LegumeLegacy

SS5 Data Science for biodiversity experiments

Funded by the European Union

Racines d'avenir
LABORATOIRE VIVANT

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Swiss Confederation

Federal Department of Economic Affairs, Education and Research EAER
State Secretariat for Education, Research and Innovation SERI

UK Research and Innovation

General issues on simplex designs and DI models

- Origin of the simplex
- DI models and linear regression
- Sown versus realised proportions as predictor

Origin of the simplex?

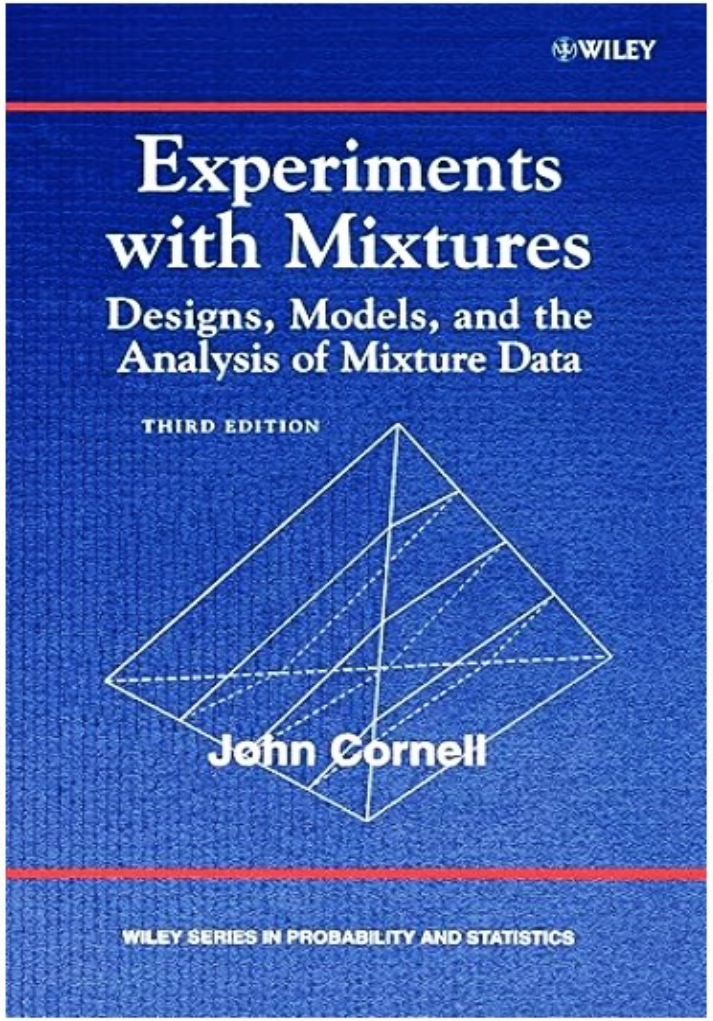
Mixture problems

- Construction of concrete: mix of sand, water, cement
- Tobacco blends: mix of processed tobacco, turkish blend, burley
- Tyres: mix of rubbers of varying consistency
- Cake formulations: mix of flour, baking pouder, sugar, water
- …

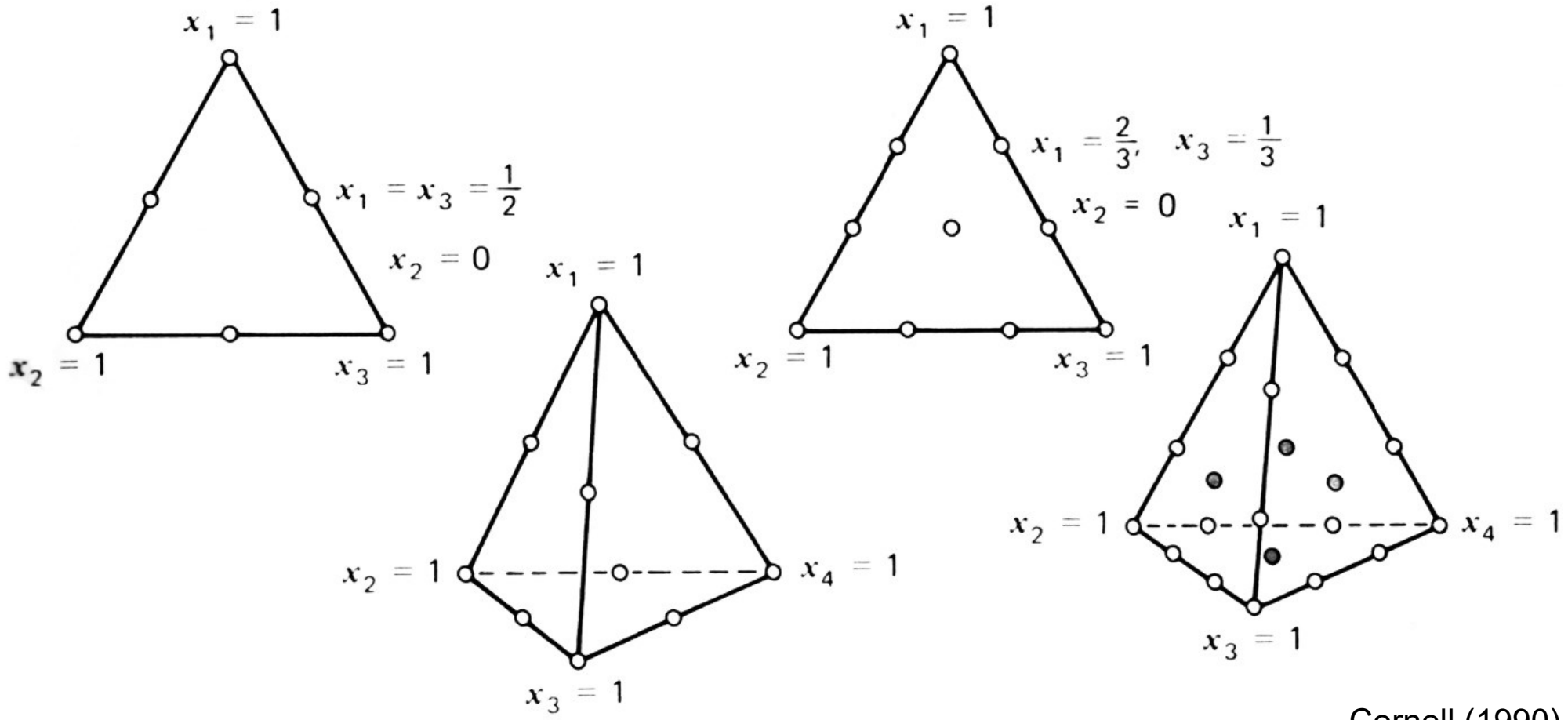
⇨ In the general mixture problem, the measured response is assumed to depend only on the proportions of the ingredients …

Cornell (1990) Wiley

THE book on simplex designs

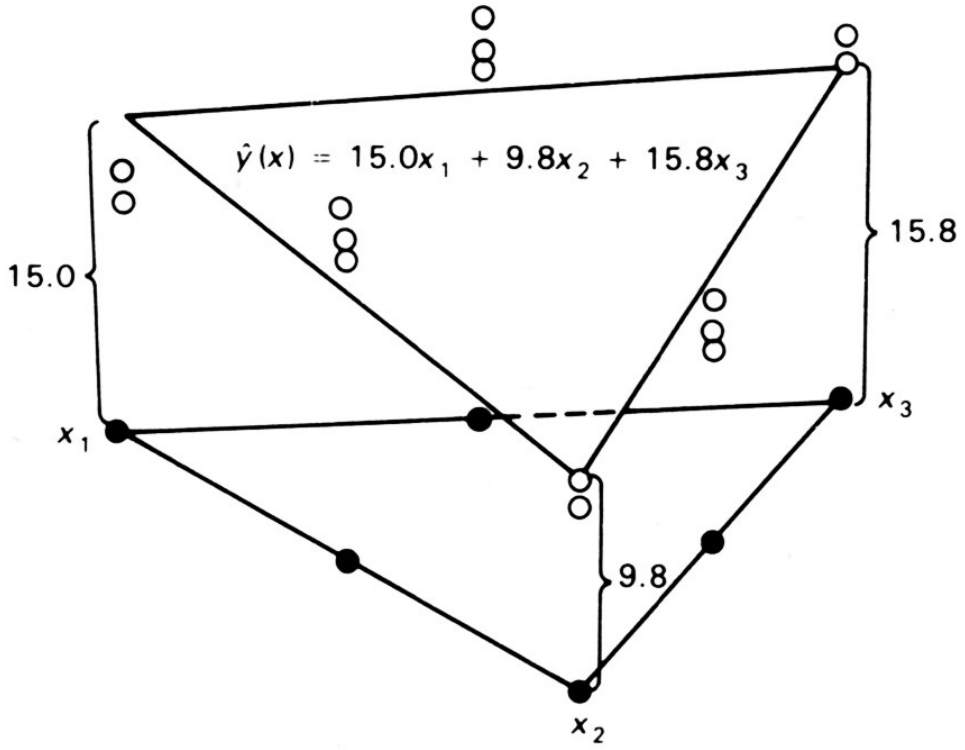


Simplex lattice designs



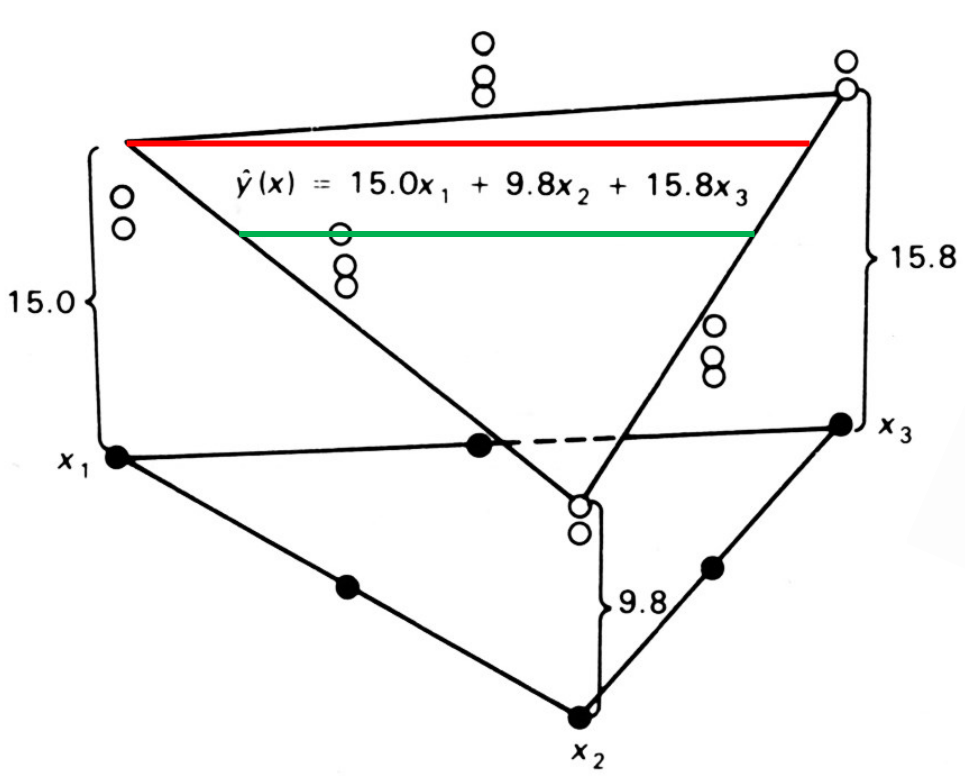
Cornell (1990) Wiley

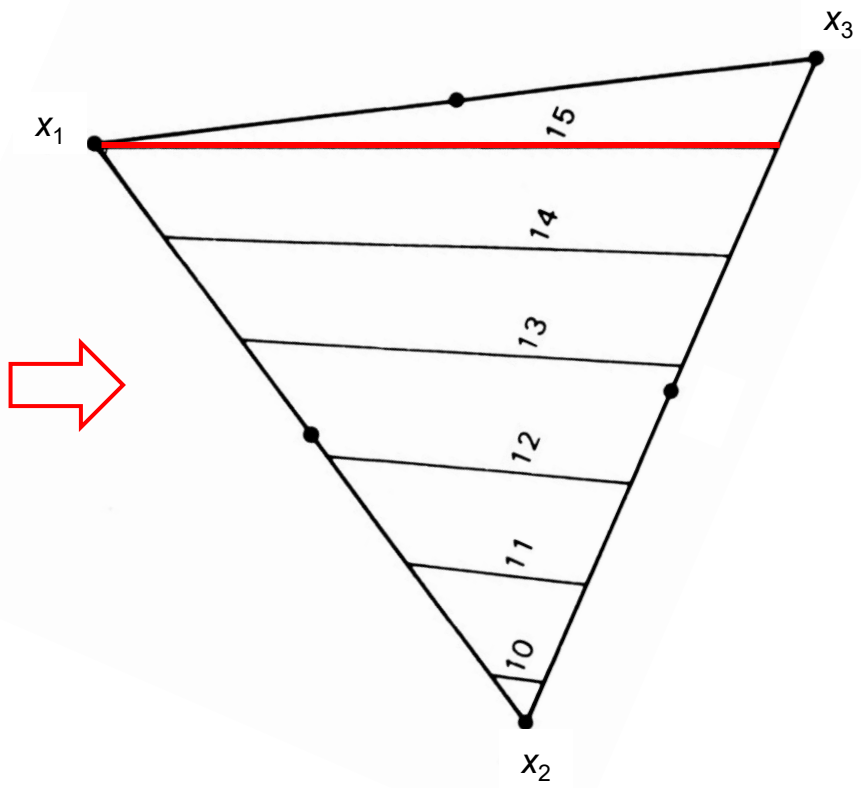
Estimated response surface and its contour



Cornell (1990) Wiley

Estimated response surface and its contour

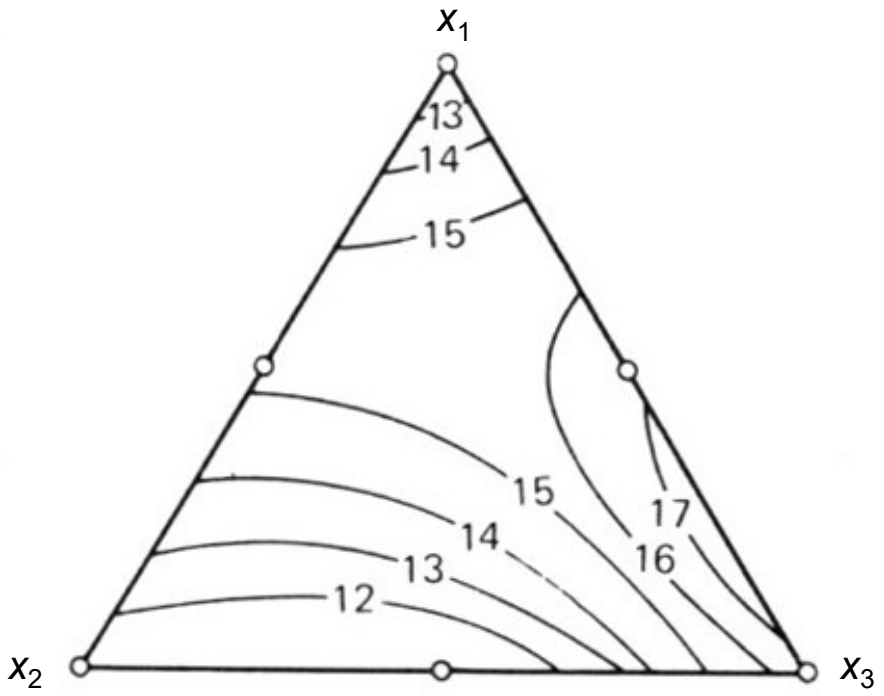




Cornell (1990) Wiley

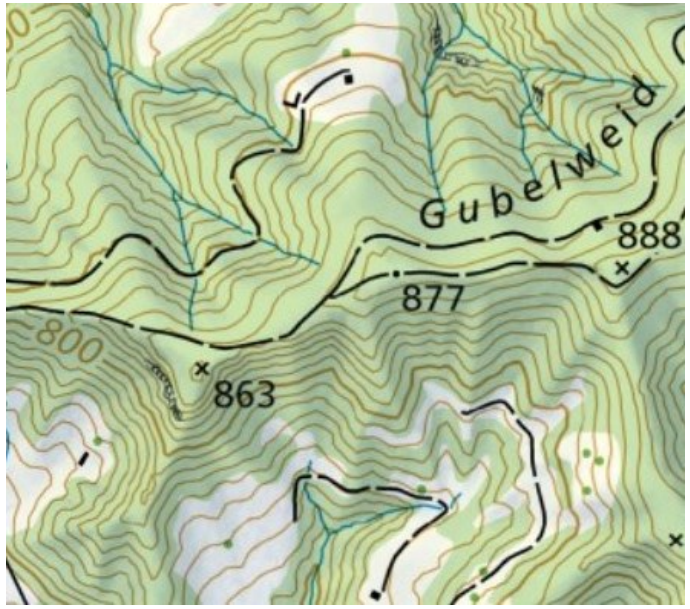
Complex response surface from polynomial equation

Contour lines or Isolines

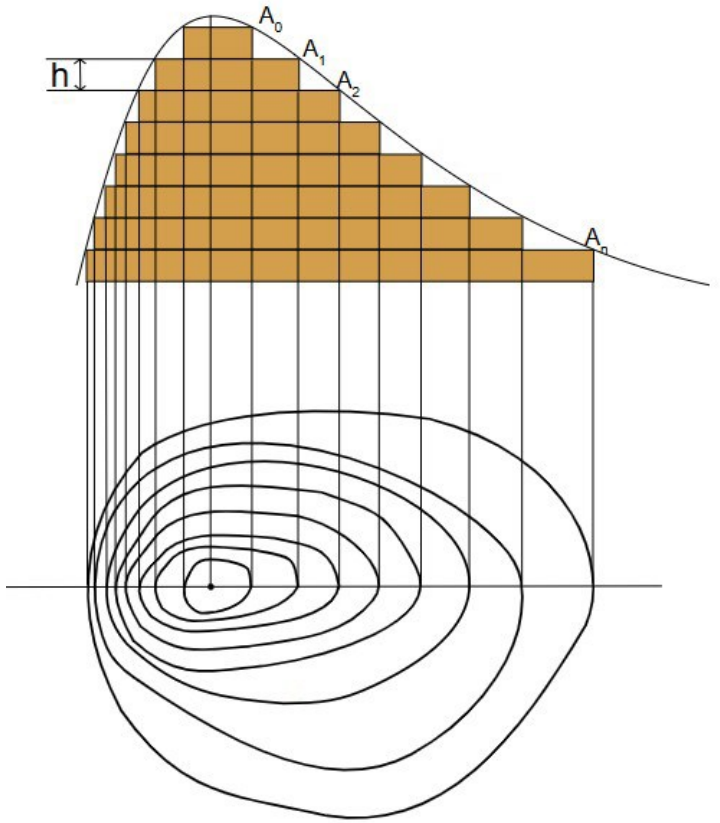


Cornell (1990) Wiley

Contour lines



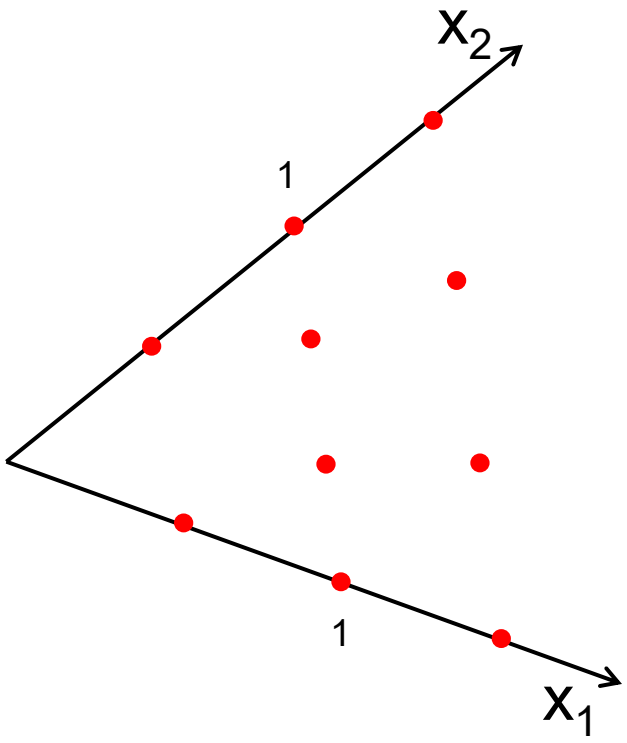
Swisstopo



“Romary” on https://commons.wikimedia.org

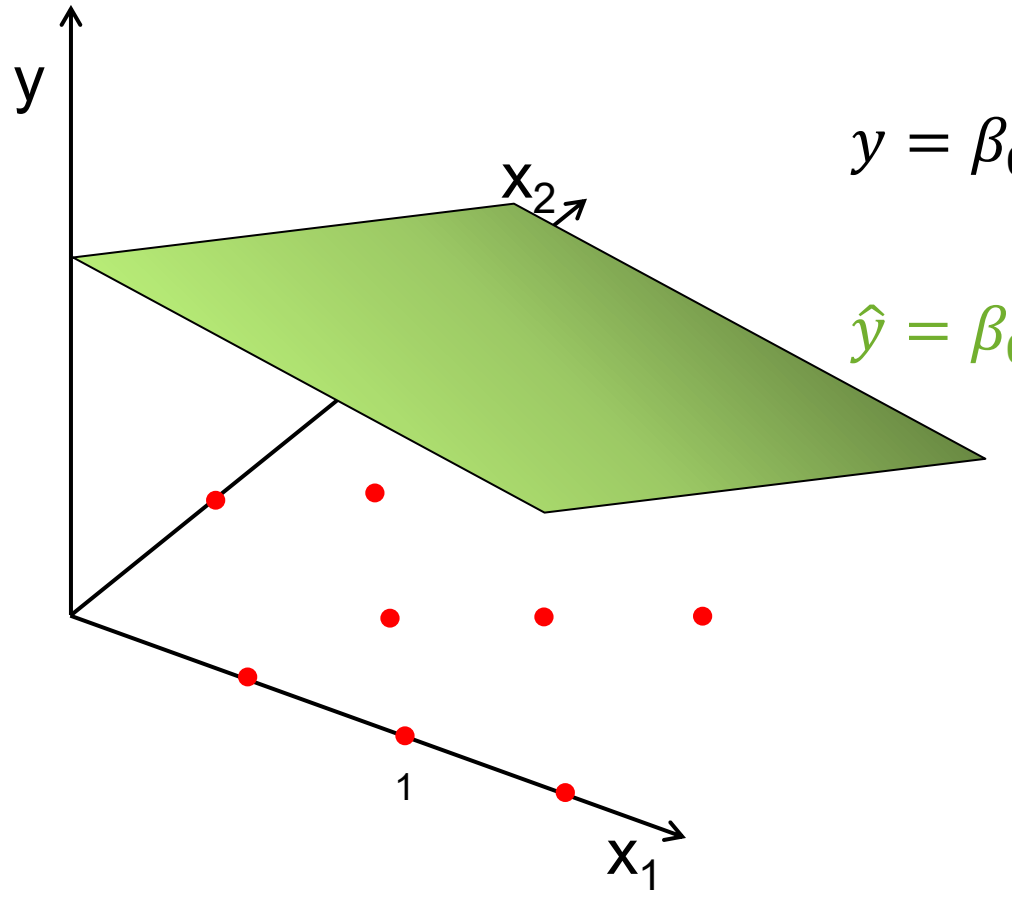
Design space

Two dimensions



Design space and response surface

Two dimensions

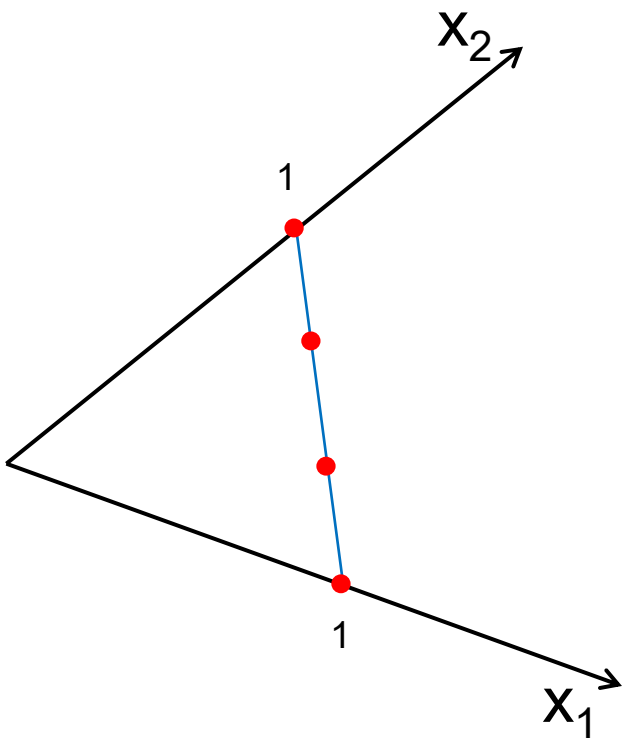


$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

Design space of a simplex

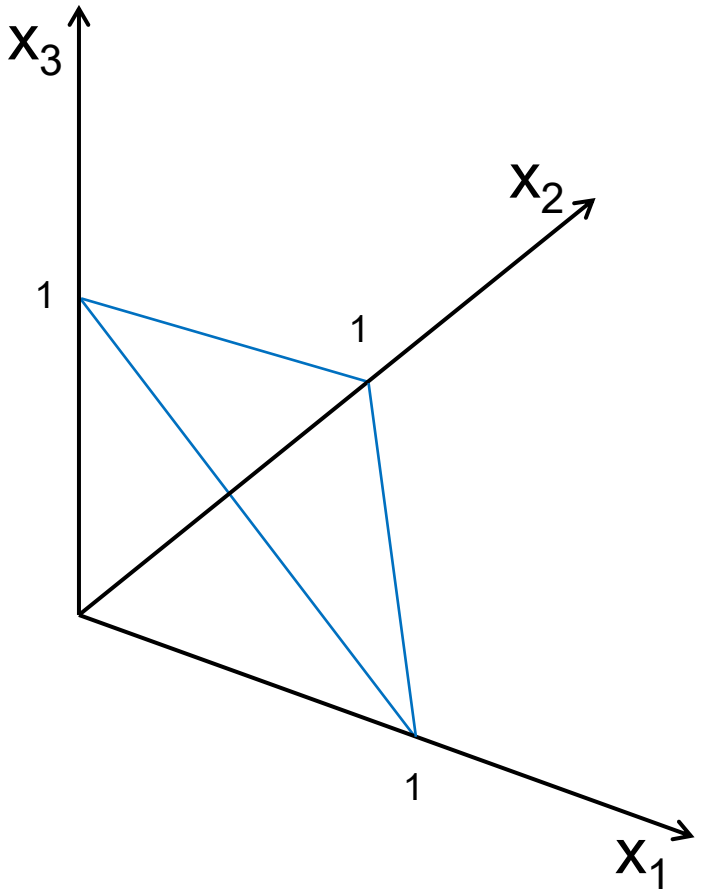
Two dimensions



Constrain the total density to a constant and scale to unit-sum

Design space of a simplex

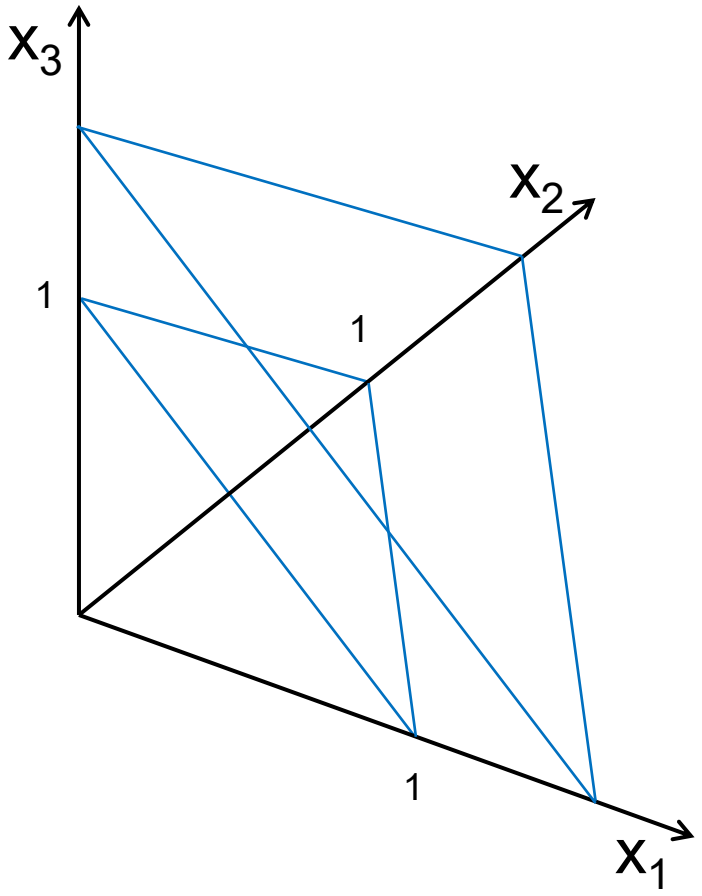
Three dimensions



Constrain the total density to a constant and scale to unit-sum

Design space of a simplex

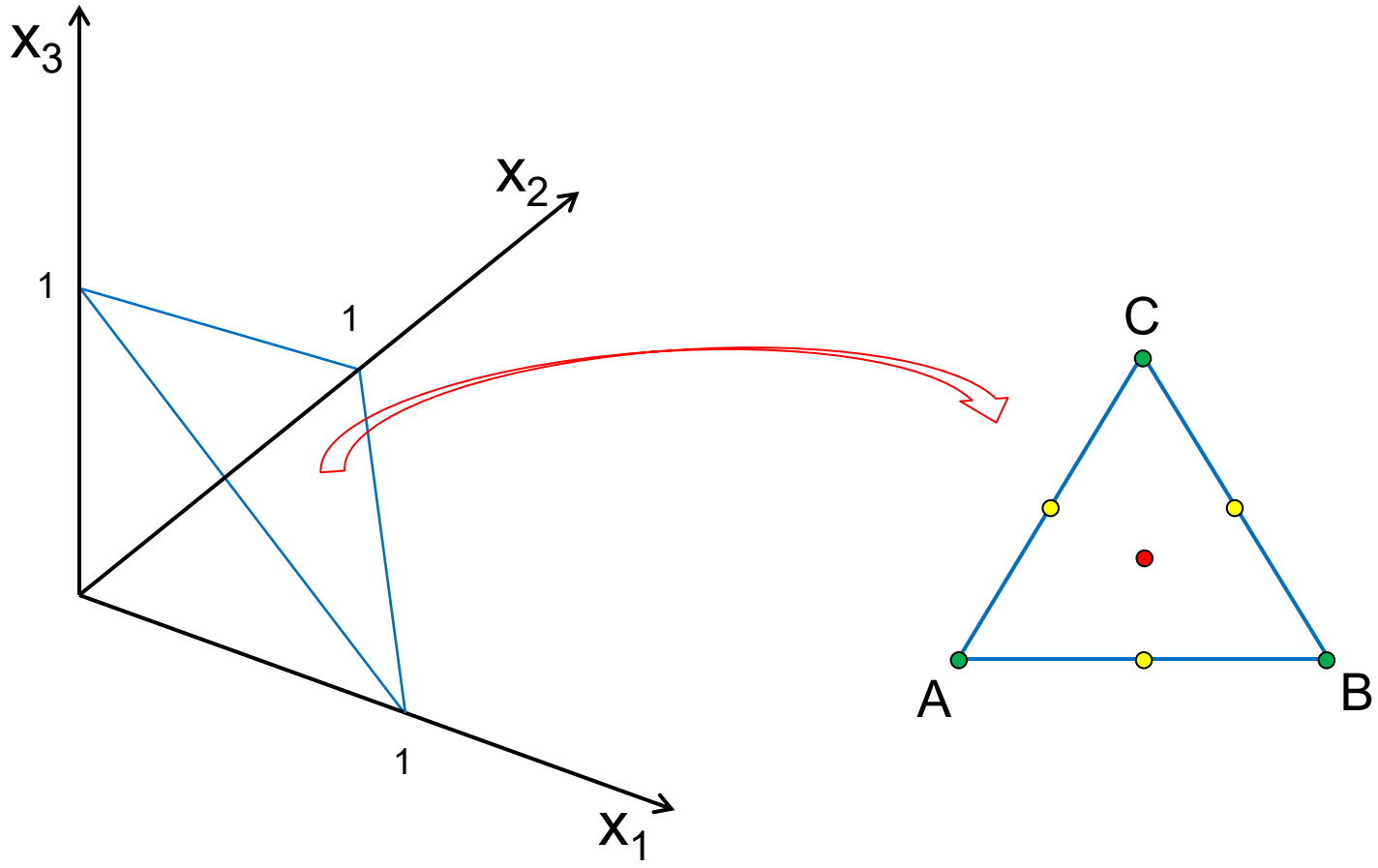
Three dimensions



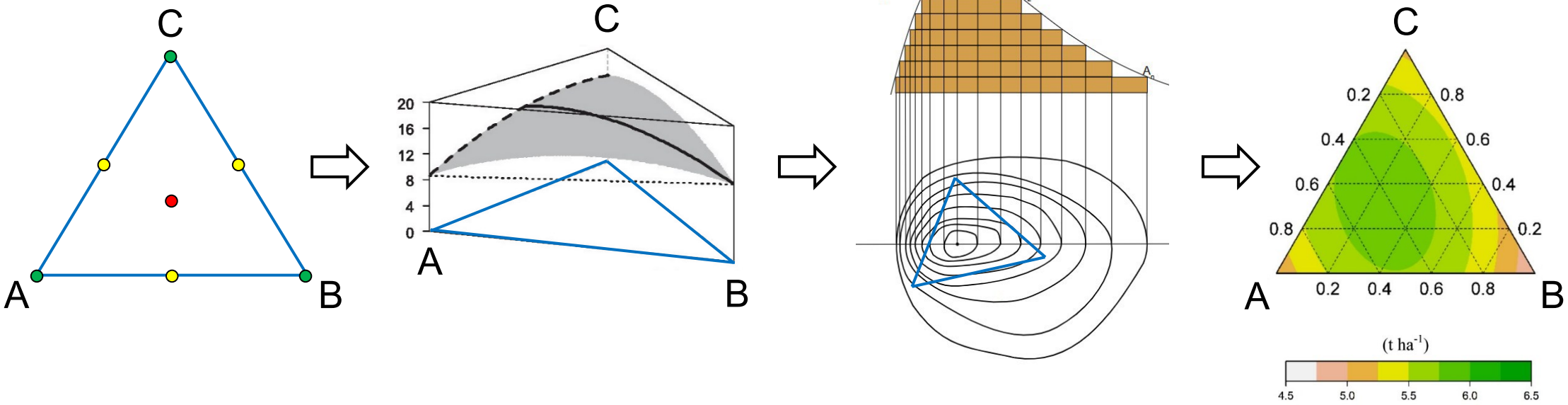
Set-up with higher density
⇨ constrain the total to unit-sum for analysis

Design space of a simplex

Three dimensions



Design space – Response surface – Contour lines



Cong *et al.* (2018) AGEE

"Romary" on https://commons.wikimedia.org

Grange *et al.* (2021) J Appl Ecol

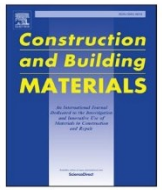
Current examples beyond grassland science

Construction and Building Materials 418 (2024) 135439

Contents lists available at ScienceDirect

Construction and Building Materials

journal homepage: www.elsevier.com/locate/conbuildmat



Design of all solid waste red mud-based cementitious materials based on the simplex centroid method

Wenwen Cui [a], Xiaoqiang Dong [a,b,*], Wei Duan [a], Jiajiang Liu [a], Ruiyang Zhao [a], Gaole He [a]

Bioresource Technology 341 (2021) 125746

Contents lists available at ScienceDirect

Bioresource Technology

journal homepage: www.elsevier.com/locate/biortech

Optimization of the proportion of multi-component rural solid wastes in mixed composting using a simplex centroid design

Yi Gao, Lu Tan, Fang Liu, Qian Li, Xiaocheng Wei, Liyuan Liu, Houyu Li, Xiangqun Zheng, Yan Xu *

Current examples

Design

Experimental design with four components

Run	Mixing ratio (VS basis)			
	SM(A)	HF(B)	RS(C)	KW(D)
1	1.000	0.000	0.000	0.000
2	0.000	1.000	0.000	0.000
3	0.000	0.000	1.000	0.000
4	0.000	0.000	0.000	1.000
5	0.500	0.500	0.000	0.000
6	0.500	0.000	0.500	0.000
7	0.500	0.000	0.000	0.500
8	0.000	0.500	0.500	0.000
9	0.000	0.500	0.000	0.500
10	0.000	0.000	0.500	0.500
11	0.333	0.333	0.333	0.000
12	0.333	0.333	0.000	0.333
13	0.333	0.000	0.333	0.333
14	0.000	0.333	0.333	0.333
15	0.250	0.250	0.250	0.250
16	0.625	0.125	0.125	0.125
17	0.125	0.625	0.125	0.125
18	0.125	0.125	0.625	0.125
19	0.125	0.125	0.125	0.625
20	1.000	0.000	0.000	0.000
21	0.000	1.000	0.000	0.000
22	0.000	0.000	1.000	0.000
23	0.000	0.000	0.000	1.000
24	0.500	0.500	0.000	0.000

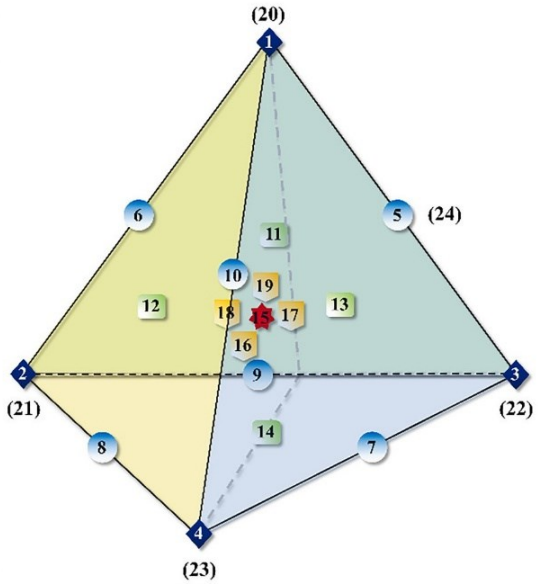


Fig 1. Experimental design with four components and schematic diagram.

Results

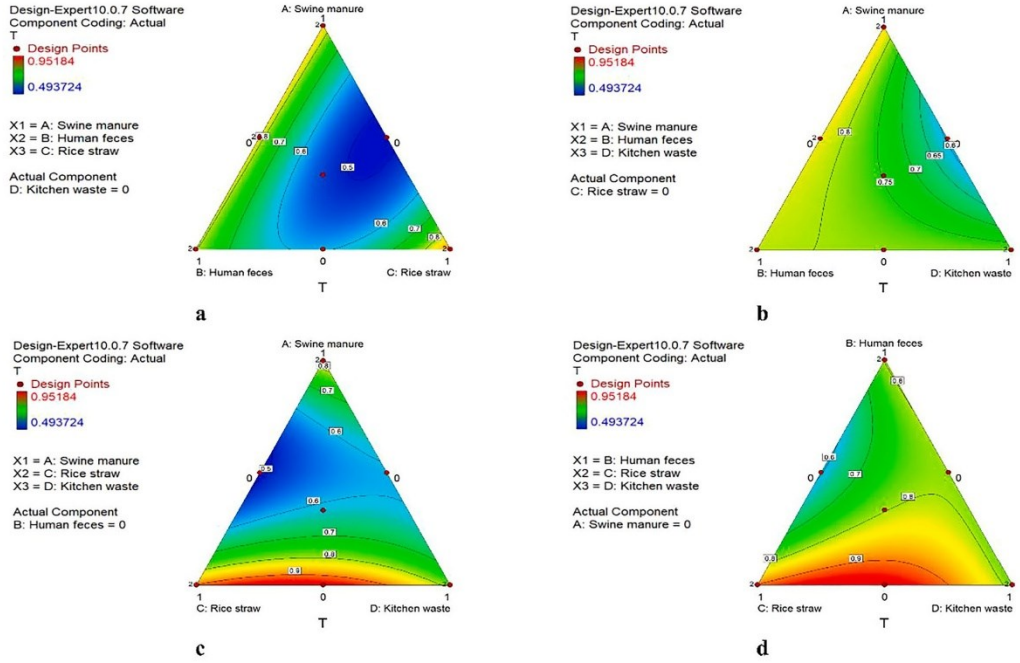
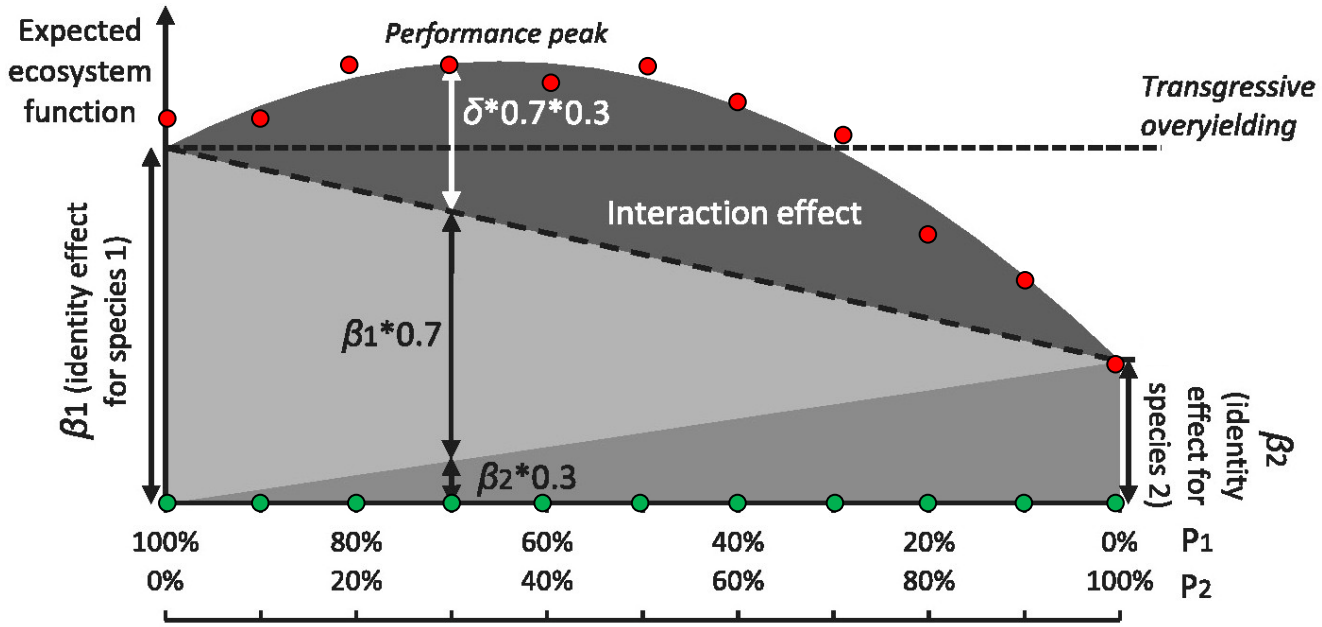


Fig 5. T contours with different proportions of a) Swine manure (SM), Human feces (HF), and Rice straw (RS), with Kitchen waste (KW) level = 0; b) SM, HF, KW, with RS level = 0; c) SM, RS, and KW, with HF level = 0; d) HF, and RS, and KW, with SM level = 0.

Gao *et al.* (2021) Bioresour Technol

DI Models and regression

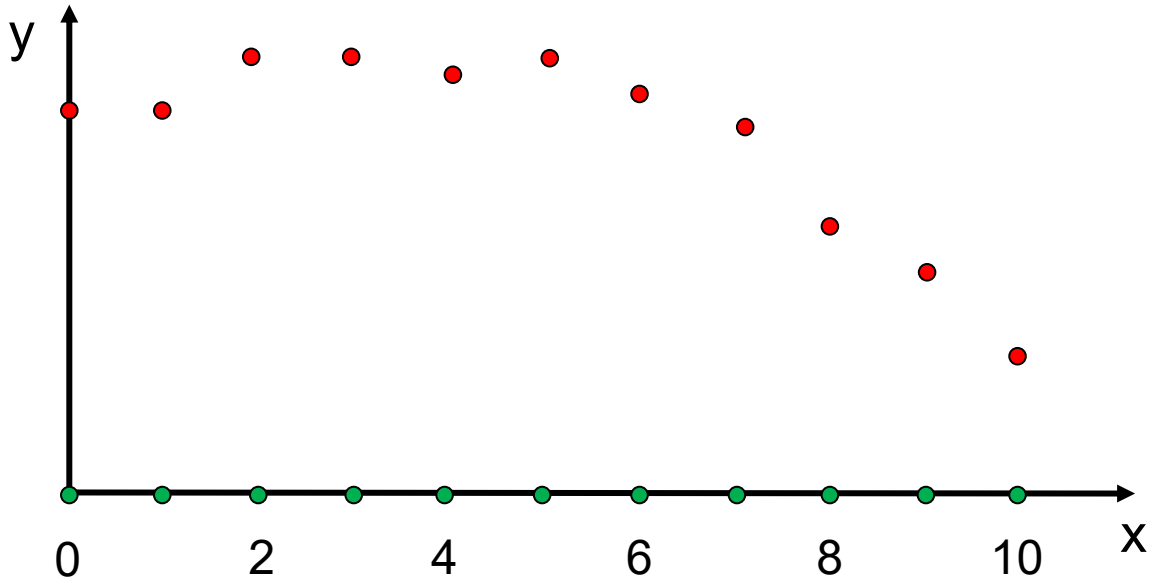


Measured yield (assumed)

$$y = \beta_1 P_1 + \beta_2 P_2 + \delta P_1 P_2 + \varepsilon$$

Grange *et al.* (2021) J Appl Ecol

Linear regression



$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$$

DI Model ⇨ re-parametrised regression

The general second-degree polynomial in q variables is

$$\eta = \beta_0 + \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{ii} x_i^2 + \sum\sum_{i<j}^{q} \beta_{ij} x_i x_j$$

and if we apply the identities $x_1 + x_2 + \cdots + x_q = 1$ and

$$x_i^2 = x_i\left(1 - \sum_{\substack{j=1 \\ j \neq i}}^{q} x_j\right)$$

then for $m = 2$

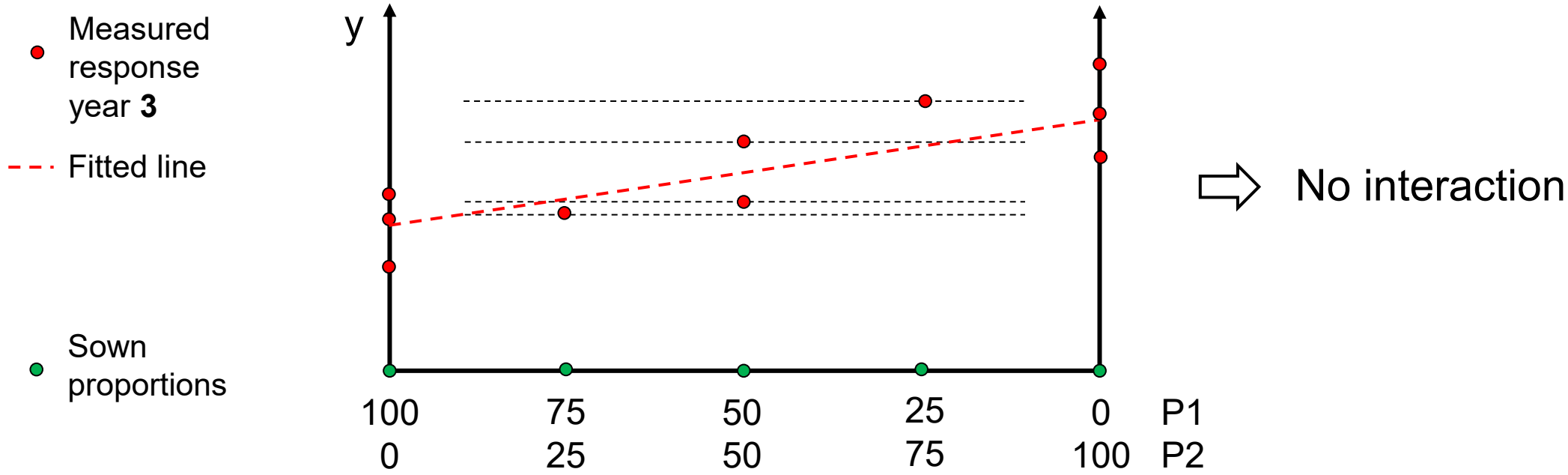
$$\eta = \beta_0\left(\sum_{i=1}^{q} x_i\right) + \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{ii} x_i\left(1 - \sum_{j \neq i}^{q} x_j\right) + \sum\sum_{i<j}^{q} \beta_{ij} x_i x_j$$

$$= \sum_{i=1}^{q} (\beta_0 + \beta_i + \beta_{ii}) x_i - \sum_{i=1}^{q} \beta_{ii} x_i \sum_{j \neq i}^{q} x_j + \sum\sum_{i<j}^{q} \beta_{ij} x_i x_j$$

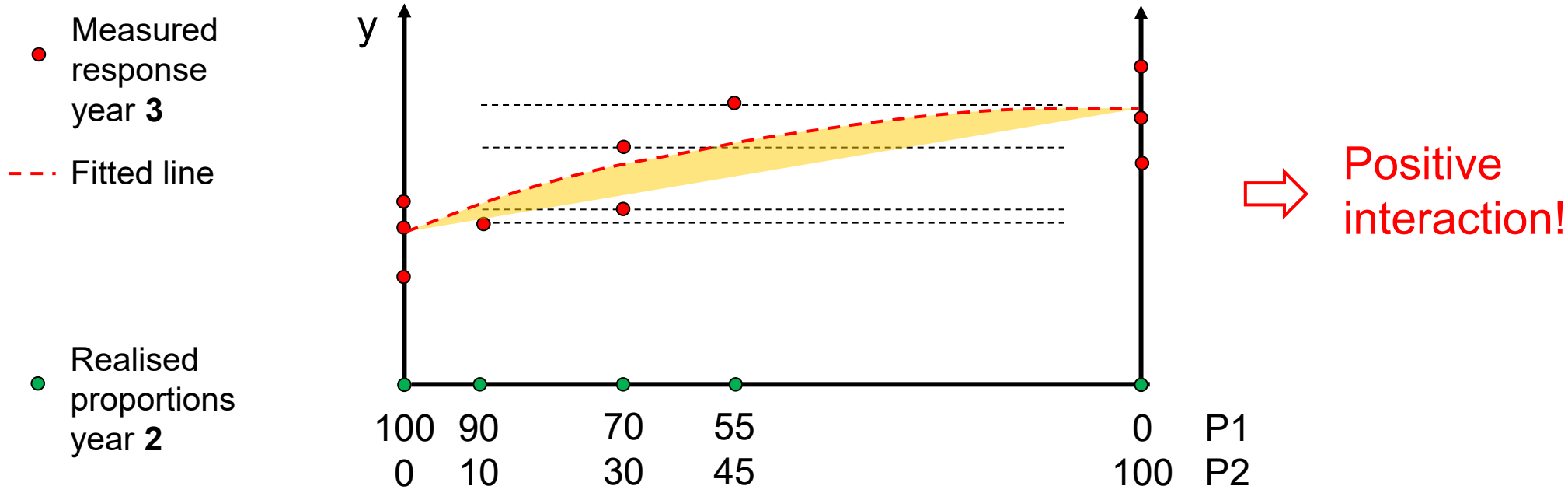
$$= \sum_{i=1}^{q} \beta_i^* x_i + \sum\sum_{i<j}^{q} \beta_{ij}^* x_i x_j$$

Cornell (1990) Wiley

Sown versus realised proportions

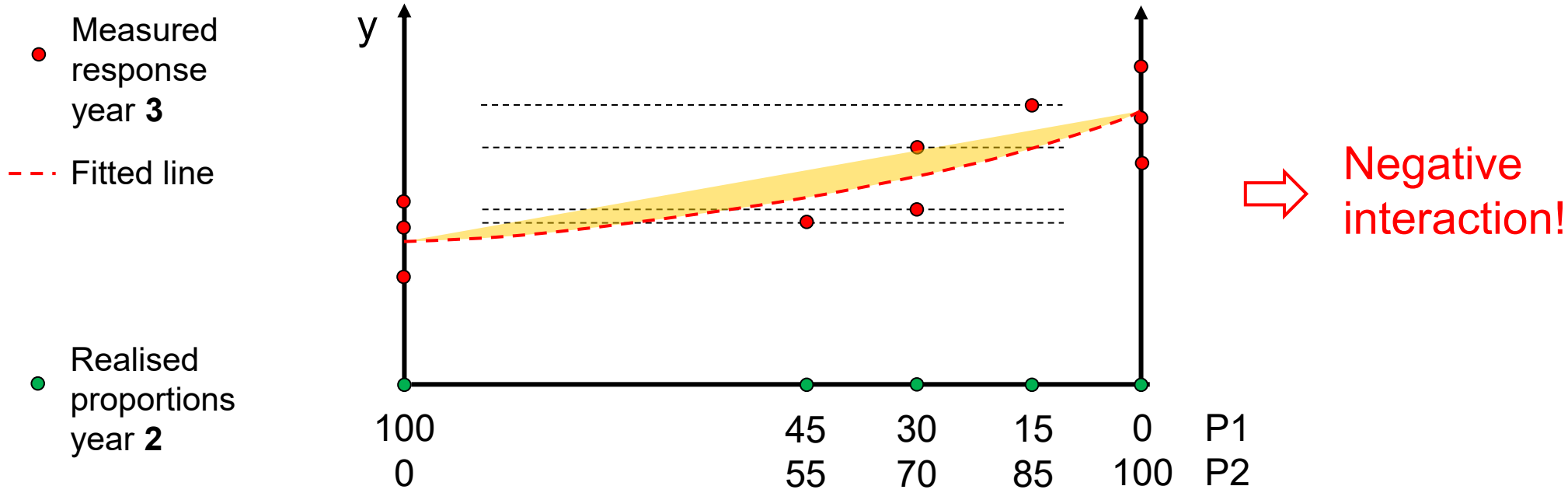


Sown versus realised proportions



Community shift towards species 1

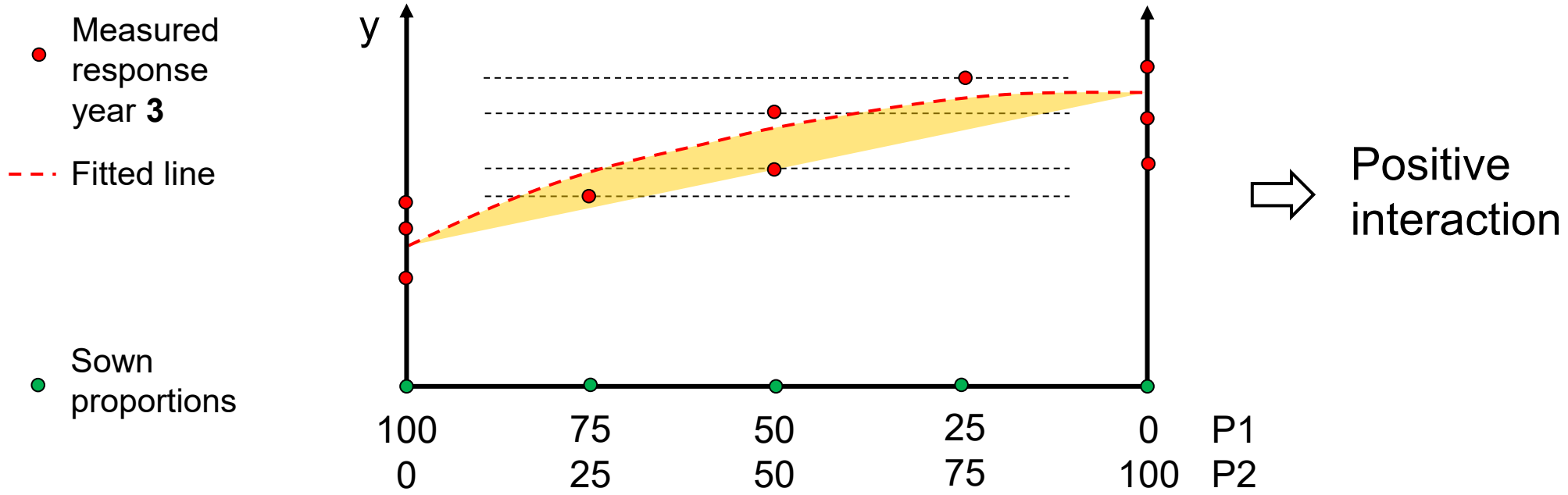
Sown versus realised proportions



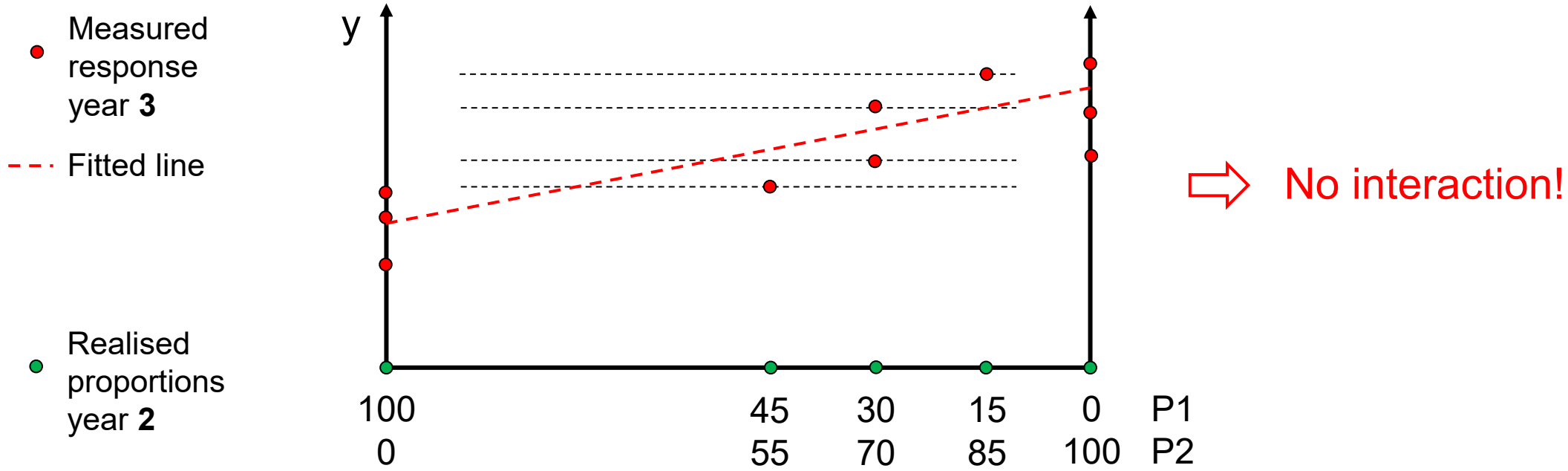
Community shift towards species 2

Sown versus realised proportions

Start with positive interaction



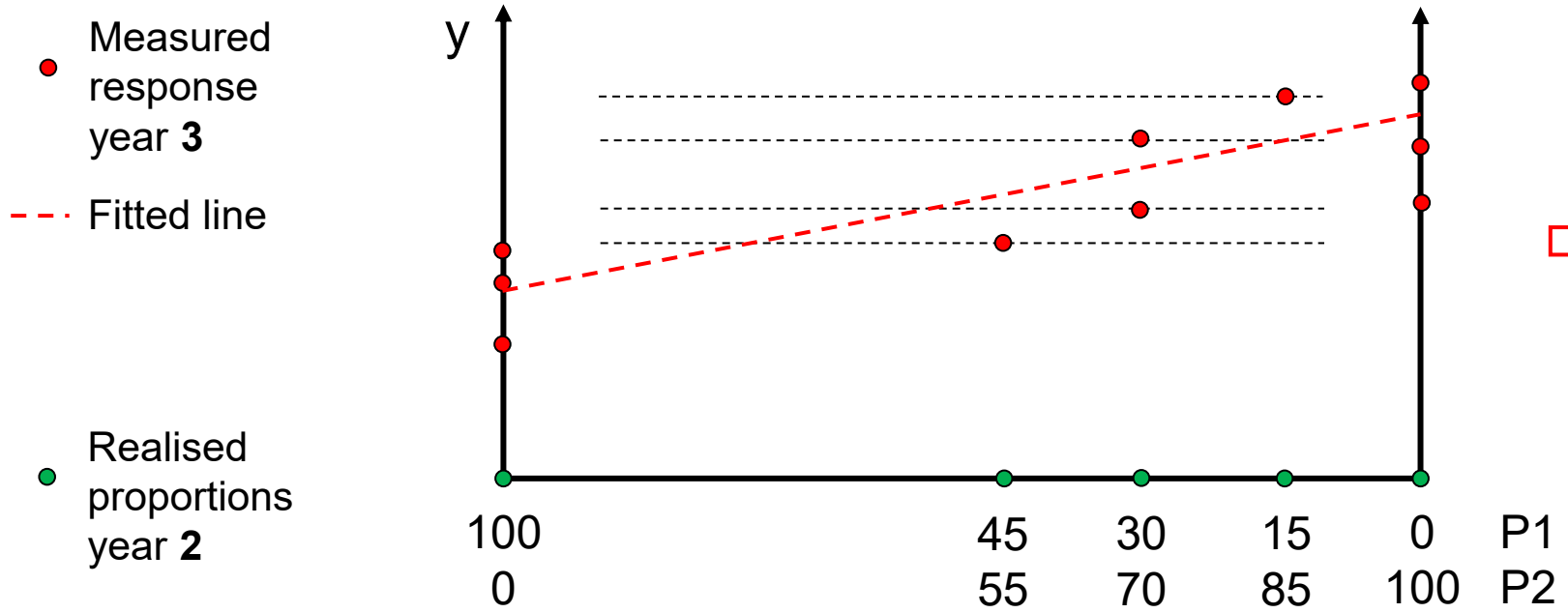
Sown versus realised proportions



⇨ No interaction!

Community shift towards species 2

Sown versus realised proportions



⇨ No interaction!

⇨ There is no black and white, but be aware of what you are doing!

Take home

- Literature on simplex designs since ~ 1950
- Basic DI model ⇨ linear regression under sum-to-one constraint
- Interpretation may vary depending on sown or realised proportions as predictor












Thank you for your attention

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