

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)



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?

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 <u>mistakes</u>...

imposing structures on data, observing the outcomes, and reasoning from what we observe.

How we infer...

* 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*).



Aristotle invented the syllogism...

١F

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!
- **Transformation Zero Constitution Zero Con**
- 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



Abduction (Hypothesis)

- 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 GI Science...



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 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 preexisting 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.



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

i In direct contrast to deduction, they:

- ** Can produce <u>new knowledge</u>*
- **#** Recognize the importance of <u>learning</u> and <u>refinement</u>
- **#** Respond to the <u>individual situation</u> 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



Graph-based methods

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

***** Exploration, detection of clusters, dominant trends and outliers:





Conographic Methods (Pickett & Grinstein)



Map-based methods



'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



Knowledge driven

Summary of various approaches...

	Databases	Statistics	A. I.	Visualization
Finding	Association rules	Local pattern analysis and global inferential tests	Neural networks, decision trees	Exploratory visualization Visual data mining
Reporting	Rule lists	Significance and power	Likelihood estimation, information gain	A stimulus within the visual domain
Representing	Schema update, metadata	Fitted statistical models, local or global	Conceptual graphs, meta models	Shared between the scene and the observer
Validating	Weak significance testing	Significance tests	Learning followed by verification	Human subjects testing.
Optimizing	Reducing computational complexity	Data reduction and stratified sampling strategies	Stochastic search, gradient ascent methods	Hierarchical and adaptive methods, grand tours

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)

I f 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 <u>could</u> 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...

Æ Even if we could control for all perceptual effects, users will still understand what they see differently...



BUT



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 <u>Intelligence Augmentation</u> (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.

