Discovery

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New uses for old hardware...
What is 'Discovery'?

- A TV channel?
- A type of Landrover?
- A famous sailing ship?
- finding something new or unexpected...?
"Modern approaches to data analysis... have clarified the fact, known to practicing scientists, that the hypotheses do not always precede the data."

(Velleman & Wilkinson, 1993)
Themes

⛅ Why do we need help with discovery?
⛅ How is new knowledge inferred?
⛅ What tools and techniques are available to help us with inference?
A previous life...Discovering gold deposits

★ Don’t know exactly how gold deposits are signified in data.
★ Don’t know exactly how mineralization occurs in the world.
★ So, discovery is a combination of looking for clues and using what is found to extend or modify theory accordingly.
Why do we need help with discovery?

 suffice

Geography has moved from being data poor to data rich in a short space of time...

- Geographic datasets are becoming large, complex and heterogeneous (highly multivariate)...

- We are beginning to address problems that span across several domains of expertise (e.g. impact of Lyme Disease), and we do not fully understand cause and effect.

Despite enormous efforts in quantification, our understanding of many of the earth’s systems remain non-axiomatic; the systems are ‘open’ and consequently it is not possible to deduce all outcomes from known laws.
Where do we begin?

“Discovery commences with the awareness of anomaly, i.e., with the recognition that nature has somehow violated the paradigm-induced expectations that govern normal science.” (Kuhn, 1962)

“Truth emerges more readily from error than from confusion.” (Francis Bacon, 1869)

... so we need to make mistakes...

... by imposing structures on data, observing the outcomes, and reasoning from what we observe.
“To know what we think, to be masters of our own meaning, will make a solid foundation for great and weighty thought.” (C.S Peirce, 1878)

Several styles of inference are possible:

- expert or model driven (deductive),
- Learning from examples (inductive),
- Hypothesis creation (abductive).
Origins of Scientific Reasoning: 
It’s all Greek to Me!

Socrates claimed to be certain of very little, his relentless questioning challenged existing, widely-held philosophical beliefs, based on: Truth, Beauty, Virtue and Justice.

Plato (Socrates’ student) established epistemology (the study of the nature of knowledge and its justification) based on Socrates’ ideas.

Aristotle (Plato’s student) proposed ways to represent knowledge and a nomenclature for describing it (including inventing the terms: metaphor & hypothesis).
Deduction

Aristotle invented the syllogism...

IF

Nothing absent minded is an elephant

AND

All professors are absent-minded

THEREFORE

No professor is an elephant
Deduction ≠ Science

- Deduction is often treated as the only legitimate form of inference for a respectable scientist...
- BUT it cannot generate new knowledge!
- Deduction is what computers are good at.
- In many situations, deductive rules get too messy, and besides, we (people) do not usually describe objects and categories according to precise values of their attributes.
Induction

Induction operates by “learning from known examples”.

The inductive learning hypothesis: “A hypothesis constructed from enough training examples will generalize to unseen examples”

A large portion of human knowledge is thought to be captured and formed inductively: e.g. we synthesize models of categories from examples given and use these models to identify new examples.
Learning via Induction

Labeled examples

Learning Phase

Input vector of $p$ attributes: the training values for a single ‘case’

Desired outcome: continuous number or categorical value

Generalized model for mapping $K$ to $P$

Inductive Learning

TRAINING PHASE: model is learned

APPLICATION PHASE: model is applied

Generalization phase
Abduction (Hypothesis)

In abduction, an artifact is observed and simultaneously, a hypothesis is offered to explain it.

For example, an anthropologist researching the customs and behaviors of a society..., a geologist in the field working on an evolutionary explanation.

A hypothesis may draw from existing knowledge, or may extend it... e.g. by using analogy.

The 'Aha!' Moment...

In exploratory visualization, this artifact is a visual stimulus.
Doing GIScience...
Examples of computational tools for discovery

- **Association rules:**
  - Use joint-count statistics to assess likelihood of occurrence of some pattern A given pattern B.

- **Unsupervised pattern analysis (AutoClust, AutoClass):**
  - Use measures of local and global density to form clusters or classes.

- **Decision trees: (C4.5, RIPPER, BOAT)**
  - Decision rules are used to carve up feature space
  - Search is hierarchical, only 1 dimension at each iteration.
More examples

Feedforward neural networks:
- hyperplanes are positioned in feature space.

Genetic algorithms (artificial life):
- search by simulating a population of organisms evolving within an environment.

Bayesian networks:
- work from a model of concepts provided by the expert, linked via a network of conditional dependencies.
How current tools infer...

Most computational data mining and knowledge discovery tools either attempt to locate pre-defined patterns (using *deduction*) or else learn from examples that are presented or selected (induction)...

Others use a weaker form of *abduction*: a pattern is 'discovered' along with an explaining hypothesis, but this hypothesis is defined in terms of the data alone.

So computers can build new descriptions of pre-existing concepts, but not new concepts themselves, or theories that employ them...

...or can build only syntactic description of concepts that need still to be given meaning in human terms.
Inference

Notice that induction and abduction do not enforce an entirely deterministic structure on a problem.

In direct contrast to deduction, they:

- Can produce new knowledge
- Recognize the importance of learning and refinement
- Respond to the individual situation of a given problem or dataset
Why visualize?

*Machines do deduction well, people do not*

*Machines do induction well, but only with attributes (and more recently relationships); people use additional types of knowledge (e.g. procedural, tacit)*

*It is very difficult to perform computational abduction, it requires the encoding of detailed domain knowledge).*

*"The more realistic the model of abduction required, the less computationally tractable it becomes." (Psillos, 2000)*

*We visualize because visualization attempts to connect with the inferential abilities of humans, rather than replace them.*
Abduction and Visualization

Visual Display: Computer

Brain: Person
Graph-based methods

Employ traditional 'quantitative' graphing methods, based around numerical axes.

 Exploration, detection of clusters, dominant trends and outliers:
Iconographic Methods (Pickett & Grinstein)

Make use of 'pre-attentive' visual mechanisms that notice subtle differences in shape, orientation and texture...

Allow us to examine covariance across many variables.
Map-based methods

Show data within their spatial context

Population Growth and Immigrant Populations in Major US Cities
1890 - 1990

Living Conditions for Pennsylvania by County

Income
Unemployment
Population Density

Gulf of Mexico

Population Density is represented by the size of the county. The image above is a reference.

Unemployment

<table>
<thead>
<tr>
<th>Unemployment</th>
<th>0.1-2</th>
<th>2.3-4.5</th>
<th>5.6-6.8</th>
<th>7.1-11.9</th>
<th>25-38.3</th>
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</thead>
<tbody>
<tr>
<td>Value</td>
<td>21286-25788</td>
<td>25789-30291</td>
<td>30292-39009</td>
<td>39010-47728</td>
<td></td>
</tr>
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‘Landscape’ Metaphors...
tap into our experience at interpreting natural vistas.
Landscape draped with icons.

This scene depicts 10 dimensions of data.
Data driven... knowledge driven

Cluster Detection (GAM, AUTOCLUST)

Unsupervised classifiers (AutoClass, SOM)

Scatterplot / PCP Visualization

Visual Data Mining

Neural Networks & Decision Trees

Map-based Visualization

Iconographic Visualization

Genetic Algorithms

Cellular Automata

Bayesian Inference Networks

Rule-based Expert Systems

Visual Scene Composition

Case-Based Reasoning

Visualization methods

Computation methods
Summary of various approaches...

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<td>Data reduction and stratified sampling strategies</td>
<td>Stochastic search, gradient ascent methods</td>
<td>Hierarchical and adaptive methods, grand tours</td>
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Problems with discovery

- We need a way of saying what it is we already know...
- We need a mechanism to subtract what we do know from the data—otherwise obvious patterns dominate...
- We need mechanisms to search for the 'peculiarly geographic'?
  - (signatures of geographic processes such as diffusion, clustering, interaction)
- If each display represents a hypothesis (this data, shown that way, might show useful structure) then we are producing a lot of hypotheses to evaluate...
- The hypotheses we produce contain all kinds of implicit biases...
More problems with discovery

- The number of ways we could visualize the data is computationally explosive ($n$ data variables mapped to $v$ visual variables)... we cannot test them all.
- Generally speaking, we do not know enough about how different visual variables support or interfere with each other...
- We need to be able to specify what our current task is, and hence have the system change its behavior...
- Even if we could control for all perceptual effects, users will still understand what they see differently...
BUT
Problems  Opportunities

These problems, or similar, pervade data mining and knowledge discovery in general!

All the problems mentioned above are being addressed currently in visualization research.

The advantage of retaining the user’s expertise remains... Visualization for Intelligence Augmentation (Mixed Initiative Systems).

And most importantly, visualization facilitates abduction, whereby new theory can be created.
Almost the End...

"Science does not rest upon rock-bottom. The bold structure of theories rises, as it were, above a swamp, but does not go down to any natural or 'given' base; and when we cease our attempts to drive our piles into a deeper layer, it is not because we have reached firm ground. We simply stop when we are satisfied that they are firm enough to carry the structure, at least for the time being."

(Popper, 1959)
Challenges

★ Discovery is about building a structure that is strong enough to bear the concepts we need for our research, and no stronger.
★ We do not need to model the world in infinite detail.
★ The ancient Greek philosophers believed in ‘natural categories’ by which all things could be classified...
★ We need to discover new objects, categories, relationships and theories by which we can explain complex geographical systems.
★ We should resist urges to believe that this structure is ‘true’ and will last for ever.
Conclusions

- Inference is more than deduction.
- Deduction is good for some classes of problem, but...
- Geographical analysis that is entrenched only in deduction is unlikely to lead to new insights.
- Induction and abduction allow for human experience and the uniqueness of situations to influence outcomes. They also allow new knowledge to be created.
- Computational induction is now being used to solve many problems in physical geography, and some in urban and political geography.
- Our challenge is enable abduction via our visual methods.
The End