

Comparison of methods and models by consensus

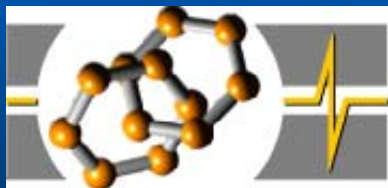
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Comparison of models

- No 'fair' procedure;
- Contradictory, (bias-variance trade-off, local minima, robustness, Occam's razor);
- Various criteria (R^2 , Q^2 , Mallows C_p , Akaike IC, etc. etc.)

Comparison of methods

- Collaborative, (round-robin) tests.
- Assumption: systematic errors follow normal distribution.
- One method is better from one point of view, the other is better from another point ...
- Cost function (weighting)

Solutions till now

- Harmonious models (between bias and variance, - John H. Kalivas).
- Principal Component Analysis of regression coefficients, - Paul Geladi).
- Its extension to classification, - Roberto Todeschini)
- and ...???

Description of the procedure

- Arrangement of data in matrix form (objects=rows, methods to be compared=columns)
- It is assumed that the **ideal** ranking is known,
- The ranking is carried out by each (individual) method,
- Calculation of absolute values for differences between **ideal** and **individual rankings** and summarizing them.
- The SRD values **orders, groups** the methods: the smaller the better.
- If the **ideal** rankings not known, **average** of all methods can be used instead (consensus).
- Validation with simulated 'methods' (generation of random numbers, and calculation of SRD values for simulated data).

Examples

- **Antioxidant activities of commercial beers**

[Zhao et al. *Food Chem.* **119** (2010) 1150-1158]

- **Evaluation of classification methods**

[R. Todeschini et al. *Chemolab* **87** (2007) 3-17]

- **Prediction of retention times by MEDV**

[Liao et al. *J. Mol Struct.* **850** (2008) 1-8]

- **Polynomial fit**

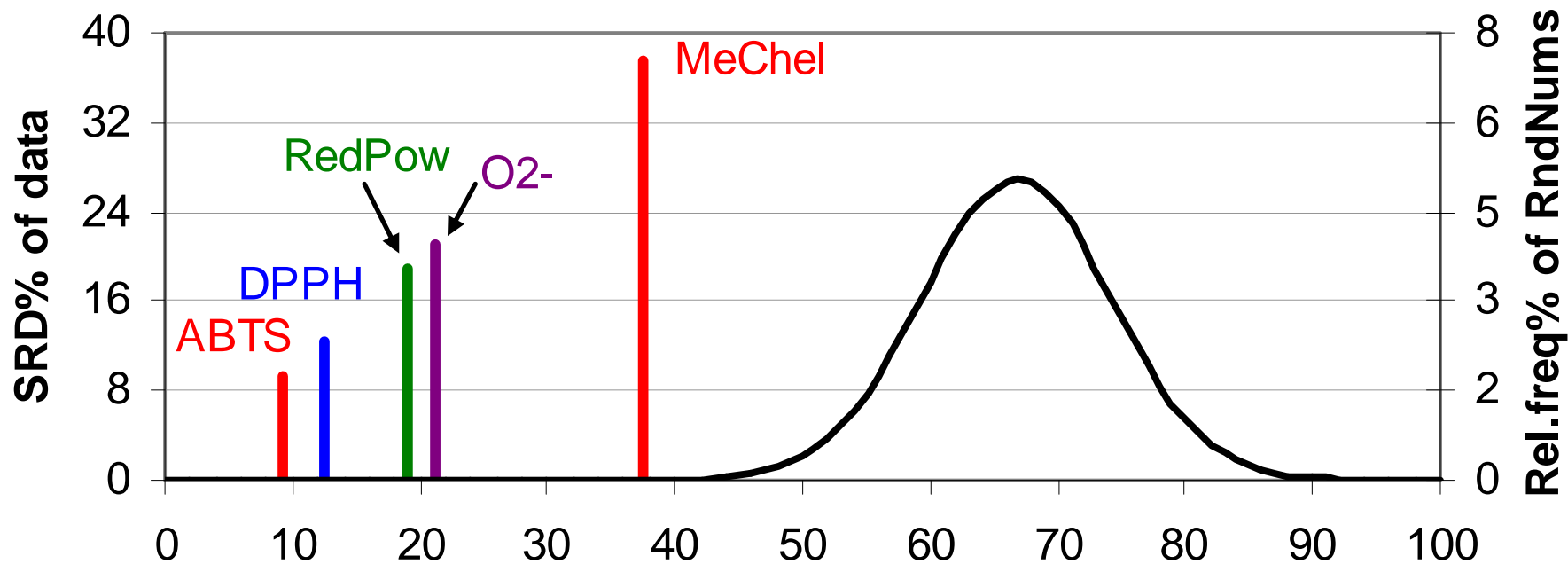
[K. Héberger et al. *J. Chromatogr. A*, **973** (2002) 135-142]

1.) Beers	Average	rnk	ABTS	rnk2	diff2
Peng Cheng	-1.46	1	-1.38183	1	0
Budweiser	-0.68	7	-0.69596	7	0
Blue Ribbon	-0.51	9	-0.84837	4	5
Corona	-0.39	13	-0.46733	12	1
Coors Light	-0.28	14	-0.65785	9	5
Tiger	-0.07	22	0.14233	23	1
Blue Lion	-0.02	23	-0.04819	22	1
Asahi	0.19	24	0.218538	25	1
Beck's	0.27	25	0.180434	24	1
Heineken	0.59	28	0.828201	29	1
Bitburger	0.61	29	0.713889	28	1
Carlsberg	0.83	30	0.866305	30	0
Grolsch	1.20	31	1.094929	31	0
Duvel	1.37	32	1.361657	32	0
Lefte	1.44	33	1.590281	33	0
Samuel	3.59	34	3.952729	34	0

2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonate) 734 nm

54

CRRN results (NormApp: n=34 ;
Mean=66.76 StD=7.41)



Ranking

results

ABTS	DPPH	RedPow	O ₂ ⁻	MeChel	XX1	Q1	Med	Q3	XX19
54	72	110	122	216	314	356	386	414	454

1.) Validation

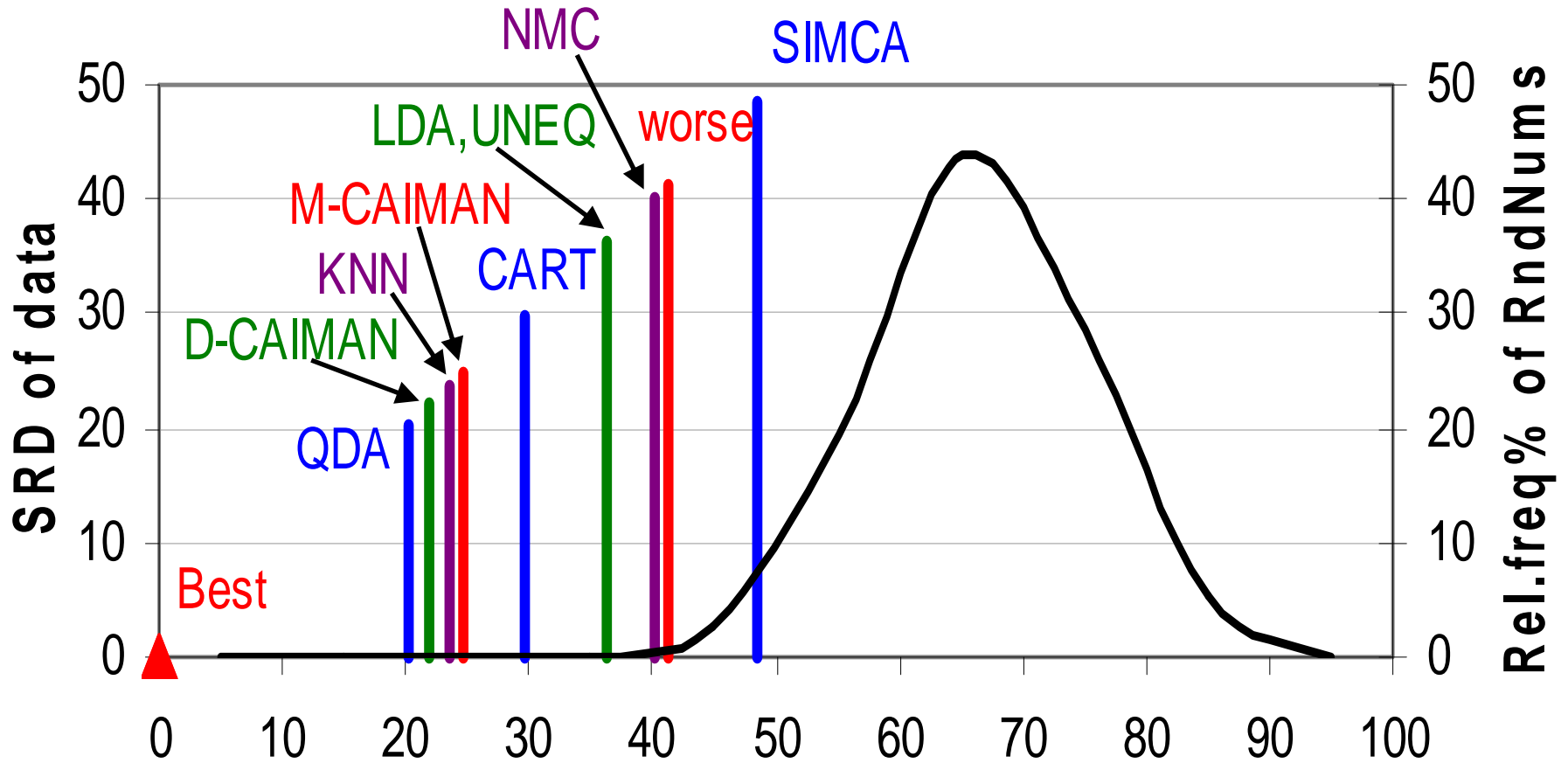
Factor Loadings (Unrotated) (ZhaoT3) Extraction: Principal components (Marked loadings are >.700000)						
Variable	Factor1 =V1^2	Factor2 =V2^2	Factor3 =V3^2	Factor4 =V4^2	Factor5 =V5^2	sum
DPPH	0.963	0.002	0.014	0.020	0.002	1
ABTS	0.976	0.004	0.008	0.000	0.012	1
O2-	0.661	0.301	0.036	0.001	0.000	1
RedPow	0.914	0.009	0.063	0.012	0.002	1
MeChel	0.739	0.148	0.112	0.000	0.000	1
SUM case 1-5	4.253	0.465	0.232	0.033	0.016	5

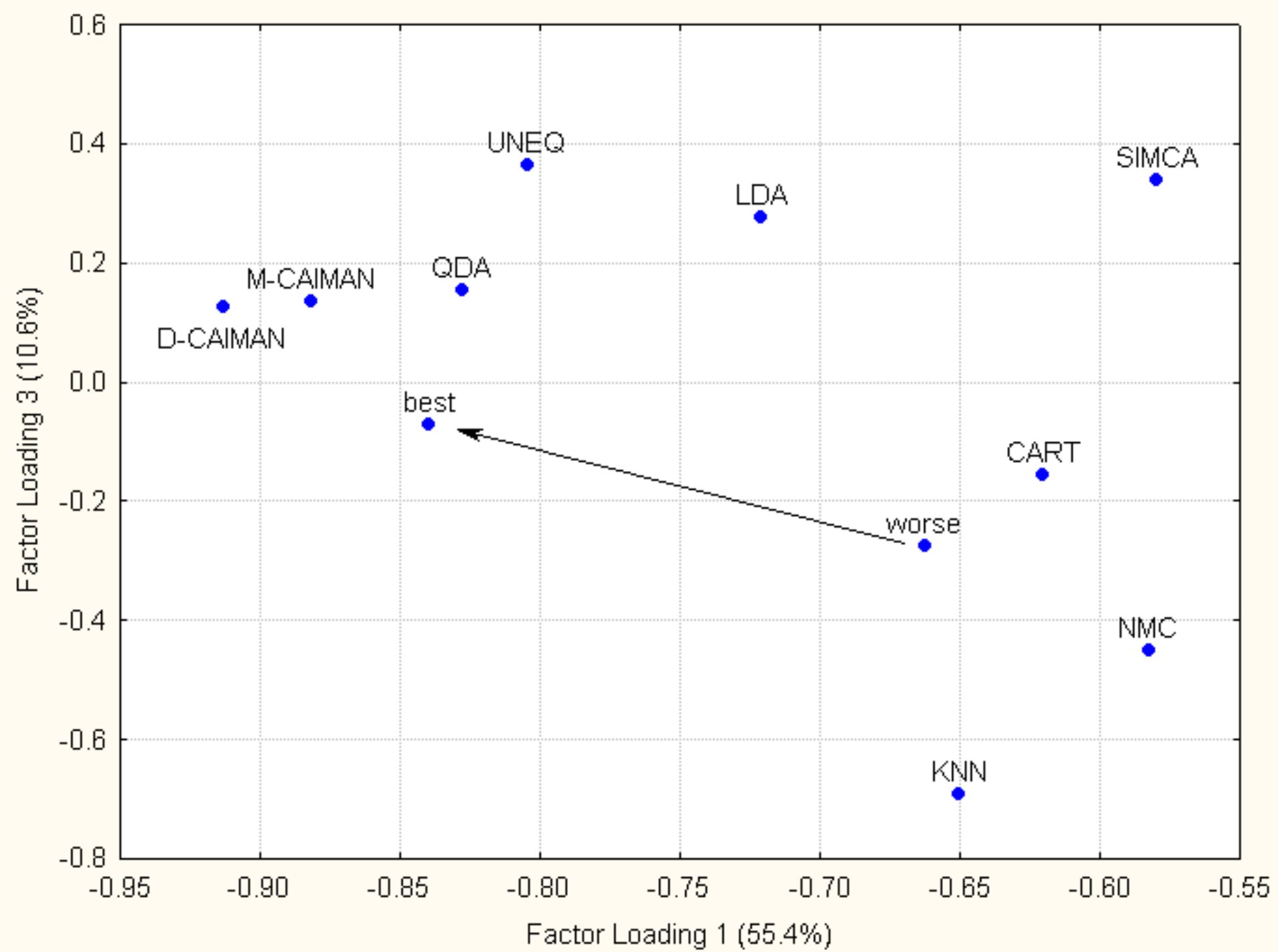
2.) Ranking of classification methods

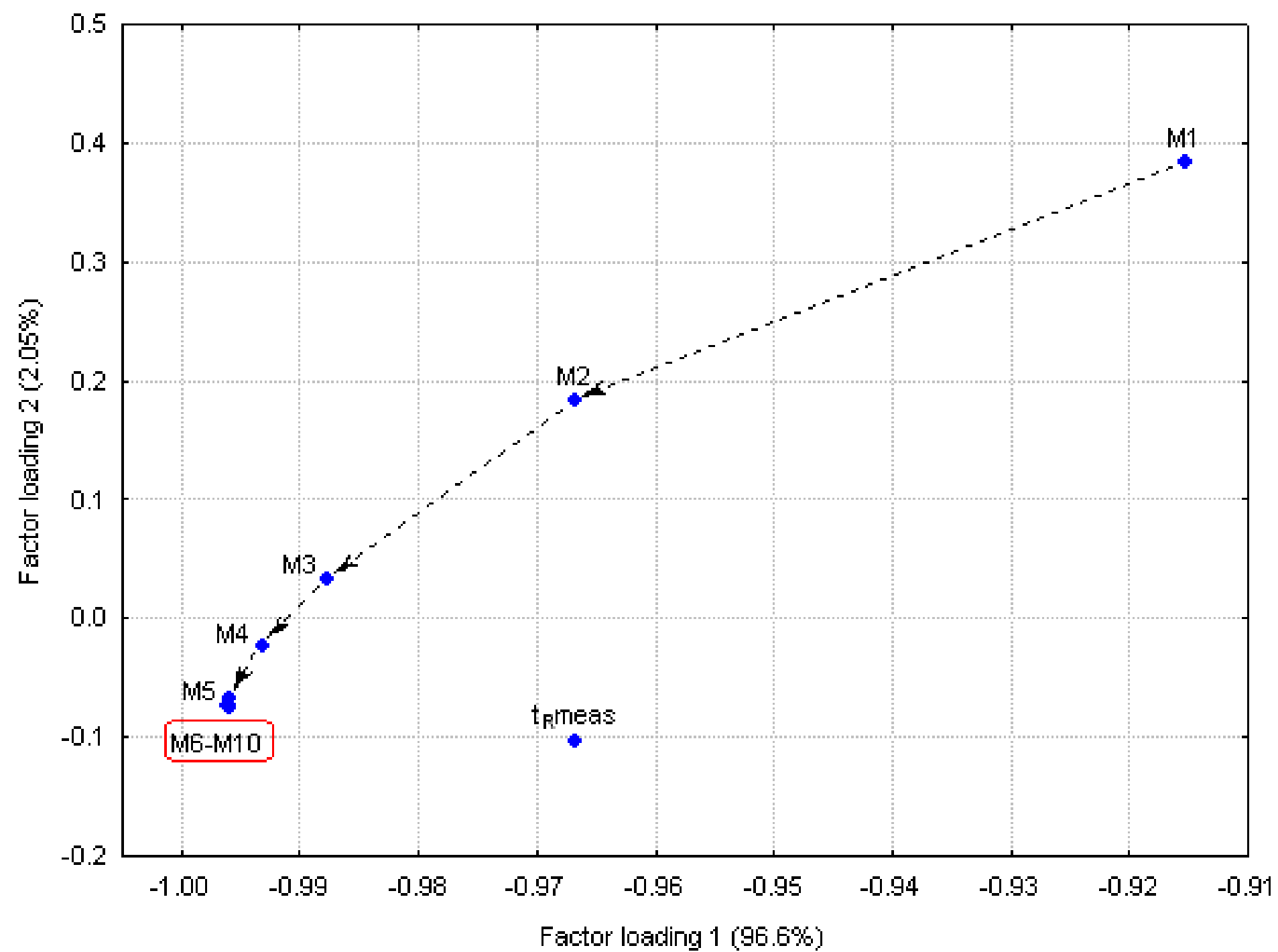
Best	0
QDA	74
D-CAIMAN	80
KNN	86
M-CAIMAN	90
CART	108
LDA	132
UNEQ	132
NMC	146
Worse	150
SIMCA	176

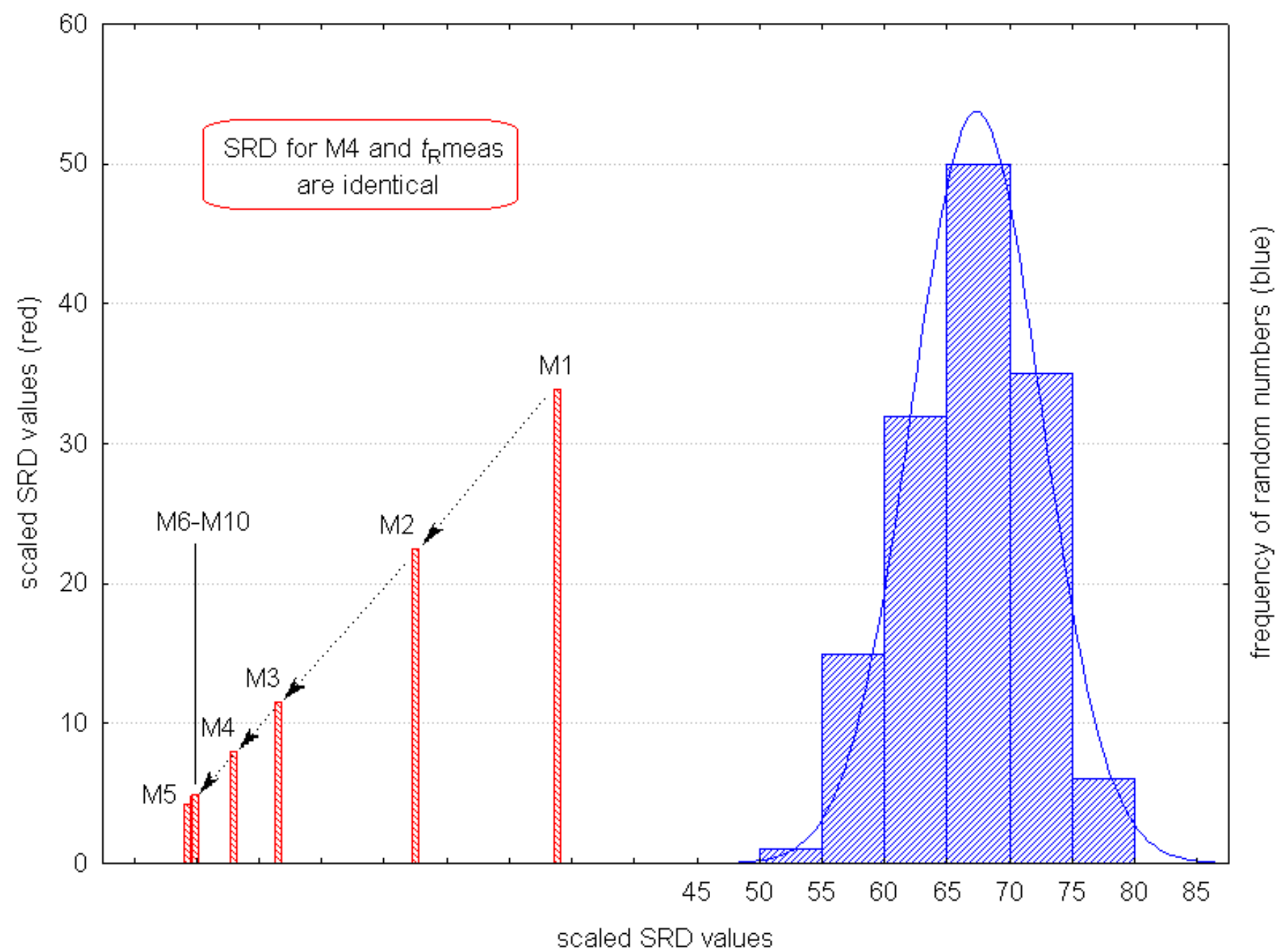
	SRD	SRDscl
XX1	191	52.5
Q1	222	61.0
Median	243	66.8
Q3	262	72.0
XX19	293	80.5

CRRN results (NormApp: n=27 ;
 Mean=66.51 StD=8.96)

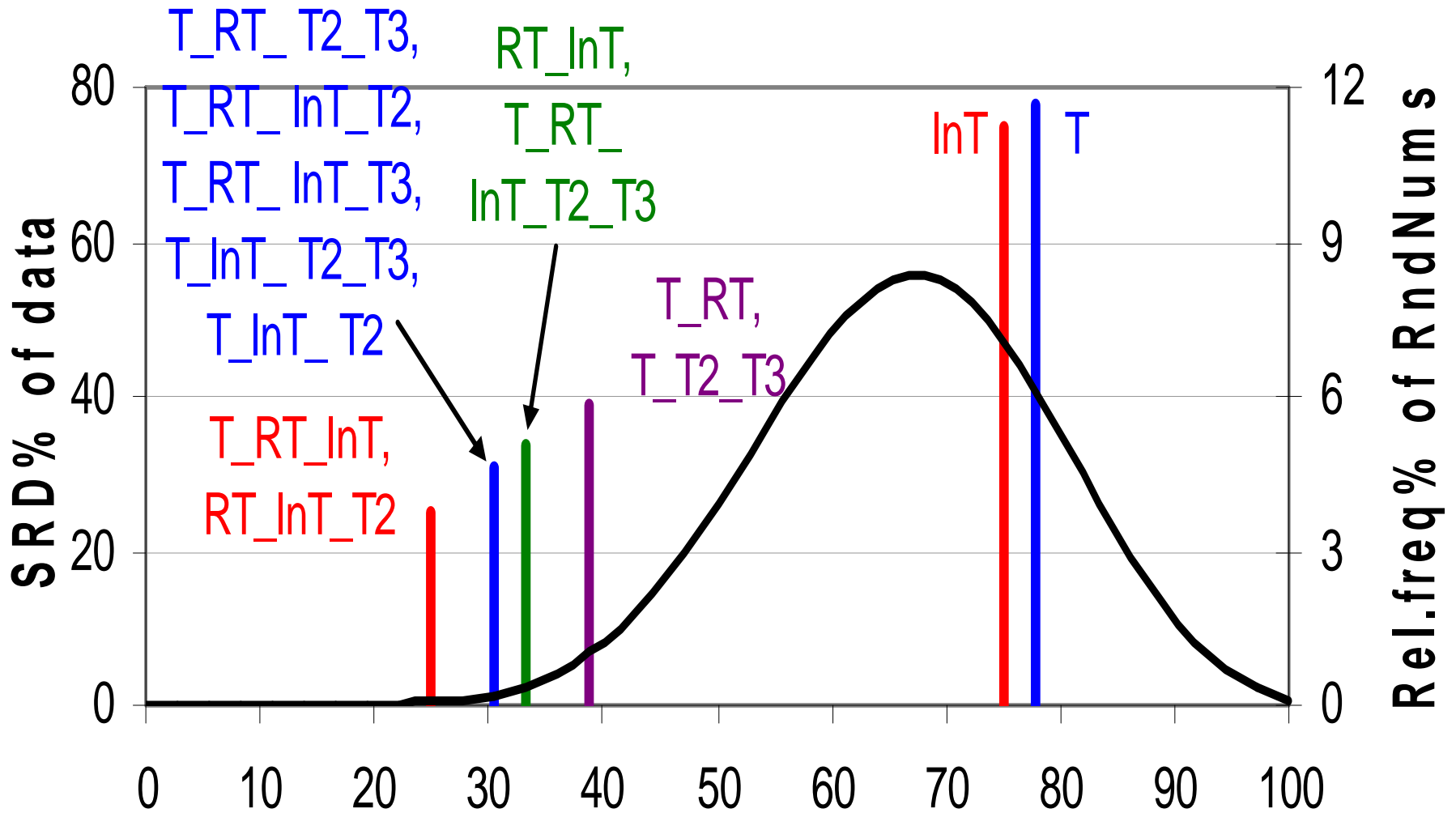






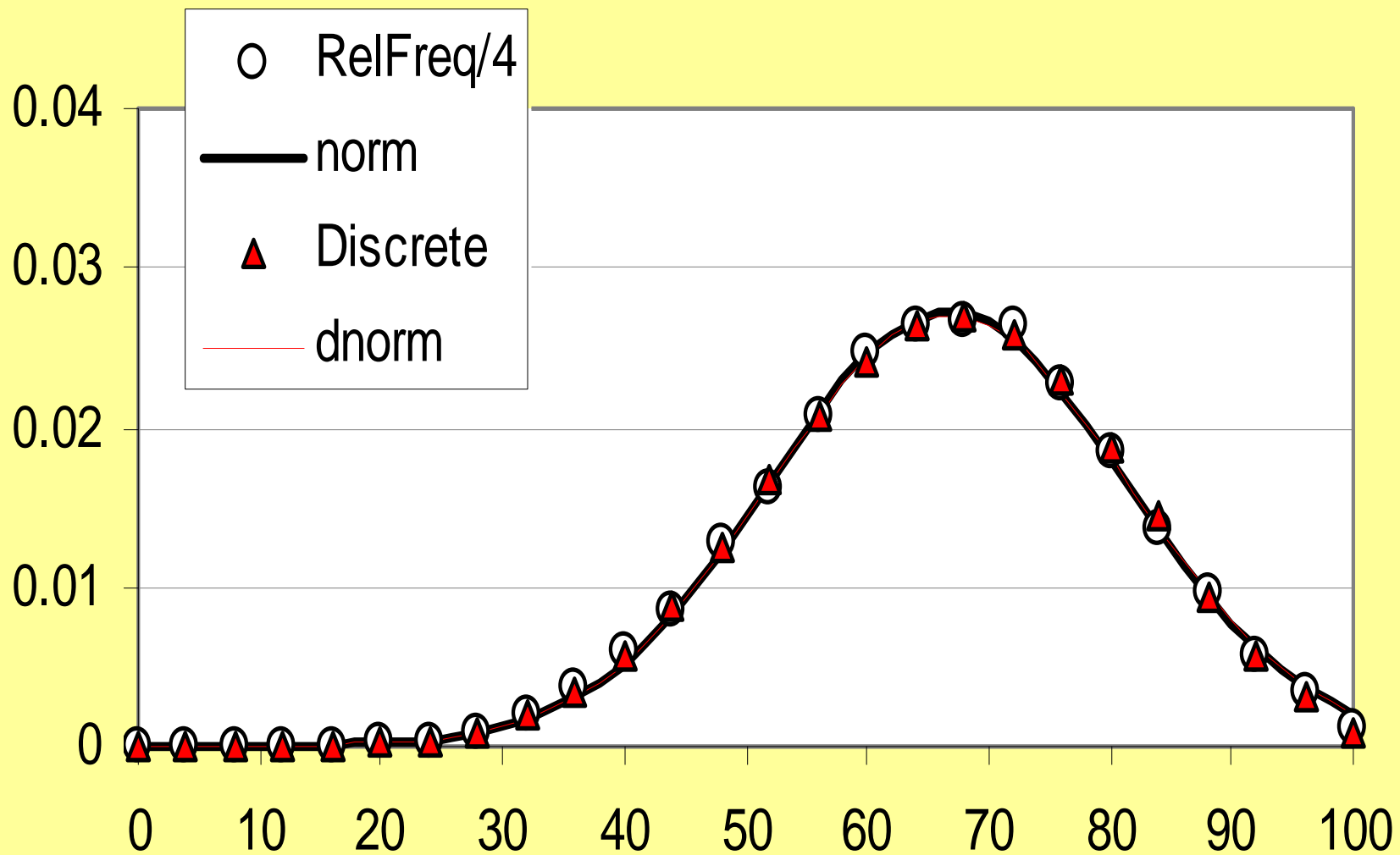


CRRN results (Discret, n=12)

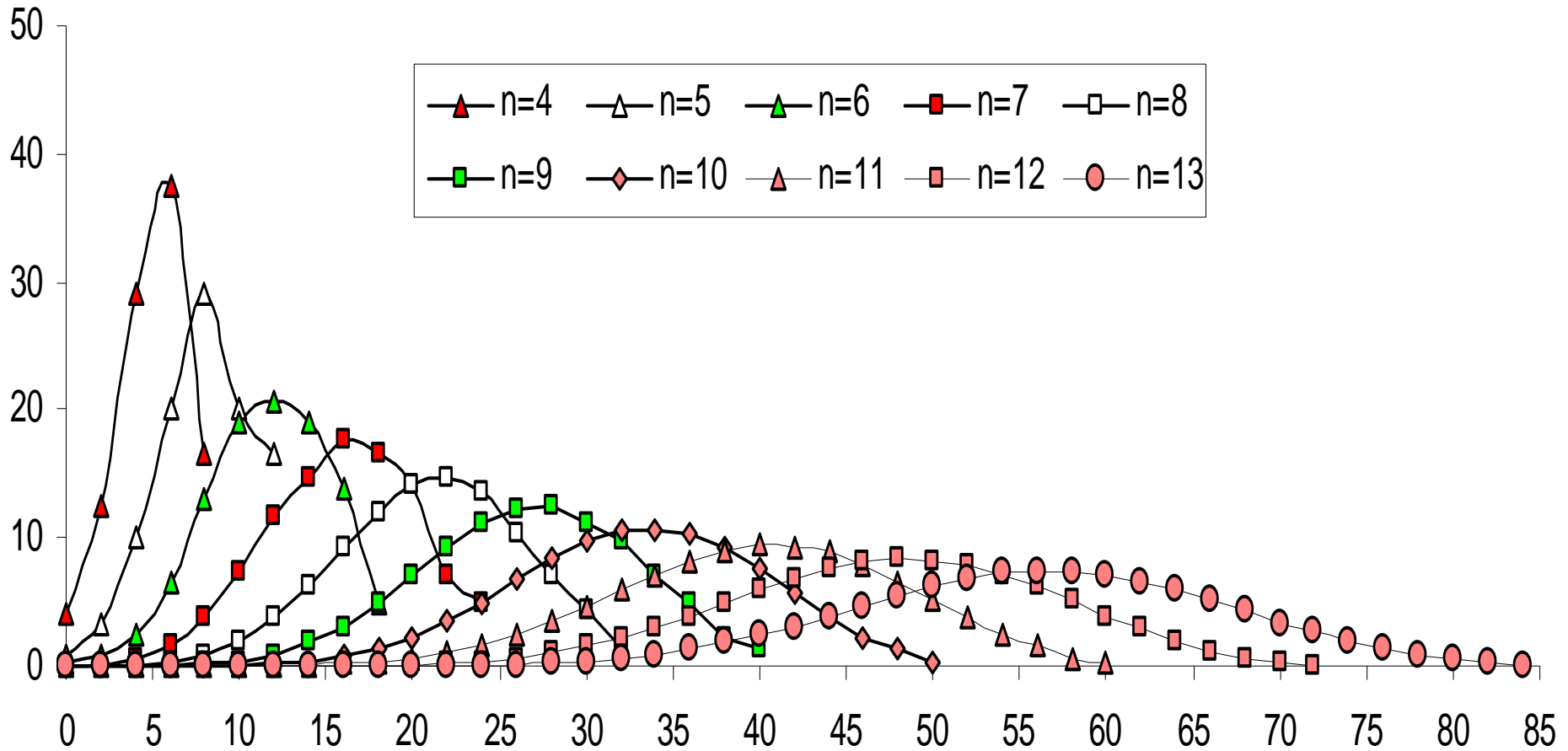


	R²adjust	SE
T	0.9874092	0.11311
T_RT	0.9999861	0.00376
T_RT_lnT	0.9999881	0.00348
RT_lnT	0.9999880	0.00349
T_T2_T3	0.9999829	0.00417
T_RT_T2_T3	0.9999907	0.00308
T_RT_lnT_T2_T3	0.9999893	0.00330
T_RT_lnT_T2	0.9999906	0.00310
T_RT_lnT_T3	0.9999906	0.00309
T_lnT_T2_T3	0.9999907	0.00307
T_lnT_T2	0.9999867	0.00367
RT_lnT_T2	0.9999880	0.00350
lnT	0.9954540	0.06797

n=10 ; MaxSRD=50 ; #RND=50000



CRRN-SRD discrete distribution for different number of objects (n)



Literature

- K. Héberger, How can multivariate data analysis be useful for chromatographers? Book of abstracts, **19th International Symposium Pharmaceutical & Biomedical Analysis**, Gdansk, Poland, June 8-12, 2008, ed.: J. Lapynska, KL07. p19.
- K. Héberger, Evaluation of Chromatographic Data. Sum of Ranking Differences, Book of abstracts, **4th International Symposium Computer Applications and Chemometrics in Analytical Chemistry**, Balatonalmádi, Hungary, Sept. 1st - 5th, 2008, ed.: T. L. Pap, KN01.
- K. Kollár-Hunek, J. Heszberger, Z. Kókai, M. Láng-Lázi, E. Papp, Testing panel consistency with GCAP method in food profile analysis, **Journal of Chemometrics 22 (2008) 218-226**.
- K. Héberger, Sum of Ranking Differences. A Novel Measure for Fair Comparison of Methods or Models, **Trends in Analytical Chemistry 29 (2010) 101-109**.
- K. Héberger, K. Kollár-Hunek, A General Ordering Method: Compare Ranks with Random Numbers. Algorithm and Validation **Journal of Chemometrics (submitted)**

Acknowledgement

Kollárné Hunek Klára,

Forlay-Frick Péter,

John H. Kalivas,

Roberto Todeschini,

Felinger Attila,

5th International Symposium on Computer Applications and Chemometrics in Analytical Chemistry

**SCAC 2010 Budapest, Hungary
21 – 25 June, 2010**

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