Pattern Recognition for Massive, Messy Data

(Data, data everywhere, and not a thought to think)

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

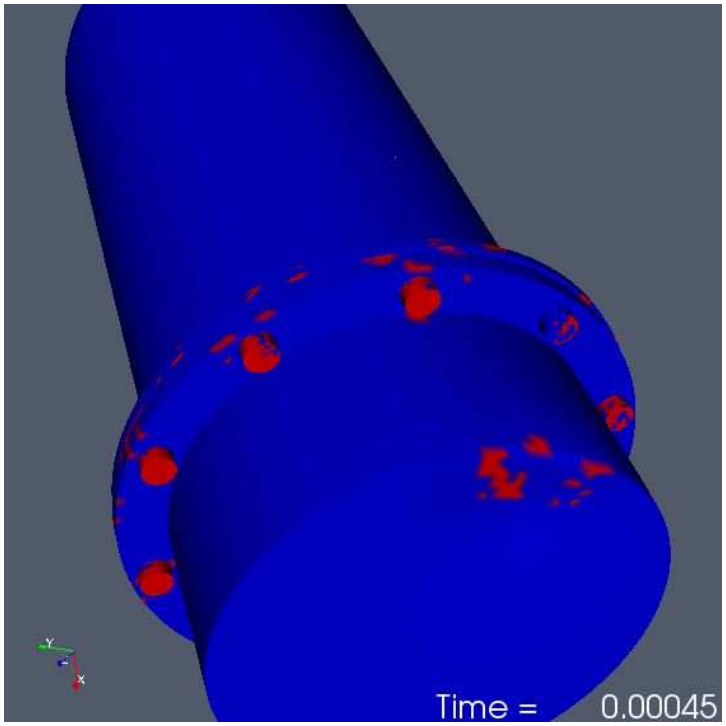
SAND Document #2006-3464, R&A #5243240

Introduction and Summary

Sandia is developing "commodity" pattern recognition methods which handle data sets that standard methods cannot.

These commodity methods:

- Accept data as is, and in situ.
- Are robust to errors in attributes and labels.
- Scale to terabyte data.
- Are crucial to Stockpile Stewardship post-processing.
- Are broadly applicable, in Sandia and out.

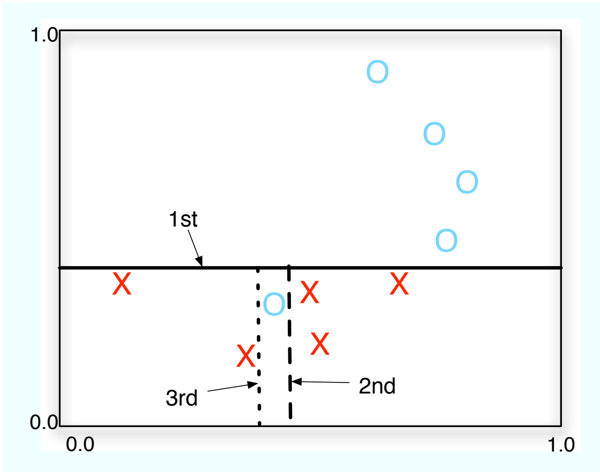


Bolt Failure Detection in ASC Data

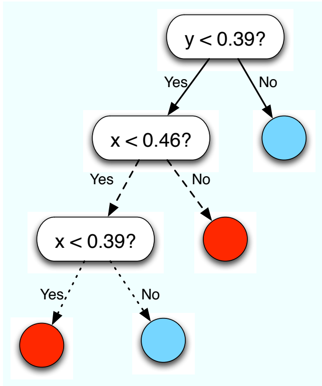
Pattern Recognition Overview

Also known as: supervised machine learning, statistical inference, data mining.

- Input: "ground truth" data.
  - Samples, with attributes, and *labels*.
  - Example ASC context:
    - Samples: nodes, elements.
    - Attributes: variable values.
    - Labels: breach, bolt failure, "interesting".
- Apply suitable method:
  decision trees, neural nets, SVMs.
- Output:
  rules for labeling new, *unlabeled* data.
  Equivalently:
  a partitioning of attribute space.

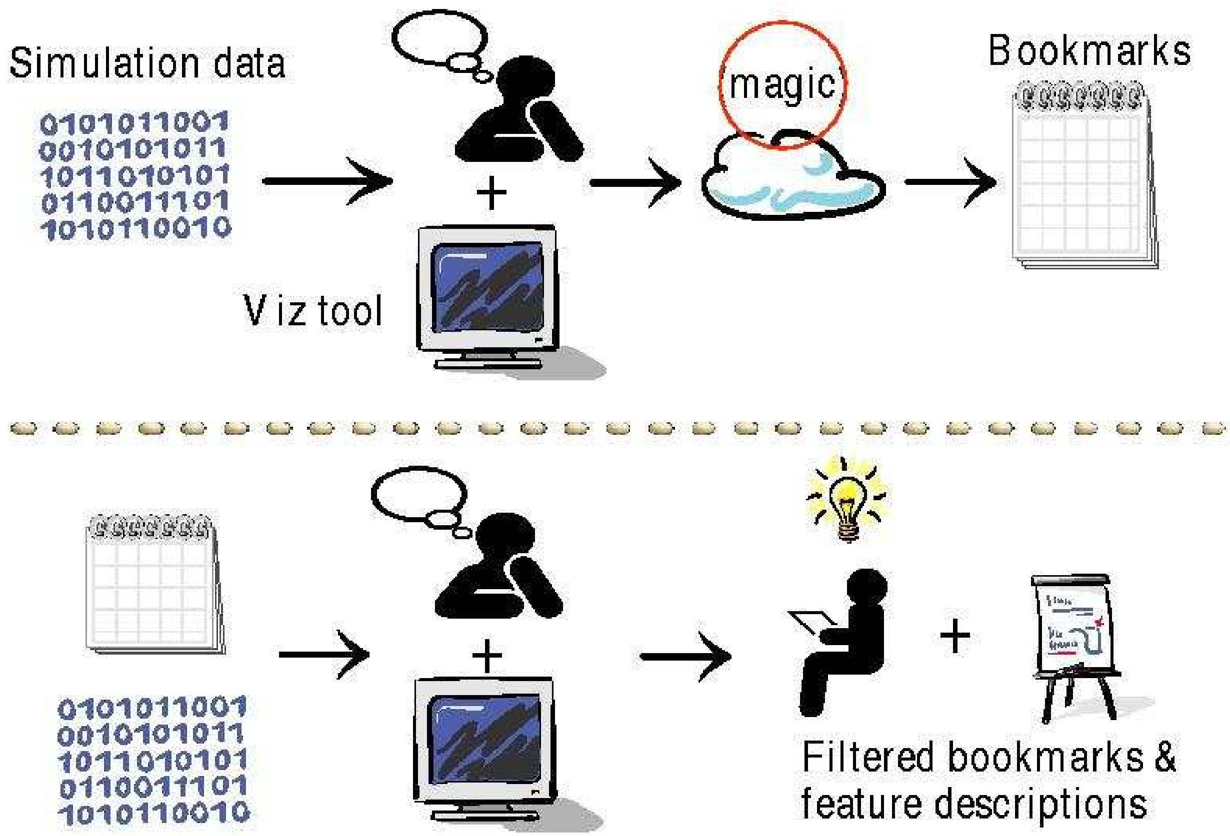


Attribute space partitioned.



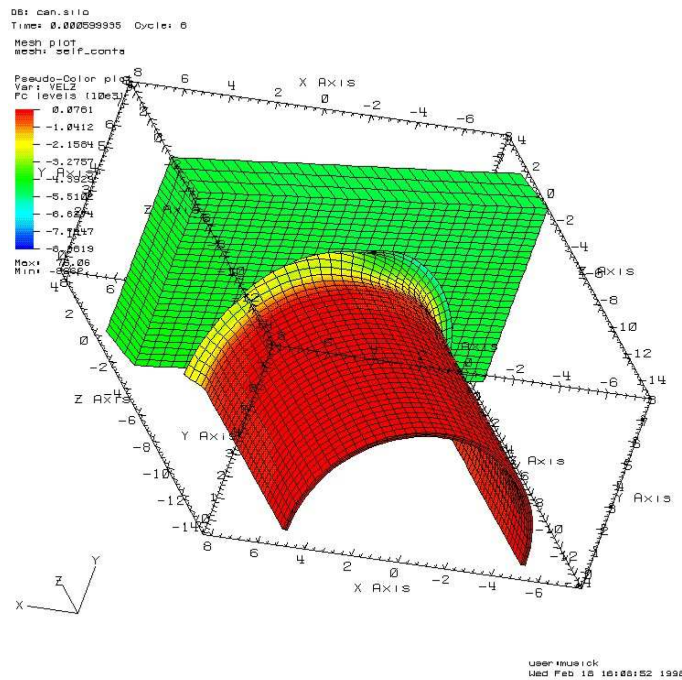
Decision tree representation.

Pattern Recognition for ASC



ASC Data is Daunting For Pattern Recognition

- Modern scientific data is:
  deeply skewed, ill-suited, noisy,
  and wrong.
- ASC data is all that and more:
  - Optimal for simulation,
    not for feature detection.
  - Highly redundant.
  - Terascale and partitioned.
  - “Interesting” is often the most useful label.
  - Unrelenting.



Simulation variables at every node in the mesh are processed by pattern recognition.

What to Do?

Give up on the craftsman model of pattern recognition.

Sandia has developed a *commodity* model:

- Accepts data as it is.
- No user tuning required.
- Robust in the face of noise.

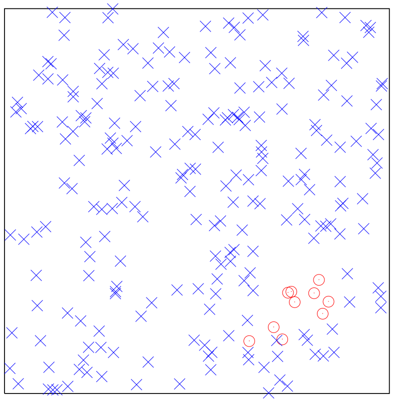
How? Some guiding principles:

1. Use *decision trees* over other methods.
2. Use *ensembles* of decision trees.
3. Embrace *redundancy.*
4. Emphasize *screening.*

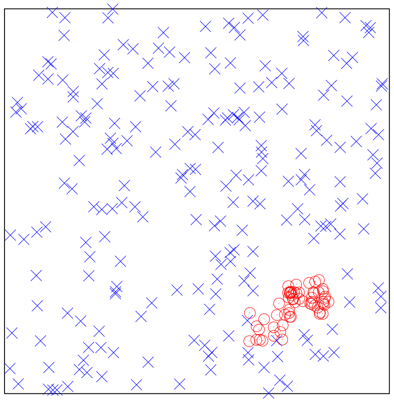
1 was mildly controversial;
2 and 3 *reverse* basic pattern recognition assumptions.

SMOTE for Skew Populations

- Synthetic Minority Oversampling TEchnique[6].
- Oversample the minority population, but ...
  ...simple oversampling induces pathologies.
  So: add *synthetic* samples.
- Method:
  - Pick minority sample.
  - Pick a nearby neighbor.
  - Add new minority sample at a random point between them.
  - Repeat.



Minority class overwhelmed.



Minority class filled out by SMOTE.

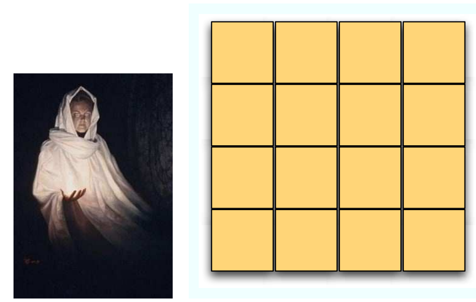
Ensembles: Democracy Over Meritocracy

Traditional: Use 100% of training data to build a sage.

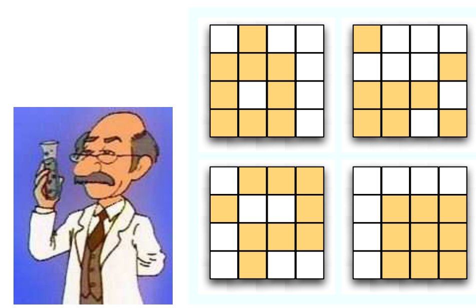
Ensembles: Use randomized 100% of training data to build an expert.
Repeat to build many experts.
Vote them.

Sandia: Use a semi-random 1% of the training data to build a "bozo".
Repeat to build very many bozos.
Vote them.

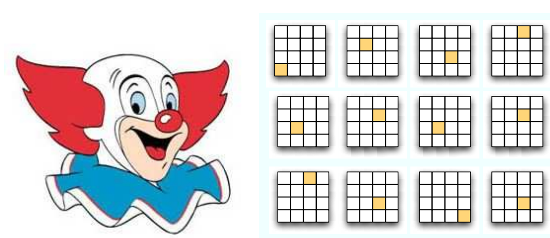
The experts beat the sage[2].
The bozos beat the experts[7].
How?
Averaging reduces measurement error.



Sage sees all the data.



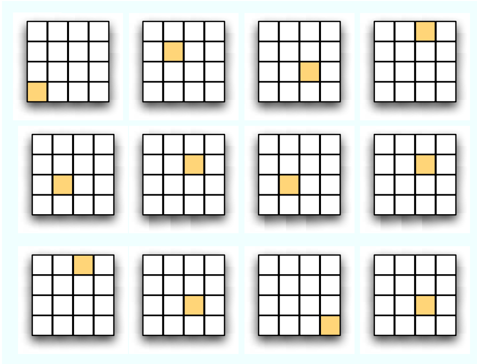
Each expert sees 2/3rds of the data.



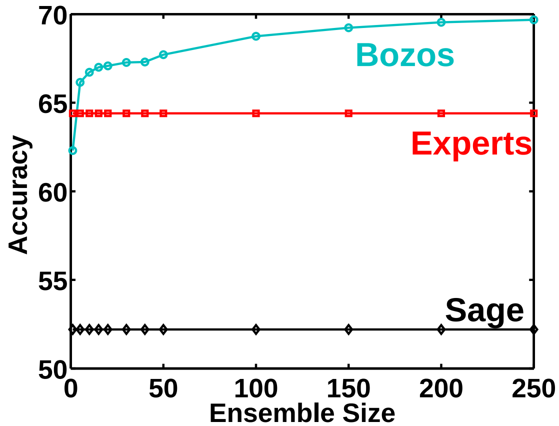
Each bozo sees a tiny fraction.

Ensembles of Bozos for Distributed Data

- Build separate ensembles on distributed data.
- Use "improvement voting" [7].
  - $e(b)$ is estimate of error rate of b bozos.
  - For (b+1)'st training set:
    - ∗ Accept all misclassified samples.
    - ∗ Accept correct samples with Prob $= e(b)/(1 - e(b))$
- Speed: $O(f \times b \times n \times \log n)$; bozos can be *faster* than sage, as well!



Bozos extracted in parallel.



Sample bozos, experts, and sage results[7].

Conclusion: Commodity Fixes for Data Challenges

Problem	Addressed by
Partitioned, terabyte data	ensembles of bozos
deeply skewed,	SMOTE
ill-suited,	decision trees, screening
noisy,	decision trees, ensembles, screening
and wrong	ensembles, redundancy, diversity

- General purpose methods (principles, algorithms, and code) to handle data sets that overwhelm standard methods.
- Broadly applicable; already in use on intelligence applications.
- Shared within Sandia via the AVATAR Tools package, more broadly via the open source OpenDT[1], and through frequent publication[10].

References

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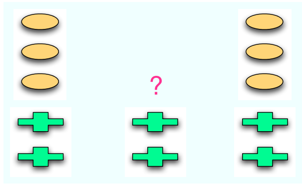
[10] Kegelmeyer, W. P., et al. AVATAR home page. http://morden.csee.usf.edu.

[11] Kolda, T., Dunlavy, D., and Kegelmeyer, W. P. Multilinear algebra for analyzing data with multiple linkages. Submitted to Twelfth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, April 2006.

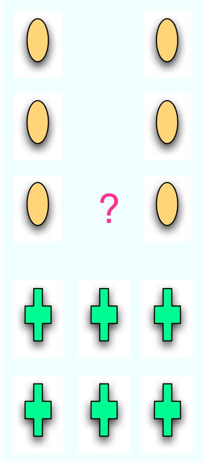
Background Slides To Follow...

Decision Trees Over Other Methods

- "No Free Lunch"[9] says the method doesn't matter . . .
  but only true for *clean* data!
- Most methods require a attribute distance metric . . .
  so attribute normalization matters.
- Decision trees don't need distance metric.
  - Use ordinal relations only.
  - Attributes need not be normalized.
  - Also, immune to noise attributes.
- With ensembles, no need to prune[7].



Unknown assigned differently . . .

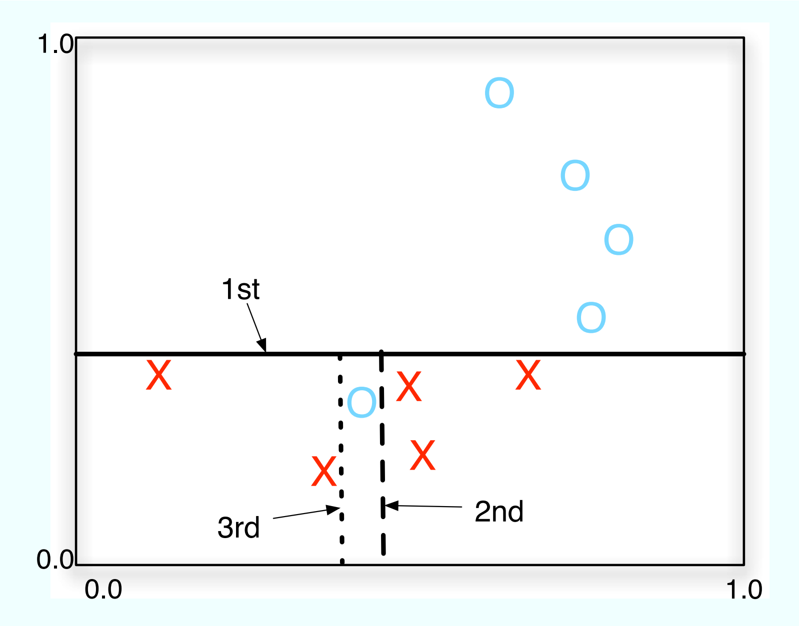


. . . depending on scaling

Decision Trees and Distance Metrics

- How to partition attribute space?
- For the current population:
  - Consider each attribute separately.
  - Consider each threshold for that attribute.
  - Pick attribute and threshold which "best decreases impurity".
  - Use them to partition the data into two child data sets.

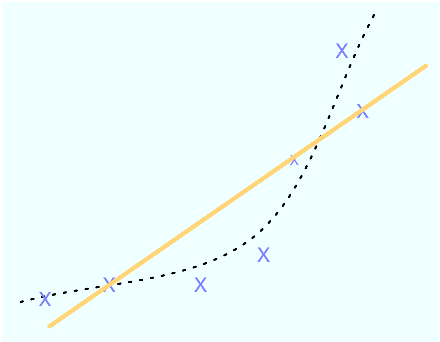
  Repeat with each child.
- Best attribute and threshold is *independent* of scaling.
- Irrelevant attributes ignored in the presence of relevant attributes.



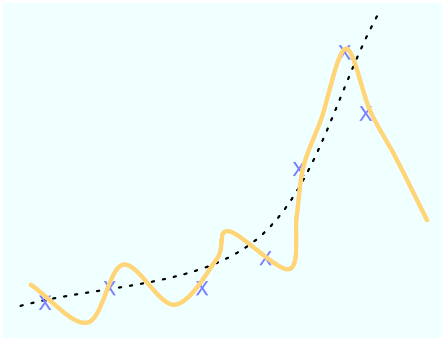
Attribute space partitioned.

Why Do Ensembles Work? (A)

- A statistical model is a *noisy* model of reality.
- Bias error:
  Model too simple, underfits.
- Variance error:
  Model too complex, overfits.
- Bias/variance is a trade-off.
- Ensembles:
  - Use methods with low bias...
    but high variance ...
    and average to reduce variance!
- Out-of-bag validation picks ensemble size[3].
- Result:
  low bias error *and* low variance error.
  No hand tuning needed.



Too simple a model underfits the data.

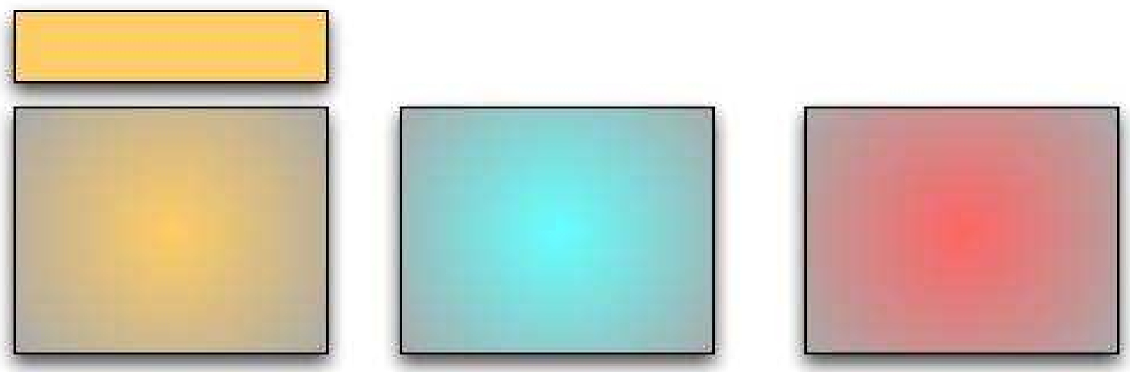


Too complex a model overfits the data.

Why Do Ensembles Work? (B)

One key is *diversity* [8].

Imagine: three classes, each bozo only 10% accurate, and when wrong, chooses at random among the three classes.
Then the horde of bozos is perfectly, 100% accurate!



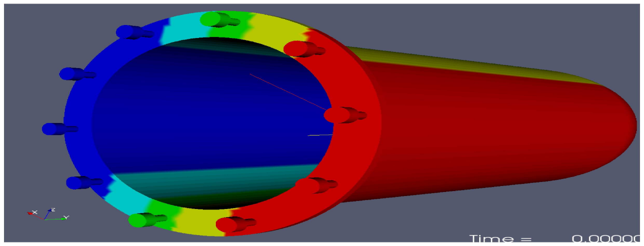
One group of unconfused bozos amid the foggy error.

Note: diverse, *random* error is difficult to achieve[4].

Next: Inconsistent Class Statistics

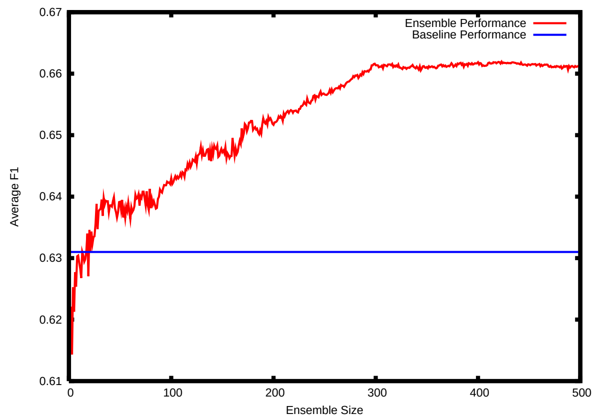
- ASC data is partitioned *and* varies in class statistics.
  - Grow ensembles of bozos on each partition.
  - *Each* ensemble generates a vote.
  - Each vote is weighted by priors:

$$
\begin{aligned}
p(w_i|x) &= \text{percentage of ensembles that vote for } w_i \text{ given } x. \\
P(w_i) &= \text{percentage of ensembles which have seen class } w_i. \\
\text{Classify as } w_m &: argmax_n\left(\frac{p(w_i|x)}{P(w_i)}\right)
\end{aligned}
$$

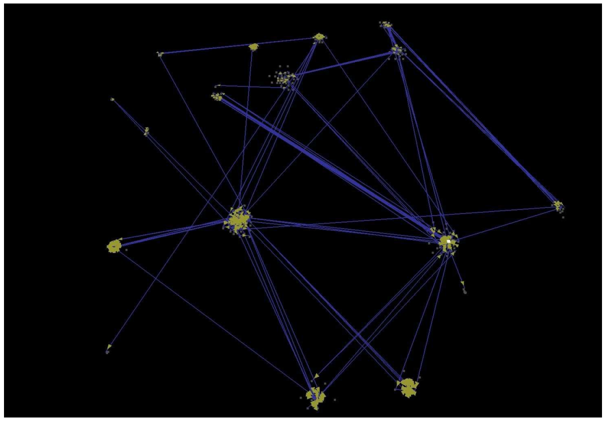


Impact: Text, Graphs, and Intelligence Analysis

- Intelligence data is often relationship data, and graphs encode relationships.
- Text pattern recognition:
  - Why? To auto-populate graphs.
  - “NER” is phrase classification.
  - Significant improvement on contest data.
- Graph pattern recognition:
  - Classify nodes, edges.
  - Find missing links, subgraphs.
  - Tensors for multilink analysis[11].
- Also, ensembles ease data sharing.



NER improves with ensemble size.



Example multilink graph.