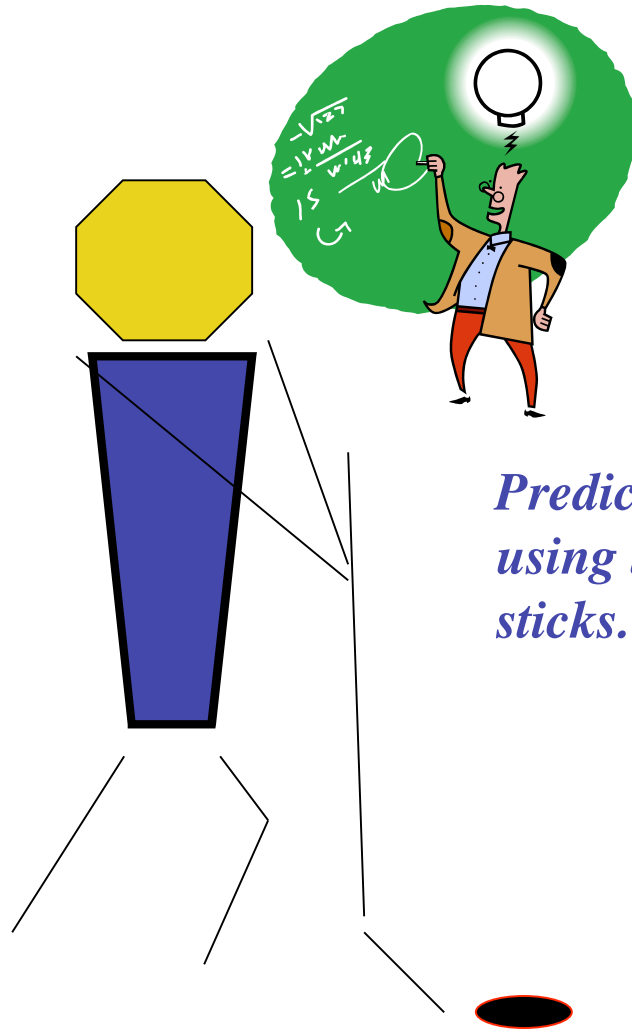


*Experimental Analysis of
Algorithms: What to Measure*

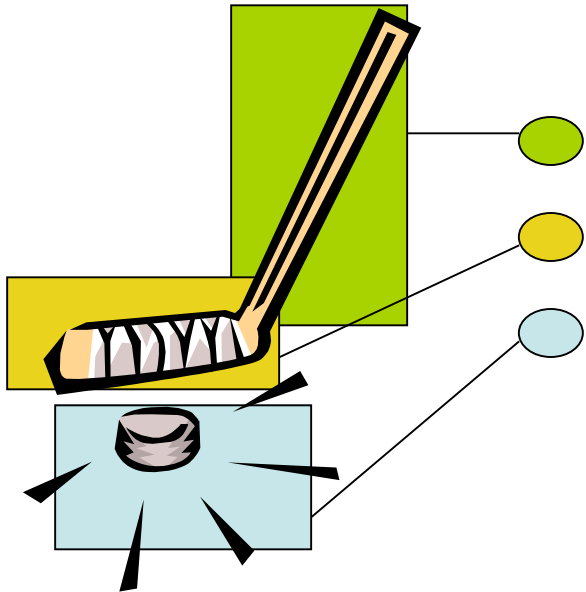
Catherine C. McGeoch
Amherst College

Theory vs Practice

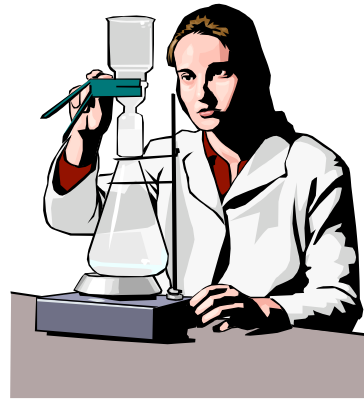


*Predict puck velocities
using the new composite
sticks.*





Isolate Components



Control Factors

Experiment



Attach Probes



Experiments on Algorithms

<i>Good news</i>	<i>Bad news</i>
<p>Easy to probe.</p> <p>Nearly total experimental control.</p> <p>Simple mechanisms.</p> <p>Model validation not a problem.</p> <p>Fast experiments (often).</p> <p>Tons of data points (often).</p>	<p>Unusual questions = few techniques.</p> <p>Unusually precise questions = need advanced techniques.</p> <p>Unusual data = parametric methods are weak.</p> <p>Large and infinite sample spaces = sampling difficulties.</p> <p>Generalization/abstraction from the computational artifact = extrapolation.</p> <p>NP-hard problems = problematic.</p>

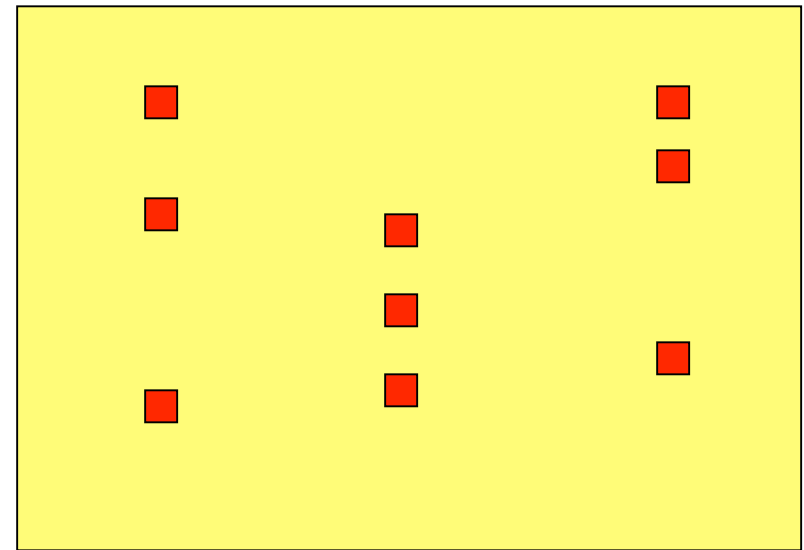
Standard statistical techniques

1. **Comparison** (*estimation and hypothesis testing*):
same/different,
bigger/smaller.

2. *Interpolation (linear and nonlinear regression -- fitting models to data.*

3. *Extrapolation (??) -- building models of data, explaining phenomena.*

cost



parameter

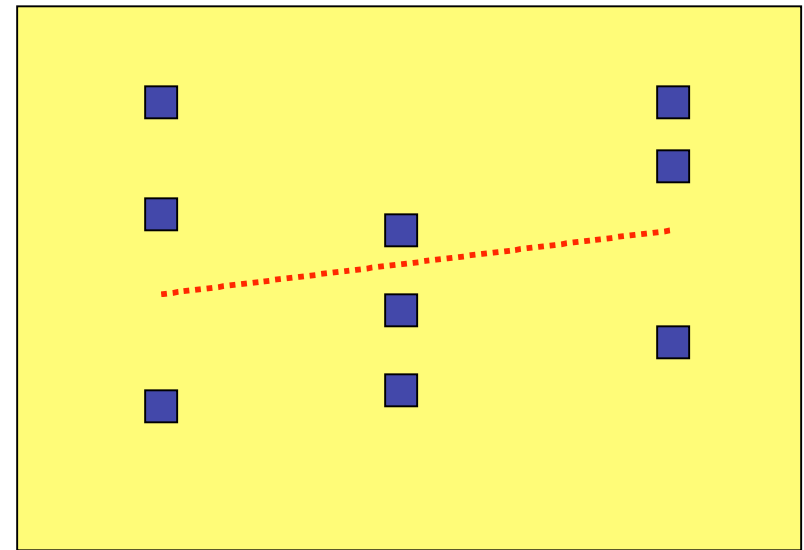
Standard statistical techniques

1. **Comparison** (*estimation and hypothesis testing*):
same/different,
bigger/smaller.

cost

2. **Interpolation** (*linear and nonlinear regression*) --
fitting models to data.

3. **Extrapolation** (*) --
building models of data,
explaining phenomena.



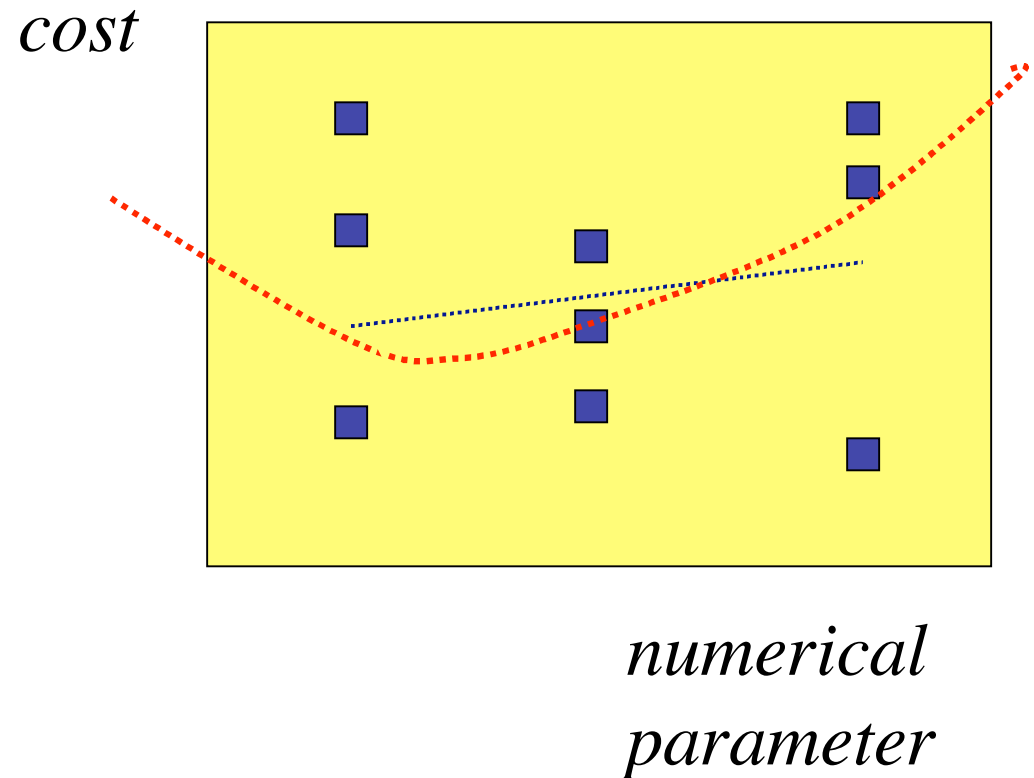
*numerical
parameter*

Standard statistical techniques

1. *Comparison* (estimation and hypothesis testing): same/different, bigger/smaller.

2. *Interpolation* (linear and nonlinear regression -- fitting models to data. Interpolation

3. *Extrapolation* (*) -- building models, explaining phenomena.

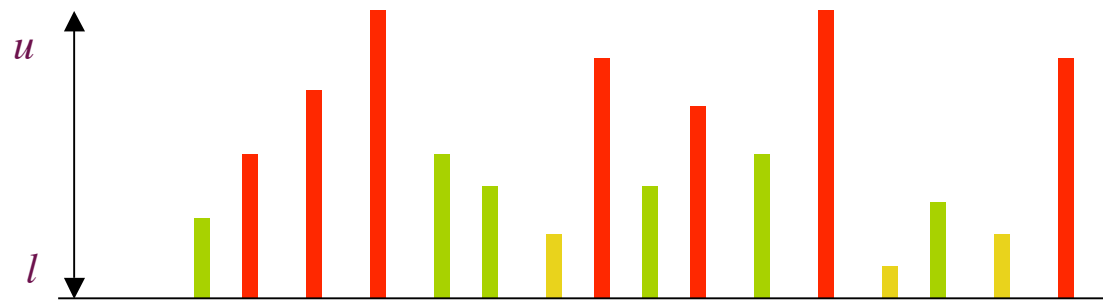


Some Nonstandard Techniques

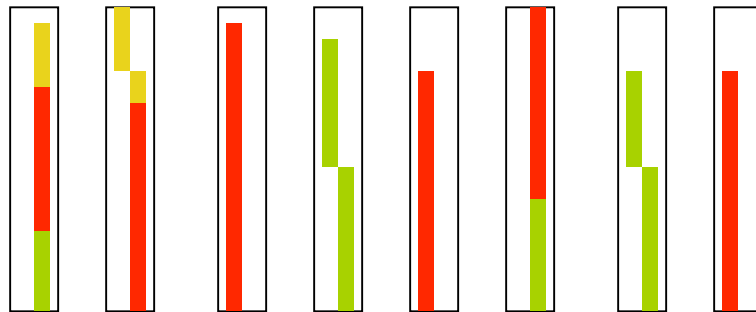
1. *Graphical analysis (GA)* -- big data sets, unusual questions, interpolation, extrapolation.
2. *Exploratory data analysis (EDA)* -- model building, unusual data sets.
3. *Variance reduction techniques* -- simple mechanisms, complete control.
4. *Biased estimators* -- NP-Hard problems, large sample spaces.



Case Study: First Fit Bin Packing



Consider weights in order of arrival; pack each into the first (leftmost) bin that can contain it.



Applications:
CD file
storage; stock
cutting; iPod
file storage;
generalizations
to 2D, 3D...

Bin packing is
NP-Hard.

How well does
the FF heuristic
perform?

Experimental Study of First Fit Bin Packing

Input categories:

- *uni1*: n reals drawn uniformly from $(0, 1]$
- *uni8*: n reals drawn uniformly from $(0, .8]$
- *file*: n file sizes (scaled to $0..1$).
- *dict*: n dictionary word sizes (in $0..1$).

Run First Fit on these inputs, analyze results....

What to Measure?

What *performance indicator* to use for assessing heuristic solution quality?

The obvious choice:

Number of Bins

Other performance indicators suggested by data analysis:

- *Graphical analysis (GA)*
- *Exploratory data analysis (EDA)*
- *Variance reduction techniques (VRT)*
- *Biased estimators*



*Today's
topic!*

First Fit

<i>input type</i>	<i>n</i>	<i>Bins</i>
<i>uni1</i>	<i>30,000</i>	<i>15,270</i>
<i>uni1</i>	<i>60,000</i>	<i>30,446</i>
<i>uni1</i>	<i>120,000</i>	<i>60,809</i>
<i>uni8</i>	<i>30,000</i>	<i>12,217</i>
<i>uni8</i>	<i>60,000</i>	<i>24,385</i>
<i>uni8</i>	<i>120,000</i>	<i>48,965</i>
<i>file</i>	<i>30,000</i>	<i>9</i>
<i>file</i>	<i>60,000</i>	<i>13</i>
<i>file</i>	<i>124,016</i>	<i>27</i>
<i>dicto</i>	<i>60,687</i>	<i>23,727</i>
<i>dicto</i>	<i>61,406</i>	<i>22,448</i>
<i>dicto</i>	<i>81,520</i>	<i>28,767</i>

Tabular data:
Good for
comparisons.

Which is
better? How
much better?
When is it
better?

Graphical Analysis

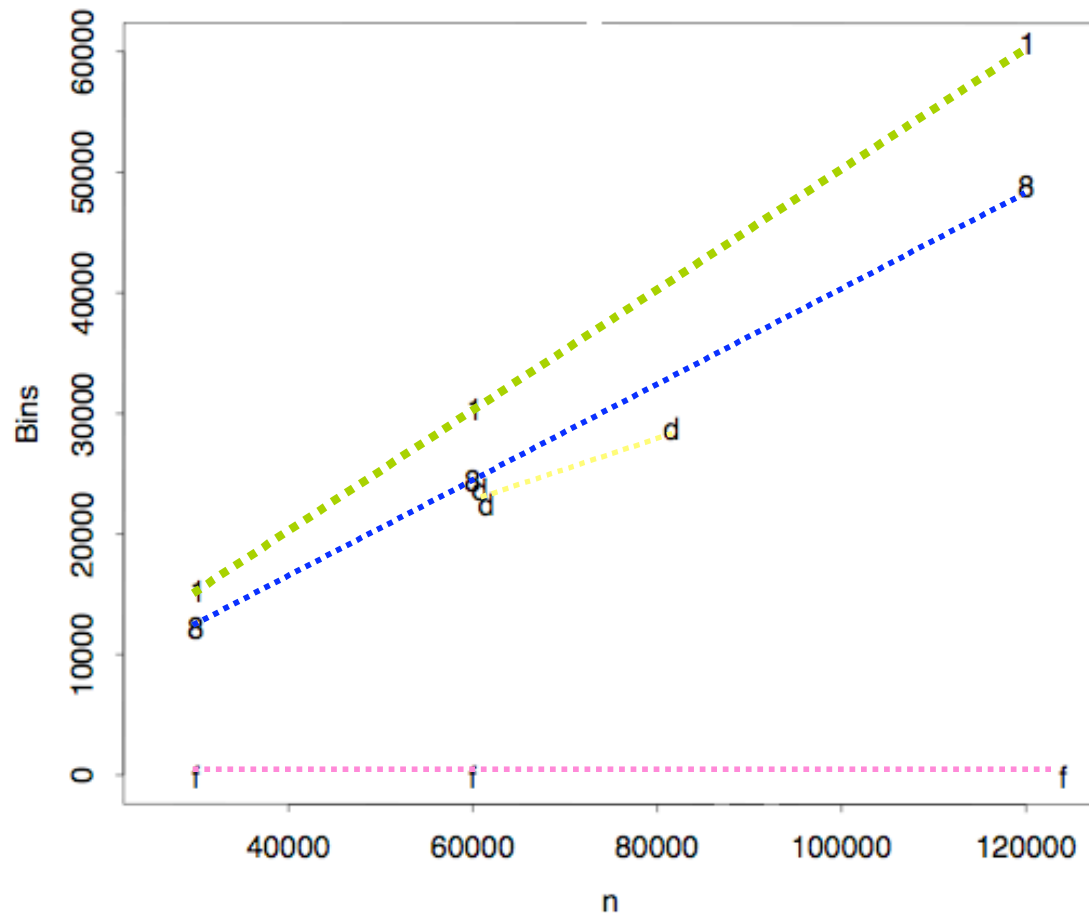
Identify trends

Find common scales

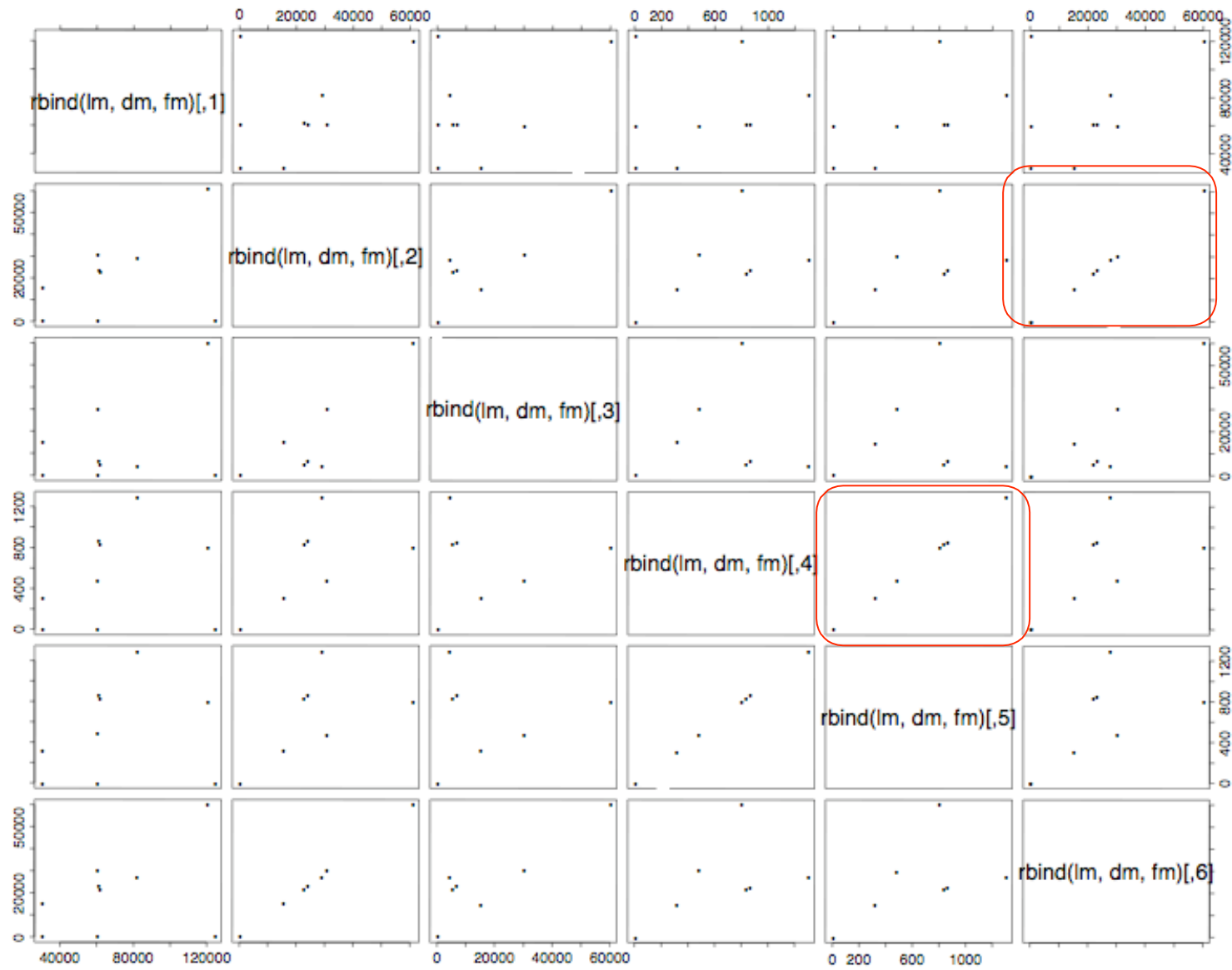
Discover anomalies

Build models/explanations

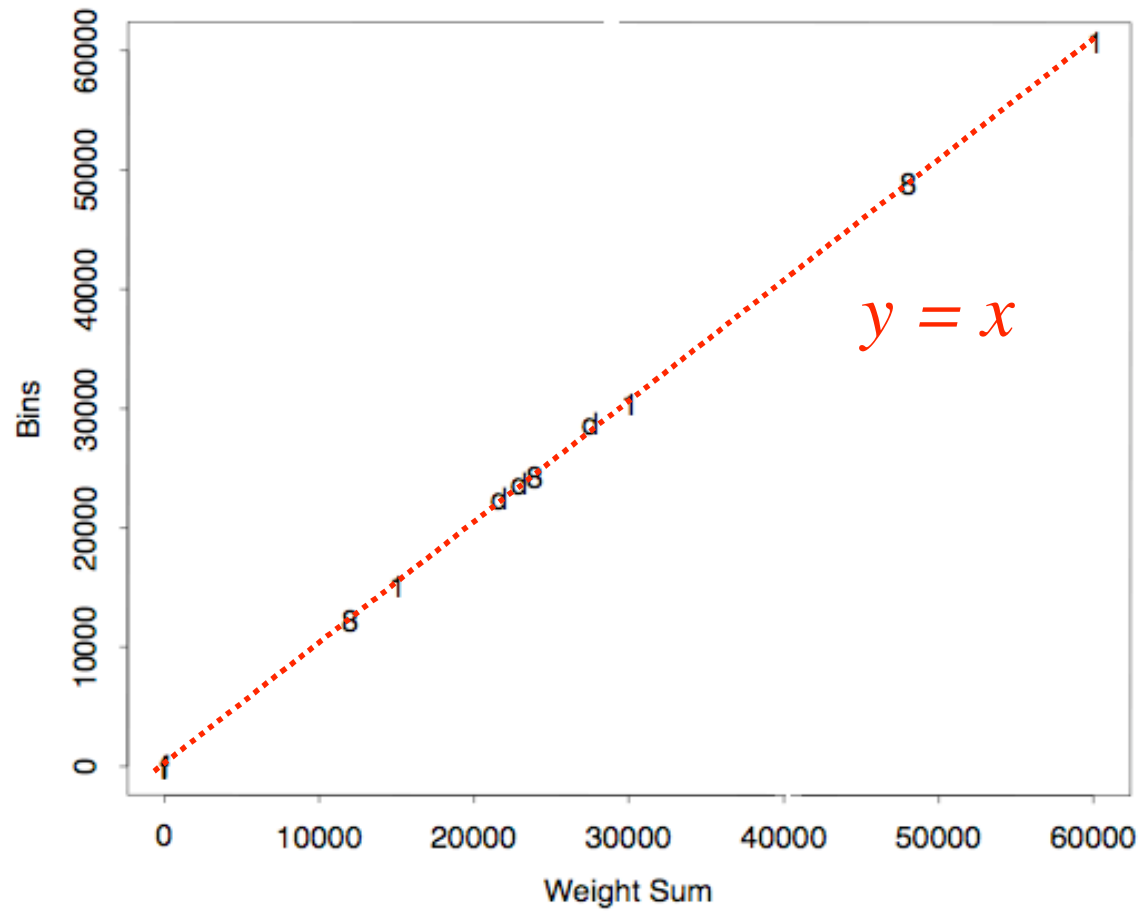




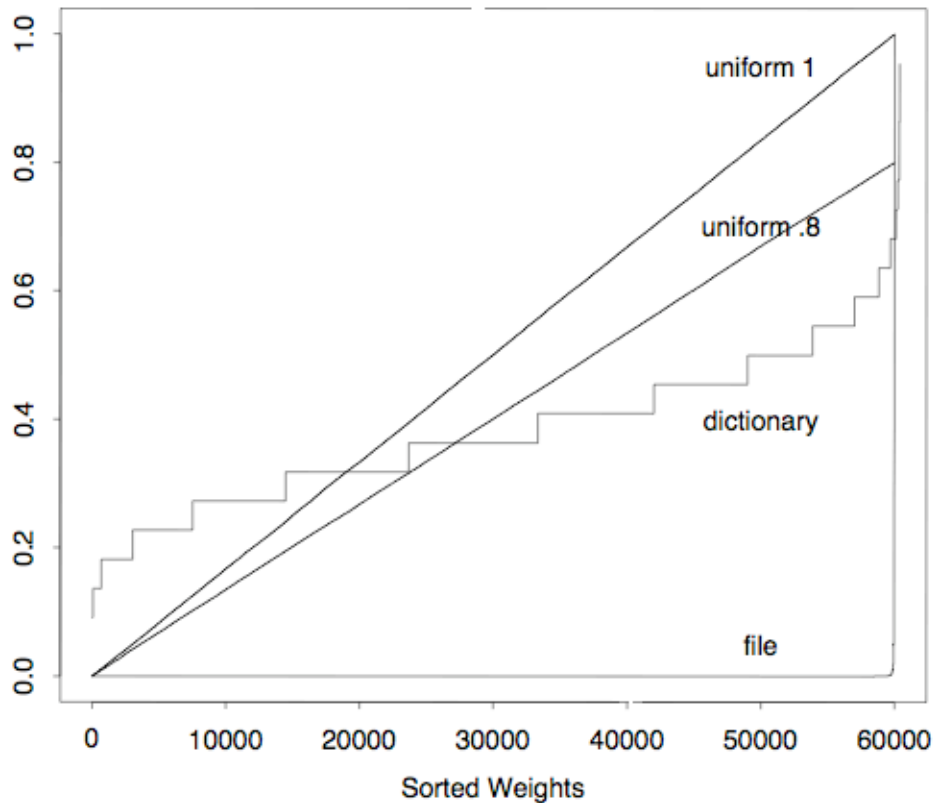
GA: Look for trends.



GA (pairs plot): Look for correlations



GA (Weight Sum vs Bins): Find a common scale



*Conjectured
input
properties
affecting FF
packing
quality:
symmetry,
discreteness,
skew.*


*GA (distribution of weights in input): look for
explanations*

Graphical Analysis: some results...

File data: FF packings are optimal! Due to extreme **skew** in the weight distribution (few big weights, many tiny weights).

Dicto data: Sorting the weights (FFD) makes the packing worse! Due to **discrete weights in bad combinations**. (Bad FFD packings can be predicted to within 100 bins.)

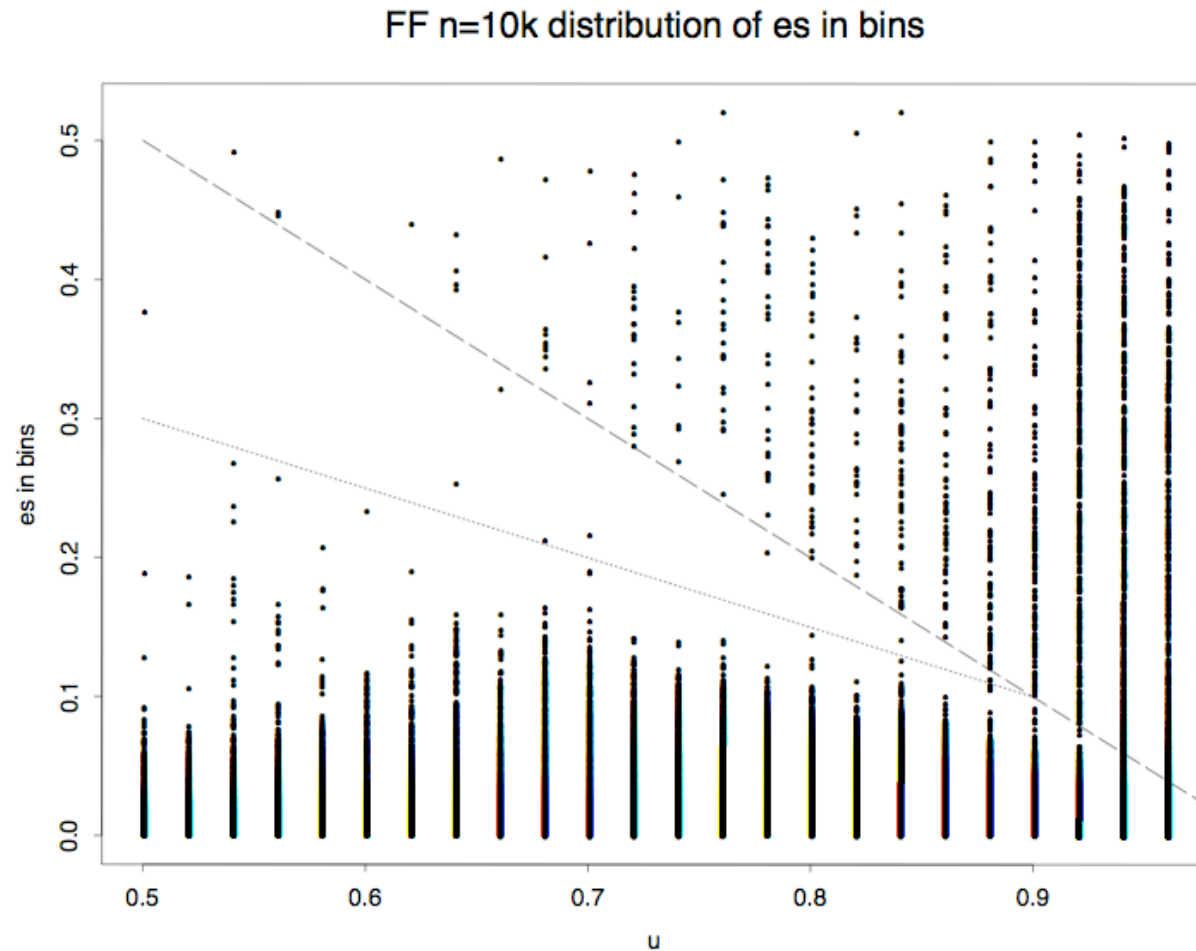
Uniform data: Smaller weight distributions (0 .8) give worse packings (compared to optimal) than larger weight distributions (0, 1). Probably due to asymmetry.

 (more)...

Top line =
 $1-u$

Bottom line
 $= .55 - u/2$

Conjecture:
The
distribution of
“empty space
per bin” has
holes when u
 $\leq .85$. These
holes cause
bad FF
packings.



GA (details): u vs distribution of es in bins

Graphical Analysis: What to Measure

Input:

Number of weights

Sum of weights

Number of weights > 0.5

Weight distribution

Output:

Number of bins

Empty space = Bins - Weight Sum

Gaps = Empty space per bin

Distribution of gaps

Animations of packings

Trends

Scale

Details

Exploratory Data Analysis

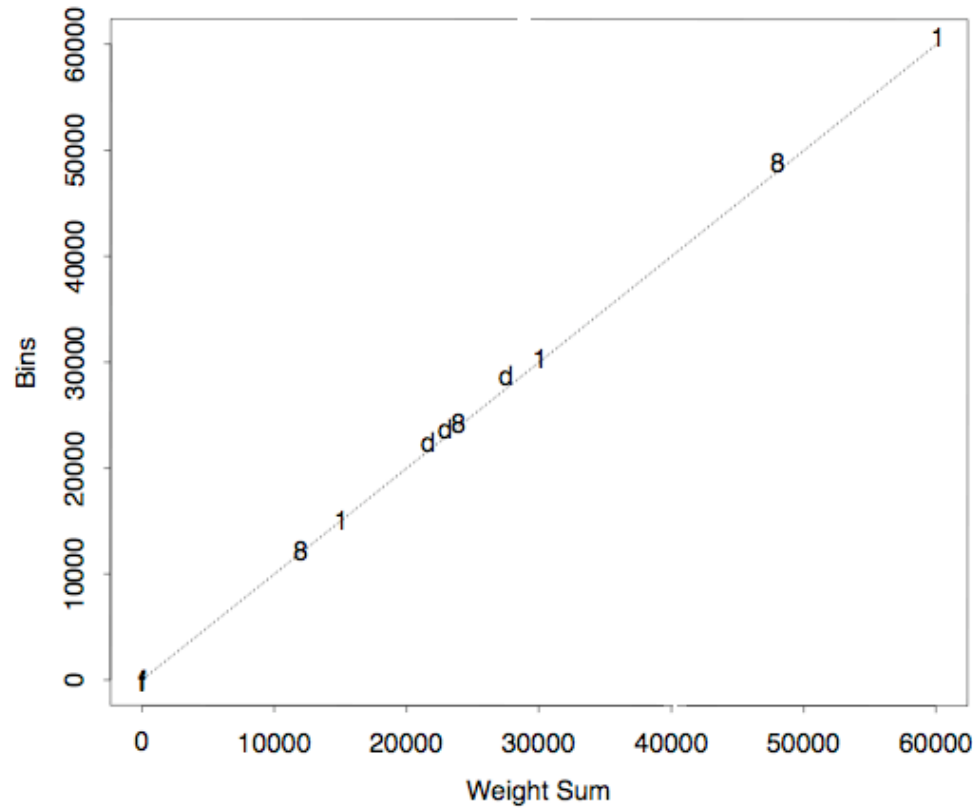
Smooth and the rough: look at general trends, and (equally important) deviation from trends.

Categories of data: tune analysis for type of data -- counts and amounts, proportions, counted fractions, percentages ...

Data transformation: adjust data properties using logarithms, powers, square roots, ratios ...

No *a priori* hypotheses,
no models, no estimators.

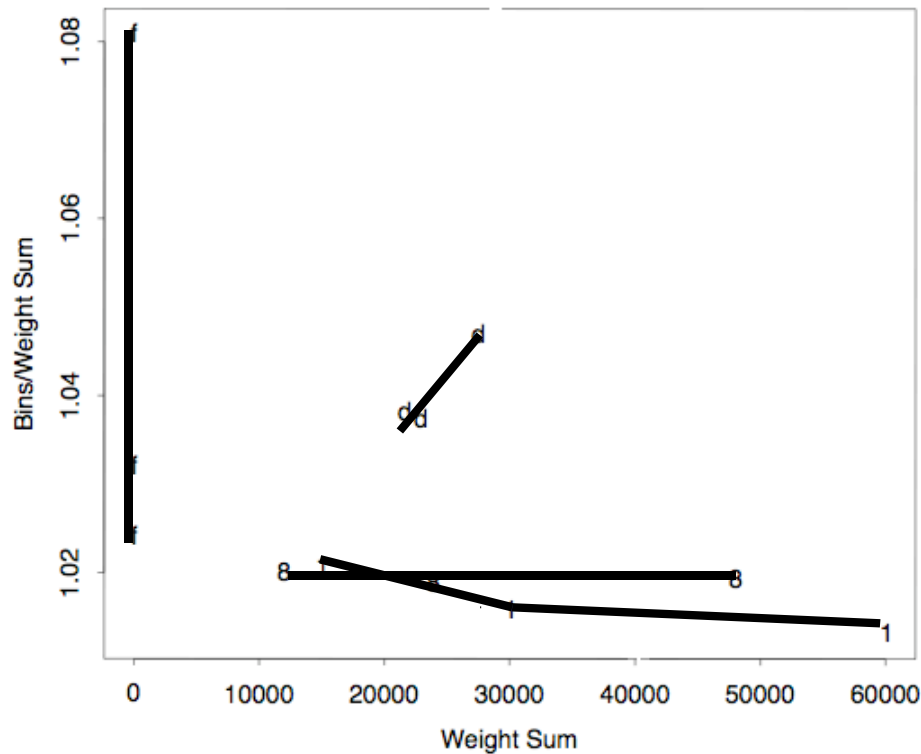




Number of bins is nearly equal to weight sum.



EDA: The smooth ...



*Deviation
of bins
from weight
sum < 8%
of bins,
depending
on input
class.
(Focus on 8
and 1 ...)*

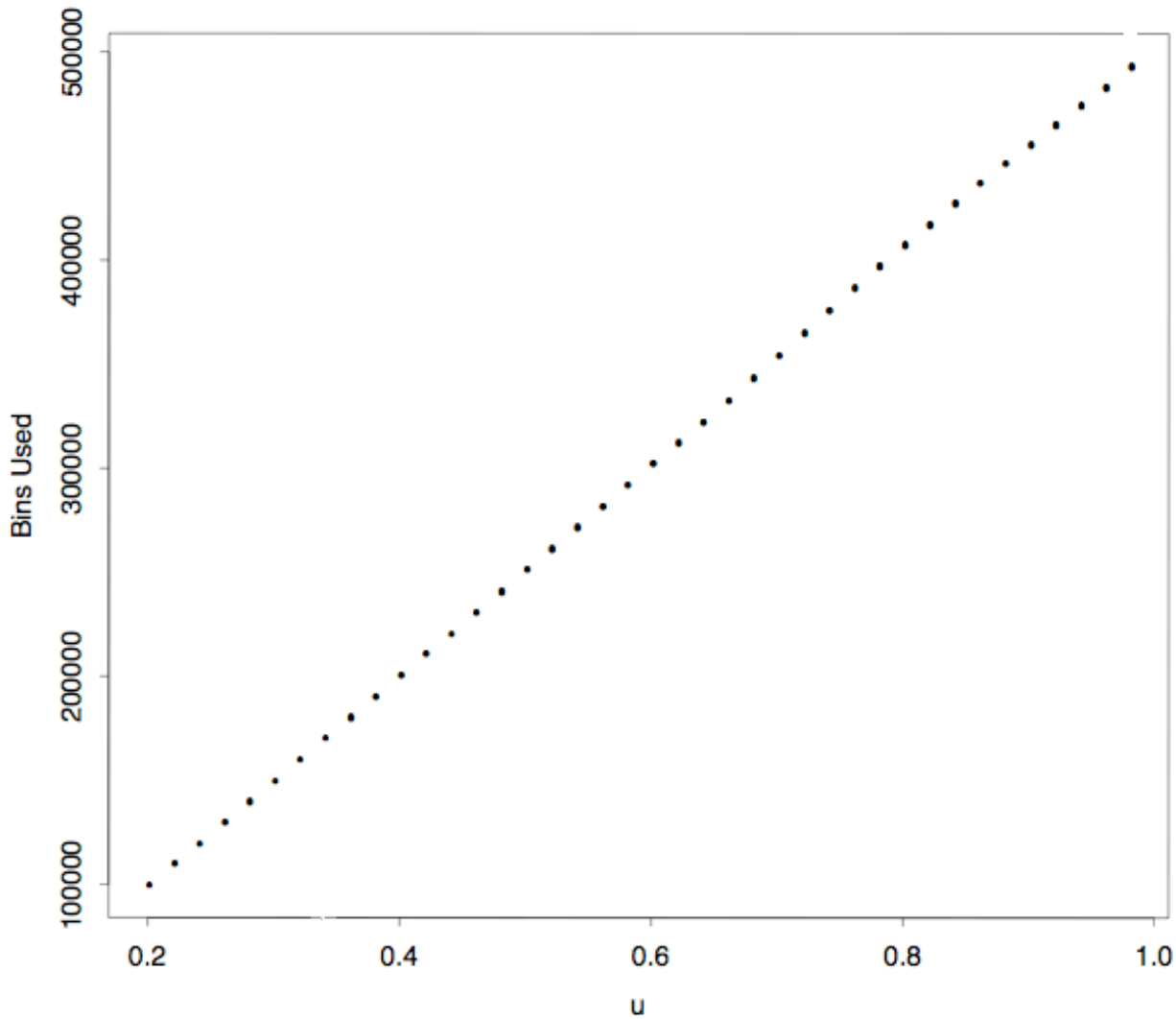
*... and the rough: Weight Sum vs
Bins/Weight Sum*



Focus on Uniform Weight Lists

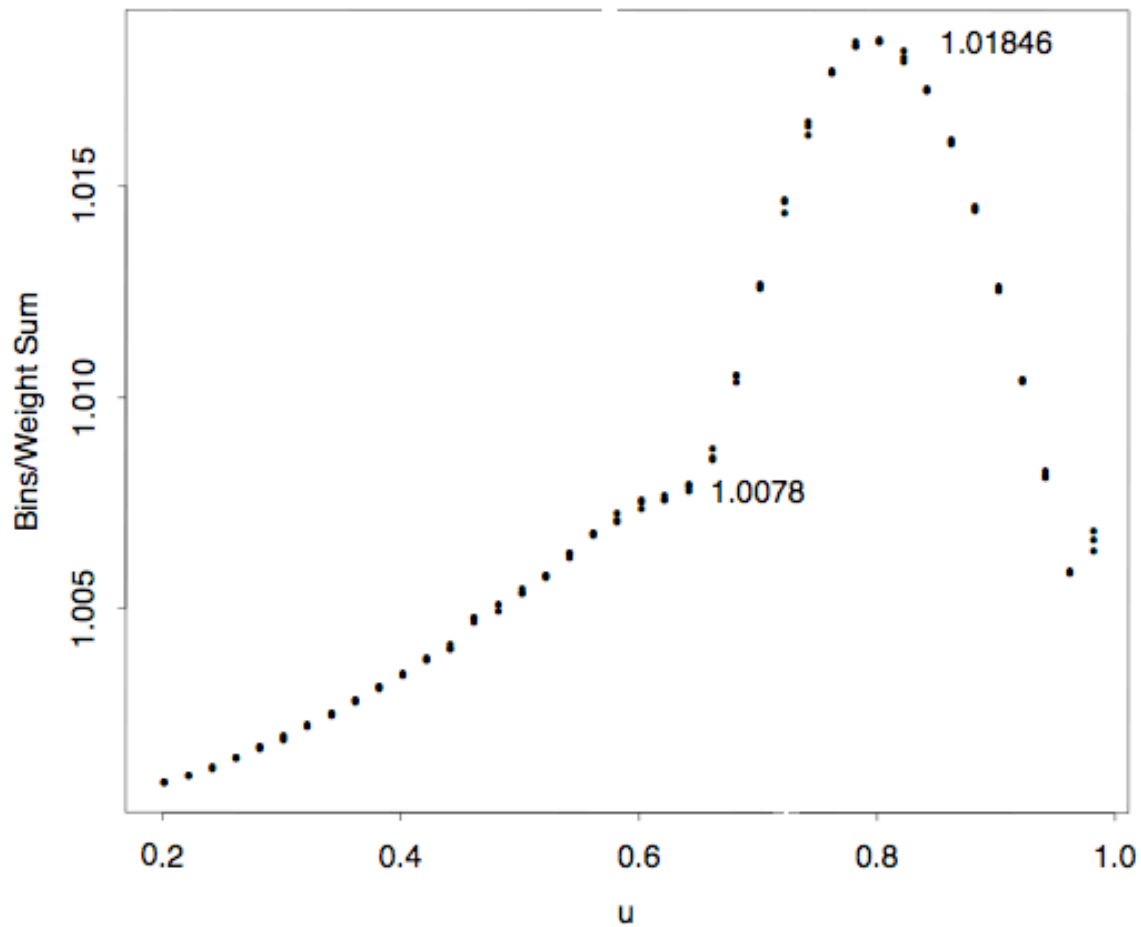
Given n weights drawn uniformly from $(0, u]$, for $0 < u \leq 1$.

Consider FF packing quality as $f(u)$, for fixed n .



Number of bins is proportional to upper bound on weights.

EDA (the smooth): u vs Bins, at $n=100,000$



EDA (the Rough): u vs Bins/Weight Sum ($\sim nu/2$).

EDA: Categories of Data

Bin efficiency = Bins/Weight Sum

a ratio

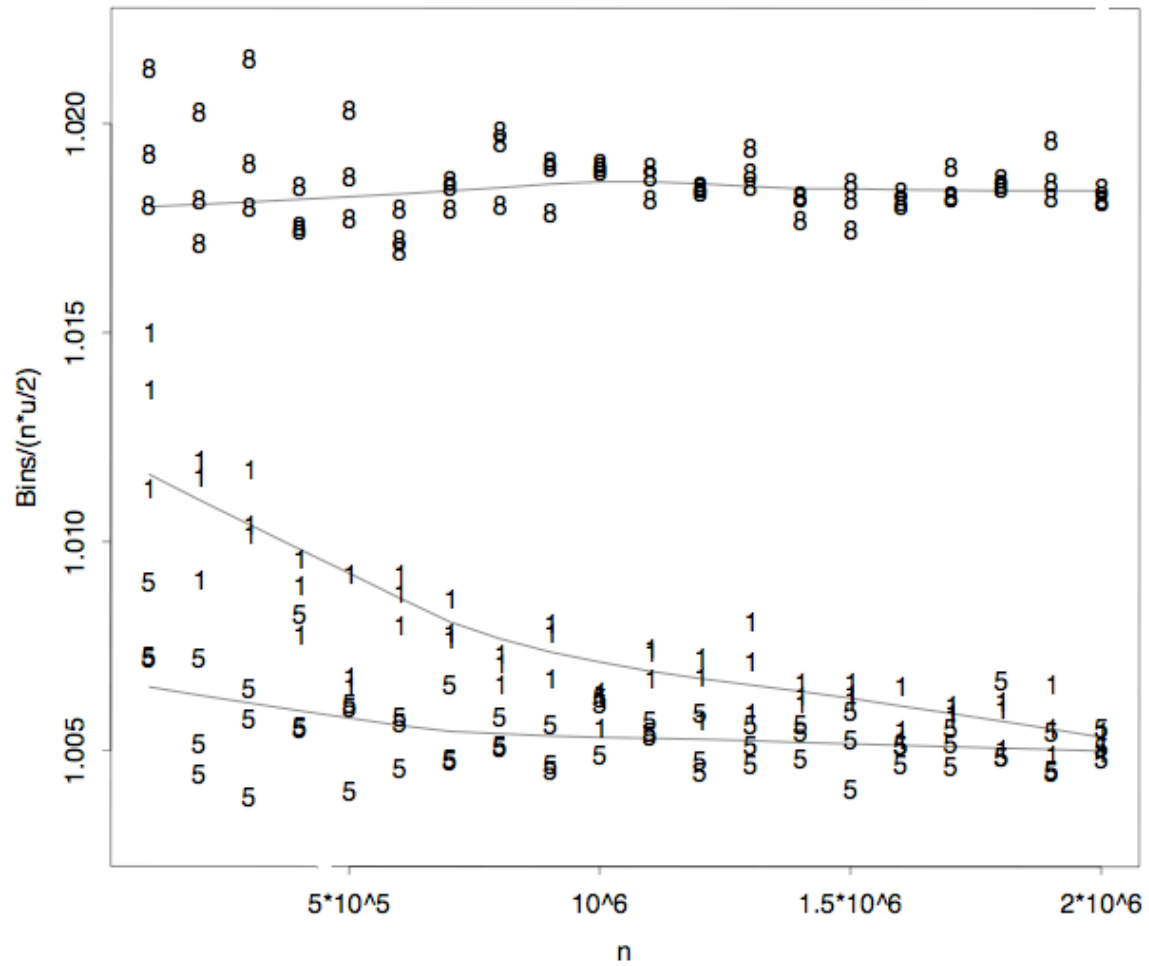
Always > 1 , mean is in $[1.0, 1.7]$, variance large but decreasing in n . Does it converge to 1 (optimal) or to $1+c$?

Empty space = Bins - Weight Sum

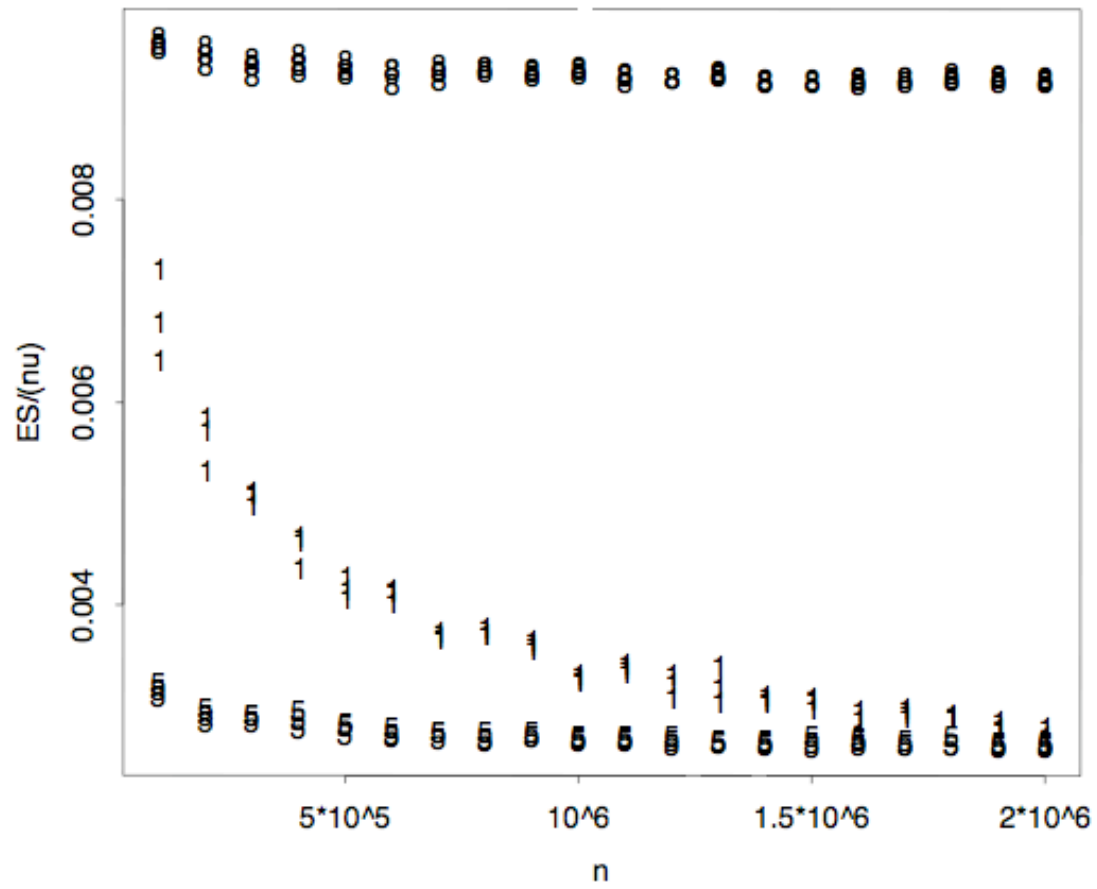
a difference

Always ≥ 0 , mean is linear or sublinear in nu , variance constant in n .) Is it linear or sublinear in n ?

Convergence in n is easier to see

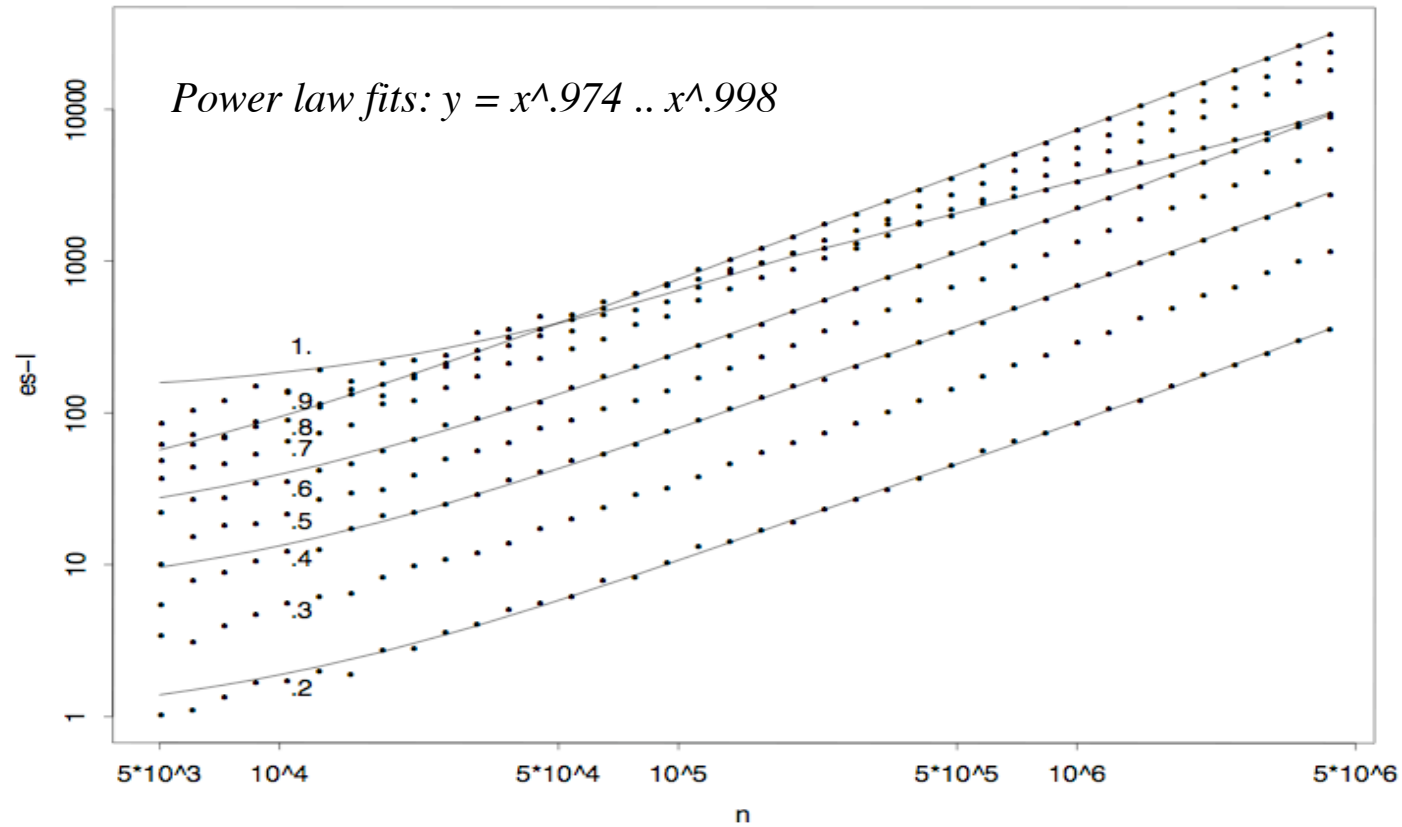


Packing efficiency: n vs $\text{Bins}/(un/2)$.



Empty Space: (Bins - Weight)/nu

ff



EDA (data transformation): Linear growth on a log-log scale.

EDA: Some Results

*Number of Bins is near
Weight Sum $\sim nu/2$, with
largest deviations near $u =$
.8.*

*Empty space (a difference)
has clearer convergence
properties than Bin
Efficiency (a ratio).*

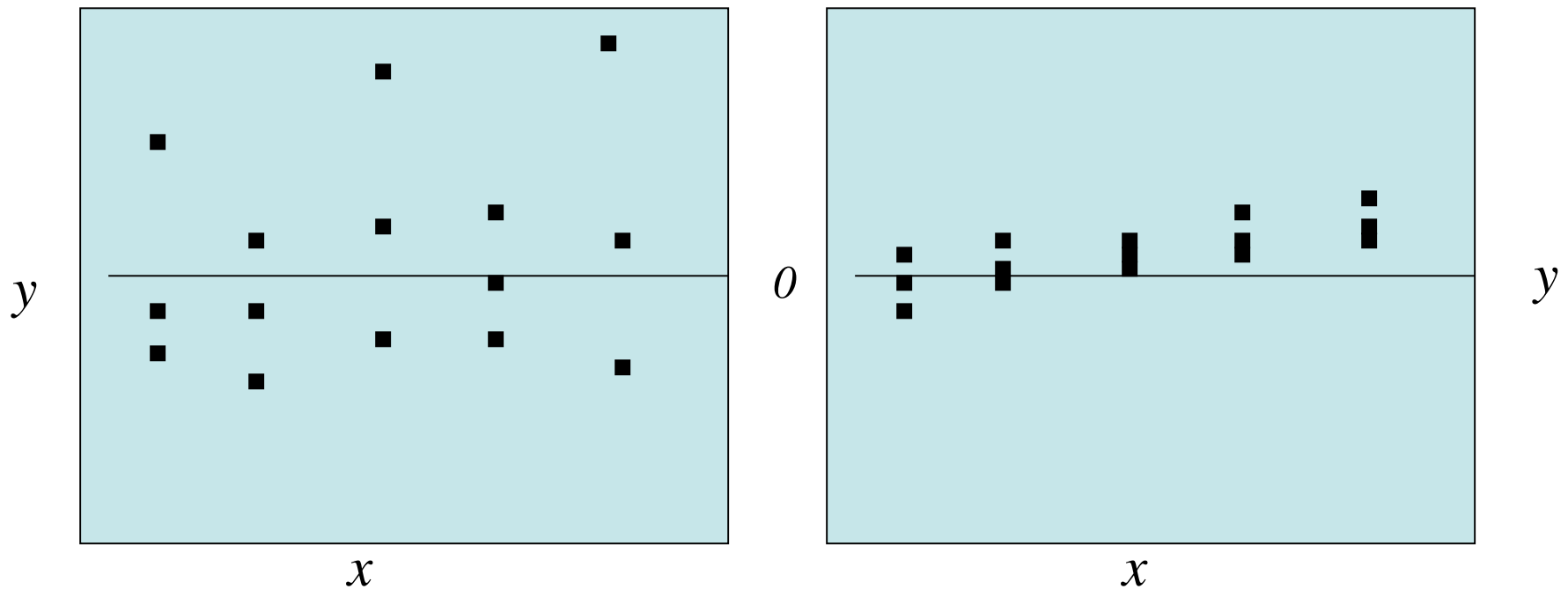
*Empty space appears to be
asymptotically linear in n -
- non-optimal -- for all u -
except 1.*

Smooth & rough

Data Categories

Transformation

Variance Reduction Techniques



Is y asymptotically positive or negative?

VRT: Control Variates

Subtract a source of noise if its expectation is known and it is positively correlated with outcome.

Expected number of bins: β

Bins = Weight Sum + Empty Space

$E[WS - nu/2] = 0$

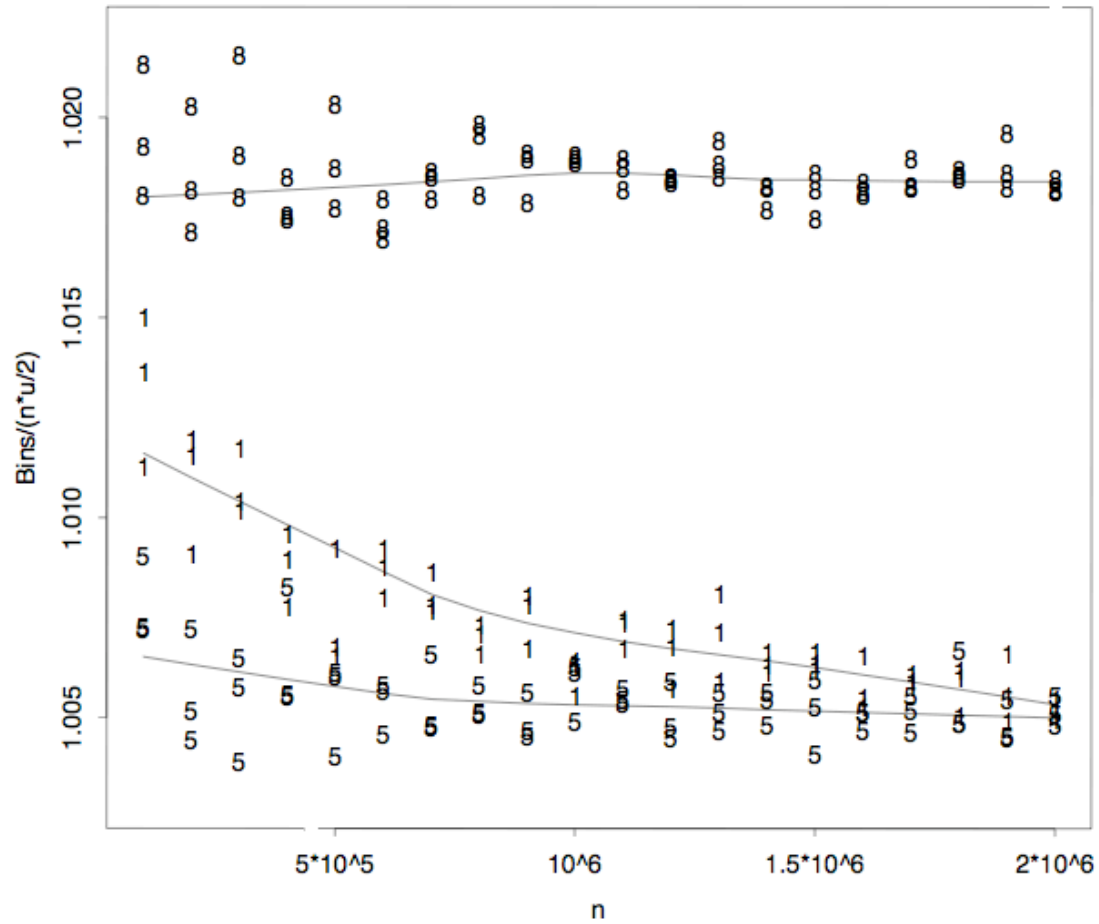
$E[B - (WS - nu/2)] = \beta$

$Var[B - (WS - nu/2)] = Var[B] + Var[(WS - nu/2)] - 2Cov[B, (WS - nu/2)].$

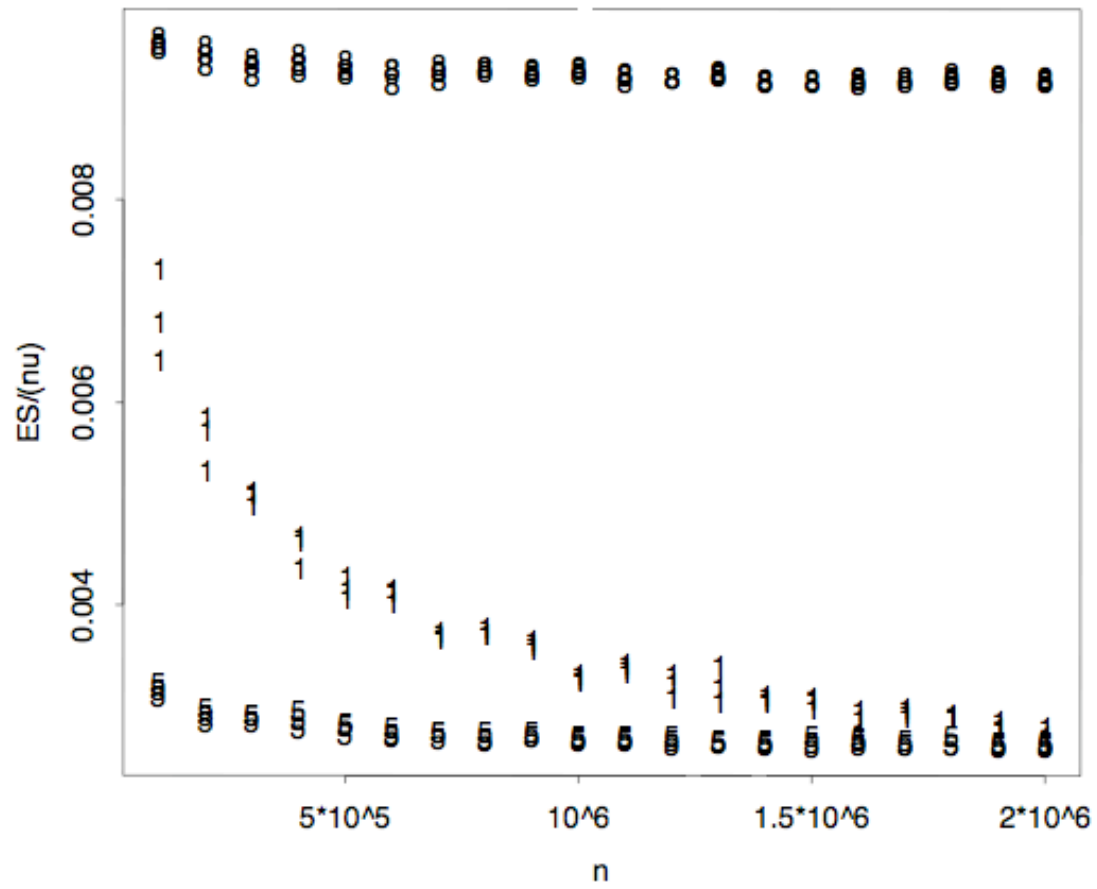
$B - WS + nu/2 = ES + nu/2.$

Weight Sum is a Control Variate for Bins.

$ES + nu/2$ is a better estimator of β .



Estimating β with B .



Estimating β with ES

More Variance Reduction Techniques

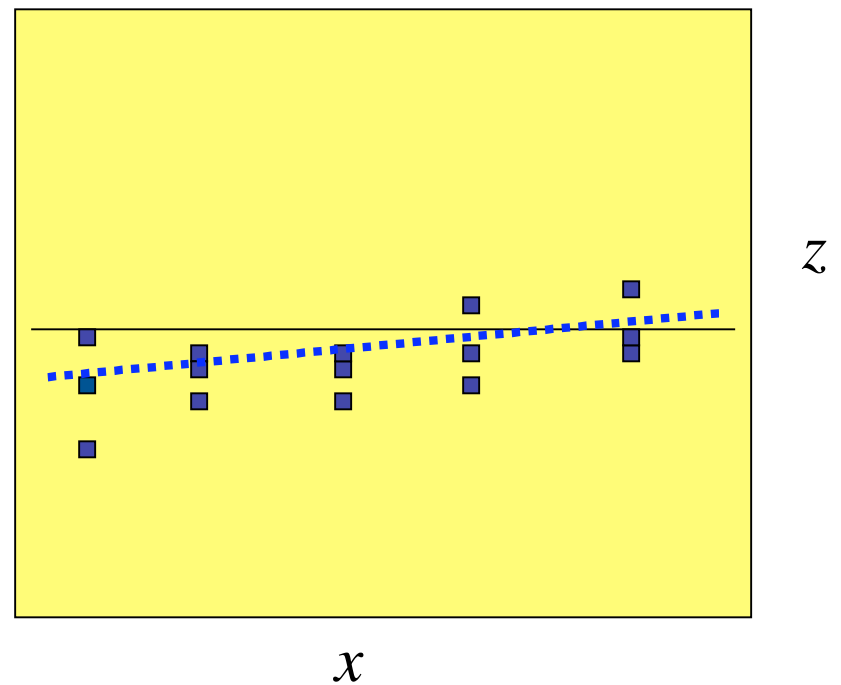
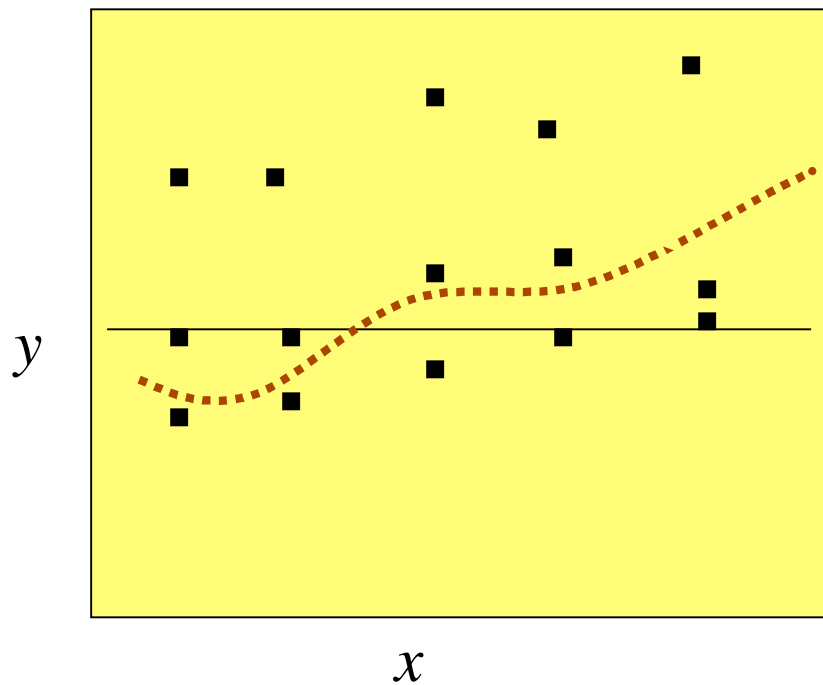
Common Random Variates: *Compare heuristics on identical inputs when performance is correlated.*

Antithetic Variates: *Exploit negative correlation in inputs.*

Stratification: *Adjust variations in output according to known variations in input.*

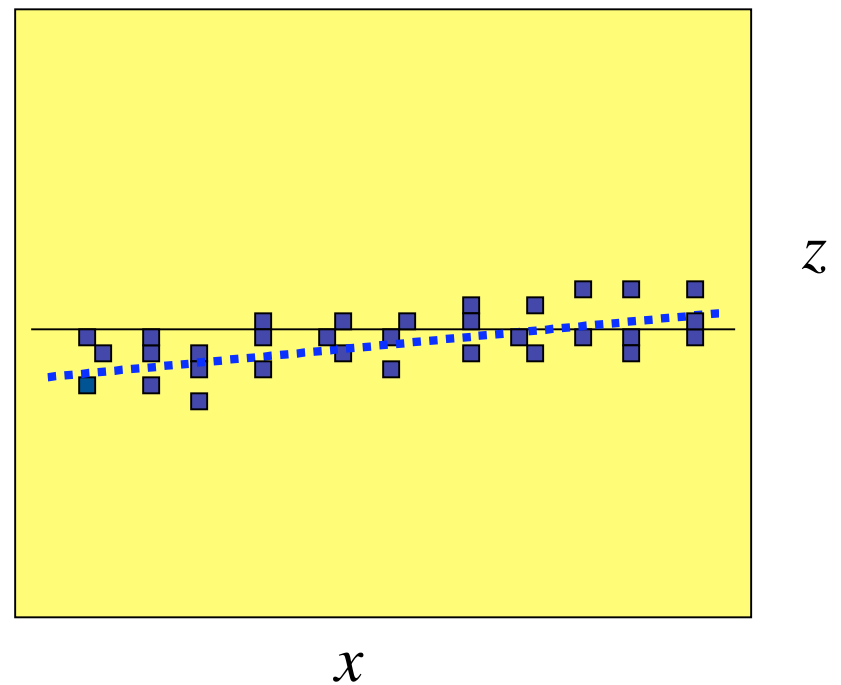
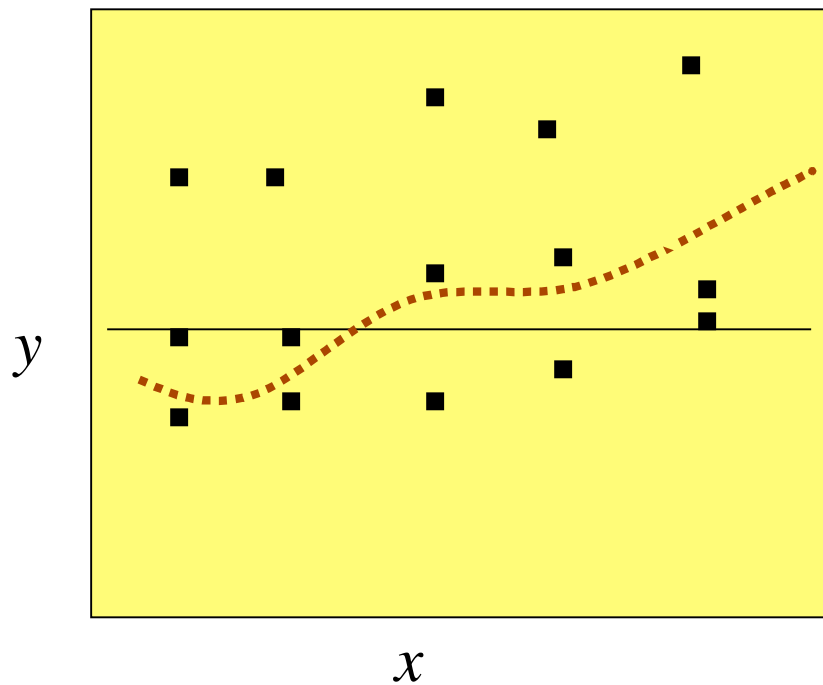
Conditional Monte Carlo: *More data per experiment, using efficient tests.*

Biased Estimators



Bad estimator of $mean(y)$ vs good estimator of $z=lb(y)$.

Biased Estimators



Bad estimator of $mean(y)$ vs cheap estimator of $z=lb(y)$.

Biased Estimators of Optimal Packing Quality

Bounds on optimal number of bins:

U: FF number of bins used (or any heuristic)

L: Weight sum

L: Number items ≥ 0.5

L: $FF/2$

L: $(FF - 2)10/17$

L: $(FFD - 4)9/11$

Summary: What to Measure

GA: *trends*

GA: *scale*

GA: *details*

EDA: *smooth and rough*

EDA: *data categories*

EDA: *data transformation*

VRT: *alternatives with same mean, lower variance*

BE: *lower/upper bounds on the interesting quantity*

First Fit Packings:

number of bins

number of weights

sum of weights

distribution of weights

number of weights $> .5$

packing efficiency

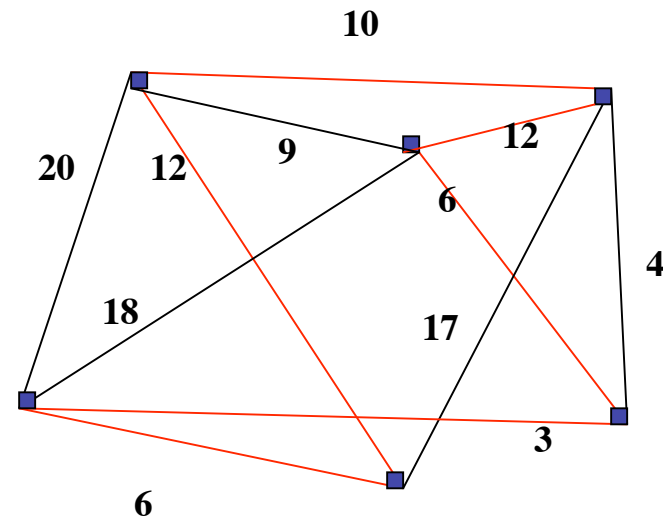
empty space

empty space per bin

bounds on bin counts

Another Example Problem

TSP: Given graph G with n vertices and m weighted edges, find the least-cost tour through all vertices.



Applications: well known.

TSP: What to Measure

VRT's and BE's:

Mean edge weight is a control variate for Tour Length.

Beginning Tour is a control variate for Final Tour, in iterative algorithms with random starts.

$f(\text{MST} + \text{Matching})$ is a biased estimator of Tour Length (lower bound).

Held-Karp Lower Bound is biased estimator of Tour Length.

Can you think of others?

TSP: Graphical Analysis

Input:

Vertices n and Edges m

... can you think of others?

Output:

Tour Length

... can you think of others?

Trends

Scale

Details

TSP: Exploratory Data Analysis

Any ideas?

Smooth & Rough

Categories

Transformation

References

Tukey, *Exploratory Data Analysis*.

Cleveland, *Visualising Data*.

Chambers, Cleveland, Kleiner,
Tukey, *Graphical Methods for
Data Analysis*.



Bratley, Fox, Schrage, *A Guide to
Simulation*.

C. C. McGeoch, “Variance
Reduction Techniques and
Simulation Speedups,” *Computing
Surveys*, June 1992.

Upcoming Events in Experimental Algorithmics



January 2007: ALENEX (Workshop on Algorithm Engineering and Experimentation), New Orleans.

Spring 2007: DIMACS/NISS joint workshop on experimental analysis of algorithms, North Carolina. (Center for Discrete Mathematics and Theoretical Computer Science, and National Institute for Statistical Sciences.)

June 2007: WEA (Workshop on Experimental Algorithmics), Rome.

(Ongoing): DIMACS Challenge on Shortest Paths Algorithms.