

Tobias Boege

# The Gaussian CI inference problem

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**Institut für Algebra und Geometrie**  
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DFG-Graduiertenkolleg  
**MATHEMATISCHE  
KOMPLEXITÄTSREDUKTION**

# Gaussian conditional independence

Consider random variables  $(\xi_i)_{i \in N}$ . The *conditional independence (CI) statement*  $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$  conveys, informally, that if  $\xi_K$  is known, then learning the value of  $\xi_i$  does not give any information about  $\xi_j$ .



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# Gaussian conditional independence

Let the random vector be normally distributed:  $(\xi_i)_{i \in N} \sim \mathcal{N}(\mu, \Sigma)$ .

## Definition

The polynomial  $\Sigma[K] := \det \Sigma_{K,K}$  is a *principal minor* of  $\Sigma$  and  $\Sigma[ij|K] := \det \Sigma_{iK,jK}$  is an *almost-principal minor*.

If  $\Sigma$  is positive-definite, then  $\Sigma[K] > 0$ , and  $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$  holds if and only if  $\Sigma[ij|K] = 0$ .



## Almost-principal minors

$$\Sigma[ij] = x_{ij}$$

$$\Sigma[ij|k] = x_{ij}x_{kk} - x_{ik}x_{jk}$$

$$\Sigma[ij|kl] = x_{ij}x_{kk}x_{ll} - x_{il}x_{jl}x_{kk} + x_{il}x_{jk}x_{kl} + x_{ik}x_{jl}x_{kl} - x_{ij}x_{kl}^2 - x_{ik}x_{jk}x_{ll}$$

$$\begin{aligned}\Sigma[ij|klm] = & x_{ij}x_{kk}x_{ll}x_{mm} + x_{im}x_{jm}x_{kl}^2 - x_{im}x_{jl}x_{kl}x_{km} - x_{il}x_{jm}x_{kl}x_{km} + x_{il}x_{jl}x_{km}^2 \\ & - x_{im}x_{jm}x_{kk}x_{ll} + x_{im}x_{jk}x_{km}x_{ll} + x_{ik}x_{jm}x_{km}x_{ll} - x_{ij}x_{km}^2x_{ll} \\ & + x_{im}x_{jl}x_{kk}x_{lm} + x_{il}x_{jm}x_{kk}x_{lm} - x_{im}x_{jk}x_{kl}x_{lm} - x_{ik}x_{jm}x_{kl}x_{lm} \\ & - x_{il}x_{jk}x_{km}x_{lm} - x_{ik}x_{jl}x_{km}x_{lm} + 2x_{ij}x_{kl}x_{km}x_{lm} + x_{ik}x_{jk}x_{lm}^2 \\ & - x_{ij}x_{kk}x_{lm}^2 - x_{il}x_{jl}x_{kk}x_{mm} + x_{il}x_{jk}x_{kl}x_{mm} + x_{ik}x_{jl}x_{kl}x_{mm} \\ & - x_{ij}x_{kl}^2x_{mm} - x_{ik}x_{jk}x_{ll}x_{mm}\end{aligned}$$

⋮



# Gaussian CI models

## Definition

A *CI constraint* is a CI statement  $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$  or its negation  $\neg(\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K)$ . They are *algebraic conditions* on the entries of  $\Sigma$ , equivalent to vanishing or non-vanishing of the almost-principal minors  $\Sigma[ij|K]$ .

## Definition

The *model* of a set of CI constraints is the set of all positive-definite matrices which satisfy the constraints.



## Gaussian CI models

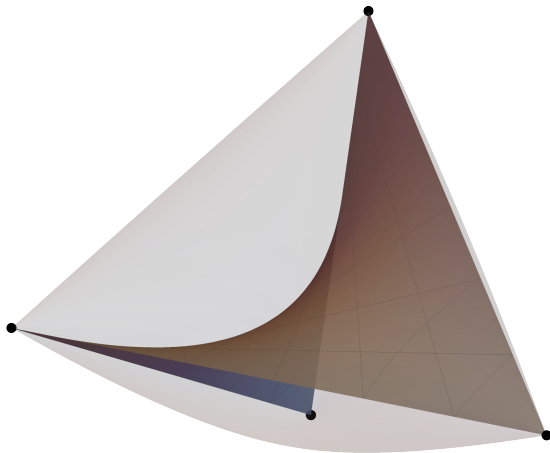


Figure: Model of  $\Sigma[12|3] = 0$  in the space of  $3 \times 3$  correlation matrices.





# Models and inference

Consider two sets of CI statements  $\mathcal{P}$  and  $\mathcal{Q}$ :

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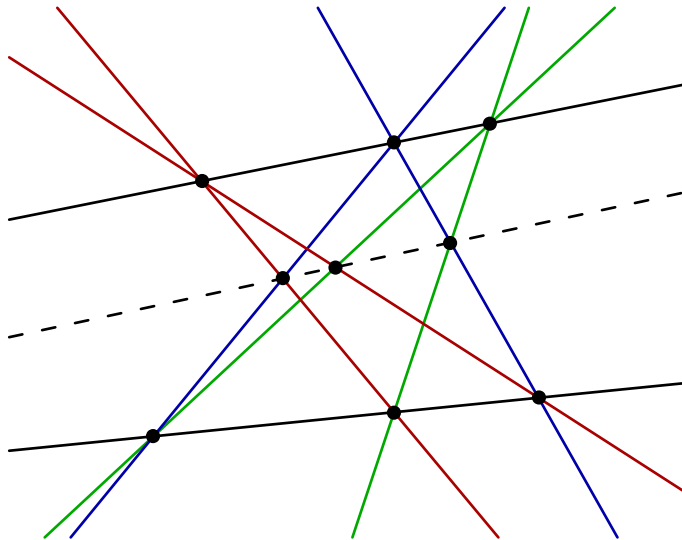
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Reasoning about relevance statements in normally distributed random variables is **the same** as reasoning about the vanishing of very special kinds of determinants on very special kinds of varieties inside the positive-definite matrices.



# For geometers: conditional independence $\approx$ collinearity



## Examples of CI inference

Consider a general positive-definite  $3 \times 3$  correlation matrix

$$\Sigma = \begin{pmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{pmatrix}.$$

- If  $\Sigma[12|3] = a - bc$  and  $\Sigma[13] = b$  vanish, then  $\Sigma[12|] = a$  and  $\Sigma[13|2] = b - ac$  must vanish as well:

$$(12|3) \wedge (13|) \Rightarrow (12|) \wedge (13|2).$$

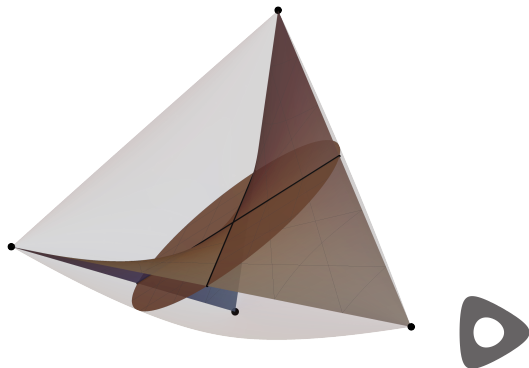


## Examples of CI inference

$$\Sigma = \begin{pmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{pmatrix}$$

- If  $\Sigma[12|] = a$  and  $\Sigma[12|3] = a - bc$  vanish, then  $bc = \Sigma[13|] \cdot \Sigma[23|]$  must vanish:

$$(12|) \wedge (12|3) \Rightarrow (13|) \vee (23|).$$



# Rational points on CI models

Šimeček's Question (2006)

*Does every non-empty Gaussian CI model contain a rational point?*

Or: can every wrong inference rule be refuted over  $\mathbb{Q}$ ?




# Rational points on CI models

## Šimeček's Question (2006)

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Or: can every wrong inference rule be refuted over  $\mathbb{Q}$ ?

**Model M85**



Where:

$$a = \frac{3}{632836} \sqrt{1107463},$$
$$b = 10c = \frac{100}{158209} \sqrt{1107463}$$
$$d = 10e = \frac{3}{4}, f = \frac{1}{10}$$

$$\begin{pmatrix} 1 & -1/17 & -49/51 & -7/17 \\ -1/17 & 1 & 1/3 & 1/7 \\ -49/51 & 1/3 & 1 & 3/7 \\ -7/17 & 1/7 & 3/7 & 1 \end{pmatrix}$$





# Complexity bounds from real geometry

Let  $f_i \in \mathbb{Z}[t_1, \dots, t_k]$  be integer polynomials in finitely many variables.

## Theorem (Tarski's transfer principle)

*If a polynomial system  $\{f_i \bowtie_i 0\}$ , where  $\bowtie_i \in \{=, \neq, <, \leq, \geq, >\}$ , has a solution over  $\mathbb{R}$ , then it has a solution in a finite real extension of  $\mathbb{Q}$ .*

→ If  $\bigwedge \mathcal{P} \Rightarrow \bigvee \mathcal{Q}$  is **false**, there exists a counterexample matrix  $\Sigma$  with algebraic entries.

$(12|) \wedge (12|3) \Rightarrow (13|)$  is false and a counterexample is

$$\begin{pmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix}.$$



## Complexity bounds from real geometry

Let  $F, f_i, g_j \in \mathbb{Z}[t_1, \dots, t_k]$  be integer polynomials in finitely many variables.

### Theorem (Positivstellensatz)

*A polynomial  $F$  vanishes on the basic semialgebraic set  $\{f_i = 0, g_j \geq 0\}$  if and only if  $-F^{2m} \in \text{ideal}(f_i) + \text{cone}(g_j)$  for  $m$  large enough.*

→ If  $\bigwedge \mathcal{P} \Rightarrow \bigvee \mathcal{Q}$  is **true**, there exists an algebraic proof for it with rational coefficients.

$(12|) \wedge (12|3) \Rightarrow (13|) \vee (23|)$  is true and a proof is the polynomial identity

$$\Sigma[13|] \cdot \Sigma[23|] = \Sigma[3] \cdot \Sigma[12|] - \Sigma[12|3].$$

The associated decision problem is the **existential theory of the reals**.



# Universality theorems

## Theorem (B. 2021)

*For every finite real extension  $\mathbb{K}/\mathbb{Q}$  there exists a Gaussian CI model  $\mathcal{M}_{\mathbb{K}}$  such that: for every  $\mathbb{L}/\mathbb{Q}$ ,  $\mathcal{M}_{\mathbb{K}}$  has an  $\mathbb{L}$ -rational point if and only if  $\mathbb{K} \subseteq \mathbb{L}$ .*

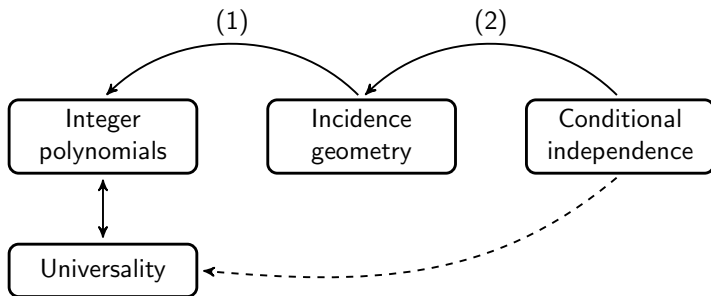
→ The answer to Šimeček's question is **NO**.

## Theorem (B. 2021)

*The problem of deciding whether a CI inference formula is valid for all Gaussian distributions is polynomial-time equivalent to the existential theory of the reals.*



## Proof sketch



### Theorem

To every polynomial system  $\{f_i \approx 0\}$  one can compute a polynomially-sized set of CI constraints which has a model over a real algebraic extension  $\mathbb{K}/\mathbb{Q}$  if and only if the polynomial system has a solution in  $\mathbb{K}$ .

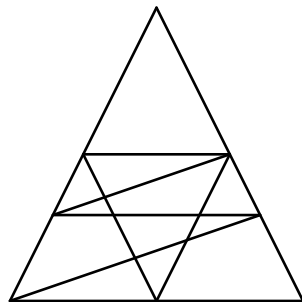


## (1) Algebra $\subseteq$ Synthetic geometry

Point and line configuration for the equation  $x^2 - 2 = 0$ .

The configuration is specified by incidences between points and lines and also the parallelities of lines.

It is realizable over  $\mathbb{Q}(\sqrt{2})$  but not over  $\mathbb{Q}$ .



Keyword for the general technique: *von Staudt constructions* (1857).



## (2) Synthetic geometry $\subseteq$ Gaussian CI

$\Sigma[ij] = x_{ij} \rightarrow$  impose  $x_{kl} = x_{km} = x_{lm} = 0$  on a correlation matrix, then:

$$\begin{aligned} \Sigma[ij|klm] &= x_{ij}x_{kk}x_{ll}x_{mm} + x_{im}x_{jm}x_{kl}^2 - x_{im}x_{jl}x_{kl}x_{km} - x_{il}x_{jm}x_{kl}x_{km} + x_{il}x_{jl}x_{km}^2 \\ &\quad - x_{im}x_{jm}x_{kk}x_{ll} + x_{im}x_{jk}x_{km}x_{ll} + x_{ik}x_{jm}x_{km}x_{ll} - x_{ij}x_{km}^2x_{ll} \\ &\quad + x_{im}x_{jl}x_{kk}x_{lm} + x_{il}x_{jm}x_{kk}x_{lm} - x_{im}x_{jk}x_{kl}x_{lm} - x_{ik}x_{jm}x_{kl}x_{lm} \\ &\quad - x_{il}x_{jk}x_{km}x_{lm} - x_{ik}x_{jl}x_{km}x_{lm} + 2x_{ij}x_{kl}x_{km}x_{lm} + x_{ik}x_{jk}x_{lm}^2 \\ &\quad - x_{ij}x_{kk}x_{lm}^2 - x_{il}x_{jl}x_{kk}x_{mm} + x_{il}x_{jk}x_{kl}x_{mm} + x_{ik}x_{jl}x_{kl}x_{mm} \\ &\quad - x_{ij}x_{kl}^2x_{mm} - x_{ik}x_{jk}x_{ll}x_{mm} \\ &= x_{ij} - \sum_{t=k,l,m} x_{it}x_{jt} = x_{ij} - \left\langle \left( \begin{array}{c} x_{ik} \\ x_{il} \\ x_{im} \end{array} \right), \left( \begin{array}{c} x_{jk} \\ x_{jl} \\ x_{jm} \end{array} \right) \right\rangle. \end{aligned}$$



# Incidence relation in a CI model

$$\begin{array}{c}
 p_1 \\
 \vdots \\
 p_n \\
 l_1 \\
 \vdots \\
 l_m \\
 x \\
 y \\
 z
 \end{array}
 \left(
 \begin{array}{ccc|ccc|ccc}
 p_1 & \dots & p_n & l_1 & \dots & l_m & x & y & z \\
 p_1^* & & \langle p, p' \rangle & & & & p_1^x & p_1^y & p_1^z \\
 & \ddots & & & \langle p, l \rangle & & & \vdots & \\
 \langle p', p \rangle & & p_n^* & & & & p_n^x & p_n^y & p_n^z \\
 \hline
 & & & l_1^* & & \langle l, l' \rangle & l_1^x & l_1^y & l_1^z \\
 & \langle l, p \rangle & & & \ddots & & & \vdots & \\
 \hline
 & & & \langle l', l \rangle & & l_m^* & l_m^x & l_m^y & l_m^z \\
 \hline
 p_1^x & & p_n^x & l_1^x & & l_m^x & 1 & 0 & 0 \\
 p_1^y & \dots & p_n^y & l_1^y & \dots & l_m^y & 0 & 1 & 0 \\
 p_1^z & & p_n^z & l_1^z & & l_m^z & 0 & 0 & 1
 \end{array}
 \right)$$



# Approximations to the inference problem





# Approximations to the inference problem

## Theorem (Matúš 2005)

*The following relations hold for every symmetric matrix  $\Sigma$ :*

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L].$$

These relations define essential geometric properties of symmetric matrices in principal and almost-principal minor coordinates. Study their combinatorics!



# The Gaussian CI configuration space

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

The *Gaussian CI configuration space*  $\mathcal{G} \subseteq \mathbb{R}^{2^n} \times \mathbb{R}^{\binom{n}{2}2^{n-2}}$  consists of all vectors of principal and almost-principal minors of  $\Sigma \in \text{PD}_n$ .



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Very wasteful encoding of a matrix, but this creates simple and useful relations on configuration vectors. The CI structure of  $\Sigma$  is encoded in the *zero pattern* of  $c(\Sigma) \in \mathcal{G}$ .



## Combinatorial compatibility

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

*Combinatorial compatibility* means **fulfilling polynomial relations under uncertainty**:

What if we only knew that all  $\Sigma[K] \neq 0$  and whether or not  $\Sigma[ij|K] = 0$  for every  $(ij|K)$ ?



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$$(ik|L) \wedge (ij|kL) \Rightarrow (ij|L)$$

⋮



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$$(ij|L) \wedge (ik|L) \Rightarrow (ij|kL) \wedge (ik|jL)$$

This yields the definition of *gaussoids*.



## CI inference via SAT solvers

Since gaussoids have a finite axiomatization, a SAT solver like CaDiCaL can deduce implications under the gaussoid axioms:

$$\begin{aligned} & (12|3) \wedge (12|34) \wedge (24|1) \wedge (34|2) \\ \Rightarrow & (12|) \wedge (12|4) \wedge (24|) \wedge (24|3) \wedge (24|13) \wedge (34|) \end{aligned}$$

These conclusions are valid for all regular Gaussian distributions.



## Oriented gaussoids

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L]$$

What if we only knew that all  $\text{sgn } \Sigma[K] = +1$  and the value of  $\text{sgn } \Sigma[ij|K]$  for every  $(ij|K)$ ?

$$+(ij|L) \wedge -(ij|kL) \Rightarrow [+(ik|L) \wedge +(jk|L)] \vee [-(ik|L) \wedge -(jk|L)]$$

→ *Oriented* and *orientable* gaussoids.





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→ *Oriented* and *orientable* gaussoids.

$$(ij|L) \wedge (kl|L) \wedge (ik|jL) \wedge (jl|ikL) \Rightarrow (ik|L)$$

$$(ij|L) \wedge (kl|iL) \wedge (kl|jL) \wedge (ij|klL) \Rightarrow (kl|L)$$

$$(ij|L) \wedge (jl|kL) \wedge (kl|iL) \wedge (ik|jL) \Rightarrow (ik|L)$$

$$(ij|kL) \wedge (ik|lL) \wedge (il|jL) \Rightarrow (ij|L)$$

$$(ij|kL) \wedge (ik|lL) \wedge (jl|iL) \wedge (kl|jL) \Rightarrow (ij|L)$$



## CI inference via SAT solvers II

Using the gaussoid axioms, we find:

$$(12|) \wedge (13|4) \wedge (14|5) \wedge (15|23) \wedge (23|5) \wedge (24|135) \wedge (34|12) \wedge (35|1) \wedge (45|2) \\ \Rightarrow \text{nothing.}$$

The structure on the left is a gaussoid.



## CI inference via SAT solvers II

Running the SAT solver CaDiCaL on the definition of **oriented** gaussoids confirms that their supports satisfy

$$(12|) \wedge (13|4) \wedge (14|5) \wedge (15|23) \wedge (23|5) \wedge (24|135) \wedge (34|12) \wedge (35|1) \wedge (45|2) \\ \Rightarrow \text{everything except } (25|K) \text{ for all } K.$$

The geometric model is that of a Markov network!



# The search for inference rules

Inference rules help characterize the *realizable* CI structures:

- 3-variate: 11 out of 64 by Matúš 2005.
- 4-variate: 629 out of 16 777 216 by Lněnička and Matúš 2007.
- 5-variate: *open!* (out of 1 208 925 819 614 629 174 706 176)
  - 254 826 gaussoids modulo symmetry
  - 87 834 of which are orientable gaussoids
  - 84 908 of which are *selfadhesive* orientable gaussoids.



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Help wanted:

- Use information inequalities and linear programming.
- Tropical approximations and valuated gaussoids.
- Compute algebraic realization spaces.
- Find and certify real solutions to polynomial systems.



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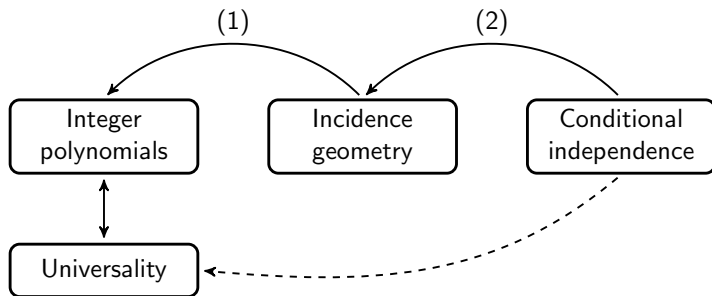


# Proof sketch





## Proof sketch



### Theorem

To every polynomial system  $\{f_i \bowtie 0\}$  one can compute a polynomially-sized set of CI constraints which has a model over a real algebraic extension  $\mathbb{K}/\mathbb{Q}$  if and only if the polynomial system has a solution in  $\mathbb{K}$ .

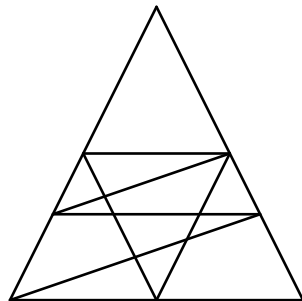


## (1) Algebra $\subseteq$ Synthetic geometry

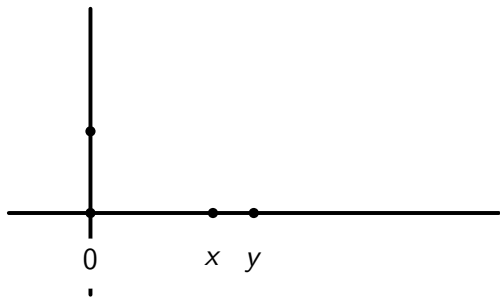
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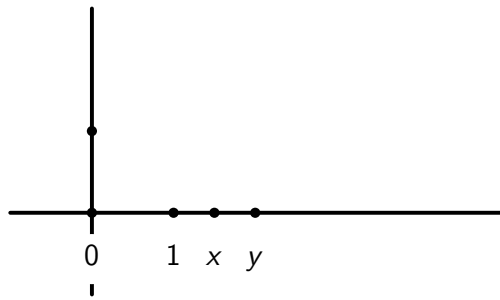
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# Von Staudt constructions



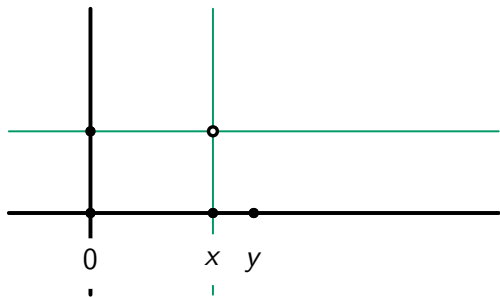
Addition



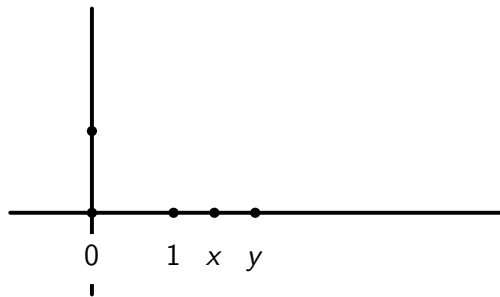
Multiplication



# Von Staudt constructions



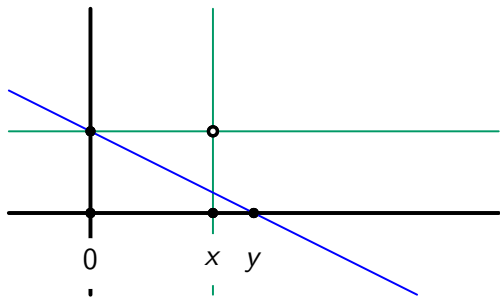
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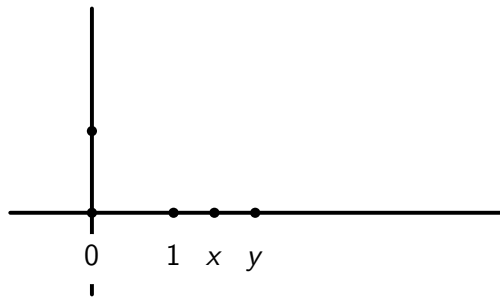
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# Von Staudt constructions



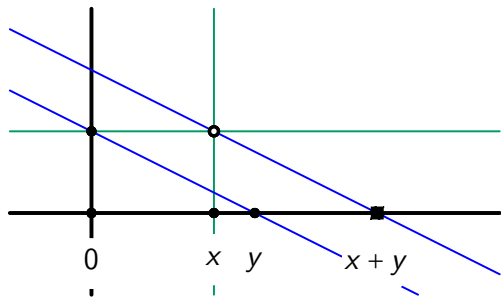
Addition



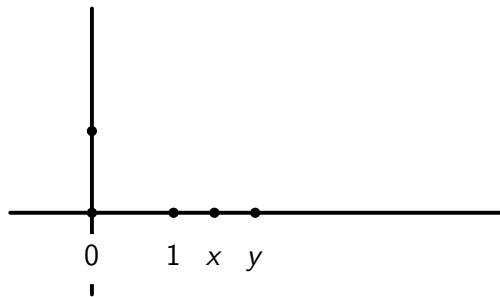
Multiplication



# Von Staudt constructions



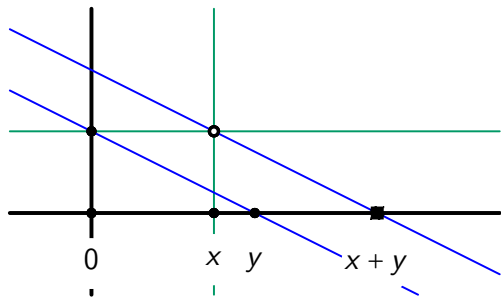
Addition



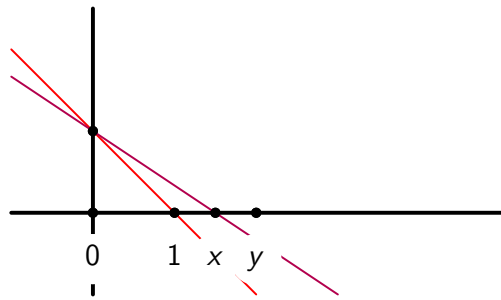
Multiplication



# Von Staudt constructions



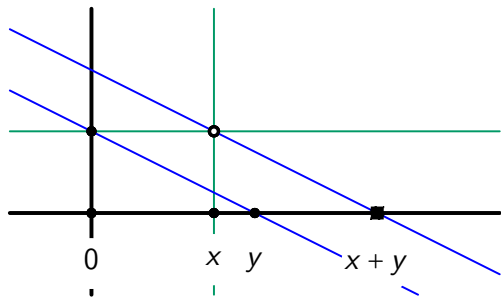
Addition



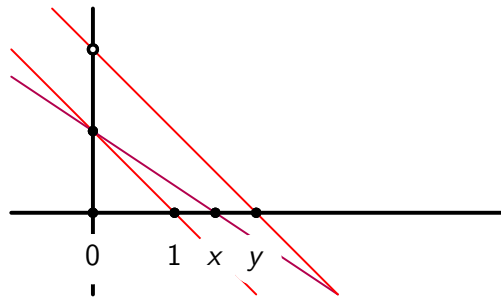
Multiplication



# Von Staudt constructions



Addition

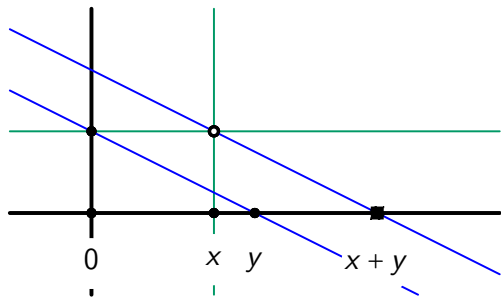


Multiplication

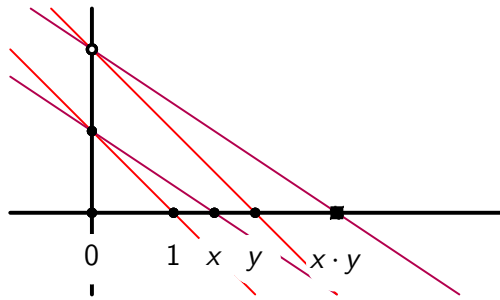




# Von Staudt constructions



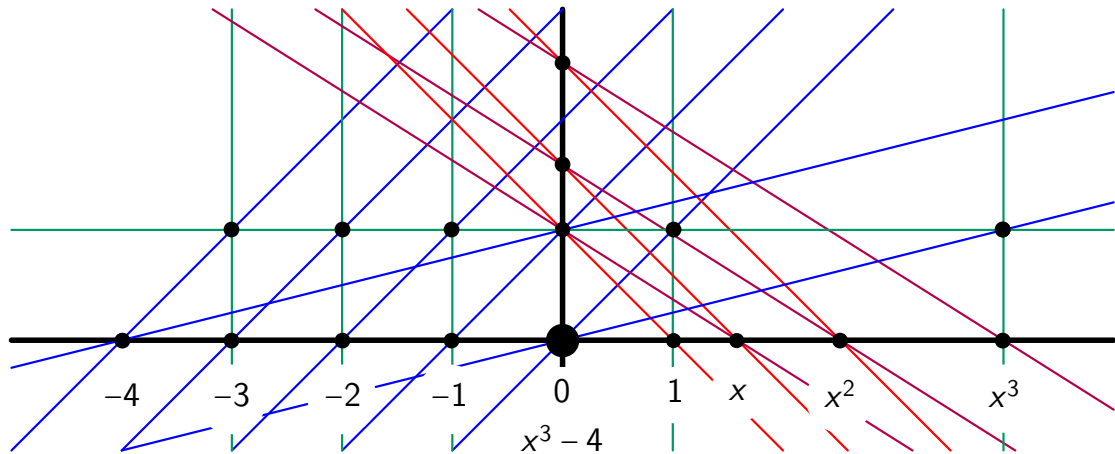
Addition



Multiplication



# The cube root of 4



## (2) Synthetic geometry $\subseteq$ Gaussian CI

$\Sigma[ij] = x_{ij} \rightarrow$  impose  $x_{kl} = x_{km} = x_{lm} = 0$  on a correlation matrix, then:

$$\begin{aligned} \Sigma[ij|klm] &= x_{ij}x_{kk}x_{ll}x_{mm} + x_{im}x_{jm}x_{kl}^2 - x_{im}x_{jl}x_{kl}x_{km} - x_{il}x_{jm}x_{kl}x_{km} + x_{il}x_{jl}x_{km}^2 \\ &\quad - x_{im}x_{jm}x_{kk}x_{ll} + x_{im}x_{jk}x_{km}x_{ll} + x_{ik}x_{jm}x_{km}x_{ll} - x_{ij}x_{km}^2x_{ll} \\ &\quad + x_{im}x_{jl}x_{kk}x_{lm} + x_{il}x_{jm}x_{kk}x_{lm} - x_{im}x_{jk}x_{kl}x_{lm} - x_{ik}x_{jm}x_{kl}x_{lm} \\ &\quad - x_{il}x_{jk}x_{km}x_{lm} - x_{ik}x_{jl}x_{km}x_{lm} + 2x_{ij}x_{kl}x_{km}x_{lm} + x_{ik}x_{jk}x_{lm}^2 \\ &\quad - x_{ij}x_{kk}x_{lm}^2 - x_{il}x_{jl}x_{kk}x_{mm} + x_{il}x_{jk}x_{kl}x_{mm} + x_{ik}x_{jl}x_{kl}x_{mm} \\ &\quad - x_{ij}x_{kl}^2x_{mm} - x_{ik}x_{jk}x_{ll}x_{mm} \\ &= x_{ij} - \sum_{k=l,m} x_{ik}x_{jk} = x_{ij} - \left\langle \begin{pmatrix} x_{ik} \\ x_{il} \\ x_{im} \end{pmatrix}, \begin{pmatrix} x_{jk} \\ x_{jl} \\ x_{jm} \end{pmatrix} \right\rangle. \end{aligned}$$



## (2) Synthetic geometry $\subseteq$ Gaussian CI

$$\left. \begin{array}{l} \Sigma[ij|klm] = 0 \Leftrightarrow \Sigma_{ij} = \langle \Sigma_{i,klm}, \Sigma_{j,klm} \rangle \\ \Sigma[ij] = 0 \Leftrightarrow \Sigma_{ij} = 0 \end{array} \right\} \Leftrightarrow \Sigma_{i,klm} \perp \Sigma_{j,klm}$$



## (2) Synthetic geometry $\subseteq$ Gaussian CI

$$\left. \begin{aligned} \Sigma[ij|klm] = 0 &\Leftrightarrow \Sigma_{ij} = \langle \Sigma_{i,klm}, \Sigma_{j,klm} \rangle \\ \Sigma[ij] = 0 &\Leftrightarrow \Sigma_{ij} = 0 \end{aligned} \right\} \Leftrightarrow \Sigma_{i,klm} \perp \Sigma_{j,klm}$$

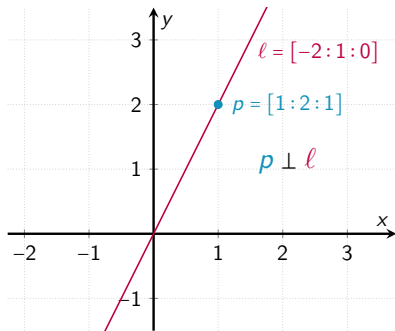
$p = \Sigma_{i,klm} = [p_x : p_y : p_z]$  and  $\ell = \Sigma_{j,klm} = [\ell_x : \ell_y : \ell_z]$   
are the *homogeneous coordinates* of a point and a line  
in the projective plane with  $p \in \ell^\perp$ .



## (2) Synthetic geometry $\subseteq$ Gaussian CI

$$\left. \begin{aligned} \Sigma[ij|klm] = 0 &\Leftrightarrow \Sigma_{ij} = \langle \Sigma_{i,klm}, \Sigma_{j,klm} \rangle \\ \Sigma[ij] = 0 &\Leftrightarrow \Sigma_{ij} = 0 \end{aligned} \right\} \Leftrightarrow \Sigma_{i,klm} \perp \Sigma_{j,klm}$$

$p = \Sigma_{i,klm} = [p_x : p_y : p_z]$  and  $l = \Sigma_{j,klm} = [l_x : l_y : l_z]$   
are the *homogeneous coordinates* of a point and a line  
in the projective plane with  $p \in l^\perp$ .



# Incidence relation in a CI model

$$\begin{array}{c}
 p_1 \\
 \vdots \\
 p_n \\
 l_1 \\
 \vdots \\
 l_m \\
 x \\
 y \\
 z
 \end{array}
 \left(
 \begin{array}{ccc|ccc|ccc}
 p_1 & \dots & p_n & l_1 & \dots & l_m & x & y & z \\
 p_1^* & & \langle p, p' \rangle & & & & p_1^x & p_1^y & p_1^z \\
 & \ddots & & & \langle p, l \rangle & & & \vdots & \\
 \langle p', p \rangle & & p_n^* & & & & p_n^x & p_n^y & p_n^z \\
 \hline
 & & & l_1^* & & \langle l, l' \rangle & l_1^x & l_1^y & l_1^z \\
 & \langle l, p \rangle & & & \ddots & & & \vdots & \\
 \hline
 & & & \langle l', l \rangle & & l_m^* & l_m^x & l_m^y & l_m^z \\
 \hline
 p_1^x & & p_n^x & l_1^x & & l_m^x & 1 & 0 & 0 \\
 p_1^y & \dots & p_n^y & l_1^y & \dots & l_m^y & 0 & 1 & 0 \\
 p_1^z & & p_n^z & l_1^z & & l_m^z & 0 & 0 & 1
 \end{array}
 \right)$$

