# Efficient Minimax Strategies for Online Prediction

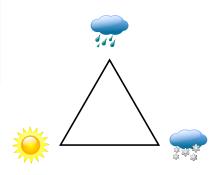
#### Peter Bartlett

Computer Science and Statistics University of California at Berkeley

Mathematical Sciences Queensland University of Technology

Joint work with Fares Hedayati, Wouter Koolen, Alan Malek, Eiji Takimoto, Manfred Warmuth.

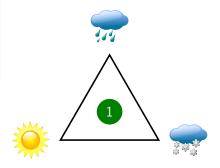
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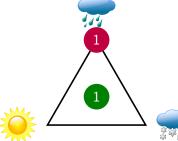
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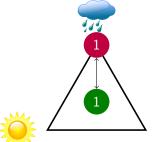




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$$\ell(a_t, y_t) = ||a_t - y_t||^2.$$







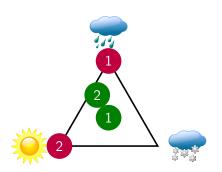
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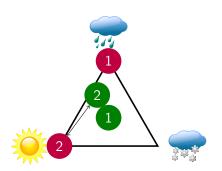
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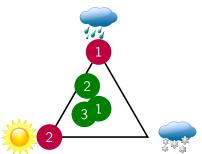
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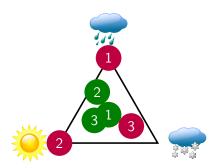
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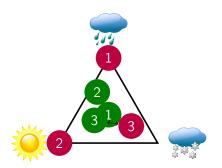
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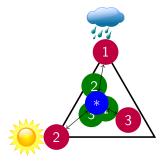
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Minimize regret:

$$\sum_{t=1}^{T} \ell(a_t, y_t) - \inf_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell(a, y_t).$$





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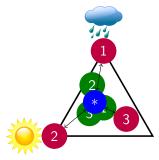
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$$\sum_{t=1}^{T} \ell(a_t, y_t) - \inf_{a \in \mathcal{A}} \sum_{t=1}^{T} \ell(a, y_t)$$

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# The value of the game: Minimax Regret

$$V_T(\mathcal{Y}, \mathcal{A}) = \inf_{a_1 \in \mathcal{A}} \sup_{y_1 \in \mathcal{Y}} \cdots \inf_{a_T \in \mathcal{A}} \sup_{y_T \in \mathcal{Y}} \left( \sum_{t=1}^T \ell(a_t, y_t) - \inf_{a \in \mathcal{A}} \sum_{t=1}^T \ell(a, y_t) \right)$$

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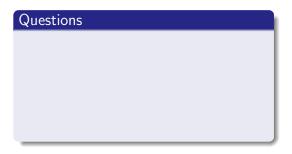
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#### Minimax Optimal Strategy:

$$\begin{split} S^* : & \bigcup_{t=0}^T \mathcal{Y}^t \to \mathcal{A}. \\ V_T(\mathcal{Y}, \mathcal{A}) &= \inf_{\mathbf{S}} \sup_{y_1^T \in \mathcal{Y}^T} \left( \sum_{t=1}^T \ell\left(\mathbf{S}\left(y_1^{t-1}\right), y_t\right) - \inf_{a \in \mathcal{A}} \sum_{t=1}^T \ell(a, y_t) \right) \\ &= \sup_{y_1^T \in \mathcal{Y}^T} \left( \sum_{t=1}^T \ell\left(\mathbf{S}^*\left(y_1^{t-1}\right), y_t\right) - \inf_{a \in \mathcal{A}} \sum_{t=1}^T \ell(a, y_t) \right). \end{split}$$



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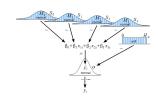
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$$a \in \{p_{\theta} : \theta \in \Theta\}.$$







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#### Efficient minimax optimal strategies

When is V a simple function of (statistics of) the history  $y_1, \ldots, y_t$ ?

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- Computation difficult in general. Efficient special cases:
  - Multinomials

[Kontkanen, Myllymäki, 2005]

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- When are simpler strategies optimal?
  - Sequential NML.
  - Bayesian prediction.



Prediction Game	Efficient optimal strategy?
Log loss	some cases ✓
Absolute loss, binary	

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$$\mathcal{Y}=\{0,1\}$$
,  $\mathcal{A}=[0,1]$ ,  $\ell(a,y)=|a-y|$ . (Also  $\mathcal{C}\subset static$  experts.)

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[Takimoto, Warmuth, 2000]

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This talk:

•  $\mathcal{Y} = \text{compact set}$ ,  $\mathcal{A} \supseteq \text{co}(\mathcal{Y})$ .

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#### Outline

- Computing minimax optimal strategies.
- Prediction games with simple minimax optimal strategies.
- Part 1: Log loss.
  - Normalized maximum likelihood.
  - SNML: predicting like there's no tomorrow.
  - Bayesian strategies.
  - Optimality = exchangeability.
- Part 2: Euclidean loss.
- Part 3: Fixed design linear regression.

Log loss  $\ell(\hat{p}, y) = -\log \hat{p}(y).$ 

#### Comparison class

Parametric family of densities:  $\mathcal{C} = \{p_{\theta} : \theta \in \Theta\}$ , where  $p_{\theta} : \mathcal{Y} \to \mathbb{R}^+$  is a parameterized probability density with respect to a reference measure  $\lambda$  on  $\mathcal{Y}$ .

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$$R(y_1^T, \hat{p}) =$$

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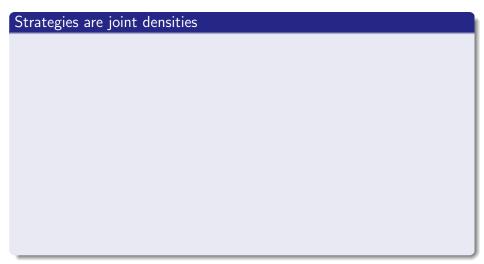
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### Strategies are joint densities

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Here, 
$$p_{\theta}(y_1^T) = \prod_{t=1}^T p_{\theta}(y_t)$$
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Many interpretations of prediction with log loss

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• Sequential probability prediction.

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Long history in several communities.

[Kelly, 1956], [Solomonoff, 1964], [Kolmogorov, 1965], [Cover, 1974], [Rissanen, 1976, 1987, 1996], [Shtarkov, 1987], [Feder, Merhav and Gutman, 1992], [Freund, 1996], [Xie and Barron, 2000], [Cesa-Bianchi and Lugosi, 2001, 2006], [Grünwald, 2007]

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NML is optimal [Shtarkov, 1987]

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**1** NML equalizes regret: for any sequence  $y_1^T$ , regret is

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Any strategy that does not equalize regret has strictly worse maximum regret.

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- When is a computationally cheaper strategy optimal?

$$\begin{aligned} p_{nml}^{(T)}(y_1 \cdots y_T) &\propto \sup_{\theta \in \Theta} p_{\theta}(y_1^T) \\ p_{nml}^{(T)}(y_t | y_1 \cdots y_{t-1}) &= \frac{\int_{\mathcal{Y}^{T-t}} \sup_{\theta \in \Theta} p_{\theta}(y_1^t z_{t+1}^T) \, d\lambda^{T-t}(z_{t+1}^T)}{\int_{\mathcal{Y}^{T-t+1}} \sup_{\theta \in \Theta} p_{\theta}(y_1^{t-1} z_{t}^T) \, d\lambda^{T-t+1}(z_{t}^T)} \end{aligned}$$

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#### Outline

- Computing minimax optimal strategies.
- Prediction games with simple minimax optimal strategies.
- Part 1: Log loss.
  - Normalized maximum likelihood.
  - SNML: predicting like there's no tomorrow.
  - Bayesian strategies.
  - Optimality = exchangeability.
- Part 2: Euclidean loss.
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Sequential Normalized Maximum Likelihood

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Pretend that this is the last prediction we'll ever make.

### Sequential Normalized Maximum Likelihood

$$p_{snml}(y_t|y_1^{t-1}) := p_{nml}^{(t)}(y_t|y_1^{t-1})$$

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$$p_{snml}(y_t|y_1^{t-1}) := p_{nml}^{\textcolor{red}{(t)}}(y_t|y_1^{t-1}) \propto \sup_{\theta \in \Theta} p_{\theta}(y_1^t)$$

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- Pretend that this is the last prediction we'll ever make.
- Simpler conditional calculation.
- Known to have asymptotically optimal regret.

[Takimoto and Warmuth, 2000], [Roos and Rissanen, 2008], [Kotłowski and Grünwald, 2011]

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#### Theorem

Sequential NML is optimal iff  $p_{snml}$  is exchangeable.

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•  $p_{snml}$  is exchangeable means  $p_{snml}(y_1, y_2, y_3, y_4) = p_{snml}(y_1, y_2, y_4, y_3) = \cdots = p_{snml}(y_4, y_3, y_2, y_1)$ .

#### Sequential Normalized Maximum Likelihood

$$p_{\mathit{snml}}\big(y_t|y_1^{t-1}\big) = p_{\mathit{nml}}^{(t)}\big(y_t|y_1^{t-1}\big) \propto \sup_{\theta \in \Theta} p_{\theta}\big(y_1^t\big)$$

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Proof idea:

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- $(\Rightarrow) p_{nml}^{(T)}(y_1^T)$  is permutation-invariant.

#### Outline

- Computing minimax optimal strategies.
- Prediction games with simple minimax optimal strategies.
- Part 1: Log loss.
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  - SNML: predicting like there's no tomorrow.
  - Bayesian strategies.
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- Jeffreys prior:

$$\pi(\theta) \propto \sqrt{|I(\theta)|},$$

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Attractive properties (e.g., invariant to parameterization).

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- Attractive properties (e.g., invariant to parameterization).
- Asymptotically optimal regret for exponential families.



### Optimality

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#### Optimality

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- If any Bayesian strategy is optimal, it uses Jeffreys prior.

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- Why?

#### Optimality

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- Why? If NML=SNML, then we can consider long time horizons, so the asymptotics emerge.

#### Optimality

For regular  $p_{\theta}$  (asymptotically normal maximum likelihood estimator, Fisher information well-behaved, integrals exist), the following are equivalent:

- NML = SNML.
- 2 p<sub>snml</sub> exchangeable.
- NML = Bayesian.
- NML = Bayesian with Jeffreys prior.
- SNML = Bayesian.
- SNML = Bayesian with Jeffreys prior.

Jeffreys prior is the only candidate.

- If we can ignore the time horizon and be optimal, that's the same as Bayesian prediction with Jeffreys prior.
- If any Bayesian strategy is optimal, it uses Jeffreys prior.
- Why? If NML=SNML, then we can consider long time horizons, so the asymptotics emerge. Asymptotic normality of the MLE implies

# Online density estimation with log loss



## Online density estimation with log loss

#### Extensions

[B., Grünwald, Harremoës, Hedayati, Kotłowski, 2013]

• One-dimensional exponential families:

$$p_{\theta}(y) = h(y) \exp(\theta y - A(\theta)).$$

#### Extensions

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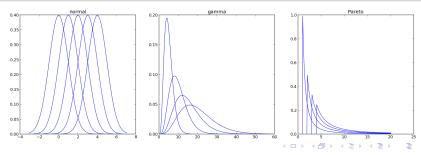
ullet  $p_{SNML}$  is exchangeable (i.e., SNML optimal, Bayesian optimal)  $\Leftrightarrow$ 

#### **Extensions**

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- $p_{SNML}$  is exchangeable (i.e., SNML optimal, Bayesian optimal)  $\Leftrightarrow$ 
  - **1** Gaussian distributions with fixed variance  $\sigma^2 > 0$ ,

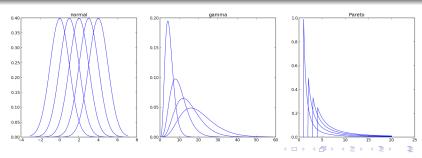


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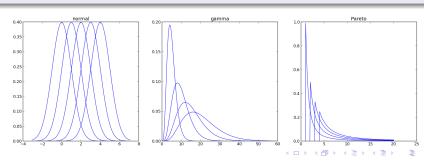


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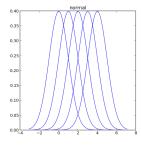


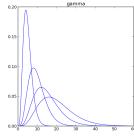
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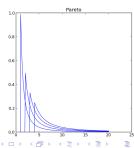
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  - **1** Gaussian distributions with fixed variance  $\sigma^2 > 0$ ,
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  - Tweedie exponential family of order 3/2,
  - Or smooth transformations.







### Outline

- Computing minimax optimal strategies.
- Prediction games with simple minimax optimal strategies.
- Part 1: Log loss.
- Part 2: Euclidean loss.
  - The role of the smallest ball.
  - The simplex and the ball.
  - Sub-game optimal strategies on ellipsoids.
- Part 3: Fixed design linear regression.

$$\ell(\hat{y}, y) = \frac{1}{2} \|\hat{y} - y\|^2.$$

#### Constraints

Adversary chooses  $y_n \in \mathcal{Y}$ , where  $\mathcal{Y} \subseteq \mathbb{R}^d$ .

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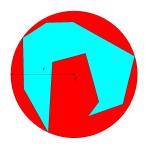
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#### Constraints

Adversary chooses  $y_n \in \mathcal{Y}$ , where  $\mathcal{Y} \subseteq \mathbb{R}^d$ . Strategy chooses  $\hat{y}_n \in \mathbb{R}^d$ .

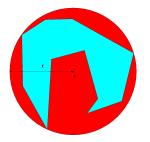
$$\ell(\hat{y}, y) = \frac{1}{2} \|\hat{y} - y\|^2.$$

$$\mathsf{Regret} \ = \sum_{t=1}^n \ell(\hat{y}_t, y_t) - \inf_{a \in \mathbb{R}^d} \sum_{t=1}^n \ell(a, y_t).$$



### The smallest ball: $B_{\mathcal{Y}}$

The smallest ball containing  $\mathcal{Y}$  is  $B_{\mathcal{Y}} = \{ y \in \mathbb{R}^d : \|y - c\| \le r \}$ , with  $c = \arg\min_c \max_{y \in \mathcal{Y}} \|y - c\|$ ,  $r = \min_c \max_{y \in \mathcal{Y}} \|y - c\|$ .



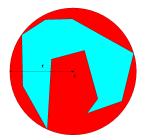
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For closed, bounded  $\mathcal{Y} \subset \mathbb{R}^d$ :

Minimax strategy is 
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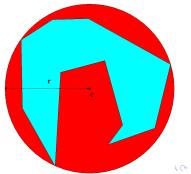
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The general case: closed, bounded  $\mathcal{Y} \subset \mathbb{R}^d$ 

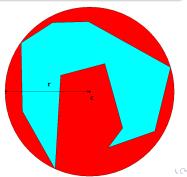
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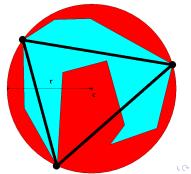


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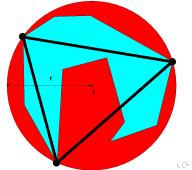
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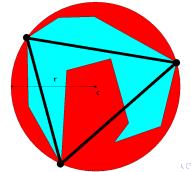
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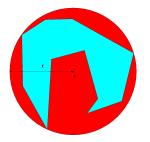
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$$\mathcal{Y} \subseteq B_{\mathcal{Y}}$$
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### Main result: the role of the smallest ball



### The smallest ball: $B_{\mathcal{Y}}$

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#### Main Theorem

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## Minimax regret

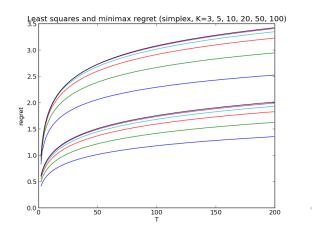
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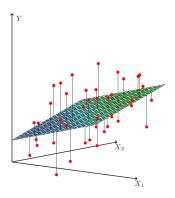
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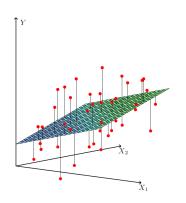
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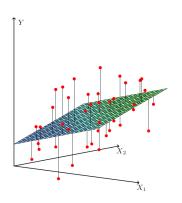
#### Outline

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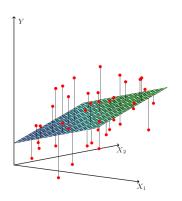






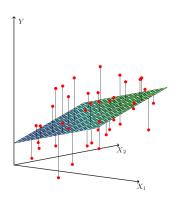
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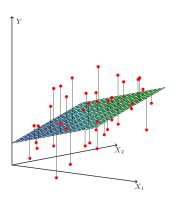
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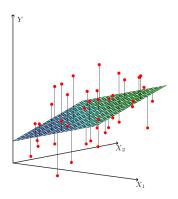
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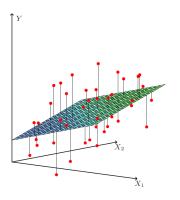


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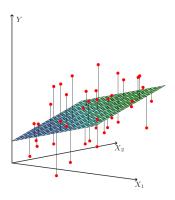
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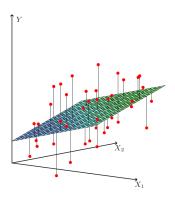
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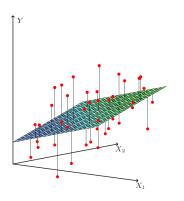
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  - SNML and Bayesian strategies: optimality = exchangeability.
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  - The role of the smallest ball.
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