Escuela Superior de Informática

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Nyström-based approximations for Kernel Logistic Regression: Application to transport choice modelling

José Ángel Martín-Baos

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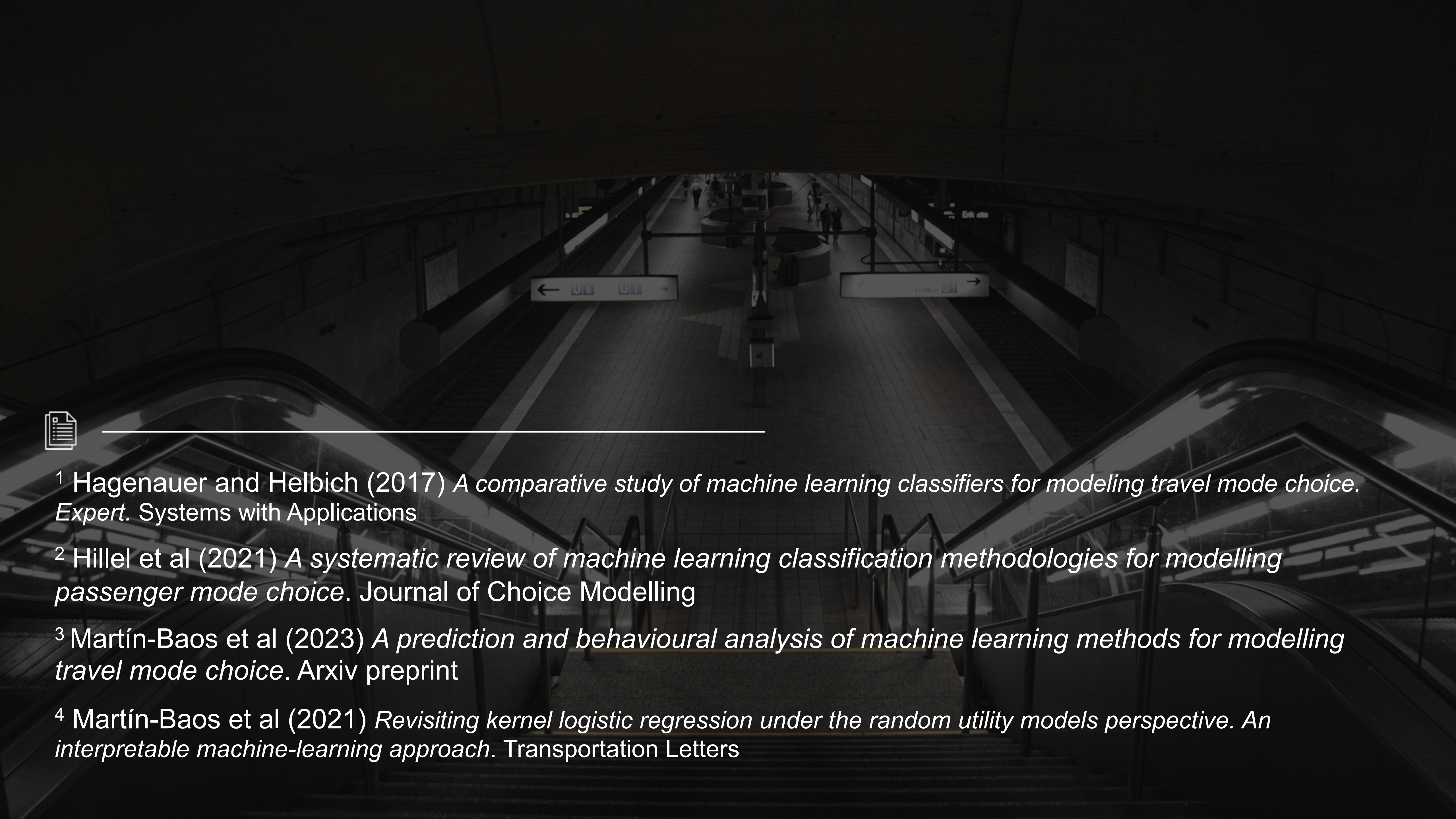
17-21 July 2023

World Conference on Transport Research



[1] Hagenauer and Helbich (2017) *A comparative study of machine learning classifiers for modeling travel mode choice. Expert.* Systems with Applications

[2] Hillel et al (2021) *A systematic review of machine learning classification methodologies for modelling passenger mode choice*. Journal of Choice Modelling

[3] Martín-Baos et al (2023) *A prediction and behavioural analysis of machine learning methods for modelling travel mode choice*. Arxiv preprint

[4] Martín-Baos et al (2021) *Revisiting kernel logistic regression under the random utility models perspective. An interpretable machine-learning approach*. Transportation Letters

$$U_{in} = V_{in} + \epsilon_{in}$$

$$U_{in} = \boxed{\text{KLR}} + \epsilon_{in}$$

KLR

$$V_i(\mathbf{x} \mid \boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_{in} k(\mathbf{x}_{in}, \mathbf{x})$$

$$[\mathbf{K}_i]_{n,n'} = k(\mathbf{x}_{in}, \mathbf{x}_{in'}) \quad \text{for } n, n' = 1, \ldots, N$$

$$V_i(\mathbf{x} \mid \boldsymbol{\alpha}) = \mathbf{K}_i^{(n)\top} \boldsymbol{\alpha}_i$$

$\mathbf{K}_i$

n	1	2	3	4	5	6
1	1.0	0.8	0.2	0.0	0.5	0.1
2	0.8	1.0	0.4	0.2	0.6	0.3
3	0.2	0.4	1.0	0.9	0.7	0.5
4	0.0	0.2	0.9	1.0	0.4	0.6
5	0.5	0.6	0.7	0.4	1.0	0.8
6	0.1	0.3	0.5	0.6	0.8	1.0

$\mathbf{K}_i$

n	1	2	3	4	5	6
1	1.0	0.8	0.2	0.0	0.5	0.1
2	0.8	1.0	0.4	0.2	0.6	0.3
3	0.2	0.4	1.0	0.9	0.7	0.5
4	0.0	0.2	0.9	1.0	0.4	0.6
5	0.5	0.6	0.7	0.4	1.0	0.8
6	0.1	0.3	0.5	0.6	0.8	1.0

$$\overset{\mathbf{K}_i}{\begin{array}{ccccccc} n & 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 1.0 & 0.8 & 0.2 & 0.0 & 0.5 & 0.1 \\ 2 & 0.8 & 1.0 & 0.4 & 0.2 & 0.6 & 0.3 \\ 3 & 0.2 & 0.4 & 1.0 & 0.9 & 0.7 & 0.5 \\ 4 & 0.0 & 0.2 & 0.9 & 1.0 & 0.4 & 0.6 \\ 5 & 0.5 & 0.6 & 0.7 & 0.4 & 1.0 & 0.8 \\ 6 & 0.1 & 0.3 & 0.5 & 0.6 & 0.8 & 1.0 \end{array}} \times \overset{\boldsymbol{\alpha}_i}{\begin{array}{c} \\ 0.82 \\ 0.14 \\ -0.26 \\ 0.91 \\ 0.74 \\ -0.6 \end{array}}$$

$$\mathbb{P}(\, i \mid \mathbf{K}_n, \boldsymbol{\alpha}\,) = \frac{e^{V_i}}{\sum_{j=1}^{I} e^{V_j}} = \frac{e^{\mathbf{K}_i^{(n)\top} \boldsymbol{\alpha}_i}}{\sum_{j=1}^{I} e^{\mathbf{K}_j^{(n)\top} \boldsymbol{\alpha}_j}}$$

Numerical results

GKLR Python package

https://github.com/JoseAngelMartinB/gklr

- Ubuntu 20.04 LTS
- 3.8 GHz 12 core AMD Ryzen
- 32 GB of RAM

LPMC

- Single day travel diary data from 2012 to 2015.
- 81,096 surveys with 31 variables.
- After pre-processing, 20 variables selected.

🚌 35% 🚗 44% 🚲 3% 🚶 18%

NTS

- ML focused dataset:
  - Data from a Dutch transport survey from 2010 to 2012.
  - Environmental data.
- 230,608 surveys with 16 variables.

🚌 4% 🚗 55% 🚲 24% 🚶 17%

KLR estimation problem

Spatial complexity to store the Gram matrix

$$\mathcal{O}(N^2)$$

Computational cost of V

$$\mathcal{O}(N^2)$$

Nyström method

$$V_i = \mathbf{K}_i \boldsymbol{\alpha}_i$$

$$\mathbf{K} \approx \mathbf{K}_{N,L} \cdot \mathbf{K}^{\dagger}_{L,L} \cdot \mathbf{K}^{\top}_{N,L}, \quad \text{with } L \ll N$$

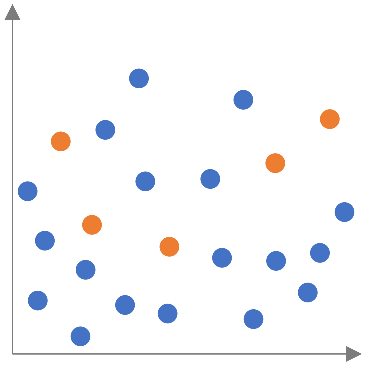
$$V_i = \mathbf{K}_{N,L} \cdot \left(\mathbf{K}^{\dagger}_{L,L} \cdot \left(\mathbf{K}^{\top}_{N,L} \cdot \boldsymbol{\alpha} \right) \right)$$

Complexity $\mathcal{O}(N \cdot L)$

Nyström method

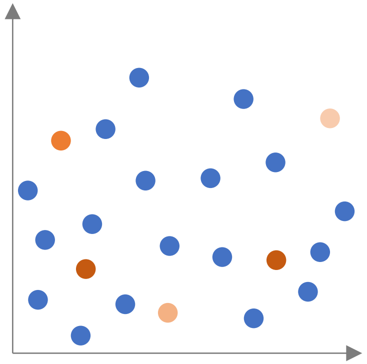
Random strategy

Nyström KLR



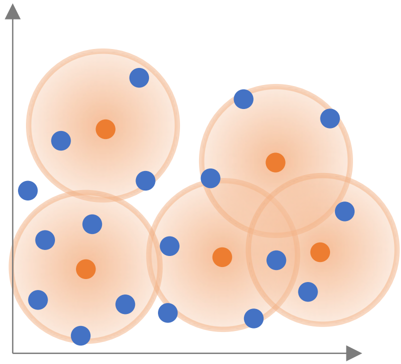
Divide-and-conquer ridge-leverage strategy

DAC ridge-leverage Nyström KLR



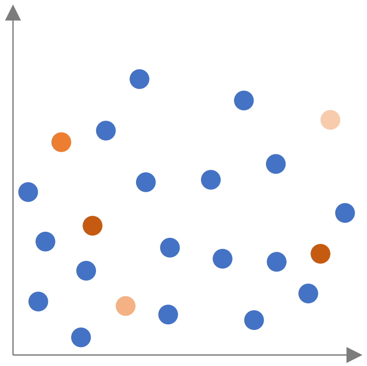
K-means strategy

K-means Nyström KLR



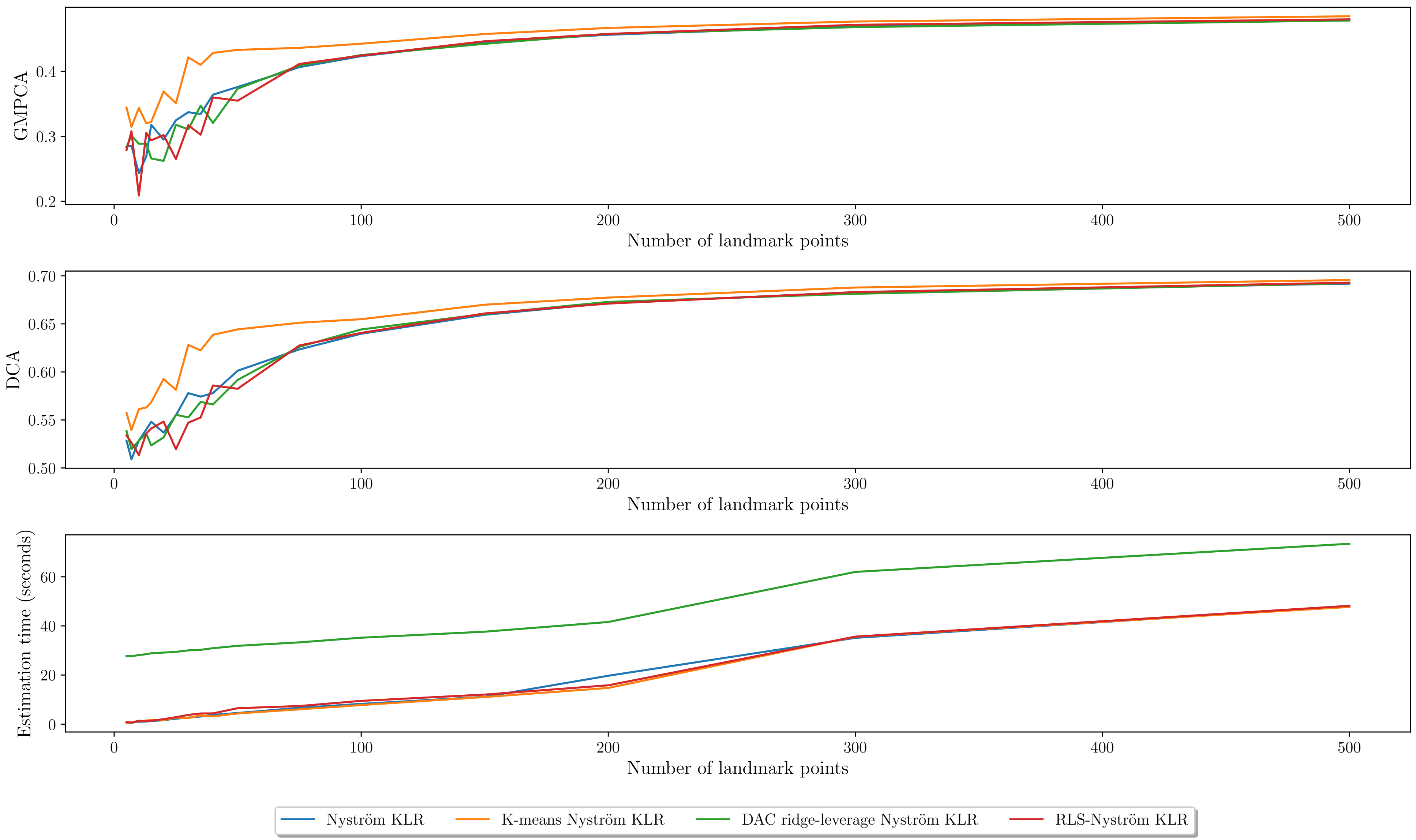
Recursive ridge-leverage strategy

RLS-Nyström KLR

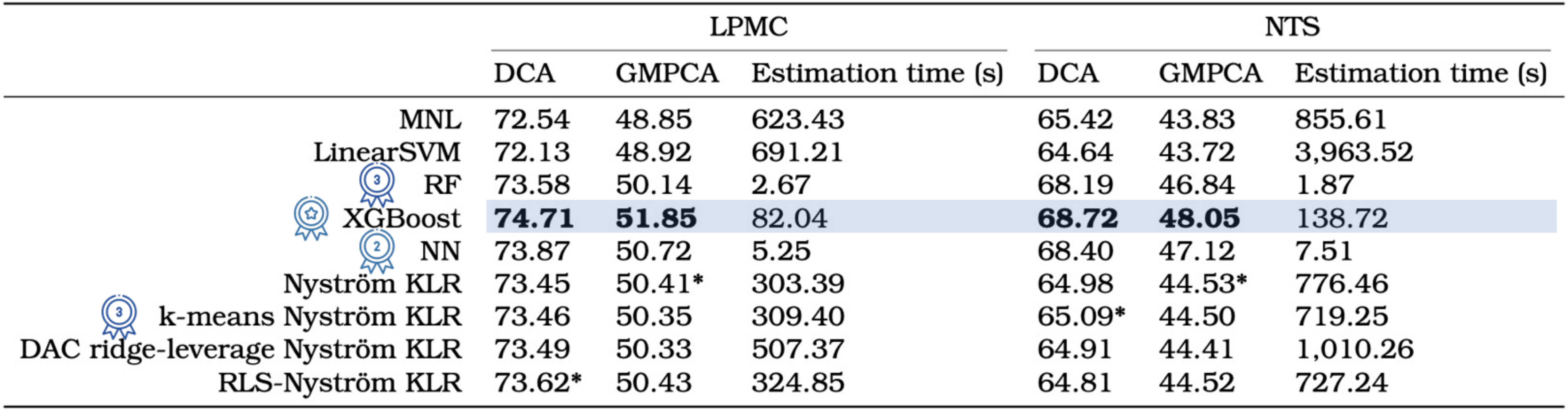


Experiment 1: Comparison Nyström KLR methods

NTS



Experiment 2: Comparison Nyström KLR and ML



	LPMC			NTS		
	DCA	GMPCA	Estimation time (s)	DCA	GMPCA	Estimation time (s)
MNL	72.54	48.85	623.43	65.42	43.83	855.61
LinearSVM	72.13	48.92	691.21	64.64	43.72	3,963.52
RF	73.58	50.14	2.67	68.19	46.84	1.87
XGBoost	**74.71**	**51.85**	82.04	**68.72**	**48.05**	138.72
NN	73.87	50.72	5.25	68.40	47.12	7.51
Nyström KLR	73.45	50.41*	303.39	64.98	44.53*	776.46
k-means Nyström KLR	73.46	50.35	309.40	65.09*	44.50	719.25
DAC ridge-leverage Nyström KLR	73.49	50.33	507.37	64.91	44.41	1,010.26
RLS-Nyström KLR	73.62*	50.43	324.85	64.81	44.52	727.24

Memory usage

LPMC

22 GB

$L = 500$

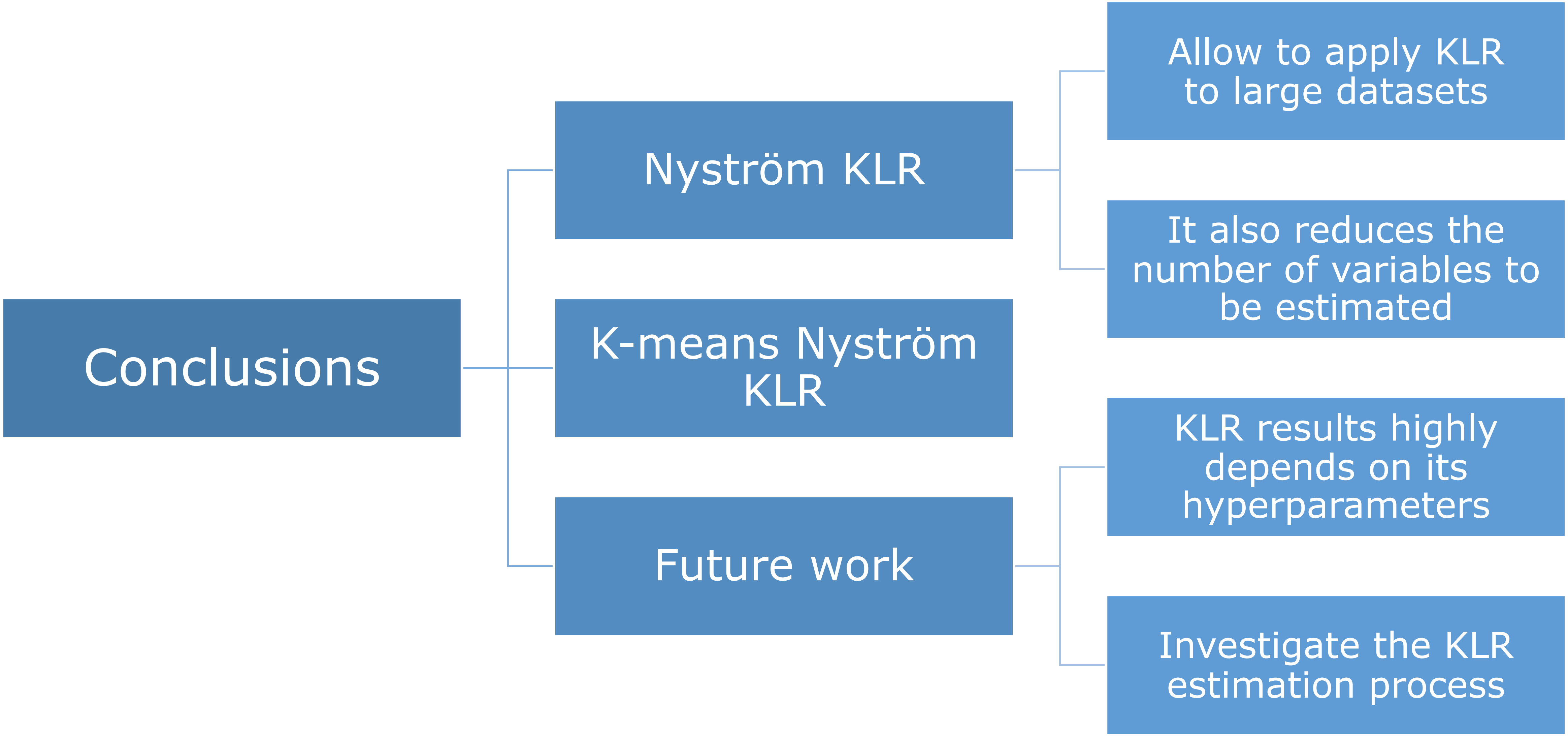
NTS

194 GB

$L = 1000$

Memory usage

LPMC	NTS
0.2 GB × **110**	1.2 GB × **160**
$L = 500$	$L = 1000$



Conclusions

Nyström KLR

- Allow to apply KLR to large datasets
- It also reduces the number of variables to be estimated

K-means Nyström KLR

Future work

- KLR results highly depends on its hyperparameters
- Investigate the KLR estimation process

Thanks for your attention!

For more information you can contact me at:

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More info of this research:

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MAT

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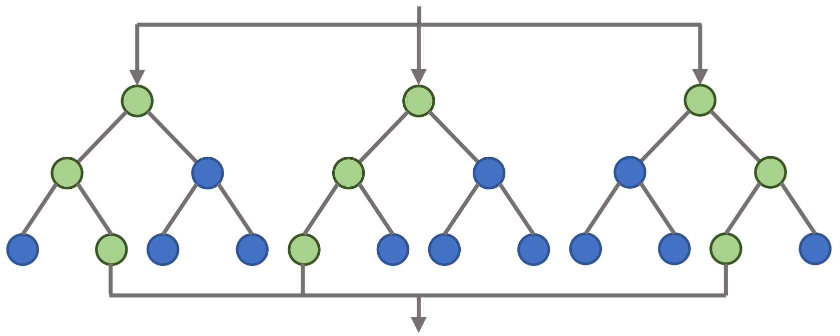
Supplementary material

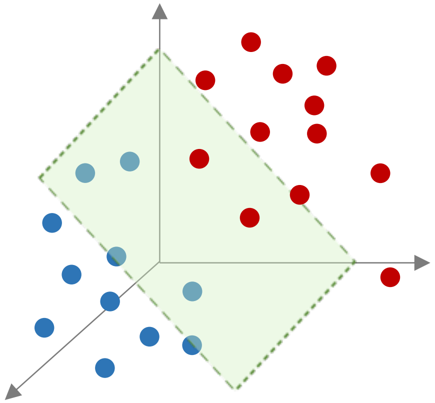
For the curious minds 😉

ML methods

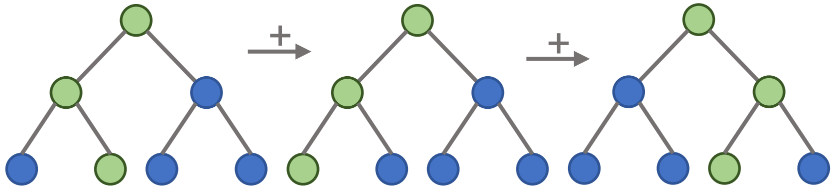
Random Forests (RF)



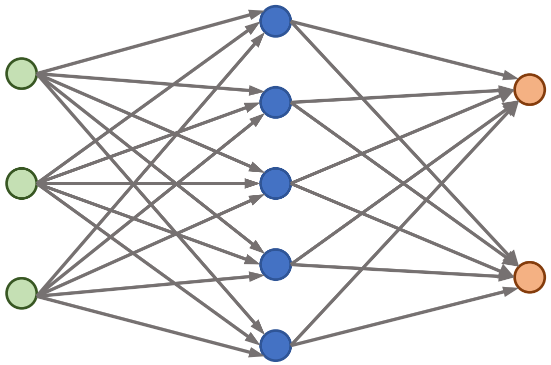
Support Vector Machines (SVM)



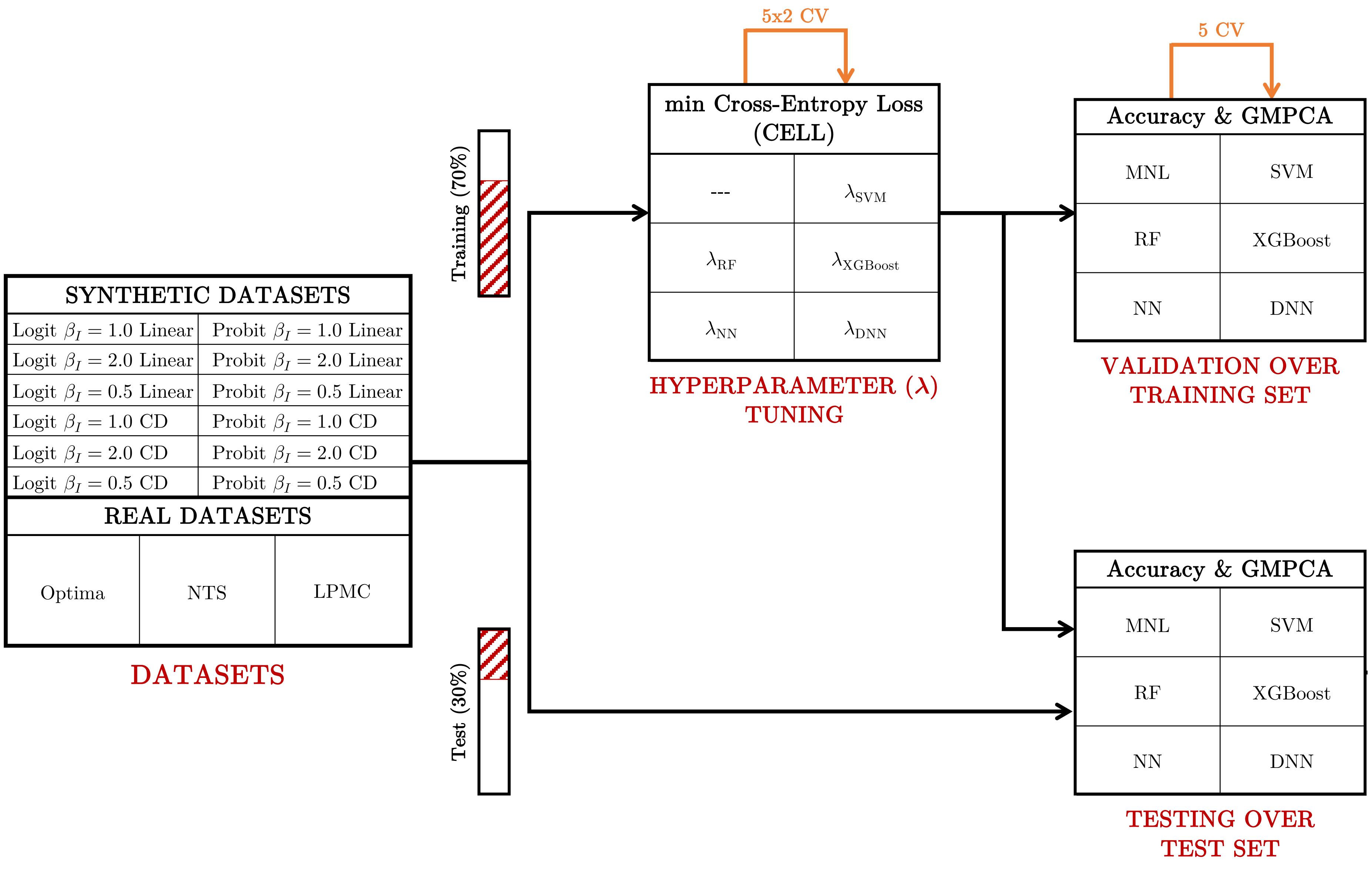
Gradient Boosting Decision Trees (GBDT)



Neural Networks (NN)



Hyperparameters tuning of ML models



SYNTHETIC DATASETS	
Logit $\beta_I = 1.0$ Linear	Probit $\beta_I = 1.0$ Linear
Logit $\beta_I = 2.0$ Linear	Probit $\beta_I = 2.0$ Linear
Logit $\beta_I = 0.5$ Linear	Probit $\beta_I = 0.5$ Linear
Logit $\beta_I = 1.0$ CD	Probit $\beta_I = 1.0$ CD
Logit $\beta_I = 2.0$ CD	Probit $\beta_I = 2.0$ CD
Logit $\beta_I = 0.5$ CD	Probit $\beta_I = 0.5$ CD

REAL DATASETS		
Optima	NTS	LPMC

DATASETS

min Cross-Entropy Loss (CELL)	
---	λ_{SVM}
λ_{RF}	λ_{XGBoost}
λ_{NN}	λ_{DNN}

HYPERPARAMETER (λ) TUNING

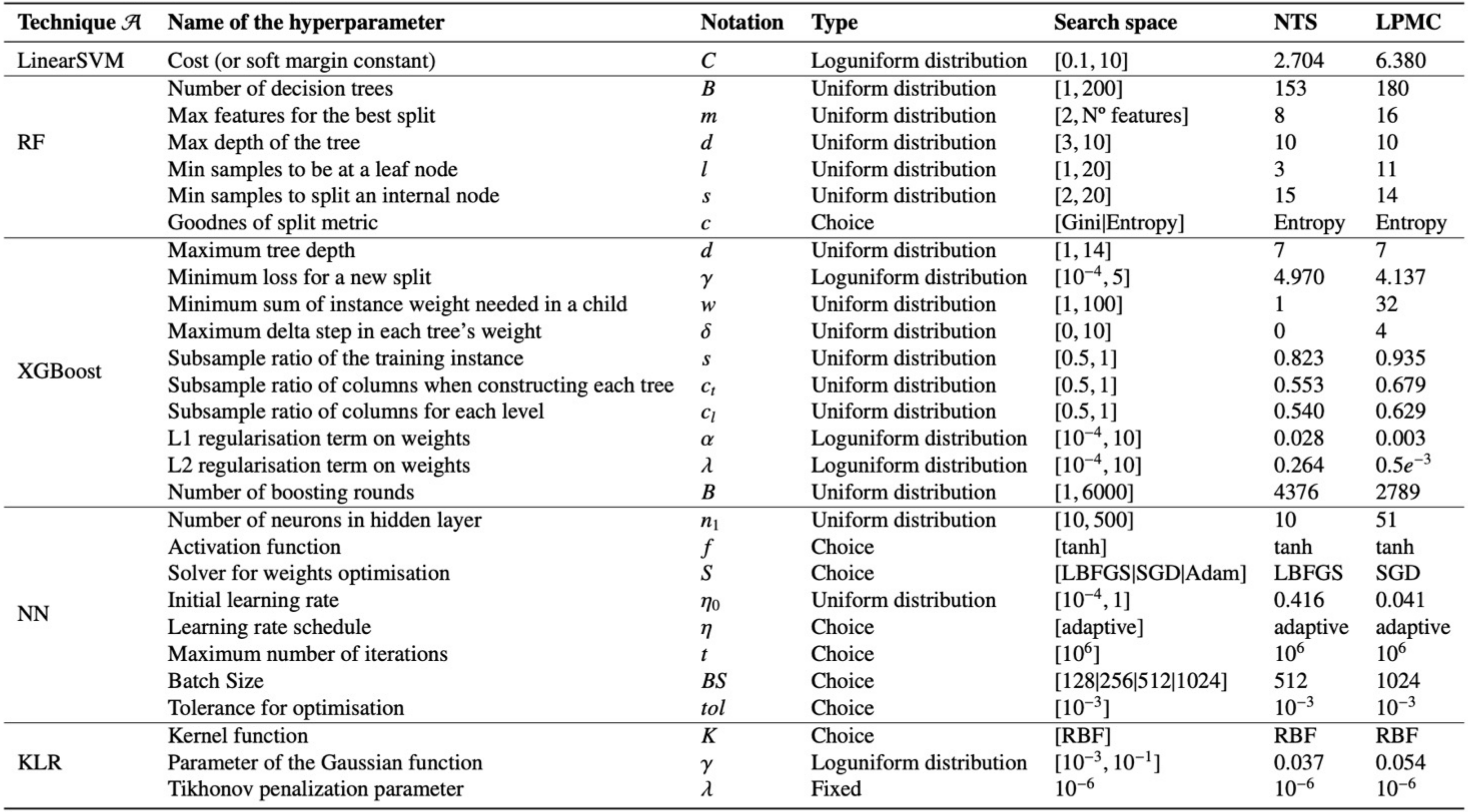
Accuracy & GMPCA	
MNL	SVM
RF	XGBoost
NN	DNN

VALIDATION OVER TRAINING SET

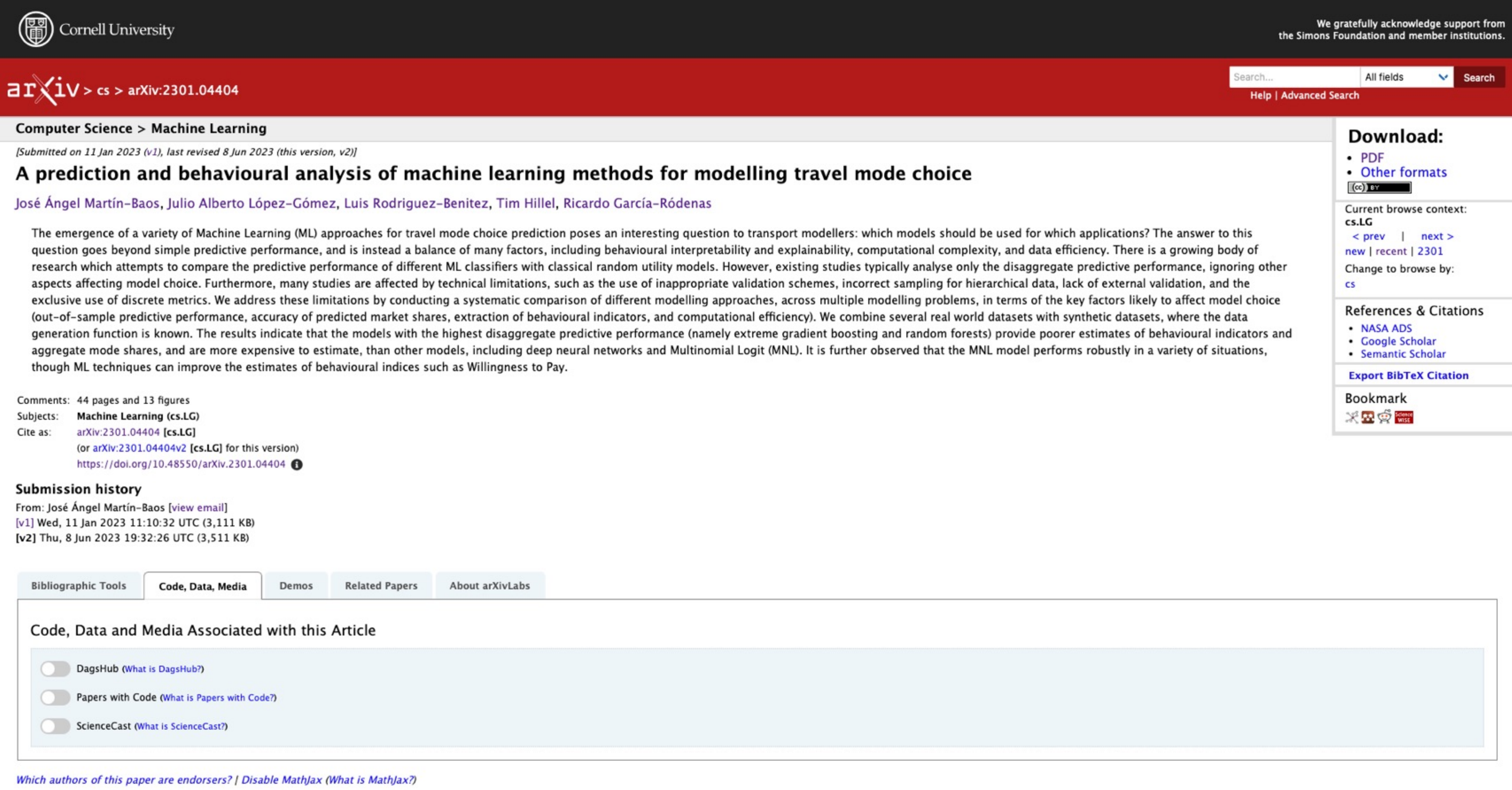
Accuracy & GMPCA	
MNL	SVM
RF	XGBoost
NN	DNN

TESTING OVER TEST SET

Hyperparameters space of ML models



Technique $\mathcal{A}$	Name of the hyperparameter	Notation	Type	Search space	NTS	LPMC
LinearSVM	Cost (or soft margin constant)	C	Loguniform distribution	$[0.1, 10]$	2.704	6.380
RF	Number of decision trees	B	Uniform distribution	$[1, 200]$	153	180
	Max features for the best split	m	Uniform distribution	[2, Nº features]	8	16
	Max depth of the tree	d	Uniform distribution	$[3, 10]$	10	10
	Min samples to be at a leaf node	l	Uniform distribution	$[1, 20]$	3	11
	Min samples to split an internal node	s	Uniform distribution	$[2, 20]$	15	14
	Goodnes of split metric	c	Choice	[Gini|Entropy]	Entropy	Entropy
XGBoost	Maximum tree depth	d	Uniform distribution	$[1, 14]$	7	7
	Minimum loss for a new split	γ	Loguniform distribution	$[10^{-4}, 5]$	4.970	4.137
	Minimum sum of instance weight needed in a child	w	Uniform distribution	$[1, 100]$	1	32
	Maximum delta step in each tree's weight	δ	Uniform distribution	$[0, 10]$	0	4
	Subsample ratio of the training instance	s	Uniform distribution	$[0.5, 1]$	0.823	0.935
	Subsample ratio of columns when constructing each tree	c_t	Uniform distribution	$[0.5, 1]$	0.553	0.679
	Subsample ratio of columns for each level	c_l	Uniform distribution	$[0.5, 1]$	0.540	0.629
	L1 regularisation term on weights	α	Loguniform distribution	$[10^{-4}, 10]$	0.028	0.003
	L2 regularisation term on weights	λ	Loguniform distribution	$[10^{-4}, 10]$	0.264	$0.5e^{-3}$
	Number of boosting rounds	B	Uniform distribution	$[1, 6000]$	4376	2789
NN	Number of neurons in hidden layer	n_1	Uniform distribution	$[10, 500]$	10	51
	Activation function	f	Choice	[tanh]	tanh	tanh
	Solver for weights optimisation	S	Choice	[LBFGS|SGD|Adam]	LBFGS	SGD
	Initial learning rate	η_0	Uniform distribution	$[10^{-4}, 1]$	0.416	0.041
	Learning rate schedule	η	Choice	[adaptive]	adaptive	adaptive
	Maximum number of iterations	t	Choice	$[10^6]$	10^6	10^6
	Batch Size	BS	Choice	[128|256|512|1024]	512	1024
	Tolerance for optimisation	tol	Choice	$[10^{-3}]$	10^{-3}	10^{-3}
KLR	Kernel function	K	Choice	[RBF]	RBF	RBF
	Parameter of the Gaussian function	γ	Loguniform distribution	$[10^{-3}, 10^{-1}]$	0.037	0.054
	Tikhonov penalization parameter	λ	Fixed	10^{-6}	10^{-6}	10^{-6}



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Computer Science > Machine Learning

[Submitted on 11 Jan 2023 (v1), last revised 8 Jun 2023 (this version, v2)]

A prediction and behavioural analysis of machine learning methods for modelling travel mode choice

José Ángel Martín-Baos, Julio Alberto López-Gómez, Luis Rodriguez-Benitez, Tim Hillel, Ricardo García-Ródenas

The emergence of a variety of Machine Learning (ML) approaches for travel mode choice prediction poses an interesting question to transport modellers: which models should be used for which applications? The answer to this question goes beyond simple predictive performance, and is instead a balance of many factors, including behavioural interpretability and explainability, computational complexity, and data efficiency. There is a growing body of research which attempts to compare the predictive performance of different ML classifiers with classical random utility models. However, existing studies typically analyse only the disaggregate predictive performance, ignoring other aspects affecting model choice. Furthermore, many studies are affected by technical limitations, such as the use of inappropriate validation schemes, incorrect sampling for hierarchical data, lack of external validation, and the exclusive use of discrete metrics. We address these limitations by conducting a systematic comparison of different modelling approaches, across multiple modelling problems, in terms of the key factors likely to affect model choice (out-of-sample predictive performance, accuracy of predicted market shares, extraction of behavioural indicators, and computational efficiency). We combine several real world datasets with synthetic datasets, where the data generation function is known. The results indicate that the models with the highest disaggregate predictive performance (namely extreme gradient boosting and random forests) provide poorer estimates of behavioural indicators and aggregate mode shares, and are more expensive to estimate, than other models, including deep neural networks and Multinomial Logit (MNL). It is further observed that the MNL model performs robustly in a variety of situations, though ML techniques can improve the estimates of behavioural indices such as Willingness to Pay.

Comments:	44 pages and 13 figures
Subjects:	**Machine Learning (cs.LG)**
Cite as:	arXiv:2301.04404 **[cs.LG]**
	(or arXiv:2301.04404v2 **[cs.LG]** for this version)
	https://doi.org/10.48550/arXiv.2301.04404

Submission history

From: José Ángel Martín-Baos [view email]
[v1] Wed, 11 Jan 2023 11:10:32 UTC (3,111 KB)
[v2] Thu, 8 Jun 2023 19:32:26 UTC (3,511 KB)

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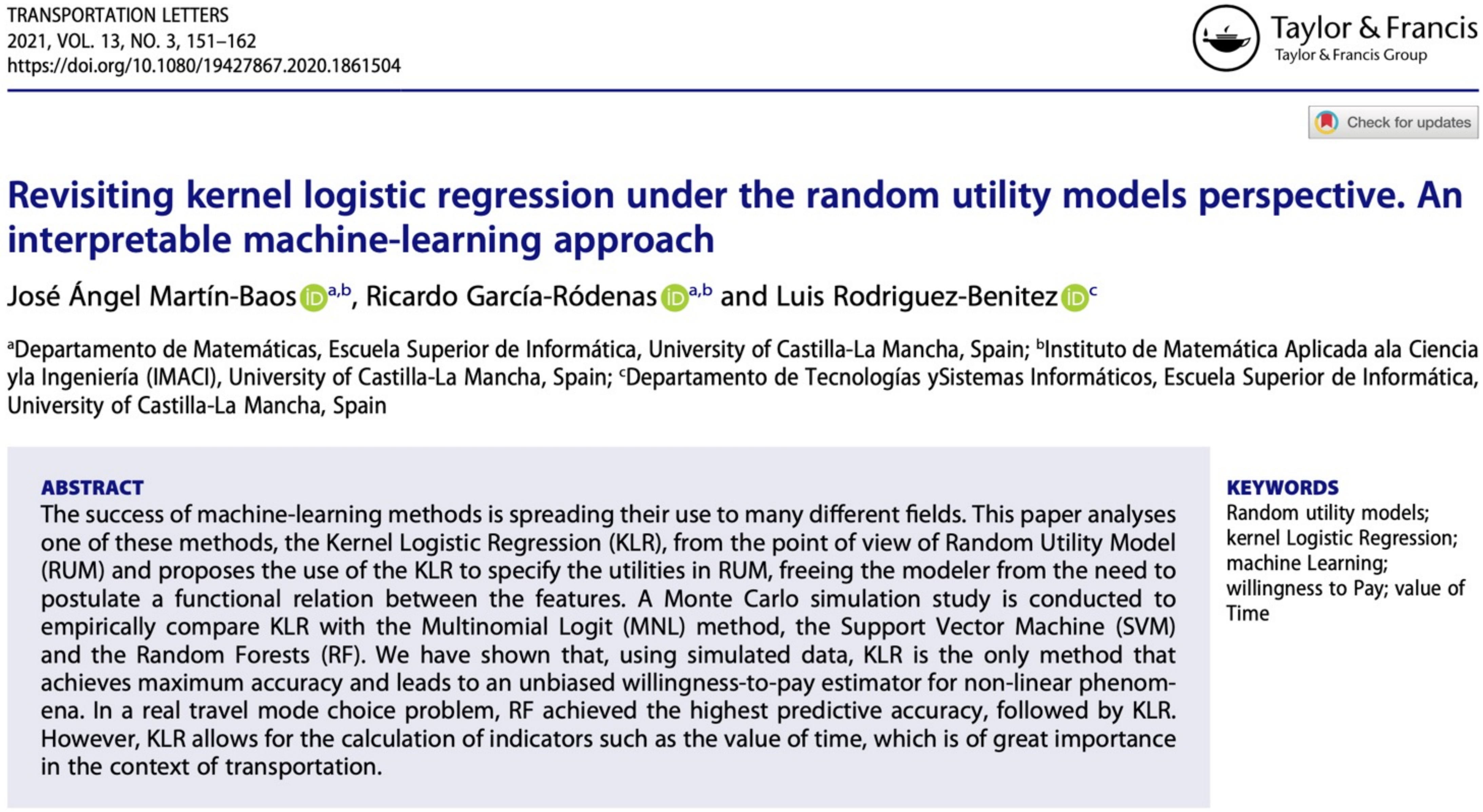

TRANSPORTATION LETTERS
2021, VOL. 13, NO. 3, 151–162
https://doi.org/10.1080/19427867.2020.1861504

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Revisiting kernel logistic regression under the random utility models perspective. An interpretable machine-learning approach

José Ángel Martín-Baos[a,b], Ricardo García-Ródenas[a,b] and Luis Rodriguez-Benitez[c]

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ABSTRACT

The success of machine-learning methods is spreading their use to many different fields. This paper analyses one of these methods, the Kernel Logistic Regression (KLR), from the point of view of Random Utility Model (RUM) and proposes the use of the KLR to specify the utilities in RUM, freeing the modeler from the need to postulate a functional relation between the features. A Monte Carlo simulation study is conducted to empirically compare KLR with the Multinomial Logit (MNL) method, the Support Vector Machine (SVM) and the Random Forests (RF). We have shown that, using simulated data, KLR is the only method that achieves maximum accuracy and leads to an unbiased willingness-to-pay estimator for non-linear phenomena. In a real travel mode choice problem, RF achieved the highest predictive accuracy, followed by KLR. However, KLR allows for the calculation of indicators such as the value of time, which is of great importance in the context of transportation.

KEYWORDS

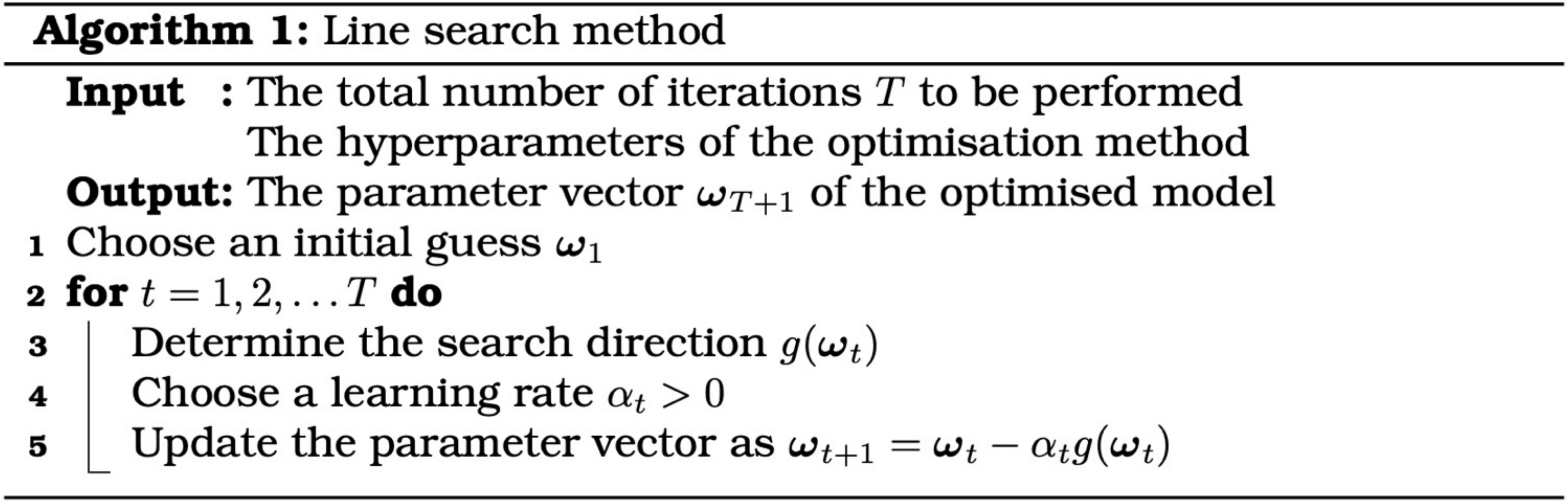
Random utility models; kernel Logistic Regression; machine Learning; willingness to Pay; value of Time

(Penalised) Maximum likelihood estimation

$$\mathcal{L}(\boldsymbol{\alpha}) = \prod_{n=1}^{N} \prod_{i=1}^{I} \mathbb{P}(\, i \mid \mathbf{x}_n, \boldsymbol{\alpha}_i \,)^{y_{in}}$$

$$\log \mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \sum_{i=1}^{I} y_{in} \log \mathbb{P}(\, i \mid \mathbf{x}_n, \boldsymbol{\alpha}_i \,)$$

$$\max_{\boldsymbol{\alpha}} \; \underbrace{\log \mathcal{L}(\boldsymbol{\alpha})}_{\text{Goodness of fit}} - \underbrace{\lambda \Omega(\boldsymbol{\alpha})}_{\text{Penalisation term}}$$



```
Algorithm 1: Line search method
Input  : The total number of iterations $T$ to be performed
         The hyperparameters of the optimisation method
Output: The parameter vector $\boldsymbol{\omega}_{T+1}$ of the optimised model
Choose an initial guess $\boldsymbol{\omega}_1$
for $t = 1, 2, \ldots T$ do
    Determine the search direction $g(\boldsymbol{\omega}_t)$
    Choose a learning rate $\alpha_t > 0$
    Update the parameter vector as $\boldsymbol{\omega}_{t+1} = \boldsymbol{\omega}_t - \alpha_t g(\boldsymbol{\omega}_t)$
```

GD:

$$g(\boldsymbol{\omega}_t) = -\nabla F(\boldsymbol{w}_t)$$

Quasi-Newton:

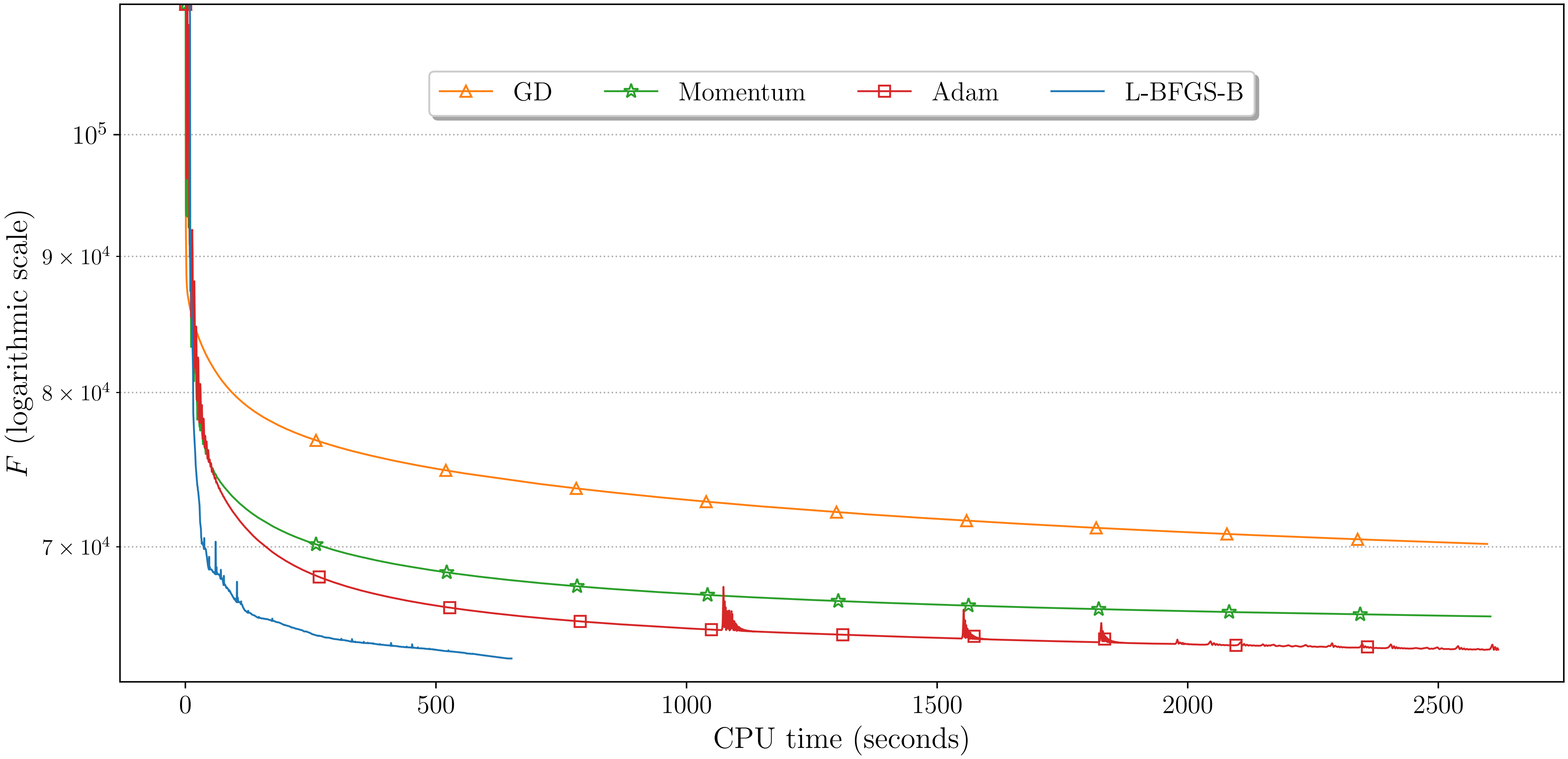
$$g(\boldsymbol{\omega}_t) = -H_t \nabla F(\boldsymbol{w}_t)$$

Newton:

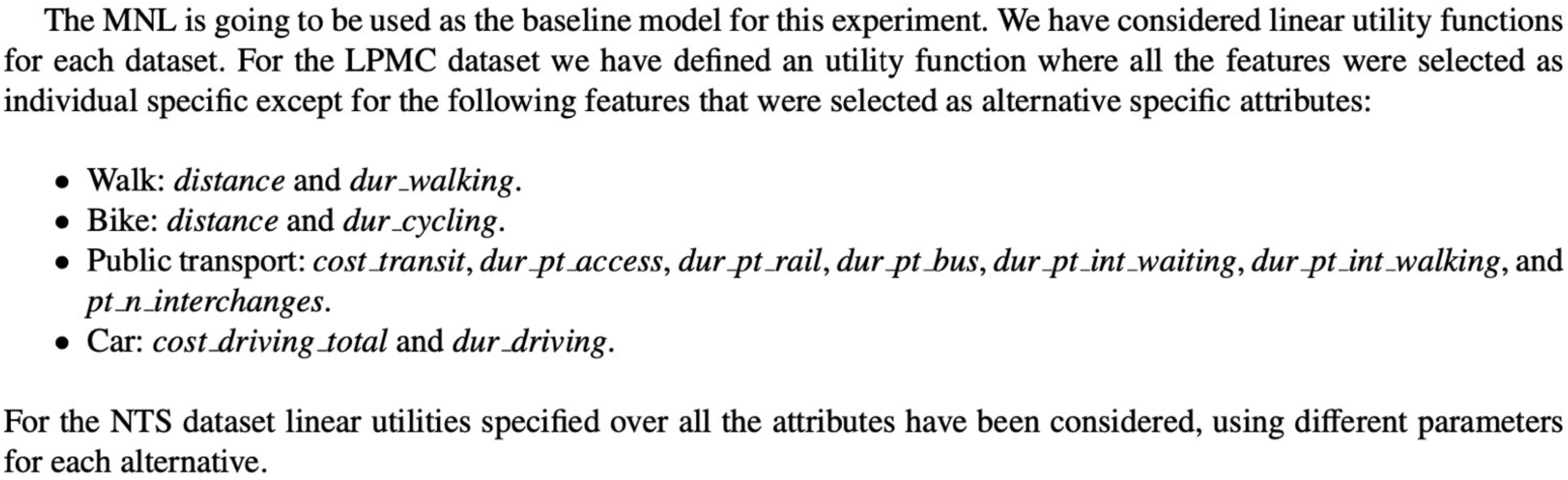
$$g(\boldsymbol{\omega}_t) = -[\nabla^2 F(\boldsymbol{w}_t)]^{-1} \nabla F(\boldsymbol{w}_t)$$

Comparison optimisation techniques

NTS



MNL model considered for the experiments

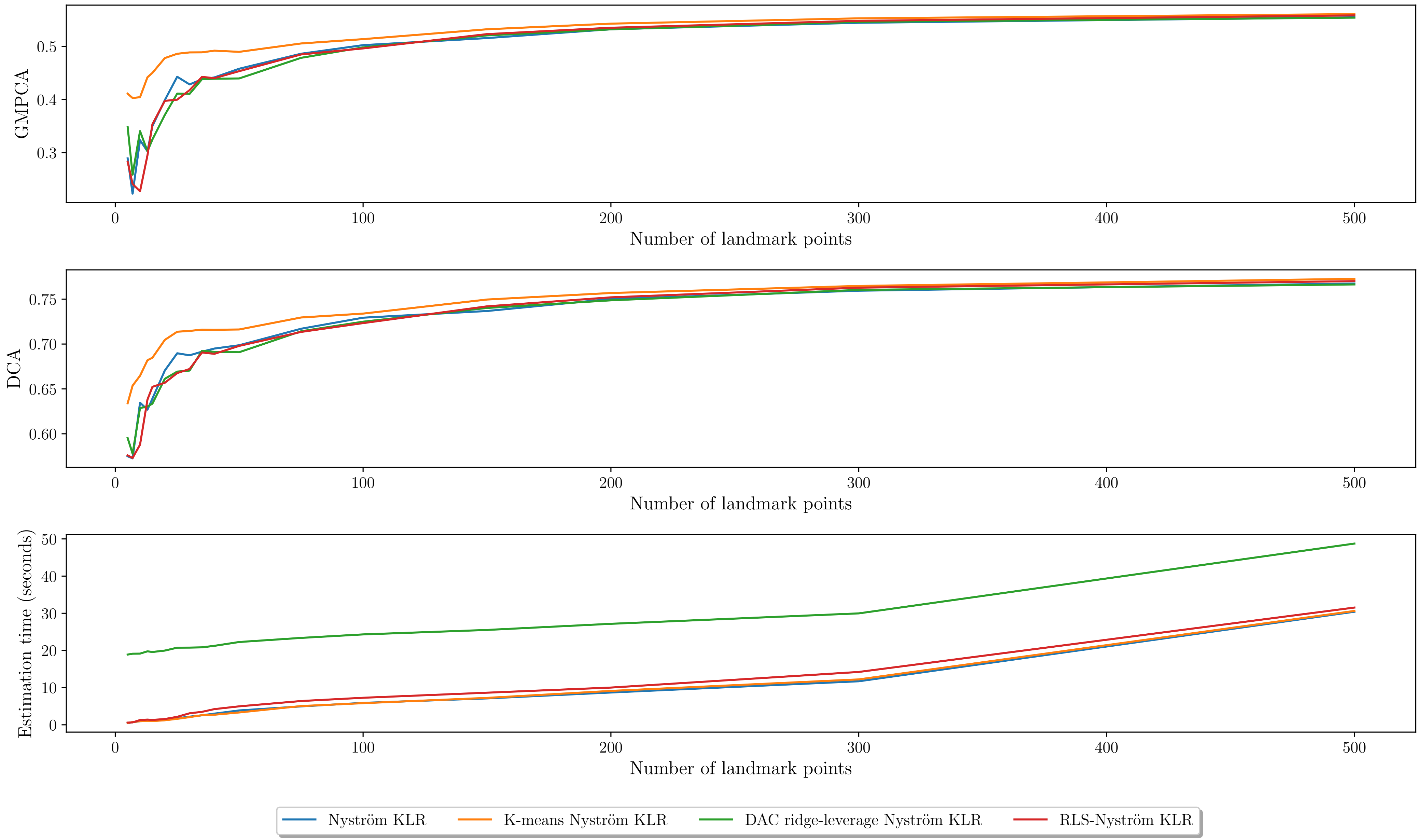


The MNL is going to be used as the baseline model for this experiment. We have considered linear utility functions for each dataset. For the LPMC dataset we have defined an utility function where all the features were selected as individual specific except for the following features that were selected as alternative specific attributes:

- Walk: *distance* and *dur_walking*.
- Bike: *distance* and *dur_cycling*.
- Public transport: *cost_transit*, *dur_pt_access*, *dur_pt_rail*, *dur_pt_bus*, *dur_pt_int_waiting*, *dur_pt_int_walking*, and *pt_n_interchanges*.
- Car: *cost_driving_total* and *dur_driving*.

For the NTS dataset linear utilities specified over all the attributes have been considered, using different parameters for each alternative.

Results for the LPMC dataset


GMPCA
DCA
Estimation time (seconds)
Number of landmark points
Nyström KLR
K-means Nyström KLR
DAC ridge-leverage Nyström KLR
RLS-Nyström KLR