Efficient Minimax Strategies for Online Prediction

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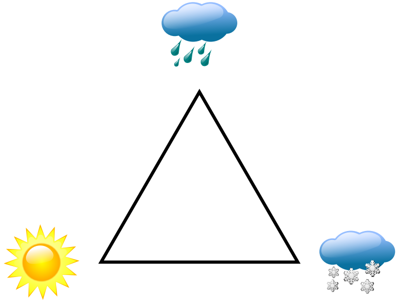
Joint work with Fares Hedayati, Wouter Koolen and Alan Malek

Online Prediction

A repeated game:

At round t:



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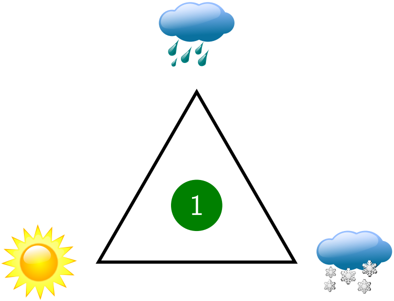

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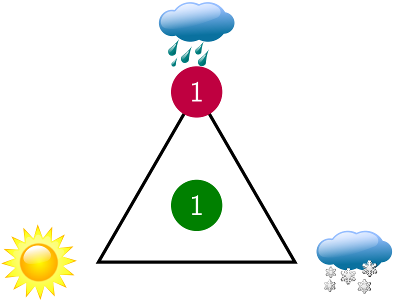

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At round t:

1. Player chooses prediction $a_t \in \mathcal{A}$.
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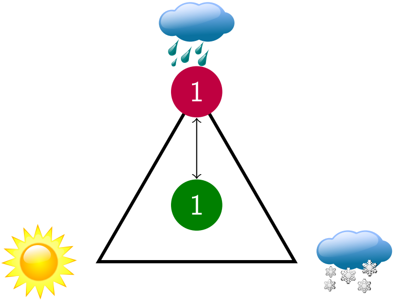
$$\ell(a_t, y_t) = \|a_t - y_t\|^2.$$



Brier loss

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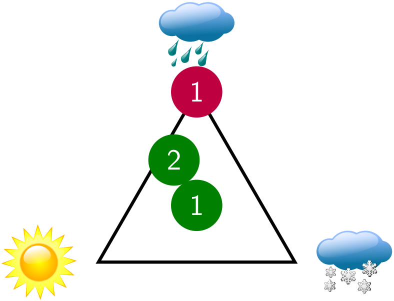

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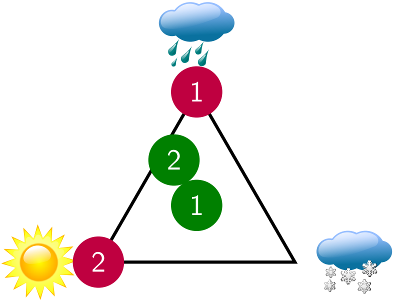

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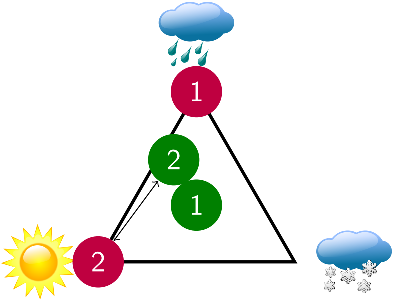

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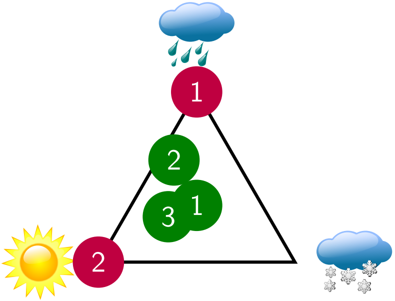

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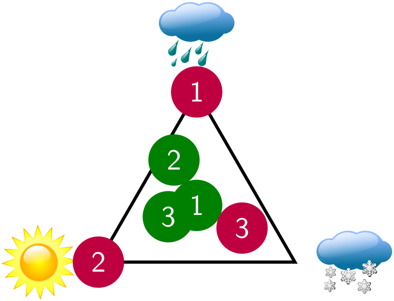

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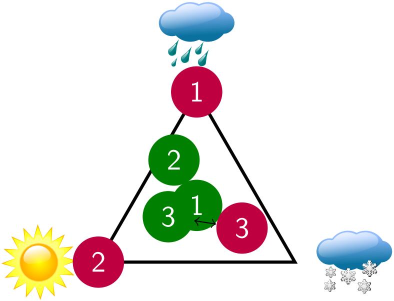

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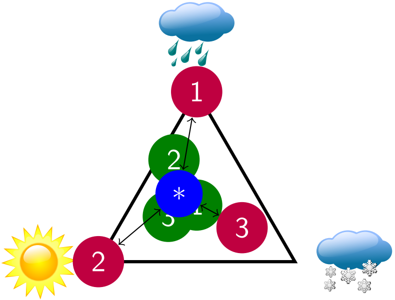
Player's aim:

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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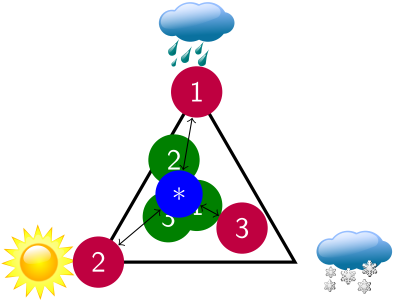

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- This talk: Minimax optimal strategies.

Online Prediction Games

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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Strategy:

$$S : \bigcup_{t=0}^{T} \mathcal{Y}^t \to \mathcal{A}.$$

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Minimax Optimal Strategy:

$$S^* : \bigcup_{t=0}^{T} \mathcal{Y}^t \to \mathcal{A}.$$

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

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1. $\frac{1}{2}\|a - y\|_2^2$,
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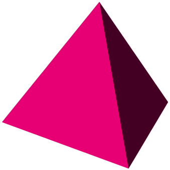

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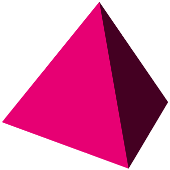

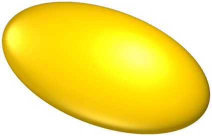

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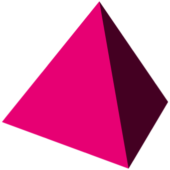

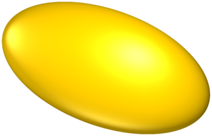

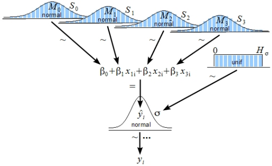

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Outline

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Computing minimax optimal strategies

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$$V_T(\mathcal{Y}, \mathcal{A}) = V().$$

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Efficient minimax optimal strategies

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

Games with simple minimax optimal strategies

Prediction Game	**Efficient** optimal strategy?

Games with simple minimax optimal strategies

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Log loss	

- Log loss: $\ell(\hat{p}, y) = -\log \hat{p}(y)$. ($\hat{p}$ a density; $\mathcal{C}$ a probability model.)

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- Minimax optimal strategy: normalized maximum likelihood. [Shtarkov, 1987]
- Computation difficult in general. Efficient special cases:
  - Multinomials [Kontkanen, Myllymäki, 2005]

Games with simple minimax optimal strategies

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This talk:

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

Games with simple minimax optimal strategies

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Absolute loss, binary	

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

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- $\mathcal{Y} = \{0,1\}$, $\mathcal{A} = [0,1]$, $\ell(a,y) = |a - y|$. (Also $\mathcal{C} \subset$ *static* experts.)
- Minimax optimal strategy: compare expected minimal cumulative loss for random futures.

[Cover, 1967], [Cesa-Bianchi, Freund, Haussler, Helmbold, Schapire, Warmuth, 1997], [Cesa-Bianchi, Shamir, 2011], [Koolen, 2011], [Gravin, Peres, Sivan, 2014]

Games with simple minimax optimal strategies

Prediction Game	**Efficient** optimal strategy?
Log loss	some cases ✓
Absolute loss, binary	can be approximated

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Experts, bounded loss	

- $\mathcal{Y} = \Delta$, linear loss, best cumulative loss is bounded.

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Prediction Game	**Efficient** optimal strategy?
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Quadratic loss	

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

Games with simple minimax optimal strategies

Prediction Game	**Efficient** optimal strategy?
Log loss	some cases ✓
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[Takimoto, Warmuth, 2000]

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This talk:

- $\ell(a, y) = \frac{1}{2}(a - y)^\top W(a - y)$, for $W \succeq 0$.
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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.
    - The role of the smallest ball.
    - The simplex and the ball.
    - Sub-game optimal strategies on ellipsoids.

Online density estimation with log loss

Online density estimation with log loss

Log loss

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

Online density estimation with log loss

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 λ on $\mathcal{Y}$.

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

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$$R(y_1^n, \hat{p}) = \sum_{t=1}^{n} \ell(\hat{p}_t, y_t) -$$

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$$R(y_1^n, \hat{p}) = \sum_{t=1}^{n} \ell(\hat{p}_t, y_t) - \inf_{p \in \mathcal{C}} \sum_{t=1}^{n} \ell(p, y_t).$$

Online density estimation with log loss

Strategies are joint densities

Online density estimation with log loss

Strategies are joint densities

- A strategy $\hat{p}$ is a mapping from histories $y_1^t = (y_1, \ldots, y_t)$ to densities $\hat{p}(\cdot|y_1^t)$ on $\mathcal{Y}$.

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$$\begin{aligned} R(y_1^n, \hat{p}) &= \sum_{t=1}^{n} \ell(\hat{p}_t, y_t) - \inf_{p \in \mathcal{C}} \sum_{t=1}^{n} \ell(p, y_t) \\ &= \sup_{\theta \in \Theta} \log p_\theta(y_1^n) - \log \hat{p}(y_1^n). \end{aligned}$$

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Here, $p_\theta(y_1^n) = \prod_{t=1}^n p_\theta(y_t)$.

Online density estimation with log loss

Many interpretations of prediction with log loss

Online density estimation with log loss

Many interpretations of prediction with log loss

- Sequential probability prediction.

Online density estimation with log loss

Many interpretations of prediction with log loss

- Sequential probability prediction.
- Sequential lossless data compression.

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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]

Normalized maximum likelihood

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NML is optimal [Shtarkov, 1987]

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1. NML equalizes regret: for any sequence y_1^n, regret is

$$\log \int_{Y^n} \sup_{\theta \in \Theta} p_\theta(z^n)\, d\lambda^n(z^n).$$

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- When is a computationally cheaper strategy optimal?

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- When is a computationally cheaper strategy optimal?
  - Horizon-independent NML?
  - Bayesian prediction?

Outline

- Computing minimax optimal strategies.
- Prediction games with simple minimax optimal strategies.
- Part 1: Log loss.
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  - Bayesian strategies.
  - Optimality = exchangeability.
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Predicting like there's no tomorrow: Sequential NML

Sequential Normalized Maximum Likelihood

Predicting like there's no tomorrow: Sequential NML

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

Predicting like there's no tomorrow: Sequential NML

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

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

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

Predicting like there's no tomorrow: Sequential NML

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Proof idea:

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- SNML's regret doesn't depend on last observation.

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- $(\Leftarrow)$ Exchangeability implies regret is independent of observations. Hence SNML is an equalizer: same as NML.

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

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Bayesian strategies

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For prior π on Θ:

$$p_\pi(x_1^t) = \int_{\theta \in \Theta} p_\theta(x_1^t)\, d\pi(\theta)$$

Bayesian strategies

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- Sequential update to prior.

Bayesian strategies

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

Bayesian strategies

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- Jeffreys prior:

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

Sequential NML and Bayesian strategies

Optimality

Sequential NML and Bayesian strategies

Optimality

For regular p_θ (asymptotically normal maximum likelihood estimator, Fisher information well-behaved, integrals exist), the following are equivalent:

Sequential NML and Bayesian strategies

Optimality

For regular p_θ (asymptotically normal maximum likelihood estimator, Fisher information well-behaved, integrals exist), the following are equivalent:

1. NML = SNML.
2. p_{snml} exchangeable.

Sequential NML and Bayesian strategies

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Sequential NML and Bayesian strategies

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5. SNML $=$ Bayesian.

Sequential NML and Bayesian strategies

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5. SNML = Bayesian.
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Sequential NML and Bayesian strategies

Optimality

For regular p_θ (asymptotically normal maximum likelihood estimator, Fisher information well-behaved, integrals exist), the following are equivalent:

1. NML = SNML.
2. p_{snml} exchangeable.
3. NML = Bayesian.
4. NML = Bayesian with Jeffreys prior.
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Online density estimation with log loss

Extensions

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

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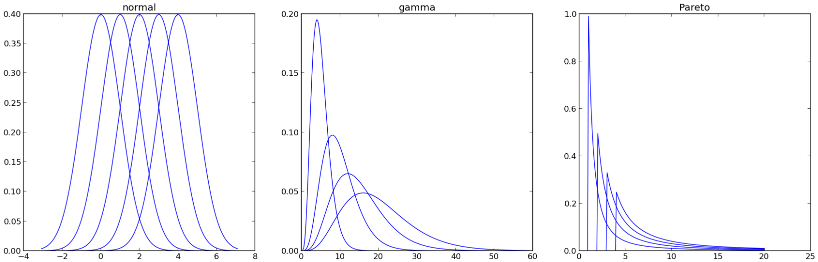

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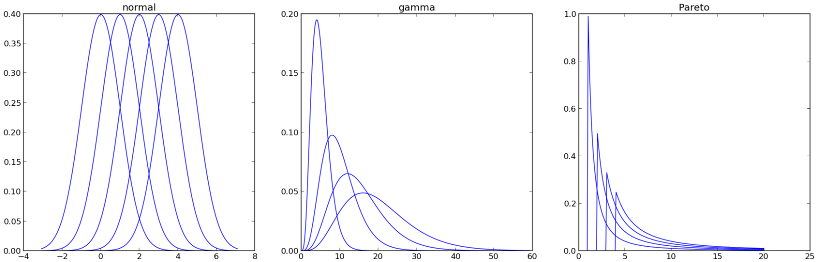

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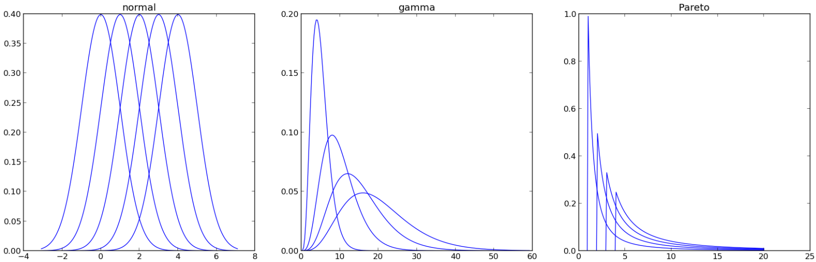

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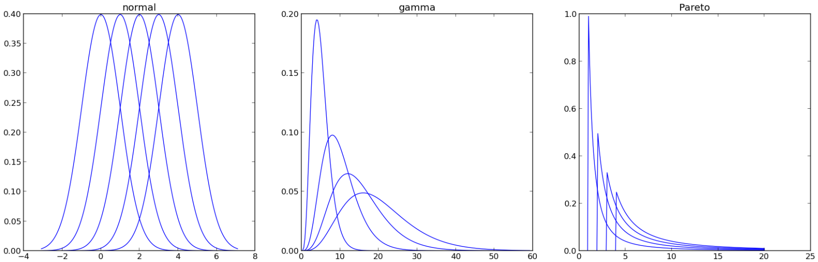
  4. Or smooth transformations
     (Pareto, Laplace, Rayleigh, Lévy, Nakagami)



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.**
  - The role of the smallest ball.
  - The simplex and the ball.
  - Sub-game optimal strategies on ellipsoids.

Mahalanobis loss and squared Euclidean loss

The value of the game: minimax regret

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

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Mahalanobis loss $\rightarrow$ quadratic loss

Since $(a - y)^\top W (a - y) = \left\| W^{1/2}(a - y) \right\|^2$, we can work with $\ell(a, y) = \frac{1}{2}\|a - y\|^2$ and $W^{1/2}\mathcal{Y}$:

$$V_T(\mathcal{Y}, \ell_W) = V_T(W^{1/2}\mathcal{Y}, \ell).$$

Main result: the role of the smallest ball

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

Define the 'minimum radius' function:
$J_{\mathcal{Y}}(c) = \max_{y \in \mathcal{Y}} \|y - c\|$,
so the smallest ball containing $\mathcal{Y}$ is
$B_{\mathcal{Y}} = \{y \in \mathbb{R}^d : \|y - c\| \leq r\}$,
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Minimax strategy is $a^*_{n+1} = n\alpha_{n+1} \frac{1}{n} \sum_{t=1}^{n} y_t + (1 - n\alpha_{n+1})c$.

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Optimal regret is $V(\mathcal{Y}) = \frac{r^2}{2} \sum_{n=1}^{T} \alpha_n$.

Online prediction with quadratic loss

The simplex case

Consider a set of $d+1$ affinely independent points in $\mathbb{R}^d$, all lying on the surface of the smallest ball.

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Value-to-go: quadratic in state

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Online prediction with quadratic loss on the simplex

Proof idea

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Use sufficient statistics: $s_n = \sum_{t=1}^n (y_t - c)$, $\sigma_n^2 = \sum_{t=1}^n \|y_t - c\|^2$.

Value-to-go: quadratic in state

$$\frac{1}{2}\left(\alpha_n \|s_n\|^2 - \sigma_n^2 + r^2 \sum_{t=n+1}^{T} \alpha_t\right).$$

Minimax strategy: affine in state

$$a_{n+1}^* - c = n\alpha_{n+1}\frac{s_n}{n}.$$

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Proof idea

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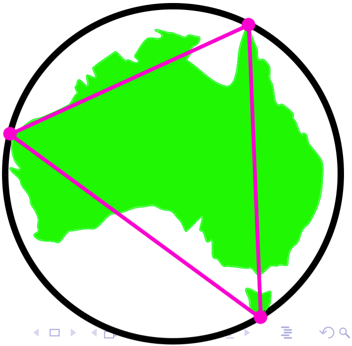
$\mathcal{Y} \supseteq S$, so

$$V(\mathcal{Y}) \geq V(S) = \frac{r^2}{2} \sum_{i=1}^{T} \alpha_i.$$



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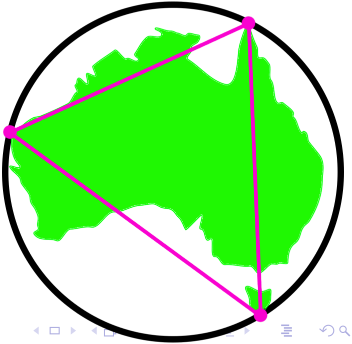

Main result: the role of the smallest ball

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

Define the 'minimum radius' function:
$J_{\mathcal{Y}}(c) = \max_{y \in \mathcal{Y}} \|y - c\|$,
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Main Theorem

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

Minimax strategy is $a^*_{n+1} = n\alpha_{n+1} \frac{1}{n} \sum_{t=1}^{n} y_t + (1 - n\alpha_{n+1})c$.

Optimal regret is $V(\mathcal{Y}) = \frac{r^2}{2} \sum_{n=1}^{T} \alpha_n$.

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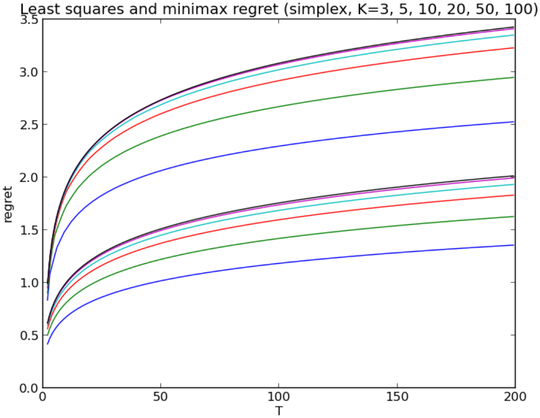

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- For $\mathcal{Y}$ an *ellipsoid*, a more complex strategy has this property...

Online prediction with quadratic loss on an ellipsoid

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Value-to-go: quadratic in state

$$V(y_1, \ldots, y_n) = \frac{1}{2} \left(s_n^\top A_n s_n - \sigma_n^2 + \lambda_{\max}(W^{-1}) \sum_{t=n+1}^{T} \alpha_t \right).$$

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other directions: more shrinkage.

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Maximin distribution: same mean, concentrated on two points along the major axis direction.

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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.
  - The role of the smallest ball.
  - The simplex and the ball.
  - Sub-game optimal strategies on ellipsoids.