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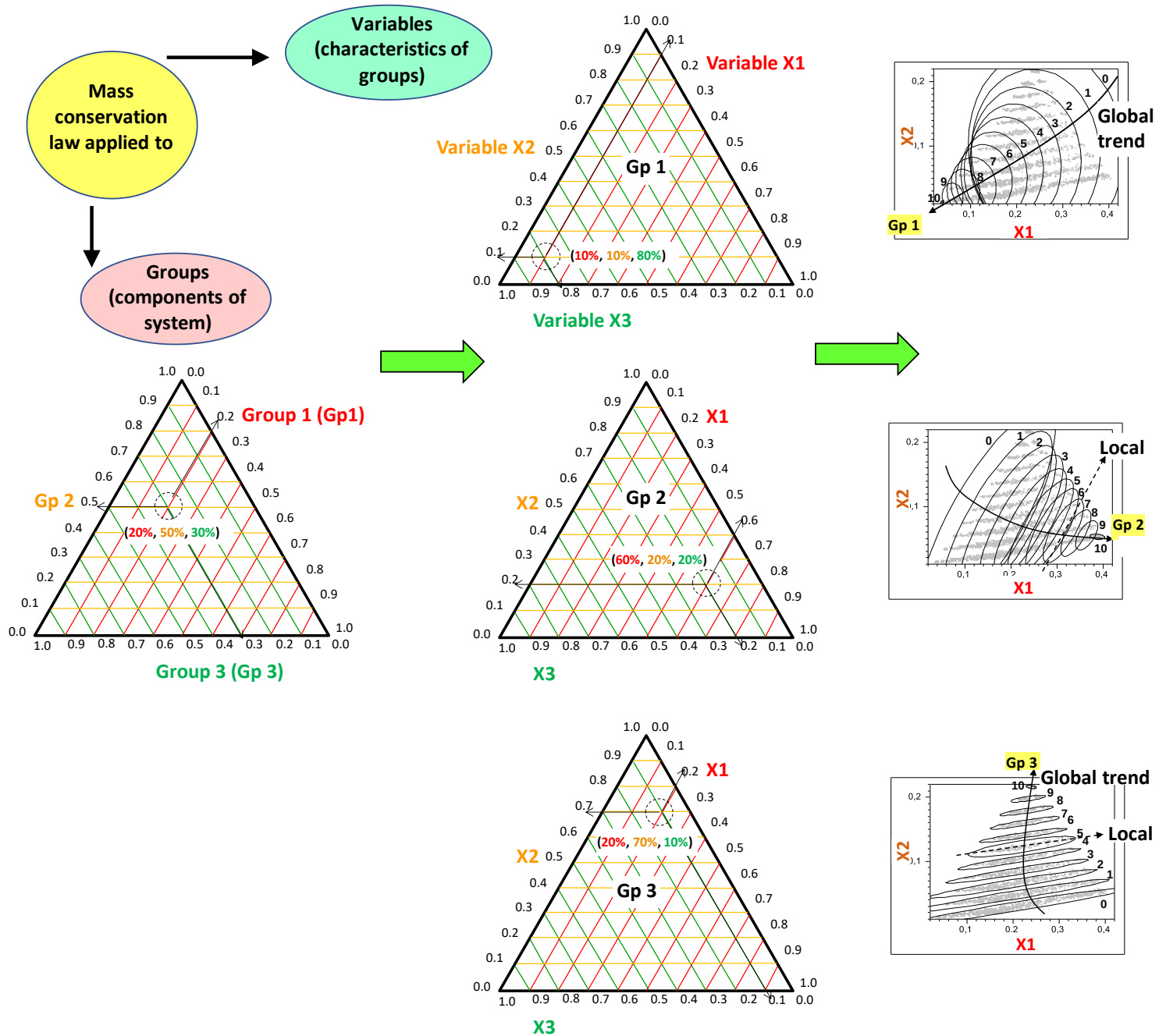
Mini-review on the applications and perspectives of a new simplex machine learning approach in chemistry and biology

Muhammad FARMAN[1], Asma HAMMAMI-SEMMAR[2], Abir SARRAJ-LAABIDI[3,4], Nabil SEMMAR[3,*]

Affiliations:

1 Quaid-i-Azam University, Department of Chemistry, Islamabad, 45320, Pakistan
2 University of Carthage, National Institute of Applied Sciences and Technologies (INSAT), 1080, Tunis, Tunisia
3 Université de Tunis El Manar, Institut Pasteur de Tunis, Laboratory of Bioinformatics, Biomathematics and Biostatistics (BIMS), 1002, Tunis, Tunisia
4 Université de Tunis El Manar, Faculté des Sciences de Tunis, Campus Universitaire, 2092 Tunis, Tunisia

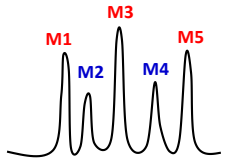
* **For correspondence**: nabilsemmar5@gmail.com


(a)
Inter-group scale
(b)
Intra-group scale
(c)
smoothed relationships
Mass conservation law applied to
Variables (characteristics of groups)
Groups (components of system)
Variable X1
Variable X2
Variable X3
Gp 1
(10%, 10%, 80%)
Global trend
Gp 1
X1
X2
Group 1 (Gp1)
Gp 2
(20%, 50%, 30%)
Group 3 (Gp 3)
X1
X2
X3
Gp 2
(60%, 20%, 20%)
Local
Gp 2
X1
X2
X3
Gp 3
(20%, 70%, 10%)
Gp 3
Global trend
Local
X1
X2

Mass conservation principle

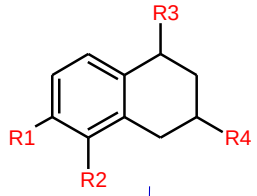
System with variables obeying to unit sum constraint

Chromatogram (Tissue)



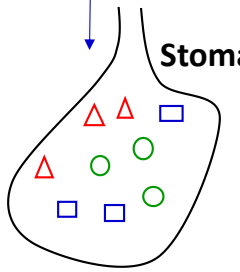
$$\mathrm{Re}\, l_{M_j} = \frac{M_j}{\sum M_j}$$

Molecule



$$\mathrm{Re}\, l_{R_j} = \frac{R_j}{\Sigma R_j}$$

Stomach



$$\mathrm{Re}\, l_{n_j} = \frac{n_j}{\sum n_j}$$

Distribution ways/processes of a whole ressource set

Metabolites' regulations

Static aspect

Dynamic aspect (in time)

Chemical groups' frequencies

Food types' frequencies

Molecular scale

Semmar et al., 2007

Semmar, 2010

Atomic scale

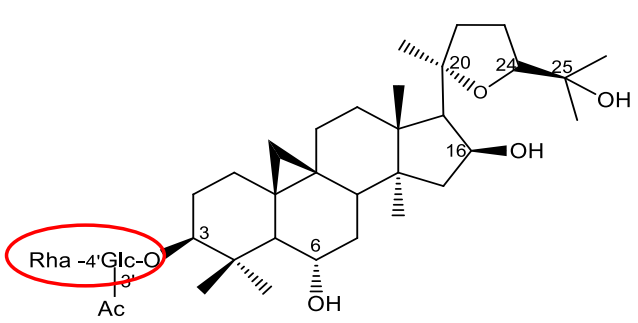
Sarraj et al., 2017

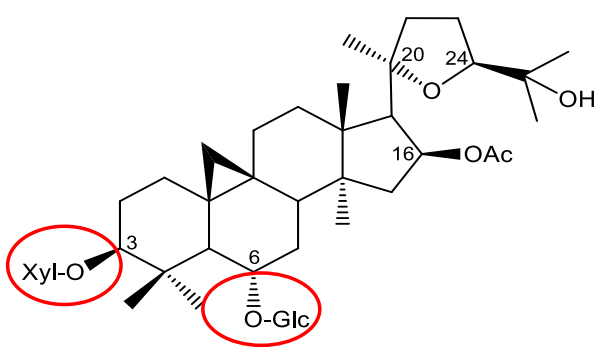
Organismal scale

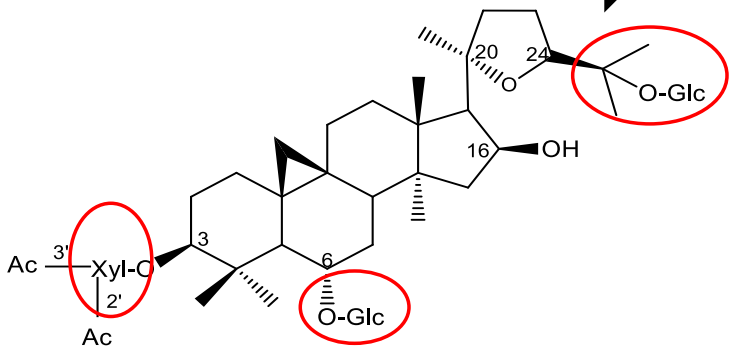
Semmar and Roux, 2014

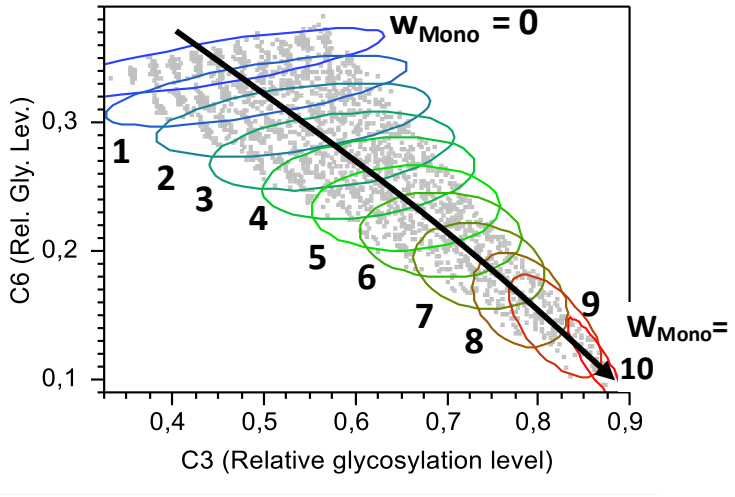
In Structural Chemistry

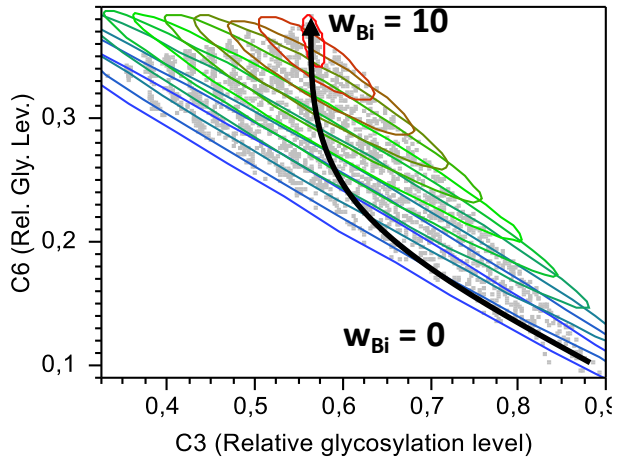
Transitions between glycosylated ramification levels

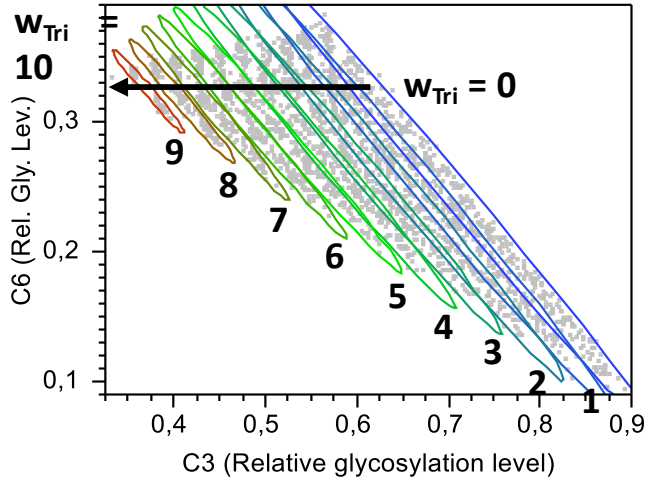






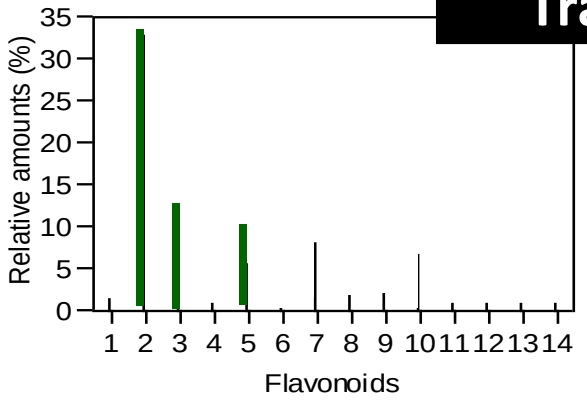




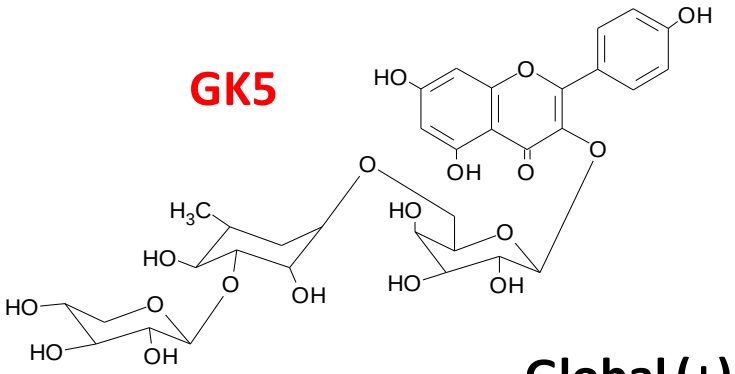


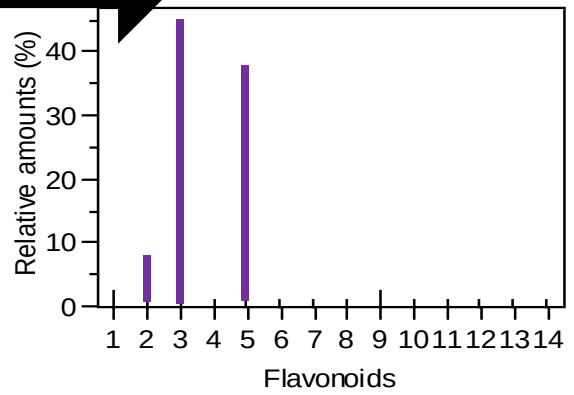
In Plant Metabolomics

Transition between metabolic profiles

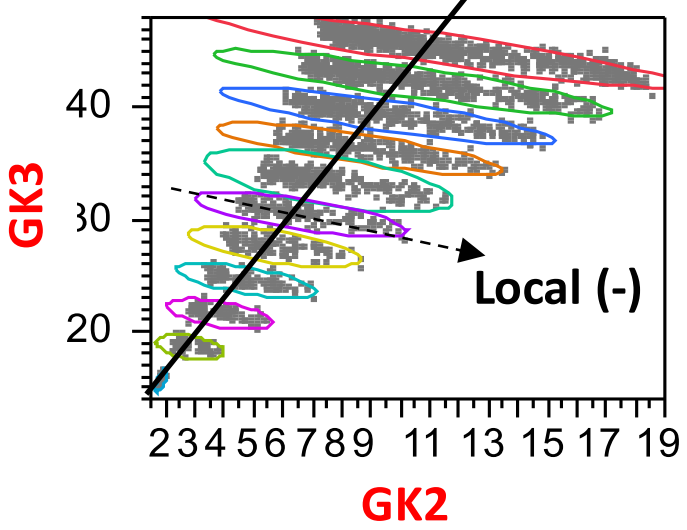


GK5

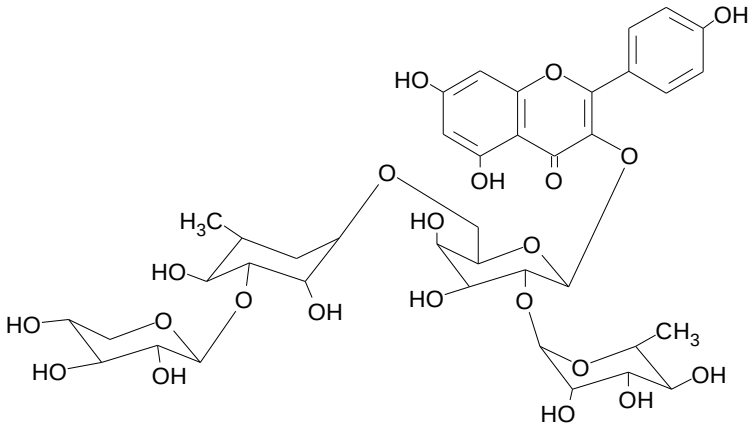




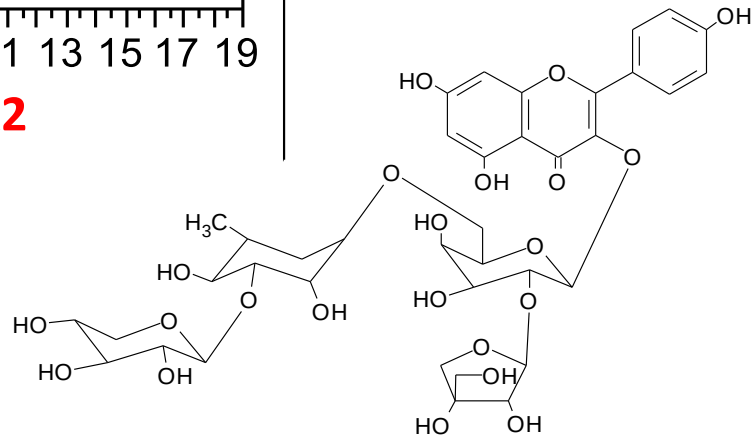
Global (+)



GK2



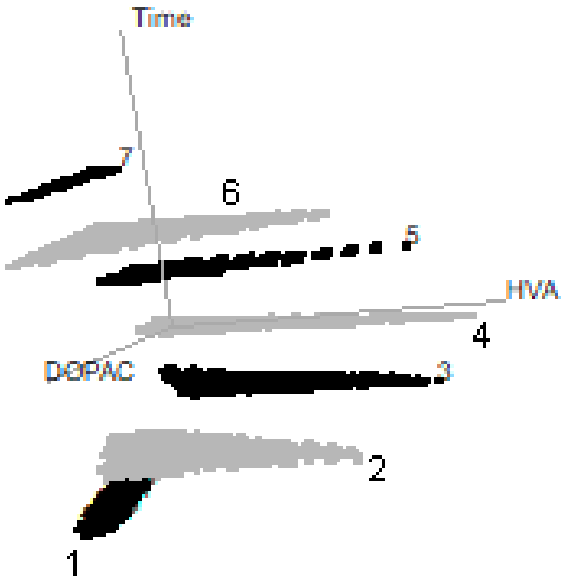
GK3

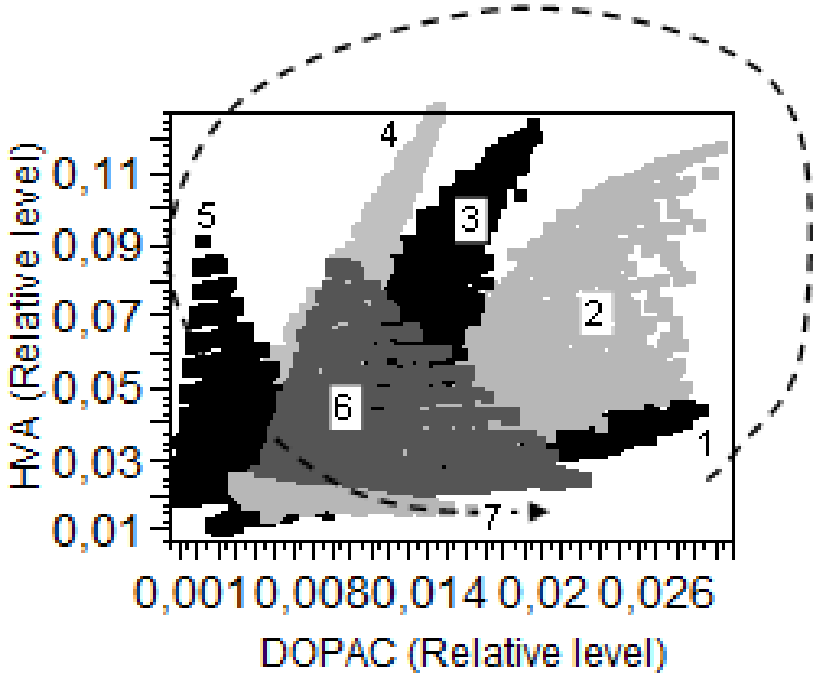


In Pharmacology

Simplex analysis of Kinetic data

Hysteretic relationship between two metabolites due to shared regulation enzymes

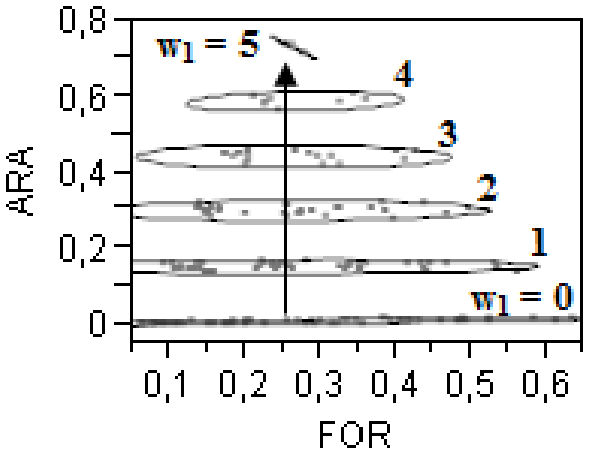


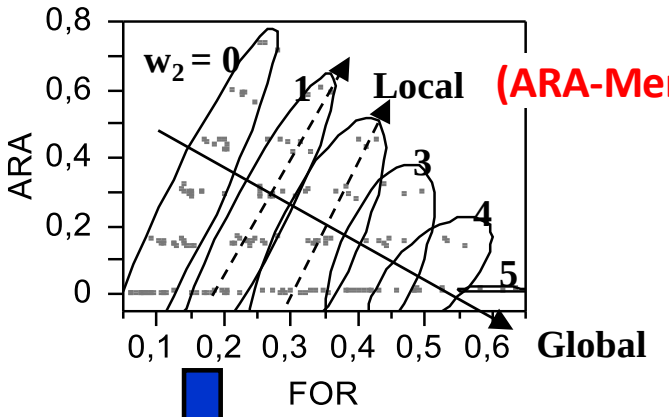


In Animal Ecology (Feeding Behavior analysis)

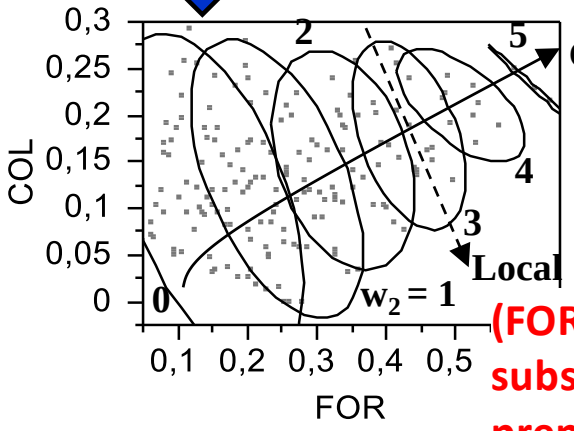
Transitions between food profiles (diets)

Diet 1 ---------- Diet 2 ---------- Diet 3



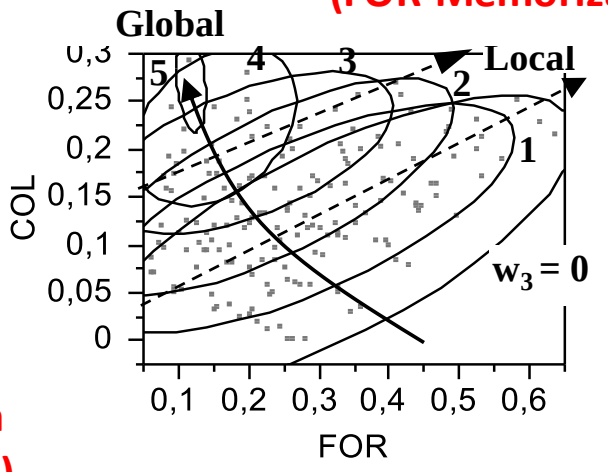


(ARA-Memorization)



(FOR-COL substitution preparation)

(FOR-Memorization)



Legend
ARA: Arachnida
FOR: Formicidae
COL: Coleoptera