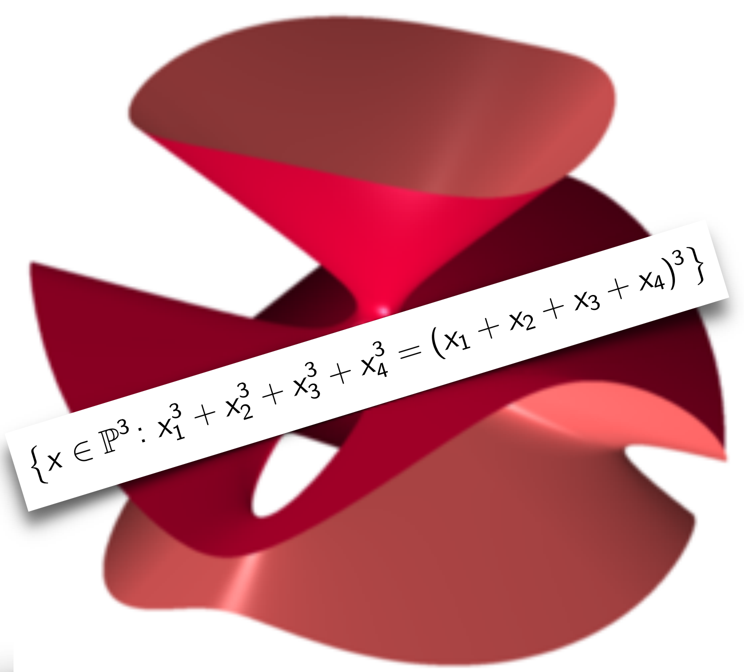
Algebraic Statistics & Quantifier Elimination

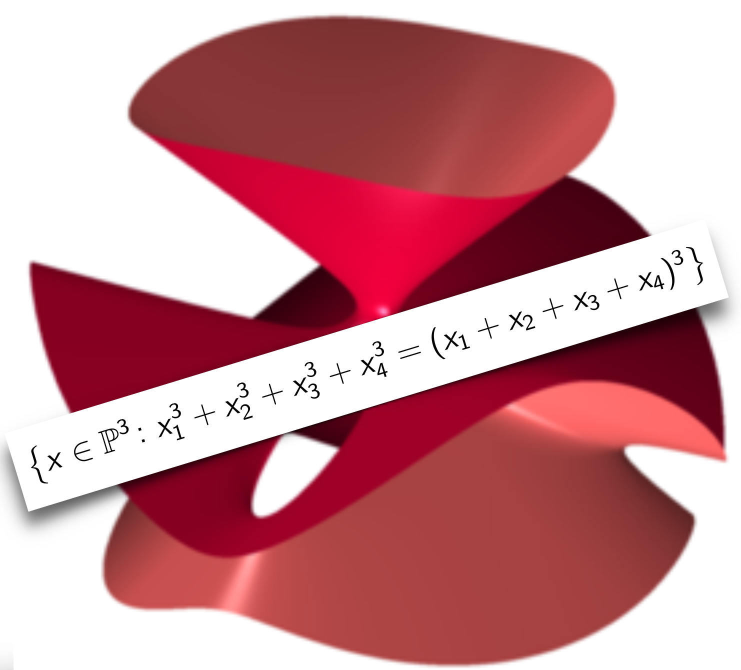
Daniel Suess

What is Algebraic Statistics?



What is Algebraic Statistics?

understand algebraic
structure of statistical models



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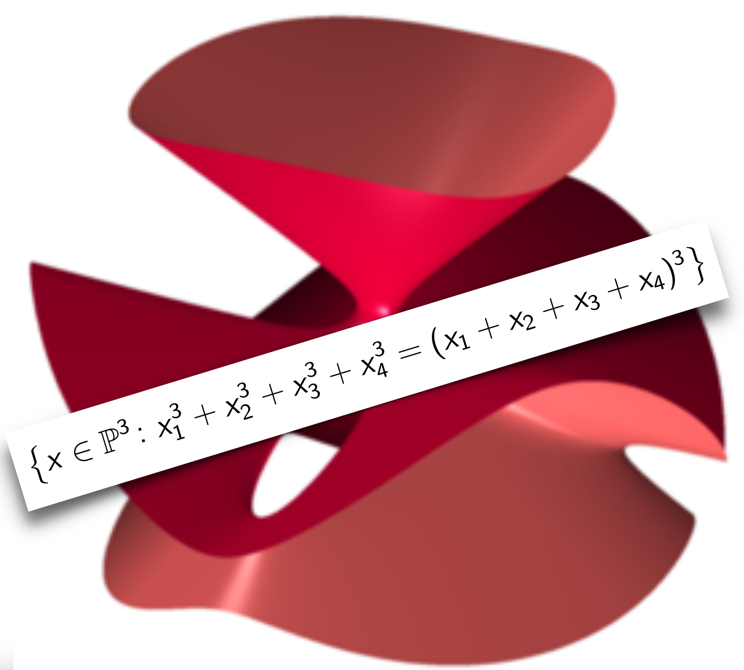
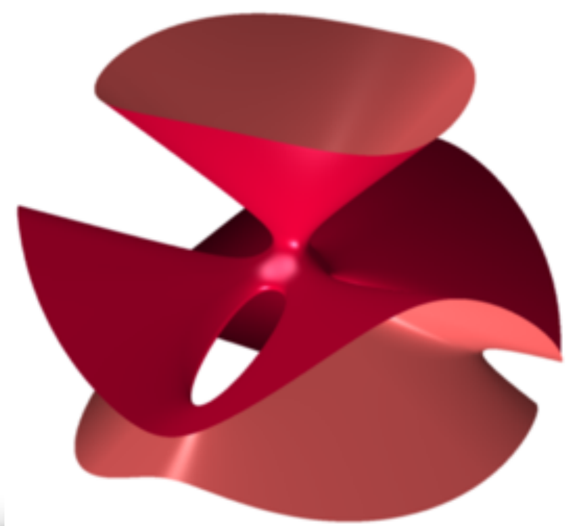


application of techniques from
computational algebra,
algebraic geometry, …

Algebraic Structure in Statistics

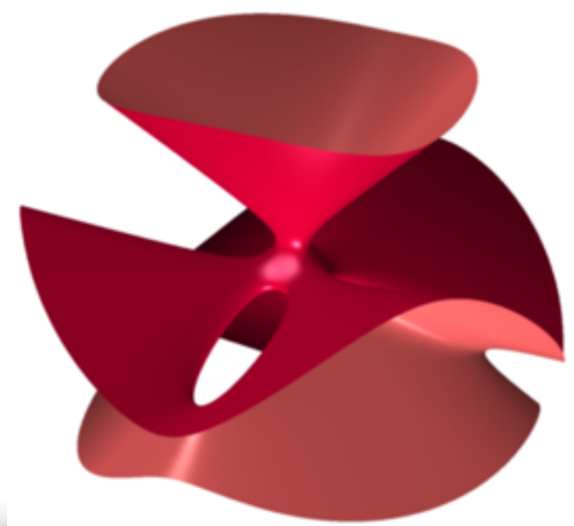


Semi-algebraic set $S \subset \mathbb{R}^n$

$$S = \Big\{x \in \mathbb{R}^n \colon\ p_i(x_1, \ldots, x_n) = 0,$$
$$q_j(x_1, \ldots, x_n) \leq 0\Big\}$$

for finitely many polynomials p_i, q_i with coefficients in $\mathbb{Q}$

Algebraic Structure in Statistics



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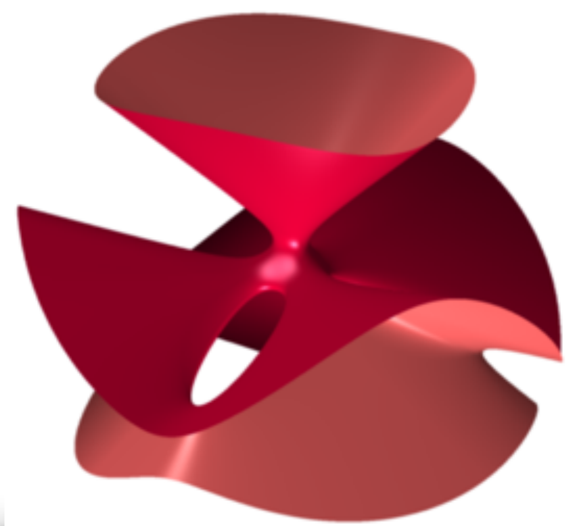
- probability simplex

  $$\Delta_{n-1} = \Big\{ x \in \mathbb{R}^n \colon\ \sum_i x_i = 1, x_i \ge 0 \Big\}$$

- joint prob. of discrete, indep. RVs
- max. likelihood estimates
- …

Algebraic Structure in Statistics



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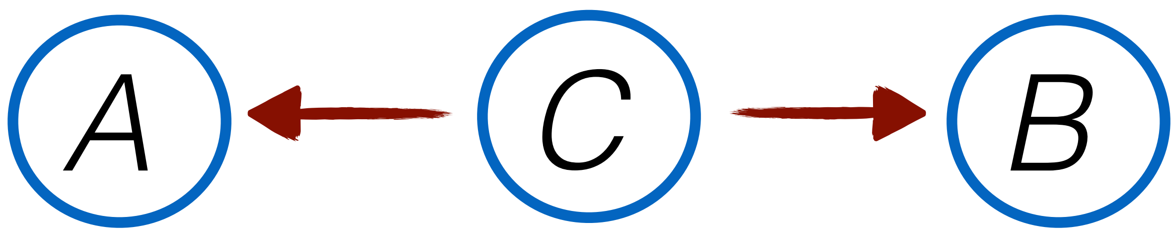
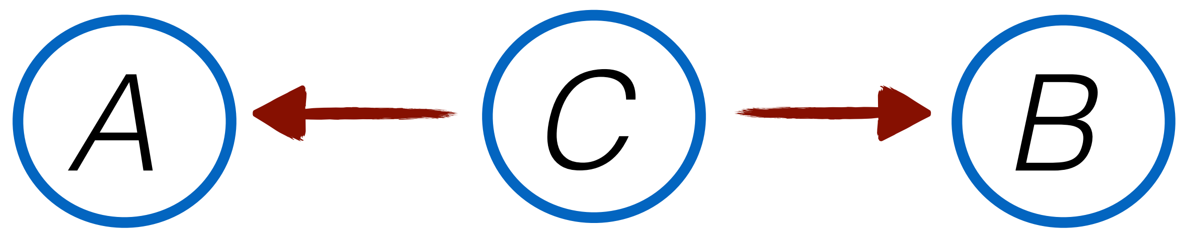
Conditional Independence: Explicit & Implicit Form



$$A \perp\!\!\!\perp B \mid C$$

Conditional Independence: Explicit & Implicit Form



$$A \perp\!\!\!\perp B \mid C$$

explicit

$$P(A, B, C) = P(A|C)\, P(B|C)\, P(C)$$

$$\Longleftrightarrow$$

$$p_{abc} = q_{ac}\, r_{bc}\, s_c$$

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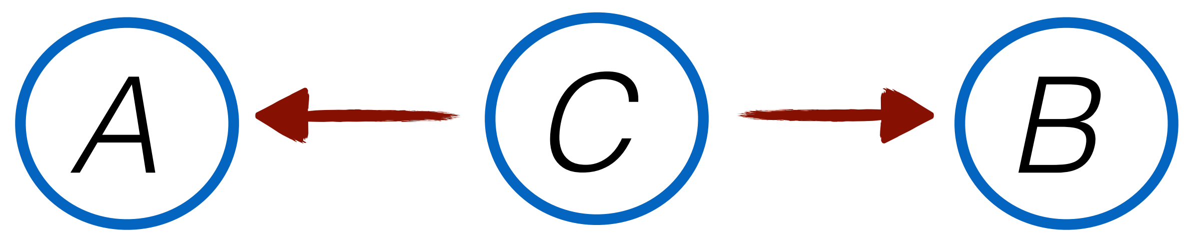

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Additional constraint for the semi-algebraic set of probabilities consistent with DAG.

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$$p_{abc} = q_{ac}\, r_{bc}\, s_c$$

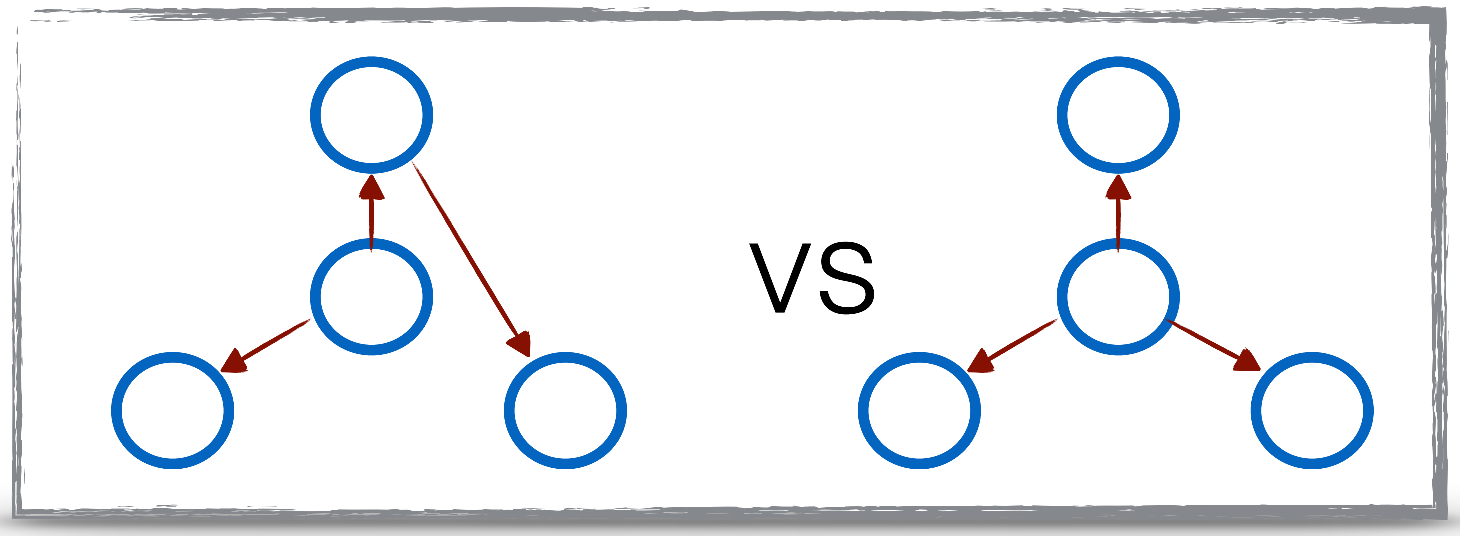
$\Longleftrightarrow$ for all c, $(p_{abc})_{ab}$ is rank 1

$\Longleftrightarrow$ $(p_{abc})_{ab}$ has determinantal rank 1

$\Longleftrightarrow$ determinant of all 2×2 minors $= 0$

$\Longleftrightarrow$ $\forall a, a', b, b', c:\ p_{abc}\, p_{a'b'c} - p_{ab'c}\, p_{a'bc} = 0$

Possible Applications



distinguishing Bayesian networks from observational data

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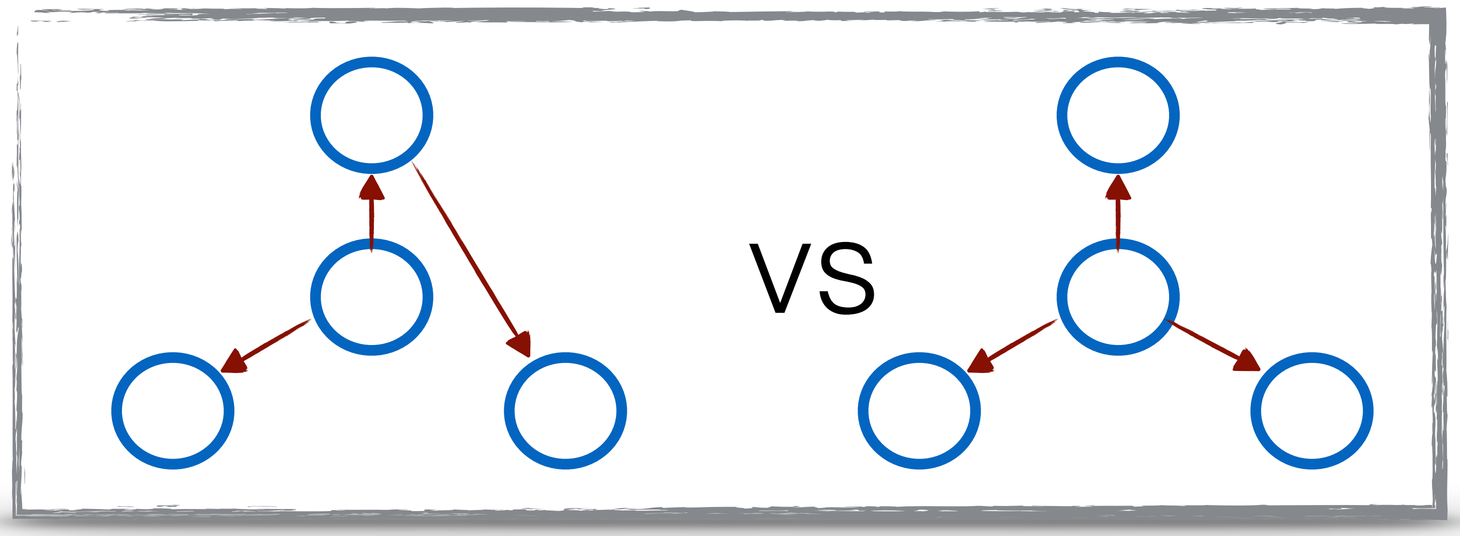

distinguishing Bayesian networks from observational data

Bell inequalities / quantum non locality

Image: http://www.belfasttelegraph.co.uk/news/northern-ireland/john-stewart-bell-belfast-city-council-to-bend-rules-on-the-naming-of-streets-to-honour-the-scientist-who-corrected-albert-einstein-30586279.html

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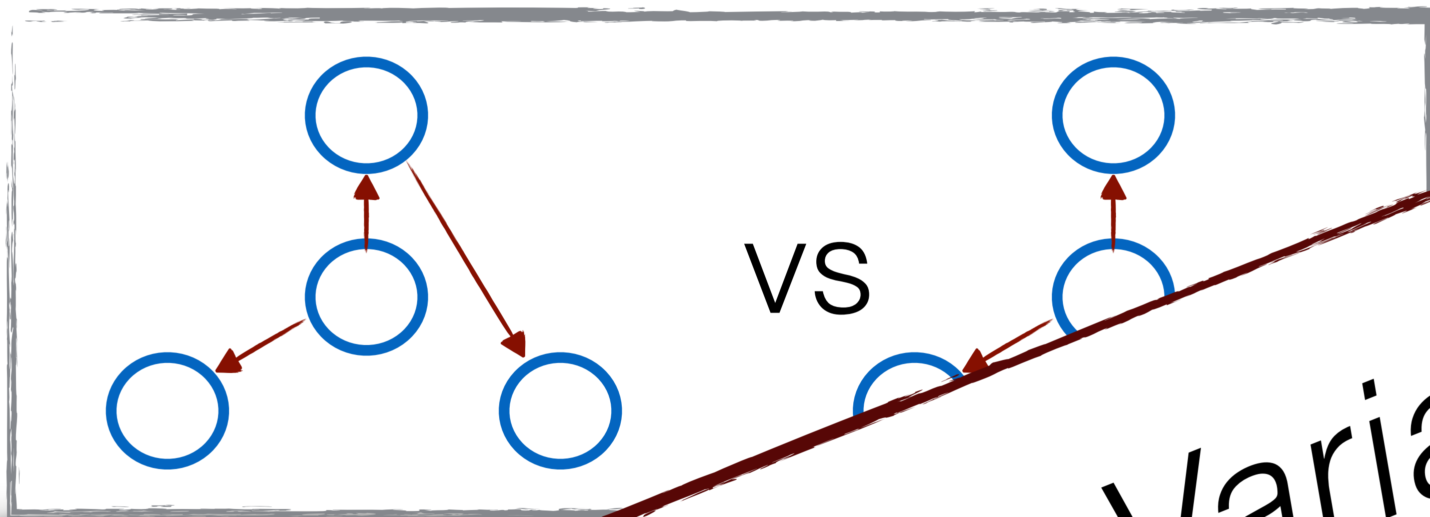
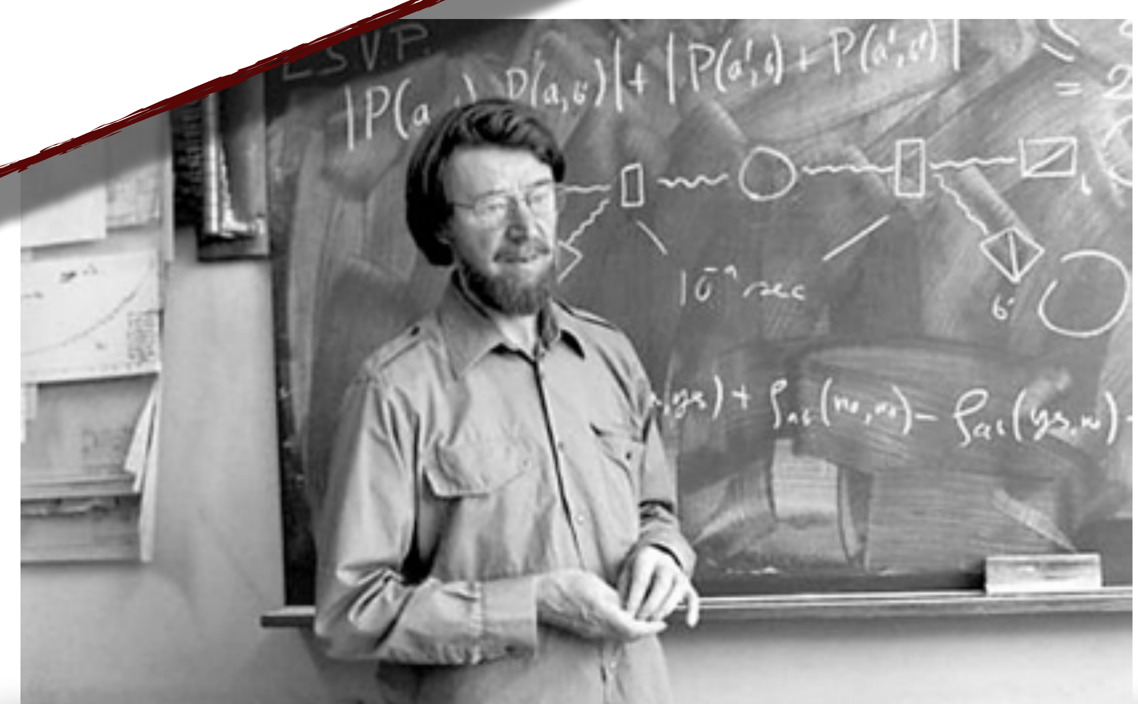


Bayesian

ata

Hidden Variables?

Bell inequa /
quantum non locality



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Quantifier Elimination: Conditional Independence

p_{abc} compatible with $A \leftarrow C \rightarrow B$

$$\left\{ \begin{array}{ll} (p_{abc}): & \exists (q_{ac}) \exists (r_{bc}) \exists (s_c) \\ & (\bigwedge_c \sum_a q_{ac} = 1) \wedge (\bigwedge_c \sum_b r_{bc} = 1) \wedge (\sum_c s_c = 1) \wedge \\ & (\bigwedge_{ac} q_{ac} \geq 0) \wedge (\bigwedge_{bc} r_{bc} \geq 0) \wedge (\bigwedge_c s_c \geq 0) \wedge \\ & (\bigwedge_{abc} p_{abc} = q_{ac} \times r_{bc} \times s_c) \end{array} \right\}$$

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$$= \pi \Big(\{ (p_{abc}, q_{ab}, r_{bc}, s_c) : \; \cdots \} \Big)$$

with $\pi : \mathbb{R}^{n_1 + n_2} \to \mathbb{R}^{n_1}, (p_{abc}, q_{ab}, r_{bc}, s_c) \mapsto (p_{abc})$

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Theorem (Tarski-Seidenberg) The image of a semi-algebraic set under a projection map π is a semi-algebraic set.

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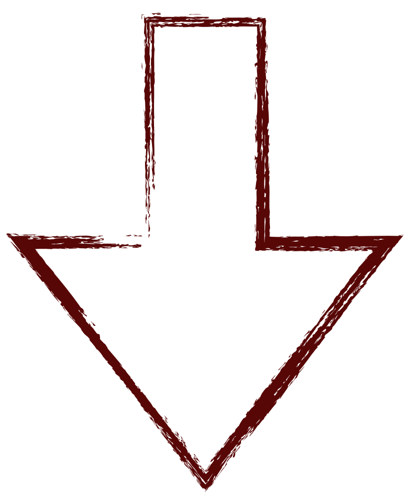
$$\boxed{\begin{array}{c} \{(p, q) \in \mathbb{R}^2 : (\exists x \in \mathbb{R})\, x^2 + px + q = 0\} \\ = \{(p, q) \in \mathbb{R}^2 : p^2 \geq 4q\} \end{array}}$$

Quantifier Elimination: Algorithms

Input: formula Ψ



Output: equivalent,
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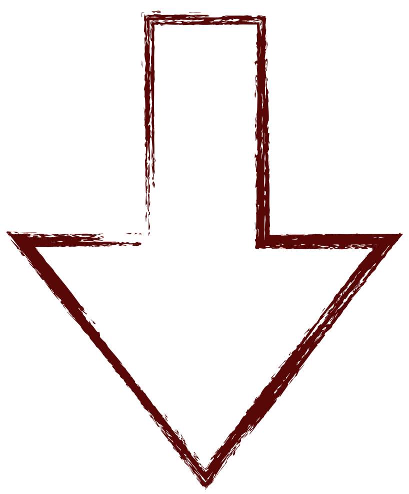

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- real valued variables
- rational constants
- operations $(+,-,\times)$
- binary relations $(=,\neq,<,\leq)$
- logical connectives $(\wedge,\vee,\neg,\Rightarrow,\Leftrightarrow)$
- quantifiers $(\forall,\exists)$

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- Tarski's algorithm
- Cylinder Algebraic decomposition

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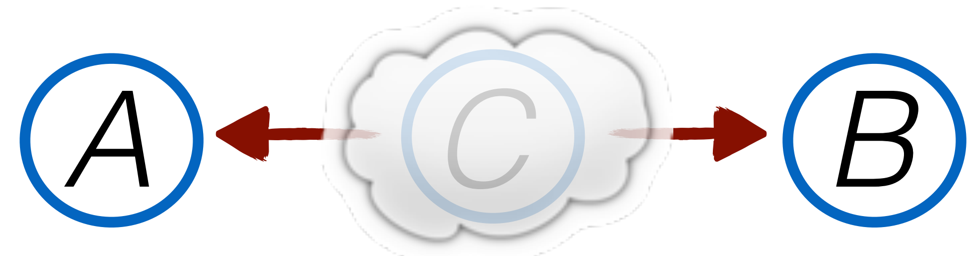
$\cancel{p_{abc}}$ compatible with 

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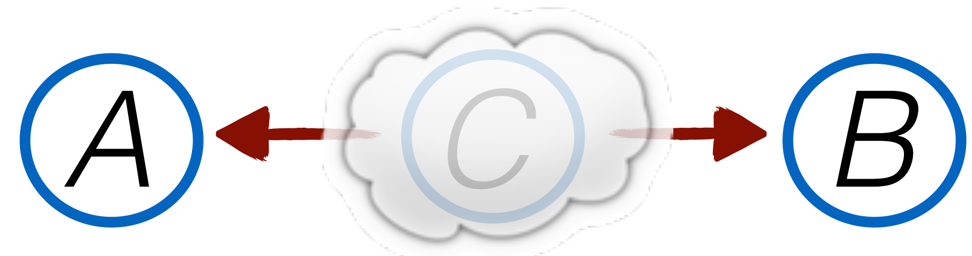

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$$\bigwedge_{ab} p_{ab} = \sum_c q_{ac} \times r_{bc} \times s_c$$

- no additional constraints on p_{ab} for $N_A = N_B = N_C = 2$
- $N_A = N_B = 3$ did not finish

Quantifier Elimination: Other Applications

Membership Problem

$$(A \perp C) \wedge (A \perp B \mid C) \Rightarrow (A \perp B)\ ?$$

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$$\underbrace{(A \perp C) \wedge (A \perp B \mid C)}_{\psi(p)} \Rightarrow \underbrace{(A \perp B)}_{\psi'(p)}\ ?$$

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Identifiability Problem

Can we uniquely identify the parameter θ in a parametric model from given observation?

Quantifier Elimination: Other Applications

Membership Problem	Identifiability Problem
$\underbrace{(A \perp C) \wedge (A \perp B \mid C)}_{\psi(p)} \Rightarrow \underbrace{(A \perp B)}_{\psi'(p)}$?	*Can we uniquely identify the parameter θ in a parametric model from given observation?*
$\forall p \colon \psi(p) \implies \psi'(p)$	$\forall \theta, \theta' \colon (\mathrm{O}(\theta) = \mathrm{O}(\theta')) \implies (\theta = \theta')$

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- CAD: best known algorithm for QE, but too slow beyond toy models
- also for continuous RV (exponential families)
- https://github.com/dseuss/algstat.git

Theorem (Tarski) Every Tarski sentence (formula without free variables) is equivalent to a quantifier-free formula.

Theorem (Tarski-Seidenberg) Let $f\colon X \to Y$ be a semi-algebraic map. Then, the image $f(X) \subseteq Y$ is a semi-algebraic set.

ALGORITHM ComputeCAD(F,j)

Input: $\mathrm{F} \subset Q[x_1, \ldots, x_j]$.

Output: (K_j, α_j) where K_j is an F-sign-invariant *CAD* of R^j and
α_j is a set of algebraic sample points, one per cell in K_j.

Recurse: If $j > 1$, then do
$\Phi(\mathrm{F}) := \Phi_1(\mathrm{F}) \cup \Phi_2(\mathrm{F}) \cup \Phi_3(\mathrm{F})$
$(K_{j-1}, \alpha_{j-1}) := ComputeCAD(\Phi(\mathrm{F}), j-1)$,
else find the roots $r_1, \ldots, r_m$ of all polynomials in F and do
$K_1 := \{[-\infty, r_1), [r_1, r_1], (r_1, r_2), \ldots, (r_m, +\infty]\}$
$\alpha_1 := \{r_1 - 1, r_1, (r_1 + r_2)/2, \ldots, r_m, r_m + 1\}$
Return (K_1, α_1)

Lift: For every cell $C_i \in K_{j-1}$ do

1. Compute the product of all polynomials in F that do not vanish at the sample point α_i of C_i and call the resulting polynomial $\pi(\alpha_i, x)$

2. Find the roots $r_1, \ldots, r_m$ of $\pi(\alpha_i, x)$

3. Set $K_{j,i} := \{\{C_i \times [-\infty, r_1)\}, \{C_i \times [r_1, r_1]\}, \{C_i \times (r_1, r_2)\}, \ldots, \{C_i \times (r_m, +\infty]\}\}$
Comment: $K_{j,i}$ are the cylinders over C_i.

4. Set $\alpha_{j,i} := \{(\alpha_i, r_1 - 1), (\alpha_i, r_1), (\alpha_i, (r_1 + r_2)/2), \ldots, (\alpha_i, r_m + 1)\ \}$
Comment: $\alpha_{j,i}$ are the algebraic sample points for the cylinders over C_i.

$K_j := \bigcup_i K_{j,i}$; $\alpha_j := \bigcup_i \alpha_{j,i}$

Return (K_j, α_j)