#### Monotone Estimation Framework and Applications for Scalable Analytics of Large Data Sets

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Outcome S(v, u): function of the data v and seed u

- Seed value *u* is available with the outcome
- S(v, u) can be interpreted as the set of all data vectors consistent with the outcome and u

**Monotonicity**: Fixing v, S(v, u) is non-increasing with u.

#### Monotone Estimation Problem (MEP)

A monotone sampling scheme (V, S):

- Data domain  $V(\subset \mathbb{R}^d)$
- Sampling scheme *S*: *V*×[0,1],
- A nonnegative function  $f: V \ge 0$



Desired properties of the estimator  $\hat{f}(S)$ :

- <u>Unbiased</u>  $\forall v, \int_{u}^{1} \hat{f}(S(v,x), x) dx = f(v)$  (useful with sums of MEPs)
- Nonnegative keep estimate  $\hat{f}$  in the same domain as f
- (Pareto) "optimal" (admissible) any estimator with smaller  $var_{u\sim U}[\hat{f}(S(v,u))]$  has for some v', larger  $var_{u\sim U[0,]}[\hat{f}(S(v',u))]$

#### Bounds on f(v) from S and u

Data v. The lower the seed u is, the more we know on v and hence on f(v).



#### **Estimators for MEPs**

- Unbiased, Nonnegative, Bounded variance
- Admissible: "Pareto Optimal" in terms of variance Results preview:

Explicit expressions for estimators for any MEP for which such estimator exists

#### Solution is not unique.

Consider some estimators with natural properties

• if we require monotonicity -  $\hat{f}(S, u)$  is non-increasing with u, we get uniqueness

Notion of "Competitiveness" of estimators

We will come back to this, but first see some applications

#### MEP applications in data analysis

Scalable computation of approximate statistics and queries over large data sets

- Data is sampled (composable, distributed scheme).
  Sample is used to estimate statistics/queries expressed as a sum of multiple MEPs
- Key-value pairs with multiple sets of values (instances)
  - Take coordinated samples of instances. We get a MEP for each key
- Sketching graph-based influence and similarity functions
  - "Distance" sketch the utility values (relations of node to all others). Get a MEP for each "target" node from sketches of seed nodes
- Sketching generalized coverage functions
  - Coordinated weighted sample of the "utility" vector of each element. MEP for each item.

## Social/Communication data

Activity value v(x) is associated with each key x = (b, c) (e.g. number of messages, communication from b to c)

 Take a weighted sample of keys. For example bottom-k ("weighed reservoir") or *PPS* (Probability Proportional to Size)



- With bottom-k, *t* is set to obtain a fixed sample size k
- Without replacement sampling:  $v(x) \ge -\tau \ln u(x)$
- Fully composable sampling scheme

## Samples of multiple days

Coordinated samples: Different values for different days. Each key is sampled with same seed u(x) in different days



#### Matrix view keys × instances

In our example: keys x = (a, b) are user pairs. Instances are days.

|       | Su | Мо | Tu | We | Th  | Fr | Sa |
|-------|----|----|----|----|-----|----|----|
| (a,b) | 40 | 30 | 10 | 43 | 55  | 30 | 20 |
| (g,c) | 0  | 5  | 0  | 0  | 4   | 0  | 10 |
| (h,c) | 5  | 0  | 0  | 60 | 3   | 0  | 2  |
| (a,z) | 20 | 10 | 5  | 24 | 15  | 7  | 4  |
| (h,f) | 0  | 7  | 6  | 3  | 8   | 5  | 20 |
| (f,s) | 0  | 0  | 0  | 20 | 100 | 70 | 50 |
| (d,h) | 13 | 10 | 8  | 0  | 0   | 5  | 6  |

## **Example Statistics**

- Specify a segment of the keys  $Y \subset X$ , examples:
  - one user in CA and one in NY
  - apple device to android

Queries/Statistics  $\sum_{x \in Y} f(v_1(x), v_2(x), \dots, v_d(x))$ 

- Total communication of segment on Wednesday.  $\sum_{x \in Y} v_1(x)$
- $L_p^p$  distance/Weighted Jaccard change in activity of segment between Friday and Saturday  $\sum_{x \in Y} |v_1(x) - v_2(x)|^p$
- $L_p^p$  increase/decrease  $\sum_{x \in Y} \max\{0, v_1(x) v_2(x)\}^p$
- Coverage of segment Y in days D :  $\sum_{x \in Y} \max_{i \in D} v_i(x)$
- Average/sum of median/max/min/top-3/concave aggregate of activity values over days D

#### We would like to compute an estimate from the sample

#### Matrix view keys × instances

Coordinated PPS sample  $\tau = 100$  for all entries

| u    |         | Su | Мо | Ти | We | Th    | Fr | Sa |
|------|---------|----|----|----|----|-------|----|----|
| 0.33 | (a,b) ( | 40 | 30 | 10 | 43 | 55    | 30 | 20 |
| 0.22 | (g,c)   | 0  | 5  | 0  | 0  | 4     | 0  | 10 |
| 0.82 | (h,c)   | 5  | 0  | 0  | 60 | 3     | 0  | 2  |
| 0.16 | (a,z) ( | 20 | 10 | 5  | 24 | 15    | 7  | 4  |
| 0.92 | (h,f)   | 0  | 7  | 6  | 3  | 8     | 5  | 20 |
| 0.16 | (f,s)   | 0  | 0  | 0  | 20 | 100 ( | 70 | 50 |
| 0.77 | (d,h)   | 13 | 10 | 8  | 0  | 0     | 5  | 6  |

#### Estimate sum statistics, one key at a time

 $\sum_{\boldsymbol{x}\in\boldsymbol{Y}}f(\boldsymbol{\boldsymbol{v}}(\boldsymbol{x}))$ 

Sum over keys  $x \in Y$  of f(v(x)), where  $v(x) = (v_1(x), v_2(x) \dots)$ 

For  $L_p$  distance:  $f(\boldsymbol{v}) = |v_1 - v_2|^p$ 

#### Estimate one key at a time:

 $\sum_{x \in Y} \hat{f}(S(v(x))) \longleftarrow$  The estimator for f(v) is applied to the sample of v

### Easy statistics: Sum over entries Estimate a single entry at a time

• Example: Total communication of segment *Y* on Monday

Inverse probability estimate (Horviz Thompson) [HT52]:

Sum over sampled  $x \in Y$  of  $\frac{v_{monday}(x)}{p_{monday}(x)}$ 

Inclusion Probability  $p_{monday}(x)$  can be computed from v(x) and  $\tau$ :

$$x \in S \leftrightarrow v(x) \ge \tau \cdot u(x)$$
$$p_i(x) = \Pr_{u \in U} [v_i(x) \ge \tau_i \cdot u(x)]$$

## HT estimator (single-instance)

Coordinated PPS sample  $\tau = 100$ 

| u    |                | Su | Мо | Tu | We | Th  | Fr | Sa |
|------|----------------|----|----|----|----|-----|----|----|
| 0.33 | (a,b) (        | 40 | 30 | 10 | 43 | 55  | 30 | 20 |
| 0.22 | (g,c)          | 0  | 5  | 0  | 0  | 4   | 0  | 10 |
| 0.82 | (h,c)          | 5  | 0  | 0  | 60 | 3   | 0  | 2  |
| 0.14 | (a,z) (        | 20 | 10 | 5  | 24 | 13  | 7  | 4  |
| 0.92 | (h,f)          | 0  | 7  | 6  | 3  | 8   | 5  | 20 |
| 0.16 | (f,s)          | 0  | 0  | 0  | 20 | 100 | 70 | 50 |
| 0.77 | (d <i>,</i> h) | 13 | 10 | 8  | 0  | 0   | 5  | 6  |

## HT estimator (single-instance)

 $\tau = 100$ . Day: Wednesday, Segment: CA-NY

| u    |         | Su | Мо | Tu | We   | Th  | Fr | Sa |
|------|---------|----|----|----|------|-----|----|----|
| 0.33 | (a,b) ( | 40 | 30 | 10 | 43   | 55  | 30 | 20 |
| 0.22 | (g,c)   | 0  | 5  | 0  | 0    | 4   | 0  | 10 |
| 0.82 | (h,c)   | 5  | 0  | 0  | 60   | 3   | 0  | 2  |
| 0.16 | (a,z) ( | 20 | 10 | 5  | 24   | 15  | 7  | 4  |
| 0.92 | (h,f)   | 0  | 7  | 6  | 3    | 8   | 5  | 20 |
| 0.16 | (f,s)   | 0  | 0  | 0  | 20 ( | 100 | 70 | 50 |
| 0.77 | (d,h)   | 13 | 10 | 8  | 0    | 0   | 5  | 6  |

# HT estimator for single-instance

 $\tau = 100$ . Day: Wednesday, Segment: CA-NY



Exact: 43 + 60 + 20 = 123p = 0.43

HT estimate is 0 for keys that are not sampled, v/p when key is sampled

HT estimate: 100 + 100 = 200

$$p = 0.20$$

### Inverse-Probability (HT) estimator

- ✓ Unbiased:  $(1 p(x)) \cdot 0 + p(x) \frac{f(v(x))}{p(x)} = f(v(x))$
- ✓ Nonnegative:  $v(x) \ge 0$  so  $\frac{v(x)}{p(x)} \ge 0$
- Sounded variance (for all v)
- ✓ **Monotone:** more information  $\Rightarrow$  higher estimate
- Optimal: UMVU The unique minimum variance (unbiased, nonnegative, sum) estimator

Works when f depends on a single entry. What about general f ?

### Queries involving multiple columns

- $L_p^p$  distance  $f(\boldsymbol{v}) = |v_1 v_2|^p$
- $L_p^p$  increase  $f(v) = \max\{0, v_1 v_2\}^p$
- HT estimate is positive only when we know  $f(v) = |v_1 v_2|$  from the sample.
- But for  $v_2 = 0$ ,  $v_1 > 0$  then f(v) > 0 but sample never reveals f(v) because second entry is never sampled. Thus, HT is biased
- Even when unbiased, HT may not be optimal. E.g. when  $v_1$  is sampled and we can deduce from  $\tau_2$  and u that  $v_2 \leq a < v_1$  then we know that  $f(v) \geq v_1 - a$ . An optimal estimator will use this incomplete information
- We want estimators with the same nice properties as HT and optimality

## Sampled data

Coordinated PPS sample  $\tau = 100$ 

| u    |                | Su | Мо | Tu | We | Th  | Fr | Sa |
|------|----------------|----|----|----|----|-----|----|----|
| 0.33 | (a,b) (        | 40 | 30 | 10 | 43 | 55  | 30 | 20 |
| 0.22 | (g,c)          | 0  | 5  | 0  | 0  | 4   | 0  | 10 |
| 0.82 | (h,c)          | 5  | 0  | 0  | 60 | 3   | 0  | 2  |
| 0.16 | (a,z) (        | 20 | 10 | 5  | 24 | 15  | 7  | 4  |
| 0.92 | (h <i>,</i> f) | 0  | 7  | 6  | 3  | 8   | 5  | 20 |
| 0.16 | (f,s)          | 0  | 0  | 0  | 20 | 100 | 70 | 50 |
| 0.77 | (d,h)          | 13 | 10 | 8  | 0  | 0   | 5  | 6  |

Want to estimate  $(55 - 43)^2 + (8 - 3)^2 + (24 - 15)^2$ Lets look at key (a,z), and estimating  $(24 - 15)^2$ 

# Information on f

Fix the data v. The lower u is, the more we know on vand on  $f(v) = (24 - 15)^2 = 81$ .

We plot the lower bound we have on f(v) as a function of the seed u.



### This is a MEP ! Monotone Estimation Problem

A monotone sampling scheme (V, S):

- Data domain  $V(\subseteq \mathbb{R}^d)$  here  $(v_1, v_2) \in \mathbb{R}^2_{\geq 0}$
- Sampling scheme S:  $V \times [0,1]$ , here  $S((v_1, v_2), u)$ reveals  $v_i$  when  $v_i > 100 u$

A nonnegative function  $f: V \ge 0$  here  $(v_1 - v_2)^2$ 

Goal: estimate f(v): specify an *estimator*  $\hat{f}(S, u)$  that is

Unbiased, Nonnegative, Bounded variance, Admissible (optimal)

Solution is not unique.

#### The optimal (admissible) range



We see S(v,u) and u. We know what S(v,x) is for all x > u. Suppose we fixed  $M = \int_{u}^{1} \hat{f}(S(v,x),x) dx$ 

### **MEP Estimators**

 Order optimal estimators: For an order < on the data domain V: Any estimator with lower variance on v, must have higher variance on z < v</li>

#### The L\* estimator:

- The unique admissible monotone estimator
- Order optimal for:  $z \prec v \Leftrightarrow f(z) < f(v)$
- 4-variance competitive (soon we define that)

#### The U\* estimator:

• Order optimal for:  $z \prec v \Leftrightarrow f(z) > f(v)$ 

Choice of estimator depends on properties we want, possibly depending on typical data distribution. L\* is a good default (monotone and competitive)

# Variance Competitiveness [CK13]

A "worst-case" over data theoretical indicator for estimator quality For each v, we can consider the minimum  $E_{u \in U[0,1]} [\hat{f}^2(S(v, u), u)]$  attainable by an estimator that is unbiased and nonnegative for all other v'

We use such "optimal" estimator  $\hat{f}^{(v)}$  for v as a reference point.

An estimator  $\hat{f}(S, u)$  is *c***-competitive** if for any data v, the expectation of the square is within a factor **c** of the minimum possible for v (by an unbiased and nonnegative estimator).

For all unbiased nonnegative  $\hat{g}$ ,  $E_{u \in U[0,1]} \left[ \hat{f}^2(\mathbf{S}(\mathbf{v},\mathbf{u})) \right] \leq c \ E_{u \in U[0,1]} \left[ \hat{g}^2(\mathbf{S}(\mathbf{v},\mathbf{u})) \right]$ 

The L<sup>\*</sup> estimator is 4-competitive and this is tight. For some MEPs, ratio is 4

Optimal estimator  $\hat{f}^{(v)}$  for data v(unbiased and nonnegative for all data) The optimal estimates  $\hat{f}^{(v)}$  are the negated derivative of the lower hull of the Lower bound function.



Intuition: The lower bound guides us on outcome S, how "high" we can go with the estimate, in order to optimize variance for v while still being nonnegative on all other consistent data vectors.

#### The L\* estimator



 $L_1$  estimation example Estimators for  $f(v_1, v_2) = |v_1 - v_2|$ Scheme:  $v_i \ge 0$  is sampled if  $v_i > u$ 

- "lower bound" (LB) on f(0.6, 0.2) from S and u The  $L^*$ ,  $U^*$ , and opt for v estimators
- The Lower hull of LB



 $U^*$  is optimized for the vector f(0.6,0.0) (always consistent with S)

 $L^*$  is optimized locally for the vector f(0.6, u) (consistent vector with smallest f

# $L_2^2$ estimation example

The  $L^*$ ,  $U^*$ , and opt for v estimators

Estimators for  $f(v_1, v_2) = |v_1 - v_2|^2$ Scheme:  $v_i \ge 0$  is sampled if  $v_i > u$ 

- "lower bound" (LB) on f(0.6, 0.2) from S and u
- The Lower hull of LB

value



 $U^*$  is optimized for the vector f(0.6,0.0) (always consistent with S)

 $L^*$  is optimized locally for the vector f(0.6, u) (consistent vector with smallest f

## Summary

- Defined Monotone Estimation Problems (MEPs) (motivated by coordinated sampling)
- Derive Pareto optimal (admissible) unbiased and nonnegative estimators (for any MEP when they exist):
  - L\* (lower end of range: unique monotone estimator, dominates HT) ,
  - U\* (upper end of range),
  - Order optimal estimators (optimized for certain data patterns)

## Applications

- Estimators for Euclidean and Manhattan distances from samples [C KDD '14]
- sketch-based closeness similarity in social networks [CDFGGW COSN '13] (similarity of the sets of longrange interactions)
- Sketching generalized coverage functions, including graph-based influence functions [CDPW '14, C' 16]

### Future

- Tighter bounds on universal ratio: L\* is 4 competitive, can do 3.375 competitive, lower bound is 1.44 competitive.
- Instance-optimal competitiveness Give efficient construction for any MEP
- Multi-dimensional MEPs: Have multiple independent seed (independent samples of "columns"), some initial derivations for d = 2 and coverage and distance functions [CK 12, C 14], but the full picture is missing

# L<sub>1</sub> distance [C KDD14]

#### Independent / Coordinated PPS sampling

#IP flows to a destination in two time periods



# $L_2^2$ distance [C KDD14]

Independent/Coordinated PPS sampling

Surname occurrences in 2007, 2008 books (Google ngrams)



var/mu^2



## **Coordination of samples**

Very powerful tool for big data analysis with applications well beyond what [Brewer, Early, Joyce 1972] could envision

- Locality Sensitive Hashing (LSH) (similar weight vectors have similar samples/sketches)
- Multi-objective samples (universal samples): A single sample (as small as possible) that provides statistical guarantees for multiple sets of weights.
- Statistics/Domain queries that span multiple "instances" (Jaccard similarity, L<sub>p</sub> distances, distinct counts, union size,...)
  - MinHash sketches are a special case with 0/1 weights.
- Facilitates faster computation of samples. Example: [C'97] Sketching/sampling reachability sets and neighborhoods of all nodes in a graph in near-linear time.