A Relaxation Approach to Feature Selection for Linear Mixed-Effects Models

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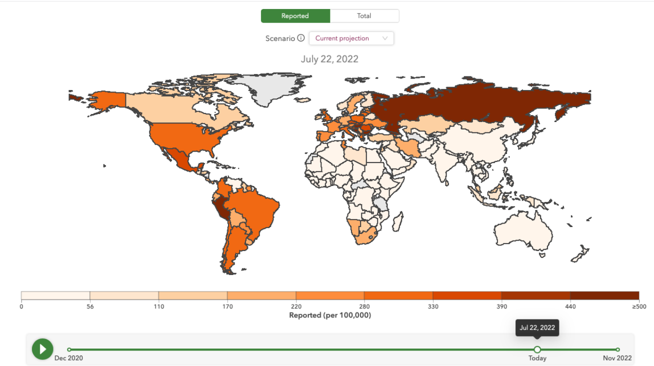
IHME

Mixed-Effect Models

- Used for analyzing **combined data** across a range of **groups**.
- Use covariates to separate the **population variability** from the **group variability**.
- **Borrow strength** across groups to estimate key statistics.
- Often seek **sparse models** that only use **most informative** covariates.



[1]

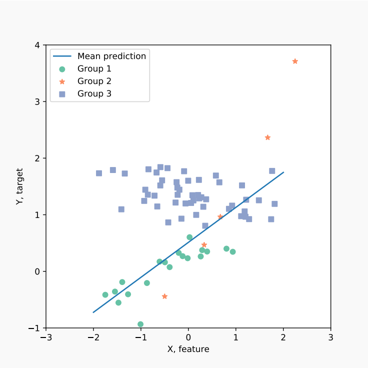
[1] Picture is taken from covid19.healthdata.org

Linear Mixed-Effect (LME) Models

Dataset: m groups (X_i, Z_i, y_i), $\quad i = 1, \ldots m$, each has n_i observations

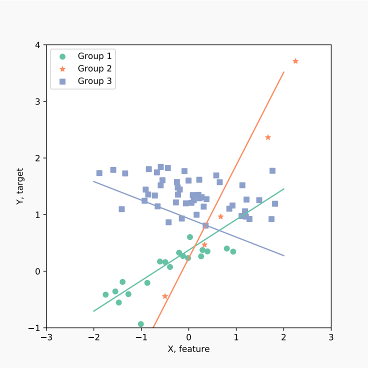
- $X_i \in \mathbb{R}^{n_i \times p}$ – group i design matrix for fixed features
- $Z_i \in \mathbb{R}^{n_i \times q}$ – group i design matrix for random effects
- $y_i \in \mathbb{R}^{n_i}$ – group i observations

Standard Linear Regression:



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

Linear Mixed-Effect Model:



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

Notation

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

- p – number of fixed features, q – number of random effects.
- $\beta \in \mathbb{R}^p$ – fixed effects, or mean effects
- $u_i \in \mathbb{R}^q$ – random effects
- $\Gamma \in \mathbb{R}^{q \times q}$ – covariance matrix of random effects, often $\Gamma = \mathrm{Diag}\,(\gamma)$
- $\varepsilon_i \in \mathbb{R}^{n_i}$ – observation noise
- $\Lambda_i \in R^{n_i \times n_i}$ – covariance matrix for noise

Unknowns: β, u_i, γ, sometimes Λ_i.

Likelihood for Mixed Models

Negative log-likelihood:

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

Maximum likelihood estimates for β and γ solve the problem:

$$\mathcal{LME} \quad \min_{\beta\in\mathbb{R}^p,\, \gamma\in\mathbb{R}^q_+} \mathcal{L}(\beta,\gamma) \tag{3}$$

To select covariates we add a sparsity-promoting regularizer $R(\beta,\gamma)$

$$\mathcal{FS} - \mathcal{LME} \quad \min_{\beta\in\mathbb{R}^p,\, \gamma\in\mathbb{R}^q_+} \mathcal{L}(\beta,\gamma) + R(\beta,\gamma) \tag{4}$$

- $\mathcal{L}(\beta,\gamma)$ is smooth on its domain, quadratic w.r.t. β and $\bar{\eta}$-weakly-convex w.r.t. γ.
- $R(\beta,\gamma)$ is closed, proper, convex, with easily computed *prox operator*

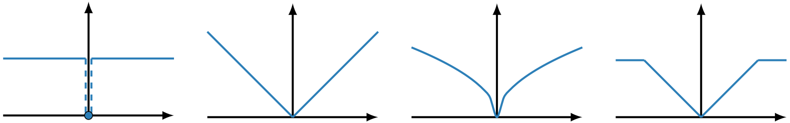
Regularization

- $R(\beta, \gamma)$ is closed, proper, with easily computed *prox operator*

$$\operatorname{prox}_{\alpha R + \delta_{\mathcal{C}}}(\tilde{\beta}, \tilde{\gamma}) := \underset{(\beta,\gamma)\in\mathcal{C}}{\operatorname{argmin}}\ R(\beta, \gamma) + \frac{1}{2\alpha}\|(\beta, \gamma) - (\tilde{\beta}, \tilde{\gamma})\|_2^2, \quad \text{where } \mathcal{C} := \mathbb{R}^p \times R_+^q \tag{5}$$

Examples:

- $R(x) = \lambda \sum_{j=1}^{p} w_j \|x_j\|_1$ – LASSO and Adaptive LASSO penalties [1, 5]
- $R(x) = \lambda \|x\|_0$ – ℓ_0 penalty [6, 4]
- $R(x)$ – SCAD penalty ([2, 3])



(a) ℓ_0 (b) ℓ_1 (c) $\ell_p,\ p = 1/2$ (d) SCAD

Figure: Four commonly-used regularizers which promote sparsity

SR3-Relaxation for Mixed-Effect Models ($\mathcal{MSR}3$)

Original problem $\mathcal{FS} - \mathcal{LME}$:

$$\min_{\beta\in\mathbb{R}^p,\, \gamma\in\mathbb{R}^q_+} \mathcal{L}(\beta,\gamma) + R(\beta,\gamma) \tag{6}$$

Relaxed problem $\mathcal{MSR}3$:

$$\min_{\beta,\tilde\beta\in\mathbb{R}^p,\, \gamma,\tilde\gamma\in\mathbb{R}^q_+} \mathcal{L}(\beta,\gamma) + \phi_\mu(\gamma) + \kappa_\eta(\beta-\tilde\beta, \gamma-\tilde\gamma) + R(\tilde\beta,\tilde\gamma) \tag{7}$$

where the *relaxation* κ_η decouples the likelihood and the regularizer

$$\kappa_\eta(\beta-\tilde\beta,\gamma-\tilde\gamma) := \frac{\eta}{2}\|\beta-\tilde\beta\|_2^2 + \frac{\eta}{2}\|\gamma-\tilde\gamma\|_2^2, \quad \eta > \bar\eta \tag{8}$$

and the *perspective mapping* ϕ_μ replaces $\gamma \geq 0$ with a log-barrier

$$\phi_\mu(\gamma) := \begin{cases} -\mu\sum_{i=1}^q \ln(\gamma_i/\mu), & \mu > 0 \\ \delta_{\mathbb{R}^q_+}(\gamma), & \mu = 0 \\ +\infty, & \mu < 0 \end{cases} \tag{9}$$

Value Function Reformulation

$\mathcal{MSR}3$-relaxation replaces the original likelihood $\mathcal{L}$ with a *value function* $u_{\eta,\mu}$:

$$\begin{aligned} u_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) &:= \min_{(\beta,\gamma)} \mathcal{L}_{\eta,\mu}((\beta,\gamma),(\tilde{\beta},\tilde{\gamma})) \\ &:= \min_{(\beta,\gamma)} \mathcal{L}(\beta,\gamma) + \phi_\mu(\gamma) + \kappa_\eta(\beta-\tilde{\beta},\gamma-\tilde{\gamma}) \end{aligned} \tag{10}$$

so $\mathcal{MSR}3$-formulation (7) becomes

$$\min_{(\tilde{\beta},\tilde{\gamma})\in\mathcal{C}} u_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) + R(\tilde{\beta},\tilde{\gamma}) \tag{11}$$

When η is larger than the weak-convexity constant

- $u_{\eta,\mu}$ is well-defined and continuously differentiable.
- As $\mu \to 0$ and $\eta \to \infty$, cluster points of solutions to $\mathcal{MSR}3$ are first-order stationary points for $\mathcal{FS}-\mathcal{LME}$

Key observation: in practice, we don't need accurate solutions for (10): a few Newton iterations keep the solution close to the central path.

Value Function Reformulation

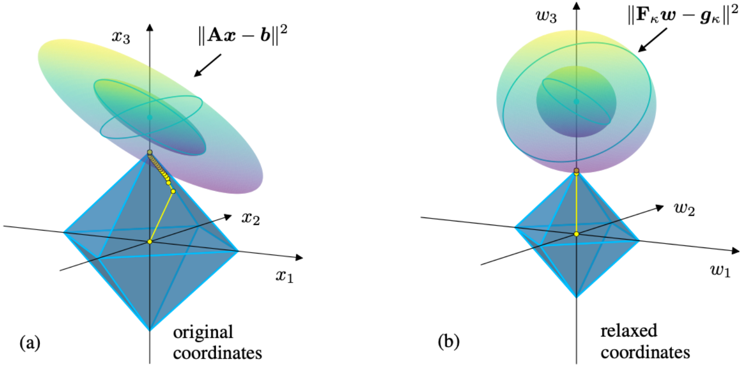


Figure: Picture from [7]: for a linear problem, value function relaxation "squashes" level-sets simplifying the optimization landscape.

Value Function Reformulation

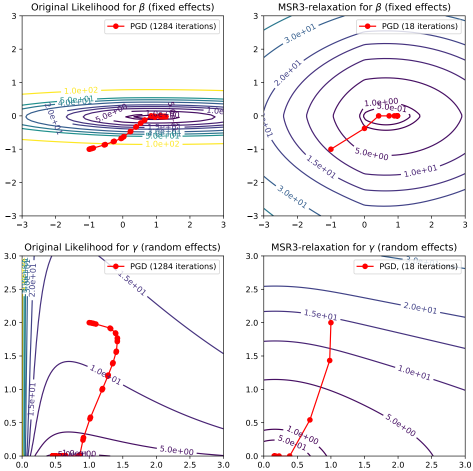


Figure: Comparison of the level-sets for the original likelihood (left) and $\mathcal{MSR}3$-likelihood (right), for fixed (top) and random (bottom) effects.

Designing an Algorithm

$G_{\nu,\eta}$ encodes both gradient of a Lagrangian (lines 1-2) and the complementarity condition (line 3):

$$G_{\nu,\eta}((\beta,\gamma,v),(\tilde{\beta},\tilde{\gamma})) := \begin{bmatrix} \nabla_\beta \mathcal{L}(\beta,\gamma) + \eta(\beta - \tilde{\beta}) \\ \nabla_\gamma \mathcal{L}(\beta,\gamma) + \eta(\gamma - \tilde{\gamma}) - v \\ v \bigodot \gamma - \mu \mathbf{1} \end{bmatrix} \tag{12}$$

We apply Newton method to G while geometrically decreasing μ.
Lemma: For every $(\mu,\eta) \in \mathbb{R}_+ \times \mathbb{R}_{++}$,

$$\begin{gathered} (\hat{\beta},\hat{\gamma}) = \operatorname*{argmin}_{(\beta,\gamma)} \mathcal{L}_{\eta,\mu}((\beta,\gamma),(\tilde{\beta},\tilde{\gamma})) \\ \iff \\ \exists \hat{v} \in \mathbb{R}^q_+ \text{ s.t. } G_{\nu,\eta}((\beta,\gamma,\hat{v}),(\tilde{\beta},\tilde{\gamma})) = 0 \end{gathered} \tag{13}$$

If $\mu > 0$, then $\hat{v} = -\nabla\phi_\mu(\hat{\gamma})$, and if $\mu = 0$, then $\hat{v}$ is the unique KKT multiplier associated with the constraint $0 \leq \gamma$.

$\mathcal{MSR}$3-fast Algorithm

$\texttt{progress} \leftarrow$ **True**; $\texttt{iter = 0}$;

$\beta^+, \tilde{\beta}^+ \leftarrow \beta_0$; $\gamma^+, \tilde{\gamma}^+ \leftarrow \gamma_0$; $v^+ \leftarrow 1 \in \mathbb{R}^q$; $\mu \leftarrow \frac{{v^+}^T \gamma^+}{10q}$

while $\underline{\texttt{iter} < \texttt{max\_iter and } \|G_\mu(\beta^+, \gamma^+, v^+)\| > \texttt{tol and progress}}$ **do**

$\quad \beta \leftarrow \beta^+$; $\gamma \leftarrow \gamma^+$; $\tilde{\beta} \leftarrow \tilde{\beta}^+$; $\tilde{\gamma} \leftarrow \tilde{\gamma}^+$

$\quad [dv, d\beta, d\gamma] \leftarrow \nabla G_\mu((\beta, \gamma, v), (\tilde{\beta}, \tilde{\gamma}))^{-1} G_\mu((\beta, \gamma, v), (\tilde{\beta}, \tilde{\gamma}))$

$\quad \alpha \leftarrow 0.99 \times \min\left(1, -\frac{\gamma_i}{d\gamma_i}, \forall i: \ d\gamma_i < 0\right)$

$\quad \beta^+ \leftarrow \beta + \alpha d\beta$; $\gamma^+ = \gamma + \alpha d\gamma$; $v^+ \leftarrow v + \alpha dv$

$\quad$ **if** $\underline{\|\gamma^+ \odot v^+ - q^{-1} {\gamma^+}^T v^+ 1\| > 0.5 q^{-1} {v^+}^T \gamma^+}$ **then** continue;

$\quad$ **else**

$\quad\quad \tilde{\beta}^+ = \text{prox}_{\alpha R}(\beta^+)$; $\tilde{\gamma}^+ = \text{prox}_{\alpha R + \delta_{\mathbb{R}_+}}(\gamma^+)$; $\mu = \frac{1}{10} \frac{{v^+}^T \gamma^+}{q}$

$\quad$ **end**

$\quad \texttt{progress} = (\|\beta^+ - \beta\| \geq \text{tol or } \|\gamma^+ - \gamma\| \geq \text{tol or } \|\tilde{\beta}^+ - \tilde{\beta}\| \geq \text{tol or } \|\tilde{\gamma}^+ - \tilde{\gamma}\| \geq \text{tol})$

$\quad \texttt{iter += 1}$

end

return $\underline{\tilde{\beta}^+, \tilde{\gamma}^+}$

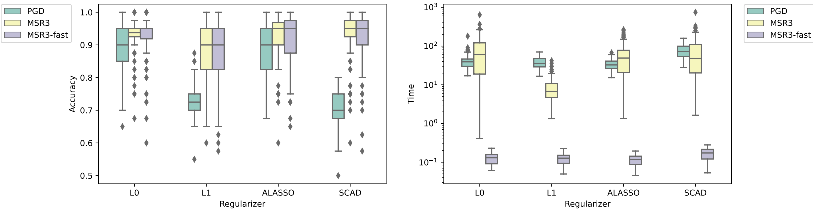
Application to Synthetic Problems

The Experiment

- The number of fixed effects p and random effects q is 20.
- $\beta = \gamma = \frac{1}{2}[1, 2, 3, \ldots, 10, 0 \ldots, 0]$
- 9 groups with sizes [10, 15, 4, 8, 3, 5, 18, 9, 6]
- $X_i \sim \mathcal{N}(0, I)^p$, $Z_i = X_i$, $\varepsilon_i \sim \mathcal{N}(0, 0.3^2 I)$
- Each experiment is repeated 100 times.
- Grid-search for $\eta \in [10^{-4}, 10^2]$, golden search for $\lambda \in [0, 10^5]$
- Final model is chosen to maximize BIC

Regularizer	Model Metric	PGD	MSR3	MSR3-fast
L0	Accuracy	0.89	**0.92**	**0.92**
	Time	41.68	88.54	**0.13**
L1	Accuracy	0.73	**0.88**	**0.88**
	Time	38.39	9.13	**0.13**
ALASSO	Accuracy	0.88	**0.92**	0.91
	Time	34.55	65.19	**0.12**
SCAD	Accuracy	0.71	**0.93**	0.92
	Time	77.62	84.67	**0.17**

Application to Synthetic Problems



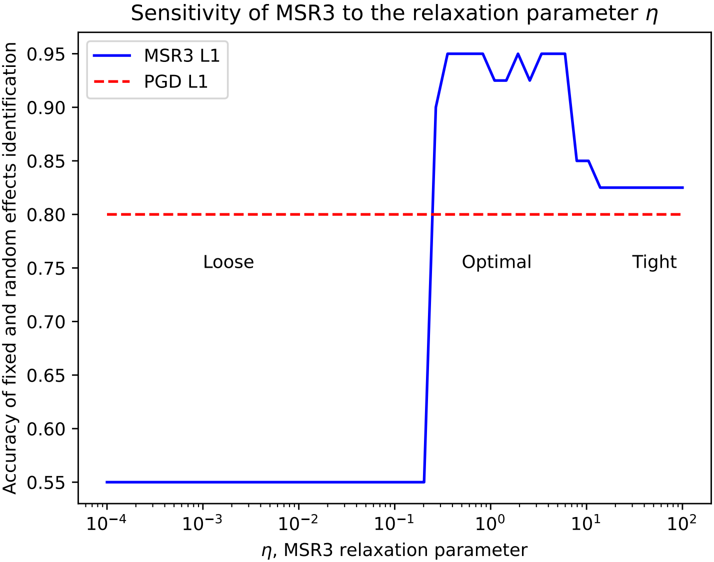
Benefits:

- $\mathcal{MSR}3$-relaxation improves feature selection performance than the original likelihood.
- $\mathcal{MSR}3$-fast optimization accelerates the compute time by $\sim 10^2$.

Challenge:

- Initialization of η is problem-specific

Choice of η



ℓ_0-based Covariate Selection for Bullying Study from GBD

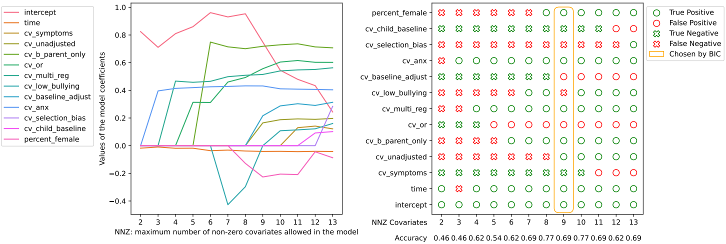


Figure: Fixed and random covariate selection for Bullying dataset from [?]. The model selected 9 covariates, 7 of which were historically significant, and did not select 4 covariates, 1 of which was historically significant.

Thank You!

The code is available on GitHub: https://github.com/aksholokhov/pysr3

- All estimators are fully compatible to `sklearn` library.
- Implements SR3 for linear, generalized-linear, and linear mixed-effect models.
- Has tutorials, tests, and documentation.

References

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