

# Applications of Information Inequalities to Database Theory Problems

Dan Suciu

University of Washington

# Motivation

- Information theory has a long history in databases, e.g. [Lee, 1987].
- Influential work by Atserias, Grohe, Marx [Atserias et al., 2013] lead to successful applications to query upper bounds, worst-case optimal join algorithms, query containment under bag semantics.
- This talk: a overview of some of the recent results, intertwined with a brief tutorial on information theory.
- The paper: contains additional details and topics left out of the talk.

# Outline

- AGM Bound and Shannon Inequalities
- Max Degree Bounds and Non-Shannon Inequalities
- Query Domination and Max-Inequalities
- Approximate Implication and Conditional Inequalities
- Conclusions

# The AGM Bound and Shannon Inequalities

## Full Conjunctive Query

Relational schema:  $R_1, \dots, R_p$ .

Definition (Full conjunctive query (CQ))

$$Q(\mathbf{X}) = R_{j_1}(\mathbf{Y}_1) \wedge \dots \wedge R_{j_m}(\mathbf{Y}_m), \quad \text{where } \mathbf{Y}_1, \dots, \mathbf{Y}_m \subseteq \mathbf{X}.$$

E.g.  $Q(X, Y, Z) = R(X, Y) \wedge S(Y, Z) \wedge T(Z, X)$

- Database instance:  $D = (R_1^D, \dots, R_p^D)$ .
- Query output:  $Q(D)$ .

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# The Output Size Problem

Given statistics on the input  $\mathbf{D}$ , e.g. cardinalities, # distinct values:

- **Estimation Problem.** Compute “estimate”  $E$ :

$$|Q(\mathbf{D})| \approx E$$

Adopted in practice, however it is ill defined.

- **Upper Bound Problem.** Compute an upper bound  $B$ :

$$|Q(\mathbf{D})| \leq B$$

Challenge: make  $B$  tight.

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## Simple Examples

Assume  $|R| \leq N$ ,  $|S| \leq N$ ,  $|T| \leq N$ .

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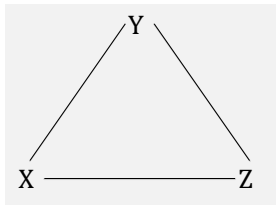
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- $Q(X, Y, Z) = R(X, Y) \wedge S(Y, Z) \wedge T(Z, X)$ .  $\max_{\mathcal{D}} |Q(\mathcal{D})| = N^{\frac{3}{2}}$

# Fractional Edge Covers

Query  $Q$  to hypograph  $G = (V, E)$ .

$$R(X, Y) \wedge S(Y, Z) \wedge T(Z, X)$$





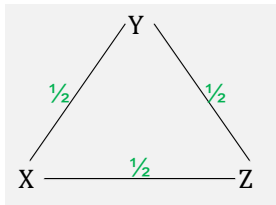
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## Definition

A fractional edge cover is  $\mathbf{w} = (w_e)_{e \in E}$ ,  $w_e \geq 0$ :  
 $\forall x \in V, \sum_{e \in E: x \in e} w_e \geq 1$ .



## The AGM Bound [Atserias et al., 2013]

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### Theorem (Upper Bound)

For every fractional edge cover  $\mathbf{w}$ :  $|Q| \leq |R_1|^{w_1} \cdots |R_m|^{w_m}$

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$$R(X, Y) \wedge S(Y, Z) \wedge T(Z, X) \quad AGM(Q) = \min \begin{pmatrix} (|R| \cdot |S| \cdot |T|)^{1/2} \\ |R| \cdot |S| \\ |R| \cdot |T| \\ |S| \cdot |T| \end{pmatrix}$$

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Proof. information inequalities.

# Entropic Vectors

## Definition

Finite probability space  $p : D \rightarrow [0, 1]$ .  $X =$  r.v. with outcomes  $D$ .

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$b$	$q$
$a$	$m$

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$X$	$Y$	$p$
$a$	$p$	$1/4$
$a$	$q$	$1/4$
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$h(XY) = \log 4$

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$h(XY) = \log 4$

$X$	$p$
$a$	$3/4$
$b$	$1/4$

$h(X) \leq \log 2$

$Y$	$p$
$p$	$1/4$
$q$	$2/4$
$m$	$1/4$

$h(Y) \leq \log 3$

$\emptyset$	$p$
	$1$

$h(\emptyset) = 0$

# Information Theory Viewed as Logic

Formulas:

$$\sum_{\alpha \subseteq [n]} c_{\alpha} h(X_{\alpha}) \geq 0$$

Information Inequality

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Information Inequality

Basic Shannon  
Inequalities:

$$h(\emptyset) = 0$$

$$h(\mathbf{U} \cup \mathbf{V}) \geq h(\mathbf{U})$$

Monotonicity

$$h(\mathbf{U}) + h(\mathbf{V}) \geq h(\mathbf{U} \cup \mathbf{V}) + h(\mathbf{U} \cap \mathbf{V})$$

Submodularity

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Model:  $\mathbf{h} \in \mathbb{R}_{+}^{2^n}$

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Classes of  
Models:

$\Gamma_n \stackrel{\text{def}}{=} \text{polymatroids}$ : satisfy Shannon inequalities

$\Gamma_n^* \stackrel{\text{def}}{=} \text{entropic vectors}$

$M_n \stackrel{\text{def}}{=} \text{modular}$ :  $h(X_1 X_2 \dots) = h(X_1) + h(X_2) + \dots$

$$M_n \subset \Gamma_n^* \subset \Gamma_n (\subset \mathbb{R}_+^{2^n})$$

# A Shannon Inequality

## Example

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Note:  $X$  is covered 2 times in each expressions. Same for  $Y$ , same for  $Z$ .

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Part 2: proof of the inequality  $\sum_j w_j h(\mathbf{Y}_j) \geq h(\mathbf{X})$ .

## Proof of the AGM Upper Bound: Part 2: $|Q| \leq |R_1|^{w_1} \dots |R_m|^{w_m}$

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### Theorem (Shearer?)

*The following are equivalent:*

- (1)  $\Gamma_n \models \mathbf{k} \cdot \mathbf{h} \geq k_0 h(\mathbf{X})$
- (2)  $\Gamma_n^* \models \mathbf{k} \cdot \mathbf{h} \geq k_0 h(\mathbf{X})$
- (3)  $M_n \models \mathbf{k} \cdot \mathbf{h} \geq k_0 h(\mathbf{X})$
- (4) Every variable is  
“covered”  $\geq k_0$  times.

[Balister and Bollobás, 2012]



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**Proof** (4)  $\Rightarrow$  (1)

Repeatedly replace  $h(\mathbf{Y}_i) + h(\mathbf{Y}_j)$   
with  $h(\mathbf{Y}_i \cup \mathbf{Y}_j) + h(\mathbf{Y}_i \cap \mathbf{Y}_j)$

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**Proof** (4)  $\Rightarrow$  (1)

Repeatedly replace  $h(\mathbf{Y}_i) + h(\mathbf{Y}_j)$   
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[Balister and Bollobás, 2012]

## Proof of the AGM Upper Bound: Part 2: $|Q| \leq |R_1|^{w_1} \dots |R_m|^{w_m}$

Consider the inequality  $k_1 h(\mathbf{Y}_1) + \dots + k_m h(\mathbf{Y}_m) \geq k_0 h(\mathbf{X})$ ,  $k_i \in \mathbb{N}$ :

### Theorem (Shearer?)

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- Thus,  $\mathbf{Y}'_1 = \mathbf{X}$  and  $k'_1 \geq k_0$ .

This proves the Upper Bound. Will skip the Lower Bound

## Summary of the AGM Bound

- AGM upper bound: apply submodularity in *any* order.
- AGM lower bound: from modular  $h^*$  to product relations.

Limitation: AGM uses only cardinality constraints.

Next: add functional dependencies and degree constraints.

# The Max-Degree Bound and Non-Shannon Inequalities



## General Statistics

Collect more statistics about the database  $D$ , such as:

- Relation cardinalities (as in the AGM bound).
- Keys and/or Functional Dependencies.
- Maximum degrees.
- $\ell_p$ -norms of degree sequences
- ...

# Max-Degrees

Fix a relation instance  $R(\mathbf{X})$ ,  $\mathbf{U}, \mathbf{V} \subseteq \mathbf{X}$

$$\text{deg}_R(\mathbf{V}|\mathbf{U} = \mathbf{u}) \stackrel{\text{def}}{=} |\{\mathbf{v} \mid (\mathbf{u}, \mathbf{v}) \in \Pi_{\mathbf{UV}}(R)\}|$$

$$\text{deg}_R(\mathbf{V}|\mathbf{U}) \stackrel{\text{def}}{=} \max_{\mathbf{u}} \text{deg}_R(\mathbf{V}|\mathbf{U} = \mathbf{u})$$

$U$	$V$
$a$	1
$a$	2
$a$	3
$b$	1
$b$	5

$R =$

$\text{deg}_R(\mathbf{V}|\mathbf{U}) = 3.$

Degree constrains generalize:

- Cardinality:  $|R| = \text{deg}_R(\mathbf{X}|\emptyset).$
- Functional Dependency  $\mathbf{U} \rightarrow \mathbf{V}$ :  $\text{deg}_R(\mathbf{V}|\mathbf{U}) = 1.$
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$$R = \begin{array}{|c|c|} \hline \mathbf{U} & \mathbf{V} \\ \hline a & 1 \\ a & 2 \\ a & 3 \\ b & 1 \\ b & 5 \\ \hline \end{array}$$

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## Information Measures

The *Conditional Entropy* and *Conditional Mutual Information* are:

$$h(\mathbf{V}|\mathbf{U}) \stackrel{\text{def}}{=} h(\mathbf{UV}) - h(\mathbf{U})$$

$$I(\mathbf{V}; \mathbf{W}|\mathbf{U}) \stackrel{\text{def}}{=} h(\mathbf{UV}) + h(\mathbf{UW}) - h(\mathbf{U}) - h(\mathbf{UVW})$$

$$\Gamma_n \models h(\mathbf{V}|\mathbf{U}) \geq 0, \quad \Gamma_n \models I(\mathbf{V}; \mathbf{W}|\mathbf{U}) \geq 0$$

If  $\mathbf{h} \in \Gamma_n^*$ , then:

$$h(\mathbf{V}|\mathbf{U}) = \mathbb{E}_{\mathbf{u}}[h(\mathbf{V}|\mathbf{U} = \mathbf{u})] \leq \log \deg(\mathbf{V}|\mathbf{U})$$

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## Max-Degree Bound by Example

### Example

$$Q(X, Y, Z, U) = R(X, Y) \wedge S(Y, Z) \wedge T(Z, U) \wedge A(\underline{X}, Z, U) \wedge B(X, Y, \underline{U})$$

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Inequality

$$h(XY) + h(YZ) + h(ZU) + h(U|XZ) + h(X|YU) \geq 2h(XYZU)$$

Implies

$$(|R| \cdot |S| \cdot |T| \cdot \deg_A(U|XZ) \cdot \deg_B(X|YU))^{1/2} \geq |Q|$$



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### Inequality

$$\log |R| + \log |S| + \log |T| + \log \deg_A(U|XZ) + \log \deg_B(X|YU) \geq h(XY) + h(YZ) + h(ZU) + h(U|XZ) + h(X|YU) \geq 2h(XYZU) = 2 \log |Q|$$

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# The Upper Bound [Khamis et al., 2017]

$$Q(\mathbf{X}) = \bigwedge_{j=1,m} R_j(\mathbf{Y}_j)$$

## Theorem

If  $\Gamma_n^* \models \sum_{i=1,s} w_i h(\mathbf{V}_i | \mathbf{U}_i) \geq h(\mathbf{X})$  then  $\prod_{i=1,s} \text{deg}_{R_j}^{w_i}(\mathbf{V}_i | \mathbf{U}_i) \geq |Q|$ .

$$M_n \models (\dots) \quad \begin{matrix} \leftarrow \\ \not\rightarrow \end{matrix} \quad \Gamma_n^* \models (\dots) \quad \begin{matrix} \leftarrow \\ \not\rightarrow \end{matrix} \quad \Gamma_n \models (\dots)$$

The  $\Gamma_n^*$ -bound is tight only “asymptotically”.

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## Summary

- Shannon inequalities are **sufficient** for the AGM bound.
- Shannon inequalities are **insufficient** for the Max-Degree bound.
- Shannon inequalities are **sufficient** for the Max-Degree bound for **simple degrees**.

$$M_n \models (\dots) \begin{matrix} \Leftarrow \\ \not\Leftarrow \end{matrix} N_n \models (\dots) \Leftrightarrow \Gamma_n^* \models (\dots) \Leftrightarrow \Gamma_n \models (\dots)$$

Moreover, the bound is tight.

# Query Domination and Max-Inequalities

## Definition

Fix two full CQs  $Q, Q'$ .

### Definition

$Q'$  *dominates*  $Q$  if  $\forall \mathbf{D}, |Q(\mathbf{D})| \leq |Q'(\mathbf{D})|$ . Write  $Q \preceq Q'$ .

Query domination problem: decide whether  $Q \preceq Q'$

Necessary condition:  $\exists \varphi : Q' \rightarrow Q$ .

E.g.  $R(U, V) \wedge R(V, W) \not\preceq R(X, Y) \wedge R(Y, Z) \wedge R(Z, X)$ .

Sufficient condition:  $\exists \varphi : Q' \rightarrow Q$  surjective.

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# History

Query domination  $Q \preceq Q'$  same as *query containment under bag semantics*.

- Introduced in [Chaudhuri and Vardi, 1993].
- Undecidable for Unions of CQ [Ioannidis and Ramakrishnan, 1995].
- Undecidable for CQs with Inequalities [Jayram et al., 2006].
- Sufficient condition [Kopparty and Rossman, 2011].
- Necessary+sufficient condition when  $Q'$  is acyclic [Khamis et al., 2021]



## Vee's Example [Kopparty and Rossman, 2011]

$$Q = R(X, Y) \wedge R(Y, Z) \wedge R(Z, X)$$



$$Q' = R(U, V) \wedge R(U, W)$$



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Three homomorphisms  $\varphi_1, \varphi_2, \varphi_3 : Q \rightarrow Q'$ ; none surjective.

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## Vee's Example [Kopparty and Rossman, 2011]

$$Q = R(X, Y) \wedge R(Y, Z) \wedge R(Z, X)$$



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We prove that  $Q \preceq Q'$

Three homomorphisms  $\varphi_1, \varphi_2, \varphi_3 : Q \rightarrow Q'$ ; none surjective.

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Assume  $E \circ \varphi_2 = h(YZ) + h(Z|Y) \geq h(XYZ)$ .

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$$\begin{aligned} \log |Q'(\mathbf{D})| &\geq h'(UVW) = h'(U) + h'(VW|U) \\ &= h'(U) + h'(V|U) + h'(W|U) \\ &= h(Y) + 2h(Z|Y) \geq h(XYZ) = \log |Q(\mathbf{D})| \end{aligned}$$

## Domination and Max-Inequalities

Fix  $Q, Q'$  and assume  $Q'$  is acyclic.

$$E_{Q'} \stackrel{\text{def}}{=} \sum_{A \in \text{atoms}(Q')} h(\text{vars}(A) | \text{vars}(A) \cap \text{vars}(\text{parent}(A)))$$

Theorem ( [Kopparty and Rossman, 2011, Khamis et al., 2021])

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- Max-inequalities and the domination problem  $Q \preceq Q'$  for  $Q'$  acyclic are computationally equivalent [Khamis et al., 2021].
- If any two atoms in  $Q'$  share at most one variable, then  $Q \preceq Q'$  is decidable.

# Approximate Implication and Conditional Inequalities

# Constraints (or Dependencies)

Fix a relation  $R(\mathbf{X})$ .

*Functional Dependency (FD)*

$$\boxed{U \rightarrow V}$$

for  $U, V \subseteq \mathbf{X}$ .

*Multivalued Dependency (MVD)*

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Goal: generalize to *Soft Constraints* (or *Soft Dependencies*).

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# The Constraint Implication Problem

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Given constraints  $\sigma_0, \sigma_1, \dots, \sigma_p$ , check if  $\sigma_1 \wedge \dots \wedge \sigma_p \Rightarrow \sigma_0$ .

[Armstrong, 1974] axiomatization for FDs.

[Beeri et al., 1977]: axiomatization for FDs and MVDs.

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## Relaxation Problem (informal)

If  $R$  satisfies  $\sigma_1, \dots, \sigma_p$  approximatively, does it satisfy  $\sigma_0$  approximatively?

## From Constraints to Information Measure

Fix  $R(\mathbf{X})$ , let  $p : R \rightarrow [0, 1]$  be uniform,  $\mathbf{h}$  its entropy.

Theorem ( [Lee, 1987])

$$R \models \mathbf{U} \rightarrow \mathbf{V} \quad \text{iff} \quad h(\mathbf{V}|\mathbf{U}) = 0$$

$$R \models \mathbf{U} \twoheadrightarrow \mathbf{V}|\mathbf{W} \quad \text{iff} \quad I(\mathbf{V}; \mathbf{W}|\mathbf{U}) = 0$$



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$$I(B; CD|A) = 0 \Rightarrow I(B; D|AC) = 0 \quad \text{conditional (in)equality!}$$

$$\text{Proof: } I(B; CD|A) = I(B; D|AC) + I(B; C|A) \geq I(B; D|AC).$$

# Conditional Information Inequalities

*Information inequality:*  $0 \geq \mathbf{c}_0 \cdot \mathbf{h}$

*Conditional information inequality:*  $\bigwedge_i (0 \geq \mathbf{c}_i \cdot \mathbf{h}) \Rightarrow (0 \geq \mathbf{c}_0 \cdot \mathbf{h})$

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Example:  $0 \geq I(B; CD|A) \Rightarrow 0 \geq I(B; D|AC)$

Because:  $I(B; CD|A) \geq I(B; D|AC)$

## The Relaxation Problem

Does the following hold?

If  $\bigwedge_i (0 \geq \mathbf{c}_i \cdot \mathbf{h}) \Rightarrow (0 \geq \mathbf{c}_0 \cdot \mathbf{h})$  then  $\exists \lambda_i \geq 0, \sum_i \lambda_i \mathbf{c}_i \cdot \mathbf{h} \geq \mathbf{c}_0 \cdot \mathbf{h}$

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- Any FD/MVD implication is a Shannon conditional inequality:

$$M_n \models (\dots) \not\Leftarrow N_n \models (\dots) \Leftrightarrow \Gamma_n^* \models (\dots) \Leftrightarrow \Gamma_n \models (\dots)$$

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$$M_n \models (\dots) \stackrel{\Leftarrow}{\neq} N_n \models (\dots) \Leftrightarrow \Gamma_n^* \models (\dots) \Leftrightarrow \Gamma_n \models (\dots)$$
- If an FD/MVD implication fails, then it fails on some  $R$  with 2 tuples.

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### Negative Results

- The following does not relax [Kaced and Romashchenko, 2013]:  
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### Negative Results

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 $I(X; Y|A) = I(X; Y|B) = I(A; B) = I(A; X|Y) = 0 \Rightarrow I(X; Y) = 0.$
- Every implication relaxes *with error* [Kenig and Suciu, 2022]:

$$\forall \epsilon > 0, \exists \lambda_i \geq 0, \quad \sum_i \lambda_i \mathbf{c}_i \cdot \mathbf{h} + \epsilon \mathbf{h}(\mathbf{X}) \geq \mathbf{c}_0 \cdot \mathbf{h}.$$

## Discussion

- Relaxation (Deduction Theorem) fails for  $\Gamma_n^*$  but holds for  $\Gamma_n$ .
- A subtle issue: semantics differs for  $\Gamma_n^*$  and for  $\bar{\Gamma}_n^*$ .
- Results on FD/MVD extend to *Approximate Acyclic Schemas* [Kenig et al., 2020].
- Open problem: “Soft Logic” based on information measures?

# Conclusions



# Summary

- AGM Bound.
- Max-Degree Bound.
- Query Domination.
- Approximate Implication.

**Information Theory:** both a logic, and a tool for logic.

## Some Open Problems

- Is  $\Gamma_n^* \models \mathbf{c} \cdot \mathbf{h} \geq 0$  decidable?
- What is the complexity of  $\Gamma_n \models \mathbf{c} \cdot \mathbf{h} \geq 0$  as a function of  $\|\mathbf{c}\|_1$ ?
- Is  $Q \preceq Q'$  decidable?
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THANK YOU!



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- The AGM bound [Atserias et al., 2013]
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## Proof of the AGM Lower Bound

$$R(X, Y) \wedge S(Y, Z) \wedge T(Z, X)$$

$$AGM(Q) = |R|^{w_1} \cdot |S|^{w_2} \cdot |T|^{w_3}$$

Primal program:

Minimize  $w_1 \log |R| + w_2 \log |S| + w_3 \log |T|$

Where  $(w_1, w_2, w_3) \in \mathbb{R}_+^3$

$\models w_1 h(XY) + w_2 h(YZ) + w_3 h(XZ) \geq h(XYZ)$

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## Brief History

- Pippenger [Pippenger, 1986]: inequalities are “*laws of information theory*”. Do Shannon inequalities form the complete laws?
- The breakthrough: a non-Shannon inequality with  $n = 4$  variables [Zhang and Yeung, 1998].
- There exists infinitely many non-equivalent non-Shannon inequalities with  $n = 4$  variable [Matús, 2007]. Hence<sup>1</sup>,  $\bar{\Gamma}_n^*$  is not a polytope.
- The characterization of  $\bar{\Gamma}_n^*$  is open to date.

---

<sup>1</sup> $\Gamma_n^*$  is not a cone, nor convex, but its topological closure  $\bar{\Gamma}_n^*$  is.

## A Non-Shannon Inequality [Zhang and Yeung, 1998]

$$\begin{aligned}
 I(X; Y) &\leq I(X; Y|A) + I(X; Y|B) + I(A; B) \\
 &\quad + I(X; Y|A) + I(A; Y|X) + I(A; X|Y) \quad (1)
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This implies  $\Gamma_n^* \models (1)$ .

$\Gamma_n \not\models (1)$ : see paper.



## Discussion

- Non-Shannon inequalities:  $\Gamma_n^* \models (\dots)$  yet  $\Gamma_n \not\models (\dots)$ .
  - ▶ Decidability of  $\Gamma_n^* \models (\dots)$  is open.
  - ▶ Lower bound holds only asymptotically:  $\mathbf{h}^* \in \Gamma_n^*$  to a worst-case instance uses the *group characterization* [Chan and Yeung, 2002].
- Shannon inequalities  $\Gamma_n \models (\dots)$  decidable in EXPTIME. But:
  - ▶ The order of submodularity steps matters.
  - ▶ The bound is not tight in general:  $\mathbf{h}^* \in \Gamma_n$  does not always correspond to a relation instance.

Next: we can recover elegant properties for “simple” inequalities.

## “Simple” Inequalities

The **step function** at  $\mathbf{V} \subseteq \mathbf{X}$  is:

$$h^{\mathbf{V}}(\mathbf{Z}) \stackrel{\text{def}}{=} \begin{cases} 0 & \text{if } \mathbf{Z} \cap \mathbf{V} = \emptyset \\ 1 & \text{otherwise} \end{cases}$$

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If all degrees are “simple”, then Max-Degree bound is computable, tight.