The Gaussian CI inference problem

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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 ξ_K is known, then learning the value of ξ_i does not give any information about ξ_j.

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Example: Let $\mathtt{c}_1$ and $\mathtt{c}_2$ be two independent coins and $\mathtt{b}$ a bell which rings if and only if $\mathtt{c}_1$ and $\mathtt{c}_2$ land with the same side up. What is the conditional independence relation of the system $(\mathtt{c}_1, \mathtt{c}_2, \mathtt{b})$ of random variables?

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Gaussian conditional independence

Let the random vector be normally distributed with covariance matrix $\Sigma \in \mathrm{PD}_N$.

Definition

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

- Σ is PD if and only if $\Sigma[K] > 0$ for all $K \subseteq N$.
- $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$ holds if and only if $\Sigma[ij|K] = 0$.

Special polynomials

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

Gaussian CI models

Definition

A *CI constraint* is a CI statement $\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K$ or its negation $\neg(\xi_i \perp\!\!\!\perp \xi_j \mid \xi_K)$.
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The *model* of a set of CI constraints is the set of all PD matrices which satisfy them.

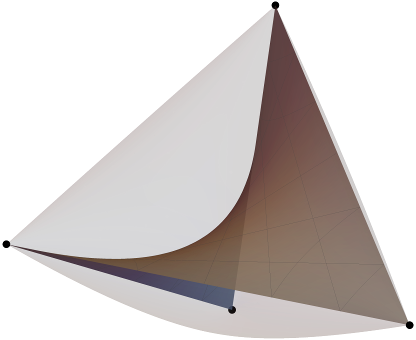

Figure: Model of $\Sigma[12 \mid 3] = 0$ in the space of 3×3 correlation matrices.

Models and inference

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

$$\bigwedge \mathcal{P} \Rightarrow \bigvee \mathcal{Q}$$

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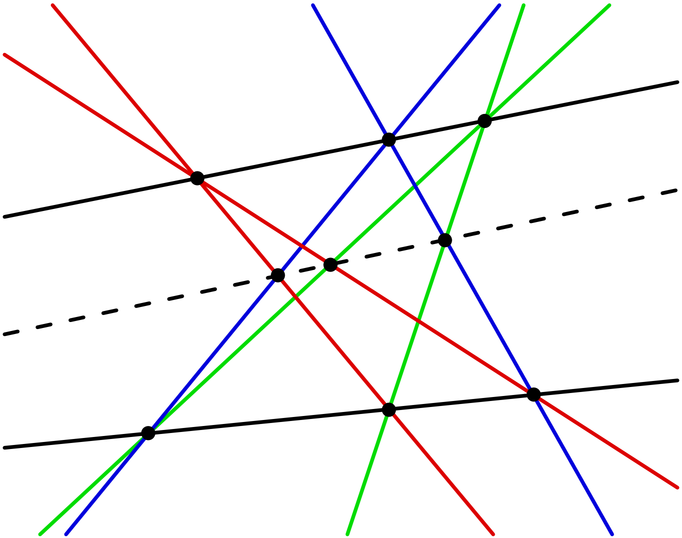
Reasoning about relevance statements in normally distributed random variables is the same as reasoning about the vanishing of very special kinds of determinants on very special kinds of varieties inside the positive-definite matrices.

For geometers: conditional independence ≈ collinearity



Examples of CI inference

Consider a general positive-definite 3×3 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:

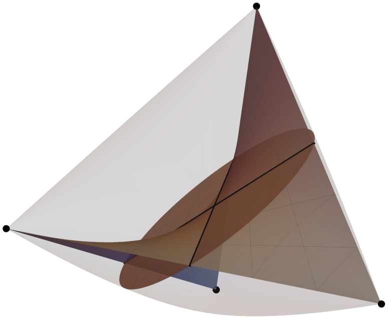
$$[12|3] \wedge [13|\,] \;\Rightarrow\; [12|\,] \wedge [13|2].$$

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 $\mathbb{Q}$?

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Model M85

$$\begin{matrix} 1 & a & b & c \\ a & 1 & d & e \\ b & d & 1 & f \\ c & e & f & 1 \end{matrix}$$

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

Theorem (Positivstellensatz)

A polynomial system $\{f_i = 0, g_j \geq 0, h_k \neq 0\}$ *is infeasible if and only if there exist* $f \in \mathrm{ideal}(f_i)$, $g \in \mathrm{cone}(g_j)$ *and* $h \in \mathrm{monoid}(h_k)$ *such that* $g + h^2 = f$.

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

A 5×5 final polynomial

The following inference rule is valid for all positive-definite 5×5 matrices:

$$[12\,|\,] \wedge [14\,|\,5] \wedge [23\,|\,5] \wedge [35\,|\,1] \wedge [45\,|\,2] \wedge [15\,|\,23] \wedge [34\,|\,12] \wedge [24\,|\,135] \;\Rightarrow\; [25\,|\,] \vee [34\,|\,].$$

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$$\begin{gathered}
[25\,|\,][34\,|\,]\cdot[1][2][3][15] = \\
\big(cd^2egr + bd^2fgr - ad^2grh - 2cd^2e^2i - 2bd^2efi - 2pdfgri + 2ad^2ehi + 2pdefi^2 - 2pdqhi^2 + 2pcqi^3 + \\
2pdqrij - 2pbqi^2j - pcegrt + pbfgrt + pagrht + 2pce^2it - 2pcqrit + 2pbqhit - 2paehit\big)\cdot[12\,|\,] + \\
\big(pdqer + pbqgr - 2pbqei\big)\cdot[14\,|\,5] - \big(pcdqr + p^2fgr - 2pbcqi + 2pb^2qj - 2p^2qrj\big)\cdot[23\,|\,5] + \\
\big(cdqgr - 2cdqei + 2pqghi - 2pqfi^2 - pqgrj + 2pqeij - 2pe^2ft + 2pqfrt\big)\cdot[35\,|\,1] + \\
\big(pd^2er - 2pbdei + p^2gri + 2pb^2et - 2p^2ert\big)\cdot[45\,|\,2] - \big(2pdfi - 2pbft\big)\cdot[15\,|\,23] - \\
\big(d^2gr - 2d^2ei - pgrt + 2peit\big)\cdot[34\,|\,12] - 2pqi\cdot[24\,|\,135].
\end{gathered}$$

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.

Approximations to the inference problem

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Theorem (Matúš 2005)

The following relations hold for every symmetric matrix Σ:

$$\Sigma[ij|L]^2 = \Sigma[iL] \cdot \Sigma[jL] - \Sigma[L] \cdot \Sigma[ijL]$$

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

Approximations to the inference problem

Theorem (Matúš 2005)

The following relations hold for every symmetric matrix Σ:

$$\Sigma[ij|L]^2 = \Sigma[iL] \cdot \Sigma[jL] - \Sigma[L] \cdot \Sigma[ijL] \quad \rightarrow \textit{semimatroids}$$

$$\Sigma[kL] \cdot \Sigma[ij|L] = \Sigma[L] \cdot \Sigma[ij|kL] + \Sigma[ik|L] \cdot \Sigma[jk|L] \quad \rightarrow \textit{gaussoids}$$

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

The Gaussian CI configuration space

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

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

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

Very wasteful encoding of a matrix, but this creates simple and useful relations on configuration vectors. The CI structure of Σ is encoded in its *zero pattern*.

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 $\Sigma[ij|K] = 0$?

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

$$\begin{aligned} [ij|L] \wedge [ij|kL] &\Rightarrow [ik|L] \vee [jk|L] \\ [ik|L] \wedge [ij|kL] &\Rightarrow [ij|L] \\ &\vdots \end{aligned}$$

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[ij|kL] \wedge [ik|jL] &\Rightarrow [ij|L] \wedge [ik|L] \\
[ij|L] \wedge [ik|L] &\Rightarrow [ij|kL] \wedge [ik|jL]
\end{aligned}$$

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 $\operatorname{sgn} \Sigma[K] = +1$ and the value of $\operatorname{sgn} \Sigma[ij|K]$?

$$[ij|L] > 0 \wedge [ij|kL] < 0 \;\Rightarrow\; \big([ik|L] > 0 \wedge [jk|L] > 0\big) \vee \big([ik|L] < 0 \wedge [jk|L] < 0\big)$$

→ *Oriented* and *orientable* gaussoids.

Oriented gaussoids

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

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→ *Oriented* and *orientable* gaussoids.

$$\begin{aligned}
[ij|\,L] \;&\wedge [kl|\,L] \;\wedge [ik|\,jlL] \wedge [jl|\,ikL] &&\Rightarrow [ik|\,L] \\
[ij|\,L] \;&\wedge [kl|\,iL] \wedge [kl|\,jL] \;\wedge [ij|\,klL] &&\Rightarrow [kl|\,L] \\
[ij|\,L] \;&\wedge [jl|\,kL] \wedge [kl|\,iL] \;\wedge [ik|\,jlL] &&\Rightarrow [ik|\,L] \\
[ij|\,kL] &\wedge [ik|\,lL] \wedge [il|\,jL] &&\Rightarrow [ij|\,L] \\
[ij|\,kL] &\wedge [ik|\,lL] \wedge [jl|\,iL] \;\wedge [kl|\,jL] &&\Rightarrow [ij|\,L]
\end{aligned}$$

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

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

The geometric model is a Gaussian graphical model!

The search for inference rules (since at least 2008!)

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.
  - 84 434 of which are selfadhesive (orientable gaussoids ∩ semimatroids).

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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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In Gabriele Kern-Isberner, Wilhelm Rödder, and Friedhelm Kulmann, editors, *Conditionals, Information, and Inference*, pages 152–161. Springer, 2005.

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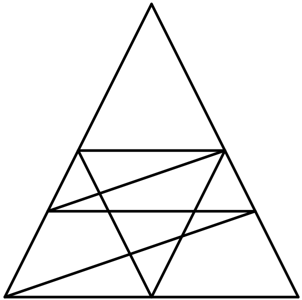
In *COMPSTAT conference*, 2006.

Proof sketch (1): Algebra ⊆ 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).

Proof sketch (2): Synthetic geometry ⊆ Gaussian CI

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

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

Incidence relation in a CI model

$$
\begin{array}{c}
\\
\mathrm{p}_1 \\ \vdots \\ \mathrm{p}_n \\ \mathrm{l}_1 \\ \vdots \\ \mathrm{l}_m \\ \mathrm{x} \\ \mathrm{y} \\ \mathrm{z}
\end{array}
\begin{array}{c}
\begin{array}{ccc|ccc|ccc}
\mathrm{p}_1 & \cdots & \mathrm{p}_n & \mathrm{l}_1 & \cdots & \mathrm{l}_m & \mathrm{x} & \mathrm{y} & \mathrm{z}
\end{array}
\\
\left(
\begin{array}{ccc|ccc|ccc}
p_1^* & & \langle p, p' \rangle & & & & p_1^x & p_1^y & p_1^z \\
& \ddots & & & \langle p, \ell \rangle & & & \vdots & \\
\langle p', p \rangle & & p_n^* & & & & p_n^x & p_n^y & p_n^z \\
\hline
& & & \ell_1^* & & \langle \ell, \ell' \rangle & \ell_1^x & \ell_1^y & \ell_1^z \\
& \langle \ell, p \rangle & & & \ddots & & & \vdots & \\
& & & \langle \ell', \ell \rangle & & \ell_m^* & \ell_m^x & \ell_m^y & \ell_m^z \\
\hline
p_1^x & & p_n^x & \ell_1^x & & \ell_m^x & 1 & 0 & 0 \\
p_1^y & \cdots & p_n^y & \ell_1^y & \cdots & \ell_m^y & 0 & 1 & 0 \\
p_1^z & & p_n^z & \ell_1^z & & \ell_m^z & 0 & 0 & 1
\end{array}
\right)
\end{array}
$$