APES: Approximated Exhaustive Search for GLM

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Acknowledgement

- This is joint work with Prof Samuel Müller, Dr Garth Tarr and Prof Jean Yang.
- `mplot` Tarr2018 is a package to assess model stability and variable selection for linear models and generalised linear models.

Background

Data and models

- $\boldsymbol{y} = (y_1, y_2, \ldots, y_n)^\top$, with independent $y_i \in \{0, 1\}$, $i = 1, \ldots, n$.
- Design matrix $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_p) \in \mathbb{R}^{n \times p}$.
- Index the columns of $\boldsymbol{X}$ by $\{1, \ldots, p\}$.
- Let α denote any subset of p_α distinct elements from $\{1, \ldots, p\}$. Use $\mathcal{A}$ to denote the collection of all α, so $|\mathcal{A}| = 2^p$.
- $\boldsymbol{X}_\alpha$ denote the $n \times p_\alpha$ matrix with columns given by the columns of $\boldsymbol{X}$ whose indices appear in α.

Logistic regression

- We model the conditional response variable $Y_i|\boldsymbol{X}$ as $\mathrm{Bernoulli}(\pi_i)$, where $\pi_i = \mathbb{P}(Y_i = 1|\boldsymbol{X})$.
- We will use the **logistic function** as our link function, so $\boldsymbol{x}_i^\top \boldsymbol{\beta} = \mathrm{logit}(\pi_i) = \ln\left(\pi_i/(1 - \pi_i)\right)$.
- Model fitting usually involves estimating $\boldsymbol{\beta}$ (or equivalently, $\boldsymbol{\pi}$).

Iterative Reweighted Least Square (IRLS)

1. Denote weights $w_i = \pi_i(1-\pi_i)$ and other estimates at the t-th iteration with a superscript (t).
2. Construct
$$z_i^{(t)} = \underbrace{\operatorname{logit}\left(\pi_i^{(t)}\right)}_{\boldsymbol{x}_i^\top \boldsymbol{\beta}^{(t)}} + \frac{y_i - \pi_i^{(t)}}{\pi_i^{(t)}(1-\pi_i^{(t)})}.$$
3. Update via
$$\widehat{\boldsymbol{\beta}}^{(t+1)} \leftarrow (\boldsymbol{X}^\top \boldsymbol{W}^{(t)} \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{W}^{(t)} \boldsymbol{z}^{(t)},$$
with $\boldsymbol{W}^{(t)} = \operatorname{diag}\left(w_i^{(t)}\right)$.
4. At convergence, $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{W} \boldsymbol{z}$, which equals to the MLE of logistic regression model.

Challenges in exhaustive GLM variable selection

For large p, exhaustive variable selection in GLM is difficult:

1. The computational cost of IRLS is $\mathcal{O}(np^2)$ per iteration.
2. We need to explore all 2^p models.

Aim of APES

Can we perform linear exhaustive variable selection (which benefits from fast algorithms) and use the results to approximate exhaustive GLM variable selection?

$$\text{GLM exhaustive} \xleftarrow{\text{Can this be done?}} \text{LM exhaustive}$$

1. Turning GLM to LM

Exhaustively computing modified MLE

- (?) described an approximation to exhaustive variable selection for logistic regression without the need for numerical optimisation.
- Their method starts with the estimated probability $\widehat{\boldsymbol{\pi}}(\alpha_f)$, from the **full** logistic model.
- Then, for each model $\alpha \in \mathcal{A}$, we calculate:

$$\widehat{\boldsymbol{\beta}}(\alpha; \widehat{\boldsymbol{\pi}}(\alpha_f)) = (\boldsymbol{X}_\alpha^\top \boldsymbol{W}(\widehat{\boldsymbol{\pi}}(\alpha_f))\boldsymbol{X}_\alpha)^{-1}\boldsymbol{X}_\alpha^\top \boldsymbol{W}(\widehat{\boldsymbol{\pi}}(\alpha_f))\boldsymbol{z}(\widehat{\boldsymbol{\pi}}(\alpha_f)).$$

- This is **NOT** the MLE for α, which should be $\widehat{\boldsymbol{\beta}}(\alpha; \widehat{\boldsymbol{\pi}}(\alpha))$.

Variable selection using the modified estimator

- Given $\widehat{\beta}(\alpha; \widehat{\boldsymbol{\pi}}(\alpha_f))$, we could **approximate** RSS or BIC for all $\alpha \in \mathcal{A}$.
- Upon selection of a small set of desired models, we can recompute the MLE and calculate other model fit statistics.

$$\text{GLM exhaustive} \xleftarrow[\text{Hosmer approx.}]{\hspace{6em}} \text{LM exhaustive}$$

2. Reducing computational time

Best subsets search

- Application of this approximation method is limited by the number of LMs we can explore.
- For $p \approx 50$, $\mathcal{A}$ is approximately 1 quadrillion in size, which is too large to explore exhaustively.
- A best subset algorithm limits our search to a subset of $\mathcal{A}$ but it guarantees to contain the global RSS-optimal model.
- **leaps** Furnival1974, Lumley2017 discard "branches" of models with insufficient fit.

Mixed Integer Optimisation

- Bertsimas2016 showed that it is feasible to perform best subset search for linear models with p in the hundreds.
- The most attractive component: guaranteed **sub-optimality** if algorithm is terminated before full convergence. Thus allowing a upper bound for real time limit.
- Current implementation in `R` is `bestsubset`, Hastie2017, which outputs the RSS-best linear model for each model size.

APES: Approximated Exhaustive Search

GLM best subset

no algorithm

GLM exhaustive

LM best subset

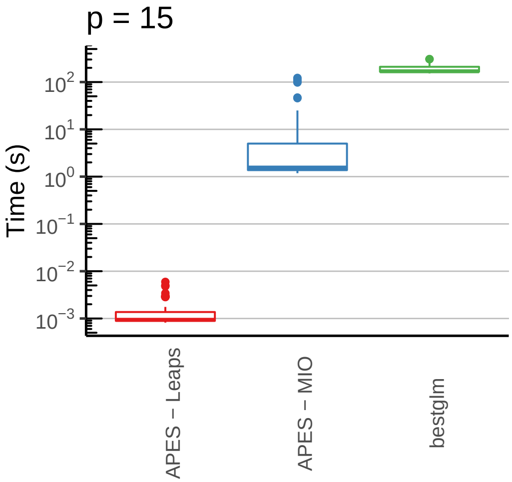
LM exhaustive

APES: Approximated Exhaustive Search

$$
\begin{tikzcd}
\text{GLM best subset} & \text{LM best subset} \arrow[d, "\text{MIO}"] \\
\text{GLM exhaustive} \arrow[u, "\text{infer}"] & \text{LM exhaustive} \arrow[l, "\text{Hosmer approx.}"']
\end{tikzcd}
$$

How fast is APES compare to genuine exhaustive search?

Very.



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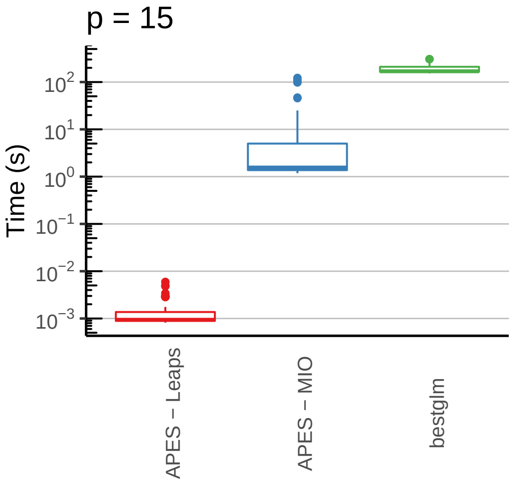
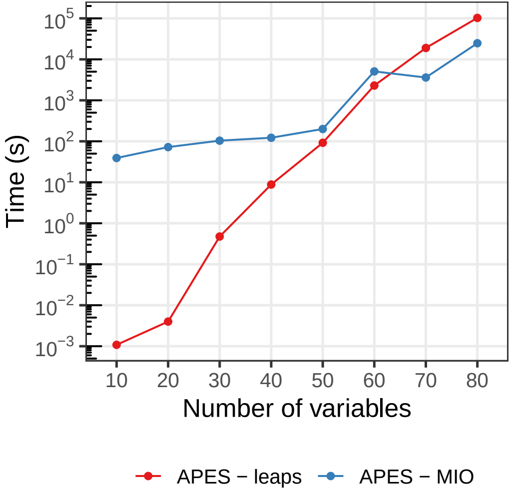




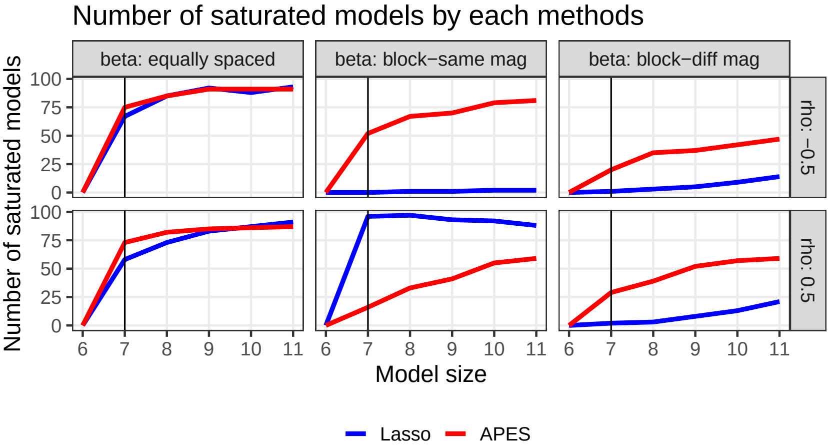
Simulation

Simulation set-up

- $n = 500, p = 100$, number of non-zero coefficient is $k = 6$.
- Intercept term is set to 0, then we tried 3 different choices of $\boldsymbol{\beta}$:
    1. Equally spaced indices: $(\frac{1}{2}, 0, \dots, 0, \frac{1}{2}, 0, \dots, 0, \frac{1}{2}, 0, \dots, 0, \frac{1}{2}, 0, \dots, 0, \frac{1}{2}, 0, \dots, \frac{1}{2})$.
    2. Block of indices, same magnitude/sign: $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, \dots, 0)$.
    3. Block of indices, different magnitude/sign: $(\frac{1}{3}, -1, 1, \frac{2}{3}, -\frac{2}{3}, -\frac{1}{3}, 0, \dots, 0)$.
- Generating $\boldsymbol{X} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$, with $\Sigma_{ij} = \rho^{|i-j|}$, $\rho = 0.5$ or -0.5. Then standardise.
- We repeated the simulation 100 times and compared APES against de-biased Lasso using various evaluation metrics.

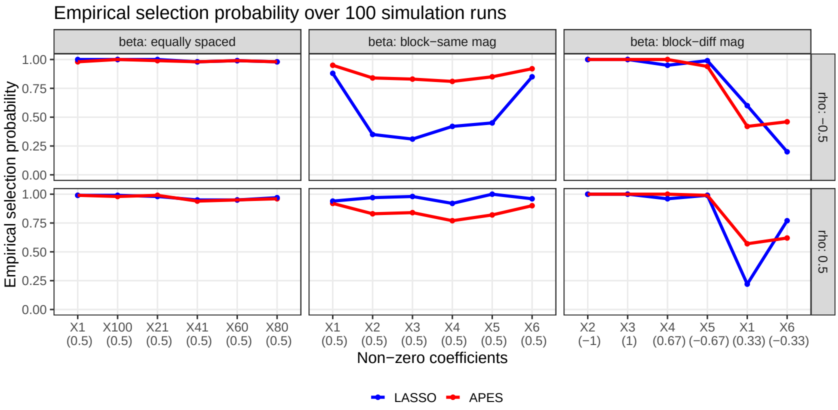
Evaluation 1: saturated models

- For each model size, APES and Lasso outputs one model.
- In most cases, APES has less false exclusion of variables than Lasso.



Evaluation 2: variable selection

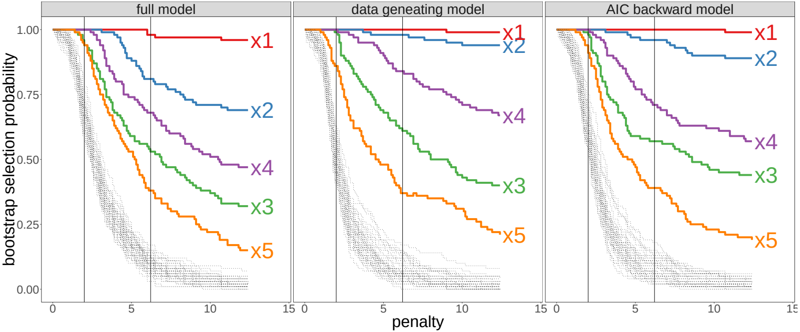
- BIC was used to select an optimal model.
- In most cases, APES has higher selection probability of active variables than Lasso.



Some extensions

The choice of $\widehat{\boldsymbol{\pi}}(\alpha_f)$ can be relaxed in two different ways:

- The full model α_f is not necessarily the best for variable selection.



- We could replace the MLE by other estimators, e.g. the Lasso or robust quasi-likelihood estimator.

Final remarks

1. APES is a **fast approximation** method for **exhaustive** variable selection in GLM.
2. APES pushes model dimensions into the hundreds/thousands and serves as a standard of comparison like a true exhaustive search.
3. APES is now published at ANZJS: `https://doi.org/10.1111/anzs.12276`.
   - https://github.com/kevinwang09/APES
   - https://github.com/garthtarr/mplot
   - Email: kevin.wang@sydney.edu.au. Twitter: @KevinWang009
4. Statistical Society of Australia has generously sponsored my travel to Taichung.

References