CS294-248 Special Topics in Database Theory Unit 4: AGM Bound, WCOJ

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Outline

• Today: the AGM bound. This is a mathematical formula that gives us $AGM(Q, \mathbf{D}) \stackrel{\text{def}}{=} \max_{\mathbf{D} \models \text{statistics}} |Q(\mathbf{D})|$.

• Thursday: Worst Case Optimal Join, by guest lecturer Hung Ngo. An algorithm that computes $Q(\mathbf{D})$ in time $\tilde{O}(AGM(Q,\mathbf{D}))$.

Background on Cardinality Estimation

Cardinality Estimation 101 (1/3)

Given:

Background

- Statistics on the input relations R_1, R_2, \dots
- A full conjunctive query Q

"Estimate":

• The size $|Q(\mathbf{D})|$.

Numerous applications: query optimization, memory provisioning, data partitioning.

Cardinality Estimation 101 (2/3)

Bottom-up on the query plan:

• Selection $\sigma_p(R)$: assume independence:

$$|\sigma_p(R)| \approx \theta_p \cdot |R|$$

$$\theta_{p_1 \wedge p_2} \approx \theta_{p_1} \cdot \theta_{p_2}$$

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- Join $J(A, B, C) = R(A, B) \land S(B, C)$: assume preservation of values
 - $|J| \approx |R| \cdot \operatorname{avg}(\operatorname{deg}_{S}(C|B)) = \frac{|R| \cdot |S|}{|\operatorname{Dom}(S.B)|}.$
 - $|J| \approx |S| \cdot \operatorname{avg}(\operatorname{deg}_R(A|B)) = \frac{|R| \cdot |S|}{|\operatorname{Dom}(R.B)|}$
 - ▶ Heuristic: take the *minimum*:

$$|J| \approx \frac{|R| \cdot |S|}{\max(|\mathsf{Dom}(R.B)| \cdot |\mathsf{Dom}(S.B)|)}$$

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Cardinality Estimation 101 (3/3)

Background

Notoriously hard to estimate cardinality of complex queries.

• No rigorous definition of the estimate: there is no probability space.

- How do we combine multiple sources of information?
 - ▶ We had two formulas for the join, why choose min?
 - ▶ Given R(A, B, C) and histograms on A, B, C, AB, AC, how do we estimate $|\sigma_{A=2,B=4,C=6}(R)|$?

Upper Bound on the Output of a Query

Given statistics on the input D, e.g. cardinalities, # distinct values,

Compute an upper bound B:

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

Challenge: make *B* tight.

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

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

$$\max_{\boldsymbol{D}} |Q(\boldsymbol{D})| = ?$$

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

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- $\max_{\boldsymbol{D}} |Q(\boldsymbol{D})| = N^2$ $\max_{\boldsymbol{D}} |Q(\boldsymbol{D})| = N$
- $Q(X, Y, Z, U) = R(X, Y) \wedge S(Y, Z) \wedge T(Z, U)$. $\max_{\mathbf{D}} |Q(\mathbf{D})| = ?$

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

• $Q(X, Y, Z) = R(X, Y) \wedge S(Y, Z)$. If S.Y is a key:

$$\max_{\boldsymbol{D}} |Q(\boldsymbol{D})| = N^2$$

 $\max_{\boldsymbol{D}} |Q(\boldsymbol{D})| = N$

• $Q(X, Y, Z, U) = R(X, Y) \wedge S(Y, Z) \wedge T(Z, U)$. $\max_{\mathbf{D}} |Q(\mathbf{D})| = \mathbb{N}^2$ Notice the role of an edge cover

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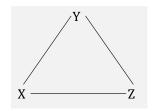
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- $\max_{\boldsymbol{D}} |Q(\boldsymbol{D})| = N^{\frac{3}{2}}$ • $Q(X, Y, Z) = R(X, Y) \wedge S(Y, Z) \wedge T(Z, X)$. Here we use a fractional edge cover

AGM Bound: The Statement

Fractional Edge Covers

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

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



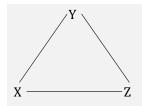
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Definition

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



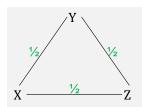
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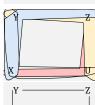
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What are fractional edge covers?





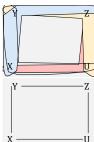
5-cycle

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

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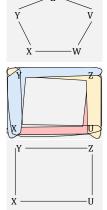




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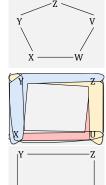


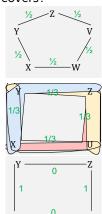


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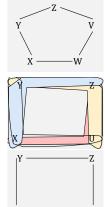


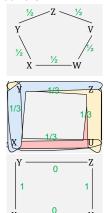


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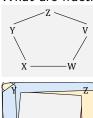


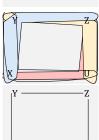
$$R(X, Y, Z) \land S(Y, Z, U)$$

$$\land T(Z, U, X) \land K(U, X, Y)$$

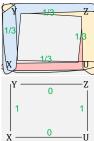
$$\begin{vmatrix} Y & & & \\ & & & \\ 0 & & & 0 \end{vmatrix}$$

What are fractional edge covers?









5-cycle

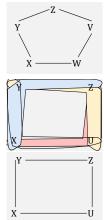
Loomis-Whitney:

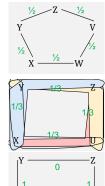
 $R(X, Y, Z) \wedge S(Y, Z, U)$ $\wedge T(Z, U, X) \wedge K(U, X, Y)$



 $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is a convex combination of (1, 0, 1, 0) and (0, 1, 0, 1).

What are fractional edge covers?







Loomis-Whitney:

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

 $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is a convex combination of (1, 0, 1, 0) and (0, 1, 0, 1). Vertex of the edge covering polytope: not > convex combination of others.

$$Q(\boldsymbol{X}) = R_1(\boldsymbol{Y}_1) \wedge \cdots \wedge R_m(\boldsymbol{Y}_m)$$

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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Theorem (Lower Bound)

$$AGM(Q) \stackrel{def}{=} \min_{\mathbf{w}} |R_1|^{w_1} \cdots |R_m|^{w_m}$$
 is "tight".

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

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

$$AGM(Q) = \min \begin{pmatrix} (|R| \cdot |S| \cdot |T|)^{1/2} \\ |R| \cdot |S| \\ |R| \cdot |T| \\ |S| \cdot |T| \end{pmatrix}$$

Minimum over vertices of the edge-covering polytope. WHY?

Proof Outline

• Proof of the upper bound: information inequalities (a.k.a. entropic inequalities).

• Proof of the lower bound: construct a worst-case database instance by using strong duality of linear optimization.



Proof of the Upper Bound

Definition

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

The *entropy* of X is:

$$h(X) \stackrel{\text{def}}{=} -\sum_{x \in D} p(x) \log p(x)$$

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R.v. X_1, \ldots, X_n . Their *entropic vector* is $\mathbf{h} = (h(X_\alpha))_{\alpha \subseteq [n]} \in \mathbb{R}^{2^n}_+$.

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X	Y	
a	р	
a	q	
Ь	q	
a	m	

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X	Y	p
а	р	1/4
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Ь	q	1/4
a	m	1/4

 $h(XY) = \log 4$

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a	m	1/4

$$\frac{a \mid m}{h(XY)} = \frac{1}{4}$$





$$h(X) < \log 2$$

$$h(Y) < \log 3$$

$$h(\emptyset) = 0$$

Shannon Inequalities

Basic Shannon Inequalities

$$h(\emptyset) = 0$$
 $h(m{U} \cup m{V}) \ge h(m{U})$ Monotonicity $h(m{U}) + h(m{V}) \ge h(m{U} \cup m{V}) + h(m{U} \cap m{V})$ Submodularity

A Shannon inequality is a consequence of these inequalities.

$$h(XY) + h(YZ) + h(XZ) \ge 2h(XYZ)$$

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$$= 2h(XYZ)$$

Example

$$h(XY) + h(YZ) + h(XZ) \ge 2h(XYZ)$$

$$\frac{h(XY) + h(YZ) + h(XZ)}{\geq h(XYZ) + h(Y) + h(XZ)}$$
$$\geq 2h(XYZ) + h(\emptyset)$$
$$= 2h(XYZ)$$

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

Proof: Upper Bound

Proof of the AGM Upper Bound: Part 1: $|Q| \leq |R_1|^{w_1} \cdots |R_m|^{w_m}$



$$|Q| \leq |R_1|^{w_1} \cdots |R_m|^{w_m}$$

From Query to Information Inequality:

$$Q(X,Y,Z) = R(X,Y) \wedge S(Y,Z) \wedge T(Z,X), \qquad |Q| \leq (|R| \cdot |S| \cdot |T|)^{1/2}.$$

From Query to Information Inequality:

Example

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Instance $\mathbf{D} = (R^D, S^D, T^D); \quad p: Q(\mathbf{D}) \to [0, 1]$ uniform; \mathbf{h} its entropy.

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$$\log |R^D| + \log |S^D| + \log |T^D|$$

$$\geq h(XY) + h(YZ) + h(XZ)$$

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$$\log |R^{D}| + \log |S^{D}| + \log |T^{D}|$$
> h(XY) + h(YZ) + h(XZ) > 2h(XYZ)

From Query to Information Inequality:

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$$= 2 \log |Q(\mathbf{D})|$$

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$$\geq h(XY) + h(YZ) + h(XZ) \geq 2h(XYZ)$$

$$= 2\log |Q(\mathbf{D})|$$

For a general query
$$Q(\boldsymbol{X}) = R_1(\boldsymbol{Y}_1) \wedge \cdots \wedge R_m(\boldsymbol{Y}_m)$$
:
If $\left[\sum_j w_j h(\boldsymbol{Y}_j) \geq h(\boldsymbol{X})\right]$ then $\left[|R_1|^{w_1} \cdots |R_m|^{w_m} \geq |Q|\right]$

$$|Q|\leq |R_1|^{w_1}\cdots |R_m|^{w_m}$$

Theorem (Generalized Shearer's Inequality)

If **w** is a frac. edge cover, then
$$w_1h(\mathbf{Y}_1) + \cdots + w_mh(\mathbf{Y}_m) \geq h(\mathbf{X})$$
.

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- We stop when $Y_1 \supset Y_2 \supset \cdots$
- Thus, $Y_1 = X$ and $k_1 > k_0$.

$$\cdots \geq k_1 h(\mathbf{Y}_1) \geq k_0 h(\mathbf{X})$$

This completes the proof of the Upper AGM Bound.

Discussion

• Shearer's inequality: apply submodularity repeatedly, in any order!

• Shearer inequalities correspond 1-1 to fractional edge covers.

• Any inequality is an upper bound on |Q|: AGM(Q) is the smallest.

How tight is AGM(Q) upper bound? Next

Proof of the Lower Bound

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By example:

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

$$AGM(Q) = \min_{\mathbf{w}} |R|^{w_R} \cdot |S|^{w_S} \cdot |T|^{w_T}$$

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Minimize

$$w_R \log |R| + w_S \log |S| + w_T \log |T|$$
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Special Case: $|R| = |S| = \cdots = N$

Definition

Fix a hypergraph (V, E); $(v_X)_{X \in V} \in \mathbb{R}_+^{|V|}$ is a fractional vertex packing if: $\forall \mathbf{Y} \in E :, \left[\sum_{X \in \mathbf{Y}} v_X \le 1 \right]$

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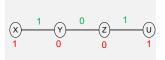
$$Q = [N^{vx}] \times [N^{vy}] \times [N^{vz}]$$

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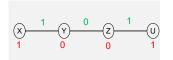
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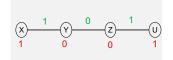
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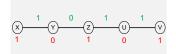
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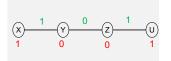
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Summary of the AGM Bound

- Upper / lower bound: fractional edge cover / vertex packing.
- Their equality follows from strong duality.
- The worst-case instance of the AGM bound is a Product Database.
- Full CQs only. Otherwise, ignore non-head variables.

Limitation of AGM: only cardinalities. Next: extensions to other stats.



Extensions of the AGM Bound

More Statistics

Statistics for a relation R(U, V, W, ...):

- Cardinality |R|.
- Same for any projection: $|R.U|, |R.UV|, \dots$
- Max degree: $\max(\deg_{R}(VW|U)), \ldots$
- Note: an FD $U \to V$ is $\max(\deg_R(V|U)) = 0$.
- ℓ_p -norm degree sequences: $||\deg_R(V|U)||_2, \dots$

Simple Functional Dependencies

Given FDs, $|Q| \ll AGM(Q)$.

E.g. $R(X, Y) \wedge S(Y, Z)$: \mathbb{N}^2 becomes \mathbb{N} when $Y \to Z$.

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 $\boldsymbol{U} \rightarrow \boldsymbol{V}$ is simple if $|\boldsymbol{U}| = 1$.

Method [Khamis et al., 2016]:

- Expand Q to Q^+ by replacing each atom R(Y) with $R'(Y^+)$.
- Return $AGM(Q^+)$.
- This bound is tight. Proof: very useful exercise.

$$Q(X,Y,Z) = R(X,Y) \land S(Y,Z) \land T(Z,X)$$

Fractional edge covers: $(1,1,0), (1,0,1), (0,1,1), (1/2,1/2,1/2)$

$$|Q| \leq \min(|R| \cdot |S|, |R| \cdot |T|, |S| \cdot |T|, \sqrt{|R| \cdot |S| \cdot |T|})$$

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Assume that S.Y is a key: $Y \rightarrow Z$ $Q^+(X,Y,Z) = R'(X,Y,Z) \land S(Y,Z) \land T(Z,X)$ Fractional edge covers: (1,0,0),(0,1,1)

$$|Q| \leq \min(|R|, |S| \cdot |T|)$$

Discussion

The expansion procedure is very easy, but limited only to simple FDs:

 $AGM(Q^{+})$ is always an upper bound on Q's output, but may not be tight.

Need to use entropic inequalities, beyond Shearer

Conditional Entropy

The Conditional Entropy

$$h(\boldsymbol{V}|\boldsymbol{U}) \stackrel{\mathsf{def}}{=} h(\boldsymbol{U}\boldsymbol{V}) - h(\boldsymbol{U})$$

Extensions

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What it means: $h(V|U) = \mathbb{E}_{\boldsymbol{u}}[h(V|U=u)]$

The submodularity inequality can be written equivalently as:

$$h(V|U) \ge h(V|UW)$$

Extensions

Example of Statistics:

$$R = \begin{bmatrix} U & V & W \\ a & 1 & m \\ a & 1 & n \\ a & 2 & m \\ a & 3 & m \\ b & 1 & m \\ b & 5 & m \end{bmatrix}$$

$$\max(\deg_R(VW|U)) = 4$$

$$h(VW|U) \le \log\max(\deg_R(VW|U))$$

$$|R| = 6$$

$$|R.U| = 2$$

$$|R.V| = 4$$

$$|R.UV| = 5$$

$$h(UVV) \le \log |R|$$

$$h(U) \le \log |R.U|$$

$$\max(\deg_R(V|U)) = 3$$

$$h(V|U) \le \log\max(\deg_R(V|U))$$

. . .

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Assume
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$$|Q| < N^{3/2}.$$

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$$\log |R| + \log |S| + \log |T| + \log \max \deg_A(U|XZ) + \log \max \deg_B(X|YU) \ge 0$$

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

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

$$\geq h(XYZ) + \underline{h(Y) + h(ZU)} + h(U|XZ) + h(X|YU)$$

$$\geq h(XYZ) + \underline{h(YZU)} + h(U|XZ) + h(X|YU)$$

$$Q = R(X, Y) \land S(Y, Z) \land T(Z, U) \land A(X, Z, U) \land B(X, Y, U)$$

Assume
$$|R| = |S| = |T| = N$$
:

$$AGM(Q) = N^2$$
.

If the FDs
$$XZ \rightarrow U$$
 and $YU \rightarrow X$ hold:

$$\frac{|Q| \leq N^{3/2}}{2\pi (X|X|X)} > \frac{|Q| \leq N^{3/2}}{2\pi (X|X|X)}$$

$$\log |R| + \log |S| + \log |T| + \log \max \deg_A(U|XZ) + \log \max \deg_B(X|YU) \ge 1$$

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

$$\geq h(XYZ) + h(Y) + h(ZU) + h(U|XZ) + h(X|YU)$$

$$\geq h(XYZ) + h(YZU) + h(U|XZ) + h(X|YU)$$

$$Q = R(X, Y) \land S(Y, Z) \land T(Z, U) \land A(X, Z, U) \land B(X, Y, U)$$

Assume
$$|R| = |S| = |T| = N$$
:

$$AGM(Q) = N^2$$
.

If the FDs
$$XZ \rightarrow U$$
 and $YU \rightarrow X$ hold:

$$\frac{|Q| \leq N^{3/2}}{2\pi (X|X|I)} >$$

$$\log |R| + \log |S| + \log |T| + \log \max \deg_A(U|XZ) + \log \max \deg_B(X|YU) \ge$$

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

$$\geq h(XYZ) + h(Y) + h(ZU) + h(U|XZ) + h(X|YU)$$

$$\geq h(XYZ) + h(YZU) + \underline{h(U|XZ)} + \underline{h(X|YU)}$$

$$\geq h(XYZ) + h(YZU) + \underline{h(U|XYZ)} + \underline{h(X|YZU)}$$

$$= 2h(XYZU) = \boxed{2 \log |Q|}$$

$$Q = R(X, Y) \land S(Y, Z) \land T(Z, U) \land A(X, Z, U) \land B(X, Y, U)$$

Assume
$$|R| = |S| = |T| = N$$
: $AGM(Q) = N^2$. If the FDs $XZ \to U$ and $YU \to X$ hold: $|Q| \le N^{3/2}$.

 $\log |R| + \log |S| + \log |T| + \log \max \deg_A(U|XZ) + \log \max \deg_B(X|YU) \ge 0$

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

$$\geq h(XYZ) + h(Y) + h(ZU) + h(U|XZ) + h(X|YU)$$

$$\geq h(XYZ) + h(YZU) + h(U|XZ) + h(X|YU)$$

$$\geq h(XYZ) + h(YZU) + h(U|XYZ) + h(X|YZU)$$

$$= 2h(XYZU) = \boxed{2 \log |Q|}$$

$$|Q| \leq \sqrt{|R| \cdot |S| \cdot |T| \cdot \max(\deg(U|XZ)) \cdot \max(\deg(X|YU))}$$

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Discussion

- AGM/Shearer limited to cardinality statistics.
- More general statistics require general entropic inequalities.
- Everything gets harder: fractional edge cover no longer sufficient, order of the submodularity matters.
- Can we compute the upper bound? Is it tight? Yes and no, it's complicated [Suciu, 2023].
- Do they work in practice? Yes, but you need to do the engineering work [Deeds et al., 2023].



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