Experiment Design for Computer Scientists

Marie desJardins (mariedj@cs.umbc.edu)

CMSC 691B

March 9, 2004

Sources

- Paul Cohen, *Empirical Methods in Artificial Intelligence*, MIT Press, 1995.
- Tom Dietterich, CS 591 class slides, Oregon State University.
- Rob Holte, "Experimental Methodology," presented at the *ICML 2003 Minitutorial on Research, 'Riting, and Reviews.*

Experiment design

- Experiment design criteria:
  - **Claims** should be **provable**
  - Contributing **factors** should be isolated and **controlled** for
  - Evaluation **criteria** should be **measurable** and **meaningful**
  - **Data** should be gathered on **convincing** domains/problems
  - **Baselines** should be **reasonable**
  - **Results** should be shown to be **statistically valid**

Provable Claims

Provable Claims

- Many research goals start out vague:
  - Build a better planner
  - Learn preference functions
- Eventually, these claims need to be made provable:
  - Concrete
  - Quantitative
  - Measurable
- Provable claims:
  - My planner can solve large, real-world planning problems under conditions of uncertainty, in polynomial time, with few execution-time repairs.
  - My learning system can learn to rank objects, producing rankings that are consistent with user preferences, measured by probability of retrieving desired objects.

More Provable Claims

- More vague claims:
  - Render painterly drawings
  - Design a better interface
- Provable claims:
  - My system can convert input images into drawings in the style of Matisse, with high user approval, and with measurably similar characteristics to actual Matisse drawings (color, texture, and contrast distributions).
  - My interface can be learned by novice users in less time than it takes to learn Matlab; task performance has equal quality, but takes significantly less time than using Matlab.

One More

- Vague claim:
  - Visualize relational data
- Provable claim:
  - My system can load and draw layouts for relational datasets of up to 2M items in less than 5 seconds; the resulting drawings exhibit efficient screen utilization and few edge crossings; and users are able to manually infer important relationships in less time than when viewing the same datasets with MicroViz.

Measurable, Meaningful Criteria

Measurable Criteria

- Ideally, your evaluation criteria should be:
  - Easy to measure
  - Reliable (i.e., replicable)
  - Valid (i.e., measuring the right thing)
  - Applicable early in the design process
  - Convincing
- Typical criteria:
  - CPU time / clock time
  - Cycles per instruction
  - Number of [iterations, search states, disk seeks, ...]
  - Percentage of correct classification
  - Number of [interface flaws, user interventions, necessary modifications, ...]

Meaningful Criteria

- Evaluation criteria must address the **claim** you are trying to make
- Need clear relationship between the **claim/goals** and the **evaluation criteria**
- Good criteria:
  - Your system *scores well iff it meets* your stated goal
- Bad criteria:
  - Your system can *score well* even though it *doesn't meet* the stated goal
  - Your system can *score badly* even though it *does meet* the stated goal

Example 1: CISC

- True goals:
  - **Efficiency** (low instruction fetch, page faults)
  - **Cost-effectiveness** (low memory cost)
  - **Ease of programming**
- Early metrics:
  - **Code size** (in **bytes**)
    Entropy of Op-code field
  - **Orthogonality** (can all modes be combined?)
- Efficient execution of the resulting programs was not being directly considered
- RISC showed that the connection between the criteria and the true goals was no longer strong
- → Metrics not appropriate! ☹

Example 2: MYCIN

- MYCIN: Expert system for diagnosing bacterial infections in the blood
- Study 1 evaluation criteria were:
  - **Expert ratings of program traces**
    - Did the patient need treatment?
    - Were the isolated organisms significant?
    - Was the system able to select an appropriate therapy?
    - What was the overall quality of MYCIN's diagnosis?
  - **Problems:**
    - Overly subjective data
    - Assumed that experts were ideal diagnosticians
    - Experts may have been biased against the computer
    - Required too much expert time
    - Limited set of experts (all from Stanford Hospital)

MYCIN Study 2

- **Evaluation criteria:**
  - **Expert ratings of treatment plan**
    - Multiple-choice rating system of MYCIN recommendations
    - Experts from several different hospitals
- **Comparison to study 1:**
  - **☺ Objective ratings**
  - **☺ More diverse experts**
  - **☹ Still have assumption that experts are right**
  - **☹ Still have possible anti-computer bias**
  - **☹ Still takes a lot of time**

MYCIN Study 3

- Evaluation criteria:
  - Multiple-choice ratings in a blind evaluation setting:
    - MYCIN recommendations
    - Novice recommendations
    - Intermediate recommendations
    - Expert recommendations
- Comparison to study 2:
  - ☺ No more anti-computer bias
  - ☹ Still assumes expert ratings are correct
  - ☹ Still time-consuming (maybe even more so!)

MYCIN Results

Prescriber	%OK (1 expert / 8)	% OK (majority)
MYCIN	65.0	70.0
Faculty-1	62.5	50.0
Faculty-2	60.0	50.0
Fellow	60.0	50.0
Faculty-3	57.5	40.0
Actual therapy	57.5	70.0
Faculty-4	55.0	50.0
Resident	45.0	30.0
Faculty-5	42.5	30.0
Student	30.0	10.0

- Experts don't always agree
- Method appears valid (more experience → higher ratings)
- MYCIN is doing well!

MYCIN Lessons Learned

- Don't assume experts are perfect
- Find out how humans are evaluated on a similar task
- Control for potential biases
  - Human vs. computer, Stanford vs. other institutions, expert vs. novice
- Don't expect superhuman performance
  - Not fair to evaluate against "right" answer
    - ...unless you evaluate humans the same way
    - ...and even then may not measure what you care about (performance under uncertainty)

Reasonable Baselines

Baseline: Point of Comparison

- Performance can't be measured in isolation
- Often have two baselines:
  - A reasonable naive method
    - Random
    - No processing
    - Manual
    - Naive Bayes
  - The current state of the art
- Ablation
  - Test the contribution of one factor
  - Compare system X to (system X – factor)

Poor Baselines

- No baseline
- The naive method, and no other alternative
- A system that was the state of the art ten years ago
- The previous version of your own system

- What if there is no existing baseline??
  - Develop reasonable baselines
  - Decompose and find baselines for the components

Establish a Need

- Try very simple approaches before complex ones
- Try off-the-shelf approaches before inventing new ones
- Try a wide range of alternatives, not just ones most similar to yours

- Make sure comparisons are fair

Thanks to Rob Holte for permission to use this slide

Test Alternative Explanations

Combinatorial auction problems

CHC = hill-climbing with a clever new heuristic

Solution Quality (% of optimal)

problem type	CHC
path	98
match	99
sched	96
r75P	83
r90P	90
r90N	89
arb	87

Thanks to Rob Holte for permission to use this slide

Is CHC Better than *Random* HC ?

Percentage of CHC solutions better than random HC solutions

problem type	% better
path	100
match	100
sched	100
r75P	63
r90P	7
r90N	6
arb	20

!

Thanks to Rob Holte for permission to use this slide

Statistically Valid Results

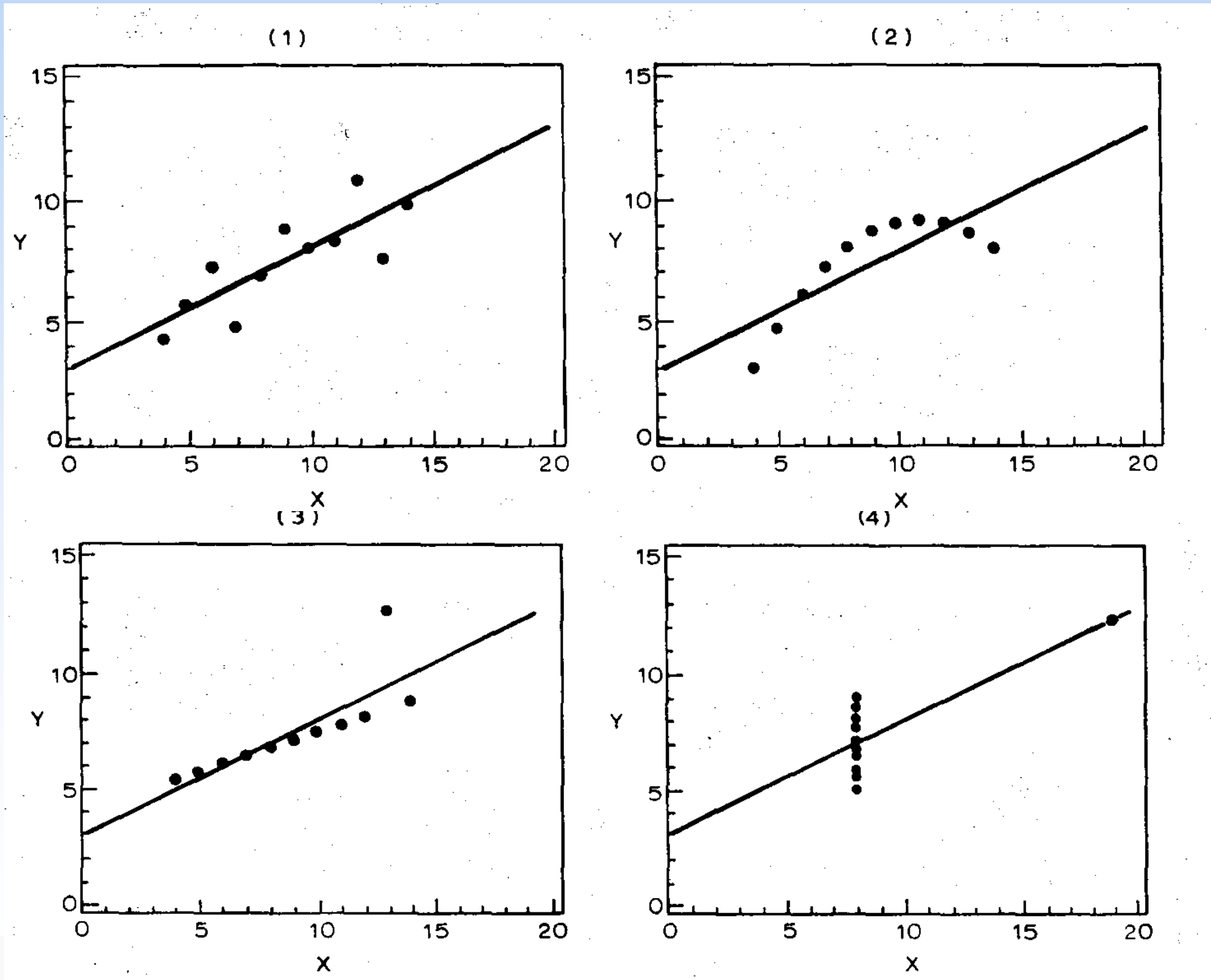
Look at Your Data

4 x-y datasets, all with the same statistics.
Are they similar ? Are they linear ?

- mean of the x values = 9.0
- mean of the y values = 7.5
- equation of the least-squared regression line is: $y = 3 + 0.5x$
- sum of squared errors (about the mean) = 110.0
- regression sum of squared errors = 27.5
- residual sum of squared errors (about the regression line) = 13.75
- correlation coefficient = 0.82
- coefficient of determination = 0.67

F.J. Anscombe (1973), "Graphs in Statistical Analysis," *American Statistician,* 27, 17-21

Anscombe Datasets Plotted



3/9/04

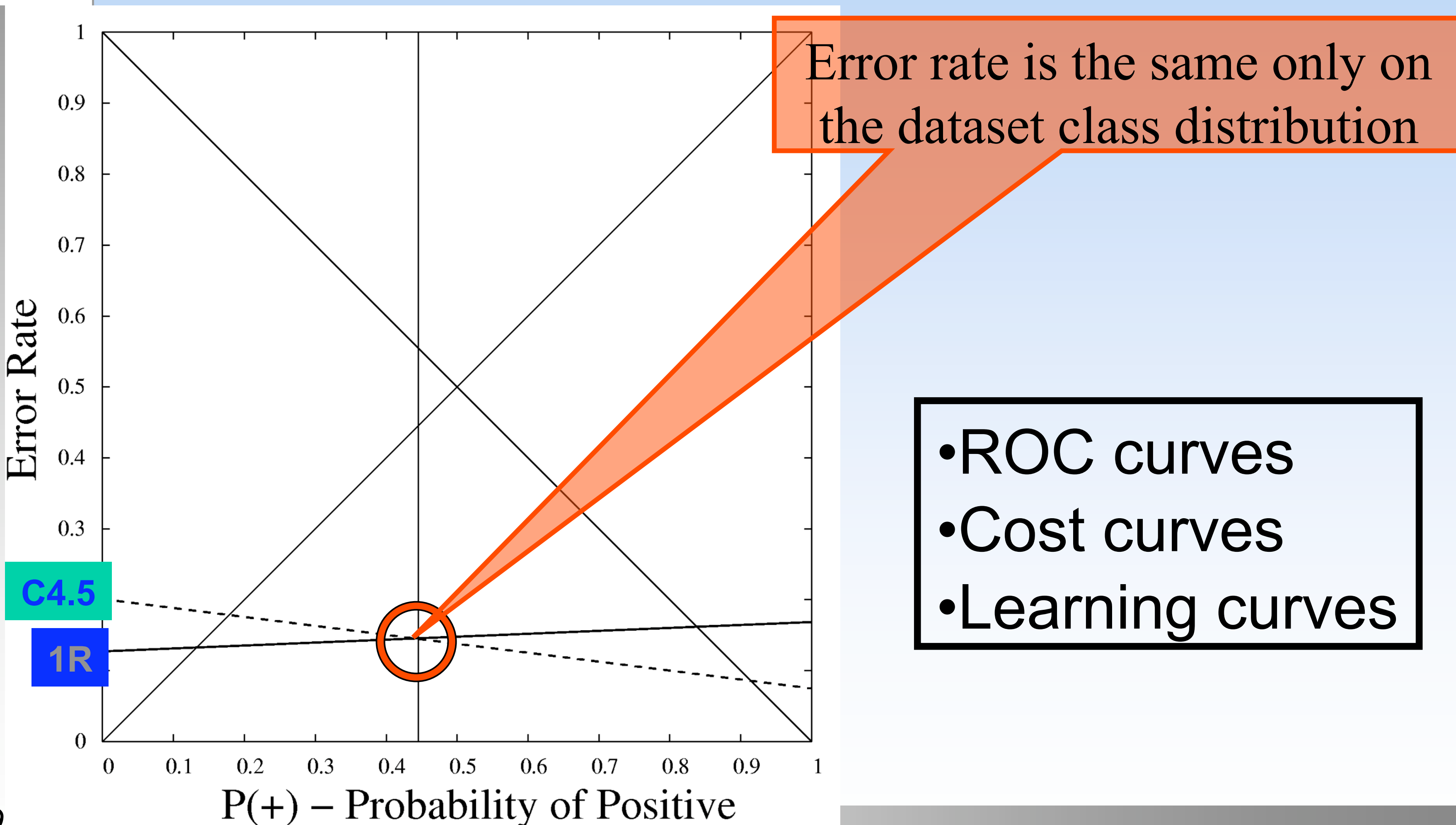
Thanks to Rob Holte for permission to use this slide

Look at Your Data, Again

- Japanese credit card dataset (UCI)
- Cross-validation error rate is identical for C4.5 and 1R

Is their performance the same ?

Closer analysis reveals…



- ROC curves
- Cost curves
- Learning curves

Thanks to Rob Holte for permission to use this slide

Statistical Methods

- Plotting the data
- Sample statistics
- Confidence intervals
  - Bootstrap, t distribution
- Comparing distributions
  - Bootstrap, t test, confidence intervals
- Learning algorithms
- Regression
- ANOVA

Lots more to come...