

# Double-stage discretization approaches for biomarker-based bladder cancer survival modeling

Mauro Nascimben<sup>1\*,2</sup>, Manolo Venturin<sup>1</sup>, Lia Rimondini<sup>2</sup>

<sup>1</sup>Enginsoft SpA, Padova, Italy

<sup>2</sup>University of Eastern Piedmont Amedeo Avogadro, Dept. of Health Sciences, Novara, Italy

\*Email address for correspondence: [m.nascimben@enginsoft.com](mailto:m.nascimben@enginsoft.com)

## Supplementary Materials

### 1. Summary tables

Value counts of the annotated data are reported in the following tables divided by age group (Table 3), human sub-populations (Table 1) and gender (Table 2).

Table 1. Patient counts based on ethnicity

Human sub-population	Counts	Frequency [%]
Unknown	16	3.95
White	323	79.75
Black and Afro-Americans	23	5.67
Asians	43	10.61

Table 2. Patient counts based on gender

Gender	Counts	Frequency [%]
Male	298	73.58
Female	107	26.41

Table 3. Patient counts based on age

Ages	Counts	Frequency [%]
≤35	1	0.24
36-65	157	38.76
66-99	247	60.98

### 2. Threshold for skewness and kurtosis selection

There are different indications regarding the threshold that should be selected to consider a heavily or moderate skewness and kurtosis in literature. A standard statistical approach to test for normality could involve the Jarque-Bera goodness of fit test. Still, it is reliable for data-set with a larger number of observations than the one under exam cause of the asymptotic  $\chi^2$  distribution with 2 degrees of freedom enclosed by the statistical test. An alternative for kurtosis evaluation is the Kolmororov-Smirnov test. Nevertheless, the mean and standard deviation of the population are not known, and Kolmororov-Smirnov test could become very sensitive to minor variations when the number of observations is large. While excessive skewness could be detected with Anderson-Darling or the Shapiro-Wilk, the latter requires the a priori knowledge of mean and standard deviation. In [46] authors suggest  $\pm 1.5$  as cut-off value while in [47] and [48], authors selected  $\pm 2$  as limits. Other researchers [49] advise for a more strict threshold of  $\pm 1$  or even smaller [50] than it. In conclusion, it could be possible to confirm that chosen range  $\pm 1.96$  finds support in various sources [51], [52], [53] and [54]. Alternatively, bootstrapping for standard error and

confidence interval calculation [55] or D’Agostino  $K^2$  test could be a way to determine if the distribution is skewed and/or kurtic.

### 3. Notes on discretization operation

Top-down methods can be subdivided into supervised and unsupervised approaches. Unsupervised splitting algorithms include the standard binning operation of interval selection based on the generations of bins by equal-width or equal-frequency. In supervised fashion, a dataset of continuous values with  $M$  samples,  $f$  features and  $c$  class labels can be discretized using a scheme that returns  $k$  discrete disjoint intervals  $\{[d_0, d_1], [d_1, d_2], \dots, [d_{k-1}, d_k]\}$  where  $d_0$  and  $d_k$  are the minimal and maximal values and the set of cut points can be written as  $\{d_1, d_2, \dots, d_k\}$ . In practical applications, users try to optimize the number of discretized values because a large number of intervals may lead to erroneous results in the learning process [56]. In supervision-based discretization, the term inconsistency stands for the number of unavoidable errors when two examples with the same values have different class labels. In general, data-sets with continuous attributes are consistent, but discretization may lead to inconsistent data if the inconsistency level is more than zero.

#### 3.1. Notes on primary discretization algorithms

Table 4. Quanta matrix

2-D matrix for each attribute and discretization scheme				
Class	$[d_0, d_1]$	$[d_{r-1}, d_r]$	$[d_{n-1}, d_n]$	Class Total
$C_1$	$q_{1l}$	$q_{1r}$	$q_{1n}$	$M_{1+}$
...	...	...	...	.
...	...	...	...	.
$C_i$	$q_{il}$	$q_{ir}$	$q_{in}$	$M_{i+}$
Interval total	$M_{+1}$	$M_{+r}$	$M_{+n}$	$M$

1. CAIM (Class-Attribute Interdependence Maximization) estimates for each feature the relation between class and discretized variable as

$$\frac{\sum_{r=1}^n \frac{\max_r^2}{M_{+r}}}{n}$$

with  $n$  being the number of intervals,  $r$  iterates through intervals  $r = 1, 2, \dots, n$  and  $\max_r$  as maximum value within the  $r^{th}$  column of the matrix exemplified in Table 4.

2. CACC (Class-Attribute Contingency Coefficient) value defined as

$$\sqrt{\frac{y'}{y' + M}} \quad \text{for } y' = \frac{M \left[ \left( \sum_{i=1}^C \sum_{r=1}^n \frac{q_{ir}^2}{M_{i+} M_{+r}} \right) - 1 \right]}{\log(n)}$$

with  $M$  total number of samples and  $n$  the number of discretized intervals.

3. Ameva minimizes the number of discrete intervals based on the contingency coefficient

$$\sqrt{\frac{y}{y + M}}, \quad y = M \left[ \left( \sum_{i=1}^C \sum_{r=1}^n \frac{q_{ir}^2}{M_{i+} M_{+r}} \right) - 1 \right]$$

to reduce the loss of class variable interdependence based on the Chi-squared statistics

$$\frac{\chi^2(k)}{k(l-1)}$$

where  $k$  is the optimal number of intervals and  $l$  the number of classes.

4. MDLP (Minimum Description Length Principle) is a splitting method that subdivides continuous attributes into discrete intervals by minimizing the conditional entropy between the feature under exam and class values. Entropy is a popular measure in splitting algorithms and it is defined as the average of the information per event  $I(x) = -\log p_x$  with  $p_x$  estimated probability of the occurring event. In general, information is high for lower probable events. MDLP algorithm uses a stopping rule based on minimum description length principle.
5. ChiMerge, a merging algorithm that uses  $\chi^2$  statistics to merge adjacent intervals (local criterion applied to two neighboring intervals). A frequency table of the intervals (single samples are evaluated during the first iteration) is built for each feature and class, and intervals with shortest  $\chi^2$  values from the frequency table are combined together.
6. Modified Chi2 (Mod Chi2) that improves the Chi2 [57] method derived from ChiMerge. Modified Chi2 replaces the stopping criterion of the inconsistency check (requires a threshold defined by the user) with a decision about quality of approximation coined from the rough sets theory [58] that takes into account the effect of degrees of freedom.
7. Extended Chi2 (Ext Chi2), an algorithm that compensates the effect of variance when two intervals are merged to better handle uncertainty in the data. Stopping criterion consists in the measures of the least upper bound.
8. In CART discretization, a decision tree model subdivides data in non-uniform bins. For each feature the desirable intervals were selected by standard cost-complexity pruning of CART. This method proved resistant to overfitting. Hyperparameters were tuned using a grid of values to keep under control tree size, ensuring maximal entropy in the searched parameter space, and separately from classifiers to avoid problems given by nested cross-validation.
9. XGB, scalable and efficient implementation of gradient boosting, creates a set of non-uniform intervals applying the extreme gradient boosting model using the information contained in the outcome variable. This kind of discretization maintains non-linear patterns as present in continuous data. Early stopping rule was set by cross-validation based on hold-out data: without improvements after a certain number of iterations, boosting ends. Hyperparameters were tuned by selecting values in equally spaced grids to cover the parameter space [59] using a design that maximizes the determinant of spatial correlation matrix between points. In general, it should be noted that there is no guarantee that hyperparameter tuning will reduce overfitting or improve performance (*overhyping* phenomenon).

#### 4. Class separability metric

Formula derived from the within  $S_W$  and between scatter  $S_B$  matrix was applied to measure class separability  $J_{B/W}$ , based on the following equations:

$$S_W = \frac{1}{N} \sum_{i=1}^C \sum_{x \in w_i} (x - m_i)(x - m_i)^T$$

$$S_B = \sum_{i=1}^C P_i (m_i - m)(m_i - m)^T$$

$$J_{B/W} = \text{tr}(S_B S_W^{-1})$$

because it is desirable to maximize  $\text{tr}(S_B)$  and minimize  $\text{tr}(S_W)$  at the same time. Equation terms are:

- all classes  $C$  of the  $M$  dimensional feature space
- $N_i$  are the number of samples in class  $w_i$  and the total number of samples is  $N = \sum_{i=1}^C N_i$
- $P_i = N_i/N$ , a priori probability of class  $w_i$
- mean vector  $m = \sum_{i=1}^C P_i m_i$

Class separability metric was organized into the following Tables 5 and 8 for PCA and NCA algorithms respectively. Values including class separability measure when  $\pm 5\%$  uniform noise was added to the

discretized data can be found in Tables 6 and 9 for PCA and NCA respectively. Values with class separability measure when  $\pm 5\%$  gaussian noise was added to the discretized data-sets are in Tables 7 and 10.

Table 5. Class separability measure with PCA dimensionality reduction

Comp.	AMEVA	CACC	CAIM	Mod Chi2	ChiMerge	Ext Chi2	MDLP	CART	XGB
2	0.992	0.584	3.858	3.519	1.448	4.045	3.623	0.276	1.566
3	0.827	0.524	3.33	3.519	1.268	3.456	3.623	0.238	1.261
4	0.904	0.502	2.963	3.519	1.19	3.067	3.623	0.233	1.172
5	0.965	0.485	2.745	3.519	1.151	2.906	3.623	0.233	1.242
6	0.921	0.485	2.558	3.519	1.131	2.838	3.623	0.242	1.151
7	0.883	0.478	2.407	3.519	1.105	2.838	3.623	0.395	1.086
8	0.862	0.471	2.285	3.519	1.084	2.838	3.623	0.377	1.032
9	0.852	0.483	2.196	3.519	1.068	2.838	3.623	0.387	0.99
10	0.858	0.477	2.112	3.519	1.057	2.838	3.623	0.387	0.954
11	0.855	0.474	2.038	3.519	1.048	2.838	3.623	0.372	0.933
12	0.85	0.472	1.978	3.519	1.038	2.838	3.623	0.368	0.91
13	0.844	0.472	1.929	3.519	1.032	2.838	3.623	0.358	0.889
14	0.843	0.471	1.881	3.519	1.027	2.838	3.623	0.349	0.872
15	0.84	0.471	1.837	3.519	1.022	2.838	3.623	0.46	0.86
16	0.839	0.471	1.802	3.519	1.018	2.838	3.623	0.452	0.846
17	0.834	0.471	1.785	3.519	1.015	2.838	3.623	0.448	0.834
18	0.832	0.471	1.767	3.519	1.013	2.838	3.623	0.443	0.825
19	0.828	0.471	1.751	3.519	1.011	2.838	3.623	0.438	0.814
20	0.824	0.471	1.734	3.519	1.009	2.838	3.623	0.435	0.804
21	0.823	0.471	1.723	3.519	1.008	2.838	3.623	0.433	0.796
22	0.822	0.471	1.712	3.519	1.007	2.838	3.623	0.43	0.788
23	0.822	0.471	1.706	3.519	1.007	2.838	3.623	0.428	0.782
24	0.821	0.471	1.702	3.519	1.006	2.838	3.623	0.428	0.776
25	0.82	0.471	1.699	3.519	1.006	2.838	3.623	0.428	0.773

Table 6. Class separability measure with PCA dimensionality reduction and  $\pm 5\%$  uniform noise

Comp.	AMEVA	CACC	CAIM	Mod Chi2	ChiMerge	Ext Chi2	MDLP	CART	XGB
2	0.99	0.585	3.904	3.511	1.449	3.973	3.556	0.278	1.598
3	0.825	0.524	3.366	3.503	1.268	3.385	3.549	0.238	1.284
4	0.909	0.502	2.994	3.497	1.19	2.999	3.54	0.233	1.2
5	0.968	0.486	2.77	3.489	1.151	2.844	3.532	0.233	1.253
6	0.923	0.485	2.58	3.481	1.131	2.779	3.526	0.242	1.161
7	0.886	0.478	2.429	3.474	1.105	2.776	3.518	0.396	1.094
8	0.865	0.471	2.306	3.467	1.084	2.774	3.511	0.377	1.04
9	0.855	0.483	2.213	3.461	1.068	2.772	3.505	0.388	0.997
10	0.86	0.477	2.13	3.455	1.057	2.77	3.499	0.387	0.961
11	0.858	0.474	2.053	3.448	1.048	2.768	3.493	0.372	0.939
12	0.852	0.472	1.991	3.442	1.038	2.766	3.487	0.368	0.915
13	0.846	0.472	1.943	3.437	1.032	2.764	3.481	0.358	0.894
14	0.846	0.471	1.893	3.431	1.027	2.762	3.476	0.349	0.877
15	0.842	0.471	1.849	3.426	1.022	2.76	3.47	0.46	0.865
16	0.84	0.471	1.811	3.42	1.019	2.759	3.465	0.451	0.851
17	0.835	0.471	1.795	3.415	1.016	2.757	3.459	0.448	0.838
18	0.834	0.471	1.778	3.41	1.013	2.755	3.455	0.443	0.828
19	0.829	0.471	1.761	3.406	1.011	2.753	3.45	0.438	0.817
20	0.826	0.471	1.743	3.401	1.009	2.752	3.446	0.435	0.808
21	0.824	0.471	1.731	3.397	1.008	2.751	3.442	0.433	0.799
22	0.823	0.471	1.72	3.393	1.007	2.749	3.438	0.43	0.791
23	0.823	0.471	1.713	3.389	1.007	2.748	3.434	0.427	0.785
24	0.822	0.471	1.709	3.385	1.007	2.746	3.431	0.428	0.779
25	0.821	0.471	1.706	3.382	1.007	2.745	3.427	0.428	0.775

## Supplementary Materials

Table 7. Class separability measure with PCA dimensionality reduction and  $\pm 5\%$  gaussian noise

Comp.	AMEVA	CACC	CAIM	Mod Chi2	ChiMerge	Ext Chi2	MDLP	CART	XGB
2	1.009	0.585	3.856	3.661	1.449	4.051	3.581	0.276	1.525
3	0.839	0.524	3.328	3.634	1.268	3.476	3.556	0.238	1.23
4	0.917	0.502	2.954	3.611	1.19	3.084	3.532	0.233	1.138
5	0.974	0.486	2.738	3.587	1.151	2.905	3.511	0.233	1.225
6	0.929	0.485	2.551	3.565	1.131	2.841	3.489	0.239	1.134
7	0.891	0.478	2.406	3.545	1.105	2.833	3.468	0.395	1.07
8	0.868	0.471	2.281	3.528	1.084	2.826	3.448	0.377	1.015
9	0.859	0.484	2.191	3.508	1.068	2.818	3.429	0.389	0.974
10	0.862	0.477	2.105	3.489	1.057	2.812	3.41	0.388	0.937
11	0.858	0.474	2.029	3.471	1.048	2.806	3.392	0.373	0.914
12	0.854	0.472	1.968	3.454	1.038	2.799	3.375	0.369	0.892
13	0.849	0.472	1.915	3.437	1.032	2.794	3.358	0.358	0.871
14	0.845	0.471	1.865	3.421	1.027	2.788	3.346	0.349	0.855
15	0.843	0.471	1.819	3.407	1.022	2.783	3.335	0.459	0.841
16	0.842	0.471	1.788	3.394	1.019	2.779	3.32	0.45	0.827
17	0.839	0.471	1.767	3.38	1.016	2.774	3.307	0.446	0.815
18	0.836	0.471	1.744	3.366	1.013	2.769	3.296	0.441	0.804
19	0.831	0.471	1.734	3.354	1.011	2.764	3.284	0.437	0.794
20	0.828	0.471	1.717	3.343	1.009	2.76	3.271	0.434	0.784
21	0.826	0.471	1.705	3.331	1.008	2.756	3.26	0.431	0.776
22	0.826	0.471	1.695	3.32	1.007	2.752	3.249	0.429	0.769
23	0.825	0.471	1.688	3.311	1.007	2.748	3.244	0.426	0.763
24	0.824	0.471	1.683	3.301	1.006	2.744	3.235	0.427	0.757
25	0.823	0.471	1.68	3.292	1.006	2.741	3.226	0.426	0.753

Table 8. Class separability measure with NCA dimensionality reduction

Comp.	AMEVA	CACC	CAIM	Mod Chi2	ChiMerge	Ext Chi2	MDLP	CART	XGB
2	1.985	0.497	4.194	4.621	1.238	5.644	4.648	0.499	3.781
3	1.584	0.546	4.766	4.621	1.31	7.856	4.648	0.342	3.025
4	1.625	0.451	4.028	4.621	1.421	6.089	4.648	0.542	3.723
5	1.724	0.466	4.93	4.621	1.534	6.015	4.648	0.265	3.215
6	1.82	0.739	4.952	4.621	1.229	4.76	4.648	0.172	3.314
7	1.666	0.664	4.963	4.621	0.654	4.76	4.648	0.522	2.801
8	1.378	0.315	5.063	4.621	1.577	4.76	4.648	0.828	2.944
9	1.523	0.484	4.918	4.621	0.978	4.76	4.648	0.515	2.205
10	1.725	0.477	4.484	4.621	0.643	4.76	4.648	0.302	2.173
11	1.137	0.369	4.84	4.621	0.955	4.76	4.648	0.467	2.747
12	1.51	0.474	4.939	4.621	1.041	4.76	4.648	0.53	2.73
13	1.235	0.464	4.861	4.621	1.473	4.76	4.648	0.499	2.262
14	1.331	0.47	4.596	4.621	1.345	4.76	4.648	0.422	2.12
15	1.163	0.471	4.467	4.621	1.628	4.76	4.648	0.676	2.106
16	0.795	0.47	4.574	4.621	1.248	4.76	4.648	0.556	2.104
17	0.952	0.47	4.659	4.621	1.012	4.76	4.648	0.609	2.074
18	1.39	0.47	4.491	4.621	1.487	4.76	4.648	0.528	2.218
19	1.639	0.47	4.864	4.621	1.207	4.76	4.648	0.672	1.728
20	2.004	0.47	5.311	4.621	0.84	4.76	4.648	0.756	1.964
21	1.778	0.471	5.029	4.621	0.736	4.76	4.648	0.813	2.034
22	1.686	0.471	5.264	4.621	1.616	4.76	4.648	0.847	1.805
23	1.858	0.471	5.049	4.621	1.167	4.76	4.648	0.737	1.971
24	1.753	0.471	5.069	4.621	1.183	4.76	4.648	0.735	1.952
25	1.862	0.471	4.988	4.621	1.485	4.76	4.648	0.628	1.791

Table 9. Class separability measure with NCA dimensionality reduction ( $\pm 5\%$  random uniform noise)

Comp.	AMEVA	CACC	CAIM	Mod Chi2	ChiMerge	Ext Chi2	MDLP	CART	XGB
2	1.829	0.566	4.476	4.705	1.738	2.57	3.702	0.453	2.813
3	1.551	0.54	5.268	4.677	2.03	3.988	3.595	0.269	2.763
4	1.612	0.501	4.266	4.696	1.321	1.605	3.585	0.263	3.345
5	1.867	0.488	4.833	4.719	1.301	4.702	3.584	0.231	3.407
6	1.791	0.504	4.221	4.725	0.721	3.291	3.584	0.175	3.308
7	1.248	0.482	4.542	4.65	0.801	3.491	3.548	0.715	2.35
8	1.103	0.408	3.806	4.65	1.165	3.334	3.547	0.536	2.679
9	1.528	0.486	3.993	4.657	0.833	3.237	3.556	0.524	2.356
10	1.685	0.476	4.077	4.644	0.751	3.47	3.578	0.369	2.107
11	1.058	0.653	4.608	4.645	0.868	3.753	3.429	0.461	2.523
12	1.457	0.472	4.203	4.63	0.967	4.127	3.449	0.494	2.677
13	1.08	0.574	4.701	4.585	1.142	4.068	3.377	0.492	2.385
14	0.952	0.471	4.972	4.573	1.068	4.45	3.36	0.406	2.179
15	0.739	0.471	5.096	4.566	1.469	4.363	3.369	0.764	2.304
16	0.853	0.471	4.664	4.565	1.255	3.236	3.396	0.589	2.069
17	1.323	0.471	4.794	4.571	0.871	3.535	3.406	0.576	2.139
18	1.192	0.471	4.717	4.567	1.401	4.016	3.443	0.48	2.214
19	1.625	0.471	5.17	4.535	1.325	3.227	3.464	0.739	1.935
20	1.694	0.471	5.119	4.533	0.89	3.445	3.484	0.724	1.774
21	1.697	0.471	4.765	4.525	1.161	2.967	3.482	0.773	1.753
22	2.016	0.471	4.649	4.564	1.233	3.197	3.498	0.629	1.847
23	1.869	0.471	4.675	4.526	1.398	3.704	3.505	0.68	1.96
24	1.63	0.471	4.495	4.539	1.134	3.413	3.506	0.651	2.005
25	1.614	0.471	4.38	4.506	1.142	3.758	3.515	0.646	1.809

Table 10. Class separability measure with NCA dimensionality reduction ( $\pm 5\%$  random gaussian noise)

Comp.	AMEVA	CACC	CAIM	Mod Chi2	ChiMerge	Ext Chi2	MDLP	CART	XGB
2	2.395	0.526	3.922	5.396	1.49	5.019	4.718	0.346	3.575
3	1.784	0.536	4.463	5.337	1.409	3.54	4.583	0.415	2.994
4	1.575	0.501	4.636	5.151	1.03	3.307	4.623	0.271	3.114
5	1.813	0.484	5.678	5.191	1.234	1.861	4.607	0.18	2.951
6	1.813	0.492	4.845	5.072	1.437	2.791	4.609	0.207	2.965
7	1.76	0.392	5.	4.989	1.223	2.77	4.54	0.48	2.979
8	1.285	0.346	5.024	4.982	1.375	2.665	4.493	0.458	2.786
9	1.066	0.484	5.002	5.046	0.734	1.817	4.52	0.383	2.604
10	1.448	0.477	4.725	5.163	0.237	1.9	4.526	0.455	2.452
11	1.041	0.428	4.558	5.145	1.023	2.229	4.54	0.403	2.104
12	1.533	0.474	4.624	5.133	0.728	2.287	4.547	0.388	2.05
13	1.109	0.34	4.242	5.135	1.362	2.31	4.53	0.4	1.989
14	1.152	0.544	4.173	5.151	1.038	2.066	4.549	0.62	1.837
15	0.917	0.492	4.024	5.142	1.441	1.675	4.558	0.58	1.657
16	0.853	0.471	3.75	5.129	1.389	2.552	4.545	0.56	2.103
17	0.687	0.465	4.274	5.126	1.011	2.469	4.542	0.539	2.006
18	1.181	0.471	4.401	5.097	1.294	2.277	4.563	0.467	1.911
19	1.357	0.471	4.612	5.085	0.803	2.266	4.556	0.57	1.663
20	1.144	0.471	4.657	5.077	1.467	2.429	4.54	0.688	1.593
21	1.227	0.471	5.286	5.086	1.018	2.593	4.565	0.727	1.609
22	1.308	0.471	5.112	5.032	1.4	2.263	4.564	0.756	1.524
23	1.212	0.471	4.919	5.033	1.528	2.399	4.582	0.679	1.455
24	1.266	0.471	4.77	5.047	1.378	2.685	4.565	0.765	1.298
25	1.111	0.471	4.648	5.034	1.586	2.459	4.56	0.861	1.165

5. Notes on Numerical Experiment 1

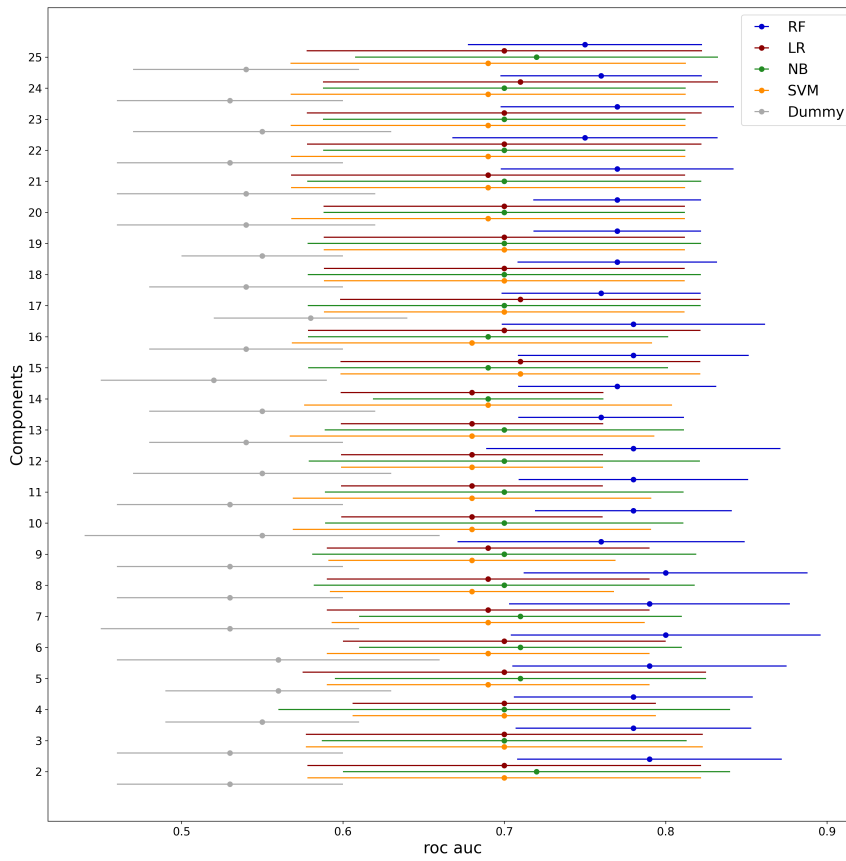


Figure 1. CV outcomes for XGB discretizer: reducing model complexity does not affect performance of RF classifier

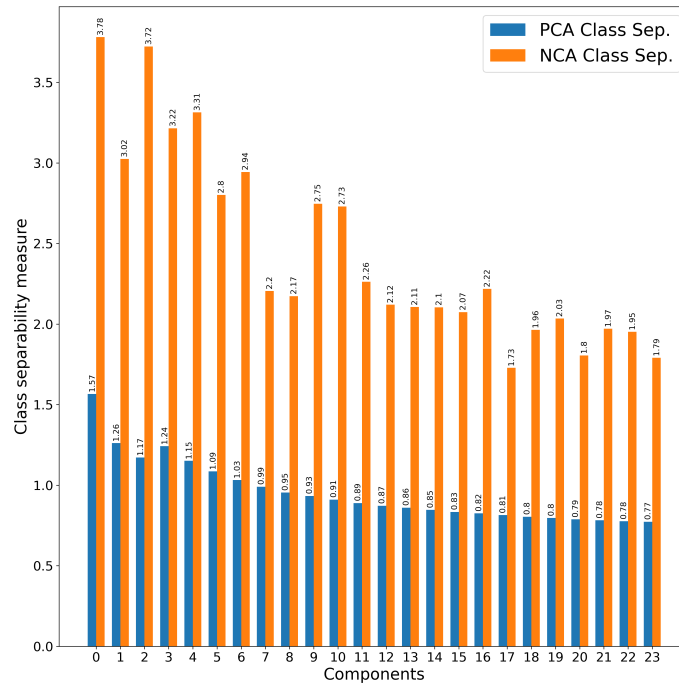


Figure 2. Class separability measure for XGB Discretizer

In this section, additional tables were included as part of the data analysis carried out during numerical experiment 1. Values describe the addition of  $\pm 5\%$  uniform or gaussian noise to discretized data after PCA and NCA dataset reduction. Values aggregating PCA data transformation and  $\pm 5\%$  uniform noise are in Table 11 while  $\pm 5\%$  gaussian noise computation is in Table 12. Table with NCA dimensionality reduction and addition of  $\pm 5\%$  uniform noise is Table 13 while addition of  $\pm 5\%$  gaussian noise can be found in Table 14. Discretizer with the highest ROC AUC at cross-validation is included to reduce the amount of information, while keeping only the most explanatory one.

Table 11. Best discretizer using different configurations of PCA components and addition of  $\pm 5$  random uniform noise

Comp.	RF	LR	NB	SVM	Dummy
2	CAIM 0.67 $\pm$ 0.07	CAIM 0.68 $\pm$ 0.11	CAIM 0.69 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.1	CACC 0.56 $\pm$ 0.09
3	CAIM 0.67 $\pm$ 0.06	CAIM 0.7 $\pm$ 0.12	CAIM 0.69 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.11	Mod Chi2 0.56 $\pm$ 0.09
4	CAIM 0.64 $\pm$ 0.07	CAIM 0.69 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.1	CAIM 0.68 $\pm$ 0.1	CACC 0.56 $\pm$ 0.07
5	AMEVA 0.65 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.1	CAIM 0.68 $\pm$ 0.09	CART 0.54 $\pm$ 0.06
6	CAIM 0.64 $\pm$ 0.06	CAIM 0.69 $\pm$ 0.11	CAIM 0.69 $\pm$ 0.09	CAIM 0.68 $\pm$ 0.1	CART 0.55 $\pm$ 0.07
7	CAIM 0.64 $\pm$ 0.07	CAIM 0.68 $\pm$ 0.12	CAIM 0.69 $\pm$ 0.1	CAIM 0.67 $\pm$ 0.11	CART 0.53 $\pm$ 0.08
8	AMEVA 0.64 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.12	CAIM 0.68 $\pm$ 0.1	CAIM 0.66 $\pm$ 0.12	XGB 0.55 $\pm$ 0.06
9	CAIM 0.64 $\pm$ 0.08	CAIM 0.68 $\pm$ 0.12	CAIM 0.68 $\pm$ 0.1	CART 0.68 $\pm$ 0.12	MDLP 0.55 $\pm$ 0.08
10	AMEVA 0.64 $\pm$ 0.08	CAIM 0.67 $\pm$ 0.12	CAIM 0.68 $\pm$ 0.1	CART 0.67 $\pm$ 0.11	MDLP 0.56 $\pm$ 0.09
11	AMEVA 0.63 $\pm$ 0.11	CART 0.68 $\pm$ 0.11	CAIM 0.67 $\pm$ 0.11	CART 0.67 $\pm$ 0.1	XGB 0.53 $\pm$ 0.06
12	AMEVA 0.64 $\pm$ 0.11	CART 0.67 $\pm$ 0.12	CAIM 0.67 $\pm$ 0.1	CART 0.67 $\pm$ 0.1	CAIM 0.54 $\pm$ 0.07
13	CART 0.64 $\pm$ 0.09	CART 0.67 $\pm$ 0.12	Ext Chi2 0.67 $\pm$ 0.08	CART 0.68 $\pm$ 0.1	MDLP 0.56 $\pm$ 0.1
14	AMEVA 0.64 $\pm$ 0.13	Ext Chi2 0.67 $\pm$ 0.08	CAIM 0.68 $\pm$ 0.11	CART 0.68 $\pm$ 0.1	CACC 0.55 $\pm$ 0.08
15	CART 0.67 $\pm$ 0.09	CART 0.72 $\pm$ 0.11	CART 0.7 $\pm$ 0.11	CART 0.7 $\pm$ 0.11	AMEVA 0.53 $\pm$ 0.1
16	CART 0.68 $\pm$ 0.08	CART 0.71 $\pm$ 0.11	CART 0.69 $\pm$ 0.12	CART 0.7 $\pm$ 0.1	Mod Chi2 0.54 $\pm$ 0.13
17	CART 0.67 $\pm$ 0.1	CART 0.71 $\pm$ 0.12	CART 0.69 $\pm$ 0.13	CART 0.7 $\pm$ 0.11	CAIM 0.57 $\pm$ 0.08
18	CART 0.68 $\pm$ 0.08	CART 0.71 $\pm$ 0.12	CART 0.69 $\pm$ 0.12	CART 0.7 $\pm$ 0.12	XGB 0.54 $\pm$ 0.06
19	CART 0.69 $\pm$ 0.1	CART 0.7 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.1	CART 0.69 $\pm$ 0.12	XGB 0.54 $\pm$ 0.08
20	CART 0.68 $\pm$ 0.08	CART 0.7 $\pm$ 0.12	CART 0.69 $\pm$ 0.12	CART 0.69 $\pm$ 0.12	CACC 0.55 $\pm$ 0.04
21	CART 0.68 $\pm$ 0.09	CART 0.7 $\pm$ 0.12	CART 0.7 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	CART 0.54 $\pm$ 0.1
22	CART 0.69 $\pm$ 0.09	CART 0.7 $\pm$ 0.12	CART 0.71 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	Mod Chi2 0.54 $\pm$ 0.07
23	CART 0.69 $\pm$ 0.09	CART 0.71 $\pm$ 0.12	CART 0.72 $\pm$ 0.09	CART 0.69 $\pm$ 0.13	XGB 0.53 $\pm$ 0.06
24	CART 0.68 $\pm$ 0.1	CART 0.71 $\pm$ 0.12	CART 0.72 $\pm$ 0.09	CART 0.69 $\pm$ 0.12	XGB 0.52 $\pm$ 0.06
25	CART 0.69 $\pm$ 0.07	CART 0.71 $\pm$ 0.12	CART 0.71 $\pm$ 0.09	CART 0.69 $\pm$ 0.13	CACC 0.55 $\pm$ 0.07



Supplementary Materials

Table 12. Best discretizer using different configurations of PCA components and addition of  $\pm 5\%$  random gaussian noise

Comp.	RF	LR	NB	SVM	Dummy
2	XGB 0.63 $\pm$ 0.09	CAIM 0.68 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.1	Ext Chi2 0.55 $\pm$ 0.1
3	Mod Chi2 0.6 $\pm$ 0.06	CAIM 0.69 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.11	Mod Chi2 0.55 $\pm$ 0.09
4	Mod Chi2 0.64 $\pm$ 0.04	CAIM 0.68 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.1	CAIM 0.67 $\pm$ 0.09	Mod Chi2 0.55 $\pm$ 0.04
5	AMEVA 0.66 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.1	CAIM 0.54 $\pm$ 0.07
6	AMEVA 0.62 $\pm$ 0.13	CAIM 0.68 $\pm$ 0.12	CAIM 0.68 $\pm$ 0.1	CAIM 0.68 $\pm$ 0.1	ChiMerge 0.54 $\pm$ 0.05
7	XGB 0.63 $\pm$ 0.13	CAIM 0.69 $\pm$ 0.12	CAIM 0.68 $\pm$ 0.1	CAIM 0.68 $\pm$ 0.1	CART 0.58 $\pm$ 0.06
8	AMEVA 0.63 $\pm$ 0.11	CAIM 0.68 $\pm$ 0.12	Ext Chi2 0.67 $\pm$ 0.08	CAIM 0.66 $\pm$ 0.12	CART 0.53 $\pm$ 0.05
9	AMEVA 0.63 $\pm$ 0.1	CAIM 0.68 $\pm$ 0.12	CAIM 0.67 $\pm$ 0.1	CART 0.68 $\pm$ 0.12	Ext Chi2 0.55 $\pm$ 0.05
10	AMEVA 0.64 $\pm$ 0.1	CART 0.67 $\pm$ 0.13	CAIM 0.67 $\pm$ 0.11	CART 0.67 $\pm$ 0.11	CART 0.54 $\pm$ 0.06
11	CART 0.64 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	CART 0.67 $\pm$ 0.12	CART 0.68 $\pm$ 0.1	XGB 0.55 $\pm$ 0.1
12	CART 0.63 $\pm$ 0.1	CART 0.67 $\pm$ 0.12	CART 0.67 $\pm$ 0.12	CART 0.68 $\pm$ 0.1	CART 0.54 $\pm$ 0.07
13	CART 0.62 $\pm$ 0.1	CART 0.68 $\pm$ 0.12	CART 0.67 $\pm$ 0.12	CART 0.68 $\pm$ 0.11	MDLP 0.55 $\pm$ 0.07
14	CART 0.67 $\pm$ 0.08	CART 0.68 $\pm$ 0.12	CART 0.66 $\pm$ 0.13	CART 0.68 $\pm$ 0.11	CART 0.53 $\pm$ 0.05
15	CART 0.7 $\pm$ 0.08	CART 0.71 $\pm$ 0.11	CART 0.69 $\pm$ 0.11	CART 0.69 $\pm$ 0.1	ChiMerge 0.54 $\pm$ 0.05
16	CART 0.67 $\pm$ 0.09	CART 0.71 $\pm$ 0.11	CART 0.69 $\pm$ 0.12	CART 0.7 $\pm$ 0.1	CART 0.56 $\pm$ 0.09
17	CART 0.68 $\pm$ 0.08	CART 0.71 $\pm$ 0.11	CART 0.69 $\pm$ 0.12	CART 0.69 $\pm$ 0.11	CAIM 0.52 $\pm$ 0.07
18	CART 0.67 $\pm$ 0.1	CART 0.7 $\pm$ 0.11	CART 0.69 $\pm$ 0.12	CART 0.69 $\pm$ 0.11	ChiMerge 0.52 $\pm$ 0.09
19	CART 0.68 $\pm$ 0.09	CART 0.7 $\pm$ 0.12	CART 0.69 $\pm$ 0.13	CART 0.69 $\pm$ 0.11	AMEVA 0.53 $\pm$ 0.07
20	CART 0.68 $\pm$ 0.09	CART 0.7 $\pm$ 0.12	CART 0.69 $\pm$ 0.12	CART 0.68 $\pm$ 0.11	MDLP 0.55 $\pm$ 0.06
21	CART 0.7 $\pm$ 0.1	CART 0.69 $\pm$ 0.12	CART 0.7 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	Ext Chi2 0.53 $\pm$ 0.04
22	CART 0.68 $\pm$ 0.1	CART 0.69 $\pm$ 0.12	CART 0.71 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	XGB 0.56 $\pm$ 0.07
23	CART 0.69 $\pm$ 0.09	CART 0.7 $\pm$ 0.12	CART 0.71 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	CART 0.54 $\pm$ 0.06
24	CART 0.71 $\pm$ 0.08	CART 0.7 $\pm$ 0.12	CART 0.71 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	CART 0.59 $\pm$ 0.05
25	CART 0.69 $\pm$ 0.08	CART 0.7 $\pm$ 0.12	CART 0.71 $\pm$ 0.1	CART 0.68 $\pm$ 0.12	MDLP 0.53 $\pm$ 0.09

Table 13. Best discretizer using different configurations of NCA components and addition of  $\pm 5\%$  random uniform noise

Comp.	RF	LR	NB	SVM	Dummy
2	XGB 0.79 $\pm$ 0.07	Ext Chi2 0.65 $\pm$ 0.09	CAIM 0.72 $\pm$ 0.1	CAIM 0.71 $\pm$ 0.11	XGB 0.54 $\pm$ 0.07
3	XGB 0.76 $\pm$ 0.08	CAIM 0.71 $\pm$ 0.11	CAIM 0.71 $\pm$ 0.1	CAIM 0.71 $\pm$ 0.11	AMEVA 0.57 $\pm$ 0.06
4	XGB 0.79 $\pm$ 0.08	CAIM 0.7 $\pm$ 0.1	CAIM 0.68 $\pm$ 0.11	CAIM 0.71 $\pm$ 0.11	CART 0.54 $\pm$ 0.1
5	XGB 0.78 $\pm$ 0.06	CAIM 0.69 $\pm$ 0.1	Ext Chi2 0.69 $\pm$ 0.08	CAIM 0.7 $\pm$ 0.1	XGB 0.56 $\pm$ 0.12
6	XGB 0.79 $\pm$ 0.07	CAIM 0.69 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.11	CAIM 0.69 $\pm$ 0.1	XGB 0.52 $\pm$ 0.07
7	XGB 0.79 $\pm$ 0.08	CAIM 0.68 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.1	Ext Chi2 0.69 $\pm$ 0.07	XGB 0.54 $\pm$ 0.06
8	XGB 0.77 $\pm$ 0.08	CAIM 0.69 $\pm$ 0.11	Ext Chi2 0.69 $\pm$ 0.09	CAIM 0.68 $\pm$ 0.08	CART 0.56 $\pm$ 0.07
9	Mod Chi2 0.76 $\pm$ 0.08	CART 0.69 $\pm$ 0.13	Ext Chi2 0.69 $\pm$ 0.09	CART 0.68 $\pm$ 0.12	Mod Chi2 0.56 $\pm$ 0.07
10	XGB 0.78 $\pm$ 0.07	Ext Chi2 0.68 $\pm$ 0.07	Ext Chi2 0.69 $\pm$ 0.1	CAIM 0.67 $\pm$ 0.09	MDLP 0.55 $\pm$ 0.06
11	XGB 0.76 $\pm$ 0.07	CART 0.68 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.11	CART 0.68 $\pm$ 0.11	XGB 0.54 $\pm$ 0.08
12	XGB 0.77 $\pm$ 0.06	CART 0.68 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.12	CART 0.68 $\pm$ 0.11	XGB 0.53 $\pm$ 0.1
13	XGB 0.77 $\pm$ 0.07	CART 0.69 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.11	CART 0.69 $\pm$ 0.1	MDLP 0.53 $\pm$ 0.07
14	XGB 0.76 $\pm$ 0.07	CART 0.68 $\pm$ 0.11	CAIM 0.69 $\pm$ 0.12	CART 0.68 $\pm$ 0.1	ChiMerge 0.53 $\pm$ 0.04
15	XGB 0.74 $\pm$ 0.06	CART 0.71 $\pm$ 0.11	CAIM 0.69 $\pm$ 0.12	CART 0.71 $\pm$ 0.11	CART 0.53 $\pm$ 0.05
16	XGB 0.76 $\pm$ 0.09	CART 0.71 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.11	CART 0.7 $\pm$ 0.11	CACC 0.56 $\pm$ 0.07
17	XGB 0.74 $\pm$ 0.07	CART 0.71 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.12	CART 0.7 $\pm$ 0.12	CART 0.56 $\pm$ 0.09
18	XGB 0.78 $\pm$ 0.06	CART 0.71 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.12	CART 0.69 $\pm$ 0.12	CACC 0.53 $\pm$ 0.07
19	XGB 0.76 $\pm$ 0.05	CART 0.67 $\pm$ 0.1	CAIM 0.7 $\pm$ 0.12	CART 0.67 $\pm$ 0.09	CART 0.53 $\pm$ 0.07
20	XGB 0.77 $\pm$ 0.04	CART 0.7 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.12	CART 0.69 $\pm$ 0.12	XGB 0.56 $\pm$ 0.06
21	XGB 0.75 $\pm$ 0.06	CART 0.7 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.12	CART 0.68 $\pm$ 0.12	AMEVA 0.53 $\pm$ 0.06
22	XGB 0.76 $\pm$ 0.06	CART 0.7 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.12	CART 0.68 $\pm$ 0.12	XGB 0.54 $\pm$ 0.07
23	XGB 0.75 $\pm$ 0.07	CART 0.7 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.11	CART 0.69 $\pm$ 0.12	CART 0.55 $\pm$ 0.07
24	XGB 0.75 $\pm$ 0.07	CART 0.71 $\pm$ 0.12	Ext Chi2 0.7 $\pm$ 0.1	CART 0.69 $\pm$ 0.12	XGB 0.53 $\pm$ 0.11
25	CART 0.76 $\pm$ 0.07	CART 0.71 $\pm$ 0.12	CAIM 0.71 $\pm$ 0.12	CART 0.69 $\pm$ 0.13	MDLP 0.54 $\pm$ 0.03

Table 14. Best discretizer using different configurations of NCA components and addition of  $\pm 5\%$  random gaussian noise

Comp.	RF	LR	NB	SVM	Dummy
2	XGB 0.8 $\pm$ 0.09	CAIM 0.7 $\pm$ 0.12	CAIM 0.73 $\pm$ 0.1	CAIM 0.71 $\pm$ 0.11	Ext Chi2 0.54 $\pm$ 0.08
3	MDLP 0.79 $\pm$ 0.07	CAIM 0.7 $\pm$ 0.13	CAIM 0.7 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.12	XGB 0.54 $\pm$ 0.11
4	MDLP 0.77 $\pm$ 0.06	CAIM 0.7 $\pm$ 0.11	CAIM 0.71 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.11	XGB 0.56 $\pm$ 0.07
5	XGB 0.81 $\pm$ 0.08	CAIM 0.7 $\pm$ 0.1	CAIM 0.71 $\pm$ 0.12	CAIM 0.7 $\pm$ 0.09	CART 0.53 $\pm$ 0.08
6	XGB 0.8 $\pm$ 0.08	CAIM 0.7 $\pm$ 0.11	CAIM 0.72 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.1	AMEVA 0.57 $\pm$ 0.04
7	XGB 0.77 $\pm$ 0.07	CAIM 0.69 $\pm$ 0.1	CAIM 0.72 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.1	CART 0.57 $\pm$ 0.05
8	CAIM 0.79 $\pm$ 0.07	CAIM 0.7 $\pm$ 0.11	CAIM 0.71 $\pm$ 0.1	CAIM 0.7 $\pm$ 0.1	XGB 0.54 $\pm$ 0.09
9	MDLP 0.77 $\pm$ 0.08	CAIM 0.69 $\pm$ 0.09	CAIM 0.71 $\pm$ 0.1	CAIM 0.69 $\pm$ 0.08	CAIM 0.54 $\pm$ 0.1
10	MDLP 0.78 $\pm$ 0.06	CART 0.68 $\pm$ 0.13	CAIM 0.71 $\pm$ 0.1	CART 0.68 $\pm$ 0.12	CART 0.55 $\pm$ 0.08
11	MDLP 0.78 $\pm$ 0.08	CART 0.68 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.1	CART 0.68 $\pm$ 0.11	AMEVA 0.55 $\pm$ 0.05
12	XGB 0.78 $\pm$ 0.07	CART 0.68 $\pm$ 0.12	CAIM 0.71 $\pm$ 0.11	CART 0.68 $\pm$ 0.11	ChiMerge 0.53 $\pm$ 0.06
13	XGB 0.79 $\pm$ 0.06	CART 0.69 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.11	CART 0.69 $\pm$ 0.11	XGB 0.55 $\pm$ 0.1
14	MDLP 0.79 $\pm$ 0.06	CART 0.68 $\pm$ 0.12	CAIM 0.71 $\pm$ 0.11	CART 0.69 $\pm$ 0.12	Ext Chi2 0.55 $\pm$ 0.06
15	XGB 0.77 $\pm$ 0.08	CART 0.71 $\pm$ 0.11	CAIM 0.71 $\pm$ 0.12	CART 0.7 $\pm$ 0.1	Ext Chi2 0.54 $\pm$ 0.12
16	MDLP 0.77 $\pm$ 0.06	CART 0.71 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.12	CART 0.7 $\pm$ 0.1	CART 0.54 $\pm$ 0.06
17	MDLP 0.77 $\pm$ 0.06	CART 0.7 $\pm$ 0.1	CAIM 0.71 $\pm$ 0.11	CART 0.68 $\pm$ 0.1	AMEVA 0.56 $\pm$ 0.06
18	XGB 0.76 $\pm$ 0.06	CART 0.7 $\pm$ 0.11	CAIM 0.7 $\pm$ 0.12	CART 0.69 $\pm$ 0.11	XGB 0.55 $\pm$ 0.07
19	Mod Chi2 0.76 $\pm$ 0.06	CART 0.7 $\pm$ 0.12	CAIM 0.71 $\pm$ 0.12	CART 0.7 $\pm$ 0.1	XGB 0.54 $\pm$ 0.06
20	MDLP 0.78 $\pm$ 0.07	CART 0.7 $\pm$ 0.12	CAIM 0.71 $\pm$ 0.12	CART 0.68 $\pm$ 0.12	Mod Chi2 0.54 $\pm$ 0.04
21	MDLP 0.78 $\pm$ 0.07	CART 0.7 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.11	CART 0.68 $\pm$ 0.12	ChiMerge 0.54 $\pm$ 0.05
22	MDLP 0.77 $\pm$ 0.06	CART 0.69 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.11	CART 0.68 $\pm$ 0.12	CAIM 0.53 $\pm$ 0.07
23	MDLP 0.77 $\pm$ 0.07	CART 0.7 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.11	CART 0.68 $\pm$ 0.12	CART 0.57 $\pm$ 0.08
24	MDLP 0.76 $\pm$ 0.07	CART 0.7 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.11	CART 0.68 $\pm$ 0.12	CAIM 0.52 $\pm$ 0.04
25	MDLP 0.76 $\pm$ 0.07	CART 0.7 $\pm$ 0.12	CAIM 0.72 $\pm$ 0.11	CART 0.68 $\pm$ 0.12	CART 0.54 $\pm$ 0.08

## 6. Notes on Numerical Experiment 2

In Figure 3, processes of tuning VFI bins for the ChiMerge and CACC data are compared together.

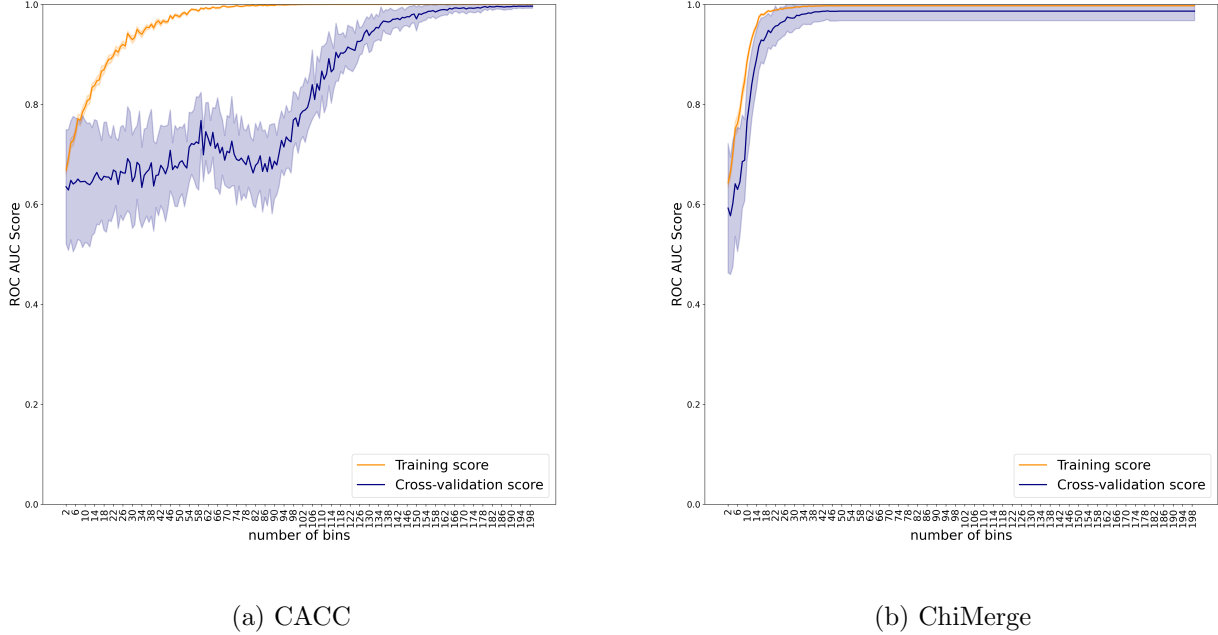


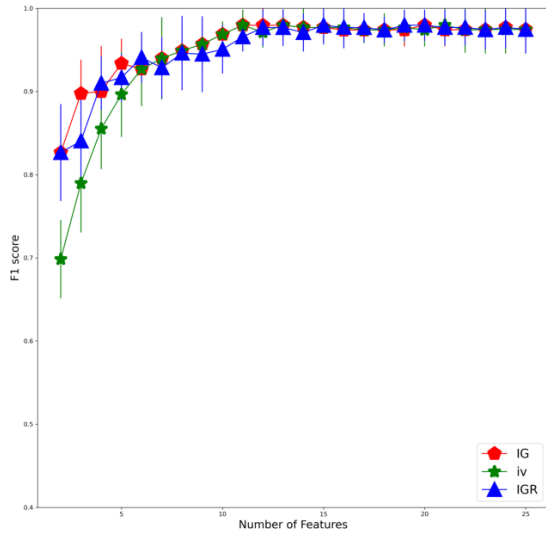
Figure 3. Selection of the optimal number of bins for the VFI model

### 6.1. Metrics from information theory

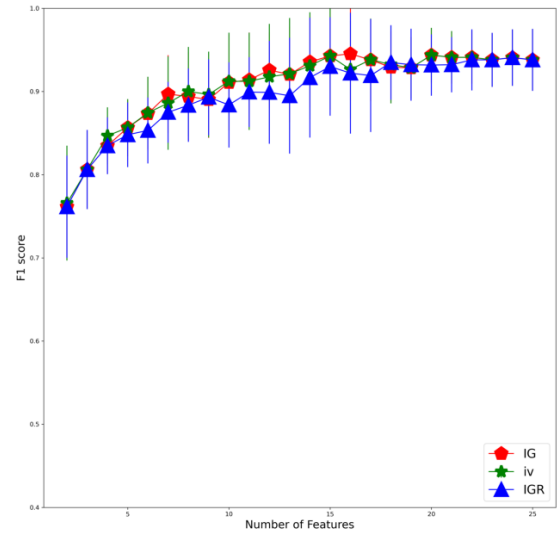
Discrete data can be handled via information theory, which quantifies the amount of information in the data distribution through probabilities. Information can be interpreted as the amount of surprise for an event measured in bits: an event with a low likelihood carries high information (is more surprising and uncertain). Information gain (IG) is a metric that can be used in machine learning to determine the gain of information of each variable in relation to the target class expressed in terms of surprise. Other information theory metrics included intrinsic value (iv) and information gain ratio (IGR), the ratio between the information gain and the intrinsic value. Measures of IG, iv, and IGR can also be intended in terms of entropy. Entropy describes the purity of a collection of examples (how balanced the distribution of classes happens to be), while information gain is the reduction in entropy one should expect when partitioning the samples according to a given attribute. Entropy of the data-set is calculated as  $-\sum_{i=1}^k P(x_i) \log_2(P(x_i))$  with  $P(x_i)$  probability of getting the  $i^{th}$  value randomly picking up one from the data-set. In the data-set under exam, entropy was 0.990 bit (almost a 50% split indeed entropy is close to 1 bit). In terms of entropy, information gain is the amount of entropy removed by knowing an input feature beforehand:  $IG(Y|X) = H(Y) - H(Y|X)$  with  $H(Y|X)$  conditional entropy or entropy in Y when X is already known. Higher information gain means that more entropy is removed, and consequently, more information the variable X carries about Y [60]. Intrinsic value measures the entropy of X.

To highlight the optimal number of features during numerical experiment 2, F1 scores were calculated by sorting in descending order all features according to IG, iv and IGR. Mean F1 score at cross-validation are plotted in Figure 4 with vertical error bars representing the standard deviation.

Highest F1 score was selected to determine the number of features to keep.



(a) CACC



(b) ChiMerge

Figure 4. F1 scores for optimal number of features detection

### 6.2. Dimensionality reduction with NCA

The possibility of working with a reduced number of NCA components was also inspected during numerical experiment 2. Number of intervals used by VFI classifier were recalculated for each fold of stratified cross-validation with mean ROC AUC score ( $\pm$ standard deviation) collected in Table 15.

Table 15. NCA dim. red. paired with VFI classifier

Comp.	CV Roc Auc
2	0.609 $\pm$ 0.05
3	0.547 $\pm$ 0.11
4	0.56 $\pm$ 0.075
5	0.571 $\pm$ 0.072
6	0.616 $\pm$ 0.122
7	0.612 $\pm$ 0.076
8	0.567 $\pm$ 0.129
9	0.601 $\pm$ 0.112
10	0.588 $\pm$ 0.109
11	0.572 $\pm$ 0.097
12	0.603 $\pm$ 0.121
13	0.631 $\pm$ 0.107
14	0.594 $\pm$ 0.088
15	0.582 $\pm$ 0.092
16	0.586 $\pm$ 0.088
17	0.596 $\pm$ 0.09
18	0.607 $\pm$ 0.095
19	0.603 $\pm$ 0.095
20	0.605 $\pm$ 0.122
21	0.603 $\pm$ 0.091
22	0.609 $\pm$ 0.089
23	0.612 $\pm$ 0.087
24	0.621 $\pm$ 0.092
25	0.997 $\pm$ 0.003

## 7. Notes on Numerical Experiment 3

### 7.1. Weight of evidence

Optimal binning based on WOE is a methodology suitable for binary classification not popular outside financial engineering. Given a data-set of features  $X_1, \dots, X_p$  and a dependent variable  $Y$  the conditional log odds are given by the equation

$$\log \frac{P(Y = 1|X_j)}{P(Y = 0|X_j)} = \log \frac{P(Y = 1)}{P(Y = 0)} + \log \frac{f(X_j|Y = 1)}{f(X_j|Y = 0)}$$

where  $f(X_j|Y)$  denotes the conditional probability density function. The expression on the right can be seen as an intercept term plus the weight of evidence term. The intercept is constant so  $Y = 1$  is highly probable when WOE term is positive and vice-versa when WOE term is negative  $Y = 0$  has more chance to be seen. If WOE term is equal to zero, the two classes have equal chance. The goodness of the fit is usually explored using the information value metric, a score typical of the credit risk industry [61], that can be defined as

$$IV_i = \int \log \frac{f(X_j|Y = 1)}{f(X_j|Y = 0)} (f(X_j|Y = 1) - f(X_j|Y = 0)) dx$$

Maximizing the information value metric also magnifies the contradistinction among bins. One characteristic of this algorithm is that it requires at least 5% of the observations in each bin and forces the controls to avoid creation of empty intervals.

Tables sum up analysis pipeline containing the sequence of a primary discretizer followed by woe-based optimization. Results after 10-fold stratified cross-validation are in Table 16 for CART technique, Table 17 for equal width intervals, Table 18 for equal frequency and Table 19 for MDLP. Values were rounded to the second decimal place to contain table length. Appraised classifiers were: k-Nearest Neighbors (k-NN), Linear SVM (LinSVM), SVM with polynomial kernel function and degree of 2 (Poly2SVM), SVM with polynomial kernel function and degree of 3 (Poly3SVM), SVM with polynomial kernel function and degree of 4 (Poly4SVM), Radial Basis Function kernel SVM (RBF SVM), Gaussian Process (Gauss Proc), Decision Tree (Dec Tree), Random Forest (RF), Neural Net based on multilayer perceptron (NNet, 1 hidden layer of 100 neurons, rectified linear unit function as activation, samples divided in two mini-batches, no iteration limit for the solver), AdaBoost (an ensemble of decision trees as base estimators), Naïve Bayes (NB), Quadratic Discriminant Analysis (QDA), Gradient Boosting (GradBoost), Dummy classifier that always predicts the most frequent label (Dummy1), Dummy classifier that generates predictions by respecting the training set’s class distribution (Dummy2).

The number of features was automatically tuned by cross-validation using CART as binning associated with WOE-based optimization “equal-width” technique as shown in Figure 5.

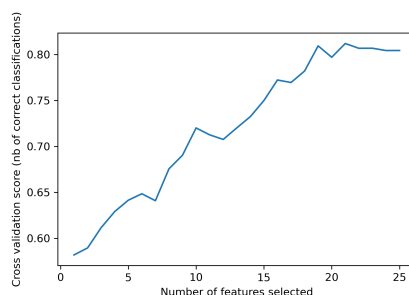


Figure 5. Recursive feature elimination by 10-fold stratified cross validation

### 7.2. Dimensionality reduction with NCA using WOE outputs

WOE features were transformed by NCA to check if model complexity could be minimized. Outcomes reported in Figure 6 are mean AUC at cross-validation plus or minus standard deviation of the AUC

Table 16. Classification results (CV, ROC AUC metric), CART WOE-based technique

Disc.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
AMEVA	0.64 ± 0.11	0.7 ± 0.1	0.64 ± 0.11	0.7 ± 0.12	0.68 ± 0.12	0.7 ± 0.1	0.7 ± 0.11	0.56 ± 0.05
CACC	0.7 ± 0.06	0.74 ± 0.08	0.67 ± 0.09	0.73 ± 0.1	0.67 ± 0.09	0.74 ± 0.09	0.73 ± 0.1	0.56 ± 0.08
CAIM	0.6 ± 0.06	0.63 ± 0.11	0.62 ± 0.11	0.6 ± 0.08	0.6 ± 0.1	0.64 ± 0.11	0.67 ± 0.11	0.54 ± 0.08
Mod Chi2	0.58 ± 0.12	0.63 ± 0.08	0.62 ± 0.04	0.63 ± 0.08	0.62 ± 0.04	0.65 ± 0.08	0.62 ± 0.07	0.62 ± 0.07
ChiMerge	0.66 ± 0.09	0.73 ± 0.09	0.66 ± 0.1	0.75 ± 0.08	0.69 ± 0.1	0.72 ± 0.09	0.71 ± 0.09	0.59 ± 0.08
Ext Chi2	0.6 ± 0.07	0.64 ± 0.09	0.61 ± 0.12	0.58 ± 0.1	0.6 ± 0.13	0.62 ± 0.1	0.65 ± 0.08	0.62 ± 0.09
MDLP	0.51 ± 0.12	0.63 ± 0.09	0.62 ± 0.09	0.6 ± 0.1	0.62 ± 0.09	0.63 ± 0.08	0.63 ± 0.09	0.62 ± 0.08
CART	0.78 ± 0.06	0.87 ± 0.07	0.73 ± 0.05	0.85 ± 0.07	0.76 ± 0.06	0.85 ± 0.06	0.83 ± 0.06	0.63 ± 0.07
XGB	0.61 ± 0.12	0.64 ± 0.09	0.58 ± 0.14	0.62 ± 0.11	0.58 ± 0.12	0.63 ± 0.13	0.65 ± 0.13	0.52 ± 0.06
Discr.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
AMEVA	0.69 ± 0.1	0.7 ± 0.08	0.69 ± 0.1	0.72 ± 0.1	0.48 ± 0.14	0.66 ± 0.11	0.5 ± 0.0	0.54 ± 0.11
CACC	0.68 ± 0.09	0.68 ± 0.09	0.68 ± 0.08	0.74 ± 0.08	0.52 ± 0.11	0.66 ± 0.07	0.5 ± 0.0	0.5 ± 0.09
CAIM	0.61 ± 0.08	0.55 ± 0.08	0.63 ± 0.12	0.68 ± 0.11	0.55 ± 0.13	0.61 ± 0.09	0.5 ± 0.0	0.55 ± 0.04
Mod Chi2	0.62 ± 0.07	0.63 ± 0.08	0.63 ± 0.08	0.63 ± 0.08	nan ± nan	0.62 ± 0.07	0.5 ± 0.0	0.54 ± 0.04
ChiMerge	0.69 ± 0.1	0.65 ± 0.12	0.69 ± 0.09	0.73 ± 0.1	0.5 ± 0.13	0.66 ± 0.09	0.5 ± 0.0	0.54 ± 0.1
Ext Chi2	0.62 ± 0.09	0.64 ± 0.09	0.65 ± 0.09	0.66 ± 0.09	nan ± nan	0.62 ± 0.1	0.5 ± 0.0	0.53 ± 0.05
MDLP	0.62 ± 0.08	0.63 ± 0.09	0.63 ± 0.09	0.63 ± 0.09	nan ± nan	0.62 ± 0.08	0.5 ± 0.0	0.46 ± 0.09
CART	0.83 ± 0.07	0.83 ± 0.08	0.83 ± 0.07	0.81 ± 0.1	0.82 ± 0.08	0.82 ± 0.08	0.5 ± 0.0	0.53 ± 0.11
XGB	0.59 ± 0.1	0.58 ± 0.11	0.58 ± 0.1	0.63 ± 0.13	0.55 ± 0.11	0.54 ± 0.09	0.5 ± 0.0	0.5 ± 0.06

Table 17. Classification results (CV, ROC AUC metric), Equal width intervals WOE-based technique

Disc.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
AMEVA	0.64 ± 0.1	0.66 ± 0.11	0.65 ± 0.09	0.72 ± 0.1	0.66 ± 0.11	0.68 ± 0.09	0.67 ± 0.09	0.58 ± 0.07
CACC	0.65 ± 0.08	0.7 ± 0.09	0.65 ± 0.07	0.71 ± 0.08	0.64 ± 0.1	0.7 ± 0.08	0.68 ± 0.07	0.57 ± 0.06
CAIM	0.59 ± 0.07	0.62 ± 0.11	0.59 ± 0.1	0.62 ± 0.1	0.64 ± 0.1	0.63 ± 0.09	0.66 ± 0.1	0.58 ± 0.08
Mod Chi2	0.58 ± 0.12	0.63 ± 0.08	0.62 ± 0.04	0.63 ± 0.08	0.62 ± 0.04	0.65 ± 0.08	0.62 ± 0.07	0.62 ± 0.07
ChiMerge	0.65 ± 0.12	0.73 ± 0.09	0.64 ± 0.11	0.71 ± 0.1	0.67 ± 0.09	0.7 ± 0.1	0.69 ± 0.09	0.59 ± 0.06
Ext Chi2	0.55 ± 0.11	0.65 ± 0.08	0.61 ± 0.12	0.61 ± 0.09	0.65 ± 0.07	0.61 ± 0.1	0.67 ± 0.08	0.63 ± 0.1
MDLP	0.51 ± 0.12	0.63 ± 0.09	0.62 ± 0.09	0.6 ± 0.1	0.62 ± 0.09	0.63 ± 0.08	0.63 ± 0.09	0.62 ± 0.08
CART	0.82 ± 0.05	0.88 ± 0.07	0.74 ± 0.06	0.86 ± 0.07	0.76 ± 0.08	0.86 ± 0.07	0.82 ± 0.08	0.68 ± 0.05
XGB	0.61 ± 0.12	0.64 ± 0.09	0.58 ± 0.14	0.62 ± 0.11	0.58 ± 0.12	0.63 ± 0.13	0.65 ± 0.13	0.51 ± 0.05
Discr.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
AMEVA	0.65 ± 0.11	0.67 ± 0.09	0.69 ± 0.1	0.71 ± 0.11	0.59 ± 0.1	0.67 ± 0.09	0.5 ± 0.0	0.47 ± 0.08
CACC	0.67 ± 0.07	0.65 ± 0.08	0.61 ± 0.07	0.72 ± 0.09	0.71 ± 0.07	0.63 ± 0.08	0.5 ± 0.0	0.51 ± 0.08
CAIM	0.6 ± 0.08	0.6 ± 0.08	0.64 ± 0.1	0.7 ± 0.11	0.5 ± 0.09	0.6 ± 0.09	0.5 ± 0.0	0.53 ± 0.05
Mod Chi2	0.62 ± 0.07	0.63 ± 0.07	0.63 ± 0.08	0.63 ± 0.08	nan ± nan	0.62 ± 0.07	0.5 ± 0.0	0.52 ± 0.06
ChiMerge	0.69 ± 0.1	0.63 ± 0.12	0.66 ± 0.11	0.73 ± 0.09	0.69 ± 0.09	0.64 ± 0.1	0.5 ± 0.0	0.48 ± 0.09
Ext Chi2	0.63 ± 0.09	0.66 ± 0.09	0.67 ± 0.09	0.68 ± 0.09	nan ± nan	0.63 ± 0.1	0.5 ± 0.0	0.47 ± 0.07
MDLP	0.62 ± 0.08	0.63 ± 0.08	0.63 ± 0.09	0.63 ± 0.09	nan ± nan	0.62 ± 0.08	0.5 ± 0.0	0.47 ± 0.1
CART	0.83 ± 0.06	0.86 ± 0.07	0.8 ± 0.08	0.83 ± 0.1	0.82 ± 0.08	0.81 ± 0.05	0.5 ± 0.0	0.49 ± 0.07
XGB	0.6 ± 0.1	0.58 ± 0.12	0.58 ± 0.1	0.63 ± 0.13	0.55 ± 0.11	0.54 ± 0.09	0.5 ± 0.0	0.52 ± 0.1

scores as vertical bar. When the regularization parameter of the linear SVM classifier is optimized by grid search (grid of four values) after each NCA transformation, ROC AUC scores remain stable until reaching a dimension of two NCA components Figure 6. If the number of features is small, the model is highly simplified, and paired with a linear SVM classifier could produce a decision boundary in the form of a straight line, suitable for visual interpretation. This abridged model reaches  $0.848 \pm 0.064$  balanced accuracy at CV (Table 20).

Supplementary Materials

Table 18. Classification results (CV, ROC AUC metric), Equal frequency intervals WOE-based technique

Disc.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
AMEVA	0.61 ± 0.11	0.64 ± 0.1	0.58 ± 0.09	0.66 ± 0.09	0.63 ± 0.07	0.61 ± 0.05	0.64 ± 0.08	0.57 ± 0.08
CACC	0.66 ± 0.09	0.7 ± 0.1	0.66 ± 0.08	0.71 ± 0.1	0.66 ± 0.08	0.7 ± 0.11	0.68 ± 0.11	0.57 ± 0.05
CAIM	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
Mod Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
ChiMerge	0.7 ± 0.07	0.71 ± 0.12	0.66 ± 0.1	0.73 ± 0.09	0.66 ± 0.08	0.72 ± 0.11	0.69 ± 0.09	0.59 ± 0.07
Ext Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
MDLP	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
CART	0.78 ± 0.05	0.86 ± 0.08	0.71 ± 0.06	0.84 ± 0.05	0.73 ± 0.05	0.85 ± 0.07	0.81 ± 0.06	0.6 ± 0.07
XGB	0.5 ± 0.09	0.52 ± 0.1	0.55 ± 0.12	0.56 ± 0.12	0.52 ± 0.11	0.54 ± 0.11	0.56 ± 0.11	0.47 ± 0.08
Discr.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
AMEVA	0.59 ± 0.12	0.64 ± 0.11	0.65 ± 0.1	0.64 ± 0.11	nan ± nan	0.64 ± 0.12	0.5 ± 0.0	0.51 ± 0.07
CACC	0.68 ± 0.11	0.64 ± 0.1	0.6 ± 0.11	0.71 ± 0.1	0.55 ± 0.13	0.62 ± 0.12	0.5 ± 0.0	0.55 ± 0.06
CAIM	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.46 ± 0.06
Mod Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.51 ± 0.07
ChiMerge	0.7 ± 0.11	0.7 ± 0.11	0.66 ± 0.13	0.71 ± 0.11	0.57 ± 0.11	0.65 ± 0.13	0.5 ± 0.0	0.54 ± 0.09
Ext Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.51 ± 0.06
MDLP	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.52 ± 0.05
CART	0.81 ± 0.08	0.84 ± 0.07	0.82 ± 0.08	0.8 ± 0.1	0.8 ± 0.08	0.8 ± 0.07	0.5 ± 0.0	0.49 ± 0.1
XGB	0.48 ± 0.08	0.56 ± 0.11	0.54 ± 0.11	0.54 ± 0.1	0.49 ± 0.09	0.48 ± 0.09	0.5 ± 0.0	0.48 ± 0.07

Table 19. Classification results (CV, ROC AUC metric), MDLP WOE-based technique

Disc.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
AMEVA	0.58 ± 0.1	0.56 ± 0.04	0.55 ± 0.08	0.54 ± 0.06	0.55 ± 0.08	0.55 ± 0.06	0.54 ± 0.05	0.55 ± 0.08
CACC	0.53 ± 0.09	0.61 ± 0.08	0.58 ± 0.11	0.6 ± 0.11	0.61 ± 0.1	0.6 ± 0.11	0.63 ± 0.1	0.55 ± 0.11
CAIM	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
Mod Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
ChiMerge	0.54 ± 0.1	0.63 ± 0.1	0.57 ± 0.11	0.63 ± 0.09	0.62 ± 0.1	0.62 ± 0.1	0.64 ± 0.12	0.49 ± 0.09
Ext Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
MDLP	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0
CART	0.68 ± 0.1	0.69 ± 0.08	0.65 ± 0.1	0.67 ± 0.09	0.65 ± 0.1	0.68 ± 0.07	0.7 ± 0.09	0.6 ± 0.07
XGB	0.5 ± 0.09	0.52 ± 0.1	0.55 ± 0.12	0.56 ± 0.12	0.52 ± 0.11	0.54 ± 0.11	0.56 ± 0.11	0.47 ± 0.08
Discr.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
AMEVA	0.55 ± 0.07	0.54 ± 0.05	0.54 ± 0.05	0.51 ± 0.08	nan ± nan	0.54 ± 0.07	0.5 ± 0.0	0.5 ± 0.06
CACC	0.55 ± 0.1	0.54 ± 0.11	0.62 ± 0.07	0.61 ± 0.13	nan ± nan	0.56 ± 0.1	0.5 ± 0.0	0.46 ± 0.07
CAIM	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.54 ± 0.07
Mod Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.46 ± 0.05
ChiMerge	0.57 ± 0.1	0.54 ± 0.12	0.6 ± 0.11	0.6 ± 0.11	nan ± nan	0.56 ± 0.12	0.5 ± 0.0	0.5 ± 0.11
Ext Chi2	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.49 ± 0.09
MDLP	0.5 ± 0.0	0.5 ± 0.0	0.5 ± 0.0	nan ± nan	nan ± nan	0.5 ± 0.0	0.5 ± 0.0	0.51 ± 0.08
CART	0.66 ± 0.09	0.62 ± 0.1	0.67 ± 0.1	0.67 ± 0.1	0.54 ± 0.1	0.62 ± 0.1	0.5 ± 0.0	0.5 ± 0.07
XGB	0.48 ± 0.08	0.56 ± 0.11	0.54 ± 0.11	0.54 ± 0.1	0.49 ± 0.09	0.48 ± 0.09	0.5 ± 0.0	0.47 ± 0.09

Table 20. Linear SVM classifier with CART pre-binning and optimized binning based on equal width intervals, using 2 NCA components

	precision	recall	f1-score	test set samples
class: "Alive"	0.88	0.85	0.86	226
class: "Dead"	0.82	0.85	0.83	179
accuracy			0.85	405
macro avg	0.85	0.85	0.85	405
weighted avg	0.85	0.85	0.85	405

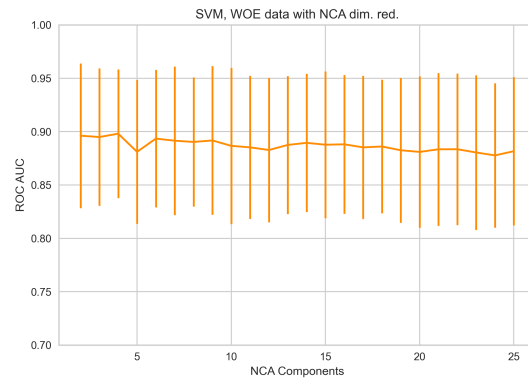


Figure 6. AUC of linear SVM classifier at different NCA components as mean and std of 10-fold stratified cross validation



### 8. Notes on Numerical Experiment 4

This section collects cross-validation values for each quantile transformation attempted using five landmarks as cut points to discretize the cumulative distribution function. Results included for uniform (Tables 21, 22, 23, 24, 25) or normal (Tables 26, 27, 28, 29, 30) mapping. After uniform or normal mapping data was discretized with CART algorithm and reduced by NCA. Included Classifiers were: k-Nearest Neighbors (k-NN), Linear SVM (LinSVM), SVM with polynomial kernel function and degree of 2 (Poly2SVM), SVM with polynomial kernel function and degree of 3 (Poly3SVM), SVM with polynomial kernel function and degree of 4 (Poly4SVM), Radial Basis Function kernel SVM (RBF SVM), Gaussian Process (Gauss Proc), Decision Tree (Dec Tree), Random Forest (RF), Neural Net based on multilayer perceptron (NNet, 1 hidden layer of 100 neurons, rectified linear unit function as activation, samples divided in two mini-batches, no iteration limit for the solver), AdaBoost (an ensemble of decision trees as base estimators), Naïve Bayes (NB), Quadratic Discriminant Analysis (QDA), Gradient Boosting (Grad-Boost), Dummy classifier that always predicts the most frequent label (Dummy1), Dummy classifier that generates predictions by respecting the training set’s class distribution (Dummy2). No further optimization of classifiers’ hyper-parameters was performed. Class separability metric seems to increase when the dimension of the data-set is reduced both with PCA and NCA in uniform and normal mapping (Figures 7 and 8). PCA landmark evaluation is shown in Figures 9 and 10.

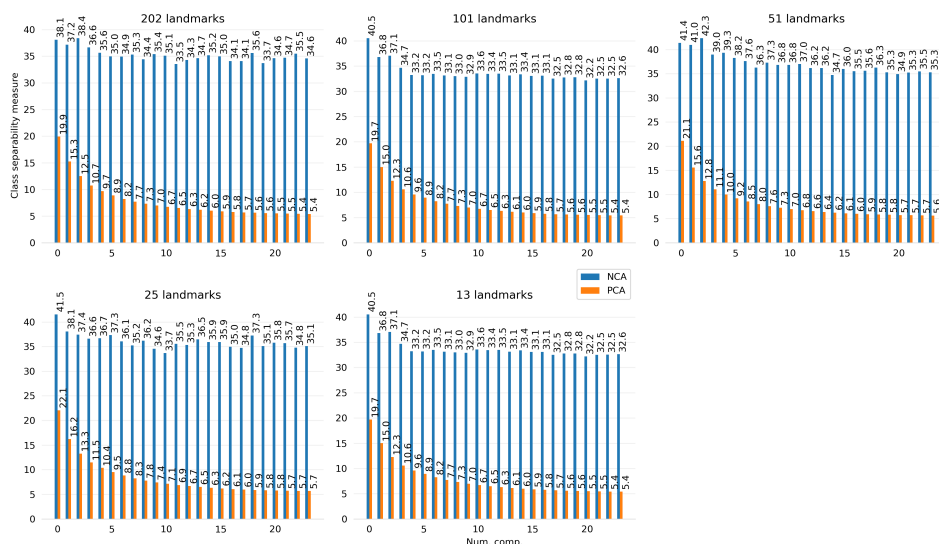


Figure 7. Class separability measure for different cut points of Uniform transformation

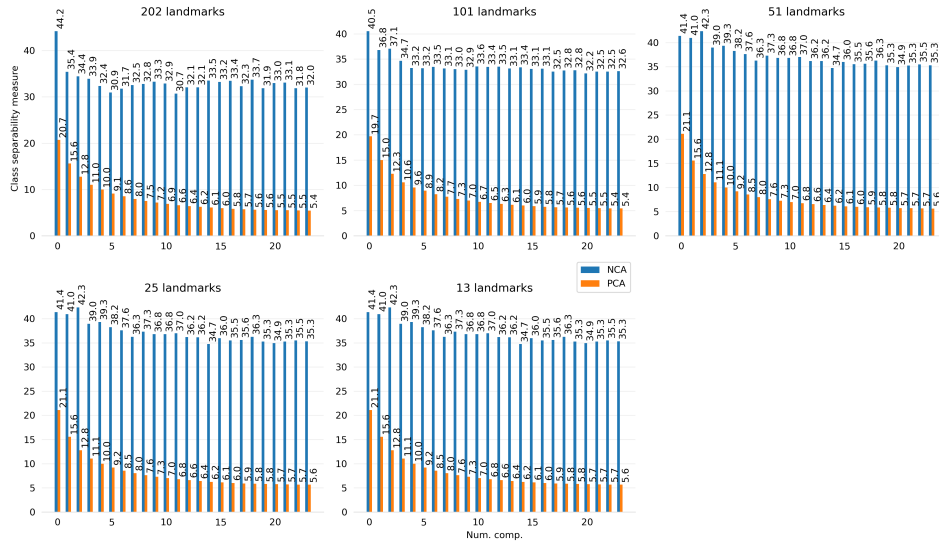


Figure 8. Class separability measure for different cut points of Normal transformation

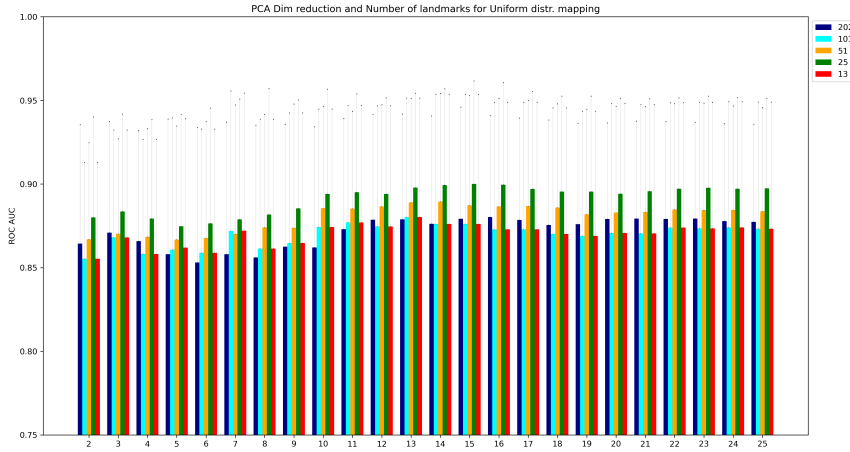


Figure 9. Uniform transf. PCA dim. red.

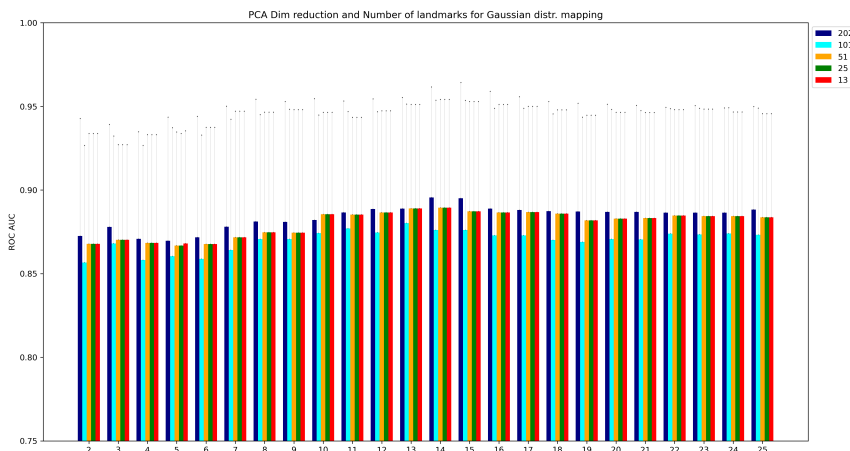


Figure 10. Normal transf. PCA dim. red.

Supplementary Materials

Table 21. Uniform quantile transformation, NCA ROC AUC CV outcomes for 202 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.89 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.07	0.83 ± 0.07
3	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.76 ± 0.06	0.82 ± 0.06
4	0.91 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.85 ± 0.04	0.8 ± 0.05
5	0.92 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.87 ± 0.05	0.8 ± 0.11
6	0.91 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.87 ± 0.04	0.78 ± 0.07
7	0.91 ± 0.04	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.76 ± 0.03	0.8 ± 0.06
8	0.9 ± 0.06	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.06	0.77 ± 0.08
9	0.9 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.07	0.77 ± 0.08
10	0.88 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.75 ± 0.05	0.8 ± 0.1
11	0.87 ± 0.08	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.08	0.77 ± 0.08
12	0.89 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.08	0.76 ± 0.05
13	0.87 ± 0.08	0.88 ± 0.08	0.88 ± 0.07	0.88 ± 0.07	0.88 ± 0.07	0.88 ± 0.07	0.74 ± 0.08	0.75 ± 0.06
14	0.89 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.54 ± 0.03	0.76 ± 0.09
15	0.87 ± 0.08	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.75 ± 0.06	0.74 ± 0.08
16	0.88 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.07	0.78 ± 0.08
17	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.73 ± 0.08	0.77 ± 0.09
18	0.88 ± 0.07	0.87 ± 0.07	0.89 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.71 ± 0.08	0.76 ± 0.08
19	0.87 ± 0.08	0.87 ± 0.07	0.89 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.74 ± 0.09	0.72 ± 0.06
20	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.08	0.78 ± 0.1
21	0.88 ± 0.07	0.87 ± 0.07	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.65 ± 0.08	0.76 ± 0.08
22	0.88 ± 0.06	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.07	0.77 ± 0.07
23	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.76 ± 0.08	0.73 ± 0.07
24	0.88 ± 0.06	0.87 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.08	0.76 ± 0.07
25	0.89 ± 0.05	0.87 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.62 ± 0.06	0.75 ± 0.07
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.9 ± 0.06	0.65 ± 0.04	0.86 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.5 ± 0.0	0.5 ± 0.05
3	0.9 ± 0.06	0.64 ± 0.06	0.86 ± 0.07	0.87 ± 0.06	0.88 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.47 ± 0.07
4	0.91 ± 0.06	0.64 ± 0.07	0.86 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.09
5	0.92 ± 0.05	0.69 ± 0.07	0.87 ± 0.07	0.89 ± 0.06	0.89 ± 0.05	0.9 ± 0.05	0.5 ± 0.0	0.49 ± 0.08
6	0.91 ± 0.05	0.69 ± 0.07	0.9 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.9 ± 0.05	0.5 ± 0.0	0.49 ± 0.1
7	0.9 ± 0.05	0.66 ± 0.08	0.87 ± 0.08	0.88 ± 0.05	0.87 ± 0.08	0.88 ± 0.07	0.5 ± 0.0	0.44 ± 0.07
8	0.89 ± 0.07	0.7 ± 0.07	0.83 ± 0.07	0.88 ± 0.05	0.86 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.49 ± 0.09
9	0.9 ± 0.06	0.7 ± 0.09	0.82 ± 0.09	0.88 ± 0.05	0.86 ± 0.08	0.87 ± 0.07	0.5 ± 0.0	0.45 ± 0.08
10	0.89 ± 0.07	0.69 ± 0.05	0.84 ± 0.06	0.88 ± 0.05	0.84 ± 0.07	0.89 ± 0.07	0.5 ± 0.0	0.55 ± 0.08
11	0.9 ± 0.06	0.69 ± 0.08	0.84 ± 0.07	0.88 ± 0.06	0.85 ± 0.08	0.87 ± 0.07	0.5 ± 0.0	0.49 ± 0.07
12	0.9 ± 0.05	0.67 ± 0.09	0.87 ± 0.06	0.88 ± 0.05	0.85 ± 0.07	0.89 ± 0.06	0.5 ± 0.0	0.46 ± 0.08
13	0.88 ± 0.08	0.68 ± 0.08	0.85 ± 0.09	0.87 ± 0.06	0.85 ± 0.08	0.85 ± 0.09	0.5 ± 0.0	0.48 ± 0.08
14	0.9 ± 0.06	0.7 ± 0.06	0.85 ± 0.08	0.88 ± 0.06	0.83 ± 0.07	0.88 ± 0.07	0.5 ± 0.0	0.5 ± 0.09
15	0.9 ± 0.06	0.71 ± 0.07	0.85 ± 0.06	0.88 ± 0.06	0.82 ± 0.09	0.87 ± 0.07	0.5 ± 0.0	0.47 ± 0.1
16	0.91 ± 0.06	0.71 ± 0.06	0.86 ± 0.06	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.06	0.5 ± 0.0	0.51 ± 0.1
17	0.91 ± 0.04	0.72 ± 0.06	0.87 ± 0.07	0.88 ± 0.06	0.82 ± 0.08	0.9 ± 0.05	0.5 ± 0.0	0.48 ± 0.05
18	0.9 ± 0.06	0.69 ± 0.09	0.84 ± 0.07	0.88 ± 0.06	0.81 ± 0.09	0.85 ± 0.08	0.5 ± 0.0	0.48 ± 0.04
19	0.9 ± 0.06	0.71 ± 0.09	0.84 ± 0.09	0.88 ± 0.06	0.8 ± 0.1	0.86 ± 0.07	0.5 ± 0.0	0.54 ± 0.06
20	0.91 ± 0.06	0.74 ± 0.07	0.87 ± 0.07	0.88 ± 0.06	0.8 ± 0.1	0.88 ± 0.07	0.5 ± 0.0	0.52 ± 0.05
21	0.9 ± 0.06	0.71 ± 0.07	0.86 ± 0.07	0.88 ± 0.06	0.8 ± 0.1	0.88 ± 0.06	0.5 ± 0.0	0.48 ± 0.04
22	0.91 ± 0.06	0.69 ± 0.05	0.86 ± 0.08	0.88 ± 0.06	0.8 ± 0.1	0.88 ± 0.07	0.5 ± 0.0	0.49 ± 0.08
23	0.9 ± 0.06	0.71 ± 0.05	0.86 ± 0.07	0.88 ± 0.06	0.8 ± 0.1	0.88 ± 0.06	0.5 ± 0.0	0.51 ± 0.1
24	0.89 ± 0.05	0.73 ± 0.08	0.85 ± 0.07	0.87 ± 0.06	0.79 ± 0.09	0.87 ± 0.06	0.5 ± 0.0	0.48 ± 0.09
25	0.91 ± 0.05	0.69 ± 0.06	0.84 ± 0.04	0.88 ± 0.06	0.79 ± 0.09	0.89 ± 0.04	0.5 ± 0.0	0.49 ± 0.08

Table 22. Uniform quantile transformation, NCA ROC AUC CV outcomes for 101 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.83 ± 0.06	0.8 ± 0.04
3	0.9 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.06	0.81 ± 0.05
4	0.88 ± 0.07	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.82 ± 0.05	0.78 ± 0.08
5	0.89 ± 0.04	0.89 ± 0.07	0.89 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.59 ± 0.05	0.74 ± 0.06
6	0.9 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.74 ± 0.04	0.75 ± 0.07
7	0.91 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.75 ± 0.05	0.8 ± 0.04
8	0.91 ± 0.04	0.88 ± 0.07	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.81 ± 0.06	0.76 ± 0.05
9	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.78 ± 0.06
10	0.89 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.8 ± 0.05	0.78 ± 0.07
11	0.89 ± 0.03	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.05	0.78 ± 0.05
12	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.76 ± 0.05	0.77 ± 0.06
13	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.06	0.79 ± 0.05
14	0.89 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.75 ± 0.07
15	0.89 ± 0.04	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.04	0.78 ± 0.06
16	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.75 ± 0.08
17	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.81 ± 0.04	0.79 ± 0.05
18	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.03	0.77 ± 0.07
19	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.03	0.8 ± 0.07
20	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.05	0.77 ± 0.06
21	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.05	0.78 ± 0.07
22	0.88 ± 0.04	0.87 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.58 ± 0.04	0.75 ± 0.07
23	0.88 ± 0.04	0.88 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.59 ± 0.06	0.77 ± 0.08
24	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.77 ± 0.08
25	0.89 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.81 ± 0.04	0.79 ± 0.07
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.9 ± 0.05	0.62 ± 0.07	0.84 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.87 ± 0.05	0.5 ± 0.0	0.46 ± 0.06
3	0.91 ± 0.04	0.65 ± 0.09	0.86 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.9 ± 0.05	0.5 ± 0.0	0.49 ± 0.08
4	0.9 ± 0.07	0.68 ± 0.08	0.86 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.51 ± 0.08
5	0.89 ± 0.06	0.67 ± 0.07	0.81 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.87 ± 0.05	0.5 ± 0.0	0.48 ± 0.1
6	0.9 ± 0.05	0.67 ± 0.1	0.86 ± 0.06	0.88 ± 0.06	0.88 ± 0.07	0.87 ± 0.06	0.5 ± 0.0	0.51 ± 0.09
7	0.92 ± 0.04	0.63 ± 0.09	0.88 ± 0.05	0.89 ± 0.07	0.86 ± 0.08	0.91 ± 0.05	0.5 ± 0.0	0.49 ± 0.11
8	0.9 ± 0.05	0.67 ± 0.07	0.84 ± 0.06	0.89 ± 0.07	0.86 ± 0.08	0.85 ± 0.08	0.5 ± 0.0	0.48 ± 0.08
9	0.9 ± 0.06	0.67 ± 0.11	0.85 ± 0.06	0.89 ± 0.07	0.86 ± 0.08	0.89 ± 0.05	0.5 ± 0.0	0.53 ± 0.07
10	0.9 ± 0.05	0.68 ± 0.1	0.85 ± 0.09	0.89 ± 0.07	0.85 ± 0.07	0.87 ± 0.07	0.5 ± 0.0	0.51 ± 0.09
11	0.91 ± 0.05	0.72 ± 0.08	0.85 ± 0.08	0.89 ± 0.07	0.84 ± 0.08	0.88 ± 0.06	0.5 ± 0.0	0.49 ± 0.09
12	0.9 ± 0.06	0.71 ± 0.09	0.86 ± 0.05	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.06	0.5 ± 0.0	0.5 ± 0.1
13	0.91 ± 0.05	0.72 ± 0.08	0.85 ± 0.05	0.89 ± 0.07	0.84 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.51 ± 0.07
14	0.9 ± 0.04	0.72 ± 0.06	0.87 ± 0.05	0.89 ± 0.06	0.83 ± 0.08	0.88 ± 0.05	0.5 ± 0.0	0.52 ± 0.08
15	0.92 ± 0.05	0.75 ± 0.08	0.88 ± 0.05	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.44 ± 0.1
16	0.91 ± 0.06	0.77 ± 0.05	0.86 ± 0.06	0.89 ± 0.07	0.81 ± 0.09	0.88 ± 0.06	0.5 ± 0.0	0.51 ± 0.08
17	0.91 ± 0.05	0.76 ± 0.05	0.84 ± 0.06	0.89 ± 0.06	0.8 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.46 ± 0.1
18	0.9 ± 0.06	0.77 ± 0.06	0.85 ± 0.06	0.89 ± 0.06	0.81 ± 0.1	0.87 ± 0.06	0.5 ± 0.0	0.47 ± 0.09
19	0.92 ± 0.04	0.75 ± 0.06	0.87 ± 0.06	0.89 ± 0.06	0.81 ± 0.09	0.9 ± 0.05	0.5 ± 0.0	0.44 ± 0.08
20	0.91 ± 0.07	0.74 ± 0.07	0.86 ± 0.07	0.88 ± 0.06	0.81 ± 0.09	0.88 ± 0.08	0.5 ± 0.0	0.52 ± 0.08
21	0.91 ± 0.06	0.74 ± 0.07	0.86 ± 0.07	0.88 ± 0.06	0.81 ± 0.08	0.89 ± 0.07	0.5 ± 0.0	0.54 ± 0.04
22	0.89 ± 0.06	0.77 ± 0.04	0.87 ± 0.05	0.88 ± 0.06	0.8 ± 0.1	0.89 ± 0.06	0.5 ± 0.0	0.54 ± 0.07
23	0.89 ± 0.05	0.76 ± 0.07	0.83 ± 0.07	0.89 ± 0.06	0.79 ± 0.11	0.87 ± 0.07	0.5 ± 0.0	0.48 ± 0.08
24	0.91 ± 0.05	0.79 ± 0.06	0.85 ± 0.06	0.89 ± 0.06	0.78 ± 0.11	0.88 ± 0.06	0.5 ± 0.0	0.51 ± 0.07
25	0.91 ± 0.05	0.71 ± 0.08	0.85 ± 0.06	0.88 ± 0.06	0.79 ± 0.11	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.07

Supplementary Materials

Table 23. Uniform quantile transformation, NCA ROC AUC CV outcomes for 51 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.9 ± 0.1	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.86 ± 0.07	0.82 ± 0.1
3	0.91 ± 0.09	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.81 ± 0.09
4	0.91 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.85 ± 0.06	0.81 ± 0.06
5	0.93 ± 0.05	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.05	0.82 ± 0.09
6	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.05	0.78 ± 0.1
7	0.91 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.81 ± 0.03	0.78 ± 0.08
8	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.04	0.81 ± 0.09
9	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.06	0.8 ± 0.06
10	0.9 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.86 ± 0.05	0.81 ± 0.07
11	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.8 ± 0.05	0.8 ± 0.06
12	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.82 ± 0.07
13	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.06	0.82 ± 0.07
14	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.07	0.82 ± 0.06
15	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.06	0.84 ± 0.05
16	0.92 ± 0.04	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.72 ± 0.06	0.8 ± 0.06
17	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.8 ± 0.09
18	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.83 ± 0.06	0.81 ± 0.1
19	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.8 ± 0.06
20	0.92 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.84 ± 0.06	0.78 ± 0.07
21	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.05	0.77 ± 0.08
22	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.71 ± 0.06	0.82 ± 0.05
23	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.78 ± 0.08
24	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.05	0.78 ± 0.09
25	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.05	0.77 ± 0.1
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.89 ± 0.08	0.58 ± 0.09	0.84 ± 0.09	0.89 ± 0.06	0.88 ± 0.07	0.85 ± 0.09	0.5 ± 0.0	0.47 ± 0.07
3	0.92 ± 0.06	0.64 ± 0.11	0.86 ± 0.09	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.52 ± 0.07
4	0.91 ± 0.06	0.68 ± 0.09	0.85 ± 0.08	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.09	0.5 ± 0.0	0.46 ± 0.09
5	0.92 ± 0.07	0.68 ± 0.08	0.9 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.91 ± 0.07	0.5 ± 0.0	0.47 ± 0.08
6	0.91 ± 0.07	0.68 ± 0.1	0.86 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.87 ± 0.08	0.5 ± 0.0	0.46 ± 0.06
7	0.91 ± 0.07	0.71 ± 0.08	0.87 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.5 ± 0.07
8	0.91 ± 0.08	0.71 ± 0.07	0.86 ± 0.06	0.89 ± 0.07	0.86 ± 0.07	0.89 ± 0.1	0.5 ± 0.0	0.49 ± 0.09
9	0.91 ± 0.06	0.72 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.08	0.89 ± 0.06	0.5 ± 0.0	0.5 ± 0.08
10	0.91 ± 0.05	0.72 ± 0.09	0.88 ± 0.05	0.89 ± 0.07	0.85 ± 0.08	0.9 ± 0.06	0.5 ± 0.0	0.52 ± 0.08
11	0.92 ± 0.05	0.72 ± 0.07	0.88 ± 0.06	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.05	0.5 ± 0.0	0.47 ± 0.06
12	0.92 ± 0.05	0.73 ± 0.08	0.87 ± 0.07	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.07	0.5 ± 0.0	0.48 ± 0.09
13	0.92 ± 0.06	0.72 ± 0.07	0.88 ± 0.08	0.89 ± 0.07	0.82 ± 0.11	0.91 ± 0.07	0.5 ± 0.0	0.5 ± 0.07
14	0.92 ± 0.05	0.74 ± 0.07	0.86 ± 0.08	0.89 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.45 ± 0.07
15	0.92 ± 0.06	0.71 ± 0.07	0.88 ± 0.06	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.06
16	0.92 ± 0.06	0.76 ± 0.09	0.86 ± 0.09	0.88 ± 0.07	0.82 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.07
17	0.92 ± 0.06	0.74 ± 0.09	0.85 ± 0.08	0.88 ± 0.07	0.82 ± 0.09	0.89 ± 0.07	0.5 ± 0.0	0.5 ± 0.07
18	0.91 ± 0.06	0.76 ± 0.07	0.87 ± 0.08	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.52 ± 0.1
19	0.91 ± 0.07	0.74 ± 0.08	0.86 ± 0.07	0.88 ± 0.07	0.83 ± 0.1	0.9 ± 0.06	0.5 ± 0.0	0.48 ± 0.08
20	0.92 ± 0.06	0.74 ± 0.08	0.89 ± 0.05	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.52 ± 0.06
21	0.91 ± 0.06	0.75 ± 0.09	0.88 ± 0.06	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.04
22	0.92 ± 0.06	0.76 ± 0.08	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.09
23	0.92 ± 0.06	0.78 ± 0.06	0.87 ± 0.09	0.88 ± 0.07	0.81 ± 0.1	0.9 ± 0.05	0.5 ± 0.0	0.49 ± 0.06
24	0.91 ± 0.07	0.78 ± 0.08	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.11	0.9 ± 0.07	0.5 ± 0.0	0.54 ± 0.05
25	0.91 ± 0.07	0.76 ± 0.08	0.86 ± 0.05	0.88 ± 0.07	0.8 ± 0.11	0.89 ± 0.07	0.5 ± 0.0	0.52 ± 0.08

Table 24. Uniform quantile transformation, NCA ROC AUC CV outcomes for 25 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.89 ± 0.07	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.86 ± 0.07	0.81 ± 0.07
3	0.9 ± 0.04	0.9 ± 0.05	0.9 ± 0.06	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.06	0.87 ± 0.03	0.78 ± 0.07
4	0.91 ± 0.04	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.05	0.85 ± 0.05	0.79 ± 0.1
5	0.91 ± 0.05	0.9 ± 0.06	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.05	0.78 ± 0.06	0.83 ± 0.06
6	0.91 ± 0.04	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.05	0.81 ± 0.05	0.78 ± 0.08
7	0.92 ± 0.04	0.89 ± 0.06	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.05	0.9 ± 0.06	0.82 ± 0.07	0.78 ± 0.08
8	0.9 ± 0.05	0.89 ± 0.05	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.05	0.77 ± 0.06	0.78 ± 0.09
9	0.89 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.81 ± 0.09	0.8 ± 0.08
10	0.9 ± 0.07	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.86 ± 0.06	0.81 ± 0.07
11	0.9 ± 0.06	0.9 ± 0.05	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.77 ± 0.07	0.75 ± 0.1
12	0.9 ± 0.05	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.72 ± 0.07	0.75 ± 0.08
13	0.91 ± 0.05	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.73 ± 0.09	0.74 ± 0.07
14	0.9 ± 0.06	0.89 ± 0.07	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.77 ± 0.09	0.78 ± 0.09
15	0.91 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.84 ± 0.06	0.81 ± 0.09
16	0.91 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.78 ± 0.09	0.74 ± 0.09
17	0.91 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.81 ± 0.08	0.79 ± 0.08
18	0.92 ± 0.05	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.78 ± 0.08	0.79 ± 0.08
19	0.91 ± 0.07	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.79 ± 0.07	0.78 ± 0.08
20	0.91 ± 0.07	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.86 ± 0.06	0.8 ± 0.09
21	0.91 ± 0.07	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.81 ± 0.05	0.77 ± 0.11
22	0.92 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.85 ± 0.05	0.79 ± 0.08
23	0.91 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.83 ± 0.05	0.77 ± 0.1
24	0.92 ± 0.05	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.74 ± 0.06	0.83 ± 0.07
25	0.92 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.61 ± 0.05	0.78 ± 0.08
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.9 ± 0.06	0.62 ± 0.09	0.89 ± 0.05	0.9 ± 0.06	0.89 ± 0.06	0.92 ± 0.05	0.5 ± 0.0	0.48 ± 0.08
3	0.91 ± 0.05	0.53 ± 0.15	0.87 ± 0.06	0.9 ± 0.05	0.9 ± 0.06	0.89 ± 0.04	0.5 ± 0.0	0.51 ± 0.09
4	0.91 ± 0.06	0.6 ± 0.08	0.89 ± 0.05	0.9 ± 0.06	0.9 ± 0.06	0.89 ± 0.07	0.5 ± 0.0	0.49 ± 0.05
5	0.92 ± 0.04	0.61 ± 0.07	0.87 ± 0.07	0.9 ± 0.05	0.9 ± 0.06	0.9 ± 0.04	0.5 ± 0.0	0.51 ± 0.07
6	0.91 ± 0.06	0.62 ± 0.1	0.87 ± 0.06	0.9 ± 0.05	0.89 ± 0.06	0.88 ± 0.07	0.5 ± 0.0	0.5 ± 0.04
7	0.92 ± 0.06	0.68 ± 0.07	0.86 ± 0.06	0.9 ± 0.06	0.88 ± 0.06	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.12
8	0.92 ± 0.05	0.69 ± 0.07	0.86 ± 0.07	0.9 ± 0.05	0.88 ± 0.07	0.9 ± 0.06	0.5 ± 0.0	0.5 ± 0.08
9	0.92 ± 0.06	0.68 ± 0.06	0.86 ± 0.06	0.89 ± 0.06	0.87 ± 0.06	0.89 ± 0.06	0.5 ± 0.0	0.5 ± 0.07
10	0.91 ± 0.06	0.75 ± 0.05	0.87 ± 0.07	0.89 ± 0.05	0.87 ± 0.07	0.9 ± 0.06	0.5 ± 0.0	0.51 ± 0.07
11	0.89 ± 0.06	0.76 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.86 ± 0.07	0.87 ± 0.06	0.5 ± 0.0	0.49 ± 0.09
12	0.9 ± 0.07	0.76 ± 0.07	0.87 ± 0.07	0.89 ± 0.06	0.86 ± 0.06	0.89 ± 0.07	0.5 ± 0.0	0.49 ± 0.07
13	0.9 ± 0.06	0.7 ± 0.07	0.85 ± 0.07	0.89 ± 0.07	0.86 ± 0.07	0.88 ± 0.07	0.5 ± 0.0	0.48 ± 0.09
14	0.9 ± 0.06	0.75 ± 0.06	0.86 ± 0.08	0.89 ± 0.06	0.84 ± 0.08	0.87 ± 0.07	0.5 ± 0.0	0.49 ± 0.07
15	0.91 ± 0.06	0.73 ± 0.07	0.86 ± 0.08	0.9 ± 0.06	0.85 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.56 ± 0.03
16	0.91 ± 0.06	0.71 ± 0.1	0.84 ± 0.07	0.9 ± 0.06	0.85 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.46 ± 0.11
17	0.91 ± 0.06	0.79 ± 0.06	0.88 ± 0.05	0.9 ± 0.06	0.83 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.08
18	0.91 ± 0.05	0.77 ± 0.06	0.88 ± 0.05	0.89 ± 0.06	0.82 ± 0.1	0.9 ± 0.05	0.5 ± 0.0	0.51 ± 0.09
19	0.91 ± 0.05	0.74 ± 0.07	0.87 ± 0.07	0.89 ± 0.06	0.82 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.48 ± 0.07
20	0.92 ± 0.06	0.76 ± 0.06	0.87 ± 0.06	0.89 ± 0.06	0.81 ± 0.08	0.9 ± 0.07	0.5 ± 0.0	0.47 ± 0.07
21	0.92 ± 0.06	0.74 ± 0.07	0.87 ± 0.07	0.89 ± 0.06	0.82 ± 0.08	0.89 ± 0.06	0.5 ± 0.0	0.56 ± 0.08
22	0.92 ± 0.06	0.77 ± 0.08	0.87 ± 0.07	0.89 ± 0.06	0.81 ± 0.08	0.9 ± 0.06	0.5 ± 0.0	0.52 ± 0.12
23	0.91 ± 0.06	0.78 ± 0.07	0.88 ± 0.06	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.06	0.5 ± 0.0	0.45 ± 0.06
24	0.91 ± 0.06	0.78 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.81 ± 0.09	0.89 ± 0.08	0.5 ± 0.0	0.49 ± 0.07
25	0.92 ± 0.06	0.77 ± 0.08	0.86 ± 0.04	0.9 ± 0.06	0.81 ± 0.09	0.92 ± 0.06	0.5 ± 0.0	0.51 ± 0.06

Supplementary Materials

Table 25. Uniform quantile transformation, NCA ROC AUC CV outcomes for 13 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.83 ± 0.06	0.8 ± 0.05
3	0.9 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.06	0.81 ± 0.05
4	0.88 ± 0.07	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.82 ± 0.05	0.78 ± 0.06
5	0.89 ± 0.04	0.89 ± 0.07	0.89 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.59 ± 0.05	0.74 ± 0.07
6	0.9 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.74 ± 0.04	0.75 ± 0.07
7	0.91 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.75 ± 0.05	0.79 ± 0.04
8	0.91 ± 0.04	0.88 ± 0.07	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.81 ± 0.06	0.75 ± 0.07
9	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.78 ± 0.07
10	0.89 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.8 ± 0.05	0.79 ± 0.08
11	0.89 ± 0.03	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.05	0.78 ± 0.04
12	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.76 ± 0.05	0.78 ± 0.05
13	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.06	0.8 ± 0.07
14	0.89 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.75 ± 0.06
15	0.89 ± 0.04	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.04	0.78 ± 0.07
16	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.77 ± 0.06
17	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.81 ± 0.04	0.81 ± 0.06
18	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.03	0.78 ± 0.08
19	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.03	0.8 ± 0.07
20	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.05	0.77 ± 0.06
21	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.05	0.79 ± 0.06
22	0.88 ± 0.04	0.87 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.58 ± 0.04	0.78 ± 0.07
23	0.88 ± 0.04	0.88 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.59 ± 0.06	0.78 ± 0.09
24	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.75 ± 0.09
25	0.89 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.81 ± 0.04	0.78 ± 0.08
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.9 ± 0.06	0.56 ± 0.12	0.84 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.87 ± 0.05	0.5 ± 0.0	0.47 ± 0.07
3	0.91 ± 0.04	0.66 ± 0.1	0.86 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.9 ± 0.05	0.5 ± 0.0	0.49 ± 0.08
4	0.9 ± 0.06	0.66 ± 0.09	0.86 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.53 ± 0.09
5	0.9 ± 0.06	0.67 ± 0.08	0.81 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.87 ± 0.05	0.5 ± 0.0	0.49 ± 0.07
6	0.91 ± 0.05	0.69 ± 0.11	0.86 ± 0.06	0.88 ± 0.06	0.88 ± 0.07	0.87 ± 0.06	0.5 ± 0.0	0.55 ± 0.1
7	0.91 ± 0.05	0.64 ± 0.08	0.88 ± 0.05	0.89 ± 0.07	0.86 ± 0.08	0.91 ± 0.04	0.5 ± 0.0	0.56 ± 0.09
8	0.9 ± 0.06	0.67 ± 0.08	0.84 ± 0.06	0.89 ± 0.07	0.86 ± 0.08	0.85 ± 0.09	0.5 ± 0.0	0.5 ± 0.1
9	0.9 ± 0.05	0.68 ± 0.09	0.85 ± 0.06	0.89 ± 0.07	0.86 ± 0.08	0.89 ± 0.06	0.5 ± 0.0	0.48 ± 0.07
10	0.9 ± 0.06	0.67 ± 0.09	0.85 ± 0.09	0.89 ± 0.07	0.85 ± 0.07	0.87 ± 0.07	0.5 ± 0.0	0.5 ± 0.08
11	0.9 ± 0.06	0.72 ± 0.1	0.85 ± 0.08	0.89 ± 0.07	0.84 ± 0.08	0.88 ± 0.06	0.5 ± 0.0	0.47 ± 0.06
12	0.9 ± 0.05	0.72 ± 0.08	0.86 ± 0.05	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.06	0.5 ± 0.0	0.47 ± 0.05
13	0.91 ± 0.05	0.73 ± 0.08	0.85 ± 0.05	0.89 ± 0.07	0.84 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.52 ± 0.07
14	0.9 ± 0.05	0.74 ± 0.07	0.87 ± 0.05	0.89 ± 0.06	0.83 ± 0.08	0.87 ± 0.05	0.5 ± 0.0	0.52 ± 0.06
15	0.92 ± 0.04	0.75 ± 0.07	0.88 ± 0.05	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.55 ± 0.05
16	0.91 ± 0.05	0.75 ± 0.05	0.86 ± 0.06	0.89 ± 0.07	0.81 ± 0.09	0.88 ± 0.06	0.5 ± 0.0	0.47 ± 0.06
17	0.91 ± 0.05	0.76 ± 0.06	0.84 ± 0.06	0.89 ± 0.06	0.8 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.48 ± 0.05
18	0.91 ± 0.06	0.78 ± 0.05	0.85 ± 0.06	0.89 ± 0.06	0.81 ± 0.1	0.87 ± 0.06	0.5 ± 0.0	0.49 ± 0.07
19	0.91 ± 0.05	0.76 ± 0.07	0.87 ± 0.06	0.89 ± 0.06	0.81 ± 0.09	0.9 ± 0.05	0.5 ± 0.0	0.51 ± 0.07
20	0.91 ± 0.06	0.72 ± 0.1	0.86 ± 0.07	0.88 ± 0.06	0.81 ± 0.09	0.88 ± 0.08	0.5 ± 0.0	0.51 ± 0.06
21	0.91 ± 0.06	0.74 ± 0.06	0.86 ± 0.07	0.88 ± 0.06	0.81 ± 0.08	0.89 ± 0.07	0.5 ± 0.0	0.51 ± 0.06
22	0.89 ± 0.06	0.74 ± 0.09	0.87 ± 0.05	0.88 ± 0.06	0.8 ± 0.1	0.89 ± 0.05	0.5 ± 0.0	0.5 ± 0.07
23	0.89 ± 0.05	0.76 ± 0.06	0.83 ± 0.07	0.89 ± 0.06	0.79 ± 0.11	0.87 ± 0.07	0.5 ± 0.0	0.52 ± 0.07
24	0.9 ± 0.05	0.79 ± 0.06	0.85 ± 0.06	0.89 ± 0.06	0.78 ± 0.11	0.88 ± 0.06	0.5 ± 0.0	0.48 ± 0.03
25	0.9 ± 0.06	0.75 ± 0.07	0.85 ± 0.06	0.88 ± 0.06	0.79 ± 0.11	0.9 ± 0.05	0.5 ± 0.0	0.51 ± 0.09

Table 26. Normal quantile transformation, NCA ROC AUV CV outcomes for 202 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.92 ± 0.06	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.83 ± 0.03	0.81 ± 0.09
3	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.79 ± 0.05	0.73 ± 0.09
4	0.91 ± 0.06	0.9 ± 0.06	0.9 ± 0.07	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.07	0.81 ± 0.05	0.77 ± 0.11
5	0.91 ± 0.03	0.9 ± 0.07	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.86 ± 0.04	0.8 ± 0.03
6	0.92 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.78 ± 0.04	0.76 ± 0.07
7	0.91 ± 0.06	0.9 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.63 ± 0.05	0.77 ± 0.07
8	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.9 ± 0.06	0.72 ± 0.07	0.74 ± 0.09
9	0.89 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.9 ± 0.06	0.83 ± 0.06	0.77 ± 0.07
10	0.9 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.76 ± 0.06	0.73 ± 0.1
11	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.06	0.9 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.77 ± 0.06	0.73 ± 0.08
12	0.88 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.06	0.77 ± 0.0
13	0.89 ± 0.06	0.88 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.72 ± 0.07	0.78 ± 0.0
14	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.79 ± 0.06	0.77 ± 0.1
15	0.91 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.81 ± 0.05	0.75 ± 0.06
16	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.84 ± 0.04	0.79 ± 0.06
17	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.81 ± 0.06	0.79 ± 0.09
18	0.91 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.06	0.81 ± 0.06	0.74 ± 0.07
19	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.83 ± 0.06	0.76 ± 0.08
20	0.9 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.82 ± 0.06	0.78 ± 0.08
21	0.9 ± 0.08	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.65 ± 0.05	0.73 ± 0.07
22	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.9 ± 0.07	0.78 ± 0.06	0.77 ± 0.07
23	0.9 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.77 ± 0.08	0.78 ± 0.08
24	0.9 ± 0.07	0.88 ± 0.07	0.9 ± 0.06	0.9 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.7 ± 0.08	0.75 ± 0.08
25	0.9 ± 0.07	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.75 ± 0.08	0.81 ± 0.04
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.9 ± 0.07	0.54 ± 0.1	0.87 ± 0.07	0.89 ± 0.07	0.9 ± 0.07	0.87 ± 0.08	0.5 ± 0.0	0.54 ± 0.08
3	0.91 ± 0.06	0.57 ± 0.12	0.84 ± 0.06	0.89 ± 0.06	0.9 ± 0.06	0.87 ± 0.06	0.5 ± 0.0	0.49 ± 0.09
4	0.9 ± 0.07	0.6 ± 0.09	0.83 ± 0.08	0.89 ± 0.06	0.9 ± 0.06	0.87 ± 0.06	0.5 ± 0.0	0.48 ± 0.07
5	0.9 ± 0.06	0.68 ± 0.08	0.83 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.49 ± 0.06
6	0.9 ± 0.07	0.65 ± 0.08	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.5 ± 0.0	0.46 ± 0.08
7	0.89 ± 0.06	0.69 ± 0.07	0.86 ± 0.04	0.88 ± 0.07	0.88 ± 0.08	0.87 ± 0.07	0.5 ± 0.0	0.46 ± 0.07
8	0.89 ± 0.06	0.69 ± 0.1	0.84 ± 0.04	0.88 ± 0.07	0.87 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.5 ± 0.06
9	0.89 ± 0.07	0.68 ± 0.1	0.83 ± 0.06	0.88 ± 0.07	0.86 ± 0.08	0.88 ± 0.07	0.5 ± 0.0	0.48 ± 0.07
10	0.88 ± 0.08	0.63 ± 0.11	0.85 ± 0.1	0.88 ± 0.08	0.86 ± 0.07	0.86 ± 0.08	0.5 ± 0.0	0.52 ± 0.11
11	0.9 ± 0.07	0.61 ± 0.1	0.83 ± 0.07	0.89 ± 0.07	0.84 ± 0.07	0.85 ± 0.07	0.5 ± 0.0	0.51 ± 0.08
12	0.9 ± 0.07	0.72 ± 0.09	0.86 ± 0.07	0.88 ± 0.07	0.85 ± 0.07	0.87 ± 0.08	0.5 ± 0.0	0.48 ± 0.09
13	0.9 ± 0.07	0.73 ± 0.07	0.83 ± 0.06	0.88 ± 0.07	0.83 ± 0.09	0.87 ± 0.08	0.5 ± 0.0	0.51 ± 0.08
14	0.9 ± 0.06	0.71 ± 0.09	0.87 ± 0.07	0.88 ± 0.07	0.83 ± 0.09	0.89 ± 0.08	0.5 ± 0.0	0.51 ± 0.07
15	0.9 ± 0.07	0.73 ± 0.06	0.85 ± 0.06	0.89 ± 0.07	0.83 ± 0.09	0.87 ± 0.06	0.5 ± 0.0	0.45 ± 0.05
16	0.9 ± 0.07	0.72 ± 0.07	0.9 ± 0.06	0.89 ± 0.07	0.85 ± 0.08	0.89 ± 0.06	0.5 ± 0.0	0.49 ± 0.05
17	0.9 ± 0.07	0.74 ± 0.09	0.88 ± 0.09	0.89 ± 0.07	0.83 ± 0.08	0.88 ± 0.08	0.5 ± 0.0	0.49 ± 0.05
18	0.9 ± 0.08	0.7 ± 0.07	0.9 ± 0.05	0.89 ± 0.07	0.81 ± 0.09	0.89 ± 0.07	0.5 ± 0.0	0.51 ± 0.05
19	0.9 ± 0.07	0.73 ± 0.08	0.87 ± 0.06	0.89 ± 0.07	0.81 ± 0.09	0.89 ± 0.07	0.5 ± 0.0	0.52 ± 0.06
20	0.91 ± 0.07	0.76 ± 0.05	0.87 ± 0.07	0.88 ± 0.07	0.82 ± 0.1	0.87 ± 0.08	0.5 ± 0.0	0.47 ± 0.1
21	0.89 ± 0.07	0.72 ± 0.08	0.87 ± 0.08	0.88 ± 0.07	0.82 ± 0.1	0.88 ± 0.06	0.5 ± 0.0	0.52 ± 0.06
22	0.9 ± 0.07	0.72 ± 0.1	0.87 ± 0.05	0.88 ± 0.07	0.81 ± 0.09	0.89 ± 0.04	0.5 ± 0.0	0.49 ± 0.07
23	0.91 ± 0.05	0.74 ± 0.11	0.87 ± 0.06	0.88 ± 0.07	0.81 ± 0.09	0.9 ± 0.09	0.5 ± 0.0	0.48 ± 0.07



Supplementary Materials

Table 27. Normal quantile transformation, NCA ROC AUC CV outcomes for 101 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.83 ± 0.06	0.8 ± 0.05
3	0.9 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.06	0.82 ± 0.06
4	0.88 ± 0.07	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.82 ± 0.05	0.8 ± 0.07
5	0.89 ± 0.04	0.89 ± 0.07	0.89 ± 0.07	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.59 ± 0.05	0.75 ± 0.06
6	0.9 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.74 ± 0.04	0.76 ± 0.08
7	0.91 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.75 ± 0.05	0.79 ± 0.03
8	0.91 ± 0.04	0.88 ± 0.07	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.81 ± 0.06	0.76 ± 0.06
9	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.78 ± 0.07
10	0.89 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.88 ± 0.06	0.8 ± 0.05	0.78 ± 0.08
11	0.89 ± 0.03	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.05	0.78 ± 0.04
12	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.76 ± 0.05	0.78 ± 0.05
13	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.06	0.79 ± 0.08
14	0.89 ± 0.05	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.75 ± 0.07
15	0.89 ± 0.04	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.04	0.78 ± 0.07
16	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.76 ± 0.07
17	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.81 ± 0.04	0.78 ± 0.06
18	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.03	0.79 ± 0.06
19	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.03	0.8 ± 0.06
20	0.9 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.78 ± 0.05	0.75 ± 0.06
21	0.9 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.05	0.77 ± 0.08
22	0.88 ± 0.04	0.87 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.58 ± 0.04	0.77 ± 0.05
23	0.88 ± 0.04	0.88 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.59 ± 0.06	0.76 ± 0.08
24	0.89 ± 0.04	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.75 ± 0.09
25	0.89 ± 0.05	0.88 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.81 ± 0.04	0.79 ± 0.07
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.9 ± 0.05	0.62 ± 0.09	0.84 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.87 ± 0.05	0.5 ± 0.0	0.51 ± 0.06
3	0.91 ± 0.04	0.65 ± 0.1	0.86 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.9 ± 0.05	0.5 ± 0.0	0.53 ± 0.08
4	0.9 ± 0.06	0.68 ± 0.1	0.86 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.88 ± 0.06	0.5 ± 0.0	0.52 ± 0.06
5	0.9 ± 0.06	0.65 ± 0.07	0.81 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.87 ± 0.05	0.5 ± 0.0	0.53 ± 0.08
6	0.9 ± 0.04	0.67 ± 0.09	0.86 ± 0.06	0.88 ± 0.06	0.88 ± 0.07	0.87 ± 0.06	0.5 ± 0.0	0.54 ± 0.07
7	0.92 ± 0.05	0.67 ± 0.08	0.88 ± 0.05	0.89 ± 0.07	0.86 ± 0.08	0.91 ± 0.04	0.5 ± 0.0	0.45 ± 0.05
8	0.9 ± 0.05	0.68 ± 0.07	0.84 ± 0.06	0.89 ± 0.07	0.86 ± 0.08	0.85 ± 0.09	0.5 ± 0.0	0.47 ± 0.07
9	0.9 ± 0.05	0.68 ± 0.11	0.85 ± 0.06	0.89 ± 0.07	0.86 ± 0.08	0.89 ± 0.05	0.5 ± 0.0	0.54 ± 0.05
10	0.9 ± 0.06	0.71 ± 0.1	0.85 ± 0.09	0.89 ± 0.07	0.85 ± 0.07	0.87 ± 0.07	0.5 ± 0.0	0.48 ± 0.08
11	0.91 ± 0.05	0.7 ± 0.08	0.85 ± 0.08	0.89 ± 0.07	0.84 ± 0.08	0.88 ± 0.06	0.5 ± 0.0	0.55 ± 0.06
12	0.9 ± 0.05	0.71 ± 0.08	0.86 ± 0.05	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.06	0.5 ± 0.0	0.49 ± 0.04
13	0.9 ± 0.05	0.68 ± 0.09	0.85 ± 0.05	0.89 ± 0.07	0.84 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.57 ± 0.08
14	0.9 ± 0.05	0.72 ± 0.06	0.87 ± 0.05	0.89 ± 0.06	0.83 ± 0.08	0.88 ± 0.05	0.5 ± 0.0	0.56 ± 0.09
15	0.92 ± 0.04	0.76 ± 0.08	0.88 ± 0.05	0.89 ± 0.06	0.82 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.5 ± 0.05
16	0.9 ± 0.06	0.76 ± 0.05	0.86 ± 0.06	0.89 ± 0.07	0.81 ± 0.09	0.88 ± 0.06	0.5 ± 0.0	0.54 ± 0.07
17	0.91 ± 0.05	0.76 ± 0.04	0.84 ± 0.06	0.89 ± 0.06	0.8 ± 0.09	0.89 ± 0.05	0.5 ± 0.0	0.46 ± 0.06
18	0.91 ± 0.05	0.76 ± 0.08	0.85 ± 0.06	0.89 ± 0.06	0.81 ± 0.1	0.87 ± 0.07	0.5 ± 0.0	0.53 ± 0.05
19	0.91 ± 0.05	0.75 ± 0.07	0.87 ± 0.06	0.89 ± 0.06	0.81 ± 0.09	0.9 ± 0.05	0.5 ± 0.0	0.56 ± 0.07
20	0.91 ± 0.06	0.75 ± 0.08	0.86 ± 0.07	0.88 ± 0.06	0.81 ± 0.09	0.88 ± 0.07	0.5 ± 0.0	0.51 ± 0.09
21	0.91 ± 0.06	0.71 ± 0.09	0.86 ± 0.07	0.88 ± 0.06	0.81 ± 0.08	0.89 ± 0.07	0.5 ± 0.0	0.51 ± 0.08
22	0.9 ± 0.05	0.77 ± 0.08	0.87 ± 0.05	0.88 ± 0.06	0.8 ± 0.1	0.89 ± 0.06	0.5 ± 0.0	0.49 ± 0.04
23	0.89 ± 0.05	0.74 ± 0.06	0.83 ± 0.07	0.89 ± 0.06	0.79 ± 0.11	0.87 ± 0.07	0.5 ± 0.0	0.45 ± 0.07
24	0.9 ± 0.05	0.76 ± 0.08	0.85 ± 0.06	0.89 ± 0.06	0.78 ± 0.11	0.88 ± 0.06	0.5 ± 0.0	0.49 ± 0.05
25	0.91 ± 0.05	0.7 ± 0.09	0.85 ± 0.06	0.88 ± 0.06	0.79 ± 0.11	0.9 ± 0.06	0.5 ± 0.0	0.52 ± 0.05

Table 28. Normal quantile transformation, NCA ROC AUC CV outcomes for 51 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.9 ± 0.1	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.86 ± 0.07	0.81 ± 0.11
3	0.91 ± 0.09	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.81 ± 0.09
4	0.91 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.85 ± 0.06	0.82 ± 0.06
5	0.93 ± 0.05	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.05	0.82 ± 0.06
6	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.05	0.77 ± 0.1
7	0.91 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.81 ± 0.03	0.81 ± 0.08
8	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.04	0.82 ± 0.1
9	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.06	0.78 ± 0.06
10	0.9 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.86 ± 0.05	0.81 ± 0.07
11	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.8 ± 0.05	0.79 ± 0.04
12	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.81 ± 0.08
13	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.06	0.82 ± 0.07
14	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.07	0.83 ± 0.05
15	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.06	0.82 ± 0.05
16	0.92 ± 0.04	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.72 ± 0.06	0.81 ± 0.06
17	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.81 ± 0.08
18	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.83 ± 0.06	0.8 ± 0.12
19	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.79 ± 0.06
20	0.92 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.84 ± 0.06	0.78 ± 0.09
21	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.05	0.79 ± 0.08
22	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.71 ± 0.06	0.83 ± 0.05
23	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.8 ± 0.07
24	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.05	0.78 ± 0.07
25	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.05	0.76 ± 0.12
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.89 ± 0.09	0.58 ± 0.11	0.84 ± 0.09	0.89 ± 0.06	0.88 ± 0.07	0.85 ± 0.09	0.5 ± 0.0	0.49 ± 0.09
3	0.92 ± 0.05	0.6 ± 0.12	0.86 ± 0.09	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.49 ± 0.13
4	0.92 ± 0.05	0.67 ± 0.1	0.85 ± 0.08	0.89 ± 0.07	0.89 ± 0.07	0.88 ± 0.1	0.5 ± 0.0	0.48 ± 0.09
5	0.92 ± 0.07	0.68 ± 0.08	0.9 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.91 ± 0.07	0.5 ± 0.0	0.49 ± 0.09
6	0.91 ± 0.06	0.68 ± 0.1	0.86 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.87 ± 0.08	0.5 ± 0.0	0.51 ± 0.06
7	0.91 ± 0.07	0.72 ± 0.08	0.87 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.52 ± 0.09
8	0.91 ± 0.08	0.73 ± 0.07	0.86 ± 0.06	0.89 ± 0.07	0.86 ± 0.07	0.88 ± 0.1	0.5 ± 0.0	0.48 ± 0.06
9	0.91 ± 0.06	0.72 ± 0.09	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.08	0.89 ± 0.07	0.5 ± 0.0	0.53 ± 0.06
10	0.92 ± 0.06	0.71 ± 0.07	0.88 ± 0.05	0.89 ± 0.07	0.85 ± 0.08	0.9 ± 0.06	0.5 ± 0.0	0.5 ± 0.06
11	0.92 ± 0.05	0.74 ± 0.08	0.88 ± 0.06	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.05	0.5 ± 0.0	0.49 ± 0.05
12	0.91 ± 0.06	0.74 ± 0.07	0.87 ± 0.07	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.08
13	0.92 ± 0.05	0.73 ± 0.08	0.88 ± 0.08	0.89 ± 0.07	0.82 ± 0.11	0.91 ± 0.07	0.5 ± 0.0	0.48 ± 0.07
14	0.91 ± 0.06	0.75 ± 0.08	0.86 ± 0.08	0.89 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.47 ± 0.04
15	0.92 ± 0.06	0.71 ± 0.08	0.88 ± 0.06	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.48 ± 0.08
16	0.91 ± 0.06	0.78 ± 0.09	0.86 ± 0.09	0.88 ± 0.07	0.82 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.45 ± 0.07
17	0.91 ± 0.06	0.76 ± 0.07	0.85 ± 0.08	0.88 ± 0.07	0.82 ± 0.09	0.89 ± 0.07	0.5 ± 0.0	0.47 ± 0.11
18	0.91 ± 0.06	0.75 ± 0.08	0.87 ± 0.08	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.53 ± 0.08
19	0.91 ± 0.06	0.75 ± 0.08	0.86 ± 0.08	0.88 ± 0.07	0.83 ± 0.1	0.9 ± 0.06	0.5 ± 0.0	0.51 ± 0.06
20	0.91 ± 0.07	0.77 ± 0.07	0.89 ± 0.05	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.47 ± 0.06
21	0.91 ± 0.06	0.74 ± 0.09	0.88 ± 0.06	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.08	0.5 ± 0.0	0.5 ± 0.08
22	0.92 ± 0.06	0.77 ± 0.09	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.54 ± 0.08
23	0.92 ± 0.07	0.77 ± 0.07	0.87 ± 0.09	0.88 ± 0.07	0.81 ± 0.1	0.9 ± 0.05	0.5 ± 0.0	0.52 ± 0.08
24	0.92 ± 0.06	0.78 ± 0.1	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.11	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.1
25	0.91 ± 0.07	0.77 ± 0.09	0.86 ± 0.05	0.88 ± 0.07	0.8 ± 0.11	0.89 ± 0.07	0.5 ± 0.0	0.49 ± 0.05

Supplementary Materials

Table 29. Normal quantile transformation, NCA ROC AUC CV outcomes for 25 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.9 ± 0.1	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.86 ± 0.07	0.82 ± 0.11
3	0.91 ± 0.09	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.81 ± 0.09
4	0.91 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.85 ± 0.06	0.82 ± 0.05
5	0.93 ± 0.05	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.05	0.82 ± 0.08
6	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.05	0.77 ± 0.11
7	0.91 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.81 ± 0.03	0.78 ± 0.09
8	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.04	0.81 ± 0.1
9	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.06	0.8 ± 0.07
10	0.9 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.86 ± 0.05	0.82 ± 0.08
11	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.8 ± 0.05	0.79 ± 0.05
12	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.81 ± 0.09
13	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.06	0.82 ± 0.07
14	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.07	0.82 ± 0.06
15	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.06	0.82 ± 0.04
16	0.92 ± 0.04	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.72 ± 0.06	0.79 ± 0.06
17	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.8 ± 0.09
18	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.83 ± 0.06	0.79 ± 0.09
19	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.78 ± 0.06
20	0.92 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.84 ± 0.06	0.76 ± 0.09
21	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.05	0.78 ± 0.07
22	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.71 ± 0.06	0.8 ± 0.07
23	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.8 ± 0.06
24	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.05	0.79 ± 0.08
25	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.05	0.76 ± 0.1
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.89 ± 0.09	0.56 ± 0.08	0.84 ± 0.09	0.89 ± 0.06	0.88 ± 0.07	0.85 ± 0.09	0.5 ± 0.0	0.51 ± 0.1
3	0.92 ± 0.06	0.64 ± 0.12	0.86 ± 0.09	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.5 ± 0.07
4	0.92 ± 0.06	0.66 ± 0.1	0.85 ± 0.08	0.89 ± 0.07	0.89 ± 0.07	0.88 ± 0.1	0.5 ± 0.0	0.52 ± 0.09
5	0.92 ± 0.07	0.67 ± 0.09	0.9 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.91 ± 0.07	0.5 ± 0.0	0.51 ± 0.08
6	0.91 ± 0.06	0.68 ± 0.1	0.86 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.87 ± 0.08	0.5 ± 0.0	0.46 ± 0.07
7	0.91 ± 0.07	0.72 ± 0.08	0.87 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.5 ± 0.05
8	0.91 ± 0.07	0.7 ± 0.06	0.86 ± 0.06	0.89 ± 0.07	0.86 ± 0.07	0.89 ± 0.1	0.5 ± 0.0	0.47 ± 0.06
9	0.91 ± 0.07	0.72 ± 0.08	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.08	0.89 ± 0.06	0.5 ± 0.0	0.53 ± 0.09
10	0.91 ± 0.05	0.71 ± 0.08	0.88 ± 0.05	0.89 ± 0.07	0.85 ± 0.08	0.9 ± 0.06	0.5 ± 0.0	0.51 ± 0.07
11	0.92 ± 0.05	0.74 ± 0.08	0.88 ± 0.06	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.05	0.5 ± 0.0	0.51 ± 0.04
12	0.92 ± 0.06	0.72 ± 0.07	0.87 ± 0.07	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.07	0.5 ± 0.0	0.49 ± 0.07
13	0.92 ± 0.06	0.73 ± 0.09	0.88 ± 0.08	0.89 ± 0.07	0.82 ± 0.11	0.91 ± 0.07	0.5 ± 0.0	0.5 ± 0.07
14	0.92 ± 0.06	0.74 ± 0.07	0.86 ± 0.08	0.89 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.56 ± 0.08
15	0.92 ± 0.05	0.72 ± 0.07	0.88 ± 0.06	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.48 ± 0.05
16	0.91 ± 0.06	0.78 ± 0.07	0.86 ± 0.09	0.88 ± 0.07	0.82 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.54 ± 0.08
17	0.92 ± 0.06	0.76 ± 0.09	0.85 ± 0.08	0.88 ± 0.07	0.82 ± 0.09	0.89 ± 0.07	0.5 ± 0.0	0.49 ± 0.05
18	0.92 ± 0.06	0.75 ± 0.07	0.87 ± 0.08	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.52 ± 0.07
19	0.91 ± 0.06	0.76 ± 0.08	0.86 ± 0.07	0.88 ± 0.07	0.83 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.56 ± 0.05
20	0.92 ± 0.05	0.77 ± 0.09	0.89 ± 0.05	0.88 ± 0.07	0.82 ± 0.09	0.91 ± 0.07	0.5 ± 0.0	0.53 ± 0.07
21	0.91 ± 0.07	0.76 ± 0.07	0.88 ± 0.06	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.48 ± 0.08
22	0.91 ± 0.06	0.76 ± 0.07	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.52 ± 0.08
23	0.92 ± 0.06	0.77 ± 0.11	0.87 ± 0.09	0.88 ± 0.07	0.81 ± 0.1	0.9 ± 0.05	0.5 ± 0.0	0.47 ± 0.11
24	0.91 ± 0.06	0.78 ± 0.08	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.11	0.9 ± 0.06	0.5 ± 0.0	0.48 ± 0.07
25	0.92 ± 0.07	0.77 ± 0.06	0.86 ± 0.05	0.88 ± 0.07	0.8 ± 0.11	0.89 ± 0.07	0.5 ± 0.0	0.52 ± 0.08

Table 30. Normal quantile transformation, NCA ROC AUC CV outcomes for 13 landmark points as pre-binning

Comp.	k-NN	LinSVM	Poly2SVM	Poly3SVM	Poly4SVM	RBF SVM	Gauss Proc	Dec Tree
2	0.9 ± 0.1	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.86 ± 0.07	0.8 ± 0.1
3	0.91 ± 0.09	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.79 ± 0.04	0.8 ± 0.09
4	0.91 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.85 ± 0.06	0.81 ± 0.06
5	0.93 ± 0.05	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.05	0.82 ± 0.08
6	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.05	0.76 ± 0.09
7	0.91 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.81 ± 0.03	0.79 ± 0.09
8	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.87 ± 0.04	0.81 ± 0.1
9	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.74 ± 0.06	0.79 ± 0.06
10	0.9 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.86 ± 0.05	0.81 ± 0.06
11	0.9 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.8 ± 0.05	0.79 ± 0.05
12	0.91 ± 0.05	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.05	0.81 ± 0.07
13	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.06	0.81 ± 0.07
14	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.83 ± 0.07	0.82 ± 0.06
15	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.85 ± 0.06	0.82 ± 0.04
16	0.92 ± 0.04	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.72 ± 0.06	0.81 ± 0.06
17	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.82 ± 0.09
18	0.91 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.83 ± 0.06	0.81 ± 0.1
19	0.91 ± 0.05	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.07	0.78 ± 0.06
20	0.92 ± 0.06	0.88 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.84 ± 0.06	0.77 ± 0.09
21	0.92 ± 0.05	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.81 ± 0.05	0.78 ± 0.09
22	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.07	0.71 ± 0.06	0.8 ± 0.06
23	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.8 ± 0.04	0.8 ± 0.06
24	0.91 ± 0.06	0.88 ± 0.06	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.06	0.89 ± 0.07	0.82 ± 0.05	0.8 ± 0.08
25	0.92 ± 0.06	0.88 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.89 ± 0.06	0.82 ± 0.05	0.75 ± 0.12
Comp.	Random Forest	NNet	AdaBoost	NB	QDA	GradBoost	Dummy1	Dummy2
2	0.89 ± 0.09	0.57 ± 0.09	0.84 ± 0.09	0.89 ± 0.06	0.88 ± 0.07	0.85 ± 0.09	0.5 ± 0.0	0.47 ± 0.07
3	0.92 ± 0.06	0.61 ± 0.08	0.86 ± 0.09	0.89 ± 0.07	0.89 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.49 ± 0.1
4	0.91 ± 0.07	0.68 ± 0.09	0.85 ± 0.08	0.89 ± 0.07	0.89 ± 0.07	0.88 ± 0.1	0.5 ± 0.0	0.51 ± 0.04
5	0.92 ± 0.06	0.67 ± 0.08	0.9 ± 0.06	0.89 ± 0.06	0.88 ± 0.06	0.91 ± 0.07	0.5 ± 0.0	0.51 ± 0.06
6	0.9 ± 0.06	0.68 ± 0.11	0.86 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.87 ± 0.08	0.5 ± 0.0	0.5 ± 0.1
7	0.91 ± 0.06	0.72 ± 0.07	0.87 ± 0.08	0.89 ± 0.06	0.88 ± 0.07	0.89 ± 0.08	0.5 ± 0.0	0.46 ± 0.04
8	0.91 ± 0.07	0.72 ± 0.08	0.86 ± 0.06	0.89 ± 0.07	0.86 ± 0.07	0.88 ± 0.1	0.5 ± 0.0	0.44 ± 0.04
9	0.92 ± 0.06	0.7 ± 0.07	0.89 ± 0.06	0.89 ± 0.06	0.86 ± 0.08	0.89 ± 0.06	0.5 ± 0.0	0.51 ± 0.1
10	0.92 ± 0.06	0.7 ± 0.09	0.88 ± 0.05	0.89 ± 0.07	0.85 ± 0.08	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.06
11	0.92 ± 0.05	0.74 ± 0.08	0.88 ± 0.06	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.05	0.5 ± 0.0	0.52 ± 0.07
12	0.92 ± 0.05	0.72 ± 0.08	0.87 ± 0.07	0.89 ± 0.07	0.84 ± 0.08	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.1
13	0.92 ± 0.05	0.74 ± 0.09	0.88 ± 0.08	0.89 ± 0.07	0.82 ± 0.11	0.91 ± 0.07	0.5 ± 0.0	0.5 ± 0.06
14	0.91 ± 0.06	0.73 ± 0.09	0.86 ± 0.08	0.89 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.56 ± 0.07
15	0.92 ± 0.06	0.74 ± 0.05	0.88 ± 0.06	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.06	0.5 ± 0.0	0.53 ± 0.06
16	0.92 ± 0.05	0.74 ± 0.09	0.86 ± 0.09	0.88 ± 0.07	0.82 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.46 ± 0.08
17	0.92 ± 0.06	0.74 ± 0.07	0.85 ± 0.08	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.48 ± 0.06
18	0.92 ± 0.06	0.75 ± 0.08	0.87 ± 0.08	0.88 ± 0.07	0.83 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.48 ± 0.08
19	0.91 ± 0.06	0.76 ± 0.07	0.86 ± 0.07	0.88 ± 0.07	0.83 ± 0.1	0.9 ± 0.07	0.5 ± 0.0	0.5 ± 0.06
20	0.92 ± 0.07	0.76 ± 0.08	0.89 ± 0.05	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.07	0.5 ± 0.0	0.48 ± 0.05
21	0.91 ± 0.07	0.74 ± 0.1	0.88 ± 0.06	0.88 ± 0.07	0.82 ± 0.09	0.9 ± 0.08	0.5 ± 0.0	0.53 ± 0.06
22	0.92 ± 0.06	0.74 ± 0.09	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.1	0.89 ± 0.07	0.5 ± 0.0	0.54 ± 0.08
23	0.91 ± 0.06	0.79 ± 0.07	0.87 ± 0.09	0.88 ± 0.07	0.81 ± 0.1	0.9 ± 0.05	0.5 ± 0.0	0.52 ± 0.09
24	0.91 ± 0.06	0.78 ± 0.07	0.87 ± 0.08	0.88 ± 0.07	0.8 ± 0.11	0.9 ± 0.06	0.5 ± 0.0	0.5 ± 0.07
25	0.91 ± 0.07	0.78 ± 0.07	0.86 ± 0.05	0.88 ± 0.07	0.8 ± 0.11	0.89 ± 0.07	0.5 ± 0.0	0.47 ± 0.09

Supplementary Materials

Table 31. Best discretizer ROC AUC using different configurations of NCA components and Uniform transformation

Comp.	RF	LR	NB	SVM	Dummy
2	CART 0.89±0.09	CART 0.89±0.06	CART 0.88±0.06	CART 0.89±0.07	XGB 0.53±0.08
3	CART 0.92±0.06	CART 0.89±0.06	CART 0.89±0.07	CART 0.89±0.06	ChiMerge 0.53±0.08
4	CART 0.92±0.07	CART 0.89±0.07	CART 0.89±0.07	CART 0.89±0.06	Mod Chi2 0.54±0.08
5	CART 0.92±0.07	CART 0.89±0.07	CART 0.89±0.06	CART 0.89±0.07	AMEVA 0.54±0.07
6	CART 0.9±0.06	CART 0.89±0.06	CART 0.89±0.06	CART 0.89±0.06	CACC 0.54±0.07
7	CART 0.91±0.07	CART 0.89±0.06	CART 0.89±0.06	CART 0.89±0.06	CACC 0.54±0.07
8	CART 0.91±0.08	CART 0.89±0.06	CART 0.89±0.07	CART 0.88±0.06	CART 0.51±0.09
9	CART 0.91±0.06	CART 0.88±0.06	CART 0.89±0.06	CART 0.88±0.06	Mod Chi2 0.52±0.06
10	CART 0.91±0.06	CART 0.88±0.06	CART 0.89±0.07	CART 0.88±0.06	CART 0.53±0.08
11	CART 0.92±0.05	CART 0.88±0.06	CART 0.89±0.07	CART 0.88±0.06	Mod Chi2 0.54±0.09
12	CART 0.92±0.06	CART 0.88±0.06	CART 0.89±0.07	CART 0.89±0.06	CART 0.54±0.06
13	CART 0.92±0.06	CART 0.88±0.06	CART 0.89±0.07	CART 0.88±0.06	ChiMerge 0.55±0.08
14	CART 0.92±0.07	CART 0.89±0.06	CART 0.89±0.07	CART 0.88±0.06	XGB 0.55±0.07
15	CART 0.92±0.05	CART 0.89±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.54±0.08
16	CART 0.92±0.06	CART 0.88±0.07	CART 0.88±0.07	CART 0.88±0.07	XGB 0.54±0.1
17	CART 0.92±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	CAIM 0.55±0.06
18	CART 0.92±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	CART 0.54±0.06
19	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.54±0.05
20	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.07	CACC 0.56±0.08
21	CART 0.92±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.54±0.03
22	CART 0.91±0.07	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.53±0.08
23	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	Mod Chi2 0.52±0.05
24	CART 0.91±0.07	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	CAIM 0.54±0.08
25	CART 0.91±0.07	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	CAIM 0.54±0.1

Table 32. Best discretizer ROC AUC using different configurations of NCA components and Normal transformation

Comp.	RF	LR	NB	SVM	Dummy
2	ChiMerge 0.89±0.04	CART 0.89±0.06	CART 0.88±0.06	CART 0.89±0.07	Mod Chi2 0.53±0.09
3	CART 0.92±0.06	CART 0.89±0.06	CART 0.89±0.07	CART 0.89±0.06	MDLP 0.53±0.07
4	CART 0.92±0.06	CART 0.89±0.07	CART 0.89±0.07	CART 0.89±0.06	ChiMerge 0.54±0.1
5	CART 0.93±0.06	CART 0.89±0.07	CART 0.89±0.06	CART 0.89±0.07	XGB 0.53±0.09
6	CART 0.9±0.06	CART 0.89±0.06	CART 0.89±0.06	CART 0.89±0.06	Ext Chi2 0.54±0.05
7	CART 0.91±0.07	CART 0.89±0.06	CART 0.89±0.06	CART 0.89±0.06	MDLP 0.53±0.06
8	CART 0.91±0.07	CART 0.89±0.06	CART 0.89±0.07	CART 0.88±0.06	XGB 0.53±0.07
9	CART 0.91±0.06	CART 0.88±0.06	CART 0.89±0.06	CART 0.88±0.06	CART 0.53±0.09
10	CART 0.91±0.06	CART 0.88±0.06	CART 0.89±0.07	CART 0.88±0.06	CART 0.53±0.08
11	CART 0.92±0.06	CART 0.88±0.06	CART 0.89±0.07	CART 0.88±0.06	XGB 0.52±0.06
12	CART 0.91±0.05	CART 0.88±0.06	CART 0.89±0.07	CART 0.89±0.06	Ext Chi2 0.54±0.08
13	CART 0.91±0.06	CART 0.88±0.06	CART 0.89±0.07	CART 0.88±0.06	XGB 0.54±0.05
14	CART 0.92±0.05	CART 0.89±0.06	CART 0.89±0.07	CART 0.88±0.06	MDLP 0.55±0.08
15	CART 0.92±0.05	CART 0.89±0.06	CART 0.88±0.07	CART 0.88±0.06	CART 0.54±0.08
16	CART 0.91±0.05	CART 0.88±0.07	CART 0.88±0.07	CART 0.88±0.07	CAIM 0.56±0.06
17	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	CART 0.53±0.06
18	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.52±0.09
19	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	Mod Chi2 0.57±0.07
20	CART 0.92±0.05	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.07	Ext Chi2 0.56±0.08
21	CART 0.91±0.07	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	AMEVA 0.56±0.12
22	CART 0.91±0.07	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.54±0.09
23	CART 0.92±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	CART 0.55±0.11
24	CART 0.91±0.06	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	XGB 0.55±0.07
25	CART 0.91±0.07	CART 0.88±0.06	CART 0.88±0.07	CART 0.88±0.06	ChiMerge 0.52±0.06

Table 33. Best discretizer ROC AUC using different configurations of PCA components and Uniform transformation

Comp.	RF	LR	NB	SVM	Dummy
2	CART 0.81±0.09	CART 0.86±0.07	CART 0.86±0.07	CART 0.86±0.07	Mod Chi2 0.55±0.05
3	CART 0.84±0.07	CART 0.86±0.07	CART 0.86±0.07	CART 0.86±0.07	XGB 0.56±0.08
4	CART 0.82±0.07	CART 0.86±0.07	CART 0.86±0.07	CART 0.86±0.07	ChiMerge 0.55±0.07
5	CART 0.84±0.07	CART 0.87±0.07	CART 0.86±0.06	CART 0.87±0.07	MDLP 0.55±0.04
6	CART 0.83±0.07	CART 0.87±0.07	CART 0.86±0.06	CART 0.87±0.07	CACC 0.53±0.08
7	CART 0.84±0.08	CART 0.87±0.07	CART 0.86±0.08	CART 0.87±0.07	XGB 0.55±0.06
8	CART 0.85±0.08	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	ChiMerge 0.55±0.06
9	CART 0.86±0.07	CART 0.88±0.07	CART 0.84±0.1	CART 0.87±0.07	XGB 0.54±0.06
10	CART 0.85±0.06	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	Mod Chi2 0.55±0.08
11	CART 0.85±0.06	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	CACC 0.54±0.07
12	CART 0.85±0.07	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	CAIM 0.55±0.08
13	CART 0.86±0.08	CART 0.88±0.07	CART 0.82±0.11	CART 0.88±0.07	AMEVA 0.55±0.06
14	CART 0.84±0.08	CART 0.88±0.07	CART 0.82±0.1	CART 0.88±0.07	XGB 0.55±0.08
15	CART 0.84±0.08	CART 0.88±0.07	CART 0.82±0.1	CART 0.88±0.07	CACC 0.53±0.07
16	CART 0.85±0.09	CART 0.88±0.07	CART 0.82±0.1	CART 0.87±0.07	MDLP 0.56±0.07
17	CART 0.85±0.08	CART 0.88±0.07	CART 0.81±0.09	CART 0.87±0.07	CART 0.53±0.07
18	CART 0.84±0.08	CART 0.88±0.07	CART 0.81±0.09	CART 0.88±0.07	AMEVA 0.54±0.07
19	CART 0.85±0.07	CART 0.88±0.07	CART 0.81±0.1	CART 0.87±0.07	Ext Chi2 0.54±0.11
20	CART 0.84±0.08	CART 0.88±0.06	CART 0.81±0.09	CART 0.88±0.07	XGB 0.53±0.08
21	CART 0.85±0.07	CART 0.88±0.06	CART 0.81±0.09	CART 0.88±0.07	AMEVA 0.54±0.08
22	CART 0.84±0.07	CART 0.88±0.06	CART 0.82±0.08	CART 0.88±0.07	XGB 0.54±0.12
23	CART 0.84±0.06	CART 0.88±0.06	CART 0.81±0.09	CART 0.88±0.07	CART 0.55±0.08
24	CART 0.84±0.07	CART 0.88±0.06	CART 0.81±0.09	CART 0.88±0.07	XGB 0.52±0.08
25	CART 0.84±0.08	CART 0.88±0.06	CART 0.8±0.09	CART 0.88±0.07	CACC 0.55±0.07

Table 34. Best discretizer ROC AUC using different configurations of PCA components and Normal transformation

Comp.	RF	LR	NB	SVM	Dummy
2	CART 0.81±0.09	CART 0.86±0.07	CART 0.86±0.07	CART 0.86±0.07	ChiMerge 0.54±0.06
3	CART 0.84±0.07	CART 0.86±0.07	CART 0.86±0.07	CART 0.86±0.07	XGB 0.55±0.05
4	CART 0.82±0.08	CART 0.86±0.07	CART 0.86±0.07	CART 0.86±0.07	XGB 0.53±0.06
5	CART 0.83±0.09	CART 0.87±0.07	CART 0.86±0.06	CART 0.87±0.07	XGB 0.52±0.07
6	CART 0.83±0.07	CART 0.87±0.07	CART 0.86±0.06	CART 0.87±0.07	Ext Chi2 0.55±0.07
7	CART 0.84±0.08	CART 0.87±0.07	CART 0.86±0.08	CART 0.87±0.07	MDLP 0.54±0.04
8	CART 0.84±0.08	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	CACC 0.54±0.06
9	CART 0.84±0.07	CART 0.88±0.07	CART 0.84±0.1	CART 0.87±0.07	XGB 0.54±0.08
10	CART 0.85±0.08	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	XGB 0.56±0.06
11	CART 0.86±0.06	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	CACC 0.52±0.09
12	CART 0.84±0.08	CART 0.88±0.07	CART 0.84±0.1	CART 0.88±0.07	MDLP 0.55±0.08
13	CART 0.85±0.08	CART 0.88±0.07	CART 0.82±0.11	CART 0.88±0.07	MDLP 0.56±0.06
14	CART 0.84±0.08	CART 0.88±0.07	CART 0.82±0.1	CART 0.88±0.07	CACC 0.55±0.03
15	CART 0.85±0.08	CART 0.88±0.07	CART 0.82±0.1	CART 0.88±0.07	XGB 0.56±0.05
16	CART 0.84±0.08	CART 0.88±0.07	CART 0.82±0.1	CART 0.87±0.07	Mod Chi2 0.53±0.1
17	CART 0.84±0.09	CART 0.88±0.07	CACC 0.81±0.1	CART 0.87±0.07	XGB 0.55±0.06
18	CART 0.84±0.08	CART 0.88±0.07	CART 0.81±0.09	CART 0.88±0.07	CAIM 0.55±0.04
19	CART 0.84±0.08	CART 0.88±0.07	CACC 0.81±0.1	CART 0.87±0.07	CART 0.57±0.08
20	CART 0.84±0.07	CART 0.88±0.06	CACC 0.82±0.08	CART 0.88±0.07	ChiMerge 0.54±0.06
21	CART 0.86±0.06	CART 0.88±0.06	CART 0.81±0.09	CART 0.88±0.07	XGB 0.52±0.06
22	CART 0.83±0.07	CART 0.88±0.06	CART 0.82±0.08	CART 0.88±0.07	XGB 0.55±0.06
23	CART 0.84±0.07	CART 0.88±0.06	CART 0.81±0.09	CART 0.88±0.07	Ext Chi2 0.53±0.08
24	CART 0.84±0.07	CART 0.88±0.06	CACC 0.81±0.08	CART 0.88±0.07	ChiMerge 0.54±0.05
25	CART 0.84±0.07	CART 0.88±0.06	CACC 0.81±0.08	CART 0.88±0.07	MDLP 0.56±0.05

9. Notes on Statistical Tests

This section collects the outcomes of the statistical evaluations. Abbreviations are NS for not significant, \*  $p < 0.05$ , \*\* when  $p < 0.01$  and \*\*\* for  $p < 0.001$ .

Table 35. Relationship between categorical variables and target variable

Associations between cat. var.			
Variable	$\chi^2$	p	
Gender	0.492	0.482	
Human sub-popul.	13.400	0.001	*
Age	10.706	0.004	*

9.1. Statistical Tests on Numerical Experiment 1

Kruskal-Wallis test is used to compare NCA and PCA data for the discretizer with the best AUC at cross-validation (Table 36).

Table 36. Kruskal-Wallis test

Data	H	p
NCA without noise addition	97.46	***
NCA with unif. noise	93.58	***
NCA with gaussian noise	107.43	***
PCA without noise addition	81.16	***
PCA with unif. noise	73.19	***
PCA with gaussian noise	68.22	***

Following tables include the multicomparison test for PCA (Table 37) and NCA (Table 40) without addition of noise. Addition of noise was assembled in Tables 38, 39, 41, 42. In following tables “Dummy” is abbreviated as “D.” to save space.

Table 37.

PCA					
	RF	LR	NB	SVM	D.
RF	-	***	**	**	*
LR	***	-	NS	NS	***
NB	**	NS	-	NS	***
SVM	**	NS	NS	-	***
D.	*	***	***	***	-

Table 38.

PCA Unif. noise					
	RF	LR	NB	SVM	D.
RF	-	**	*	NS	**
LR	**	-	NS	NS	***
NB	*	NS	-	NS	***
SVM	NS	NS	NS	-	***
D.	**	***	***	***	-

Table 39.

PCA Gauss. noise					
	RF	LR	NB	SVM	D.
RF	-	*	NS	NS	***
LR	*	-	NS	NS	***
NB	NS	NS	-	NS	***
SVM	NS	NS	NS	-	***
D.	***	***	***	***	-

Table 40.

NCA					
	RF	LR	NB	SVM	D.
RF	-	***	**	***	***
LR	***	-	NS	NS	***
NB	**	NS	-	NS	***
SVM	***	NS	NS	-	**
D.	***	***	***	**	-

Table 41.

NCA Unif. noise					
	RF	LR	NB	SVM	D.
RF	-	***	***	***	***
LR	***	-	NS	NS	***
NB	***	NS	-	NS	***
SVM	***	NS	NS	-	***
D.	***	***	***	***	-

Table 42.

NCA Gauss. noise					
	RF	LR	NB	SVM	D.
RF	-	***	NS	***	***
LR	***	-	*	NS	***
NB	NS	*	-	**	***
SVM	***	NS	**	-	*
D.	***	***	***	*	-

Table 43. Class separability H-test on series without, with uniform and gaussian noise

NCA			PCA		
Discr.	Kruskal-Wallis H	p	Discr.	Kruskal-Wallis H	p
AMEVA	5.3201	0.0699	AMEVA	0.7183	0.6982
CACC	4.6283	0.0988	CACC	0.002	0.9988
CAIM	3.8807	0.1436	CAIM	0.4328	0.8054
Mod Chi2	49.27585	***	Mod Chi2	25.7482	***
ChiMerge	1.2342	0.5394	ChiMerge	0.0138	0.9930
Ext Chi2	53.3260	***	Ext Chi2	23.2916	***
MDLP	62.9361	***	MDLP	54.9739	***
CART	1.2161	0.5443	CART	0.0241	0.9879
XGB	3.0429	0.2183	XGB	0.8061	0.6682

Table 44. NCA vs PCA Class separability metric comparison

Mann-Whitney rank test			
Discr.	Without noise	Unif. noise	Gaussian noise
AMEVA	26.0 ***	35.0 ***	37.5 ***
CACC	182.0 *	272.5 NS	259.5 NS
CAIM	0.0 ***	1.0 ***	1.0 ***
Mod Chi2	0.0 ***	0.0 ***	0.0 ***
ChiMerge	188.0 *	226.5 NS	177.0 *
Ext Chi2	0.0 ***	71.0 ***	89.0 ***
MDLP	0.0 ***	251.0 NS	0.0 ***
CART	93.0 ***	116.0 **	149.5 **
XGB	0.0 ***	0.0 ***	6.0 ***

Table 45. Kruskal-Wallis H-test test to highlight differences in performance after addition of noise

NCA, p values of Kruskal-Wallis test					
Comp.	RF	LR	NB	SVM	Dummy
2	0.425	0.707	0.927	0.828	0.686
3	0.686	0.798	0.937	0.67	0.618
4	0.948	0.984	0.975	0.985	0.503
5	0.634	0.909	0.925	0.864	0.313
6	0.825	0.994	0.98	0.917	0.198
7	0.698	0.624	0.738	0.672	0.972
8	0.692	0.968	0.939	0.972	0.398
9	0.821	0.941	0.921	0.95	0.464
10	0.635	0.783	0.965	0.924	0.841
11	0.553	0.974	0.984	0.996	0.482
12	0.605	0.814	0.875	0.851	0.374
13	0.684	0.931	0.927	0.995	0.176
14	0.632	0.925	0.686	0.973	0.106
15	0.377	0.903	0.885	0.838	0.613
16	0.622	0.766	0.461	0.844	0.806
17	0.521	0.871	0.892	0.561	0.291
18	0.55	0.78	0.879	0.559	0.928
19	0.7	0.865	0.952	0.83	0.732
20	0.597	0.945	0.928	0.979	0.981
21	0.381	0.978	0.855	0.776	0.853
22	0.7	0.908	0.974	0.888	0.523
23	0.655	0.883	0.917	0.73	0.998
24	0.388	0.98	0.975	0.842	0.122
25	0.55	0.879	0.632	0.633	0.592



## Supplementary Materials

Table 46. Kruskal-Wallis H-test test to highlight differences in performance after addition of noise

PCA, p values of Kruskal-Wallis test					
Comp.	RF	LR	NB	SVM	Dummy
2	0.786	0.871	0.966	0.999	0.346
3	0.597	0.937	0.963	0.989	0.277
4	0.824	0.993	0.948	0.989	0.443
5	0.749	0.995	0.828	0.975	0.654
6	0.933	0.988	0.886	0.953	0.544
7	0.996	0.995	0.978	0.956	0.2
8	0.811	0.997	0.897	0.935	0.891
9	0.815	0.98	0.922	0.955	0.349
10	0.909	0.988	0.898	0.927	0.217
11	0.859	0.98	0.971	0.89	0.288
12	0.796	0.98	0.853	0.893	0.691
13	0.879	0.984	0.961	0.881	0.467
14	0.67	0.984	0.952	0.974	0.957
15	0.993	0.985	0.984	0.936	0.561
16	0.91	0.996	0.978	0.952	0.769
17	0.7	0.975	0.984	0.974	0.741
18	0.918	0.993	0.988	0.991	0.065
19	0.722	0.998	0.968	0.953	0.235
20	0.883	0.956	0.955	0.892	0.193
21	0.737	0.99	0.891	0.879	0.911
22	0.413	0.98	0.978	0.95	0.302
23	0.844	0.936	0.947	0.954	0.576
24	0.459	0.991	0.968	0.994	0.351
25	0.991	0.989	0.851	0.987	0.073

## 9.2. Statistical Tests on Numerical Experiment 4

Statistical assessments were sub-divided in two sections: one for the Uniform (Section 9.2.1) and one for the Normal (Section 9.2.2) transformation.

### 9.2.1. Uniform mapping

Class separability metric was tested to highlight differences between the number of landmarks while performing NCA and PCA transformations. Kruskal-Wallis one-way analysis of variance by ranks (NCA  $H=58.48$   $p < 0.0001$ , PCA  $H=2.34$   $p > 0.05$ ) and post-hoc test for NCA transformation is in Table 47.

Table 47. Class separability Post-hoc test on NCA series for different landmarks (Uniform)

NCA					
	202	101	51	25	13
202	-	**	NS	NS	**
101	**	-	***	***	NS
51	NS	***	-	NS	***
25	NS	***	NS	-	***
13	**	NS	***	***	-

In Table 48, class separability series from NCA and PCA data were tested against each other with the Mann-Whitney U test. Values showed a statistically significant difference between NCA and PCA in the class separability metric.

Table 48. Table to test NCA and PCA for each landmark (Uniform mapping)

Landmarks	U	p
202	0.0	***
101	0.0	***
51	0.0	***
25	0.0	***
13	0.0	***

### 9.2.2. Normal mapping

Kruskal-Wallis one-way analysis of variance by ranks on class separability metric after normal distribution mapping was significant for NCA serie ( $H=64.22$ ,  $p < 0.0001$ ) but not for PCA ( $H=1.48$ ,  $p > 0.05$ ). Post-hoc multicomparison is in Table 49.

Table 49. Class separability Post-hoc test on NCA series for different landmarks (Normal)

NCA					
	202	101	51	25	13
202	-	NS	***	***	***
101	NS	-	***	***	***
51	***	***	-	NS	NS
25	***	***	NS	-	NS
13	***	***	NS	NS	-

In Table 50, class separability series from NCA and PCA data were tested with Mann-Whitney U test. Statistics showed a significant difference between NCA and PCA in the class separability metric for the Normal mapping of the data.

## Supplementary Materials

Table 50. Table to test NCA and PCA for each landmark (Normal mapping)

Landmarks	U	p
202	0.0	***
101	0.0	***
51	0.0	***
25	0.0	***
13	0.0	***

### 10. Notes on Discussion

Dunn post-hoc test [62] between data transformations used for analyzing gene expression data is shown in (Table 51).

Table 51. Post-hoc test for difference between data transformations across NCA dimensions

	Log-transf	Unif-transf	Norm-transf
Log-transf	-	***	***
Unif-transf	***	-	NS
Norm-transf	***	NS	-

### References

46. B. G. Tabachnick, L. S. Fidell, and J. B. Ullman, *Using multivariate statistics*, vol. 5. Pearson Boston, MA, 2007.
47. D. Joanes and C. Gill, Comparing measures of sample skewness and kurtosis, *Journal of the Royal Statistical Society: Series D (The Statistician)*, vol. 47, no. 1, pp. 183–189, 1998.
48. C. Duncan, *Fundamental Statistics for Social Research*. Routledge, 1997.
49. M. G. Bulmer, *Principles of statistics*. Courier Corporation, 1979.
50. D. K. Hildebrand, *Statistical thinking for behavioral scientists*. Brooks/Cole, 1986.
51. W. Trochim and J. Donnelly, The research methods knowledge base, 3rd, *Mason, OH: Atomic Dog Publishing*, 2006.
52. F. J. Gravetter, L. B. Wallnau, L.-A. B. Forzano, and J. E. Witnauer, *Essentials of statistics for the behavioral sciences*. Cengage Learning, 2020.
53. F. Andy, *Discovering statistics using spss for windows: Advanced techniques for the beginner*, 2000.
54. A. Field, *Discovering statistics using IBM SPSS statistics*. sage, 2013.
55. D. B. Wright and J. A. Herrington, Problematic standard errors and confidence intervals for skewness and kurtosis, *Behavior Research Methods*, vol. 43, no. 1, pp. 8–17, 2011.
56. S. Ramírez-Gallego, S. García, H. Mouriño-Talín, D. Martínez-Rego, V. Bolón-Canedo, A. Alonso-Betanzos, J. M. Benítez, and F. Herrera, Data discretization: taxonomy and big data challenge, *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, vol. 6, no. 1, pp. 5–21, 2016.
57. H. Liu and R. Setiono, Feature selection via discretization, *IEEE Transactions on knowledge and Data Engineering*, vol. 9, no. 4, pp. 642–645, 1997.
58. Z. Pawlak, Rough sets, *International journal of computer & information sciences*, vol. 11, no. 5, pp. 341–356, 1982.
59. T. J. Santner, B. J. Williams, W. I. Notz, and B. J. Williams, *The design and analysis of computer experiments*, vol. 1. Springer, 2003.
60. K. P. Murphy, *Machine learning: a probabilistic perspective*. MIT press, 2012.
61. N. Siddiqi, *Credit risk scorecards: developing and implementing intelligent credit scoring*, vol. 3. John Wiley & Sons, 2012.

62. O. J. Dunn, Multiple comparisons using rank sums, *Technometrics*, vol. 6, no. 3, pp. 241–252, 1964.