

THE PROFICIENCY TESTING OF LABORATORIES: A FIRST APPROACH TO IMPLEMENT BAYESIAN METHODS IN THE ASSESSMENT OF PERFORMANCE

Rafael Núñez-Lagos⁽¹⁾, Manuel Barrera⁽²⁾, M. Lourdes Romero⁽²⁾

(1) Facultad de Ciencias. Universidad de Zaragoza. C/ Cerbuna 12, 50009
Zaragoza

(2) CIEMAT. Av. Complutense 22, 28040 Madrid

PRESENT SITUATION

Periodical Intercomparison exercises among Environmental Radioactivity Laboratories in Spain, have shown that the recommendations of the IUPAC protocol, the z-score, is the best working method to assess laboratory performance

$$\mathbf{z - score} = \frac{(b - a)}{S_{ffp}}$$

Reference $a \pm S$

Laboratory $b \pm t$

**S_{ffp} fitness for purpose
uncertainty**

A more precise assessment of performance, should require a better estimation of the quality of the measurement

Inclusion of the laboratory uncertainty

$$u - \text{score} = \frac{|a - b|}{\sqrt{s^2 + t^2}}$$

Problem: Large t disguises the results

GOAL: The Development of an objective methodology which takes into account **the laboratory value and its uncertainty** not giving advantage to extreme values of τ

BAYESIAN METHODOLOGY

Intrinsic Discrepancy, $d(p,q)$, is a very general objective measure of the divergence between two probability distributions $p(x)$ and $q(x)$

$$d(p,q) = \text{Min}_{All x} \int p(x) \ln \frac{p(x)}{q(x)} dx, \int q(x) \ln \frac{q(x)}{p(x)} dx$$

When $p(x)$ is supposed to be a true probability distribution then

$$d(p,q) = \int_{All x} p(x) \ln \frac{p(x)}{q(x)} dx$$

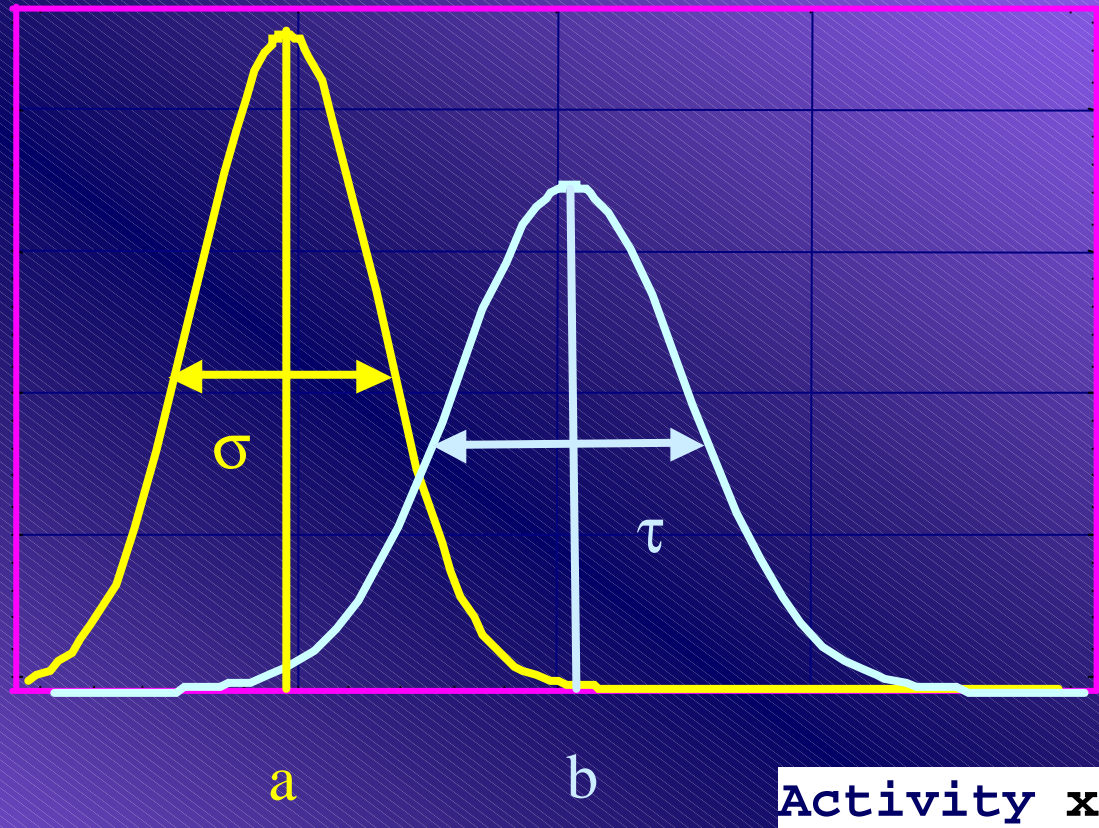
Methodology: Associate probability distribution functions (pdf) to reference $p(x)$ and laboratory $q(x)$ results

First approach associate normal distribution functions

Reference: Normal distribution $p(x|a,s)$ with expected value a and width s

Laboratory: Normal distribution $q(x|b,t)$ with expected value b and width t

Probability



Reference $p(x|a,s)$

Laboratory $q(x|b,t)$

Reference $p(x|a, S_{ffp})$? True distribution

Use σ_{ffp} as the width of $p(x)$. The intrinsic discrepancy, $\delta(p, q)$, of laboratory pdf, $q(x)$, respect the reference (true) pdf, $p(x)$, is then:

$$d(p, q) = \int_{All\ x} p(x) \ln \frac{p(x)}{q(x)} dx = \ln \frac{t}{S_{ffp}} - \frac{1}{2} + \frac{S_{ffp}^2}{2t^2} + \frac{(a-b)^2}{2t^2}$$

Use the new variables, τ^* and z

$$t^* = \frac{t}{S_{ffp}} \quad z = \frac{(b-a)}{S_{ffp}}$$

The intrinsic discrepancy
becomes

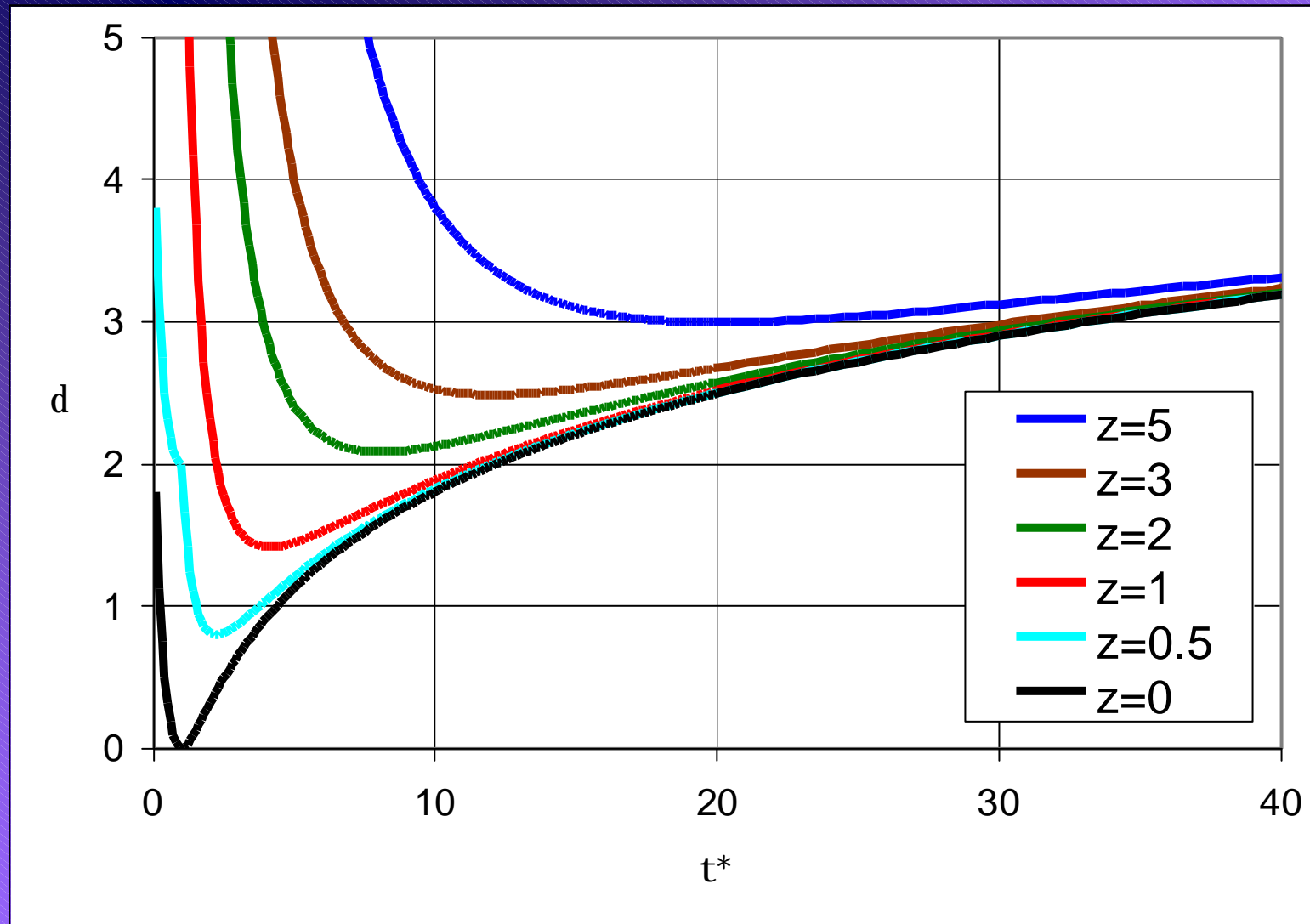
$$d(\mathbf{z}, t^*) = \ln t^* - \frac{1}{2} + \frac{1}{2t^{*2}} (1 + \mathbf{z}^2)$$

$$\text{Minimum value } t^* = \sqrt{1 + \mathbf{z}^2}$$

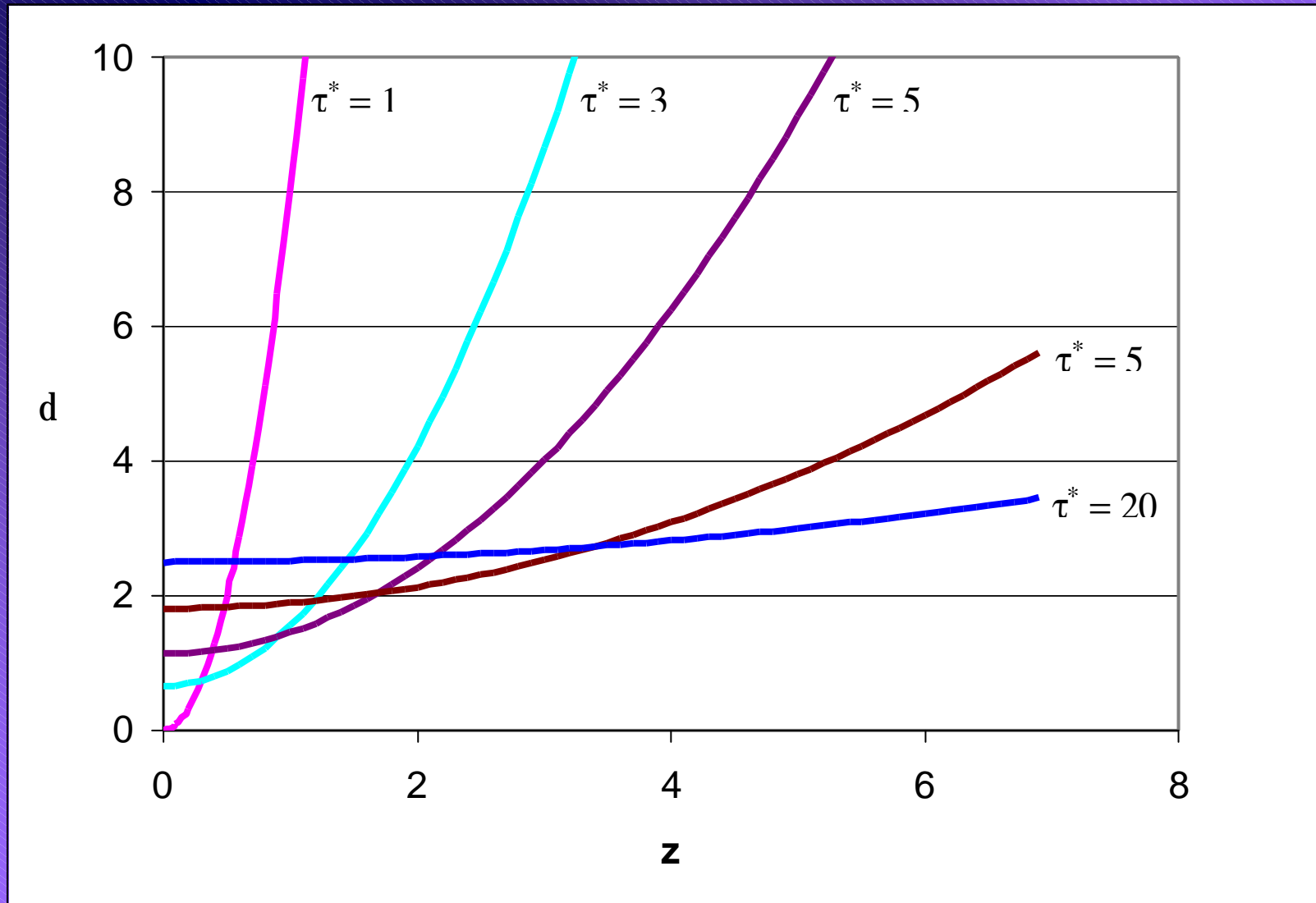
Good d vs t behaviour

Lower and larger t^* values *increases* d

Intrinsic discrepancy $d(p,q)$ as a function of t^* for different z values



Intrinsic discrepancy $d(p,q)$ as a function of z for different τ^* values



APPLICATION

2004 Ciemat proficiency test

Aqueous synthetic solution with certified amounts of radionuclides

39 laboratories

Data on ^{137}Cs

Reference Activity $a = 498,8 \text{ Bq/m}^3$

Reference uncertainty $s = 10 \text{ Bq/m}^3 (2\%)$

Fitness for purpose uncertainty

$S_{\text{ffp}} = 39,9 \text{ Bq/m}^3 (8\%)$

Labs with z-score < 0,5 and their d(p,q) values

Last two columns labs ordered by |z| and $\delta(p,q)$

Lab	Lab act b Bq/m ³	Lab unc t Bq/m ³	z	t*	d(p,q)	Ord z	Ord d(p,q)
1	515	48	0,41	1,2	0,09	25	22
2	486	36	-0,32	0,9	0,07	22	27
9	486	206	-0,32	5,16	1,16	30	25
17	506	25	0,18	0,63	0,35	34	21
19	503	54,2	0,11	1,36	0,08	27	9
20	516	86	0,43	2,16	0,4	19	1
21	514	24,4	0,38	0,61	0,54	29	17
22	500	21	0,03	0,53	0,66	32	34
25	500	73	0,03	1,83	0,25	17	19
27	495,6	59	-0,08	1,48	0,12	2	2
29	493,7	23,2	-0,13	0,58	0,46	9	29
30	496	114	-0,07	2,86	0,61	36	36
32	492	56	-0,17	1,4	0,1	21	32
34	502	64	0,08	1,6	0,17	1	30
36	485	10	-0,35	0,25	7,03	20	20

Ref (Bq/m³)

$$a = 498,8$$

$$\sigma = 9,98$$

$$\sigma_{ffp} = 39,9$$

Intrinsic Discrepancy, d , and z-score classification of laboratory performance are different.

Best z-score laboratories

Lab 25 $b = 500,0 \text{ Bq/l}$ $t = 73,0 \text{ Bq/l}$ is 7th in d classification

Lab 22 $b = 500,0 \text{ Bq/l}$ $t = 21,0 \text{ Bq/l}$ is 17th in d classification

Best d laboratories

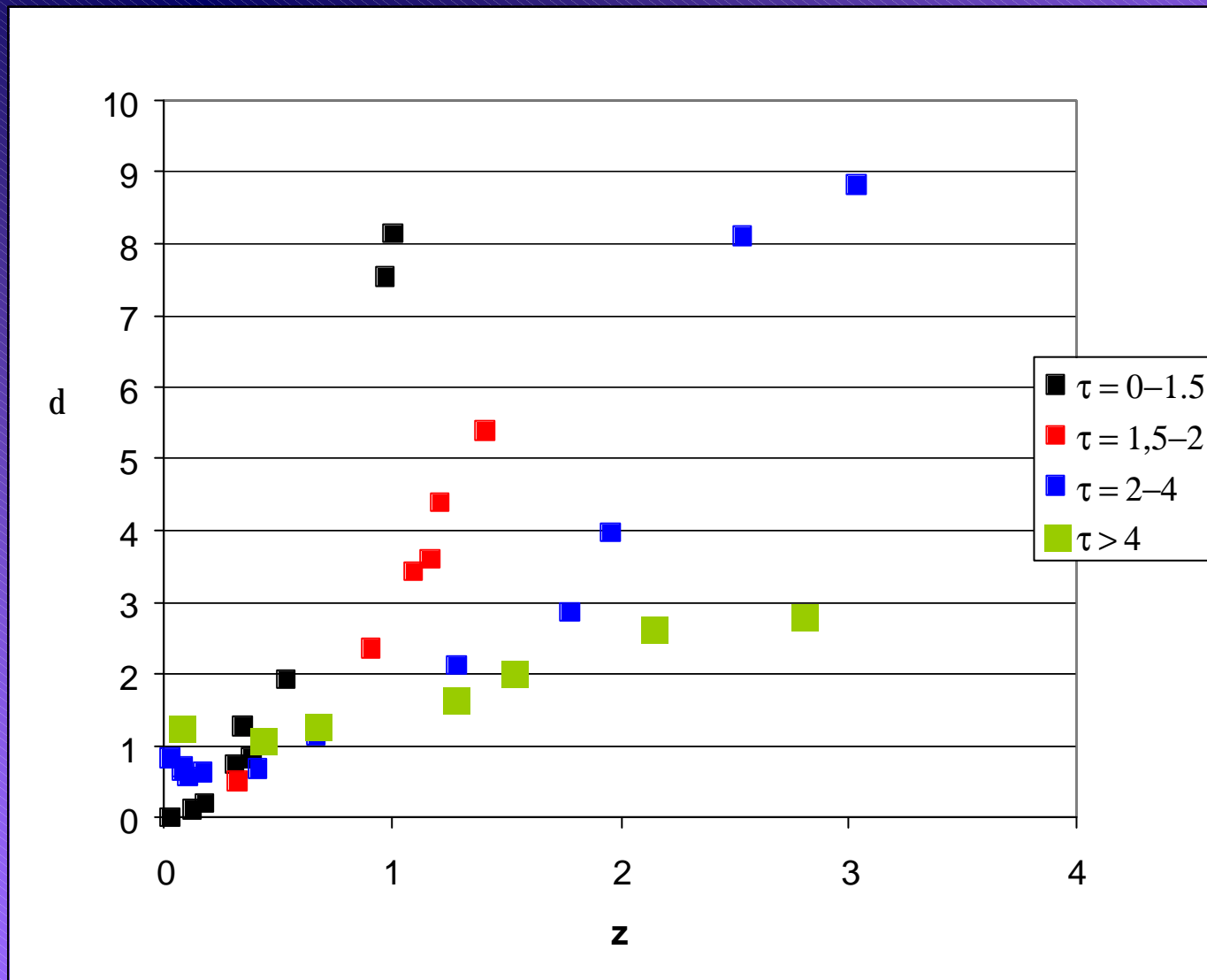
Lab 2 $b = 515,0 \text{ Bq/l}$ $t = 48,0 \text{ Bq/l}$ is 10 th in z classification

Lab 19 $b = 486,0 \text{ Bq/l}$ $t = 36,0 \text{ Bq/l}$ is 6 th in z classification

The laboratory uncertainty plays an important rule in the intrinsic discrepancy classification

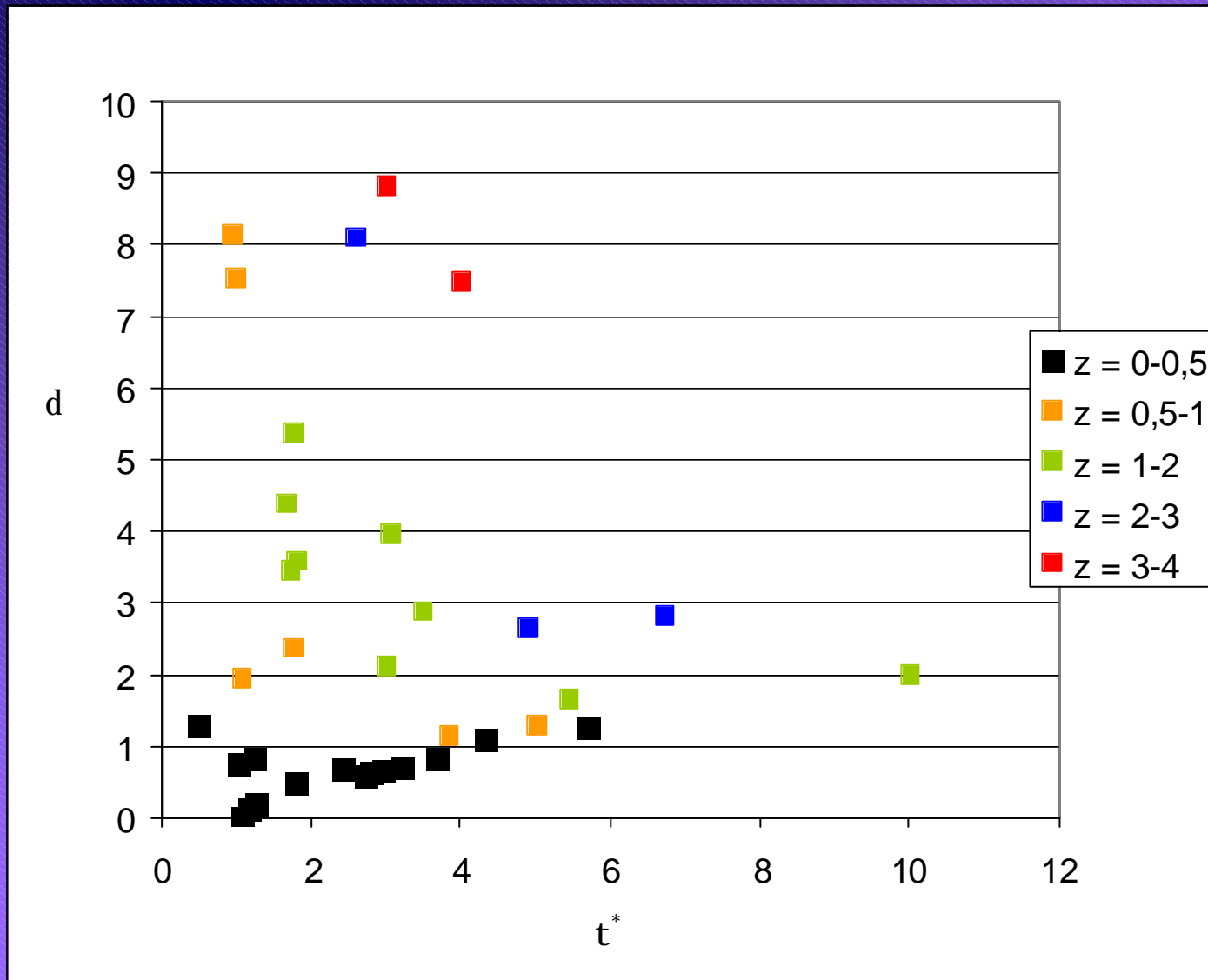
Proficiency test CSN/CIEMAT 2004 : ^{137}Cs Data

$d(p,q)$ versus z for different t^* values



Proficiency test CSN/CIEMAT 2004 : ^{137}Cs Data

$d(p,q)$ versus t^* for different z values



CONCLUSIONS

The methodology could be used as an adequate tool to evaluate the results of proficiency testing.

The intrinsic discrepancy d considers the laboratory value and its uncertainty in a suitable way.

Future developments:

Classification intervals for d

Optimum S_{ffp} value

Use of non-normal distributions

Thank you for your attention

Contact:

Rafael Núñez-Lagos: nlagos@unizar.es

Lourdes Romero: lourdes.romero@ciemat.es

Manuel Barrera: manuel.barrera@ciemat.es