Addressing Complex Sampling Designs in the Development of Regression Models

Amaia Iparragirre¹, Irantzu Barrio^{1,2}, Inmaculada Arostegui^{1,2}

¹ University of the Basque Country (UPV/EHU)

² BCAM-Basque Center for Applied Mathematics



1 Introduction

- 2 Methodological proposals
- 3 Software development
- **4** Discussion and further research

1 Introduction

2 Methodological proposals

- 3 Software development
- 4
- Discussion and further research

|1



|1



|1

Prediction models

Based on known past behavior ...

... what is most likely to happen in the future?

Purpose: To make future predictions by means of known past results.

Prediction models

Based on known past behavior ...

... what is most likely to happen in the future?

Purpose: To make future predictions by means of known past results.

Development of prediction models

Several steps should be considered in the development of prediction models in order to end up with a **valid model**:



Prediction models

Based on known past behavior ...

... what is most likely to happen in the future?

Purpose: To make future predictions by means of known past results.

Development of prediction models

Several steps should be considered in the development of prediction models in order to end up with a **valid model**:



Existing techniques: data need to satisfy iid conditions

Survey data





Motivation

Complex sampling designs | 3



Complex sampling designs

One-stage stratified sampling

Complex sampling designs

One-stage stratified sampling



One-stage stratified sampling

One-stage stratified sampling



One-stage stratified sampling



One-stage stratified sampling

Population U (of size N):

$$U = \bigcup_{h=1}^{H} U_h$$
, each U_h of size $N_h, \forall h \in \{1, \dots, H\}.$

Inclusion probabilities:

$$\pi_i = \frac{n_h}{N_h}, \quad \forall i \in U_h, \quad \forall h \in \{1, \dots, H\}.$$

Sampling weights

$$w_i = \frac{1}{\pi_i} = \frac{N_h}{n_h}, \quad \forall i \in S_h, \quad \forall h \in \{1, \dots, H\}, \ S = \cup_{h=1}^H S_h.$$

Complex sampling designs



4

Complex sampling designs



4

Complex sampling designs



4

Complex sampling designs



4

Complex sampling designs



Two-stage stratified cluster sampling



Complex sampling designs



Two-stage stratified cluster sampling

Population U (of size N):

$$U = \bigcup_{h=1}^{H} \bigcup_{\alpha=1}^{A_h} U_{h,\alpha} \text{ , each } U_{h,\alpha} \text{ of size } N_{h,\alpha}, \forall h \in \{1, \dots, H\}, \forall \alpha = 1, \dots, A_h.$$

Inclusion probabilities:

$$\pi_i = \frac{a_h}{A_h} \cdot \frac{n_{h,\alpha}}{N_{h,\alpha}}, \quad \forall i \in U_{h,\alpha}, \quad \forall \alpha \in \{1, \dots, A_h\}, \ \forall h \in \{1, \dots, H\}.$$

Sampling weights

$$w_i = \frac{1}{\pi_i} = \frac{A_h}{a_h} \cdot \frac{N_{h,\dot{\alpha}}}{n_{h,\dot{\alpha}}}, \quad \forall i \in S_{h,\dot{\alpha}}, \forall \dot{\alpha} \in \mathbb{A}_h, \forall h \in \{1,\ldots,H\},$$

where $\dot{\alpha}$ is the index of each selected cluster (grouped in the set \mathbb{A}_h).

Prediction models Complex Survey Design Data

Prediction models

PROBLEM:

complex survey data do not satisfy iid conditions

Complex Design Survey Data

Objectives





Variable selection with LASSO regression for complex survey data



Estimation of the ROC curve and AUC with complex survey data

Basic notation

Y: dichotomous response variable $\mathbf{X} = (1, X_1, ..., X_p)$: vector of covariates. U: finite population of N units $S \subset U$: sample of n observations, $(y_i, \mathbf{x}_i, w_i), \forall i \in S$ $\boldsymbol{\beta} = (\beta_0, \beta_1, ..., \beta_p)^T$: model coefficients.

Focus: Logistic regression model

$$logit(p_i) = ln\left[\frac{p_i}{1-p_i}\right] = \beta_0 + \beta_1 x_{1i} + \ldots + \beta_p x_{pi}$$

where $p_i = p(\mathbf{x}_i) = P(Y = 1 | \mathbf{X} = \mathbf{x}_i)$.

Basic notation

Y: dichotomous response variable $\mathbf{X} = (1, X_1, \dots, X_p)$: vector of covariates. U: finite population of N units $S \subset U$: sample of n observations, $(y_i, \mathbf{x}_i, w_i), \forall i \in S$ $\mathbf{\beta} = (\beta_0, \beta_1, \dots, \beta_p)^T$: model coefficients.

Focus: Logistic regression model

$$logit(p_i) = ln\left[\frac{p_i}{1-p_i}\right] = \beta_0 + \beta_1 x_{1i} + \ldots + \beta_p x_{pi}$$

where $p_i = p(\mathbf{x}_i) = P(Y = 1 | \mathbf{X} = \mathbf{x}_i)$.

Likelihood function

$$L(oldsymbol{eta}) = \prod_{i\in S} p_i^{y_i} (1-p_i)^{1-y_i} \Longrightarrow \hat{oldsymbol{eta}}$$

Basic notation

Y: dichotomous response variable $\boldsymbol{X} = (1, X_1, \dots, X_p)$: vector of covariates. U: finite population of N units $S \subset U$: sample of n observations, $(y_i, \boldsymbol{x}_i, w_i), \forall i \in S$ $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_p)^T$: model coefficients.

Focus: Logistic regression model

$$logit(p_i) = ln\left[\frac{p_i}{1-p_i}\right] = \beta_0 + \beta_1 x_{1i} + \ldots + \beta_p x_{pi}$$

where $p_i = p(x_i) = P(Y = 1 | X = x_i)$.

Pseudo-likelihood function (Binder, 1983)

$$PL(\boldsymbol{\beta}) = \prod_{i \in S} p_i^{y_i \mathbf{w}_i} (1 - p_i)^{(1 - y_i) \mathbf{w}_i} \Longrightarrow \hat{\boldsymbol{\beta}}$$



2 Methodological proposals

3 Software development



Variable selection with LASSO regression

Introduction

Variable selection | 7

- Development of prediction models
 - > Variable selection
 - > LASSO regression models \implies Tuning parameter (λ)
- Development of prediction models
 - > Variable selection
 - > LASSO regression models \Longrightarrow Tuning parameter (λ)
 - > Select λ that minimizes the error: validation methods (train/test sets)
 - > Cross-validation (CV)

Variable selection | 7

- Development of prediction models
 - > Variable selection
 - > LASSO regression models \Longrightarrow Tuning parameter (λ)
 - > Select λ that minimizes the error: validation methods (train/test sets)
 - > Cross-validation (CV)

▶ **PROBLEMS:** sampling design is not considered

- > Estimation of regression coefficients
- > Validation techniques

Variable selection | 7

- Development of prediction models
 - > Variable selection
 - > LASSO regression models \Longrightarrow Tuning parameter (λ)
 - > Select λ that minimizes the error: validation methods (train/test sets)
 - > Cross-validation (CV)
- ► **PROBLEMS:** sampling design is not considered
 - > Estimation of regression coefficients
 - Validation techniques
- Complex survey data framework:

Validation techniques \implies **Replicate weights methods**

Replicate weights methods

Modify the sampling weights (w_i^*) to define new subsamples that replicate the original sample and properly represent the finite population.

Variable selection | 8

Goals

- 1 Analyze the performance of replicate weights methods to select λ .
- 2 Propose new methods based on replicate weights: design-based cross-validation (dCV).

Variable selection | 8

Goals

- 1 Analyze the performance of replicate weights methods to select λ .
- 2 Propose new methods based on replicate weights: design-based cross-validation (dCV).

We compare the performance of the methods with respect to the traditional cross-validation

Variable selection | 9

► Logistic regression model:
$$p(\mathbf{x}_i) = \frac{e^{\mathbf{x}_i \beta}}{1 + e^{\mathbf{x}_i \beta}}$$

$$\ell(\boldsymbol{\beta}) = \sum_{i \in S} \left[y_i \ln(p(\boldsymbol{x}_i)) + (1 - y_i) \ln(1 - p(\boldsymbol{x}_i)) \right] \Longrightarrow \hat{\boldsymbol{\beta}}$$

For a given value of λ , logistic LASSO regression models:

$$\min\left\{-\ell(\boldsymbol{\beta}) + \lambda \sum_{j=1}^{p} |\beta_j|\right\}$$

Variable selection | 9

► Logistic regression model:
$$p(\mathbf{x}_i) = \frac{e^{\mathbf{x}_i \beta}}{1 + e^{\mathbf{x}_i \beta}}$$

$$\ell(\boldsymbol{\beta}) = \sum_{i \in S} \left[y_i \ln(p(\boldsymbol{x}_i)) + (1 - y_i) \ln(1 - p(\boldsymbol{x}_i)) \right] \Longrightarrow \hat{\boldsymbol{\beta}}$$

For a given value of λ , logistic LASSO regression models:

$$\min\left\{-\ell(\boldsymbol{\beta}) + \lambda \sum_{j=1}^{p} |\beta_j|\right\} \Longrightarrow \lambda?$$

Software development

Discussion and further research

Methods

Variable selection | 10

Unweighted cross-validation (unw-SRSCV) (K = 10)

Software development

Discussion and further research

Methods

Variable selection | 10

Unweighted cross-validation (unw-SRSCV) (K = 10)

> Define a grid for λ : λ_l , $\forall l = 1, \ldots, L$.

Variable selection | 10

Unweighted cross-validation (unw-SRSCV) (K = 10)

- > Define a grid for λ : λ_I , $\forall I = 1, \dots, L$.
- $\ > \ \textit{K} \ \text{folds} \Longrightarrow \textit{S}_{\operatorname{tr}(k)}, \ \textit{S}_{\operatorname{test}(k)}, \ \forall k = 1, \ldots, \textit{K}$

Variable selection | 10

Unweighted cross-validation (unw-SRSCV) (K = 10)

- > Define a grid for λ : λ_I , $\forall I = 1, \ldots, L$.
- $\ > \ \textit{K} \ \text{folds} \Longrightarrow \textit{S}_{\operatorname{tr}(k)}, \ \textit{S}_{\operatorname{test}(k)}, \ \forall k = 1, \ldots, \textit{K}$
- > Fit the model to the training set $S_{tr(k)}$ considering $\lambda_l \Longrightarrow \hat{p}_{tr(k)}^l(\cdot)$

Unweighted cross-validation (unw-SRSCV) (K = 10)

- > Define a grid for λ : λ_l , $\forall l = 1, ..., L$.
- $\ > \ \textit{K} \ \text{folds} \Longrightarrow \textit{S}_{\operatorname{tr}(k)}, \ \textit{S}_{\operatorname{test}(k)}, \ \forall k = 1, \ldots, \textit{K}$
- > Fit the model to the training set $S_{tr(k)}$ considering $\lambda_l \Longrightarrow \hat{p}'_{tr(k)}(\cdot)$
- > Estimate the error in the test sets:

$$\widehat{Err}'_{(k)} = \frac{1}{n_{\text{test}(k)}} \sum_{i \in S_{\text{test}(k)}} \mathcal{L}(y_i, \hat{p}'_{\text{tr}(k)}(\boldsymbol{x}_i)) \Longrightarrow \widehat{Err}_{CV}(\lambda_i) = \frac{1}{K} \sum_{k=1}^{K} \widehat{Err}'_{(k)},$$

where: $\mathcal{L}(y_i, \hat{p}'_{tr(k)}(\mathbf{x}_i)) = -y_i \ln(\hat{p}'_{tr(k)}(\mathbf{x}_i)) - (1 - y_i) \ln(1 - \hat{p}'_{tr(k)}(\mathbf{x}_i)).$

Unweighted cross-validation (unw-SRSCV) (K = 10)

- > Define a grid for λ : λ_l , $\forall l = 1, ..., L$.
- $> \quad \textit{K} \ \text{folds} \Longrightarrow \textit{S}_{\operatorname{tr}(k)}, \ \textit{S}_{\operatorname{test}(k)}, \ \forall k = 1, \ldots, \textit{K}$
- > Fit the model to the training set $S_{tr(k)}$ considering $\lambda_l \Longrightarrow \hat{p}'_{tr(k)}(\cdot)$
- > Estimate the error in the test sets:

$$\widehat{Err}'_{(k)} = \frac{1}{n_{\text{test}(k)}} \sum_{i \in S_{\text{test}(k)}} \mathcal{L}(y_i, \hat{p}'_{\text{tr}(k)}(\boldsymbol{x}_i)) \Longrightarrow \widehat{Err}_{CV}(\lambda_i) = \frac{1}{K} \sum_{k=1}^{K} \widehat{Err}'_{(k)},$$

where: $\mathcal{L}(y_i, \hat{p}'_{tr(k)}(\mathbf{x}_i)) = -y_i \ln(\hat{p}'_{tr(k)}(\mathbf{x}_i)) - (1 - y_i) \ln(1 - \hat{p}'_{tr(k)}(\mathbf{x}_i)).$

> Best value for λ :

$$\Lambda = \underset{\lambda_l: \ l=1,...,L}{\operatorname{argmin}} \{ \widehat{Err}_{CV}(\lambda_l) \}$$

Software development

Discussion and further research

Methods

Unweighted cross-validation (unw-SRSCV) (K = 10)

- Define a grid for λ : λ_l , $\forall l = 1, \ldots, L$.
- K folds $\implies S_{tr(k)}, S_{test(k)}, \forall k = 1, ..., K$ (*)
- ▶ Fit the model to the training set $S_{tr(k)}$ considering $\lambda_l \Longrightarrow \hat{p}'_{tr(k)}(\cdot)$ (*)

Estimate the error in the test sets: (*)

$$\widehat{Err}'_{(k)} = \frac{1}{n_{\text{test}(k)}} \sum_{i \in S_{\text{test}(k)}} \mathcal{L}(y_i, \hat{p}'_{\text{tr}(k)}(\mathbf{x}_i)) \Longrightarrow \widehat{Err}_{CV}(\lambda_I) = \frac{1}{K} \sum_{k=1}^{K} \widehat{Err}'_{(k)},$$

where:

$$\mathcal{L}(y_i, \hat{p}_{\mathrm{tr}(k)}^{\prime}(\boldsymbol{x}_i)) = -y_i \ln(\hat{p}_{\mathrm{tr}(k)}^{\prime}(\boldsymbol{x}_i)) - (1 - y_i) \ln(1 - \hat{p}_{\mathrm{tr}(k)}^{\prime}(\boldsymbol{x}_i)).$$

• Best value for λ :

$$\Lambda = \underset{\lambda_{l}: \ l=1,...,L}{\operatorname{argmin}} \{ \widehat{Err}_{CV}(\lambda_{l}) \}$$

Software development

Discussion and further research

Methods

Variable selection | 12

PROPOSAL: Sampling design should be considered.

Software development

Discussion and further research

Methods

Variable selection | 12

PROPOSAL: Sampling design should be considered.

• Fitting the models: \implies weighted cross-validation (w_i , w-SRSCV)

$$\min\left\{-p\ell(\boldsymbol{\beta})+\lambda\sum_{j=1}^{p}|\beta_{j}|\right\},\,$$

where,

$$p\ell(\boldsymbol{\beta}) = \sum_{i \in S} w_i \left[y_i \ln(p(\boldsymbol{x}_i)) + (1 - y_i) \ln(1 - p(\boldsymbol{x}_i)) \right].$$

Software development

Discussion and further research

Methods

Variable selection | 12

PROPOSAL: Sampling design should be considered.

• Fitting the models: \implies weighted cross-validation (w_i , w-SRSCV)

$$\min\left\{-p\ell(\boldsymbol{\beta})+\lambda\sum_{j=1}^{p}|\beta_{j}|\right\},\,$$

where,

$$p\ell(\boldsymbol{\beta}) = \sum_{i \in S} \boldsymbol{w}_i^* \left[y_i \ln(p(\boldsymbol{x}_i)) + (1 - y_i) \ln(1 - p(\boldsymbol{x}_i)) \right].$$

• Defining training and test sets \implies Replicate weights methods (w_i^*)

Software development

Discussion and further research

Methods

Variable selection | 12

PROPOSAL: Sampling design should be considered.

• Fitting the models: \implies weighted cross-validation (w_i , w-SRSCV)

$$\min\left\{-p\ell(\boldsymbol{\beta})+\lambda\sum_{j=1}^{p}|\beta_{j}|\right\},\,$$

where,

$$p\ell(\boldsymbol{\beta}) = \sum_{i \in S} \boldsymbol{w}_i^* \left[y_i \ln(p(\boldsymbol{x}_i)) + (1 - y_i) \ln(1 - p(\boldsymbol{x}_i)) \right].$$

▶ Defining training and test sets ⇒ Replicate weights methods (w_i*)
▶ Estimating the error:

$$\widehat{Err}'_{(k)} = \frac{1}{\sum_{i \in S_{\text{test}(k)}} \mathbf{w}_i^*} \sum_{i \in S_{\text{test}(k)}} \mathbf{w}_i^* \mathcal{L}(y_i, \hat{p}'_{\text{tr}(k)}(\mathbf{x}_i)).$$

Discussion and further research

Methods

Variable selection | 13

Replicate weights methods:

Existing methods

- Jackknife Repeated Replication (JKn)
- Rescaling Bootstrap (Bootstrap)
- Balanced Repeated Replication (BRR)

New methods

- Design-based cross-validation (dCV)
- Split-sample Repeated Replication (split)
- Extrapolation (extrap)

Software development

Discussion and further research

Methods

Variable selection | 13

Replicate weights methods:

Existing methods

- Jackknife Repeated Replication (JKn)
- Rescaling Bootstrap (Bootstrap)
- Balanced Repeated Replication (BRR)

New methods

- Design-based cross-validation (dCV)
- Split-sample Repeated Replication (split)
- Extrapolation (extrap)

Software development

Discussion and further research

Methods

Variable selection | 14

Jackknife Repeated Replication (JKn)



Software development

Discussion and further research

Methods

Variable selection | 15

Design-based cross-validation (dCV)



Simulation study

- Generate population covariates (x_i) and design variables (z_i) following a multivariate normal distribution.
- Pre-define β (some values = 0) \Longrightarrow $y_i \sim Bernoulli(p(\mathbf{x}_i, \mathbf{z}_i)) \Longrightarrow U$

- Generate population covariates (x_i) and design variables (z_i) following a multivariate normal distribution.
- Pre-define β (some values = 0) \Longrightarrow $y_i \sim Bernoulli(p(\mathbf{x}_i, \mathbf{z}_i)) \Longrightarrow U$
- p = 50 covariates (\mathbf{x}_i) are considered to fit the models.

- Generate population covariates (x_i) and design variables (z_i) following a multivariate normal distribution.
- Pre-define β (some values = 0) \Longrightarrow $y_i \sim Bernoulli(p(\mathbf{x}_i, \mathbf{z}_i)) \Longrightarrow U$
- p = 50 covariates (\mathbf{x}_i) are considered to fit the models.
- ▶ S1 (d = 0 cluster-level variables), S2 (d = 5).

- Generate population covariates (x_i) and design variables (z_i) following a multivariate normal distribution.
- Pre-define β (some values = 0) \Longrightarrow $y_i \sim Bernoulli(p(\mathbf{x}_i, \mathbf{z}_i)) \Longrightarrow U$
- p = 50 covariates (\mathbf{x}_i) are considered to fit the models.
- ▶ S1 (d = 0 cluster-level variables), S2 (d = 5).
- H = 5 strata, $A_h = 20, \forall h = 1, \dots, H$ clusters

Variable selection | 16

- Generate population covariates (x_i) and design variables (z_i) following a multivariate normal distribution.
- Pre-define β (some values = 0) \Longrightarrow $y_i \sim Bernoulli(p(\mathbf{x}_i, \mathbf{z}_i)) \Longrightarrow U$
- p = 50 covariates (\mathbf{x}_i) are considered to fit the models.
- ▶ S1 (d = 0 cluster-level variables), S2 (d = 5).
- H = 5 strata, $A_h = 20, \forall h = 1, \dots, H$ clusters
- Sample (S):
 - > $a_h = 4, \forall h = 1, \dots, H$ clusters
 - > $n_{h,\alpha}$ units per cluster:

S1: (5, 10, 25, 50, 500), **S2:** $(5, 25, 50, 100, 250) \implies w_i$





Discussion and further research

Simulation study

Differences between Λ parameters





Variable selection | 18

Number of variables



Discussion and further research

Simulation study

Differences between Λ parameters



oftware development

Discussion and further research

Variable selection | 18

Number of variables



Conclusions

- Weights need to be incorporated to fit LASSO models.
- The greater the cluster-effects, the greater the difference between dCV and w-SRSCV.
- Similar results for linear regression models.

Conclusions

Variable selection | 19

- ▶ Weights need to be incorporated to fit LASSO models.
- ► The greater the cluster-effects, the greater the difference between dCV and w-SRSCV.
- Similar results for linear regression models.

Recommendation

The use of dCV is recommended: parsimonious models and the best method in terms of computational efficiency.

Conclusions

Variable selection | 19

- ► Weights need to be incorporated to fit LASSO models.
- ► The greater the cluster-effects, the greater the difference between dCV and w-SRSCV.
- Similar results for linear regression models.

Recommendation

The use of dCV is recommended: parsimonious models and the best method in terms of computational efficiency.

Extended to elastic nets
Estimation of the ROC curve and the AUC

Introduction

Estimation of ROC and AUC | 21

 S_0 : subset of units with Y = 0; S_1 : subset of units with Y = 1.

Introduction

Estimation of ROC and AUC | 21

 S_0 : subset of units with Y = 0; S_1 : subset of units with Y = 1.

Area under the ROC curve (\mathcal{A}_{unw})

$$\widehat{ROC}(\cdot) = \left\{ (1 - \widehat{Sp}(c), \ \widehat{Se}(c)), \ c \in (-\infty, \infty) \right\} :$$
$$\widehat{Sp}(c) = \frac{1}{n} \sum_{i_0 \in S_0} I(\hat{p}_{i_0} < c) \quad ; \quad \widehat{Se}(c) = \frac{1}{n} \sum_{i_1 \in S_1} I(\hat{p}_{i_1} \ge c)$$

Introduction

Estimation of ROC and AUC|21

 S_0 : subset of units with Y = 0; S_1 : subset of units with Y = 1.

Area under the ROC curve (\mathcal{A}_{unw})

$$\widehat{ROC}(\cdot) = \left\{ (1 - \widehat{Sp}(c), \ \widehat{Se}(c)), \ c \in (-\infty, \infty) \right\} :$$
$$\widehat{Sp}(c) = \frac{1}{n} \sum_{i_0 \in S_0} I(\hat{p}_{i_0} < c) \quad ; \quad \widehat{Se}(c) = \frac{1}{n} \sum_{i_1 \in S_1} I(\hat{p}_{i_1} \ge c)$$

Mann-Whitney U-statistic (Bamber, 1975)

$$\widehat{AUC}_{unw} = \frac{1}{n_0 \cdot n_1} \sum_{i_0 \in S_0} \sum_{i_1 \in S_1} \left[I(\hat{p}_{i_0} < \hat{p}_{i_1}) + 0.5I(\hat{p}_{i_0} = \hat{p}_{i_1}) \right]$$

 $\mathcal{A}_{unw} = \widehat{AUC}_{unw}$

Estimation of ROC and AUC | 22

 S_0 : subset of units with Y = 0; S_1 : subset of units with Y = 1.

Area under the ROC curve (\mathcal{A})

$$\widehat{ROC}_{w}(\cdot) = \left\{ (1 - \widehat{Sp}_{w}(c), \ \widehat{Se}_{w}(c)), \ c \in (-\infty, \infty) \right\} :$$

$$\widehat{Sp}_{w}(c) = \frac{\sum_{i_{0} \in S_{0}} w_{i_{0}} \cdot l(\hat{p}_{i_{0}} < c)}{\sum_{i_{0} \in S_{0}} w_{i_{0}}} \quad ; \quad \widehat{Se}_{w}(c) = \frac{\sum_{i_{1} \in S_{1}} w_{i_{1}} \cdot l(\hat{p}_{i_{1}} \ge c)}{\sum_{i_{1} \in S_{1}} w_{i_{1}}}$$

Estimation of ROC and AUC | 22

 S_0 : subset of units with Y = 0; S_1 : subset of units with Y = 1.

Area under the ROC curve (\mathcal{A})

$$\widehat{ROC}_{w}(\cdot) = \left\{ (1 - \widehat{Sp}_{w}(c), \ \widehat{Se}_{w}(c)), \ c \in (-\infty, \infty) \right\} :$$

$$\widehat{Sp}_{w}(c) = \frac{\sum_{i_{0} \in S_{0}} w_{i_{0}} \cdot l(\hat{p}_{i_{0}} < c)}{\sum_{i_{0} \in S_{0}} w_{i_{0}}} \quad ; \quad \widehat{Se}_{w}(c) = \frac{\sum_{i_{1} \in S_{1}} w_{i_{1}} \cdot l(\hat{p}_{i_{1}} \ge c)}{\sum_{i_{1} \in S_{1}} w_{i_{1}}}$$

Based on the Mann-Whitney U-statistic

$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} \left[l(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot l(\hat{p}_{i_{0}} = \hat{p}_{i_{1}}) \right]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$

Estimation of ROC and AUC | 22

 S_0 : subset of units with Y = 0; S_1 : subset of units with Y = 1.

Area under the ROC curve (\mathcal{A})

$$\widehat{ROC}_{w}(\cdot) = \left\{ (1 - \widehat{Sp}_{w}(c), \ \widehat{Se}_{w}(c)), \ c \in (-\infty, \infty) \right\} :$$

$$\widehat{Sp}_{w}(c) = \frac{\sum_{i_{0} \in S_{0}} w_{i_{0}} \cdot l(\hat{p}_{i_{0}} < c)}{\sum_{i_{0} \in S_{0}} w_{i_{0}}} \quad ; \quad \widehat{Se}_{w}(c) = \frac{\sum_{i_{1} \in S_{1}} w_{i_{1}} \cdot l(\hat{p}_{i_{1}} \ge c)}{\sum_{i_{1} \in S_{1}} w_{i_{1}}}$$

Based on the Mann-Whitney U-statistic

$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} \left[I(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot I(\hat{p}_{i_{0}} = \hat{p}_{i_{1}}) \right]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$

$$\mathcal{A} = \widehat{AUC}_{\mathsf{M}}$$

Estimation of ROC and AUC | 23

Q probabilities \implies Cut-off points: $c_Q < c_{Q-1} < \ldots < c_1 < c_0$

$$\begin{array}{l} Q \text{ probabilities} \Longrightarrow \text{Cut-off points: } c_Q < c_{Q-1} < \ldots < c_1 < c_0 \\ \Longrightarrow \forall q \in \{0, 1, \ldots, Q\}, \quad (1 - \widehat{Sp}_w(c_q), \widehat{Se}_w(c_q)) \Longrightarrow \widehat{ROC}_w(\cdot) \end{array}$$



$$\begin{array}{l} Q \text{ probabilities} \Longrightarrow \text{Cut-off points: } c_Q < c_{Q-1} < \ldots < c_1 < c_0 \\ \Longrightarrow \forall q \in \{0, 1, \ldots, Q\}, \quad (1 - \widehat{Sp}_w(c_q), \widehat{Se}_w(c_q)) \Longrightarrow \widehat{ROC}_w(\cdot) \end{array}$$



$$\mathcal{A}_1 = rac{(1-\widehat{Sp}_w(c_1))\cdot\widehat{Se}_w(c_1)}{2}$$

$$\begin{array}{l} Q \text{ probabilities} \Longrightarrow \text{Cut-off points: } c_Q < c_{Q-1} < \ldots < c_1 < c_0 \\ \Longrightarrow \forall q \in \{0, 1, \ldots, Q\}, \quad (1 - \widehat{Sp}_w(c_q), \widehat{Se}_w(c_q)) \Longrightarrow \widehat{ROC}_w(\cdot) \end{array}$$



$$\begin{array}{l} Q \text{ probabilities} \Longrightarrow \mathsf{Cut-off points:} \ c_Q < c_{Q-1} < \ldots < c_1 < c_0 \\ \Longrightarrow \forall q \in \{0, 1, \ldots, Q\}, \quad (1 - \widehat{Sp}_w(c_q), \widehat{Se}_w(c_q)) \Longrightarrow \widehat{ROC}_w(\cdot) \end{array}$$



$$\begin{array}{l} Q \text{ probabilities} \Longrightarrow \text{Cut-off points: } c_Q < c_{Q-1} < \ldots < c_1 < c_0 \\ \Longrightarrow \forall q \in \{0, 1, \ldots, Q\}, \quad (1 - \widehat{Sp}_w(c_q), \widehat{Se}_w(c_q)) \Longrightarrow \widehat{ROC}_w(\cdot) \end{array}$$

$$\mathcal{A} = \mathcal{A}_1 + \ldots + \mathcal{A}_Q$$



$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} \left[I(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot I(\hat{p}_{i_{0}} = \hat{p}_{i_{1}}) \right]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$

$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} \left[I(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot I(\hat{p}_{i_{0}} = \hat{p}_{i_{1}}) \right]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$









$$I(\hat{p}_{i_0} < \hat{p}_{i_1}) = \sum_{q=1}^Q I(\hat{p}_{i_0} < c_q) \cdot [I(\hat{p}_{i_1} \ge c_q) - I(\hat{p}_{i_1} \ge c_{q-1})]$$







$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} [I(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot I(\hat{p}_{i_{0}} = \hat{p}_{i_{1}})]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$

$$I(\hat{p}_{i_0}=\hat{p}_{i_1})=\sum_{q=1}^Q \left[I(\hat{p}_{i_0} < c_{q-1}) - I(\hat{p}_{i_0} < c_q)
ight] \cdot \left[I(\hat{p}_{i_1} \geq c_q) - I(\hat{p}_{i_1} \geq c_{q-1})
ight]$$

$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} [I(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot I(\hat{p}_{i_{0}} = \hat{p}_{i_{1}})]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$

$$I(\hat{p}_{i_0} < \hat{p}_{i_1}) = \sum_{q=1}^Q I(\hat{p}_{i_0} < c_q) \cdot [I(\hat{p}_{i_1} \ge c_q) - I(\hat{p}_{i_1} \ge c_{q-1})]$$

$$I(\hat{p}_{i_0} = \hat{p}_{i_1}) = \sum_{q=1}^Q \left[I(\hat{p}_{i_0} < c_{q-1}) - I(\hat{p}_{i_0} < c_q) \right] \cdot \left[I(\hat{p}_{i_1} \ge c_q) - I(\hat{p}_{i_1} \ge c_{q-1}) \right]$$

Software development

Discussion and further research

Proposal

$$\widehat{AUC}_{w} = \frac{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}} \left[l(\hat{p}_{i_{0}} < \hat{p}_{i_{1}}) + 0.5 \cdot l(\hat{p}_{i_{0}} = \hat{p}_{i_{1}}) \right]}{\sum_{i_{0} \in S_{0}} \sum_{i_{1} \in S_{1}} w_{i_{0}} w_{i_{1}}}$$
$$\mathcal{A} = \frac{1}{2} \sum_{q=1}^{Q} \left[\widehat{Sp}_{w}(c_{q-1}) \widehat{Se}_{w}(c_{q}) - \widehat{Sp}_{w}(c_{q}) \widehat{Se}_{w}(c_{q-1}) \right]$$

Estimation of ROC and AUC | 25

Data generation

Step 1. Generate U with covariates following a normal distribution.

Estimation of ROC and AUC | 25

Data generation

Step 1. Generate U with covariates following a normal distribution.

Step 2. Generate the response for a given β following Bernoulli's distribution.

Estimation of ROC and AUC $\space{25}$

- Step 1. Generate U with covariates following a normal distribution.
- Step 2. Generate the response for a given β following Bernoulli's distribution.
- Step 3. Define the sampling design:
 - > Strata
 - > Clusters within strata

Estimation of ROC and AUC | 25

- Step 1. Generate U with covariates following a normal distribution.
- Step 2. Generate the response for a given β following Bernoulli's distribution.
- Step 3. Define the sampling design:
 - > Strata
 - > Clusters within strata
- Step 4. Sample the population and calculate the weights:

Estimation of ROC and AUC $\space{25}$

- Step 1. Generate U with covariates following a normal distribution.
- Step 2. Generate the response for a given β following Bernoulli's distribution.
- Step 3. Define the sampling design:
 - > Strata
 - > Clusters within strata
- Step 4. Sample the population and calculate the weights:
 - One-stage stratified sampling (SH)
 - > Two-stage stratified cluster sampling (SC)
 - 0 cluster-level variables (SC.0)
 - 1 cluster-level variable (SC.1)
 - > Two sampling schemes: (a) and (b)

Estimation of ROC and AUC $\space{25}$

- Step 1. Generate U with covariates following a normal distribution.
- Step 2. Generate the response for a given β following Bernoulli's distribution.
- Step 3. Define the sampling design:
 - > Strata
 - > Clusters within strata
- Step 4. Sample the population and calculate the weights:
 - > One-stage stratified sampling (SH)
 - > Two-stage stratified cluster sampling (SC)
 - 0 cluster-level variables (SC.0)
 - 1 cluster-level variable (SC.1)
 - > Two sampling schemes: (a) and (b)

Set-up

Estimation of ROC and AUC $\scriptstyle | \, 26$

 $\widehat{ROC}^1_{\text{true}}$ \widehat{ROC}_{true}^r $\widehat{ROC}_{\text{true}}^{500}$ \widehat{AUC}^{1}_{true} \widehat{AUC}^{r}_{true} \widehat{AUC}^{500} $\widehat{p}_i^{500}, \forall i \in U$ $\widehat{p}_i^1, \forall i \in U$ $\widehat{p}_i^r, \forall i \in U$ $\boldsymbol{\beta}^{\mathrm{pop}}, p_i^{\mathrm{pop}}, \forall i \in U$ POPULATION (U) ROC_{pop} S⁵⁰⁰ S^1 S^r AUC_{pop} \widehat{A}^{500} $\widehat{p}_i^1, \forall i \in S^1$ $\widehat{p}_i^r, \forall i \in S^r$ $\widehat{p}_i^{500}, \forall i \in S^{500}$ $\widehat{ROC}^1_{\rm unw} \ \widehat{AUC}^1_{\rm unw}$ $\widehat{ROC}^r_{\mathrm{unw}} \ \widehat{AUC}^r_{\mathrm{unw}}$ \widehat{AUC}^{1}_{w} \widehat{ROC}_{w}^{r} \widehat{AUC}_{w}^{r} \widehat{AUC}_{w}^{500} \widehat{ROC}^1_w \widehat{ROC}^{500} $\widehat{AUC}^{1}_{nairs}$ $\widehat{AUC}^r_{\text{pairs}}$ AUC 500

Software development

Discussion and further research

Simulation study

Estimation of ROC and AUC|27

Estimated ROC curves



Software development

Discussion and further research

Simulation study

Estimation of ROC and AUC|27

Differences between the estimated and true AUCs



Software development

Discussion and further research

Problem

Estimation of ROC and AUC | 28



 \downarrow

Optimistic estimates

 \downarrow

Correction needed

Optimism correction of the $\ensuremath{\mathsf{AUC}}$
Introduction

Optimism correction AUC | 30

Same data: (1) fit the model, (2) estimate the AUC \Longrightarrow **Optimism**

- In line with traditional simple random sample (SRS) context See, e.g: Austin and Steyerberg (2017), Iparragirre et al (2019).
- Recommendation in SRS: validation techniques
 - > split-sample validation
 - > Bootstrap
 - > cross-validation
- ▶ In general, in complex survey data context, to define training and test sets
 - > Validation techniques \implies **Replicate weights**

Goal

Analyze the performance of replicate weights methods for optimism correction of the AUC.

Optimism correction AUC | 31

Rescaling Bootstrap (RB) (Rao and Wu, 1988)



RBn: another variant in which the same number of units (one-stage) or clusters (two-stage) are in both, training and test (original) set.

Optimism correction AUC | 32

Rescaling Bootstrap (RB)



Optimism correction AUC | 33

Design-based cross-validation (dCV) (lparragirre et al. (2023))



JKn: another variant in which each unit (one-stage) or cluster (two-stage) is set as the test set once.

Optimism correction AUC|34



Simulation study

Optimism correction AUC | 35

- Population U is generated in the same way as in the previous simulation study carried out for the estimation of the ROC curve.
- ► Sampling schemes: SH (one-stage), and SC.0, SC.1 (two-stage).
- ► Consider:
 - > RB, RBn: B = 200 resamples
 - > dCV: K = 10 folds, L = 20 replicates
- **Simulation set-up:** For $r = 1, \ldots, 500$:
 - > Obtain the sample S^r
 - > Fit the model to $S^r(\hat{\beta}^r)$ and estimate its AUC: $\widehat{AUC}_w^{r,app}$.
 - > Calculated the corrected AUCs : dCV.av, dCV.pool, JKn, RB, RBn
 - > Extend $\hat{\boldsymbol{\beta}}^r$ to $U: \widehat{AUC}_{true}^r$
 - ≥ For $m \in \{app, dCV.av, dCV.pool, JKn, RB, RBn\}$:, $\widehat{AUC}_w^{r,m}$

$$\mathsf{diff}^{r,m} = \widehat{\mathsf{AUC}}_w^{r,m} - \widehat{\mathsf{AUC}}_{\mathsf{true}}^r$$

Simulation study

Optimism correction AUC | 36



Simulation study

Optimism correction AUC | 37



Conclusions

Estimation of ROC and AUC | 38

Conclusions

- We propose unbiased design-based estimators for estimating the ROC curve and AUC in the context of complex survey data.
- Replicate weights recommended for the optimism correction of the AUC.

Conclusions

Estimation of ROC and AUC $_{\mid\,38}$

Conclusions

- We propose unbiased design-based estimators for estimating the ROC curve and AUC in the context of complex survey data.
- Replicate weights recommended for the optimism correction of the AUC.

Further research

- Variance estimation and confidence intervals for the ROC curve and AUC
- Extended simulation study to properly understand the behaviour of each replicate weight methods under different scenarios for optimism correction.

1 Introduction

2 Methodological proposals

3 Software development



svyVarSel R package

svyVarSel

40

Goal

Variable selection with complex survey data.

▶ Initially: LASSO regression models \implies Extended to: Elastic Nets

Available functions:

Function	Brief description
replicate.weights()	Define training and test sets with replicate weights.
wlasso()	Fit LASSO models with complex survey data.
<pre>welnet()</pre>	Fit elastic nets with complex survey data.
<pre>wlasso.plot()</pre>	Graphical visualization of the error.
<pre>welnet.plot()</pre>	Graphical visualization of the error.



svyVarSel: welnet()

Purpose

Fit elastic net models with complex survey data.

Formulation:

$$\min\left\{-p\ell(\boldsymbol{\beta})+\lambda\left(\alpha\sum_{j=1}^{p}|\beta_{j}|+(1-\alpha)\sum_{j=1}^{p}\beta_{j}^{2}\right)\right\}\Longrightarrow\lambda?$$

Steps: For a grid of values for λ_k , $k \in \{1, \ldots, K\}$,

- 1 Define train and test sets
- 2 Fit the models in the train set
- 3 Estimate the error of the fitted model in the test set

Select: $\lambda_k \in {\lambda_1, \ldots, \lambda_K}$, that minimizes the error

svyVarSel: welnet()

Usage

```
mcv <- welnet(data = simdata_lasso_binomial,</pre>
  col.y = "y", col.x = 1:50,
  family = "binomial",
  alpha = 0.5,
  cluster = "cluster", strata = "strata", weights = "weights",
  method = "dCV", k=10, R=20)
```

svyVarSel: welnet()

Output

A list containing the following elements:

- lambda:
 - > grid: All the values in the grid $\{\lambda_1, \ldots, \lambda_K\}$.
 - > min: The value of $\lambda_k \in \{\lambda_1, \dots, \lambda_K\}$ that minimizes the error.

▶ error:

- > average: average error for each $\lambda_k \in \{\lambda_1, \dots, \lambda_K\}$
- > all: error for each $\lambda_k \in \{\lambda_1, \ldots, \lambda_K\}$ in each test set.

▶ model:

- > grid: all the coefficients of all the fitted models for $\{\lambda_1, \ldots, \lambda_K\}$.
- > min: model coefficients considering the λ_k that minimizes the error.
- data.rw:
 - > Data frame with the information of the training and test sets defined with replicate weights.

Software development

Discussion and further research

svyVarSel: welnet.plot()

44

Usage and output



svyROC R package

svyROC

46

Goal

Estimation of the ROC curve, AUC and optimal cut-off points with complex survey data.

Available functions:

Function	Brief description	
<pre>wsp(), wse()</pre>	Estimate the specificity and sensitivity parameters	
wocp()	Estimate optimal cut-off points	
<pre>wauc()</pre>	Estimate the AUC	
<pre>corrected.wauc()</pre>	Corrected estimate of the AUC based on replicate weights	
wroc()	Estimate the ROC curve	
wroc.plot()	Plot the ROC curve	



https://github.com/aiparragirre/svyROC https://cran.r-project.org/web/packages/svyROC/

svyROC: wroc()

47

Usage

svyROC: wroc()

Output

A list containing the following elements:

- ▶ wroc.curve: list containing the following elements:
 - > Sew.values, Spw.values: all the values of the weighted estimate of sensitivity and specificity across all the possible cut-off points.
 - > cutoffs: all the evaluated cut-off points.
- wauc: a numeric value indicating the area under the curve.
- optimal.cutoff: list containing the following elements:
 - > method: Youden, ROC01, MaxProdSpSe or MaxEfficiency
 - > cutoff.value: optimal cut-off point
 - > Spw, Sew: sensitivity and specificity estimates for the optimal cutoff
- Other basic information

svyROC: wroc.plot()

Usage and output



svyROC: corrected.wauc()

Usage

Output

A list containing:

- corrected.AUCw: the value of the corrected AUC.
- Other basic information

1 Introduction

2 Methodological proposals





Discussion and further research

New proposals improve the development of prediction models

- Variable selection based on elastic nets
 - > Design-based cross-validation
- Unbiased estimators for the ROC curve and AUC
 - > Optimism correction based on replicate weights
- Easy to apply: implemented in svyVarSel and svyROC

Discussion and further research

New proposals improve the development of prediction models

- Variable selection based on elastic nets
 - > Design-based cross-validation
- Unbiased estimators for the ROC curve and AUC
 - > Optimism correction based on replicate weights
- Easy to apply: implemented in svyVarSel and svyROC

Further research

- ► Variable selection with **Statistical Boosting** for complex survey data.
- ► Variance estimation and confidence intervals for the ROC and AUC.
- Implement the proposals in svyVarSel and svyROC.

51

References

More methodological details

Variable selection



Iparragirre, A., Lumley, T., Barrio, I., & Arostegui, I. (2023). Variable selection with LASSO regression for complex survey data. *Stat*, 12(1), e578.

ROC curve and AUC

-			
100			

Iparragirre, A., Barrio, I., & Arostegui, I. (2023). Estimation of the ROC curve and the area under it with complex survey data. *Stat*, 12(1), e635.

	_ /

Iparragirre, A., Barrio, I., Aramendi, J. & Arostegui, I. (2022). Estimation of cut-off points under complex-sampling design data. *SORT-Statistics and Operations Research Transactions*, 46(1), 137– 158.

Iparragirre, A., Barrio, I. (2024). Optimism Correction of the AUC with Complex Survey Data. In: Einbeck, J., Maeng, H., Ogundimu, E., Perrakis, K. (eds) *Developments in Statistical Modelling. IWSM 2024. Contributions to Statistics.* Springer, Cham.

References

Related main references



Bamber, D.

The area above the ordinal dominance graph and the area below the receiver operating characteristic graph.

Journal of Mathematical Psychology, 1975; 12(4), 387-415.



Binder, D. A.

On the variances of asymptotically normal estimators from complex surveys. International Statistical Review/Revue Internationale de Statistique, 1983; 279-292.

Iparragirre, A., Barrio, I., & Rodríguez-Álvarez, M. X.

On the optimism correction of the area under the receiver operating characteristic curve in logistic prediction models.

SORT - Statistics and Operations Research Transactions, 2019; 43(1), 145-162.



Rao, J. N. K., & Wu, C. F. J.

Resampling Inference With Complex Survey Data. Journal of the American Statistical Association, 1988; 83(401), 231–241.



Tsuruta, H., & Bax, L.

Polychotomization of continuous variables in regression models based on the overall C index. BMC Medical Informatics and Decision Making, 2006; 6(1), 41.



Yao, W., Li, Z., & Graubard, B. I.

Estimation of ROC curve with complex survey data. *Statistics in Medicine*, 2015; 34(8), 1293-1303.

Thank you for your attention