i \in \mathbb{R}^q$ random effects
- $ightharpoonup \Gamma \in \mathbb{R}^{q \times q}$ covariance matrix of random effects
- \triangleright $\varepsilon_i \in \mathbb{R}^{n_i}$ observation noise
- ▶ $\Lambda_i \in R^{n_i \times n_i}$ covariance matrix for noise

$$y_{i} = X_{i}\beta + Z_{i}u_{i} + \varepsilon_{i} \quad i = 1...m$$

$$\varepsilon_{i} \sim \mathcal{N}(0, \Lambda_{i})$$

$$u_{i} \sim \mathcal{N}(0, \Gamma)$$
(1)

- ▶ $X_i \in \mathbb{R}^{n_i \times p}$ fixed features, or covariates, $Z_i \in R^{n_i \times q}$ random features
- ightharpoonup p number of fixed features, q number of random effects.
- $\triangleright \beta \in \mathbb{R}^p$ fixed effects, or mean effects
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- ▶ $\Lambda_i \in R^{n_i \times n_i}$ covariance matrix for noise
- ▶ Unknowns: β, u_i , Γ, sometimes $Λ_i$.

$$y_{i} = X_{i}\beta + Z_{i}u_{i} + \varepsilon_{i} \quad i = 1 \dots m$$

$$\varepsilon_{i} \sim \mathcal{N}(0, \Lambda_{i})$$

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- ▶ $\Lambda_i \in R^{n_i \times n_i}$ covariance matrix for noise
- ▶ Unknowns: β, u_i , Γ, sometimes $Λ_i$.

$$\Gamma = \text{Diag}(\gamma), \ \gamma \in \mathbb{R}^q$$
 and Λ_i are known.

Likelihood for Mixed Models

Suppose we have a linear mixed effects model

$$Y_{i} = X_{i}\beta + Z_{i}u_{i} + \varepsilon_{i}$$

$$u_{i} \sim \mathcal{N}(0, \Gamma), \ \Gamma = \text{Diag } \gamma$$

$$\varepsilon_{i} \sim \mathcal{N}(0, \Lambda_{i})$$
(2)

where β , γ , and u_i are unknown model parameters, and λ_i are known. Noticing that $Z_i u_i + \varepsilon_i \sim \mathcal{N}(0, Z_i \Gamma Z_i^T + \Lambda_i)$ we get the negative log-likelihood:

$$\mathcal{L}(\beta, \gamma) = \sum_{i=1}^{m} \frac{1}{2} (y_i - X_i \beta)^T (Z_i \Gamma Z_i^T + \Lambda_i)^{-1} (y_i - X_i \beta) +$$

$$+ \frac{1}{2} \log \det (Z_i \Gamma Z_i^T + \Lambda_i)$$
(3)

Feature Selection for Mixed Models

Consider the following feature selection setup:

$$\min_{\beta,\gamma} \mathcal{L}(\beta,\gamma)$$
s.t. $\|\beta\|_0 \le k$

$$\|\gamma\|_0 \le j$$

$$\gamma \ge 0$$
(4)

where k and j is the size of the sparse support for the fixed and random effects respectively.

This is a very hard problem to solve directly.

There are several ways to address this setup:

(0) Exhaustive Search:

```
\begin{aligned} \min_{\beta,\gamma} \mathcal{L}(\beta,\gamma) \\ \text{s.t.} & & \|\beta\|_0 \leq k \\ & \|\gamma\|_0 \leq j \\ & \gamma \geq 0 \\ & \text{AIC [VB05]} \\ & \text{BIC [Jon11]} \end{aligned}
```

There are several ways to address this setup:

(0) Exhaustive Search:

(1)
$$\ell_1$$
-relaxation:

$$\begin{aligned} \min_{\beta,\gamma} \mathcal{L}(\beta,\gamma) & \min_{\beta,\gamma} \mathcal{L}(\beta,\gamma) \\ \text{s.t.} & \|\beta\|_0 \leq k & \text{s.t.} & \|\beta\|_1 \leq \lambda_\beta \\ & \|\gamma\|_0 \leq j & \|\gamma\|_1 \leq \lambda_\gamma \\ & \gamma \geq 0 & \gamma \geq 0 \end{aligned}$$
 AIC [VB05] M-ALASSO [BKG10] BIC [Jon11] ALASSO [LPJ13]

There are several ways to address this setup:

(0) Exhaustive Search:

$$\min_{\beta,\gamma} \mathcal{L}(\beta,\gamma)$$

s.t.
$$\|\beta\|_0 \le k$$

 $\|\gamma\|_0 \le j$
 $\gamma > 0$

(1)
$$\ell_1$$
-relaxation:

$$\begin{aligned} \min_{\beta,\gamma} \mathcal{L}(\beta,\gamma) \\ \text{s.t. } & \|\beta\|_1 \leq \lambda_{\beta} \\ & \|\gamma\|_1 \leq \lambda_{\gamma} \end{aligned}$$

$$\gamma \geq 0$$
 M-ALASSO [BKG10]

(3) Other types of sparsity-inducing penalties
$$(\ell_P, SCAD)$$
.

SCAD [FL01] SCAD-P [FL12]

There are several ways to address this setup:

(0) Exhaustive Search:

$$\begin{aligned} \min_{\beta,\gamma} \mathcal{L}(\beta,\gamma) \\ \text{s.t.} & & \|\beta\|_0 \leq k \\ & \|\gamma\|_0 \leq j \\ & \gamma > 0 \end{aligned}$$

(1)
$$\ell_1$$
-relaxation:

$$\min_{\beta,\gamma} \mathcal{L}(\beta,\gamma)$$
s.t. $\|\beta\|_{1} \leq \lambda_{\beta}$
 $\|\gamma\|_{1} \leq \lambda_{\gamma}$
 $\gamma \geq 0$

(3) Other types of sparsity-inducing penalties $(\ell_p, SCAD)$.

(2) SR3-type Relaxation [ZAB+19]

$$\min_{\beta,\gamma,\hat{\beta},\hat{\gamma}} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}\|_{2}^{2}$$
s.t. $\|\hat{\beta}\|_{0} \le k$

$$\|\hat{\gamma}\|_{0} \le j, \ \gamma \ge 0$$
(5)

$$\min_{\beta,\gamma,\hat{\beta},\hat{\gamma}} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}\|_{2}^{2}$$
s.t. $\|\hat{\beta}\|_{0} \le k$, $\|\hat{\gamma}\|_{0} \le j$

$$\gamma \ge 0, \ \hat{\gamma} \ge 0$$
(6)

We'll find β^* , γ^* , $\hat{\beta}^*$, and $\hat{\gamma}^*$ via alternating partial minimization:

$$\min_{\beta,\gamma,\hat{\beta},\hat{\gamma}} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}\|_{2}^{2}$$
s.t. $\|\hat{\beta}\|_{0} \le k$, $\|\hat{\gamma}\|_{0} \le j$

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We'll find β^* , γ^* , $\hat{\beta}^*$, and $\hat{\gamma}^*$ via alternating partial minimization:

Minimization w.r.t. β and γ is done via **Interior Point Method**.

$$\min_{\beta,\gamma,\hat{\beta},\hat{\gamma}} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}\|_{2}^{2}$$
s.t. $\|\hat{\beta}\|_{0} \le k$, $\|\hat{\gamma}\|_{0} \le j$

$$\gamma \ge 0, \ \hat{\gamma} \ge 0$$
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We'll find β^* , γ^* , $\hat{\beta}^*$, and $\hat{\gamma}^*$ via alternating partial minimization:

- Minimization w.r.t. β and γ is done via **Interior Point Method**.
- ▶ Minimization w.r.t. $\hat{\beta}$ and $\hat{\gamma}$ is **projection** of β and γ onto ℓ_0 -balls.

$$\hat{\beta}^{(k+1)} \leftarrow \underset{\|\beta\|_{\mathbf{0}} \le k}{\operatorname{Proj}} (\beta^{(k)}) \quad \Longrightarrow \quad \text{Take max k from } \beta, \text{ rest to 0}$$

$$\hat{\gamma}^{(k+1)} \leftarrow \underset{\|\gamma\|_{\mathbf{0}} < s}{\operatorname{Proj}} (\gamma^{(k)}) \quad \Longrightarrow \quad \text{Take max j from } \gamma, \text{ rest to 0}$$

$$\min_{\beta,\gamma,\hat{\beta},\hat{\gamma}} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}\|_{2}^{2}$$
s.t. $\|\hat{\beta}\|_{0} \le k$, $\|\hat{\gamma}\|_{0} \le j$

$$\gamma \ge 0, \ \hat{\gamma} \ge 0$$
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- ▶ Minimization w.r.t. $\hat{\beta}$ and $\hat{\gamma}$ is **projection** of β and γ onto ℓ_0 -balls.
- λ_{β} and λ_{γ} are iteratively increased until $\hat{\beta} \approx \beta$ and $\hat{\gamma} \approx \gamma$.

$$\min_{\beta,\gamma,\hat{\beta},\hat{\gamma}} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}\|_{2}^{2}$$
s.t. $\|\hat{\beta}\|_{0} \le k$, $\|\hat{\gamma}\|_{0} \le j$

$$\gamma \ge 0, \ \hat{\gamma} \ge 0$$
(6)

We'll find β^* , γ^* , $\hat{\beta}^*$, and $\hat{\gamma}^*$ via alternating partial minimization:

- Minimization w.r.t. β and γ is done via **Interior Point Method**.
- Minimization w.r.t. $\hat{\beta}$ and $\hat{\gamma}$ is **projection** of β and γ onto ℓ_0 -balls.
- $ightharpoonup \lambda_{\beta}$ and λ_{γ} are iteratively increased until $\hat{\beta} \approx \beta$ and $\hat{\gamma} \approx \gamma$.

Advantages:

- 1. Interpretable hyperparameters.
- 2. No model bias when the k-subspace is chosen.

The pseudocode of the proposed algorithm:

```
\begin{array}{l} 1 \\ \lambda_{\beta} = 0; \ \lambda_{\gamma} = 0 \\ \text{repeat} \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ \text{until } \frac{\beta^{(k+1)} \leftarrow \Pr{\text{oj}}_{\parallel\beta\parallel_{\mathbf{0}} \leq k}(\beta^{(k)})}{\beta^{(k+1)} \leftarrow \Pr{\text{oj}}_{\parallel\gamma\parallel_{\mathbf{0}} \leq s}(\gamma^{(k)})} \\ \beta^{(k+1)} \leftarrow \Pr{\text{oj}}_{\parallel\gamma\parallel_{\mathbf{0}} \leq s}(\gamma^{(k)}) \\ \beta^{(k+1)}, \gamma^{(k+1)} \leftarrow \operatorname{argmin}_{\gamma \geq \mathbf{0}, \beta} \mathcal{L}(\beta, \gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}^{(k)}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}^{(k)}\|_{2}^{2} \\ \text{until } \frac{1}{\hat{\beta} \approx \beta, \hat{\gamma} \approx \gamma}; \end{array}
```

Performance in Comparison to Other Algorithms

▶ Scenario 1: n = 30, $n_i = 5$, p = 9, q = 4, with true parameters $\beta = (1, 1, 0, ..., 0)$ and the covariance matrix Γ being:

$$\Gamma = \begin{bmatrix} 9 & 4.8 & 0.6 & 0 \\ 4.8 & 4 & 1 & 0 \\ 0.6 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$
 (7)

Scenario 2: everything as in Scenario 1, but n = 60 and $n_i = 10$.

Competitors:

- ► ALASSO: 2 stage: A-LASSO+Newton and A-LASSO+PCO
- ► M-ALASSO: Adaptive LASSO + EM Algorithm
- **SCAD-P:** SCAD + Proxy Matrix for Γ
- rPQL: Quasi-Likelihood + Adaptive LASSO (for GLMMs)

Performance in Comparison to Other Algorithms

Setup	Algoritm	% C	% CF	% CR	MSE	TIME
$n = 30, n_i = 5$	R&S-Mixed	58	72	78	0.66	0.015
	rPQL	88	98	88	0.88	26-59
	M-ALASSO	71	73	79	-	-
	ALASSO	79	81	96	-	-
	SCAD-P	-	90	86	-	-
$n = 60, n_i = 10$	R&S-Mixed	98	100	98	0.69	0.018
	rPQL	98	99	98	0.97	26-59
	M-ALASSO	83	83	89	-	-
	ALASSO	95	96	99	-	-
	SCAD-P	100	100	100	-	-

Table: Comparison of feature selection algorithms. % CF – percent of models where true fixed effects were identified correctly, % CR – percent of models where true random effects were identified correctly, % C – both fixed and random effects were identified correctly.

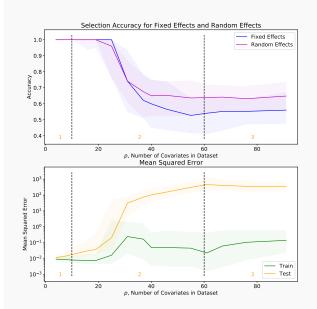
Scalability Experiment

- $n = 60, n_i = 10$
- ▶ $p = q \in [4, 7, 10, ..., 90]$, 200 experiments for each.
- $ightharpoonup X_i = Z_i$, columns are drawn form $\mathcal{N}(0, \Psi)$ where

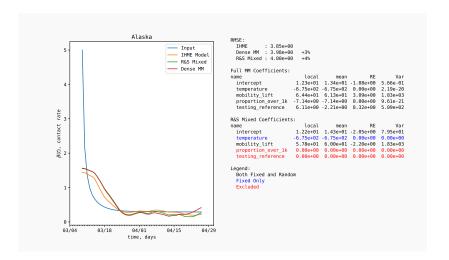
$$\Psi = \begin{bmatrix} 9 & 4.8 & 0.6 \\ 4.8 & 4 & 1 \\ 0.6 & 1 & 1 \end{bmatrix}$$

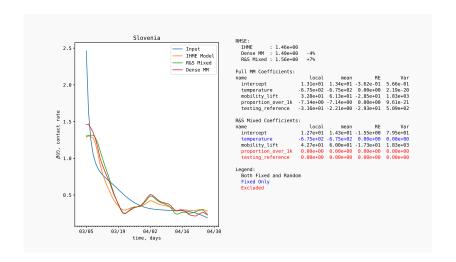
- ▶ 50% random coordinate in β are active
- \triangleright 70% of those are also active in γ

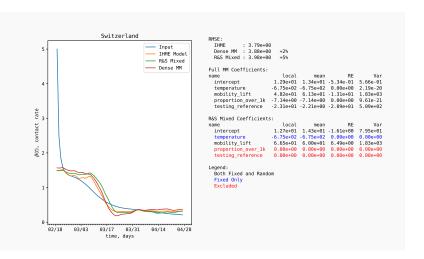
Scalability Experiment

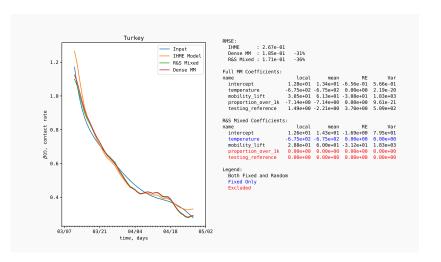


- ▶ n = 60 groups (countries and US states), $n_i \approx 50$
- ▶ Y_i contact rate for COVID SEIIR Model
- ho = q = 5 covariates related to temperature, mobility, population, testing; plus intercept.





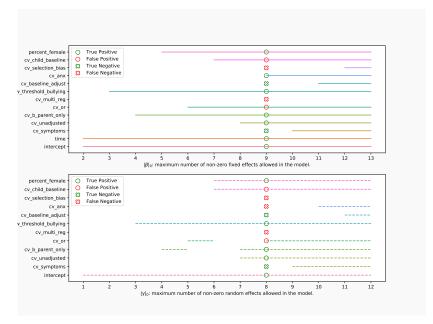




Burden of Anxiety and Depression as Result of Bullying

- ightharpoonup m = 10 cohort studies, n = 77, highly unbalanced
- ightharpoonup p = 13, q = 12 (time was preselected fixed-only)
- Covariates are related to studies' designs.

Burden of Anxiety and Depression as Result of Bullying



Future Work: Theory

Theorem (Conditions for Convergence to True Estimator)

Under certain conditions the method converges in a finite number of iterations to $(\hat{\beta}, \hat{\gamma})$ which projections $(\hat{\beta}, \hat{\gamma})$ belong to a k- and j-subspaces respectively that contain the true minimum (β^*, γ^*) .

Theorem (Consistency of Estimator)

There exists a local minimizer $(\hat{\beta}, \hat{\gamma})$ for the proposed loss function, such that it is asymptotically consistent with true minimum (β^*, γ^*) .

Theorem (Consistency in Zeros)

If some coordinates of the true minimizer (β^*, γ^*) are zero, then it is also zero in $(\hat{\beta}, \hat{\gamma})$, given that the later is sufficiently close to the former.

Theorem (Asymptotic Normality)

The proposed estimator $(\hat{\beta}, \hat{\gamma})$ asymptotically normally distributed around true minimizer (β^*, γ^*) in its true non-zero k+j-subspace.

Future work: Algorithm

Question: Will exponential smoothing of projection improve the accuracy?

```
 \begin{array}{l} 1 \\ \lambda_{\beta} = 0; \ \lambda_{\gamma} = 0 \\ \\ \text{repeat} \\ 3 \\ 4 \\ \lambda_{\gamma} \leftarrow 2(1+\lambda_{\beta}) \\ \lambda_{\gamma} \leftarrow 2(1+\lambda_{\gamma}) \\ \text{repeat} \\ 6 \\ 6 \\ 7 \\ 8 \\ 9 \\ \text{until } \frac{\hat{\beta}^{(k+1)} \leftarrow \delta \Pr{j_{\parallel\beta\parallel_{\mathbf{0}} \leq k}(\beta^{(k)}) + (1-\delta)\hat{\beta}^{(k)}}}{\hat{\beta}^{(k+1)} \leftarrow \delta \Pr{j_{\parallel\gamma\parallel_{\mathbf{0}} \leq s}(\gamma^{(k)}) + (1-\delta)\hat{\gamma}^{(k)}}} \\ \beta^{(k+1)} \leftarrow \delta \Pr{j_{\parallel\gamma\parallel_{\mathbf{0}} \leq s}(\gamma^{(k)}) + (1-\delta)\hat{\gamma}^{(k)}} \\ \beta^{(k+1)}, \gamma^{(k+1)} \leftarrow \operatorname{argmin}_{\gamma\geq\mathbf{0},\beta} \mathcal{L}(\beta,\gamma) + \frac{\lambda_{\beta}}{2} \|\beta - \hat{\beta}^{(k)}\|_{2}^{2} + \frac{\lambda_{\gamma}}{2} \|\gamma - \hat{\gamma}^{(k)}\|_{2}^{2} \\ \text{until } \frac{\hat{\beta} \approx \beta, \hat{\gamma} \approx \gamma}{2}; \end{array}
```

Future Work: Implementation

Can we increase λ_{β} and λ_{γ} in a more careful way to avoid potential stacking? The approach can be based on the theorem:

Theorem (Distance Between Minima)

For a fixed dataset (X_i,Y_i) and relaxation parameters λ_{β} , λ_{γ} the distance between (β^*,γ^*) , the unconstrained minimizers of relaxed problem, and their projections $(\hat{\beta}^*,\hat{\gamma}^*)$ is bounded by a constant M depending on (X_i,Y_i) and the relaxation parameters.

The End

Thank you for your attention!

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