

# On Sequential Designs Based on Maximum Likelihood Estimation

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## Introduction

- Nonlinear models: Information matrix and optimal design  $\xi^*$  depend on unknown parameters
- Asymptotic behavior of the maximum likelihood estimator and a sequential design  $\xi_n$  are investigated

## The Sequential Procedure

### Choose Initial Design

- Existence of the estimator depends on initial design!
- Design region  $\mathcal{X}$ : closed interval in  $\mathbb{R}^q$

### Observations: A Logistic Binary Response Model

- Sequence of observations: Modeled by binary random variables  $Y_1, \dots, Y_n, \dots$
- $n$ -th observation depends on the past through design point  $\mathbf{x}_n$  only:

$$P(Y_n = 1) = G(\mathbf{f}(\mathbf{x}_n)^\top \beta)$$

where  $\beta \in \mathbb{R} \times (\mathbb{R}^+)^q$  and  $\mathbf{f}(\mathbf{x}_n) = (1 \ x_{1n} \ \dots \ x_{qn})^\top$

### Estimate: Maximum Likelihood Estimator

- Maximum likelihood estimator based on  $n$  observations:  $\hat{\beta}_n$
- If the estimator exists:

$$\hat{\beta}_n = \hat{\beta}_{n-1} + \frac{1}{n} \underbrace{M(\xi_n, \hat{\beta}_{n-1})^{-1} \mathbf{f}(\mathbf{x}_n) (Y_n - G(\mathbf{f}(\mathbf{x}_n)^\top \hat{\beta}_{n-1}))}_{\text{Main component of recursion}} + H_n$$

- Main component of recursion:  $\leftarrow$   
Yields "mean differential equation" for proof of convergence

### Choose a new Design Point

- Information matrix: Fisher Information as in the i.i.d. case

$$M(\xi_n, \beta) = \frac{1}{n} \sum_{i=1}^n G(\mathbf{f}(\mathbf{x}_i)^\top \beta) (1 - G(\mathbf{f}(\mathbf{x}_i)^\top \beta)) \mathbf{f}(\mathbf{x}_i) \mathbf{f}(\mathbf{x}_i)^\top$$

- Criterion: D-optimality
- New design point: Maximize

$$G(\mathbf{f}(\mathbf{x})^\top \hat{\beta}_n) (1 - G(\mathbf{f}(\mathbf{x})^\top \hat{\beta}_n)) \mathbf{f}(\mathbf{x})^\top M(\xi_n, \hat{\beta}_n)^{-1} \mathbf{f}(\mathbf{x})$$

## Convergence

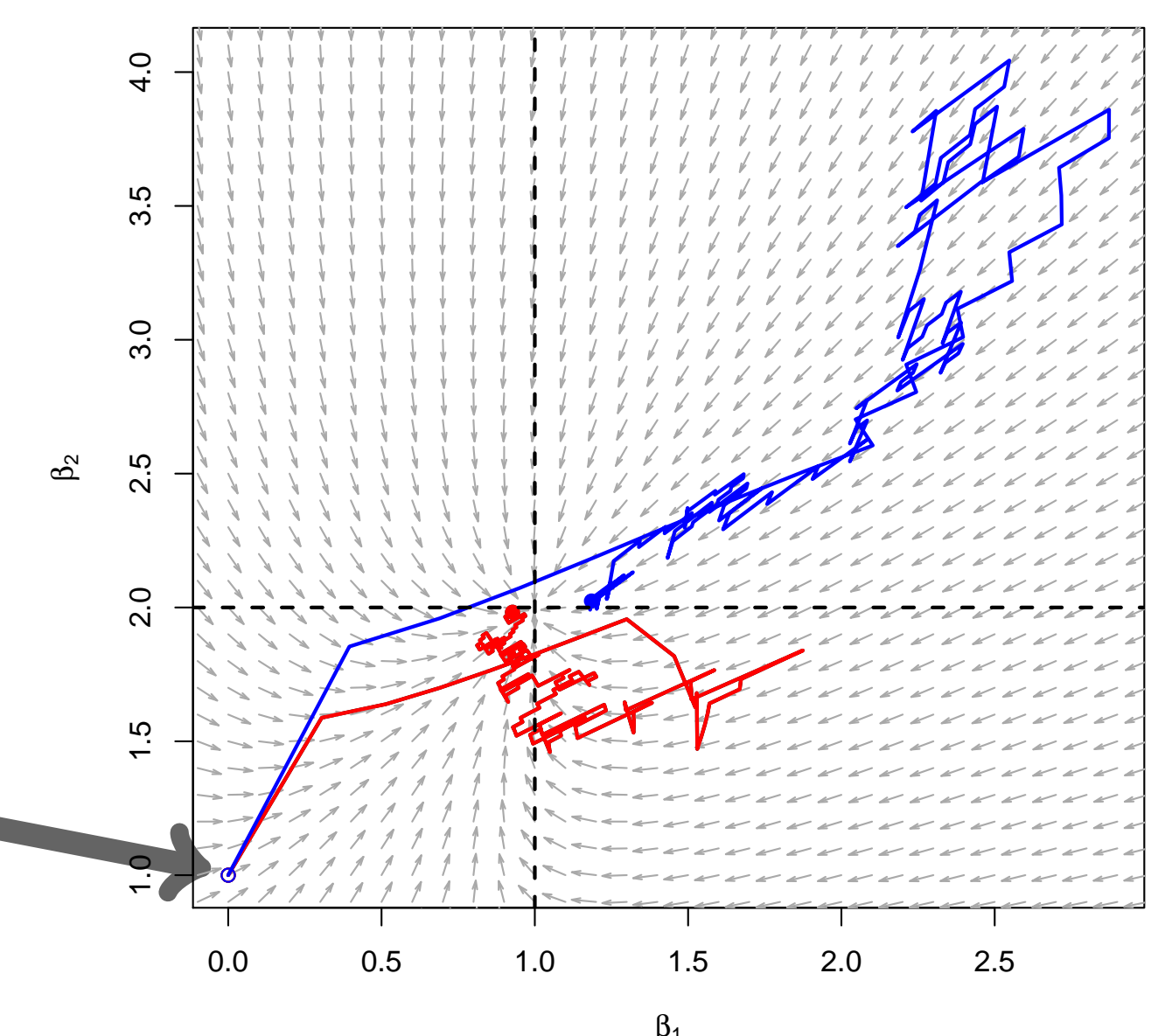
- **Estimator:**  $\hat{\beta}_n \rightarrow \beta$  a.s.
- **Design:**  $M(\xi_n, \hat{\beta}_n) \rightarrow M(\xi^*, \beta)$

## Simulations

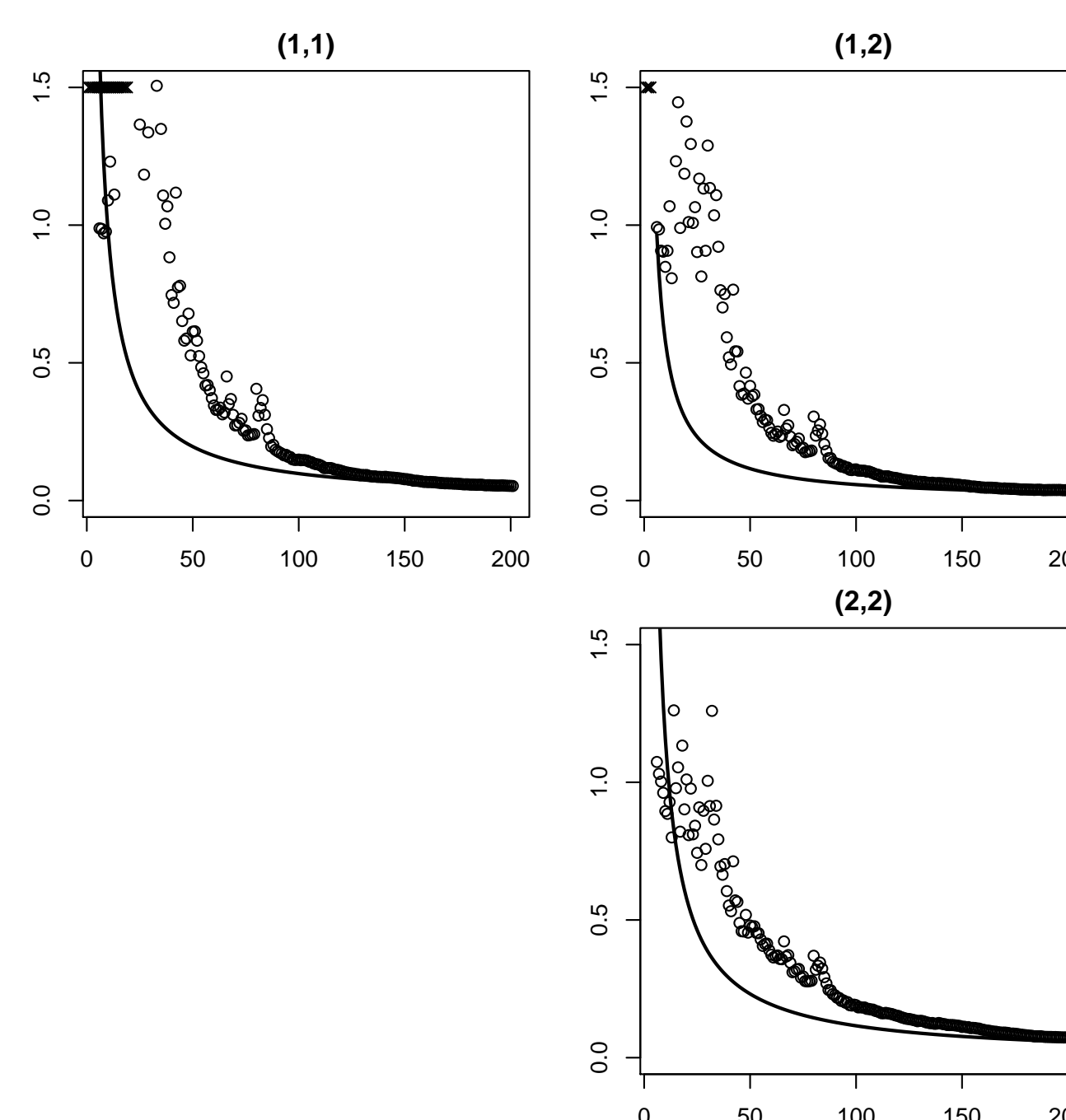
- True parameter:  $\beta = (1 \ 2)^\top$
- Design region:  $[-10, 10]$
- Number of runs: 500
- Initial design:  $0, \pm 1, \pm 5$

### Trajectories

- Solid red/blue: Simulated paths
- Dashed lines: True parameter
- Grey arrows: Directional field of the "mean differential equation"
- Initial parameter value  $\rightarrow$



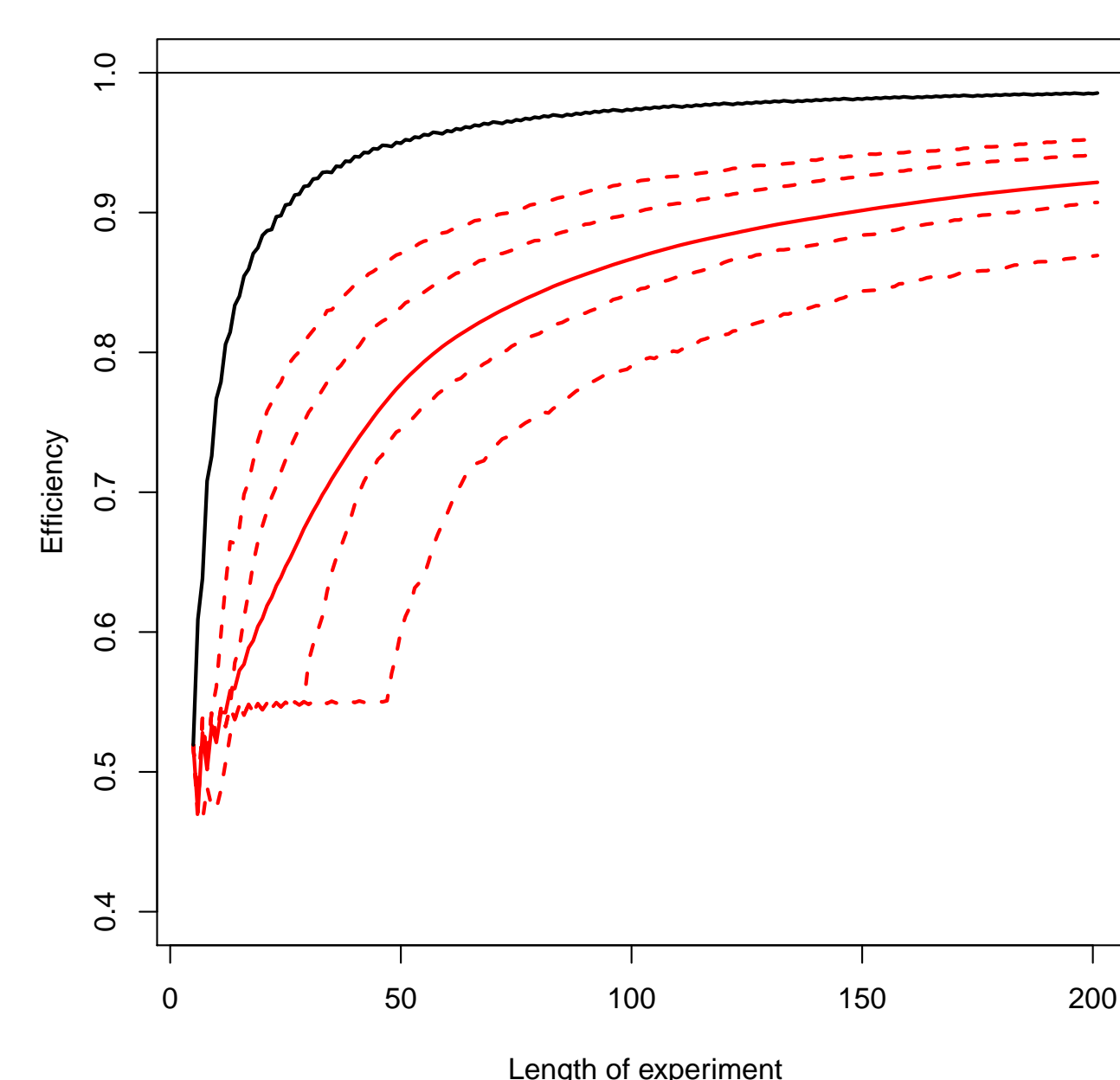
### Mean squared error



- Components of simulated MSE-matrix and asymptotic variance
- Circles: Simulated
- Solid line:  $\frac{1}{n} M(\xi^*, \beta)^{-1}$

### Efficiency

- w.r.t. D-optimal design: balanced, support at  $-1.27$  and  $0.27$



- Solid red: Mean efficiency
- Dashed red: 0.05, 0.1, 0.9, 0.95 quantiles
- Solid black: Wynn-algorithm for known true parameter

## Bibliography

- H.P. Wynn: The sequential generation of D-optimum experimental designs. Ann. Math. Statist., 41 (1970) 1655-1664.  
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H.J. Kushner and G.G. Yin: Stochastic approximation and recursive algorithms and applications. 2nd Edition. Springer, 2003