Optimal Experimental Design
An overview

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http://areaestadistica.uclm.es/

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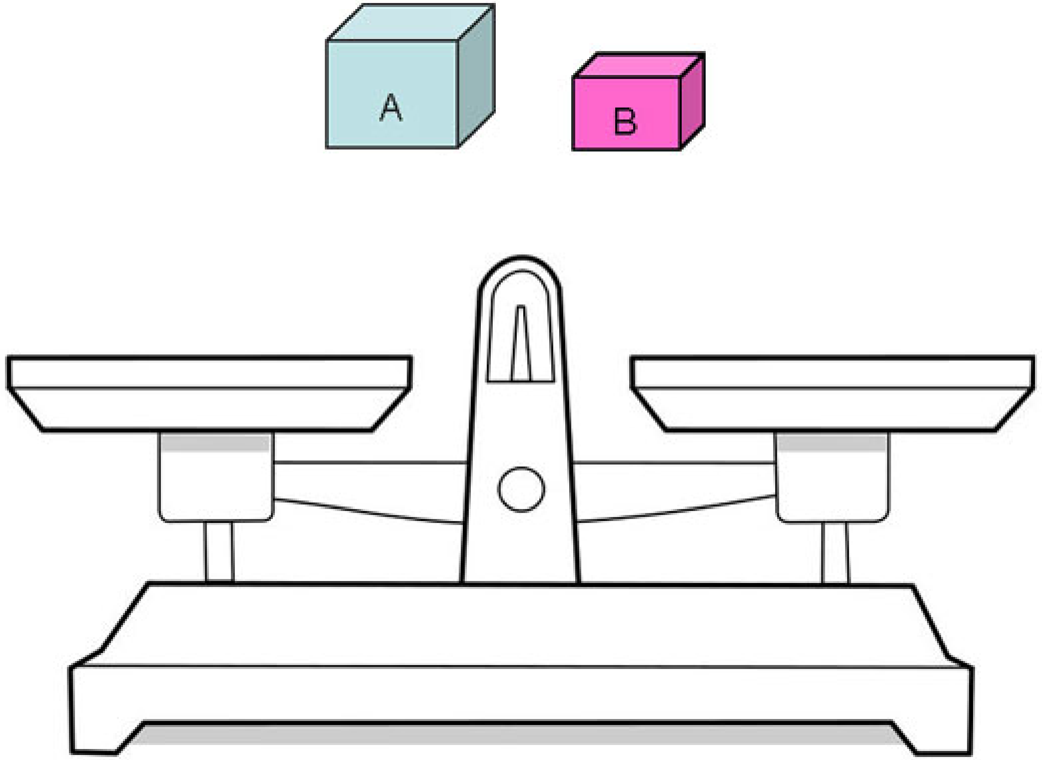
Motivating example

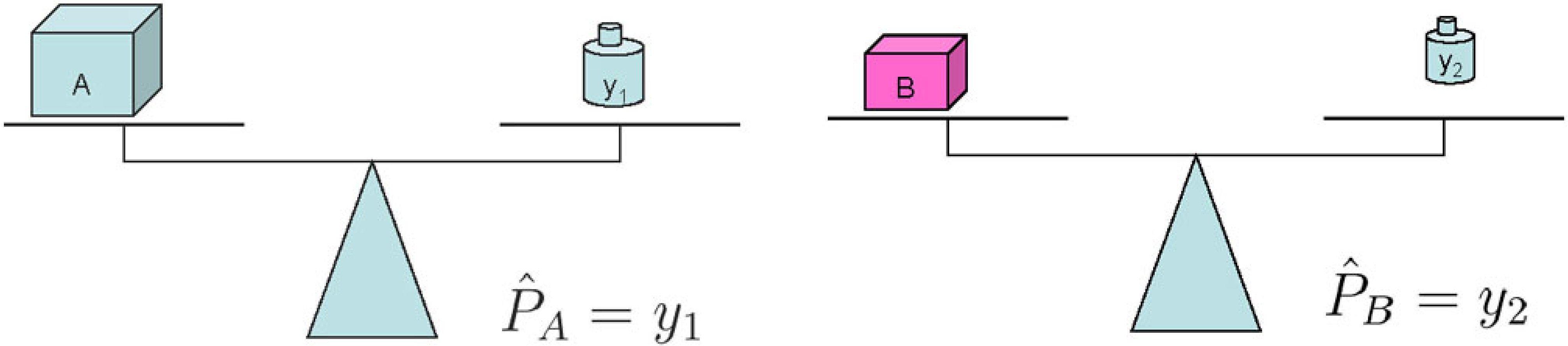


Restricción:
¡ Sólo 2 pesadas !

“Diseño“ habitual

$$y = P + \epsilon, \qquad \epsilon \equiv \mathcal{N}(0, \sigma^2)$$

Hipótesis: El error de la balanza no depende del peso de los objetos (error homocedástico).

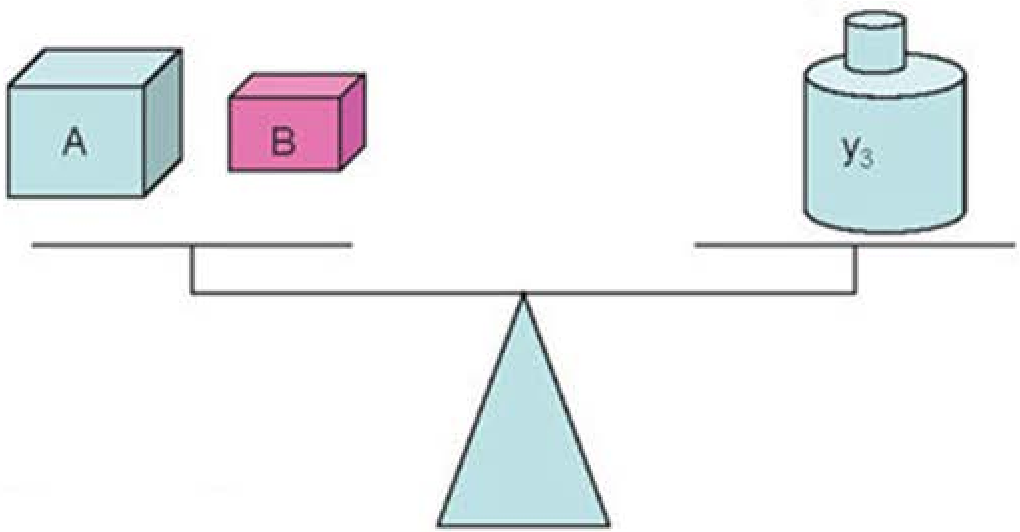


$$\hat{P}_A = y_1 \qquad \hat{P}_B = y_2$$

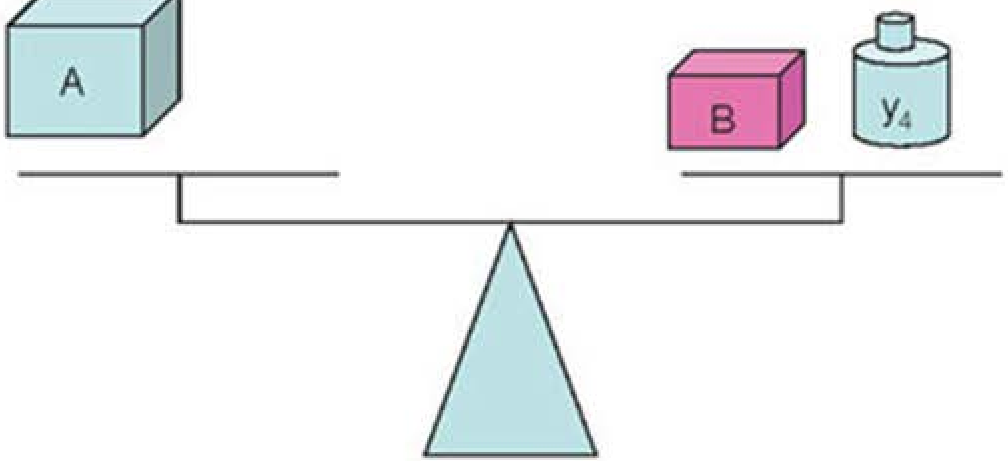
$$y_1 = P_A + \epsilon_1 \longrightarrow \mathrm{Var}(\hat{P}_A) = \sigma^2$$

$$y_2 = P_B + \epsilon_2 \longrightarrow \mathrm{Var}(\hat{P}_B) = \sigma^2$$

Diseño óptimo



$$y_3 = P_A + P_B + \epsilon_3$$



$$y_4 = P_A - P_B + \epsilon_4$$

$$\hat{P}_A = \frac{y_3 + y_4}{2} \quad \hat{P}_B = \frac{y_3 - y_4}{2} \Rightarrow \mathrm{Var}(\hat{P}_A) = \mathrm{Var}(\hat{P}_B) = \sigma^2/2$$

!!

Optimal experimental design

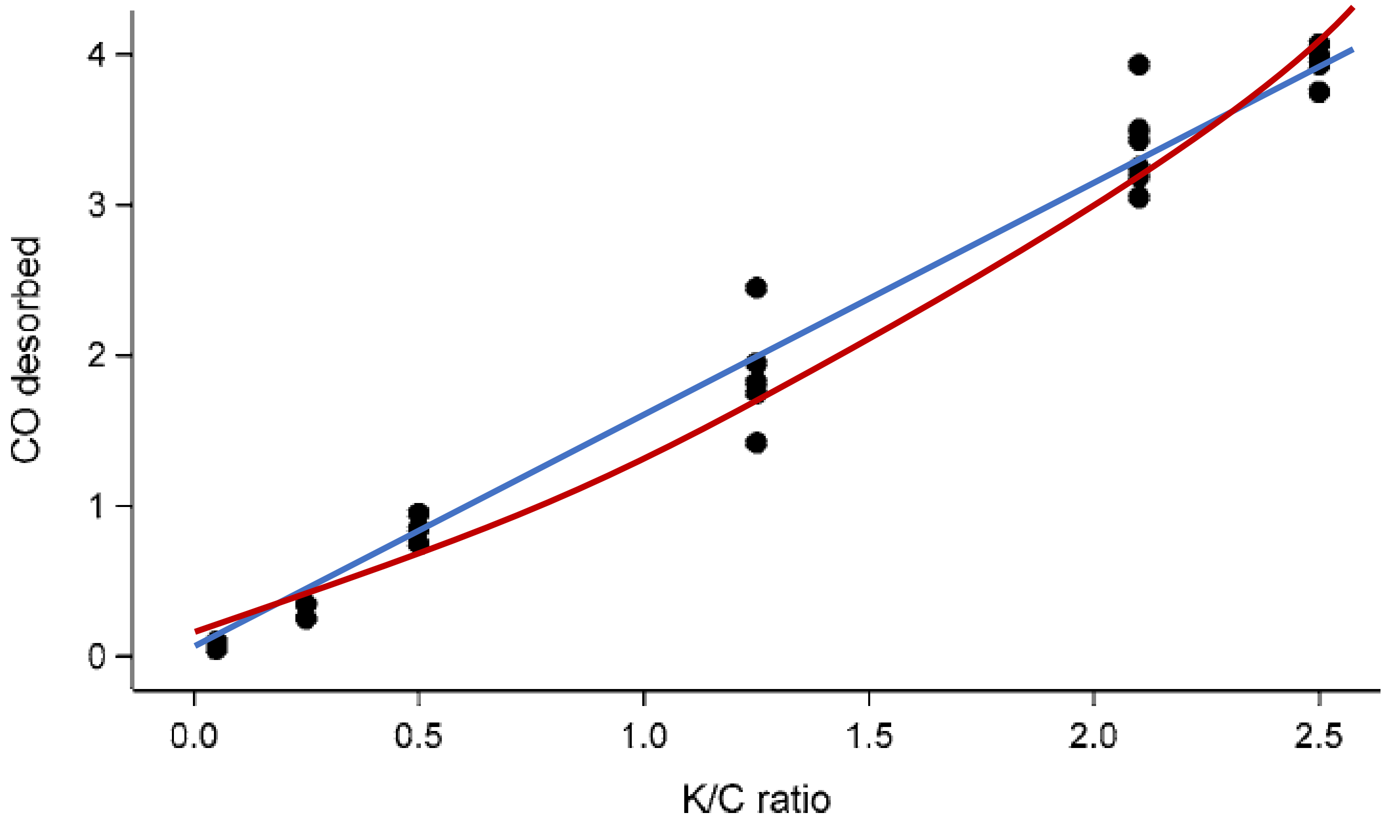


FIG. 1.1. Example 1.1 the desorption of carbon monoxide. Yield (carbon monoxide desorbed) against K/C ratio.

Atkinson, Donev and Tobias (2007). Optimum experimental designs, with SAS. Oxford University Press

Optimal designs and efficiencies

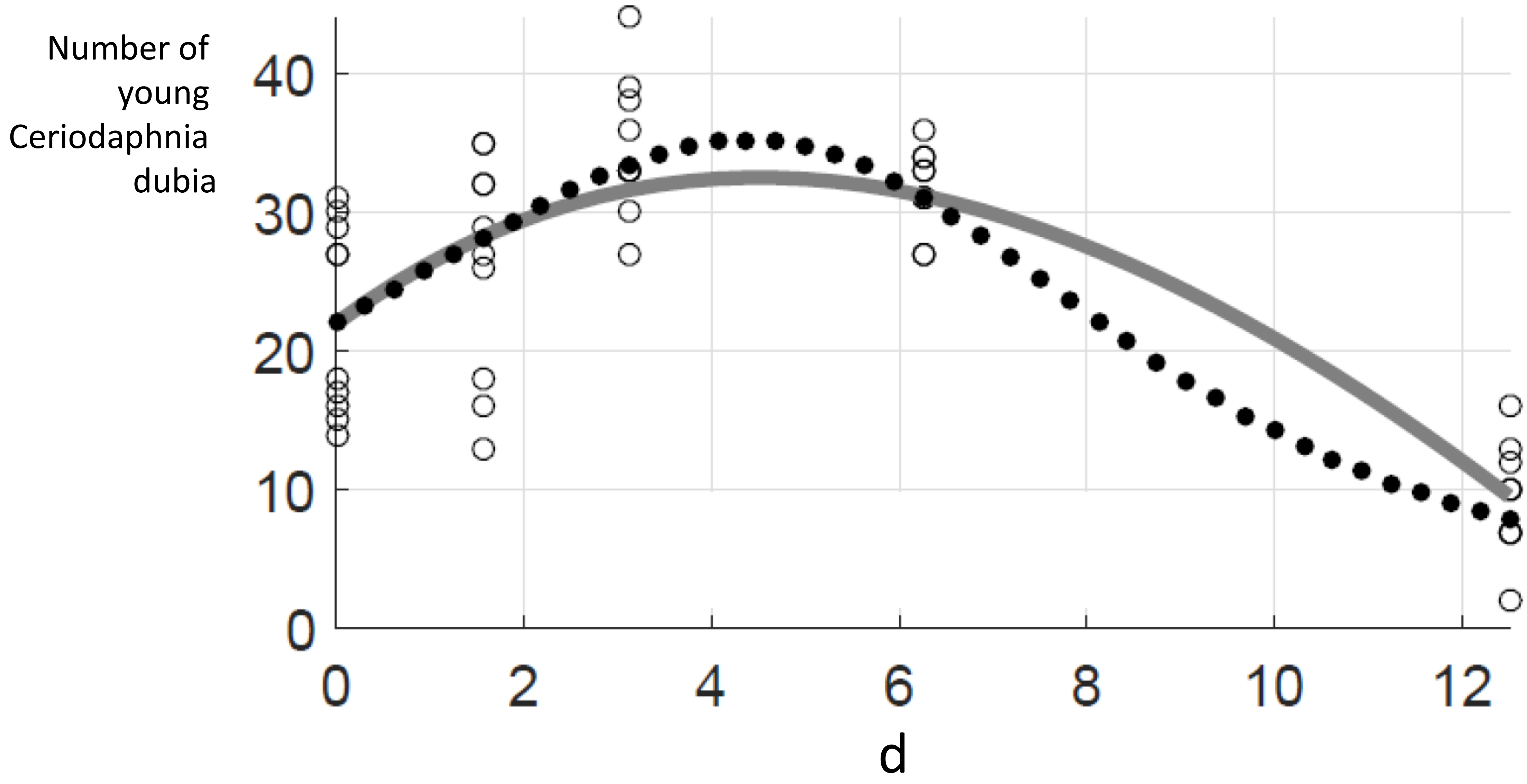
TABLE 11.2. Example 1.1. Efficiency for a variety of purposes of the design* of Table 1.1 for measuring the desorption of carbon monoxide

Model	Optimality	Weight at design points				Efficiency
$\eta(x)$	criterion	0	$\sqrt{(2)}-1$	0.5	1	(%)
$\beta_0+\beta_1 x$	D	1/2	—	—	1/2	69.5
$\beta_0+\beta_1 x+\beta_2 x^2$	D	1/3	—	1/3	1/3	81.7
$\beta_0+\beta_1 x+\beta_2 x^2$	D_S for β_2	1/4	—	1/2	1/4	47.4
$\beta_1 x$	D	—	—	—	1	43.7
$\beta_1 x+\beta_2 x^2$	D	—	—	1/2	1/2	62.4
$\beta_1 x+\beta_2 x^2$	D_S for β_2	—	$\sqrt{2}/2$	—	$1-\sqrt{2}/2$	47.2

* The design region is scaled to be $\mathcal{X}=[0,1]$. The design of Table 1.1 is then

$$\xi_{22}=\left\{\begin{array}{cccccc} 0.02 & 0.1 & 0.2 & 0.5 & 0.84 & 1.0 \\ 2/22 & 2/22 & 3/22 & 5/22 & 6/22 & 4/22 \end{array}\right\}.$$

Ongoing work... Hormesis related problems



- Model for the response: $$\mu(d,\theta)\begin{cases} = \theta_1 - \theta_2 d + \dfrac{\theta_3}{\theta_4}(1 - e^{-\theta_4 d}) \\ = \dfrac{\theta_1 + \theta_2 d}{1 + e^{-\theta_3} d^{\theta_4}} \end{cases}$$

- Approximate designs: $$\xi = \begin{Bmatrix} d_1 & d_2 & \dots & d_k \\ w_1 & w_2 & \dots & w_k \end{Bmatrix} \quad d_i \in \Omega$$

- Information matrix: $$M(\xi,\theta) = \sum_{i=1}^{k} w_i f(d_i,\theta) f^T(d_i,\theta),$$

where $f(d,\theta) = \dfrac{\partial \mu(d,\theta)}{\partial \theta}$.

Online R tools

Optimal design for detec

Es seguro | https://vcaseroalonso.shinyapps.io/OEDhormesis1/

Optimal design for detecting hormesis | Compute optimal designs for one model | Models to compare

Based on Dette, Pepelyshev and Wong (2011) and ongoing work by Casero-Alonso, Pepelyshev and Wong

Choose a model

e-Gompertz

Design interval : (values between 0 and 100)

Lower end-point: 0

Upper end-point: 12,5

Parameter values (separated by commas)

22,10,15,0.09

Design to compare (xi_p):

- Equally weigthed in 0, 1.56, 3.12, 6.25 and 12.5 (Whole Effluent Toxicity test)
- Equally weigthed in 0, 0.025, 0.05, 0.1 and 0.15 (Toxicity study of DEHP)
- Other (you must provide the support points and weights)

Support points of xi_p (separated by commas)

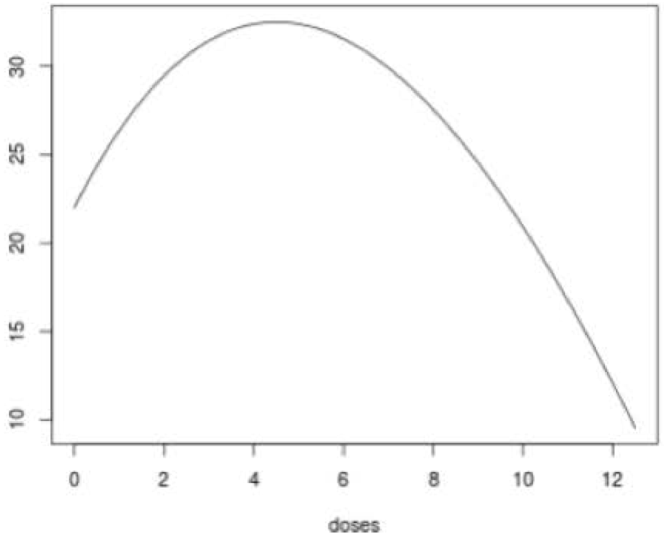
0,0.025,0.05,0.1,0.15

Corresponding weights (separated by commas, total sum=1)

0.2,0.2,0.2,0.2,0.2

Plot | Optimal designs

Response curve for the selected model



If the response curves do not have the U-shape or the inverted U-shape, please, check the right end-points and parameter values

Plot | Optimal designs

D-optimal design for the assumed model

	Supp1	Supp2	Supp3	Supp4
doses	0.0000	3.0095	8.5565	12.5000
weights	0.2500	0.2500	0.2500	0.2500

h-optimal design for the assumed model

	Supp1	Supp2	Supp3	Supp4
doses	0.0000	2.7095	8.9174	12.5000
weights	0.3550	0.4414	0.1482	0.0554

tau-optimal design for the assumed model

	Supp1	Supp2	Supp3	Supp4
doses	0.0000	0.0953	9.4220	9.7688
weights	0.4965	0.0059	0.0836	0.4140

Efficiencies of xi_p design (with respect to the above optimal designs) + tau value

D-eff(xi_p)	h-eff(xi_p)	tau-eff(xi_p)	tau value
0.0000	0.0001	0.0000	9.7135

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¡Muchas gracias por su atención!

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