

Relational Algorithms

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Relational AI

Fine-Grained Complexity, Logic, and Query Evaluation

Simons Institute

Outline

- What are Relational Algorithms?
- Technical Tools
 - Sum-Product Queries
- Example: Relational Linear Regression
- Generalizing the Example?
- Open Problems

What are Relational Algorithms?

Relational Algorithms

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- The algorithms *utilizes* relational structure for
 - *better performance*
 - *better results*

Relational Algorithms

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- The algorithms *utilizes* relational structure for
 - *better performance*
 - *better results*
- The output can be represented relationally

Example

$$Q(x_1, x_2, x_3, y) = R(x_1, x_2) \wedge S(x_2, x_3) \wedge T(x_3, y)$$

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| x_1 | x_2 |
|-------|-------|
| a | 1 |
| a | 3 |
| b | 1 |

| x_2 | x_3 |
|-------|-------|
| 1 | e |
| 4 | d |

| x_3 | y |
|-------|-----|
| d | 1.5 |
| e | 2.0 |
| e | 2.5 |

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Input

Goal: Compute
something

that depends on Q

Low-level Computation: Aggregation

$$Q(x_1, x_2, x_3, y) = R(x_1, x_2) \wedge S(x_2, x_3) \wedge T(x_3, y)$$

$$s = \sum_{(x_1, x_2, x_3, y) \in Q} y^2$$

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- **Non-relational** Algorithm
 - Compute $Q(x_1, x_2, x_3, y)$ then sum y^2
 - Time: $\tilde{O}(|R| \cdot |T|)$

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- **Non-relational** Algorithm

- Compute $Q(x_1, x_2, x_3, y)$ then sum y^2
- Time: $\tilde{O}(|R| \cdot |T|)$

- **Relational** Algorithm

- *Push* the sum *inside* the query

$$\circ s = \sum_{(x_1, x_2) \in R} \left(\sum_{x_3: (x_2, x_3) \in S} \left(\sum_{y: (x_3, y) \in T} y^2 \right) \right)$$

- Time: $\tilde{O}(|R| + |S| + |T|)$

High-level Computation: ML Training

$$Q(x_1, x_2, x_3, y) = R(x_1, x_2) \wedge S(x_2, x_3) \wedge T(x_3, y)$$

Train some ML model on $Q(x_1, x_2, x_3, y)$
to predict y from (x_1, x_2, x_3)

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 - Materialize Q (a **big** matrix)
 - Run ML

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- **Non-relational** Algorithm
 - Materialize Q (a **big** matrix)
 - Run ML
- **Relational** Algorithm
 - Operate directly on (**small**) R, S, T
 - *Push ML inside* the query?

Technical Tools

Sum-Product Queries

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- A technical tool to *describe* and *develop* (some) relational algorithms

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Sum-Product Queries

- A technical tool to *describe* and *develop* (some) relational algorithms
 - Relational Algorithm \Rightarrow Solving SPQs
- A universal language to express many problems
 - Databases
 - Linear Algebra
 - CSP
 - Logic
 - PGMs
 - ...

Sum-Product Queries

- Input

Sum-Product Queries

- Input
 - A commutative semiring $(D, \oplus, \otimes, \mathbf{0}, \mathbf{1})$
 - $\mathbf{0} \oplus a = a$
 - $\mathbf{1} \otimes a = a$
 - $\mathbf{0} \otimes a = \mathbf{0}$
 - $a \otimes (b \oplus c) = (a \otimes b) \oplus (a \otimes c)$

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 - A variable set X
 - Subsets $X_1, \dots, X_m \subseteq X$
 - Functions $\psi_1(X_1), \dots, \psi_m(X_m)$ to D
 - A subset $Y \subseteq X$
- Goal: Compute
 - $$\varphi(Y) := \bigoplus_{X-Y} \psi_1(X_1) \otimes \dots \otimes \psi_m(X_m)$$

Examples

$$\varphi(a, d) = \bigoplus_{b,c} \psi_1(a, b) \otimes \psi_2(b, c) \otimes \psi_3(c, d)$$

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- Is there a 3-path from a to d ?

- $Q_1(a, d) = \bigvee_{b,c} E(a, b) \wedge E(b, c) \wedge E(c, d)$

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- How many 3-paths?

- $Q_2(a, d) = \sum_{b,c} 1_E(a, b) \times 1_E(b, c) \times 1_E(c, d)$

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- Shortest 3-path?

- $Q_3(a, d) = \min_{b,c} W(a, b) + W(b, c) + W(c, d)$

Examples

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- Matrix multiplication

- $M(a, d) = \sum_{b,c} M_1(a, b) \times M_2(b, c) \times M_3(c, d)$

Examples

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Compute minimum ℓ_1 -norm among $(x_1, x_2, x_3, x_4) \in Q$

$$\varphi = \min_{x_1, x_2, x_3, x_4} \psi_R(x_1, x_2) + \psi_S(x_2, x_3) + \psi_T(x_3, x_4)$$

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- $\psi_R(x_1, x_2) := \begin{cases} |x_1| + |x_2| & \text{if } (x_1, x_2) \in R \\ \infty & \text{otherwise} \end{cases}$

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- $\psi_T(x_3, x_4) := \begin{cases} |x_4| & \text{if } (x_3, x_4) \in T \\ \infty & \text{otherwise} \end{cases}$

Solving SPQs using Join Algorithms

$$\varphi(x) = \bigoplus_{y,z} \psi_1(x, y) \otimes \psi_2(y, z) \otimes \psi_3(x, z)$$

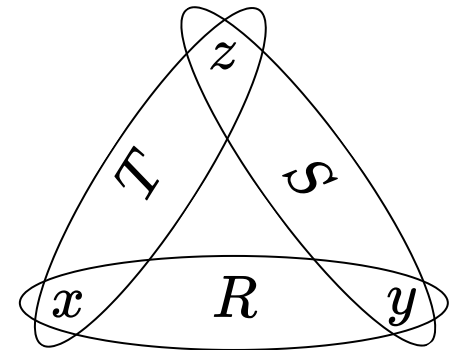
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$$Q(x, y, z) := R(x, y) \wedge S(y, z) \wedge T(x, z)$$

$$R := \{(x, y) \mid \psi_1(x, y) \neq \mathbf{0}\}$$



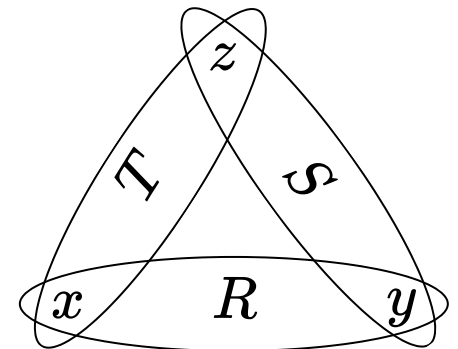
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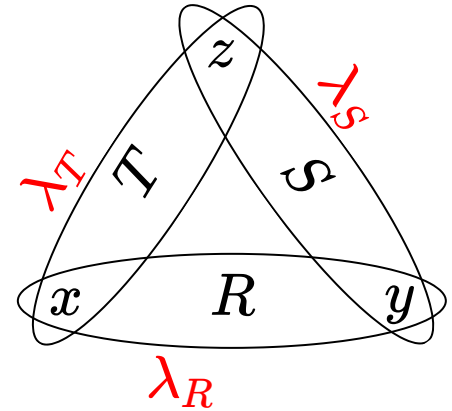
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- Use *Worst-case Optimal Joins (WCOJ)* or beyond
 - See [Logic&Algo-in-DB&AI BootCamp](#)

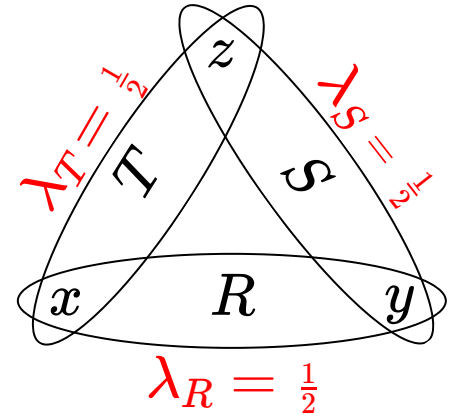
WCOJ Runtime

- $(\lambda_R, \lambda_S, \lambda_T)$ is a *fractional edge cover*



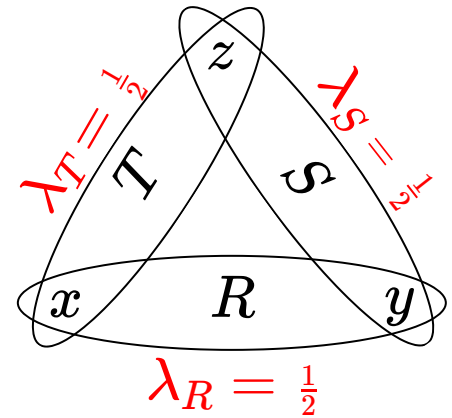
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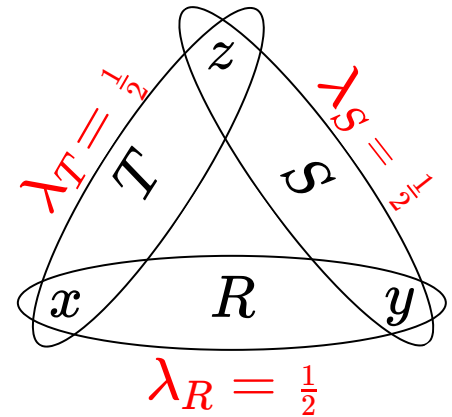
WCOJ Runtime

- $(\lambda_R, \lambda_S, \lambda_T)$ is a *fractional edge cover*
- ρ^* is the minimum $\lambda_R + \lambda_S + \lambda_T$



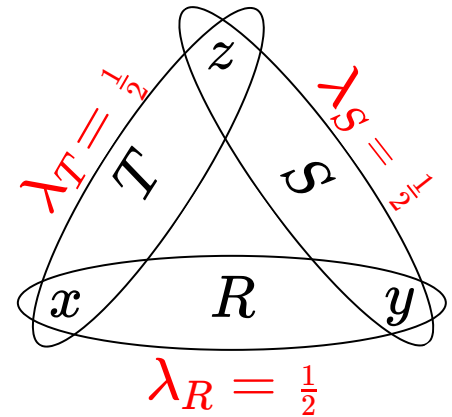
WCOJ Runtime

- $(\lambda_R, \lambda_S, \lambda_T)$ is a *fractional edge cover*
- ρ^* is the minimum $\lambda_R + \lambda_S + \lambda_T$
- \Rightarrow
 - $|Q| \leq N^{\rho^*}$ (AGM-bound)
 - Time = $\tilde{O}(N^{\rho^*})$



WCOJ Runtime

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 - $|Q| \leq N^{\rho^*}$ (AGM-bound)
 - Time = $\tilde{O}(N^{\rho^*})$



Examples:

- k -clique: $\rho^* = k/2$
- k -path: $\rho^* = \lceil k/2 \rceil$

Solving SPQs using Variable Elimination

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- Eliminate t

$$\blacksquare \varphi = \bigoplus_{x,y,z} \psi_1(x, y) \otimes \psi_2(y, z) \otimes \underbrace{\bigoplus_t \psi_3(z, t)}_{\psi_t(z)}$$

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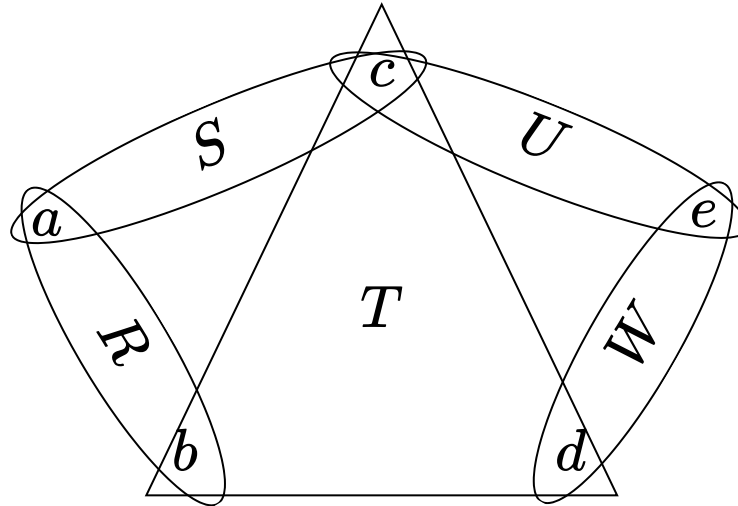
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- Eliminate z

- $\varphi = \bigoplus_{x,y} \psi_1(x,y) \otimes \underbrace{\bigoplus_z \psi_2(y,z) \otimes \psi_t(z)}_{\psi_z(y)}$

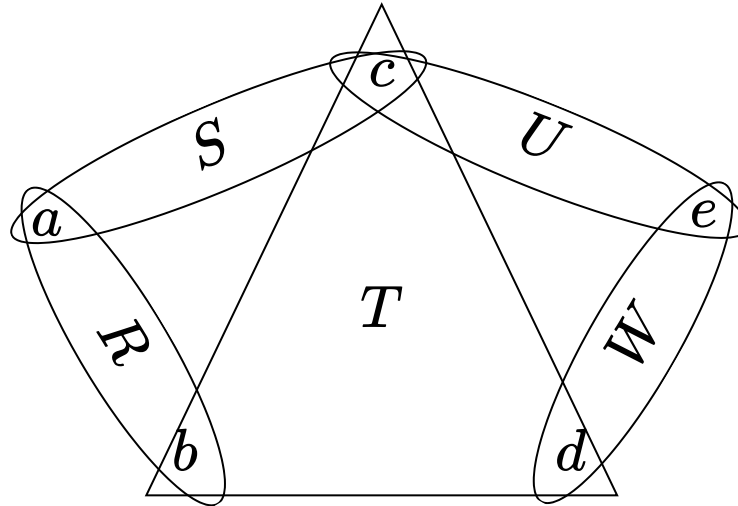
- $\varphi = \bigoplus_{x,y} \psi_1(x,y) \otimes \psi_z(y)$

Solving SPQs using Variable Elimination



$$\varphi(a) = \bigoplus_{b,c,d,e} R(a,b) \otimes S(a,c) \otimes T(b,c,d) \otimes U(c,e) \otimes W(d,e)$$

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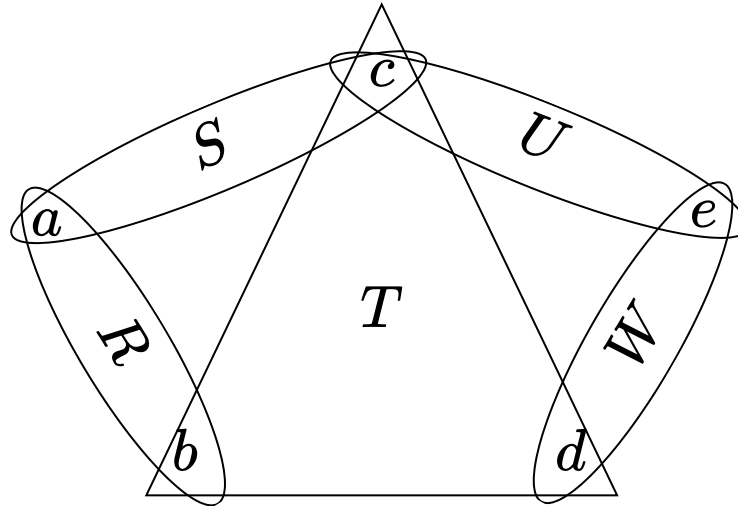


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- Eliminate d

$$= \bigoplus_{b,c,e} R(a,b) \otimes S(a,c) \otimes U(c,e) \otimes \underbrace{\bigoplus_d T(b,c,d) \otimes W(d,e)}_{\substack{\psi_d(b,c,e) \\ \tilde{O}(N^2)}}$$

Solving SPQs using Variable Elimination

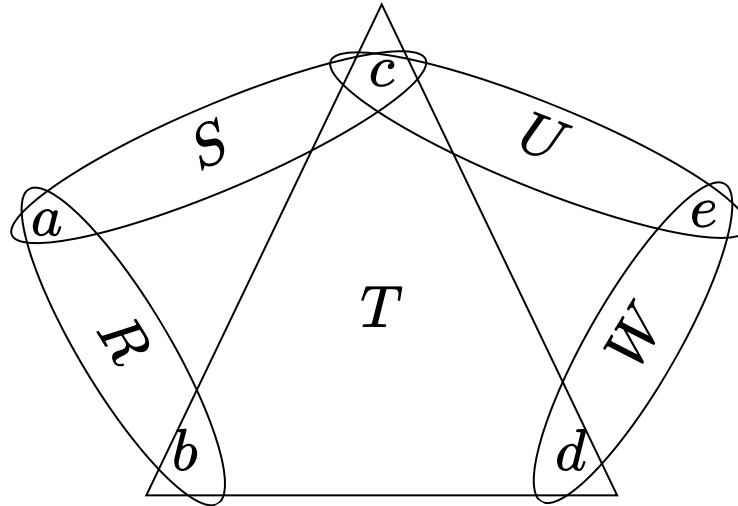


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- Eliminate e

$$= \bigoplus_{b,c,d} R(a,b) \otimes S(a,c) \otimes T(b,c,d) \otimes \underbrace{\bigoplus_e U(c,e) \otimes W(d,e)}_{\substack{\psi_e(c,d) \\ \tilde{O}(N^2)}}$$

Solving SPQs using Variable Elimination



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- Eliminate e **smarter**

$$= \bigoplus_{b,c,d} R(a,b) \otimes S(a,c) \otimes T(b,c,d) \otimes \underbrace{\bigoplus_e U(c,e) \otimes W(d,e)}_{\psi'_e(c,d)} \otimes T'(c,d)$$

$$T'(c,d) := 1_{\exists b : T(b,c,d) \neq 0}$$

$$\psi'_e(c,d)$$

$$\tilde{O}(N^{1.5})$$

SPQ Width

$$\text{spqw} \quad := \quad \min_{\substack{\sigma:\text{var} \\ \text{elimination} \\ \text{order}}} \quad \max_{v \in \sigma} \quad \rho^* \left(\underbrace{\psi_v^\sigma}_{\substack{\text{SPQ to} \\ \text{eliminate } v}} \right)$$

SPQ Width

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- Special cases
 - $\text{spqw} = 1$ for *acyclic* queries w/o free vars
 - $\text{spqw} = \text{fhtw}$ for queries w/o free vars
 - fhtw = fractional hypertree width
 - See [Logic&Algo-in-DB&AI BootCamp](#)

SPQ Width

Examples

- $Q_1 = \sum_{x,y,z,w} R(x, y) \times S(y, z) \times T(z, w)$
- $Q_2(y, z) = \sum_{x,w} R(x, y) \times S(y, z) \times T(z, w)$
- $Q_3(x, z) = \sum_y R(x, y) \times S(y, z)$ (Sparse MM)
- $Q_4(x, w) = \sum_{y,z} R(x, y) \times S(y, z) \times T(z, w)$

SPQ Width

Examples

- $Q_1 = \sum_{x,y,z,w} R(x, y) \times S(y, z) \times T(z, w)$
 - **spqw = 1**
- $Q_2(y, z) = \sum_{x,w} R(x, y) \times S(y, z) \times T(z, w)$
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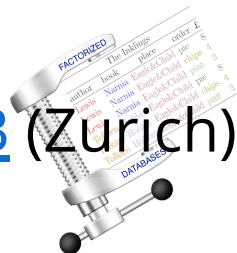
Example

Relational Linear Regression

Some References

- *"Learning Models over Relational Data using Sparse Tensors and Functional Dependencies"*, **TODS'20**
 - Abo Khamis, Ngo, Nguyen, Olteanu, Schleich
- *"A Layered Aggregate Engine for Analytics Workloads"*, **SIGMOD'19**
 - Schleich, Olteanu, Abo Khamis, Ngo, Nguyen
- *"Learning Generalized Linear Models Over Normalized Data"*, **SIGMOD'15**
 - Kumar, Naughton, Patel

FactorizedDB (Zurich)



Relational Linear Regression

Relational Linear Regression

- Input: Feature Extraction Query (FEQ)

$Q(\text{item}, \text{price}, \text{city}, \text{country} \rightarrow \text{sales}) =$

$S(\text{item}, \text{city} \rightarrow \text{sales}) \wedge P(\text{item}, \text{price}) \wedge C(\text{city} \rightarrow \text{country})$

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$Q(\text{item}, \text{price}, \text{city}, \text{country} \rightarrow \text{sales}) =$

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| item | city | sales |
|------|--------|-------|
| coat | Oxford | 1000 |
| ... | ... | ... |

| item | price |
|------|-------|
| coat | 50\$ |
| ... | ... |

| city | country |
|--------|---------|
| Oxford | UK |
| ... | ... |

Relational Linear Regression

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|--------|---------|
| Oxford | UK |
| ... | ... |

- Goal
 - Learn to predict sales from (item, price, city, country)
 - using Linear Regression with Square Loss

Traditional ML (Structure-agnostic)

Traditional ML (Structure-agnostic)

- Compute $Q(\text{item}, \text{price}, \text{city}, \text{country}, \text{sales})$

| item | price | city | country | sales |
|------|-------|--------|---------|-------|
| coat | 50\$ | Oxford | UK | 1000 |
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| coat | 50\$ | Oxford | UK | 1000 |
| ... | ... | ... | ... | ... |

- One-hot encode categorical features (item, city, country) to obtain D

| item | item | price | city | city | city | country | country | sales |
|------|-------|-------|--------|--------|--------|---------|---------|-------|
| coat | shoes | | London | Oxford | Saigon | UK | Vietnam | |
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| ... | ... | ... | ... | ... | ... | ... | ... | ... |

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| coat | shoes | | London | Oxford | Saigon | UK | Vietnam | |
| 1 | 0 | 50\$ | 0 | 1 | 0 | 1 | 0 | 1000 |
| ... | ... | ... | ... | ... | ... | ... | ... | ... |

- Feed D into an ML tool to search for θ
 - $\theta = (\theta_{\text{coat}}, \theta_{\text{shoes}}, \theta_{\text{price}}, \theta_{\text{London}}, \theta_{\text{Oxford}}, \theta_{\text{Saigon}}, \theta_{\text{UK}}, \theta_{\text{Vietnam}})$

Traditional ML (Structure-agnostic)

Traditional ML (Structure-agnostic)

- θ minimizes

- $$J(\theta) := \underbrace{\frac{1}{2|D|} \sum_{(\mathbf{x}, y) \in D} (\langle \theta, \mathbf{x} \rangle - y)^2}_{\text{least-squares loss}} + \underbrace{\frac{\lambda}{2} \|\theta\|_2^2}_{\ell_2\text{-regularizer}}$$

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- Optimal θ is found using Batch Gradient Descent (BGD)

- $$\theta \leftarrow \theta - \alpha \cdot \nabla J(\theta)$$

Drawbacks

$$Q(\text{item, price, city, country} \rightarrow \text{sales}) = \\ S(\text{item, city} \rightarrow \text{sales}) \wedge P(\text{item, price}) \wedge C(\text{city} \rightarrow \text{country})$$

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- Materializing a **doubly large** table

$$\blacksquare \quad \circ \quad \underbrace{|S| + |P| + |C|}_{\text{input tables}} \ll \underbrace{|Q|}_{\text{their join}} \ll \underbrace{|D|}_{\text{One-hot encoding}}$$

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 - ML has to rediscover structure

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- Materializing a **doubly large** table

$$\begin{array}{ccccc} \blacksquare & \circ & \underbrace{|S| + |P| + |C|}_{\text{input tables}} & \ll & \underbrace{|Q|}_{\text{their join}} & \ll & \underbrace{|D|}_{\text{One-hot encoding}} \end{array}$$

- **Destroying data structure** (e.g. JDs and FDs)
 - ML has to rediscover structure
- **Expensive data move** DB \Leftrightarrow ML
- **High maintenance cost** (updating θ after updates to input tables)
 - Recompute from scratch

Relational ML (Structure-aware)

- One Approach

Relational ML (Structure-aware)

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 - Step 1: Factor out θ -independent computations
 - i.e. only dependent on the data

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- One Approach
 - Step 1: Factor out θ -independent computations
 - i.e. only dependent on the data
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 - Step 3: Share computations across SPQs

Step 1: Factor out θ -independent computations

Step 1: Factor out θ -independent computations

$$\begin{aligned} J(\boldsymbol{\theta}) &= \frac{1}{2|D|} \sum_{(\mathbf{x}, y) \in D} \left(\langle \boldsymbol{\theta}, \mathbf{x} \rangle - y \right)^2 + \frac{\lambda}{2} \|\boldsymbol{\theta}\|_2^2 \\ &= \frac{1}{2|D|} \left(\boldsymbol{\theta}^T \underbrace{\left(\sum_{(\mathbf{x}, y) \in D} \mathbf{x} \mathbf{x}^T \right)}_{\boldsymbol{\Sigma}} \boldsymbol{\theta} - 2 \left\langle \boldsymbol{\theta}, \underbrace{\sum_{(\mathbf{x}, y) \in D} y \cdot \mathbf{x}}_{\mathbf{c}} \right\rangle + \underbrace{\sum_{(\mathbf{x}, y) \in D} y^2}_{s} \right) + \frac{\lambda}{2} \|\boldsymbol{\theta}\|_2^2 \\ &= \frac{1}{2|D|} \left(\boldsymbol{\theta}^T \boldsymbol{\Sigma} \boldsymbol{\theta} - 2 \langle \boldsymbol{\theta}, \mathbf{c} \rangle + s \right) + \frac{\lambda}{2} \|\boldsymbol{\theta}\|_2^2 \end{aligned}$$

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$$\nabla J(\boldsymbol{\theta}) = \frac{1}{|D|} \left(\boldsymbol{\Sigma} \boldsymbol{\theta} - \mathbf{c} \right) + \lambda \boldsymbol{\theta}$$

Step 2: Encode Σ, c, s as SPQs

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| item | item | price | city | city | city | country | country | sales |
|------|-------|-------|--------|--------|--------|---------|---------|-------|
| coat | shoes | | London | Oxford | Saigon | UK | Vietnam | |
| 1 | 0 | 50\$ | 0 | 1 | 0 | 1 | 0 | 1000 |
| ... | ... | ... | ... | ... | ... | ... | ... | ... |

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| | coat | shoes | price | London | Oxford | Saigon | UK | Vietnam | sales |
|---------|------|-------|-------|--------|--------|--------|----|---------|-------|
| coat | | | | | | | | | |
| shoes | | | | | | | | | |
| price | | | | | | | | | |
| London | | | | | | | | | |
| Oxford | | | | | | | | | |
| Saigon | | | | | | | | | |
| UK | | | | | | | | | |
| Vietnam | | | | | | | | | |
| sales | | | | | | | | | |

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|---------|------|-------|-------|--------|--------|--------|----|---------|-------|
| coat | | | | | | | | | |
| shoes | | | | | | | | | |
| price | | | | | | | | | |
| London | | | | | | | | | |
| Oxford | | | | | | | | | |
| Saigon | | | | | | | | | |
| UK | | | | | | | | | |
| Vietnam | | | | | | | | | |
| sales | | | | | | | | | |

Σ

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| ... | ... | ... | ... | ... | ... | ... | ... | ... |

| | coat | shoes | price | London | Oxford | Saigon | UK | Vietnam | sales |
|---------|------|-------|-------|--------|--------|--------|----|---------|-------|
| coat | | | | | | | | | |
| shoes | | | | | | | | | |
| price | | | | | | | | | |
| London | | | | | | | | | |
| Oxford | | | | | | | | | |
| Saigon | | | | | | | | | |
| UK | | | | | | | | | |
| Vietnam | | | | | | | | | |
| sales | | | | | | | | | |

Σ

c

c^T

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| | coat | shoes | price | London | Oxford | Saigon | UK | Vietnam | sales |
|---------|------|-------|-------|----------|--------|--------|----|---------|-------|
| coat | | | | | | | | | |
| shoes | | | | | | | | | |
| price | | | | | | | | | |
| London | | | | Σ | | | | | c |
| Oxford | | | | | | | | | |
| Saigon | | | | | | | | | |
| UK | | | | c^T | | | | | |
| Vietnam | | | | | | | | | |
| sales | | | | c^T | | | | | s |

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| | coat | shoes | price | London | Oxford | Saigon | UK | Vietnam | sales |
|----------------------------|--------------------------------|-------|---------------------------------|--------------------------------|--------|--------|-----------------------------------|---------|-------|
| coat shoes | $\sigma_{\text{item,item}}$ | | $\sigma_{\text{item,price}}$ | $\sigma_{\text{item,city}}$ | | | $\sigma_{\text{item,country}}$ | | |
| price | $\sigma_{\text{item,price}}$ | | $\sigma_{\text{price,price}}$ | $\sigma_{\text{price,city}}$ | | | $\sigma_{\text{price,country}}$ | | |
| London Oxford Saigon | $\sigma_{\text{item,city}}$ | | $\sigma_{\text{price,city}}$ | $\sigma_{\text{city,city}}$ | | | $\sigma_{\text{city,country}}$ | | |
| UK Vietnam | $\sigma_{\text{item,country}}$ | | $\sigma_{\text{price,country}}$ | $\sigma_{\text{city,country}}$ | | | $\sigma_{\text{country,country}}$ | | |
| sales | | | | | | | | | |

Step 2: Encode Σ, c, s as SPQs

$$\begin{aligned} Q(\text{item, price, city, country} \rightarrow \text{sales}) = \\ S(\text{item, city} \rightarrow \text{sales}) \wedge P(\text{item, price}) \wedge C(\text{city} \rightarrow \text{country}) \end{aligned}$$

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$$\sigma_{\text{item,item}}(\text{item}) = \sum_{\text{price,city,country,sales}} 1_S(\text{item, city, sales}) \cdot 1_P(\text{item, price}) \cdot 1_C(\text{city, country})$$

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$$\sigma_{\text{item,city}}(\text{item, city}) = \sum_{\text{price,country,sales}} 1_S(\text{item, city, sales}) \cdot 1_P(\text{item, price}) \cdot 1_C(\text{city, country})$$

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$$\sigma_{\text{price, price}} = \sum_{\text{item, price, city, country, sales}} 1_S(\text{item, city, sales}) \cdot 1_P(\text{item, price}) \cdot 1_C(\text{city, country}) \cdot \text{price}^2$$

Step 3: Share Computations across SPQs

$$Q(\text{item, price, city, country} \rightarrow \text{sales}) = \\ S(\text{item, city} \rightarrow \text{sales}) \wedge P(\text{item, price}) \wedge C(\text{city} \rightarrow \text{country})$$

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⇓ (Var Elimination)

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Step 3: Share Computations across SPQs

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FD-Aware Linear Regression

FD-Aware Linear Regression

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|------|-------|-------|--------|--------|--------|---------|---------|-------|
| coat | shoes | | London | Oxford | Saigon | UK | Vietnam | |
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$$J(\boldsymbol{\gamma}, \boldsymbol{\theta}_{\text{country}}) = \frac{1}{2|\mathcal{D}|} \sum_{(\mathbf{x}, y) \in \mathcal{D}} \left(\langle \boldsymbol{\gamma}, \bar{\mathbf{x}} \rangle - y \right)^2 + \frac{\lambda}{2} \left(\sum_{j \neq \text{city}} \underbrace{\|\boldsymbol{\gamma}_j\|_2^2}_{\boldsymbol{\theta}_j} + \underbrace{\|\boldsymbol{\gamma}_{\text{city}} - \mathbf{R}^T \boldsymbol{\theta}_{\text{country}}\|_2^2}_{\boldsymbol{\theta}_{\text{city}}} + \|\boldsymbol{\theta}_{\text{country}}\|_2^2 \right)$$

FD-Aware Linear Regression

$$+ \frac{\lambda}{2} \left(\sum_{j \neq \text{city}} \underbrace{\|\gamma_j\|_2^2}_{\theta_j} + \underbrace{\|\gamma_{\text{city}} - \mathbf{R}^T \theta_{\text{country}}\|_2^2}_{\theta_{\text{city}}} + \|\theta_{\text{country}}\|_2^2 \right)$$

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For a fixed γ_j , optimal θ_{country} :

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Generalizing The Linear Regression Example

(Some) Supported Models

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 - Polynomial Regression
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Open Problems

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 - Graphs \Rightarrow Graph Neural Networks
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 - impose constraints on *Model Parameters*?
 - e.g. FDs/JDs in the training data \Rightarrow constraints on NN weights?

Thank You!

Any Questions/Comments?