The Reusable Holdout: Preserving Statistical Validity in Adaptive Data Analysis

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False discovery — a growing concern

“Trouble at the Lab” – The Economist

Most published research findings are probably false. – John Ioannidis

P-hacking is trying multiple things until you get the desired result. – Uri Simonsohn

She is a p-hacker, she always monitors data while it is being collected. – *Urban Dictionary*

The p value was never meant to be used the way it's used today. – Steven Goodman

Preventing false discovery

Decade old subject in Statistics

Powerful results such as Benjamini-Hochberg work on controlling **False Discovery Rate**

Lots of tools:

Cross-validation, bootstrapping, holdout sets

Theory focuses on *non-adaptive* data analysis

Non-adaptive data analysis

Data analyst

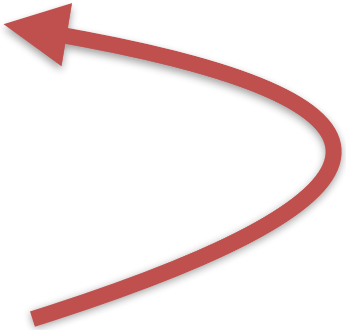
- Specify exact experimental setup
  - e.g., hypotheses to test
- Collect data
- Run experiment
- Observe outcome

Can't reuse data after observing outcome.

Adaptive data analysis

Data analyst

- Specify exact experimental setup
  - e.g., hypotheses to test
- Collect data
- Run experiment
- Observe outcome
- Revise experiment

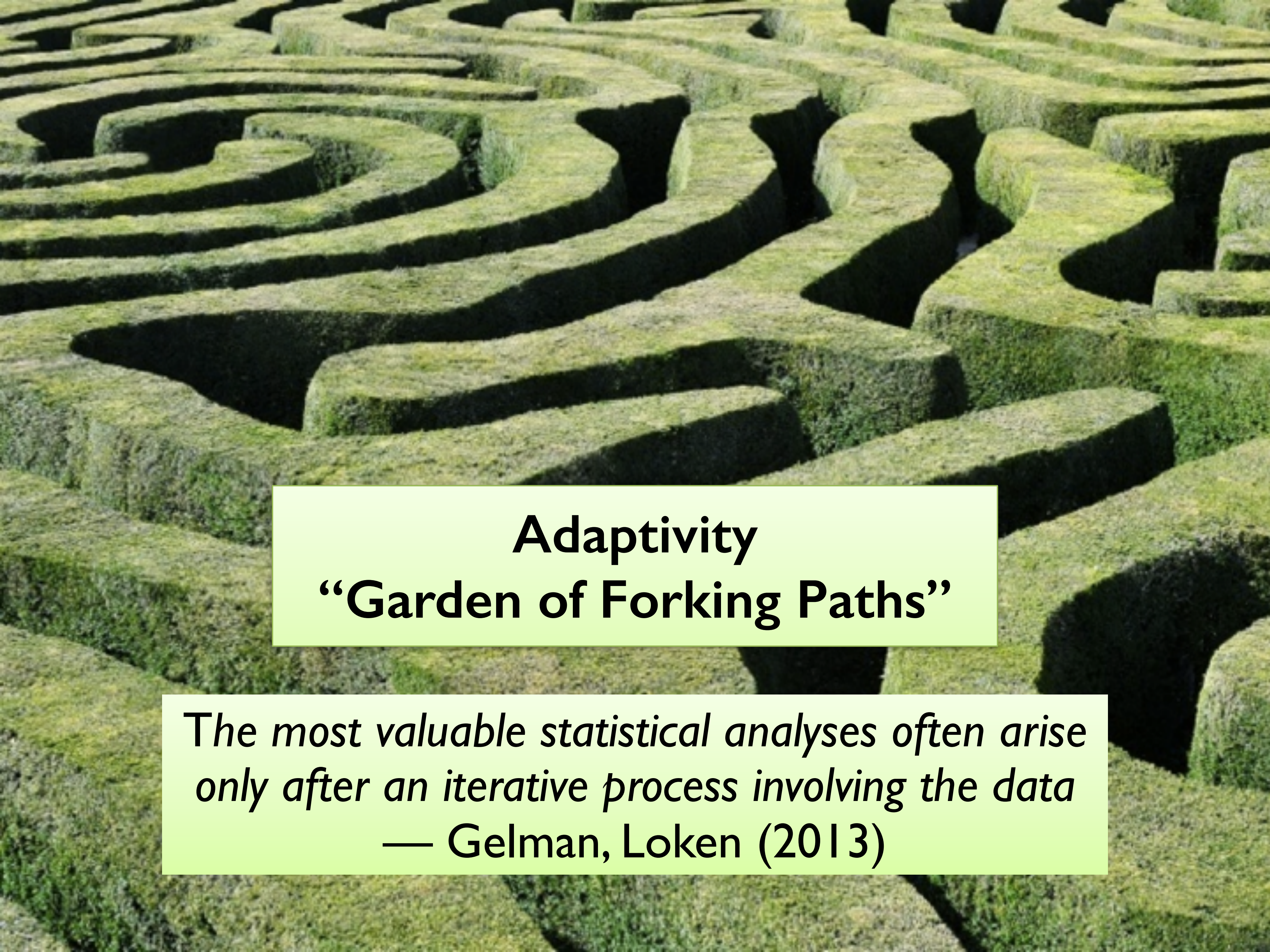


Adaptivity

Data dredging, data snooping, fishing,
p-hacking, post-hoc analysis,
garden of the forking paths

Some caution strongly against it:
“Pre-registration” — specify entire experimental setup ahead of time

Humphreys, Sanchez, Windt (2013), Monogan (2013)



Adaptivity
“Garden of Forking Paths”

The most valuable statistical analyses often arise only after an iterative process involving the data
— Gelman, Loken (2013)

From art to science

Can we guarantee statistical validity in adaptive data analysis?

Our results: To a surprising extent, yes.

Our hope: To inform discourse on false discovery.

A general approach

Main result:

The outcome of any differentially private analysis *generalizes**.

* If we sample fresh data, we will observe roughly the same outcome.

Moreover, there are powerful differentially private algorithms for adaptive data analysis.

Intuition

Differential privacy is a *stability* guarantee:

- Changing one data point doesn’t affect the outcome much

Stability implies generalization

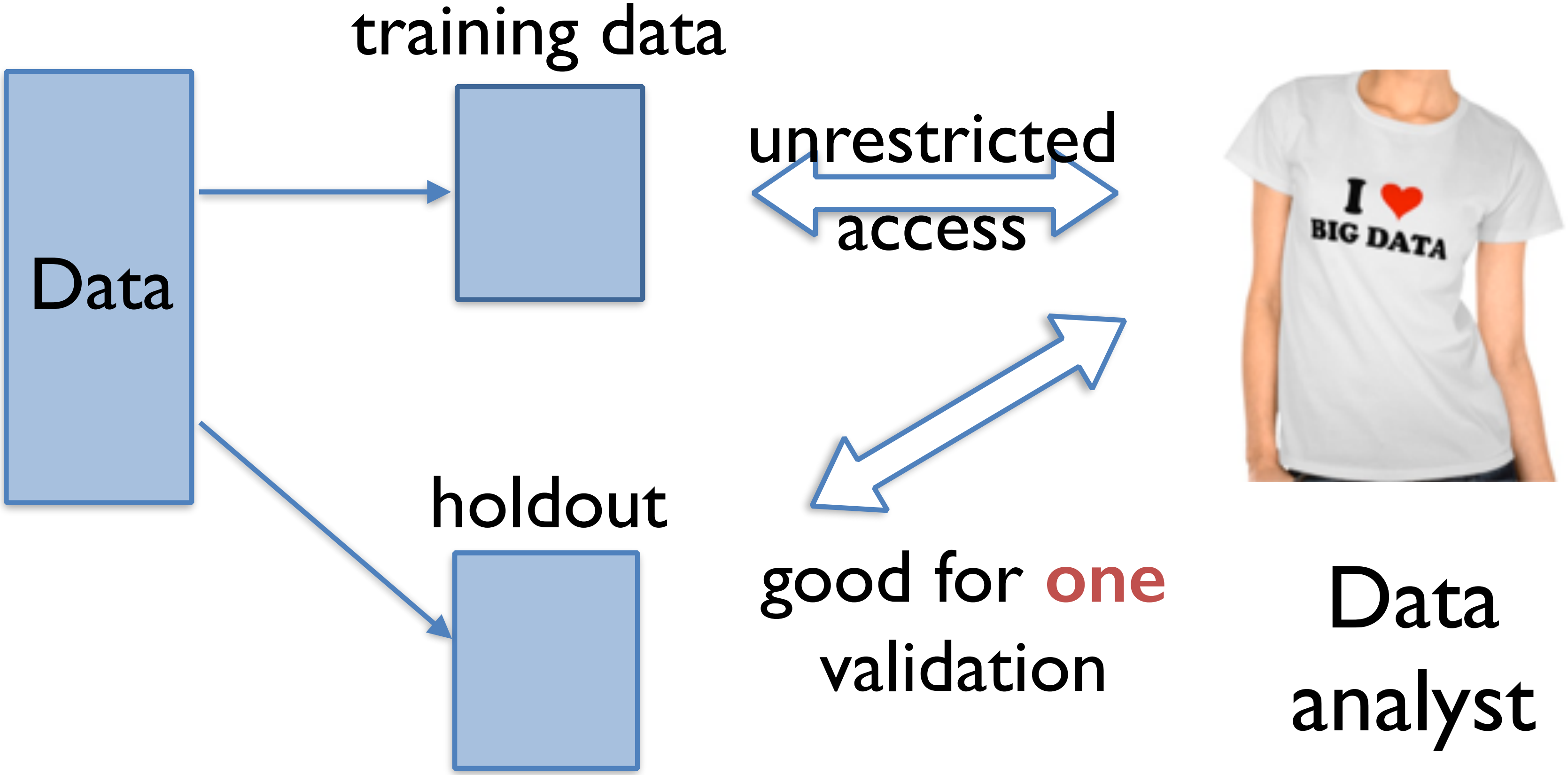
- “Overfitting is not stable”

Does this mean I have to learn how to use differential privacy?

Resoundingly, no!

Thanks to our **reusable holdout** method

Standard holdout method



training data

Data

unrestricted access

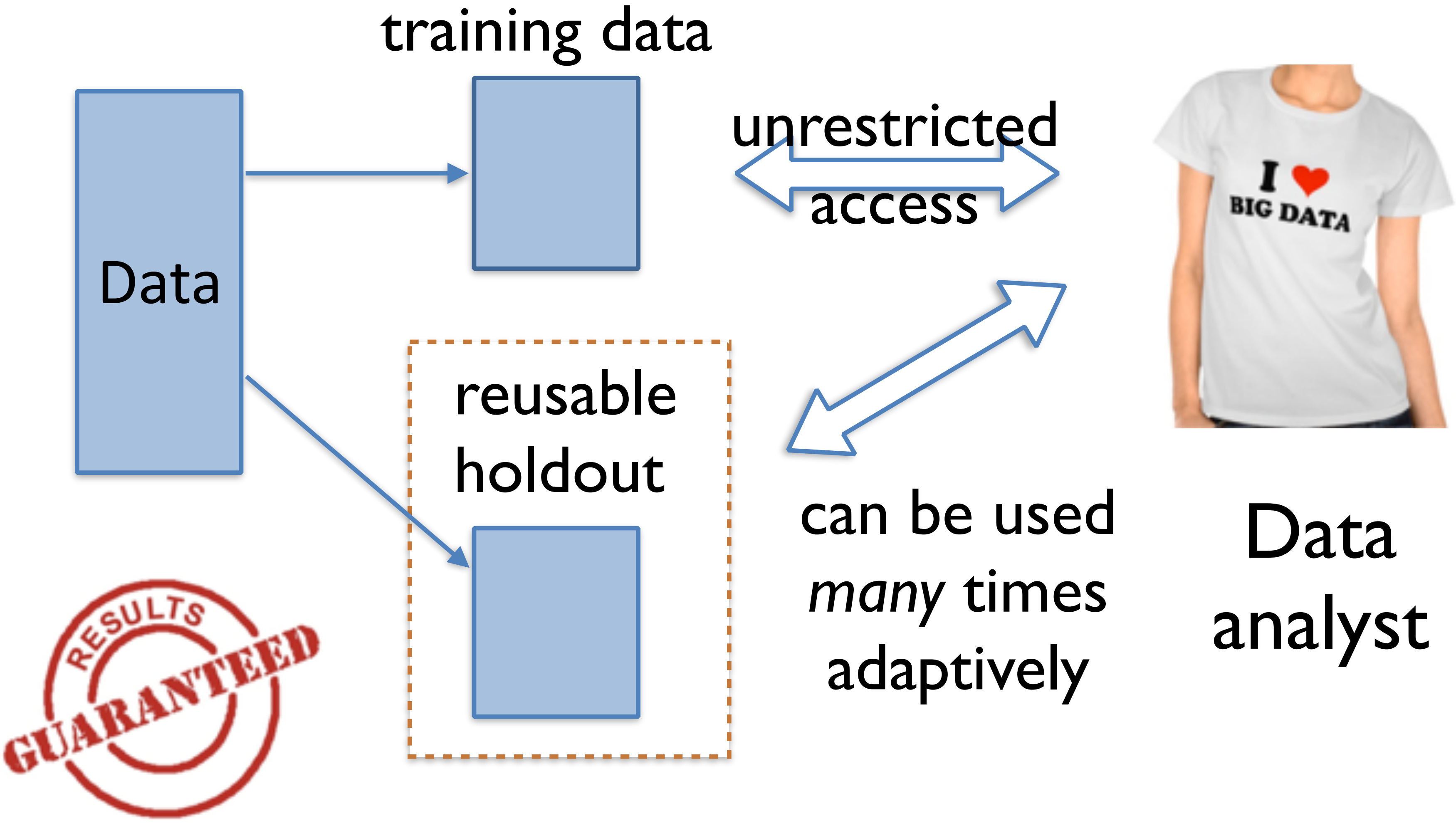
holdout

good for **one** validation

Data analyst

***Non*-reusable:** Can’t use information from holdout in training stage adaptively

One corollary: a reusable holdout



Data

training data

unrestricted access

reusable holdout

can be used *many* times adaptively

Data analyst

essentially as good as using *fresh* data each time!

More formally

Domain X. Unknown distribution D over X

Data set S of size n sampled i.i.d. from D

What the holdout will do:

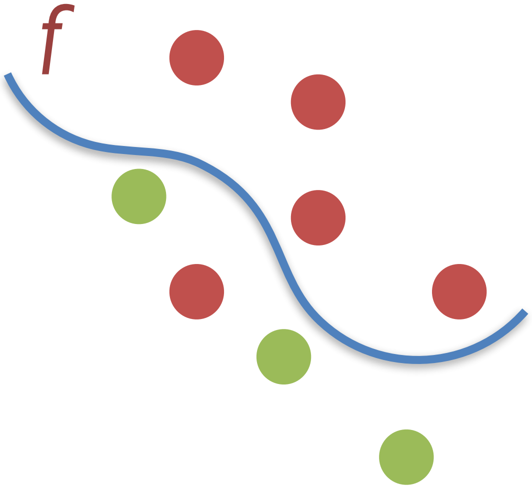
Given a *function* $q : X \longrightarrow [0,1]$, estimate the expectation $\mathbb{E}_D[q]$ from sample S

Definition: An estimate a *is valid* if $|a - \mathbb{E}_D[q]| < 0.01$

Enough for many statistical purposes, e.g.,

estimating quality of a model on distribution D

Example: Model Validation



We trained predictive model $f : Z \longrightarrow Y$
and want to know its accuracy

Put $X = Z \times Y$.
Joint distribution D over data x labels

Estimate accuracy of classifier
using the function $q(z,y) = \mathbf{1}\{ f(z) = y \}$

$\mathbb{E}_S[q]$ = accuracy with respect to sample S
$\mathbb{E}_D[q]$ = true accuracy with respect to unknown D

A reusable holdout: *Thresholdout*

Theorem. Thresholdout gives valid estimates for any sequence of adaptively chosen functions until n^2 overfitting* functions occurred.

* Function q *overfits* if $|\mathbb{E}_S[q]-\mathbb{E}_D[q]| > 0.01$.

Example: Model is good on S, bad on D.

Thresholdout

Input:

Data S, holdout H, threshold $T > 0$, tolerance $\sigma > 0$

Given function q:

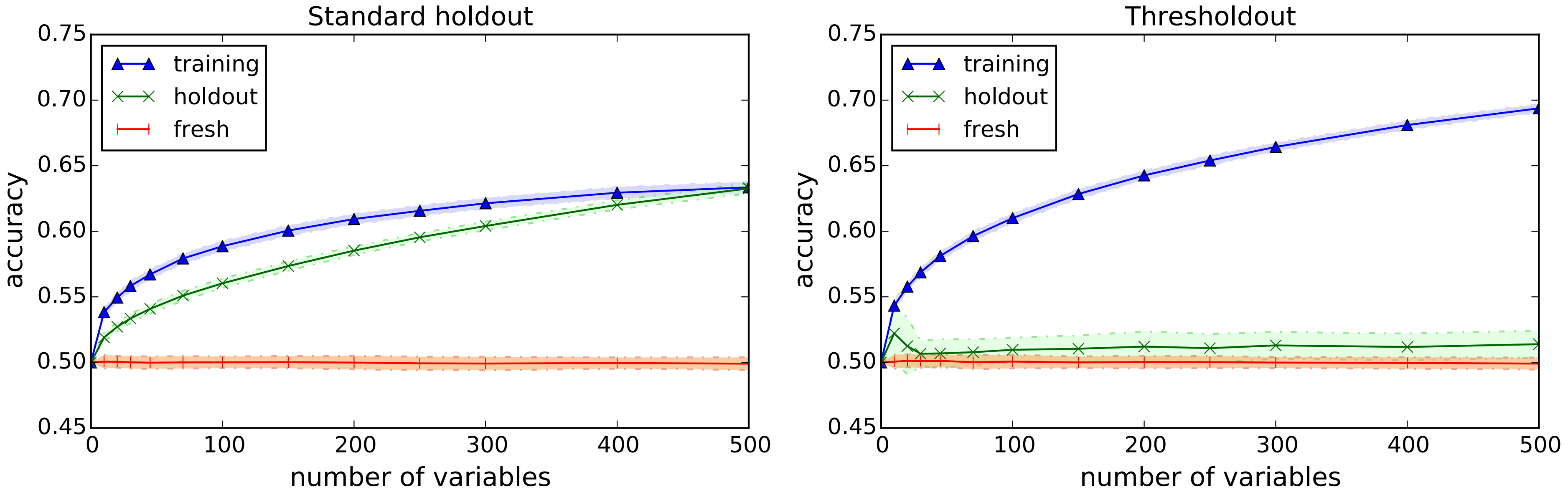
```
Sample $\eta, \eta'$ from $N(0,\sigma^2)$
If $|\mathrm{avg}_H[q] - \mathrm{avg}_S[q]| > T + \eta$:
    output $\mathrm{avg}_H[q] + \eta'$
Otherwise:
    output $\mathrm{avg}_S[q]$
```

An illustrative experiment

- Data set with $2n = 20{,}000$ rows and $d = 10{,}000$ variables. Class labels in $\{-1,1\}$
- Analyst performs **stepwise variable selection**:
    1. Split data into training/holdout of size n
    2. Select "best" k variables on training data
    3. Only use variables also good on holdout
    4. Build linear predictor out of k variables
    5. Find best $k = 10,20,30,\ldots$

No correlation
between data and labels

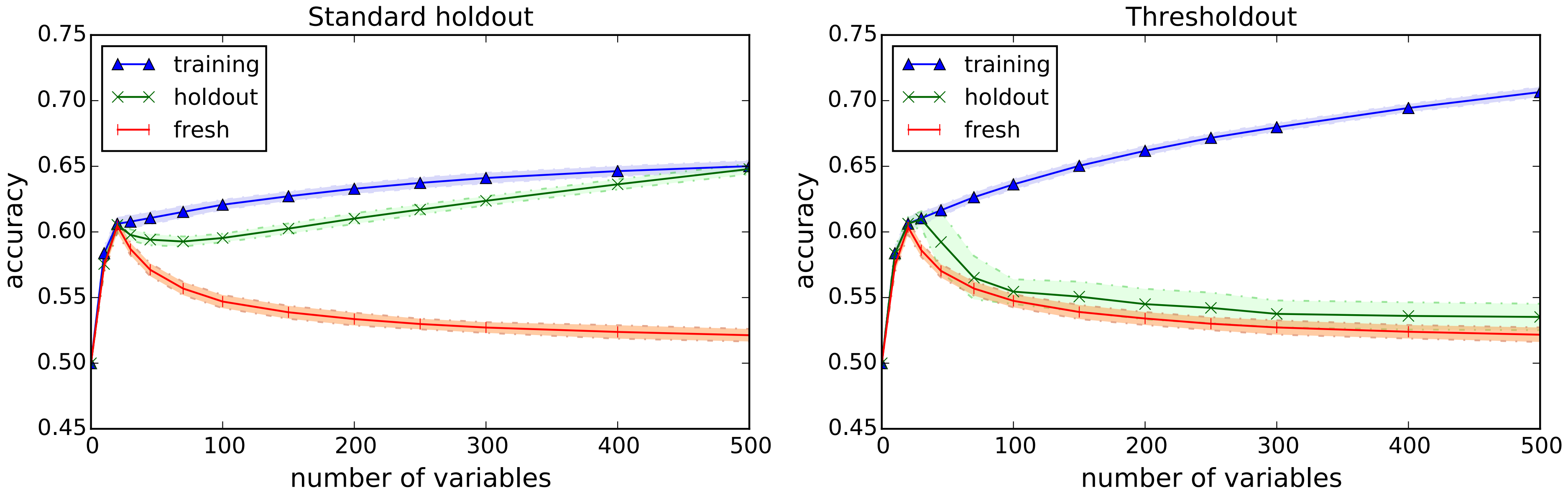
data are random gaussians
labels are drawn *independently* at random from {-1,1}



Thresholdout correctly detects overfitting!

High correlation

20 attributes are highly correlated with target
remaining attributes are uncorrelated



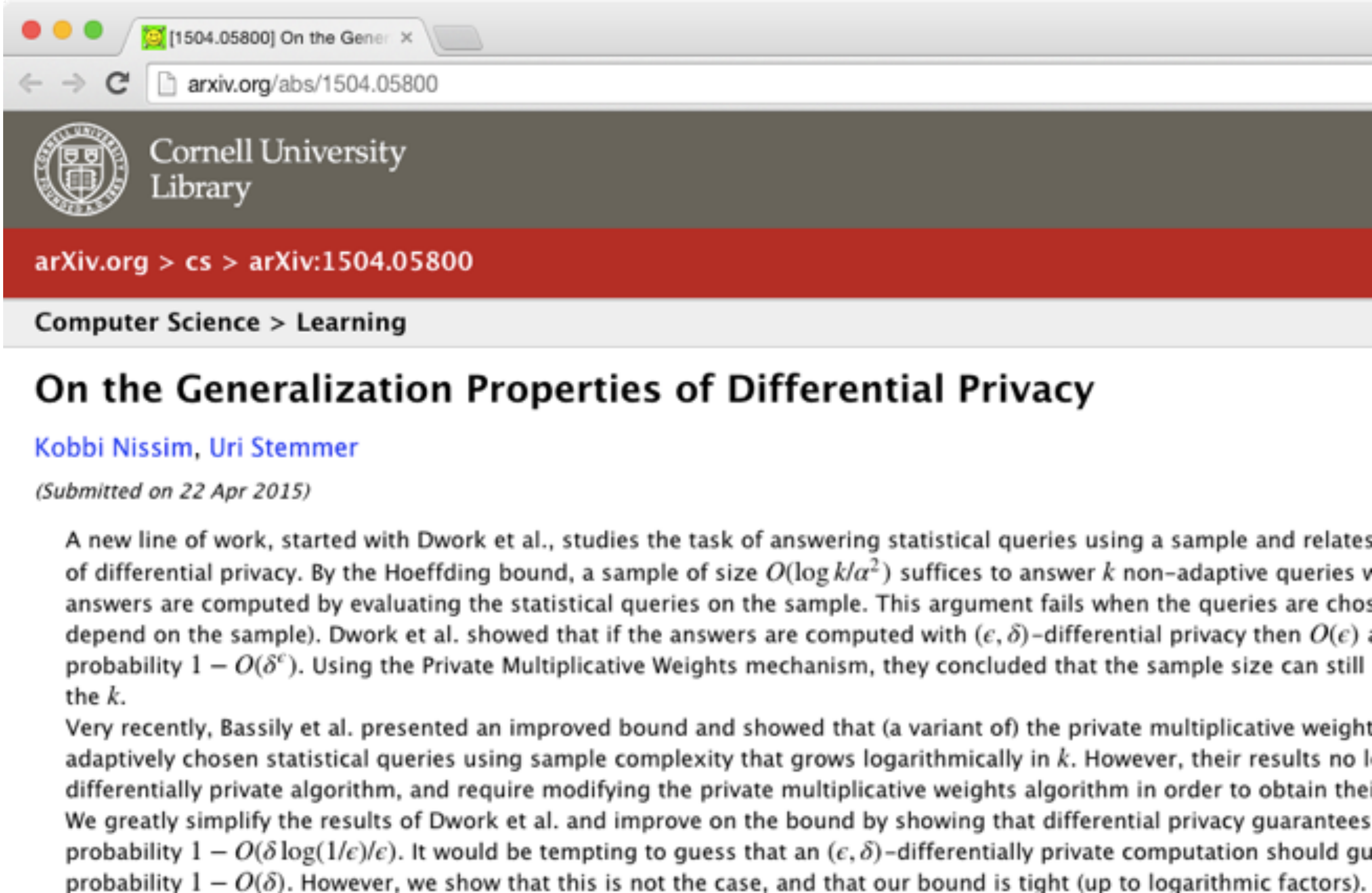
Thresholdout correctly detects right model size!

Conclusion

Powerful new approach for achieving statistical validity in adaptive data analysis building on differential privacy!

- Reusable holdout:
    - Broadly applicable
    - Complete freedom on training data
    - Guaranteed accuracy on the holdout
    - No need to understand Differential Privacy
    - Computationally fast and easy to apply

Go read this paper for a proof:



arXiv.org > cs > arXiv:1504.05800

Computer Science > Learning

On the Generalization Properties of Differential Privacy

Kobbi Nissim, Uri Stemmer

(Submitted on 22 Apr 2015)

A new line of work, started with Dwork et al., studies the task of answering statistical queries using a sample and relates
of differential privacy. By the Hoeffding bound, a sample of size $O(\log k/\alpha^2)$ suffices to answer k non-adaptive queries w
answers are computed by evaluating the statistical queries on the sample. This argument fails when the queries are chos
depend on the sample). Dwork et al. showed that if the answers are computed with (ϵ,δ)-differential privacy then $O(\epsilon)$ a
probability $1-O(\delta^\epsilon)$. Using the Private Multiplicative Weights mechanism, they concluded that the sample size can still
the k.
Very recently, Bassily et al. presented an improved bound and showed that (a variant of) the private multiplicative weight
adaptively chosen statistical queries using sample complexity that grows logarithmically in k. However, their results no l
differentially private algorithm, and require modifying the private multiplicative weights algorithm in order to obtain thei
We greatly simplify the results of Dwork et al. and improve on the bound by showing that differential privacy guarantees
probability $1-O(\delta\log(1/\epsilon)/\epsilon)$. It would be tempting to guess that an (ϵ,δ)-differentially private computation should gu
probability $1-O(\delta)$. However, we show that this is not the case, and that our bound is tight (up to logarithmic factors).

Thank you.