An algorithm for high-dimensional generalized linear mixed models using ℓ_1 -penalization

Jürg Schelldorfer

joint work with Peter Bühlmann

encouraged by Stephan Dlugosz

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data set of Stephan Dlugosz:

administrative data set about employment:

Binary response variable $Y \in \{\text{employed}, \text{unemployed}\}$

covariates X: income, sex, age group, employment duration,....

quarterly results of (Y, X) of many workers over several years

- response variable from the exponential family
- continuous covariates
- grouped observations (think of longitudinal data, repeated measures data)

Goal:

Performing variable selection in the setup where AIC, BIC, cAIC, mAIC, ... are computationally infeasible (i.e. $n \approx p, n \ll p$)

Table of Contents



2 High-dimensional Generalized Linear Mixed Models

Computational Algorithm



	n > p	n ≪ p
Generalized Linear Models (GLMs)	MLE [IRLS]	Lasso [R:glmnet]
Generalized Linear Mixed Models (GLMMs)	MLE [R:glmer]	?

n: number of observations p: number of variables

Generalized Linear Model (GLM)

For *n* observations (y_i, x_i^T)

- (y_i, x_i^T) are independent for i = 1, ..., n
- y_i has a density of the form

$$\exp\left\{\phi^{-1}\left(y_i\xi_i-b(\xi_i)\right)+c(y_i,\phi)\right\} \text{with } \boldsymbol{\mu}_i=\mathbb{E}[y_i]$$

•
$$g(\mu) = \eta$$
 with $\eta = \pmb{X}eta$

Then estimate β by

$$\hat{eta}_{\mathsf{MLE}} = \operatorname{argmin}_{eta} - \ell(eta)$$

For $n \ll p$ we should not use the MLE. Use the Lasso (Tibshirani, 1996)

$$\hat{\boldsymbol{\beta}}(\lambda) = \operatorname{argmin}_{\boldsymbol{\beta}} - \ell(\boldsymbol{\beta}) + \lambda \|\boldsymbol{\beta}\|_{1} \quad , \quad \lambda > 0$$

with the following properties:

- The Lasso does variable selection (i.e. some coefficients are set exactly to zero)
- Convex optimiziation problem, which can be solved efficiently

Generalized Linear Mixed Model (GLMM)

g = 1, ..., N independent groups/clusters/subjects $j = 1, ..., n_g$ observations for group/cluster/subject g $n = \sum_{g=1}^{N} n_g$ total number of observations

- *y* : *n*-dim response variable *b* : *q*-dim (correlated) random effects
- $\beta \in \mathbb{R}^{\rho}$ fixed-effects parameters $\theta \in \mathbb{R}^{L}$ covariance parameters ϕ dispersion parameter
- $\boldsymbol{X}: \boldsymbol{n} \times \boldsymbol{p}$ model matrix for $\boldsymbol{\beta}$
- $\boldsymbol{Z}: \boldsymbol{n} \times \boldsymbol{q}$ model matrix for \boldsymbol{b}
- ${old \Sigma}_{oldsymbol{ heta}}: q imes q$ covariance matrix, determined by ${oldsymbol{ heta}}$

Generalized Linear Mixed Model (GLMM)

Model Assumptions:

- $y_i | \boldsymbol{b}$ are independent for $i = 1, \dots, n$
- $y_i | \boldsymbol{b}$ has a density of the form

$$\exp\left\{\phi^{-1}\left(y_{i}\xi_{i}-b(\xi_{i})\right)+c(y_{i},\phi)\right\} \text{ with } \boldsymbol{\mu}_{i}=\mathbb{E}[y_{i}|\boldsymbol{b}]$$

•
$$g(\mu) = \eta$$
 with $\eta = Xeta + Zb$
• $b \sim \mathcal{N}_q(\mathbf{0}, \Sigma_{m{ heta}})$ with $\Sigma_{m{ heta}} \geq 0$ for $m{ heta} \in \mathbb{R}^L$

$$(\hat{eta}, \hat{m{ heta}}, \hat{\phi})_{\textit{MLE}} = argmin_{m{eta}, m{ heta}, \phi} - \log L(m{eta}, m{ heta}, \phi)$$

	n > p	n ≪ p
Generalized Linear Models (GLMs)	MLE [IRLS] 🖌	Lasso [R:glmnet] 🗸
Generalized Linear Mixed Models (GLMMs)	MLE [R:glmer]✔	ļ

Additionally to a GLMM, assume

•
$$n = \sum_{i=1}^{N} n_g \ll p$$

• the true β_0 is sparse

L small

Aim: Estimate β , θ , ϕ and predict **b**

Keyldea 1: Lasso-type penalty

Estimate the parameters (β, θ, ϕ) by minimizing

$$egin{aligned} & \mathcal{Q}_{\lambda}(oldsymbol{eta},oldsymbol{ heta},\phi) &:= -2\log L(oldsymbol{eta},\phi) + \lambda \|oldsymbol{eta}\|_{1}, \ & (\hat{oldsymbol{eta}},\hat{oldsymbol{ heta}},\hat{oldsymbol{\phi}}) &:= extsf{argmin}_{oldsymbol{eta},oldsymbol{ heta},\phi} & \mathcal{Q}_{\lambda}(oldsymbol{eta},oldsymbol{ heta},\phi). \end{aligned}$$

Remark: In general, $L(\beta, \theta, \phi)$ cannot be computed explicitly.

Keyldea 2: Laplace approximation to approximate the integrand of $L(\beta, \theta, \phi)$ by a quadratic function.

$$I = \int_{\mathbb{R}^q} e^{-S(\boldsymbol{b})} d\boldsymbol{b} pprox (2\pi)^{q/2} |S''(\tilde{\boldsymbol{b}})|^{-1/2} e^{-S(\tilde{\boldsymbol{b}})}$$

where $\tilde{\boldsymbol{b}} = argmin_{\boldsymbol{b}}S(\boldsymbol{b})$ is the mode of $-S(\boldsymbol{b})$.

Hence

$$oldsymbol{Q}_{\lambda}(oldsymbol{eta},oldsymbol{ heta},\phi) \rightsquigarrow ilde{oldsymbol{Q}}_{\lambda}^{Loldsymbol{A}}(oldsymbol{eta},oldsymbol{ heta},\phi)$$

The GLMMLasso estimator is defined by

$$(\hat{oldsymbol{eta}},\hat{oldsymbol{ heta}},\hat{oldsymbol{ heta}}):= argmin_{oldsymbol{eta},oldsymbol{ heta},\phi} ilde{oldsymbol{Q}}_{\lambda}^{L\!oldsymbol{A}}(oldsymbol{eta},oldsymbol{ heta},\phi)$$

Remark: It is a non-convex optimization problem!

How to calculate

$$(\hat{oldsymbol{eta}}, \hat{oldsymbol{ heta}}, \hat{oldsymbol{ heta}}) := argmin_{oldsymbol{eta}, oldsymbol{ heta}, \phi} ilde{oldsymbol{Q}}_{\lambda}^{LA}(oldsymbol{eta}, oldsymbol{ heta}, \phi)?$$

Keyldea 3: coordinate-wise optimization with inexact line search ,

i.e. optimize \tilde{Q}_{λ}^{LA} w.r.t. one coordinate keeping all other coordinates fixed (Tseng and Yun, 2009):

- Quadratic approximation of the objective function
- calculate the gradient
- Inexact line search using the Armijo rule

The GLMMLasso algorithm II

GLMMLasso algorithm

(0) Choose a starting value $(\beta^{(0)}, \theta^{(0)}, \phi^{(0)})$.

Repeat for s = 1, 2, ...

- (1) (Fixed-effects parameter optimization) For k = 1, ..., p
 - a) (Laplace approximation) Calculate the Laplace approximation $\tilde{Q}_{\lambda}^{LA}(.,.,.)$
 - b) (Quadratic approximation and inexact line search)
 - i) Approximate the second derivative by $h_k^{(s)} > 0$.
 - ii) Calculate the descent direction $d_k^{(s)} \in \mathbb{R}$
 - iii) Choose a step size $\alpha_k^{(s)} > 0$ such that there is a decrease in the objective function.

(2) (Covariance parameter optimization) For I = 1, ..., L

$$\theta_l^{(s)} = \textit{argmin}_{\theta_l} \tilde{\textit{Q}}_{\lambda}^{\textit{LA}}(.,.,.)$$

(3) (Dispersion parameter optimization)

$$\phi^{(s)} = \operatorname{argmin}_{\phi} \tilde{Q}_{\lambda}^{LA}(.,.,.)$$

until convergence.

Tools to speed up

Two ingredients which speed up the algorithm remarkably:

- **Keyldea 4a**: regard $\tilde{\boldsymbol{b}}$ as fixed for the quadratic approximation w.r.t. β_k
- **Keyldea 4b**: active-set algorithm cycle through the non-zero coefficients β_k , and only through all *p* coefficients every *D*th iteration

This two ingredients make it feasable to calculate large data sets (i.e. n = 400 and p = 4000)!

Small additional bias in the parameter estimates, and similar variable selection properties.

This is ongoing work with Stephan Dlugosz on administrative data.

Take-home message

	<i>n</i> > <i>p</i>	n≪p
Generalized Linear	MLE	Lasso
Models (GLMs)	[IRLS]	[R:glmnet]
Generalized Linear	MLE	GLMMLasso
Mixed Models (GLMMs)	[R:glmer]	Keyldea 1-4

Thank you!

Questions?

- P. Tseng and S. Yun ; A Coordinte Gradient Descent Method for Nonsmooth Separable Minimization ; Mathematical Programming (2009)
- R. Tibshirani ; Regression Shrinkage and Selection via the Lasso ; J. R. Stat. Soc. (1996)
- J. Schelldorfer, P. Bühlmann and S. van de Geer ; Estimation for High-Dimensional Linear Mixed-Effects Models Using ℓ_1 -penalization ; The Scandinavian Journal of Statistics (2011)
- D. Bates ; Ime4: Mixed-effects modeling with R (to appear)