Optimal design for the bounded log-linear model

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Motivation

The bounded log-linear regression model, an alternative to the four parameter logistic model, has a bounded response with non-homogeneous variance. In this paper, we theoretically show that an optimal design that minimizes an information based criterion consists at most five support points including the two boundaries of the design space. The **D**-optimal design does not depend on the two parameters representing the boundaries of the response but it depends on the variance of the error. Furthermore, if the error variance is known and big enough, we prove that the **D**-optimal design is the two-point design supported at boundary points with equal weights.

The model

$$\log\left(\frac{B-Y}{Y-A}\right) = a + bx + \varepsilon,$$

or equivalently,

$$Y = B - \frac{B-A}{1+e^{-(a+bx+\varepsilon)}},$$

where

Y is the response,

$x \in \mathbb{X}$ is a non-random covariate,

$\varepsilon \sim N(0, \sigma^2)$,

a, b, A and B are parameters.

For σ, two cases are considered: unknown or known.

Simulated data

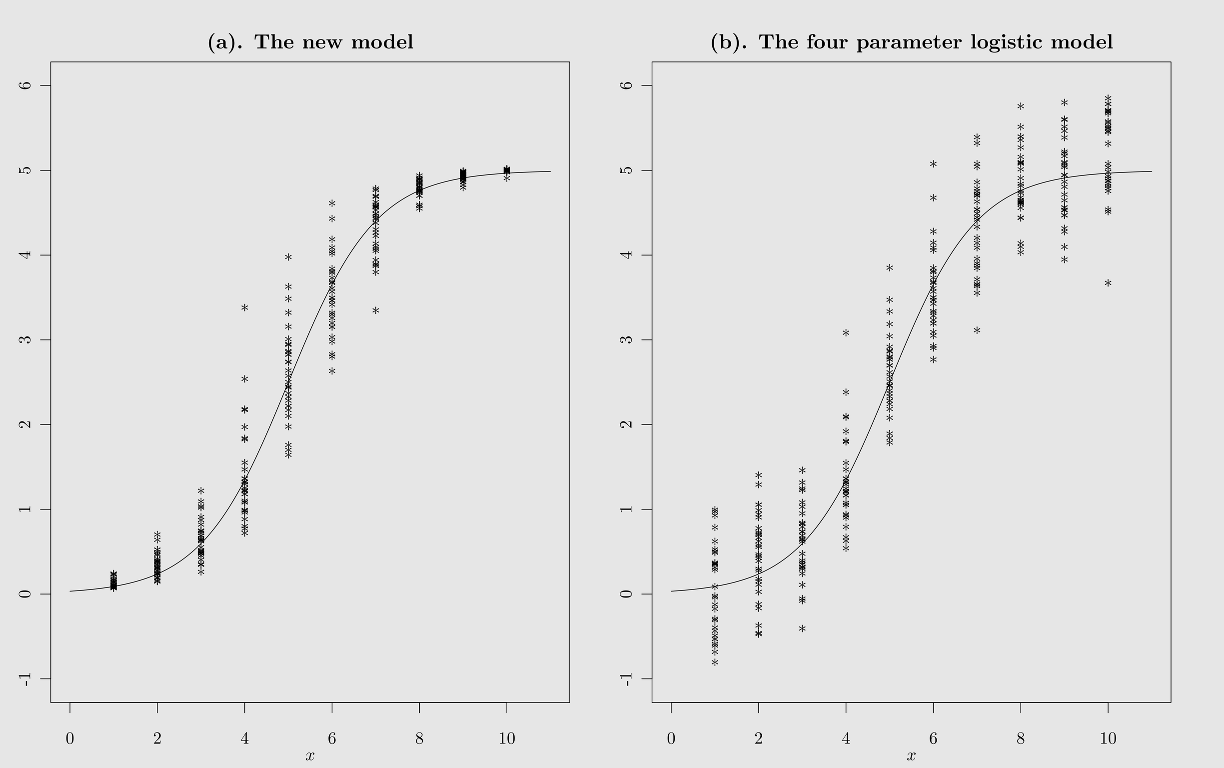


Figure: Simulated data from the bounded log-linear model and the 4 parameter logistic (4PL) model.

The information matrices

- For $\theta = (a, b, \sigma, A, B)^T$, the Fisher information matrix based on a single observation at x is

$$I(\theta, x) = \begin{bmatrix} \frac{1}{\sigma^2} & \frac{x}{\sigma^2} & 0 & \frac{-1-z_i d}{\sigma^2(B-A)} & \frac{-1-\frac{d}{z_i}}{\sigma^2(B-A)} \\ \frac{x}{\sigma^2} & \frac{x^2}{\sigma^2} & 0 & \frac{-1-z_i d}{\sigma^2(B-A)}x & \frac{-1-\frac{d}{z_i}}{\sigma^2(B-A)}x \\ 0 & 0 & \frac{2}{\sigma^2} & \frac{-2z_i d}{\sigma(B-A)} & \frac{2\frac{d}{z_i}}{\sigma(B-A)} \\ \frac{-1-z_i d}{\sigma^2(B-A)} & \frac{-1-z_i d}{\sigma^2(B-A)}x & \frac{-2z_i d}{\sigma(B-A)} & \frac{z_i^2 d^4}{(B-A)^2} + \frac{1+2z_i d+z_i^2 d^4}{\sigma^2(B-A)^2} & \frac{-1}{(B-A)^2} + \frac{2+z_i d+\frac{d}{z_i}}{\sigma^2(B-A)^2} \\ \frac{-1-\frac{d}{z_i}}{\sigma^2(B-A)} & \frac{-1-\frac{d}{z_i}}{\sigma^2(B-A)}x & \frac{2\frac{d}{z_i}}{\sigma(B-A)} & \frac{-1}{(B-A)^2} + \frac{2+z_i d+\frac{d}{z_i}}{\sigma^2(B-A)^2} & \frac{\frac{d^4}{z_i^2}}{(B-A)^2} + \frac{1+2\frac{d}{z_i}+\frac{d^4}{z_i^2}}{\sigma^2(B-A)^2} \end{bmatrix},$$

where $z_i = e^{a+bx}$ and $d = e^{\sigma^2/2}$.

- The average information matrix under a design $\xi = \begin{Bmatrix} x_1 & x_2 & \dots & x_K \\ w_1 & w_2 & \dots & w_K \end{Bmatrix}$ is

$$M(\xi, \theta) = \int_{\mathbb{X}} I(x, \theta) d\xi(x) = \sum_{i=1}^{K} w_i I(x_i, \theta)$$

Theorem (An upper bound)

For the model of interest with an unknown σ,

- *an optimal design that minimizes an information based criterion is supported at no more than* **5** *points;*
- *the optimal design is always supported at boundary points.*

Theorem (D-optimal design)

For the model of interest with known variance σ, there exists a constant $\zeta < 9$ such that if $(\sigma^2+1)e^{\sigma^2} > \zeta$ the **D***-optimal design is*

$$\xi_{2p}^* = \begin{Bmatrix} L & U \\ 0.5 & 0.5 \end{Bmatrix}$$

Numerical studies

- The sensitivity function

$$d(x; \xi, \theta) = \mathrm{tr}\{I(x, \theta) M(\xi, \theta)^{-1}\}.$$

- The D-efficiency of a design

$$\left\{\frac{|M(\xi, \theta)|}{|M(\xi^*, \theta)|}\right\}^{1/p}$$

- Relative MSE for a single parameter

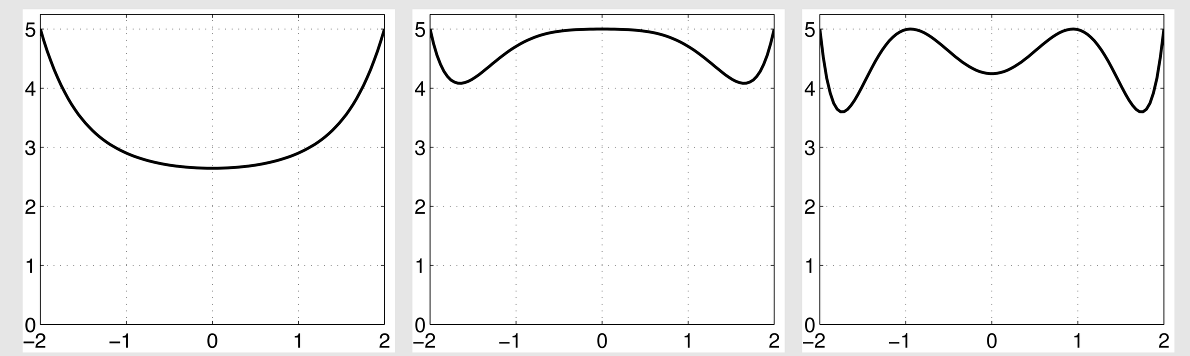
$$\mathrm{RMSE} = \frac{\mathrm{MSE}(\hat{\theta}_k | \xi_{2p}^*)}{\mathrm{MSE}(\hat{\theta}_k | \xi)} \times 100$$

Optimal designs (σ unknown)

$A = 0$, $B = 10$, $a = 0$, $b = 1$; $\mathbb{X} = [-2, 2]$

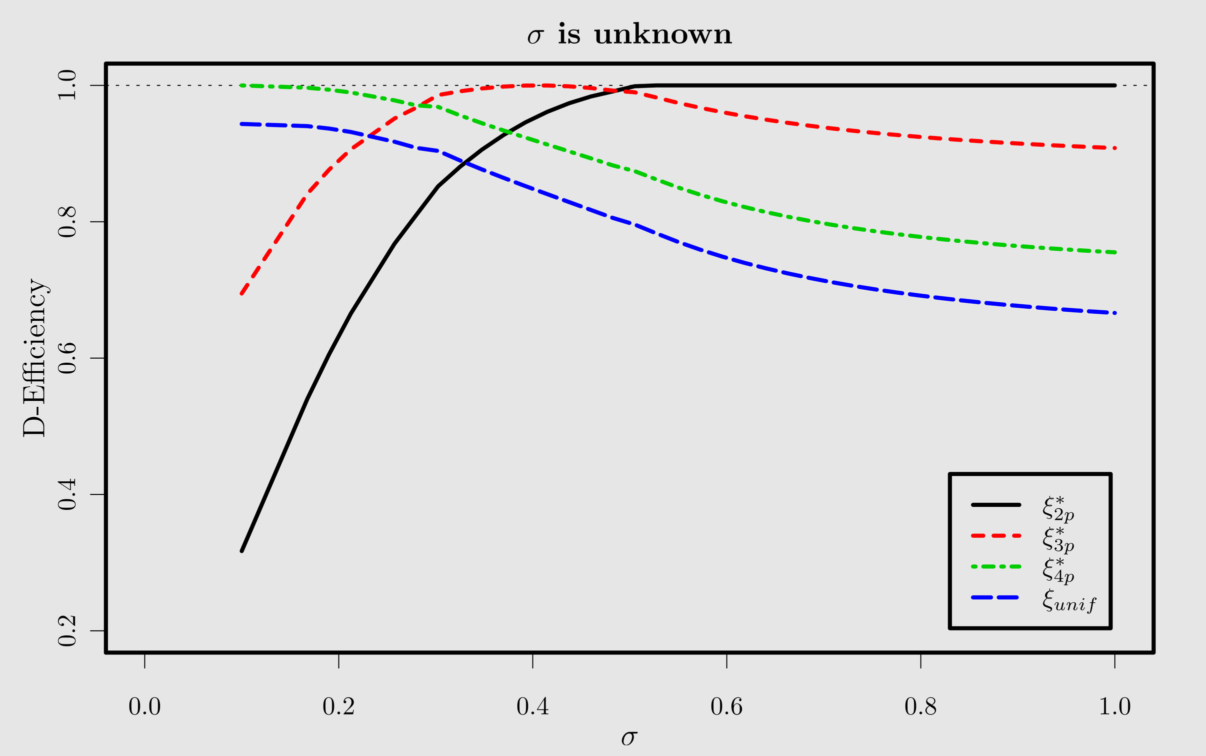
- $\sigma = 1.0$: $\xi_{2p}^* = \begin{Bmatrix} -2 & 2 \\ 0.5 & 0.5 \end{Bmatrix}$
- $\sigma = 0.4$: $\xi_{3p}^* = \begin{Bmatrix} -2 & 0 & 2 \\ 0.41 & 0.18 & 0.41 \end{Bmatrix}$
- $\sigma = 0.1$: $\xi_{4p}^* = \begin{Bmatrix} -2 & -0.94 & 0.94 & 2 \\ 0.26 & 0.24 & 0.24 & 0.26 \end{Bmatrix}$

Sensitivity function $d(x, \xi^*, \theta)$ (σ unknown)



(a) $\sigma = 1, \xi_{2p}^*$ (b) $\sigma = 0.4, \xi_{3p}^*$ (c) $\sigma = 0.1, \xi_{4p}^*$

D-efficiency



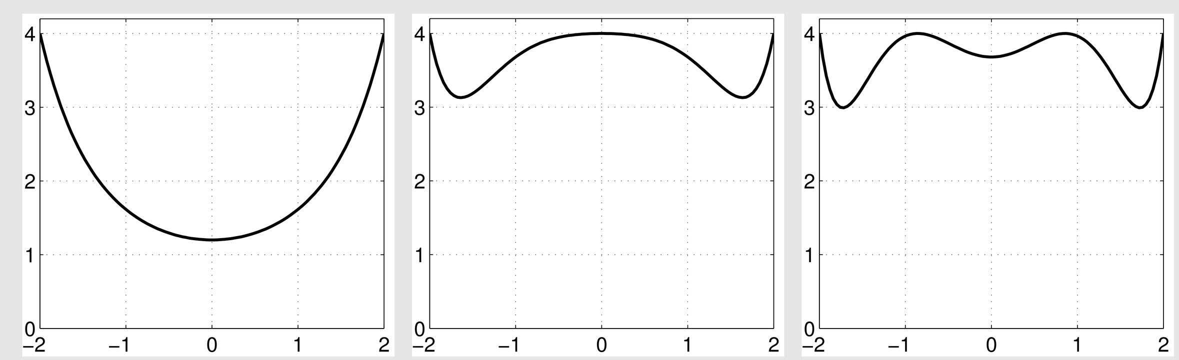
Design		a	b	σ	A	B
				$\sigma = 1.0$		
Uniform	$n = 20$	98.5	44.6	105.2	39.8	40.8
	$n = 40$	98.3	50.6	113.5	39.2	44.7
	$n = 80$	96.3	53.7	117.9	45.7	43.2
Random	$n = 20$	76.5	29.9	86.0	21.7	19.3
	$n = 40$	74.5	31.9	89.3	22.2	21.4
	$n = 80$	89.0	30.7	100.6	22.6	20.7
				$\sigma = 0.5$		
Uniform	$n = 20$	139.3	88.4	270.6	74.6	77.0
	$n = 40$	131.4	108.6	283.4	87.2	92.8
	$n = 80$	120.1	114.2	249.8	90.6	101.8
Random	$n = 20$	79.0	47.6	174.2	33.5	32.0
	$n = 40$	83.5	55.4	181.8	40.5	43.2
	$n = 80$	94.5	57.8	182.4	44.4	43.0

Optimal designs (σ known)

$A = 0$, $B = 10$, $a = 0$, $b = 1$; $\mathbb{X} = [-2, 2]$

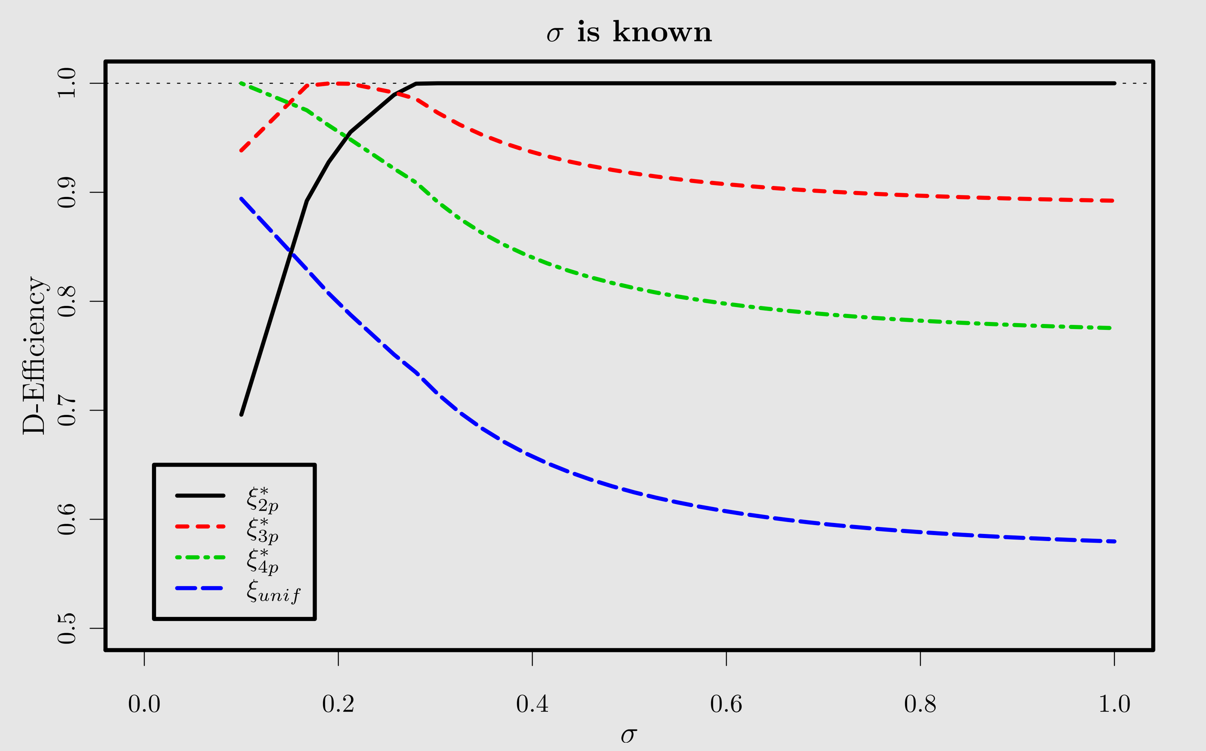
- $\sigma = 1.0$: $\xi_{2p}^* = \begin{Bmatrix} -2 & 2 \\ 0.5 & 0.5 \end{Bmatrix}$
- $\sigma = 0.2$: $\xi_{3p}^* = \begin{Bmatrix} -2 & 0 & 2 \\ 0.425 & 0.15 & 0.425 \end{Bmatrix}$
- $\sigma = 0.1$: $\xi_{4p}^* = \begin{Bmatrix} -2 & -0.86 & 0.86 & 2 \\ 0.33 & 0.17 & 0.17 & 0.33 \end{Bmatrix}$

Sensitivity function $d(x, \xi^*, \theta)$ (σ known)



(d) $\sigma = 1$, ξ_{2p}^* (e) $\sigma = 0.2$, ξ_{3p}^* (f) $\sigma = 0.1$, ξ_{4p}^*

D-efficiency



Design		a	b	A	B
			$\sigma = 1.0$		
Uniform	$n = 20$	96.5	40.6	35.3	35.3
	$n = 40$	98.6	45.2	33.7	37.3
	$n = 80$	96.3	48.5	40.7	38.6
Random	$n = 20$	74.2	28.5	19.6	17.6
	$n = 40$	75.4	31.2	20.8	19.7
	$n = 80$	90.3	30.9	21.9	21.1
			$\sigma = 0.5$		
Uniform	$n = 20$	120.9	42.4	47.4	44.0
	$n = 40$	129.0	49.0	46.2	49.1
	$n = 80$	118.4	53.6	50.8	53.0
Random	$n = 20$	75.0	32.0	21.9	19.3
	$n = 40$	81.6	33.5	24.5	23.4
	$n = 80$	94.6	34.9	27.4	26.4

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