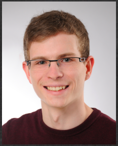
# Connections Between Invariant Theory and Statistics

Kathlén Kohn
KTH Stockholm

based on joint work with

Carlos Améndola
TU Munich

Philipp Reichenbach
TU Berlin

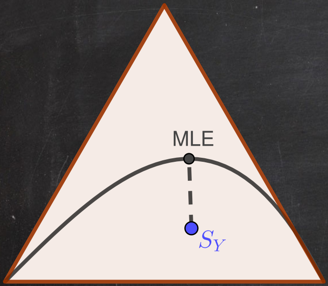


Anna Seigal
University of Oxford

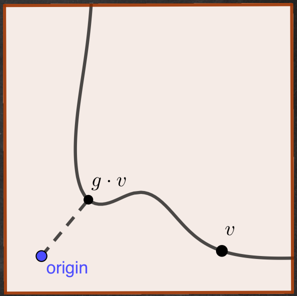
August 16, 2020

# Global picture

**Statistics**




**Invariant theory**



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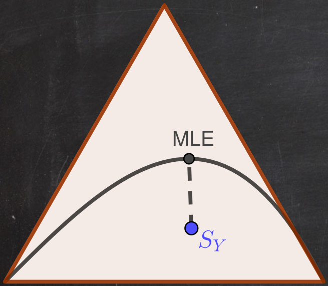


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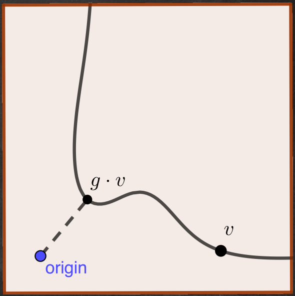


**Given:** statistical model
sample data $S_Y$

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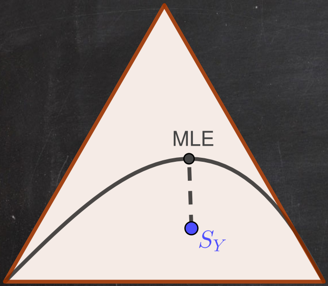


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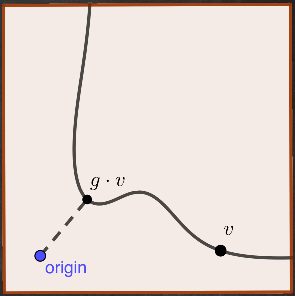


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= point in model that best fits $S_Y$

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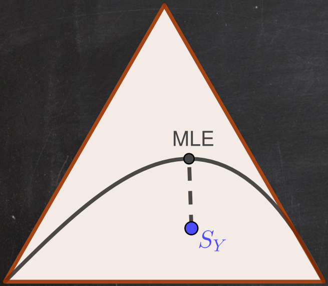


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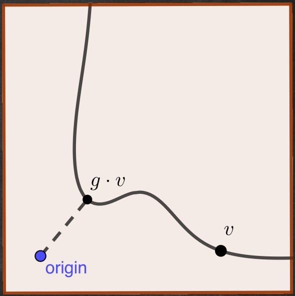


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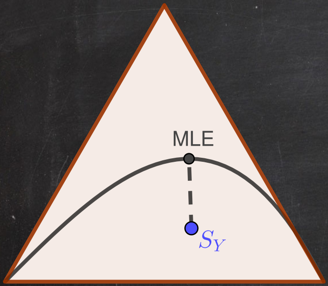


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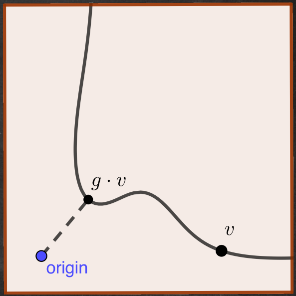



**Given:** orbit $G \cdot v = \{g \cdot v \mid g \in G\}$

**Task:** compute **capacity**

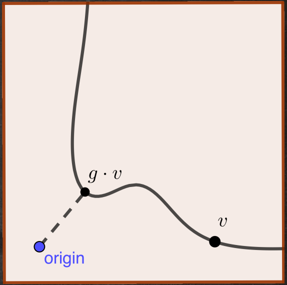
= closest distance of orbit to origin

# Invariant theory

## Stability notions

The **orbit** of a vector $v$ in a vector space $V$ under an action by a group $G$ is

$$G.v = \{g \cdot v \mid g \in G\} \subset V.$$



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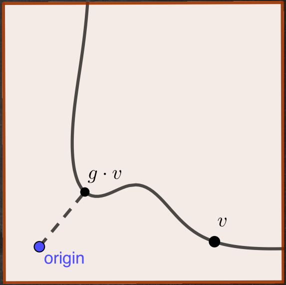


- $v$ is **unstable** iff $0 \in \overline{G.v}$ (i.e. $v$ can be scaled to 0 in the limit)

The **null cone** of the action by $G$ is the set of unstable vectors $v$.

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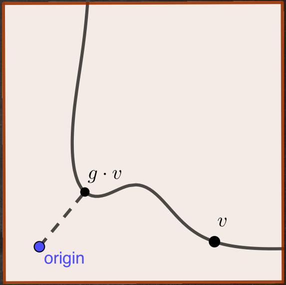


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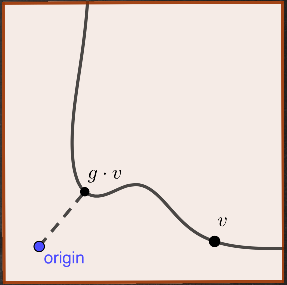


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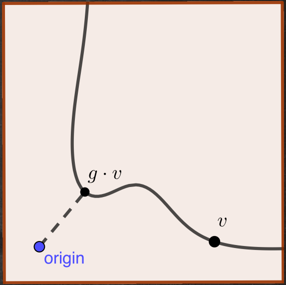


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- $v$ is **stable** iff $v$ is polystable and its stabilizer is finite

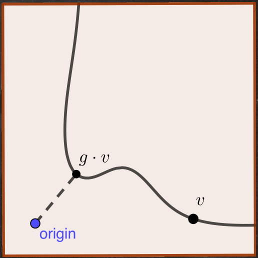
The **null cone** of the action by $G$ is the set of unstable vectors $v$.

# Invariant theory

## Null cone membership testing

Classical and often hard question: Describe null cone
(essentially equivalent to finding generators for the ring of polynomial invariants)

Modern approach: Provide a test to determine if a vector $v$ lies in null cone



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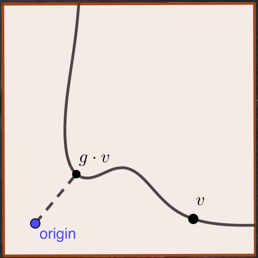
$$\operatorname{cap}_G(v) := \inf_{g \in G} \|g \cdot v\|_2^2.$$

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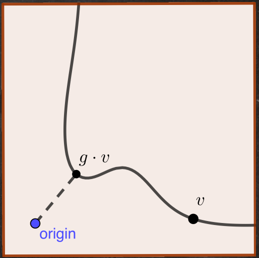


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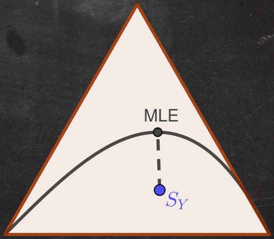
Hence: Testing null cone membership is a minimization problem.
$\rightsquigarrow$ algorithms: [series of 3 papers in 2017 – 2019 by
Bürgisser, Franks, Garg, Oliveira, Walter, Wigderson]

# Maximum likelihood estimation

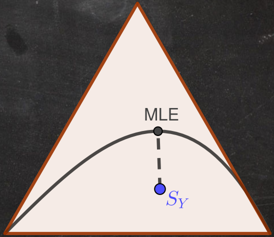


# Maximum likelihood estimation

**Given:**

- $\mathscr{M}$: a statistical **model** = a set of probability distributions
- $Y = (Y_1, \ldots, Y_n)$: $n$ samples of observed **data**

**Goal:** find a distribution in the model $\mathscr{M}$ that best fits the empirical data $Y$



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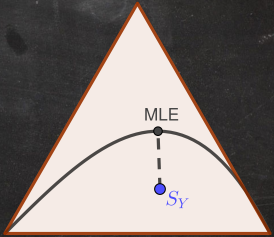
**Approach:** maximize the **likelihood function**

$$L_Y(\rho) := \rho(Y_1) \cdots \rho(Y_n), \qquad \text{where } \rho \in \mathscr{M}.$$




A **maximum likelihood estimate (MLE)** is a distribution in the model $\mathscr{M}$ that maximizes the likelihood $L_Y$.

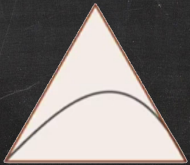
# Discrete statistical models

A probability distribution on $m$ states is determined by is **probability mass function** $\rho$, where $\rho_j$ is the probability that the $j$-th state occurs.

$\rho$ is a point in the **probability simplex**

$$\Delta_{m-1} = \left\{ q \in \mathbb{R}^m \mid q_j \geq 0 \text{ and } \sum q_j = 1 \right\}.$$

A **discrete statistical model** $\mathscr{M}$ is a subset of the simplex $\Delta_{m-1}$.

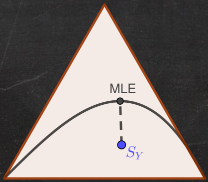


# Discrete statistical models

maximum likelihood estimation

Given data is a **vector of counts** $Y \in \mathbb{Z}^m_{\geq 0}$,
where $Y_j$ is the number of times the $j$-th state occurs.

The **empirical distribution** is $S_Y = \frac{1}{n} Y \in \Delta_{m-1}$, where $n = Y_1 + \ldots + Y_m$.



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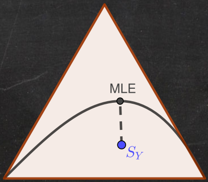
The **likelihood function** takes the form $L_Y(\rho) = \rho_1^{Y_1} \cdots \rho_m^{Y_m}$, where $\rho \in \mathscr{M}$.

An **MLE** is a point in model $\mathscr{M}$ that maximizes the likelihood $L_Y$ of observing $Y$.



# Log-linear models

= set of distributions whose logarithms lie in a fixed linear space.

Let $A \in \mathbb{Z}^{d \times m}$, and define

$$\mathcal{M}_A = \{p \in \Delta_{m-1} \mid \log p \in \mathrm{rowspan}(A)\}.$$

We assume that $\mathbb{1} := (1, \ldots, 1) \in \mathrm{rowspan}(A)$ (i.e., uniform distribution in $\mathcal{M}_A$).

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Matrix $A = [a_1 \mid a_2 \mid \dots \mid a_m]$ also defines an **action by the torus** $(\mathbb{C}^\times)^d$ on $\mathbb{C}^m$:

$g \in (\mathbb{C}^\times)^d$ acts on $x \in \mathbb{C}^m$ by left multiplication with

$$\begin{bmatrix} g^{a_1} & & \\ & \ddots & \\ & & g^{a_m} \end{bmatrix}, \qquad \text{where } g^{a_j} = g_1^{a_{1j}} \dots g_d^{a_{dj}}.$$

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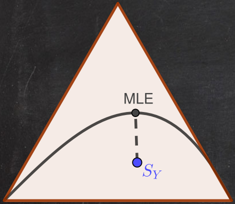
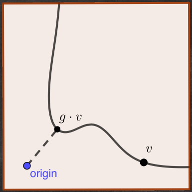
**Examples: independence model, graphical models, hierarchical models, . . .**

# Combining both worlds

**Theorem** (Améndola, Kohn, Reichenbach, Seigal)
Let $A = [a_1|\dots|a_m] \in \mathbb{Z}^{d\times m}$ and $Y \in \mathbb{Z}^m$ be a vector of counts with $n = \sum Y_j$.

MLE given $Y$ exists in $\mathscr{M}_A$ $\Leftrightarrow$ $\mathbb{1} \in \mathbb{C}^m$ is polystable under the action of $(\mathbb{C}^\times)^d$ given by the matrix $[na_1 - AY|\dots|na_m - AY]$



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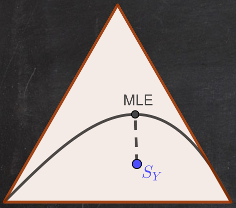


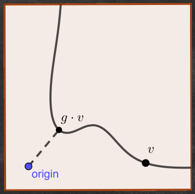


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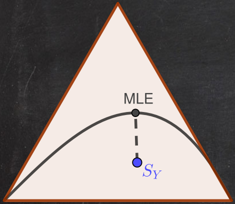


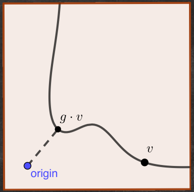


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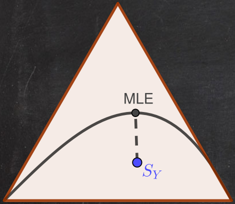


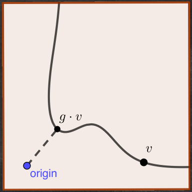


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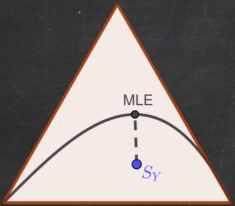
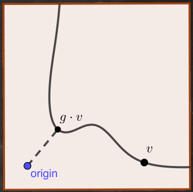
**Theorem** (cont'd)
If $x \in \mathbb{C}^m$ is a point of minimal norm in the orbit $(\mathbb{C}^\times)^d \cdot \mathbb{1}$, then the MLE is

$$\frac{x^{(2)}}{\|x\|^2}, \qquad \text{where } x^{(2)} \text{ is the vector with } j\text{-th entry } |x_j|^2.$$

# Algorithmic consequences

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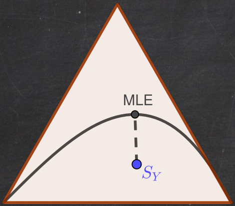


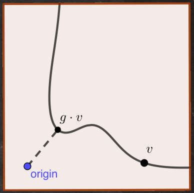


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maximize likelihood $\Leftrightarrow$ minimize KL divergence

minimize $\ell_2$-norm

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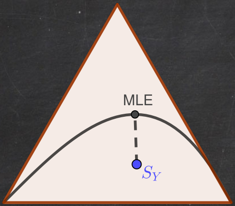


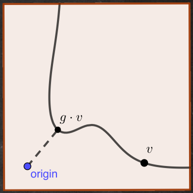


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maximize likelihood $\Leftrightarrow$ minimize KL divergence — minimize $\ell_2$-norm

model lives in $\Delta_{m-1} \cap \mathbb{R}^m_{>0}$ — orbit lives in $\mathbb{C}^m$

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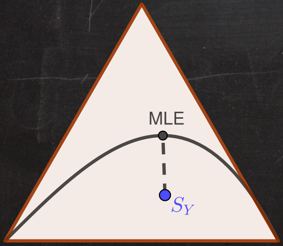

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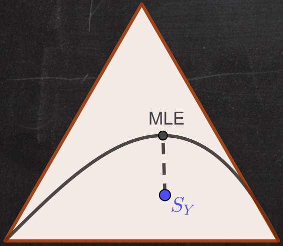

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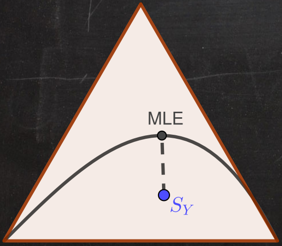


likelihood $L_Y$ can be unbounded from above

MLE might not exist

MLE might not be unique

# Combining both worlds

Invariant theory classically over $\mathbb{C}$ – can also define Gaussian models over $\mathbb{C}$

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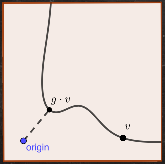


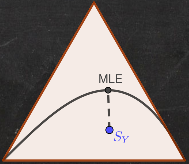

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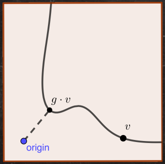


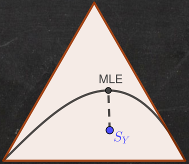

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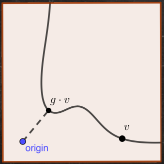


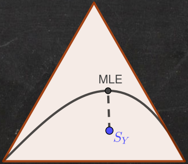


$h \cdot Y$ point of minimal norm $\Rightarrow$ $\tau h^* h$ is an MLE where $\tau = \underset{\mathbb{R}_{>0}}{\mathrm{argmin}}(\tau \|h \cdot Y\|_2^2 - nm \log \tau)$

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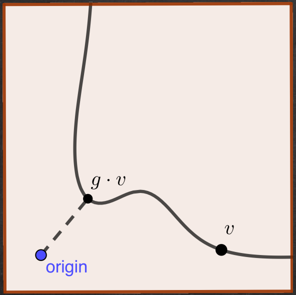
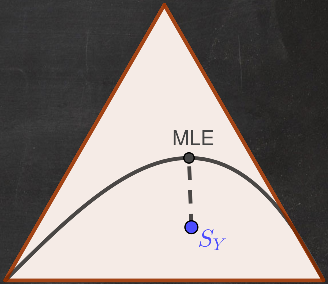
**Example:** **Gaussian graphical models**

# Summary




| | Invariant theory | | Statistics |
|---|---|---|---|
| | describe null cone | × | algorithms to find MLE |
| *historical progression* ↓ | algorithmic null cone membership testing | | convergence analysis |