#### New Cached-Sufficient Statistics Algorithms for quickly answering statistical questions



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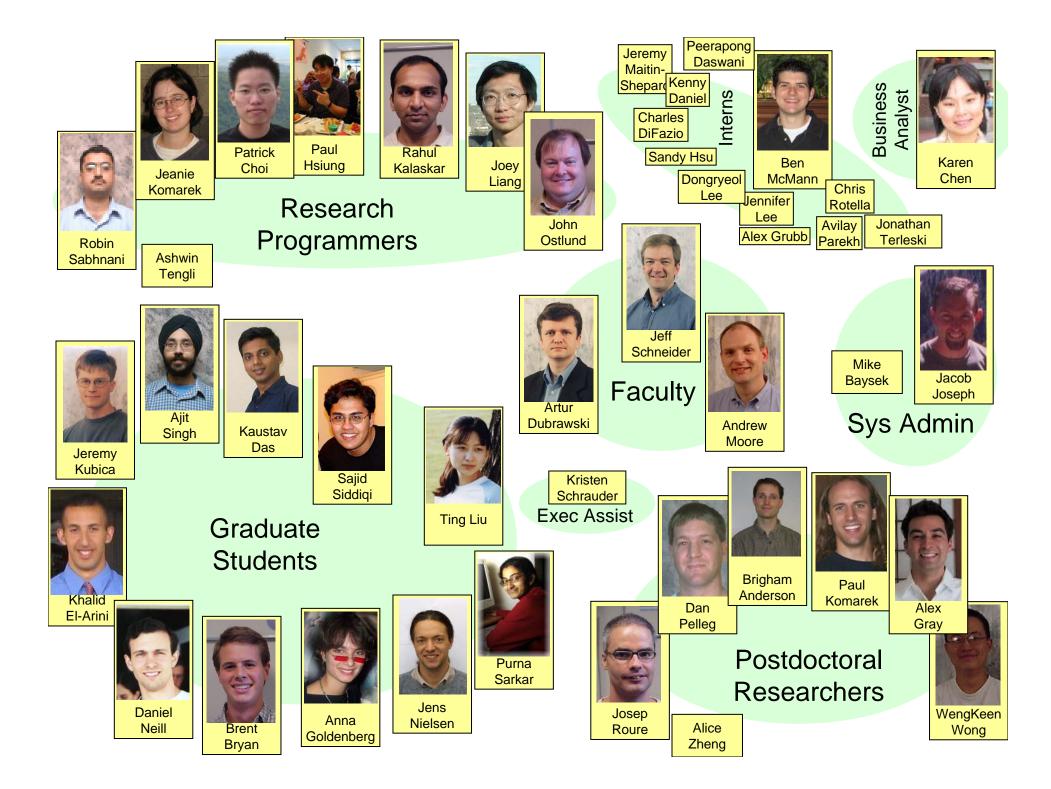
Daniel Neill <u>neill+@cs.cmu.edu</u> Auton Lab, CMU



Auton

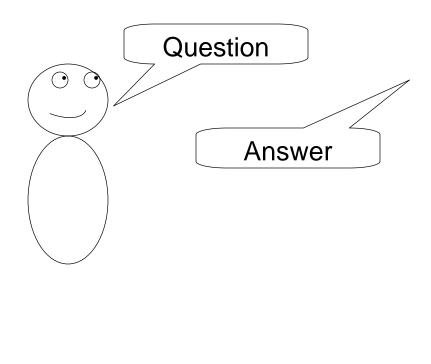


Papers, Software, Example Datasets, Tutorials: www.autonlab.org



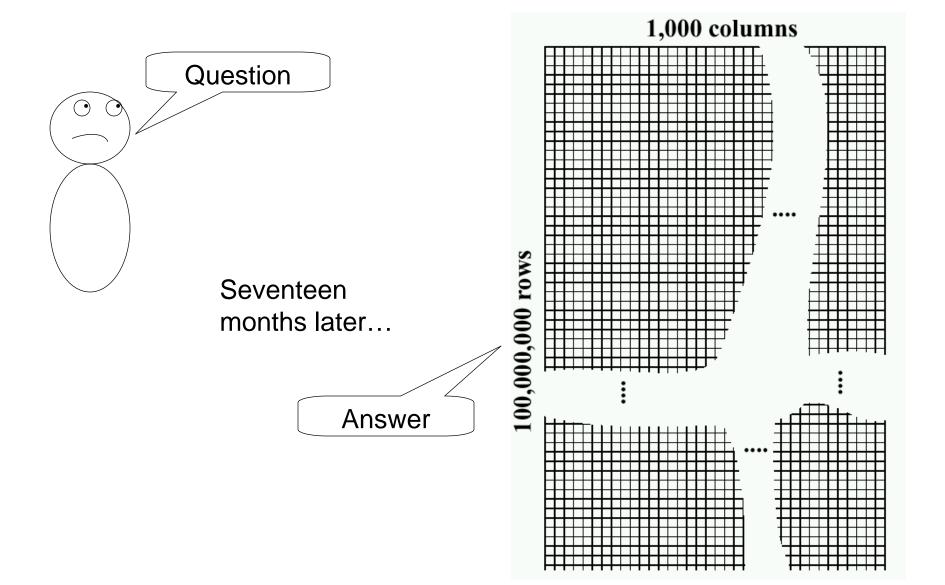
Cached Sufficient Statistics New searches over cached statistics **Biosurveillance and Epidemiology Scan Statistics Cached Scan Statistics Branch-and-Bound Scan Statistics** Retail data monitoring Brain monitoring **Entering Google** 

# Data Analysis: The old days

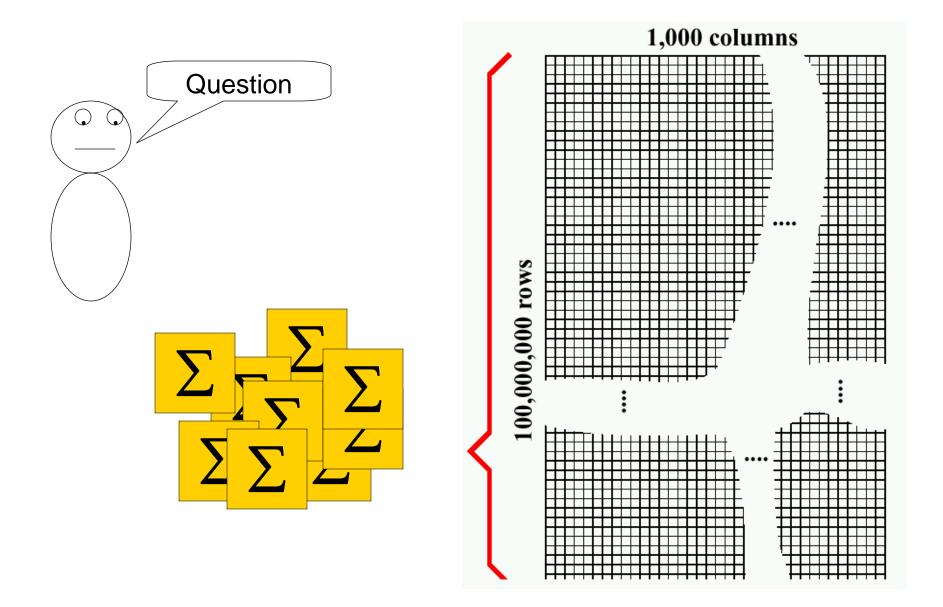


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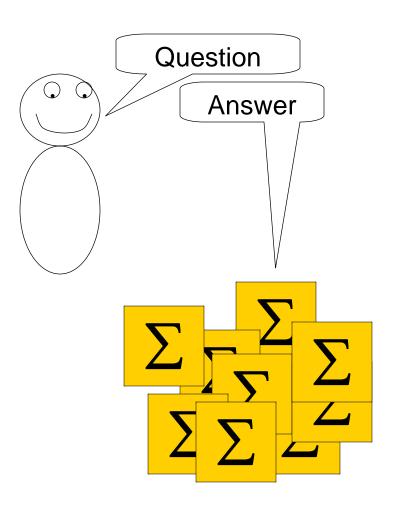
# Data Analysis: The new days

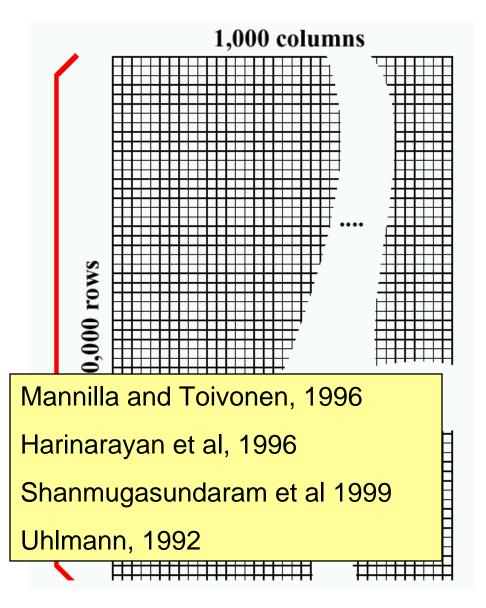


# **Cached Sufficient Statistics**



# **Cached Sufficient Statistics**





Frequent Sets (Agrawal et al)

KD-trees (Friedman, Bentley, Finkel)

Multi-resolution KD-trees (Deng, Moore)

All-Dimensions Trees (Moore, Lee)

Multi-resolution metric trees (Liu, Moore)

Well-Separated Pairwise Decomposition (Callahan 1995)

TimeCube (Sabhnani, Moore)

**Cached Sufficient Statistics** New searches over cached statistics **Biosurveillance and Epidemiology Scan Statistics Cached Scan Statistics Branch-and-Bound Scan Statistics** Retail data monitoring Brain monitoring **Entering Google** 

#### **Cached Sufficient Statistics**

New searches over cached statistics

Biosurveillance Scan Statistics Cached Scan S Branch-and-Bot

Retail data monitoring

Brain monitoring

**Entering Google** 

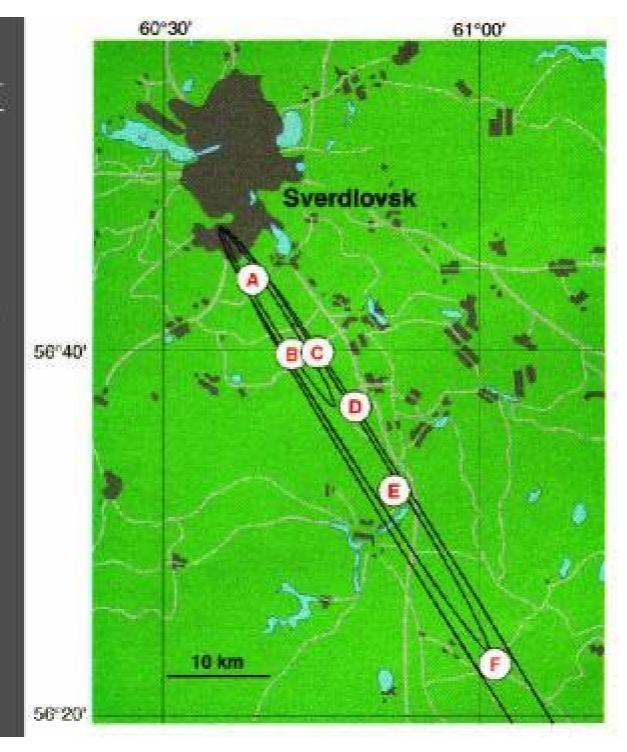
**Cached Sufficient Statistics** New searches over cached statistics **Biosurveillance and Epidemiology Scan Statistics Cached Scan Statistics Branch-and-Bound Scan Statistics** Retail data monitoring Brain monitoring **Entering Google** 

#### ...Early Thursday Morning. Russia. April 1979...



collaboration with Daniel Neill <neill@cs.cmu.edu>

Sverdlovsk Region: Epi-map





# **Biosurveillance Algorithms**

#### **Specific Detectors**

CityDiagnosis (DBN-based surveillance): [Anderson, Moore]

EPFC: Emerging Patterns from food complaints: [Dubrawski, Sabhnani, Moore]

PANDA2: Patient-based Bayesian Network [Cooper, Levander et. al]

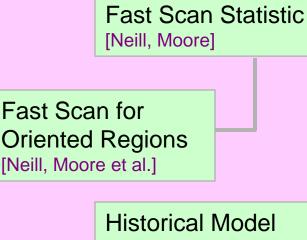


BARD: Airborne Attack Detection [Hogan, Cooper et al.]



#### **General Detectors**

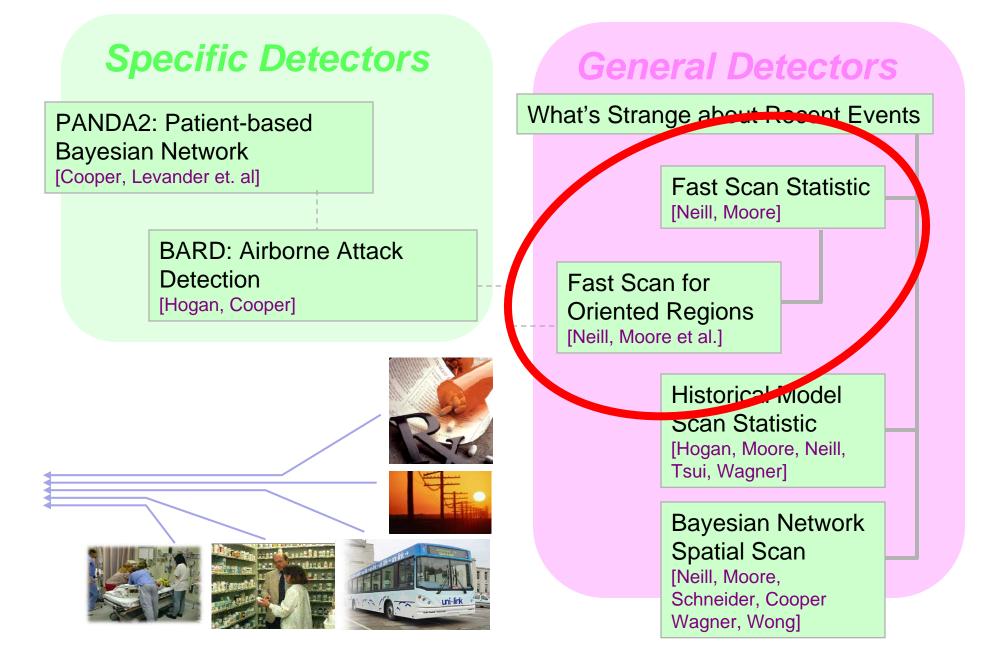
What's Strange about Recent Events [Wong, Moore, Wagner and Cooper]

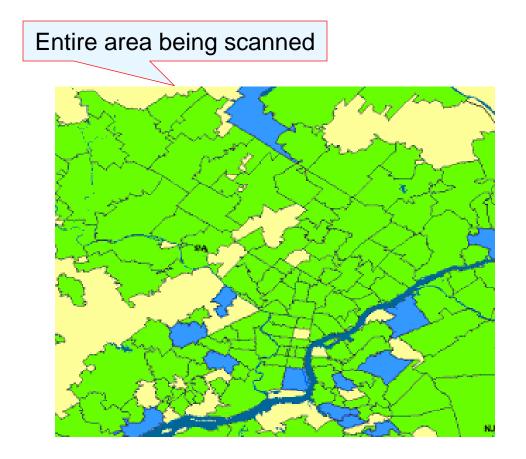


Historical Model Scan Statistic [Hogan, Moore, Neill, Tsui, Wagner]

Bayesian Network Spatial Scan [Neill, Moore, Schneider, Cooper Wagner, Wong]

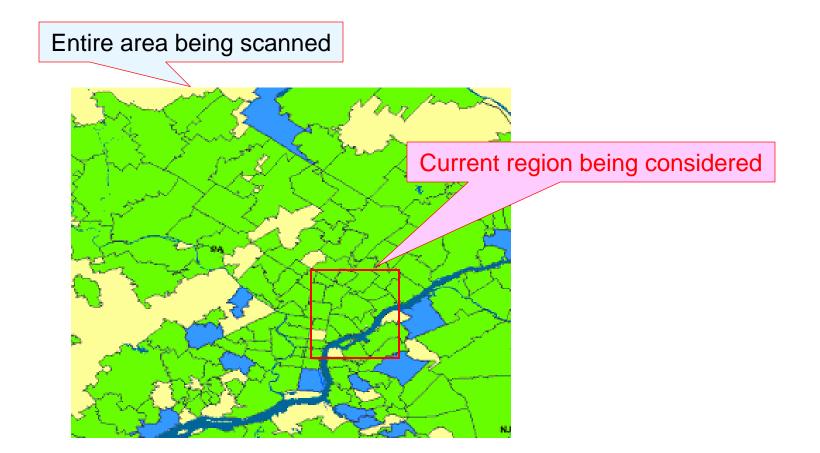
# **Biosurveillance Algorithms**





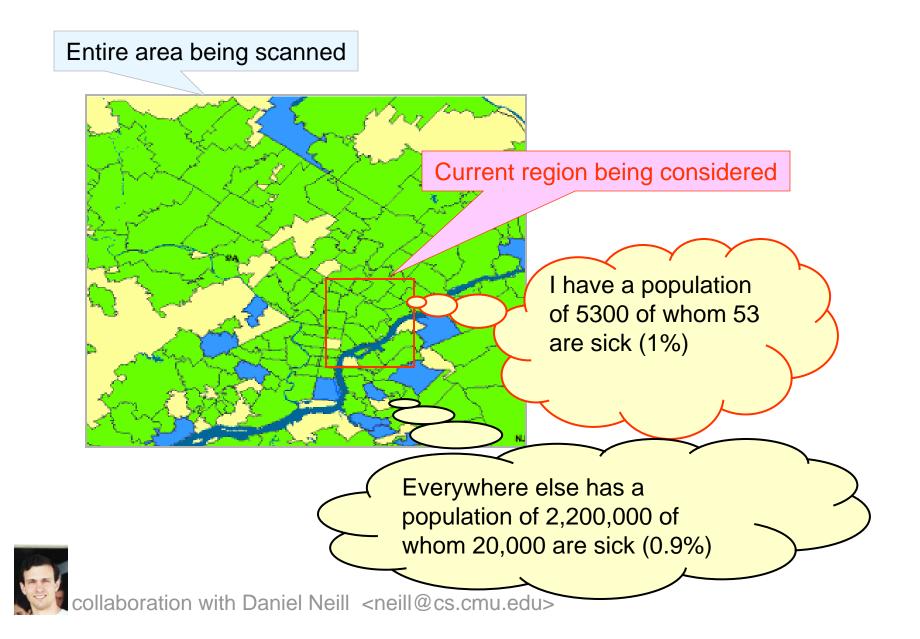


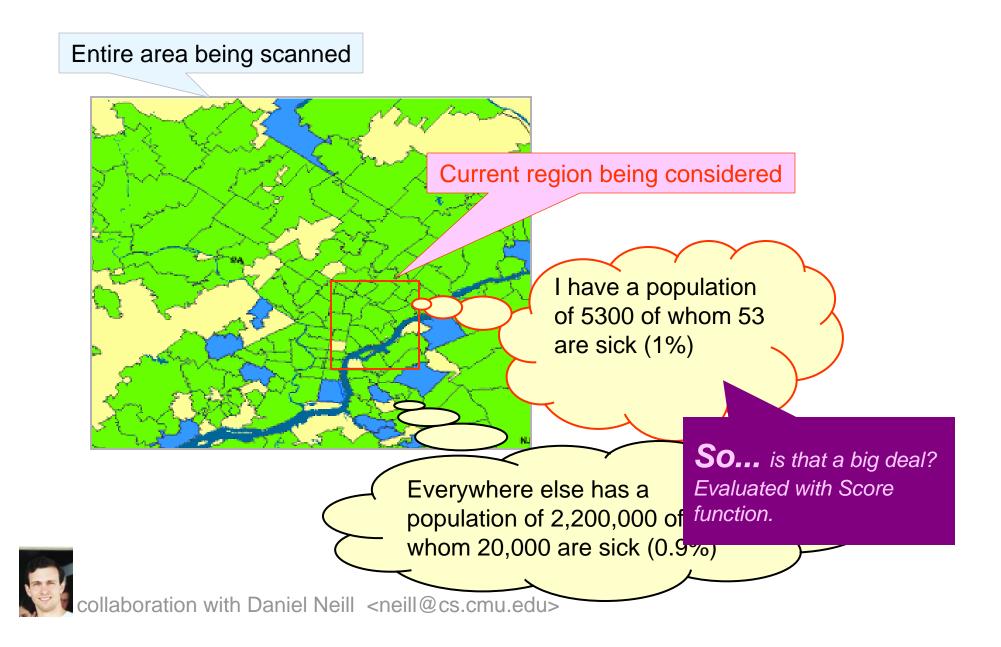
collaboration with Daniel Neill <neill@cs.cmu.edu>





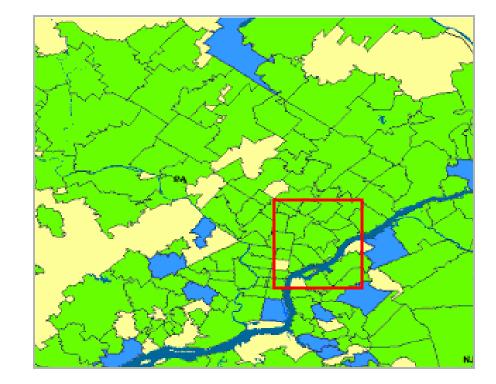
collaboration with Daniel Neill <neill@cs.cmu.edu>





- Define <u>models</u>:

   of the null hypothesis
   H<sub>0</sub>: no attacks.
  - of the alternative hypotheses H<sub>1</sub>(S): attack in region S.



(Individually Most Powerful statistic for detecting significant increases) (but still...just an example)

- Define <u>models</u>:
  - of the null hypothesis  $H_0$ : no attacks.
  - of the alternative hypotheses H<sub>1</sub>(S): attack in region S.
- Derive a <u>score function</u> Score(S) = Score(C, B).
  - Likelihood ratio:
  - To find the most significant region:

Score(S) = 
$$\frac{L(\text{Data} | H_1(S))}{L(\text{Data} | H_0)}$$
  
S\* = arg max Score(S)

S

(Individually Most Powerful statistic for detecting significant increases) (but still...just an example)

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  - Likelihood ratio:
  - To find the most significant region:

Example: Kulldorf's score Assumption:  $c_i \sim Poisson(qb_i)$  $H_0$ :  $q = q_{all}$  everywhere  $H_1$ :  $q = q_{in}$  inside region,  $q = q_{out}$  outside region

 $S^* = \arg \max \operatorname{Score}(S)$ 

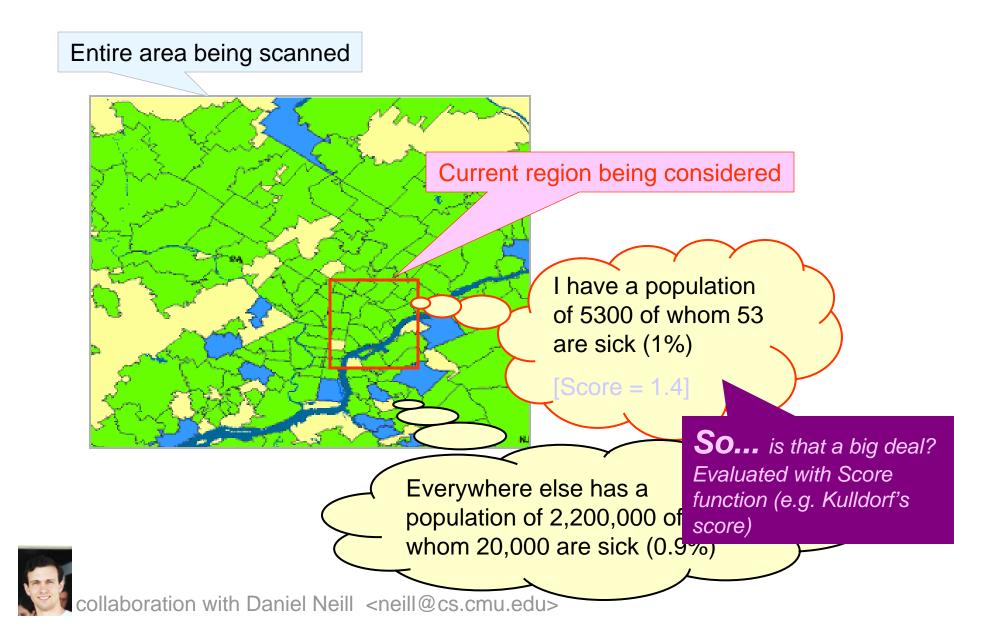
S

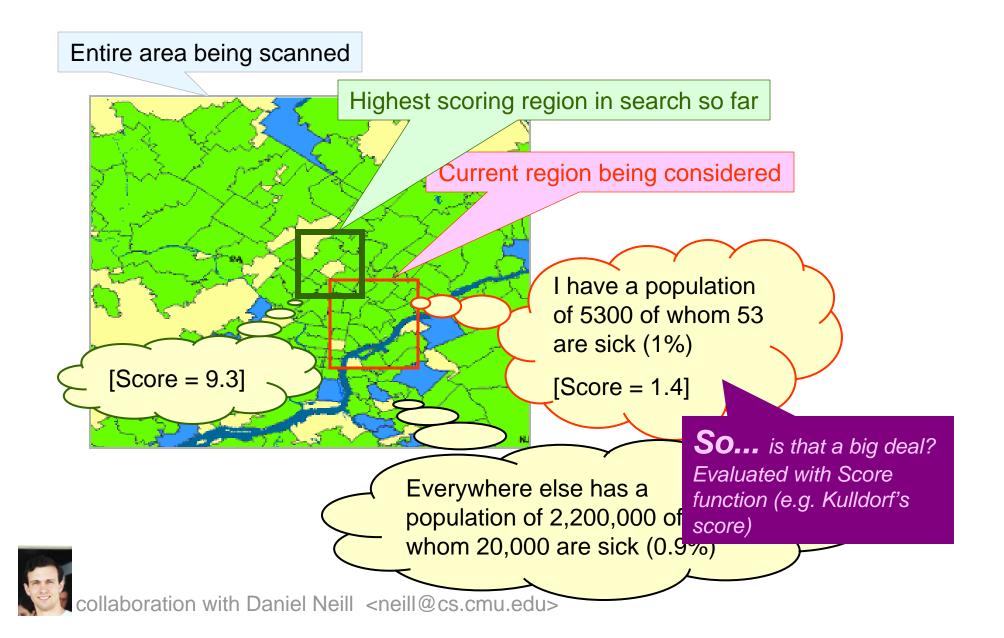
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- Derive a <u>score function</u> Score(S) = Score(C, B).
  - Likelihood ratio:  $Score(S) = \frac{1}{2}$  To find the most significant region:  $S^* = \arg \max_{S}$

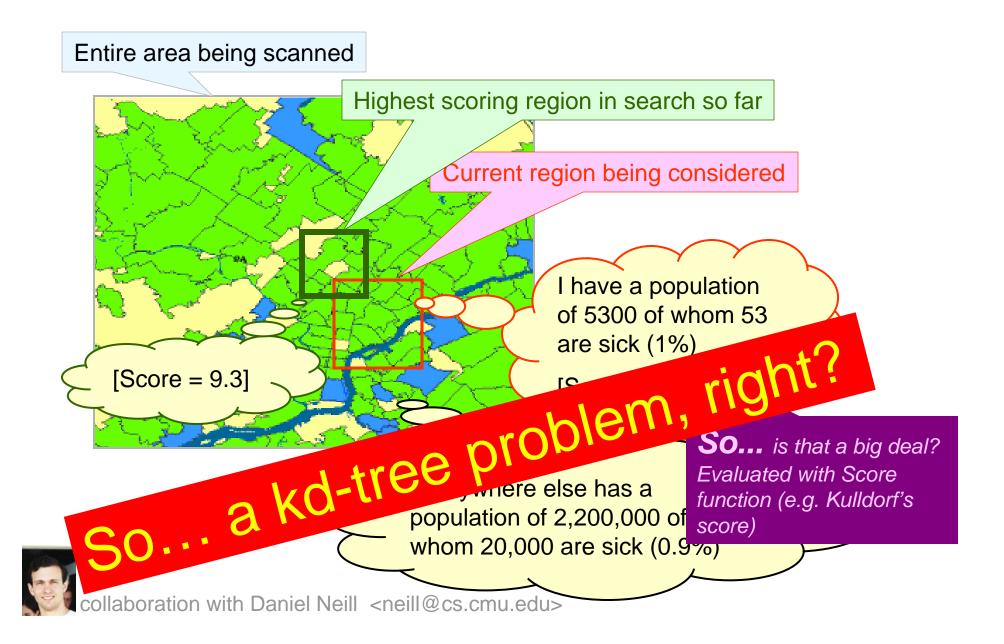
Example: Kulldorf's score  
Assumption: 
$$c_i \sim \text{Poisson}(qb_i)$$
  
 $H_0: q = q_{all}$  everywhere  
 $H_1: q = q_{in}$  inside region,  
 $q = q_{out}$  outside region  
 $Score(S) = \frac{L(\text{Data} | H_1(S))}{L(\text{Data} | H_0)}$   
 $S^* = \arg\max Score(S)$ 

$$D(S) = C \log \frac{C}{B} + (C_{tot} - C) \log \frac{C_{tot} - C}{B_{tot} - B} - C_{tot} \log \frac{C_{tot}}{B_{tot}}$$

(Individually Most Powerful statistic for detecting significant increases) (but still...just an example)







#### **Computational framework**

# Data is aggregated to a grid.

B=25	B=18	B=22	B=14	B=5
C=27	C=14	C=22	C=15	C=5
B=25	B=20	B=6	B=20	B=5
C=26	C=17	C=9	C=12	C=4
B=25	B=25	B=20	B=15	B=20
C=19	C=26	C=43	C=37	C=20
B=24	B=24	B=19	B=15	B=19
C=18	C=20	C=40	C=32	C=16
B=23	B=15	B=14	B=10	B=2
C=20	C=17	C=8	C=10	C=3



collaboration with Daniel Neill <neill@cs.cmu.edu>

#### **Computational framework**

Data is aggregated to a grid.

Cost of obtaining sufficient statistics for an arbitrary rectangle: O(1)

B=25	B=18	B=22	B=14	B=5
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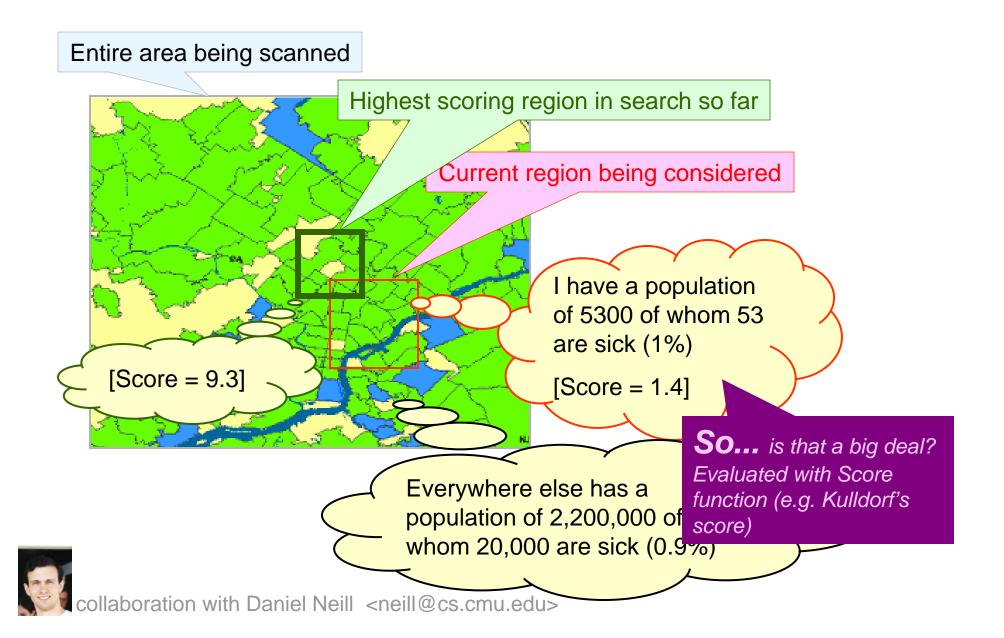
*n x n* grid has

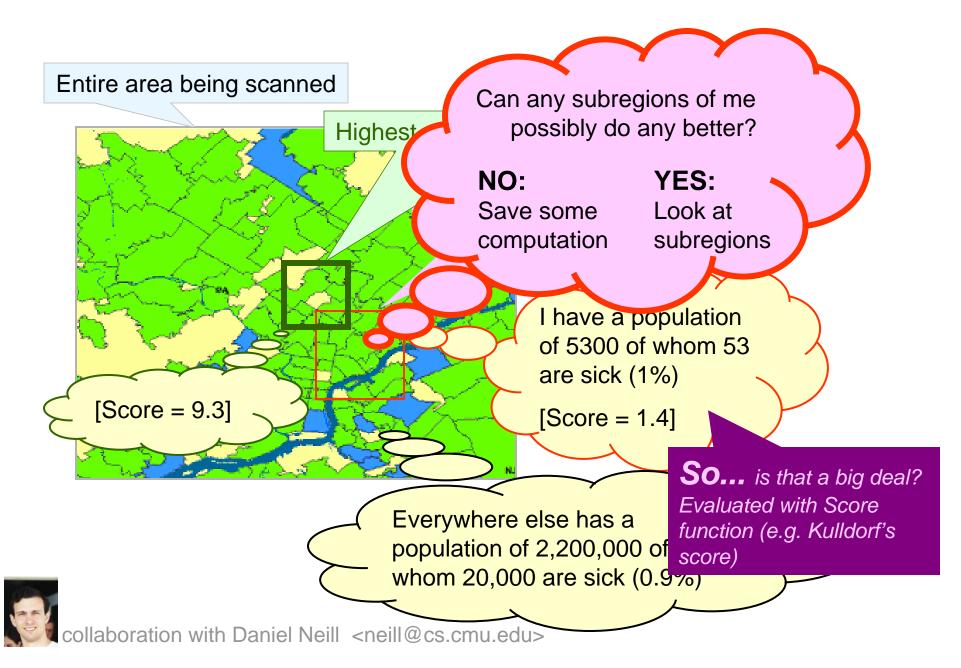
$$\left[\binom{n+1}{2}\right]^2 = O(n^4)$$

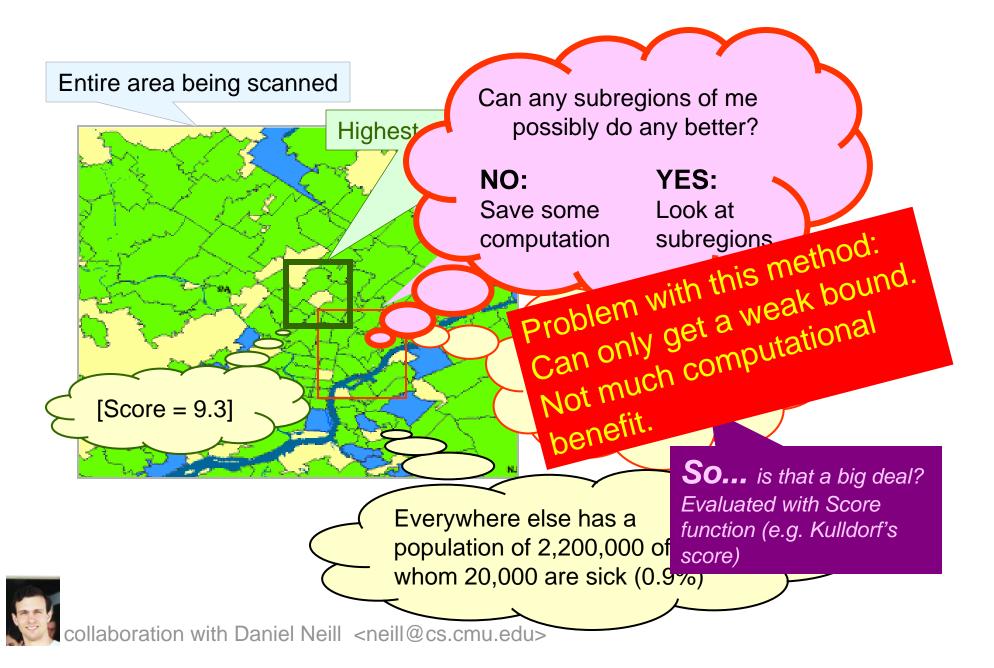
rectangles to search

B=25	B=18	B=22	B=14	B=5
C=27	C=14	C=22	C=15	C=5
B=25	B=20	B=6	B=20	B=5
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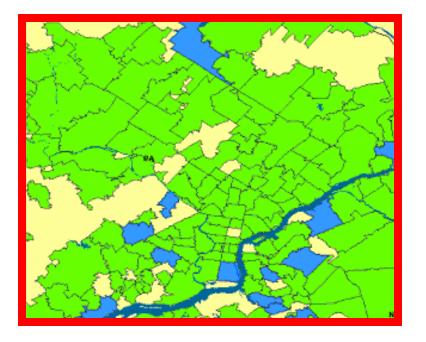






#### Gridded then Exhaustive

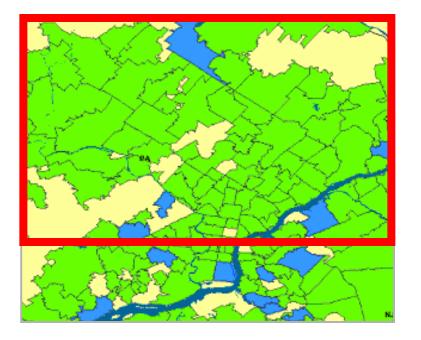
#### Step 1: Gridded



Check a specific recursive overlapping set of regions called 'Gridded Regions" collaboration with Daniel Neill <neill@cs.cmu.edu>

#### Gridded then Exhaustive

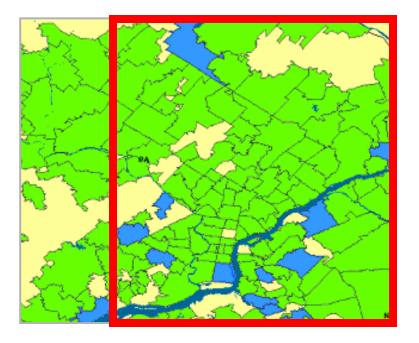
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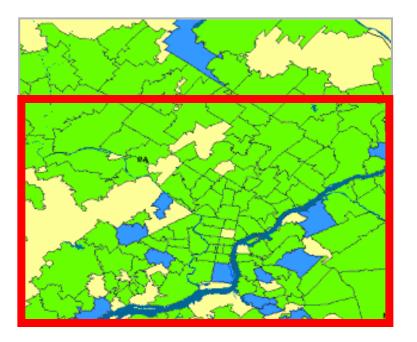
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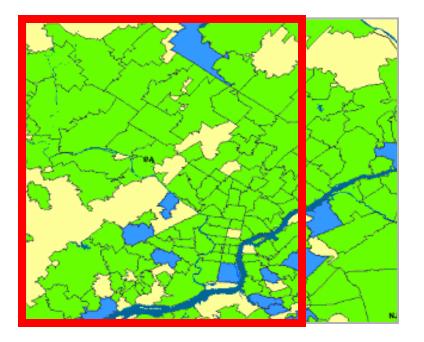


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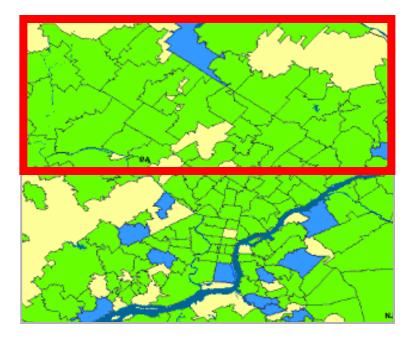
#### Step 1: Gridded



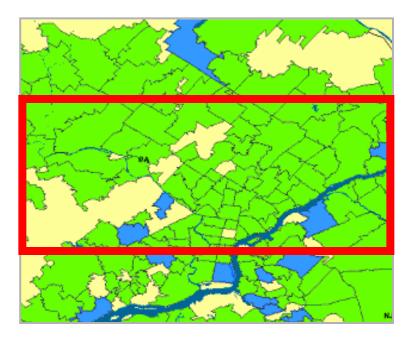
#### Step 1: Gridded



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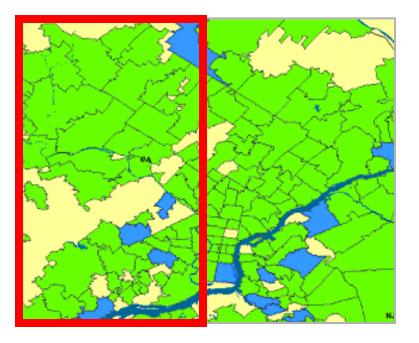
#### Step 1: Gridded



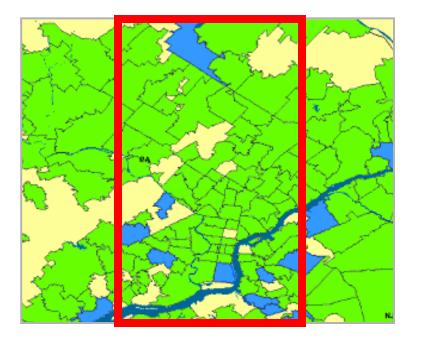
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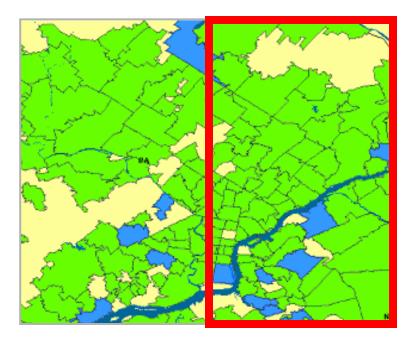
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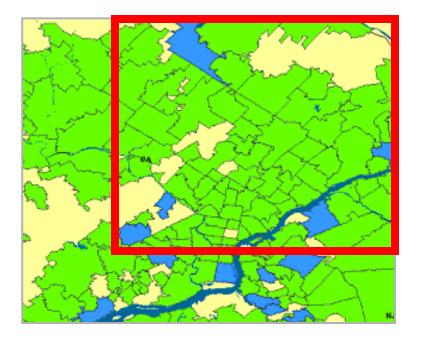
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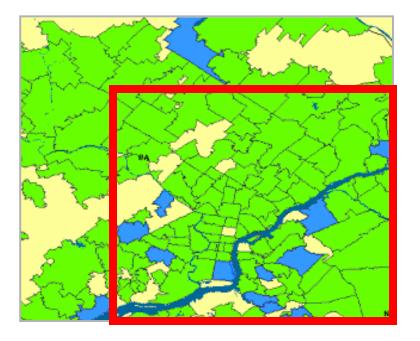
#### Step 1: Gridded



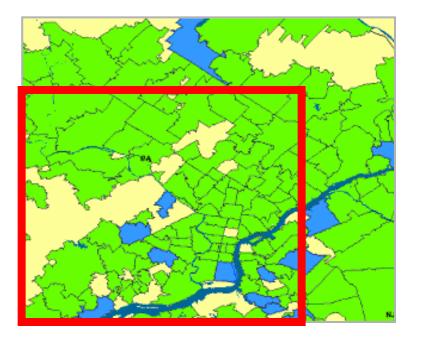
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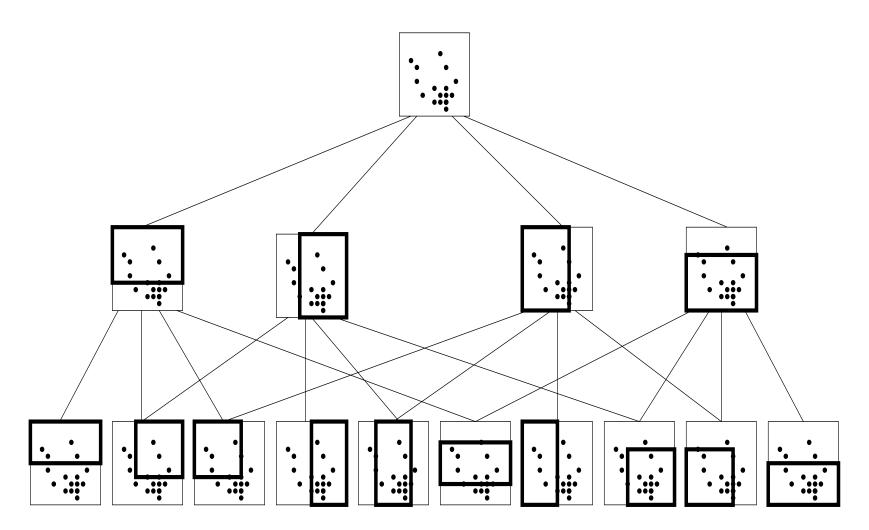
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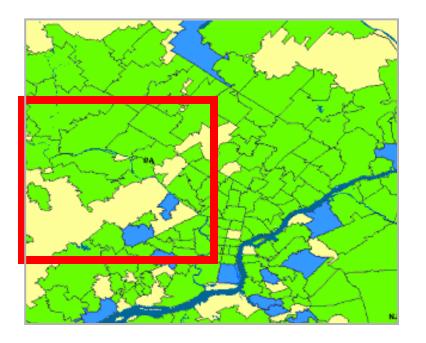
# The multi-resolution tree for rectangular regions





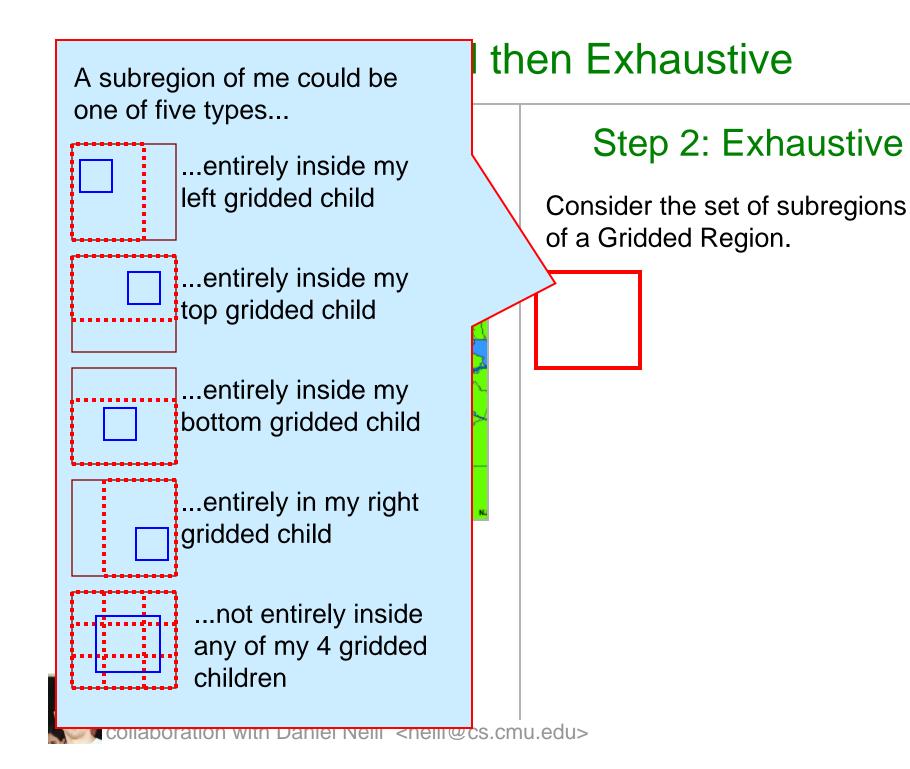
collaboration with Daniel Neill <neill@cs.cmu.edu>

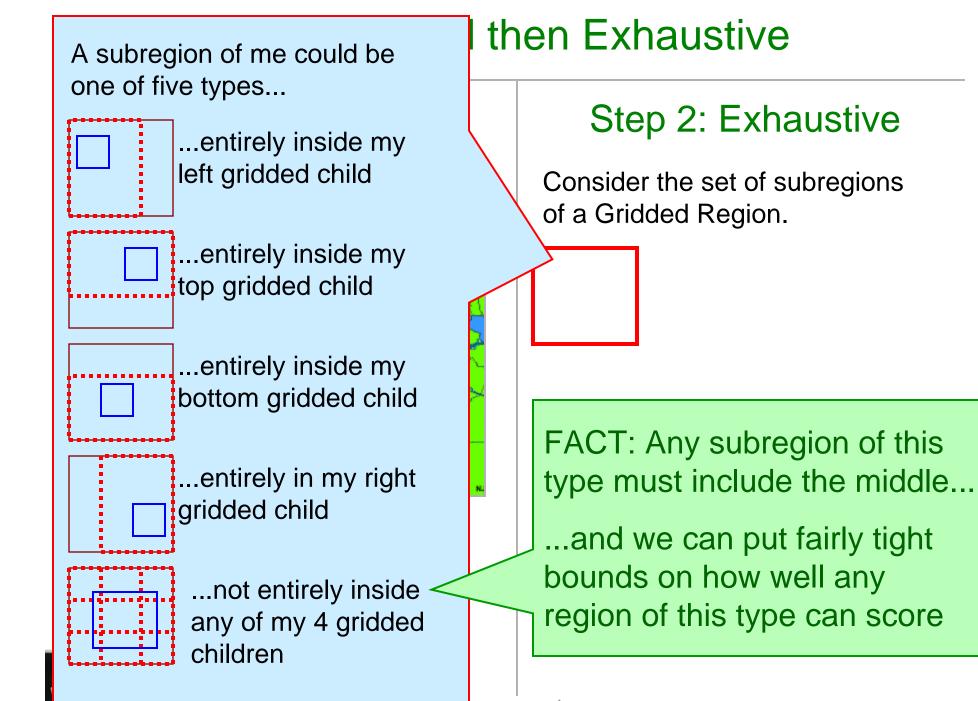
#### Step 1: Gridded

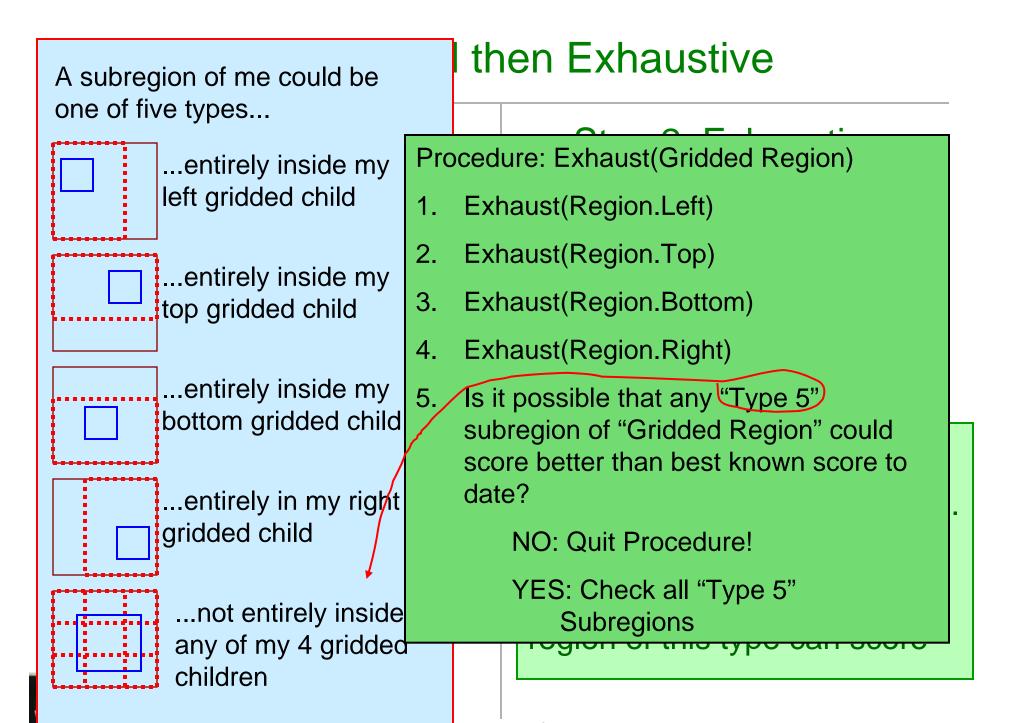


#### Step 2: Exhaustive

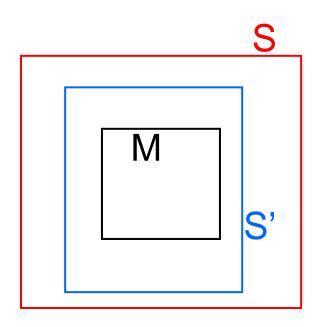
Consider the set of subregions of a Gridded Region.







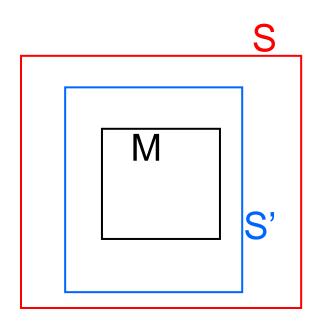
collaboration with Daniel Nelli <nelli@cs.cmu.edu>



5. Is it possible that any "Type 5" subregion of "Gridded Region" could score better than best known score to date?



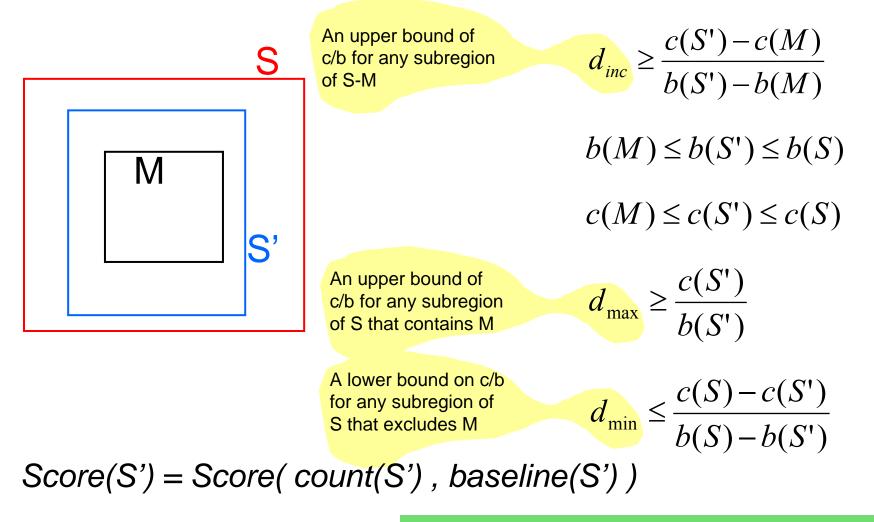
collaboration with Daniel Neill <neill@cs.cmu.edu>



#### Score(S') = Score( count(S') , baseline(S') )

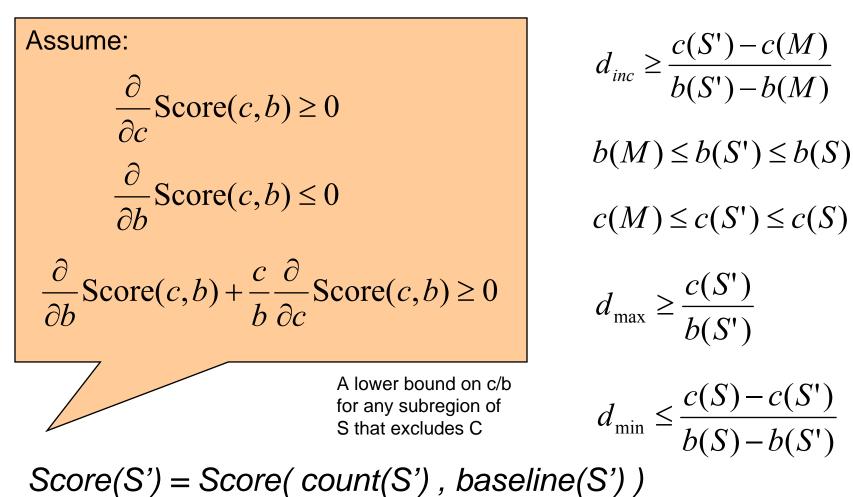
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collaboration with Daniel Neill <neill@cs.cmu.edu>



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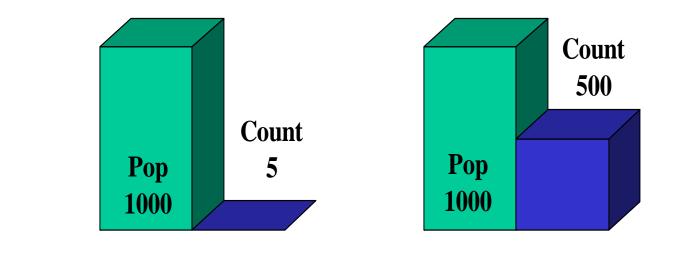


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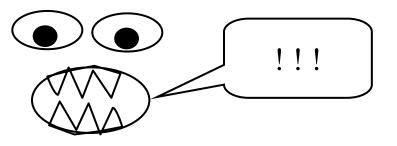
Score(S) increases with the total count of S,  $C(S) = \sum_{S} c_{i}$ .





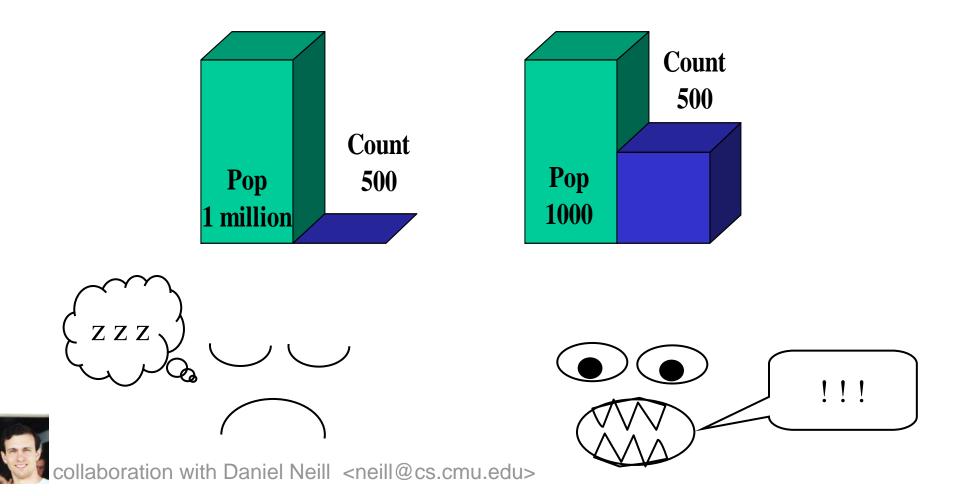


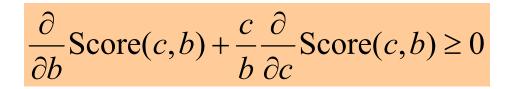
collaboration with Daniel Neill <neill@cs.cmu.edu>





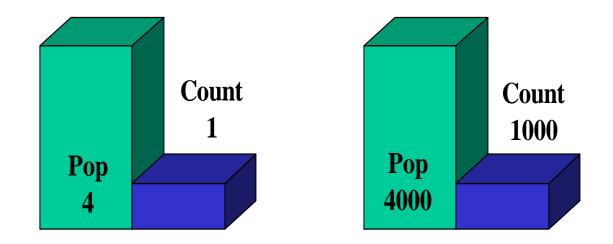
Score(S) decreases with total baseline of S,  $B(S) = \sum_{S} b_{i}$ .





## Properties of D(S)

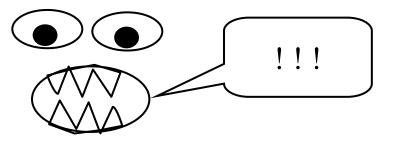
For a constant ratio C / B, Score(S) increases with C and B.

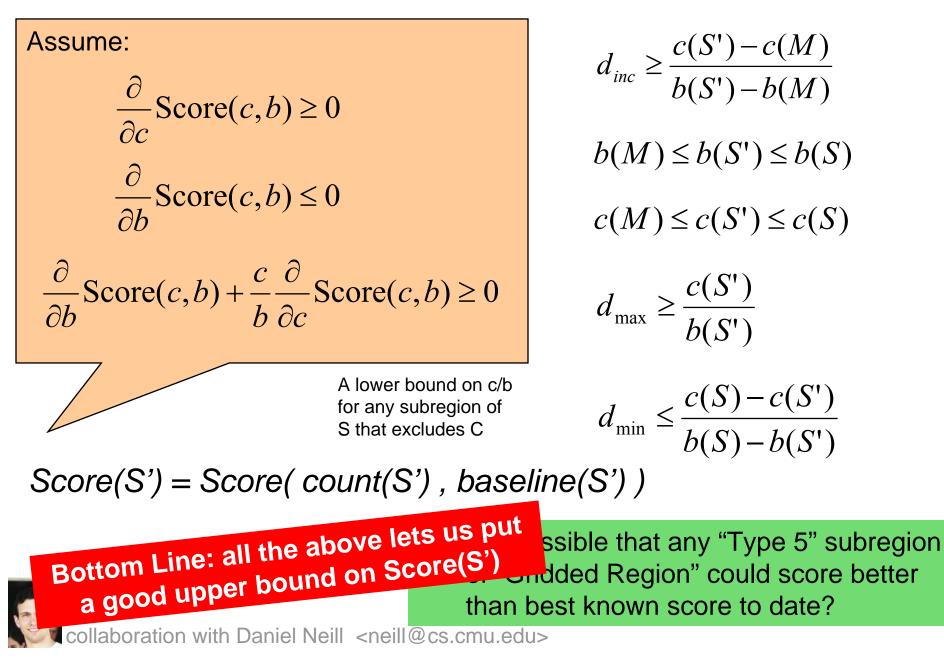






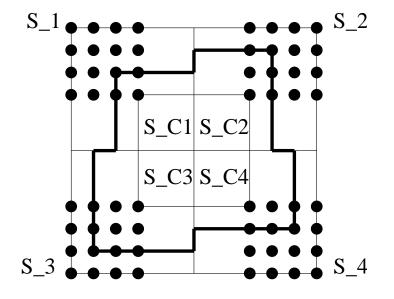
collaboration with Daniel Neill <neill@cs.cmu.edu>





# Tighter score bounds by quartering

- We precompute global bounds on populations  $p_{ij}$  and ratios  $c_{ij}$  /  $p_{ij}$ , and use these for our initial pruning.
- If we cannot prune the outer regions of S using the global bounds, we do a second pass which is more expensive but allows much more pruning.
- We can use quartering to give much tighter bounds on populations and ratios, and compute a better score bound using these.
  - Requires time quadratic in region size; in effect, we are computing bounds for all irregular but rectanglelike outer regions. Inter with Daniel Neill <neill@cs.cmu.edu>



# Where are we?

- So we can find the <u>most significant</u> region by searching over the desired set of regions S, and finding the highest D(S).
- Now how can we find whether this region actually is a significant cluster?



# Where are we?

- So we can find the <u>most significant</u> region by searching over the desired set of regions S, and finding the highest D(S).
- Now how can we find whether this region actually is a significant cluster?
- Randomization testing

Can sometimes cost us 1000 times more computation!

Though there are further tricks...



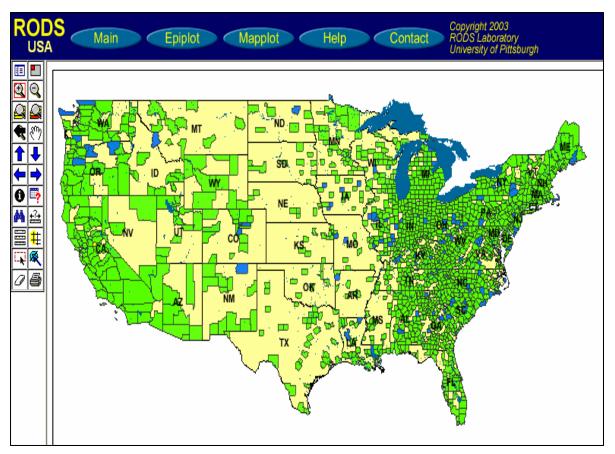
# Why the Scan Statistic speed obsession?



collaboration with Daniel Neill <neill@cs.cmu.edu>

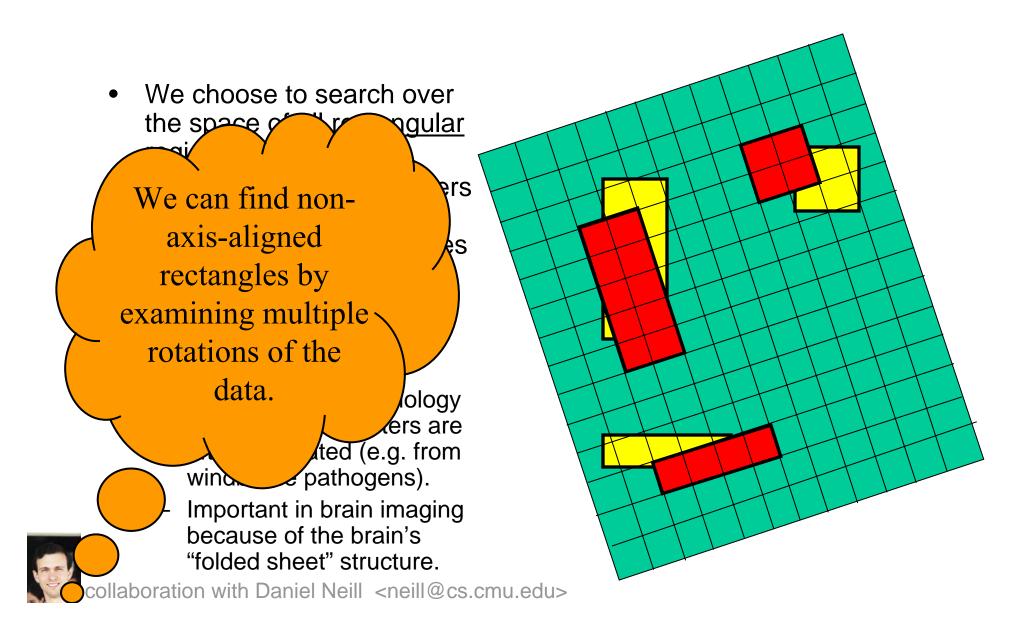
# Why the Scan Statistic speed obsession?

- Traditional Scan Statistics very expensive, especially with Randomization tests
- Going national
- A few hours could actually matter!



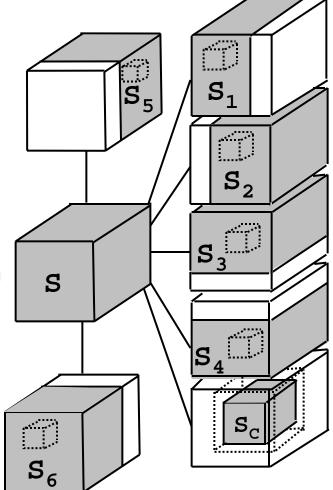


# Which regions to search?



# d-dimensional partitioning

- Parent region S is divided into 2d overlapping children: an "upper child" and a "lower child" in each dimension.
- Then for any rectangular subregion S' of S, exactly one of the following is true:
  - S' is contained entirely in (at least) one of the children  $S_1 \dots S_{2d}$ .
  - S' contains the center region S<sub>C</sub>, which is common to all the children.
- Starting with the entire grid G and repeating this partitioning recursively, we obtain the overlap-kd tree structure.

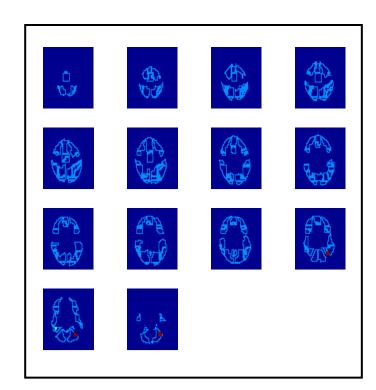




• Algorithm: Neill, Moore and Mitchell NIPS 2005

# Results: OTC, fMRI

- fMRI data (64 x 64 x 14 grid):
  - 7-148x speedups as compared to exhaustive search approach.



fMRI data from noun/verb word recognition task



# Limitations of the algorithm

- Data must be aggregated to a grid.
- Not appropriate for very highdimensional data.
- Assumes that we are interested in finding (rotated) rectangular regions.
- Less useful for special cases (e.g. square regions, small regions only).
- Slower for finding multiple regions.



# **Density-based cluster detection**

- Kernel density based detection
- Spatial statistics
- Connected component approaches
- Density optima
- Linear scan approximations



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- Kernel density based detection
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- Linear scan
   approximations

- DBSCAN (Ester, Kriegel, Sander and Xu)
- CFF Clustering (Cuevas, Febrero and Fraiman)
- CLIQUE (Agrawal, Gehrke, Gunopulus, and Raghavan)
- Priebe's method (Priebe)
- MAFIA (Goil, Nagesh and Choudhary)
- DENCLUE (Hinneburg and Keim)
- STING (Wang, Yang, and Muntz)
- Bump Hunting (Friedman and Fisher)



#### Density-based cluster detection

- Account for varying baseline?
- Are the hotspots significant?
- Is there a small rise over a large stripe?

- Kernel density based detection
- Spatial statistics
- Connected component approaches
- Density optima
- Linear scan
   approximations

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#### For more information and references to related work...

<u>http://www.autonlab.org/autonweb/14667.html</u>

```
@inproceedings{neill-rectangles,
Howpublished = {Conference on Knowledge Discovery in Databases (KDD)
2004},
Month = {August},
Year = {2004},
Editor = {J. Guerke and W. DuMouchel},
Author = {Daniel Neill and Andrew Moore},
Title = {Rapid Detection of Significant Spatial Clusters}
}
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http://www.autonlab.org/autonweb/15868.html

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    Booktitle = {Proceedings of the KDD 2005 Workshop on Data Mining Methods
    for Anomaly Detection},
        Author = {Robin Sabhnani and Daniel Neill and Andrew Moore},
        Title = {Detecting Anomalous Patterns in Pharmacy Retail Data}
    }
```

Software: <u>http://www.autonlab.org/autonweb/10474.html</u>

**Cached Sufficient Statistics** New searches over cached statistics **Biosurveillance and Epidemiology Scan Statistics Cached Scan Statistics Branch-and-Bound Scan Statistics** Retail data monitoring Brain monitoring **Entering Google** 

Asteroids

Multi (and I mean multi) object target tracking Multiple-tree search Entering Google

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#### Asteroids

Multi (and I mean multi) object target tracking Multiple-tree search Entering Google

#### Asteroid Tracking

#### <u>Ultimate Goal</u>: Find all asteroids large enough to do significant damage, calculate their orbits, and determine risk.





### Why Is This Hard/Interesting?

#### **Partial Observability:**

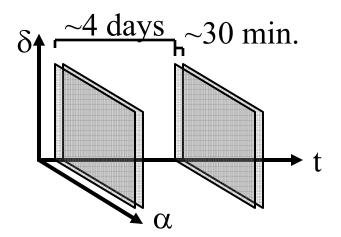
- Positions are in 3-d space.
- We see observations from earth.
- We see two angular coordinates  $(\alpha, \delta) \leq$
- We do **not** see the distance (r).

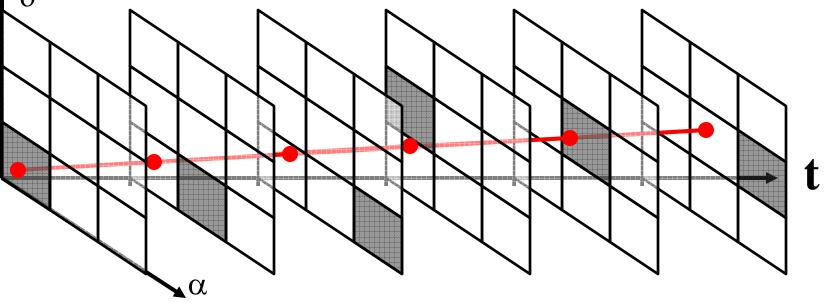


### Why Is This Hard/Interesting?

#### **Temporally sparse:**

- Each region viewed infrequently.
- Each viewing only covers a fraction of the sky.



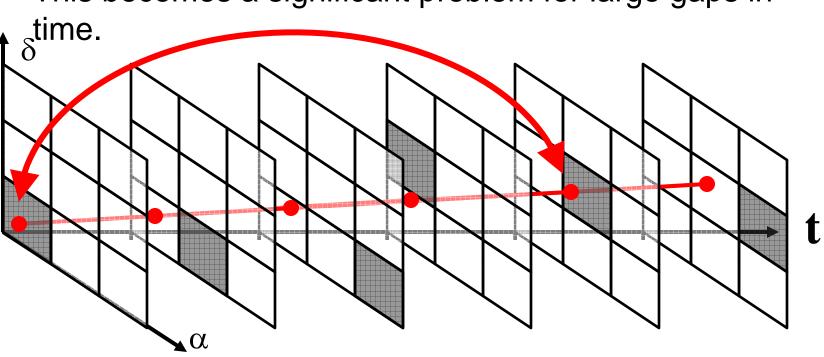




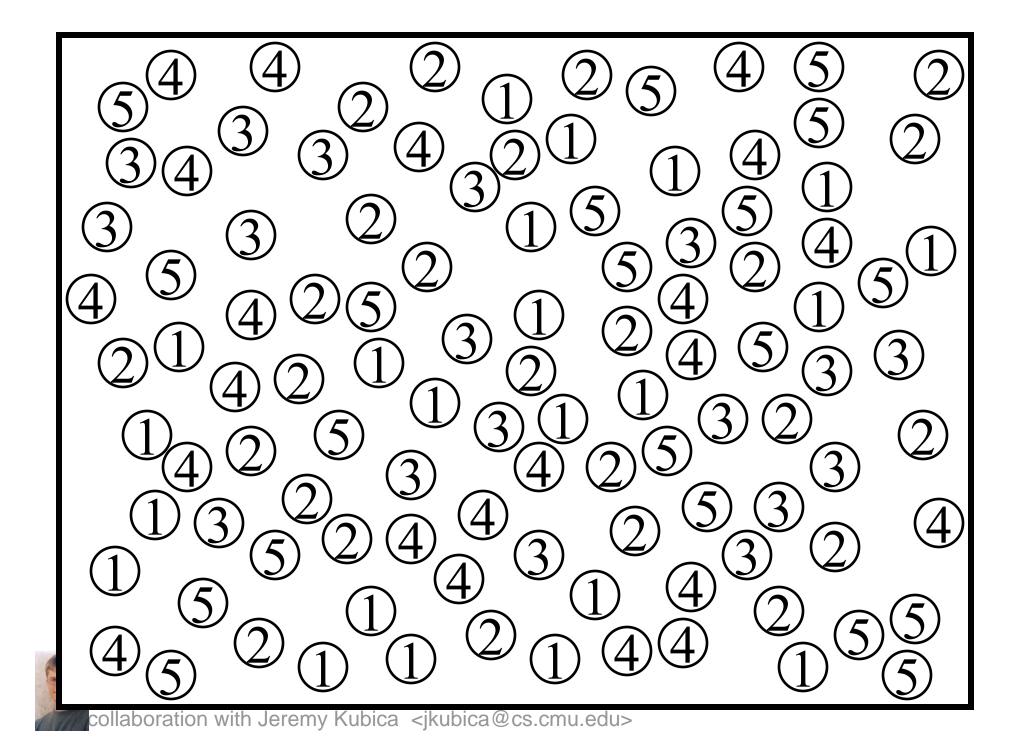
# Why Is This Hard/Interesting?

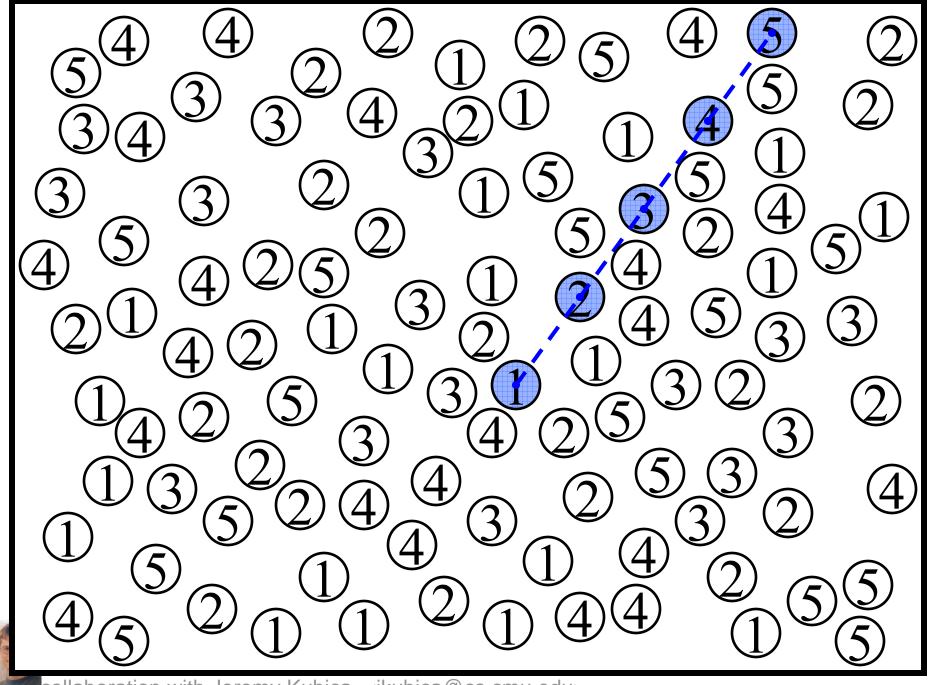
# Lack of initial parameter information (and temporally sparse):

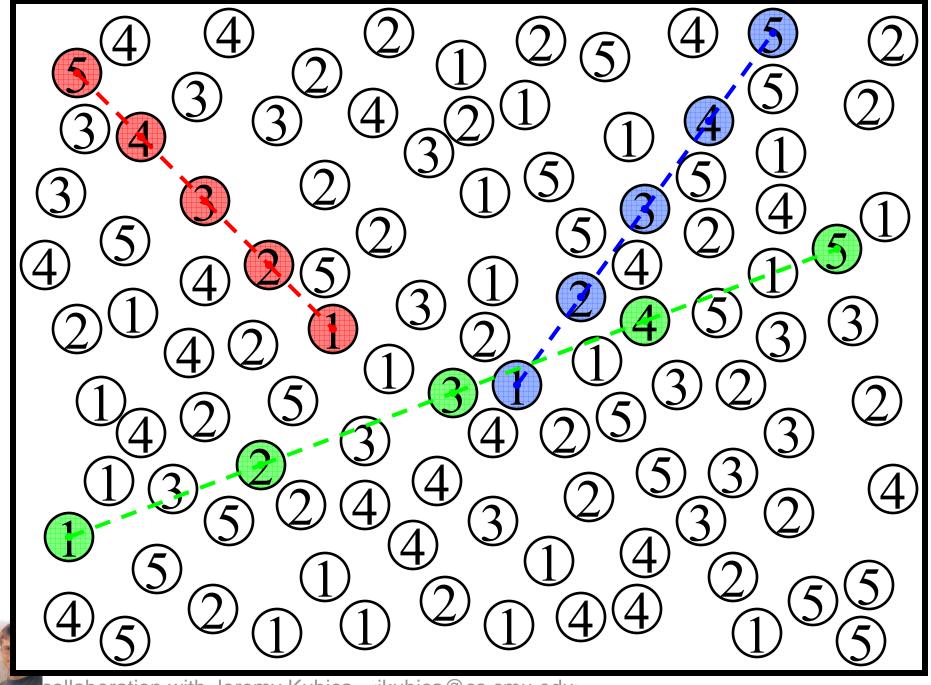
- We do not have initial estimates of all of the motion parameters.
- This becomes a significant problem for large gaps in time

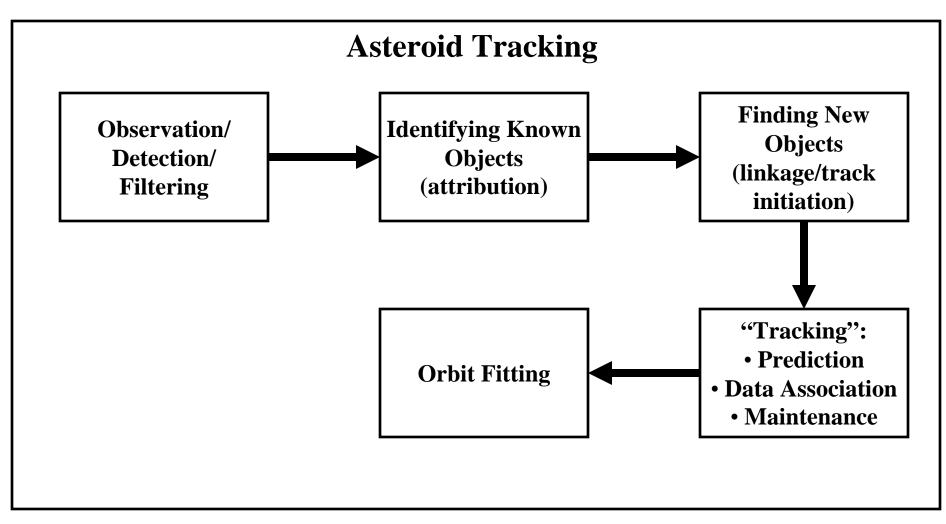




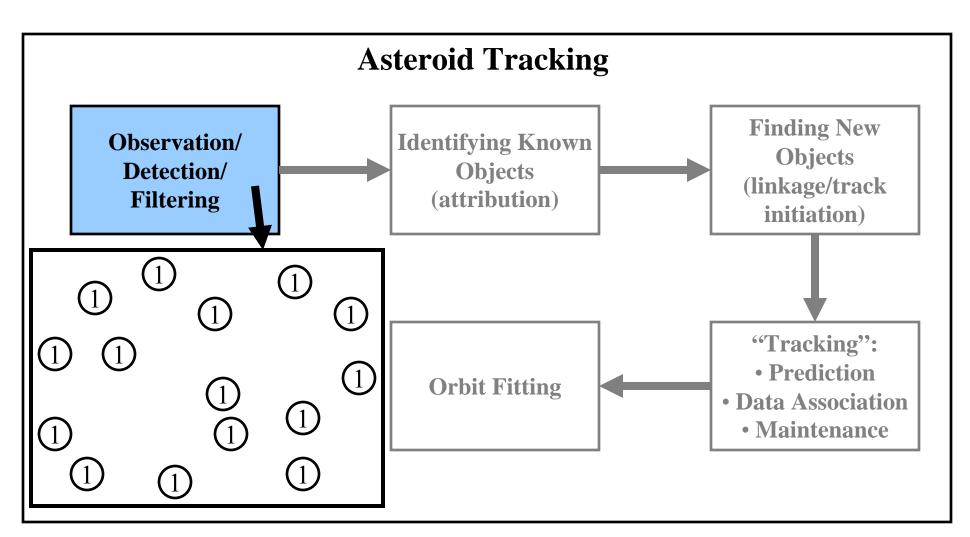




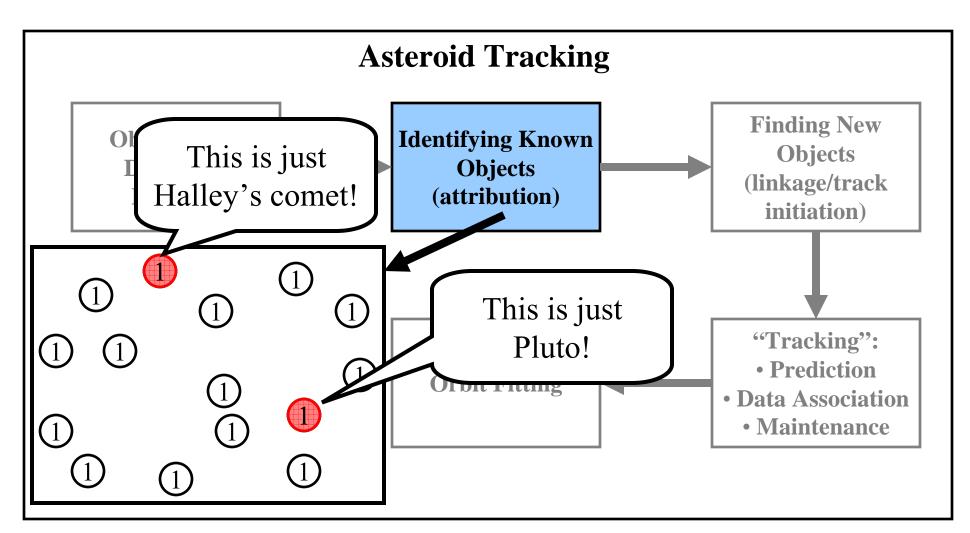




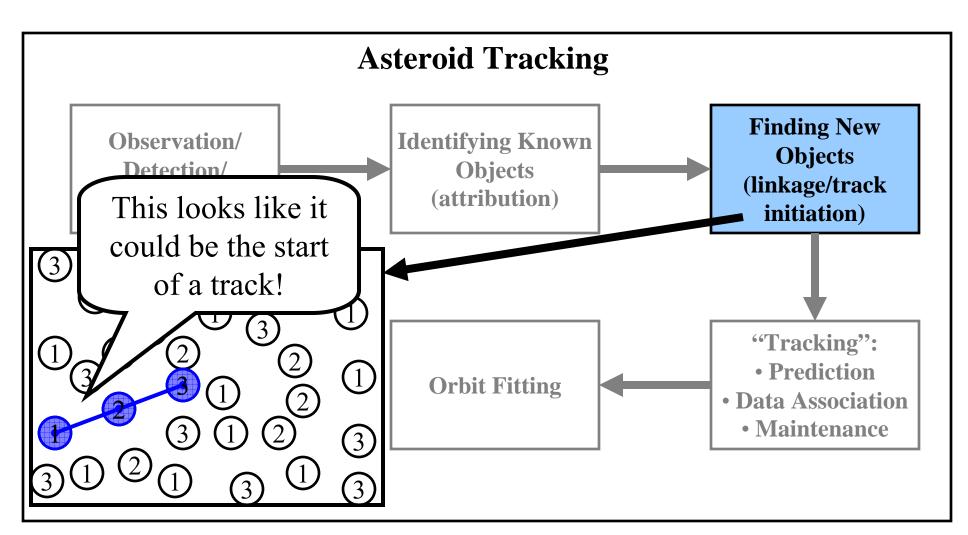




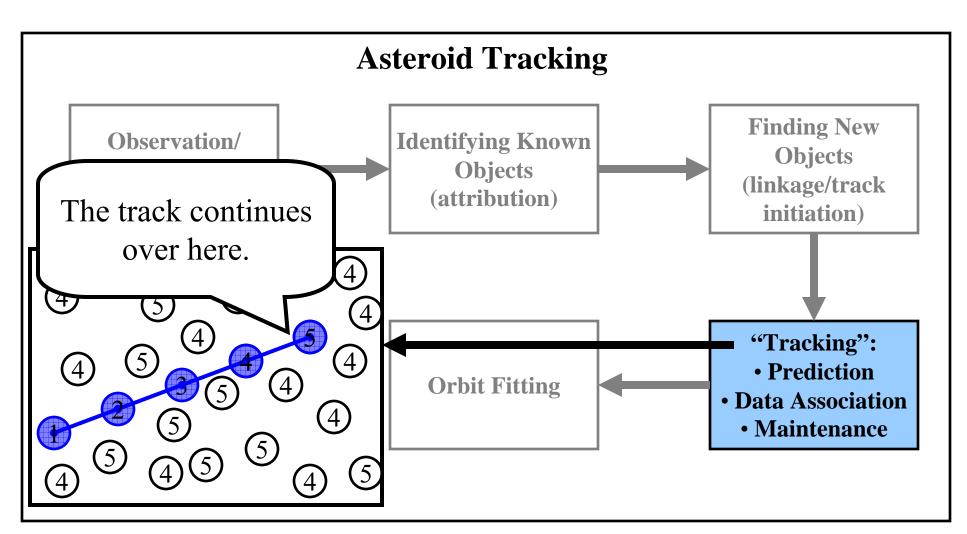




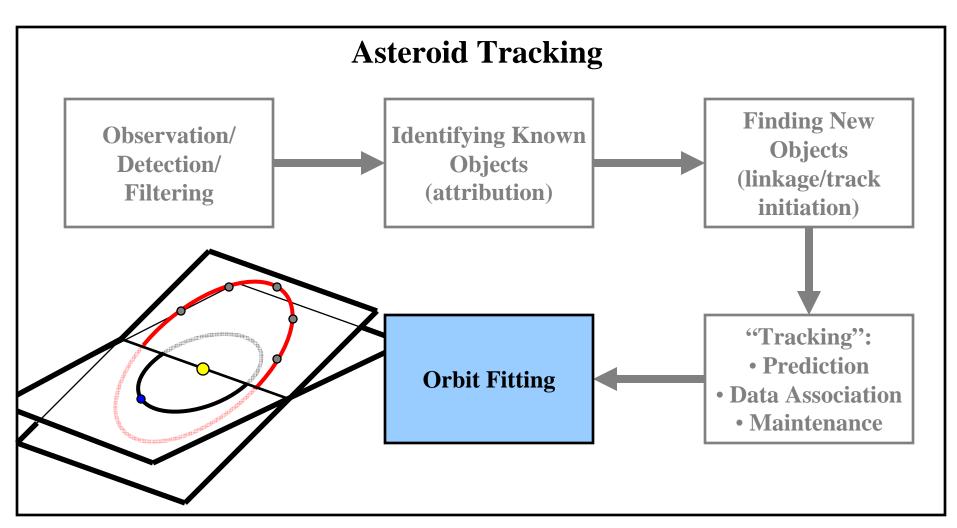




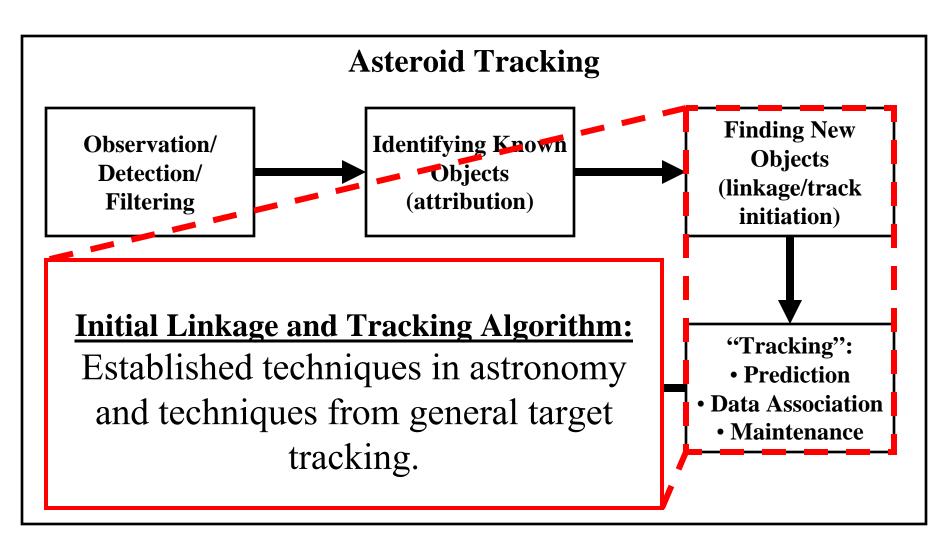








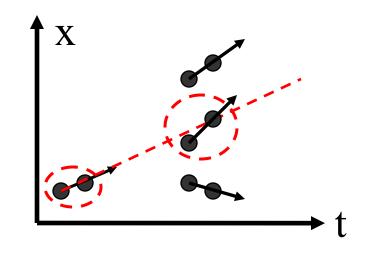






#### **Previous Approaches**

- Look for sets with linear movement over a short time span (Kristensen 2003, Milani 2004).
- "Close" observations from same night linked and used to estimate line (Marsden 1991, Milani 2004).
- Asteroid is projected to later nights and associated with other observations.



• Proposed sets of observations are tested by fitting an orbit.



### **Previous Approaches:** Drawbacks

- Linear projections will only be valid 1. over a short time span.
- Checking every neighbor can be 2. expensive.
- Orbit fitting is only applied after sets 3. are found with linear approximation.
  - May need to fit many orbits to incorrect sets.
  - May incorrectly reject true linkages based on linear model.















#### **Initial Improvements**

- We can improve accuracy and tractability by using techniques from general target tracking:
  - Sequential tracking,
  - Multiple hypothesis tracker,
  - Use of spatial structure via kd-trees, and
  - Quadratic track models.



#### **Evaluation**

Model	kd-	Time	Percent	Percent
	trees?	(sec)	Found	Correct
Linear	No	93	96.22	2.06
Linear	Yes	6	96.22	2.06
Quadratic	No	59	96.38	88.67
Quadratic	Yes	3	96.38	88.67

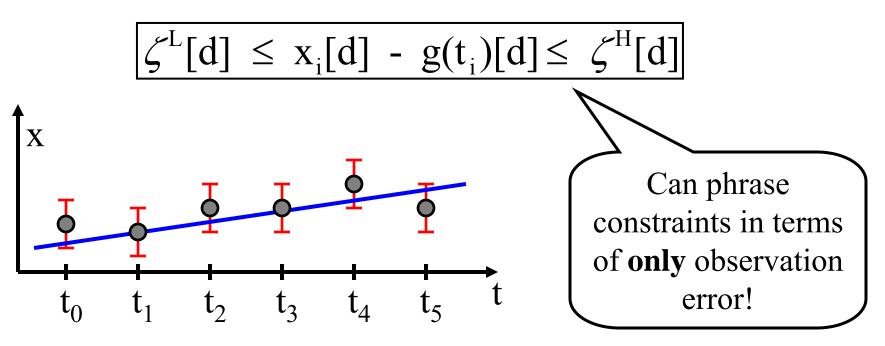


### Why "M-trees" method?

- Sequential approach is heuristic. We could end up doing a significant amount of work for "bad pairs".
- Early associations may be done with incomplete and/or noisy parameters.
- Next observation may be far from predicted position.
- dist
- Problem gets much worse as gap between
  observations increases.

### Motivation 2: Constrained Feasibility

- Find all tuples of observations such that:
  - We have exactly one observation per time, and
  - a track can exist that passes "near" the observations:





### Feasibility

- "Can any track exist that is near all of the observations?"
- Each observation's bounds give constraints on track's position at that time:

$$a[d]t_i^2 + v[d]t_i + p[d] \ge x_i[d] - \varepsilon$$
$$a[d]t_i^2 + v[d]t_i + p[d] \le x_i[d] + \varepsilon$$

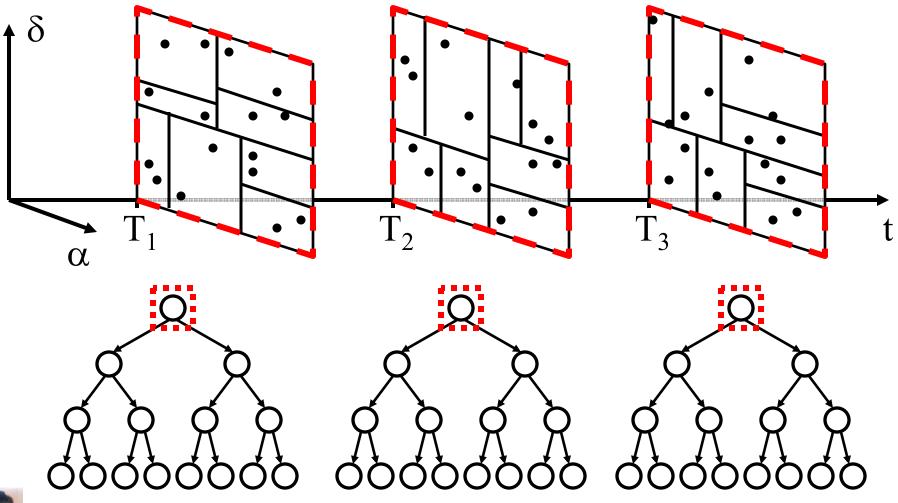
- We must either:
  - Find parameters satisfying these equations, OR
  - Prove that no such parameters exist.



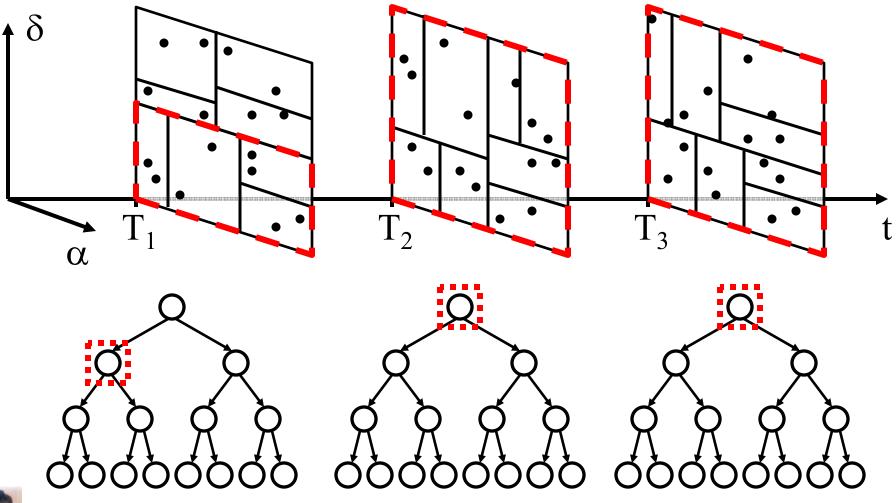
### Multiple Tree Approach

- <u>Our approach</u>: Use a multi-tree algorithm (Gray and Moore 2001):
  - -Build *multiple* kd-trees over observations.
  - -Do a depth first search of *combinations* of tree nodes.

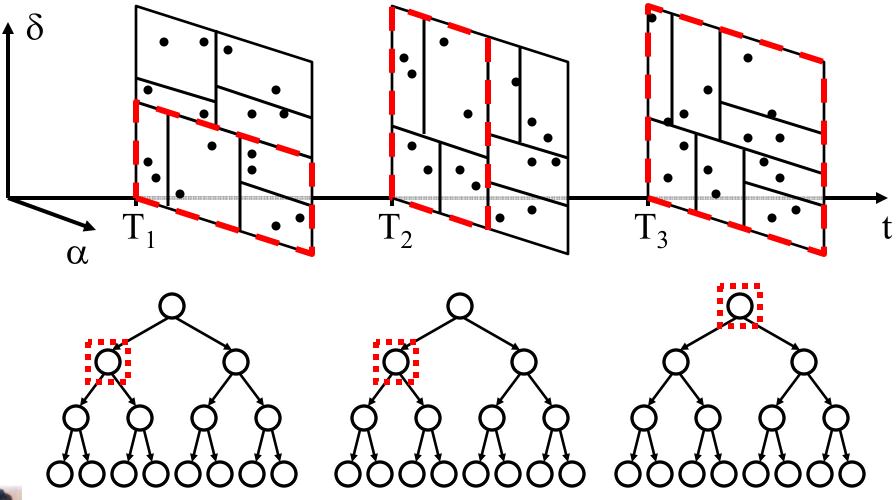




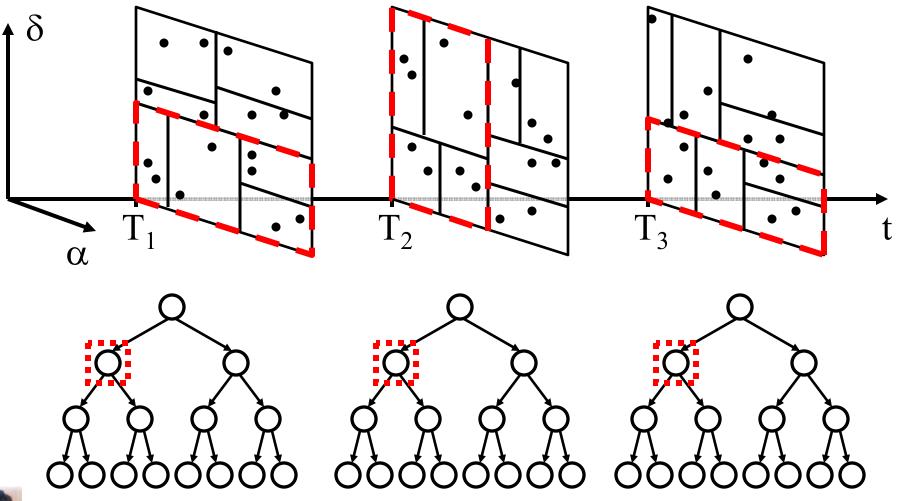




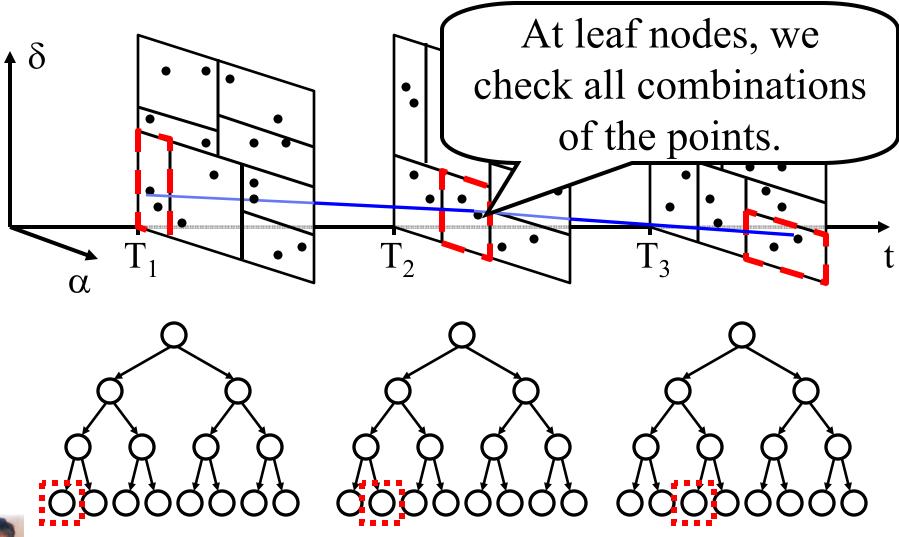




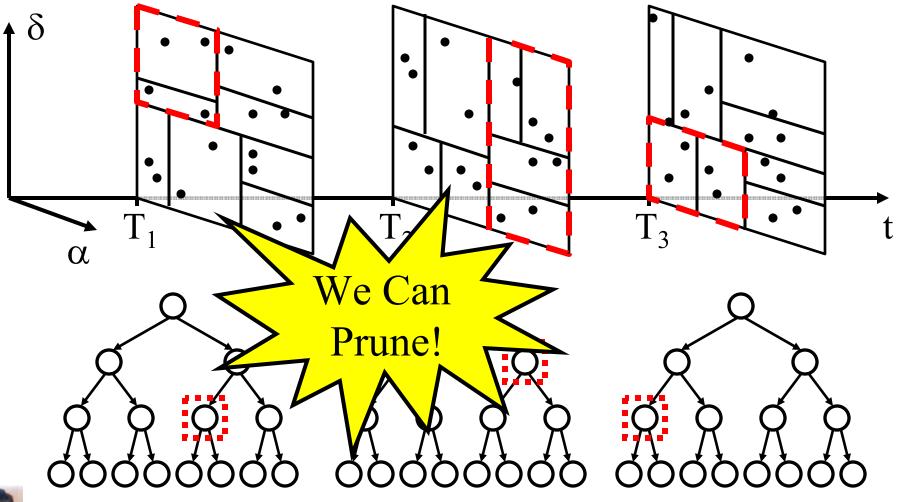














# Pruning

"Can any track exist that hits all nodes?"

Given times  $t_1, t_2, ..., t_M$ , and given kdtree bounding boxes  $(L_1, H_1), (L_2, H_2), ..., (L_M, H_M)$ , at those times, we ask...  ${}^{ii} \exists \mathbf{a}, \mathbf{v}, \mathbf{p}. \forall i \in \{1, 2, \cdots M\}, \forall d \in \{1, 2 \cdots D\},$  $a[d]t_i^2 + v[d]t_i + p[d] \ge L_i[d] - \varepsilon$  $a[d]t_i^2 + v[d]t_i + p[d] \le H_i[d] + \varepsilon$ 

Pruning = proving that such parameters do not exist.

#### **Pruning: Independent Dimensions**

<u>**Theorem 1**</u>: (*a*,*v*,*p*) is a feasible track if and only if (*a*[*i*],*v*[*i*],*p*[*i*]) satisfies the constraints in the i-th dimension for all i.

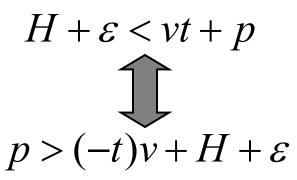
- Allows us to check the dimensions separately.
- Breaks query on 2MD constraints into D sub-queries of MD constraints.
- Each sub-query consists of significantly fewer variables.

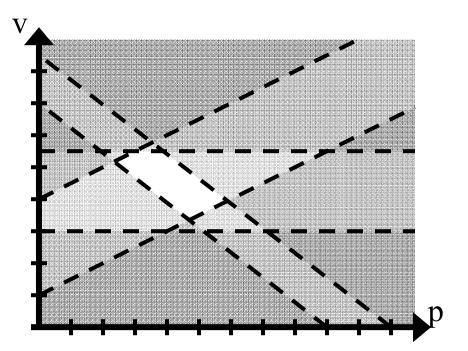


M = Number of timesteps (eg 4-6), D = Number of obs. dim'ns (eg 2), C = # Track params (eg 3)

#### **Constraints as Hyper-planes**

 Each constraint specifies a C dimensional hyperplane and half-space in parameter space:



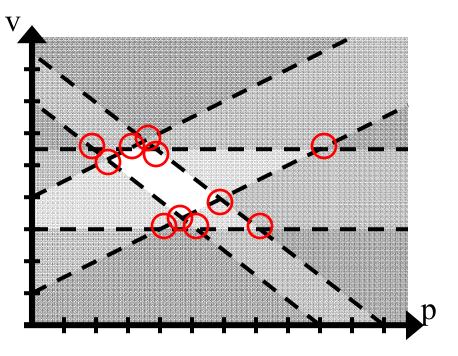


 If the intersection of the feasible half-spaces is not empty, then there exists a track that satisfies all of the constraints.



#### **Smart Brute Force Search**

- Search "corners" of constraint hyper-planes for feasible point.
- C nonparallel Cdimensional hyper-planes intersect at a point ("Corner").



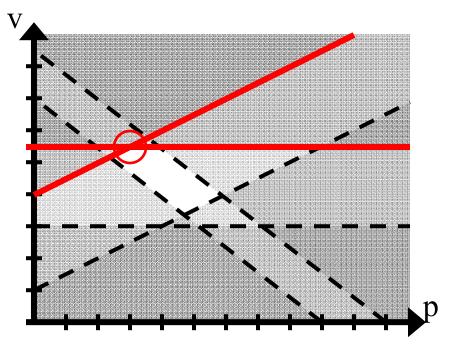
 <u>Theorem 2</u>: The intersection of M half-spaces defined by at least C nonparallel C-dimensional hyper-planes is not empty if and only if there exists a point (a,v,p) such that (a,v,p) is feasible and lies on at least C hyper-planes.



M = Number of timesteps (eg 4-6), D = Number of obs. dim'ns (eg 2), C = # Track params (eg 3)

# **Smart Brute Force Search**

- For each set of C nonparallel hyperplanes:
  - Calculate the point of intersection.
  - Test point for feasibility against other constraints.



- Positives: Simple, exact
- Negatives: Painfully slow -> O(DM<sup>(C+1)</sup>)



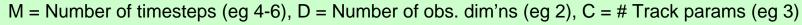
- The tree search provides a significant amount of structure that can be exploited:
  - At each level of the search, the constraints for all tree nodes except one are identical to the previous level

We can save the feasible track from previous level and test it against new (tighter)

constraints.



- The tree search provides a significant amount of structure that can be exploited:
  - At each level of the search, the constraints for all tree nodes except one are identical to the previous level.
  - At each level of the search, the constraints for the one tree node that changed are *tighter* than at the previous We can look for a new feasible point on hyper-planes from new constraints.

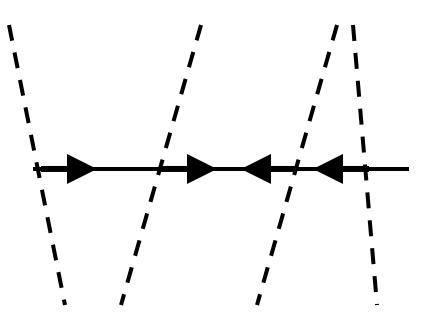


**Theorem 3**: If the feasible track from the previous level is not compatible with a new constraint then either the new set of constraints is not compatible or a new feasible point lies on the plane defined by the new constraint.

- Allows us to only check corners containing new constraints -> O(DM<sup>C</sup>)
- Allows us to check new constraints one at a time.



- We can combine search and test steps.
  - C-1 hyper-planes intersect at a line.
  - Remaining hyperplanes intersect the line at *signed* points.



 There is feasible point on those C-1 constraints if and only if there is a feasible point on the line.



Reduces cost to O(DM<sup>(C-1)</sup>).

# **Additional Constraints**

 This formulation of constraints allows us to add additional (non-node-based) constraints:

$$v_{\min[d]} \le v[d] \le v_{\max}[d]$$
$$a_{\min[d]} \le a[d] \le a_{\max}[d]$$

 This allows us to encode additional domain knowledge!



# Multiple Trees: Advantages

 Allows us to consider pruning opportunities resulting from future time-steps.

repeated over similar

observations/initial

Reduces work

tracks.



ollaboration with Jeremy Kubica <jkubica@cs.cmu.edu>

# Experiments

Experiment	Num Points	Seq secs	Seq P(C)	Singletree secs	Singletree P(C)	V-Tree secs	V-tree P(C)
BIGOBS	205424	66	0.18	31	0.46	15	0.46
Gap134	184016	31	0.07	24	0.83	6	0.90
Gap124	184016	28	0.10	12	0.69	6	0.69
61T.10.10	147244	102	0.3	5	0.77	2	0.77
61T.10.100	187178	451	0.22	7	0.76	7	0.76
61T.10.opp	179090	>2000	?	72	0.03	38	0.03
61T.1af	1433269	>2000	?	213	0.18	66	0.18



collaboration with Jeremy Kubica <jkubica@cs.cmu.edu>

### For more information and references to related work...

<u>http://www.autonlab.org/autonweb/14667.html</u>

```
@inproceedings{neill-rectangles,
Howpublished = {Conference on Knowledge Discovery in Databases (KDD)
2004},
Month = {August},
Year = {2004},
Editor = {J. Guerke and W. DuMouchel},
Author = {Daniel Neill and Andrew Moore},
Title = {Rapid Detection of Significant Spatial Clusters}
}
```

http://www.autonlab.org/autonweb/15868.html

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@inproceedings{sabhnani-pharmacy,
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    Year = {2005},
    Booktitle = {Proceedings of the KDD 2005 Workshop on Data Mining Methods
    for Anomaly Detection},
        Author = {Robin Sabhnani and Daniel Neill and Andrew Moore},
        Title = {Detecting Anomalous Patterns in Pharmacy Retail Data}
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#### For more information and references to related work...

<u>http://www.autonlab.org/autonweb/16063.html</u> @inproceedings{kubicaNIPS05,

```
Month = {December},
Year = {2005},
Booktitle = {Advances in Neural Information Processing Systems},
Author = {Jeremy Kubica and Andrew Moore},
Title = {Variable KD-Tree Algorithms for Spatial Pattern Search and Discovery}
```

- <u>http://www.autonlab.org/autonweb/14715.html</u>
- @inproceedings{kubicaKDD2005,

Month = {August}, Year = {2005}, Pages = {138-146}, Publisher = {ACM Press}, Booktitle = {The Eleventh ACM SIGKDD International Conference on Knowledge Discovery and Data Mining}, Author = {Jeremy Kubica and Andrew Moore and Andrew Connolly and Robert Jedicke}, Title = {A Multiple Tree Algorithm for the Efficient Association of Asteroid Observations}

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- <u>http://www.autonlab.org/autonweb/14680.html</u>
- @inproceedings{kubicaSPIE05,

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Month = {August},
Year = {2005},
Publisher = {SPIE},
Booktitle = {Proc. SPIE Signal and Data Processing of Small Targets},
Editor = {Oliver E. Drummond},
Author = {Jeremy Kubica and Andrew Moore and Andrew Connolly and Robert Jedicke},
Title = {Efficiently Identifying Close Track/Observation Pairs in Continuous Timed Data}
```

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**Justifiable Conclusions** 

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- Geometry can help tractability of Massive Statistical Data Analysis
- Cached sufficient statistics are one approach
- Not merely for simple friendly aggregates

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Fluffy Conclusion "Theorem of Statistical Computation Benevolence"

If Statistics thinks you're going the right way, it will throw in computational opportunities for you

Papers, Software, Example Datasets, Tutorials: www.autonlab.org

#### For more information and references to related work...



- - Author = {Jeremy Kubica and Andrew Moore and Andrew Connolly and Robert Jedicke}, Title = {Efficiently Identifying Close Track/Observation Pairs in Continuous Timed Data}