A Practical Algorithm for Exact Inference on Tables

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Motivation

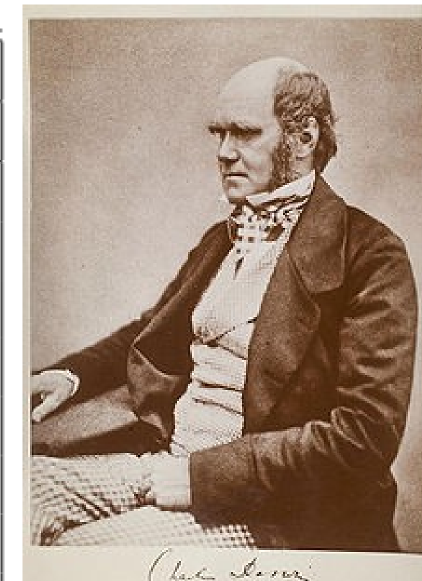
Suppose you are an ecologist, and observe...

Darwin's Finches on the Galápagos Islands

	Island																
Finch	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
Large ground finch	0	0	1	1	1	1	1	1	1	1	0	1	1	1	1	1	1
Medium ground finch	1	1	1	1	1	1	1	1	1	1	0	1	0	1	1	0	0
Small ground finch	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	0	0
Sharp-beaked ground finch	0	0	1	1	1	0	0	1	0	1	0	1	1	0	1	1	1
Cactus ground finch	1	1	1	0	1	1	1	1	1	1	0	1	0	1	1	0	0
Large cactus ground finch	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0
Large tree finch	0	0	1	1	1	1	1	1	1	0	0	1	0	1	1	0	0
Medium tree finch	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Small tree finch	0	0	1	1	1	1	1	1	1	1	0	1	0	0	1	0	0
Vegetarian finch	0	0	1	1	1	1	1	1	1	1	0	1	0	1	1	0	0
Woodpecker finch	0	0	1	1	1	0	1	1	0	1	0	0	0	0	0	0	0
Mangrove finch	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Warblerfinch	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Islands: A = Seymour, B = Baltra, C = Isabella, D = Fernandina, E = Santiago, F = Rábida, G = Pinzón, H = Santa Cruz, I = Santa Fe, J = San Cristóbal, K = Española, L = Floreana, M = Genovesa, N = Marchena, O = Pinta, P = Darwin, Q = Wolf.

Chen et al. 2005



Motivation

This arrangement of finches seems unusual to you. To analyze it, you formulate a statistical test:

- Null hypothesis: uniform distribution given fixed row and column sums
- Test statistic: $$\bar{S}^2 = \frac{1}{m(m-1)} \sum_{i \neq j} c_{ij}^2,$$

  where m is the number of species, $\mathbf{C} = (c_{ij}) = \mathbf{A}\mathbf{A}^T$

  and $\mathbf{A}$ is the occurrence matrix.
- Estimate the p-value

How to sample?

Motivation

Fixing the row and column sums makes the distribution very complicated.

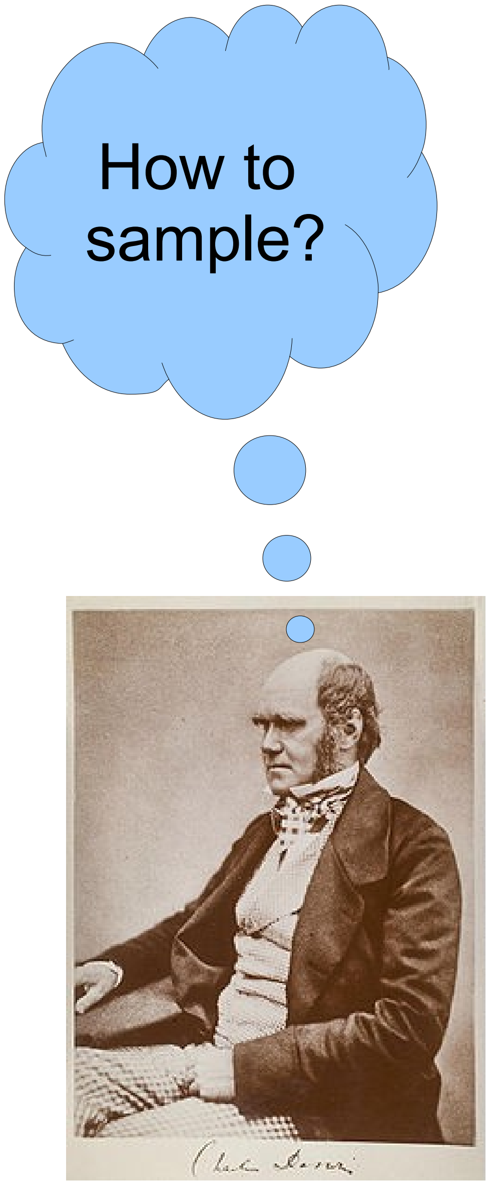
Trivial example:

Row sums = (2, 2, 1, 1), Column sums = (3, 2, 1)

There are 8 such binary matrices:

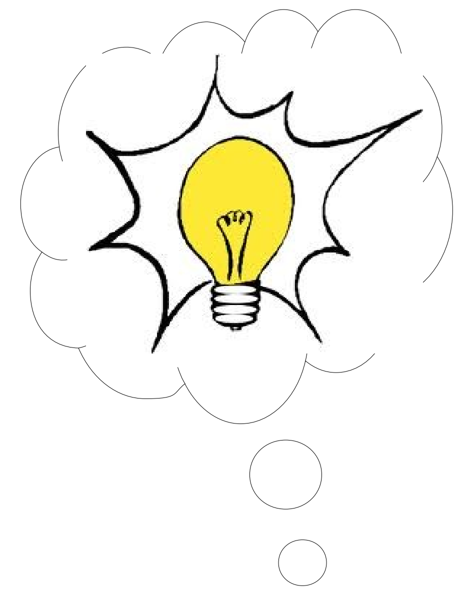
$$\begin{matrix}1&1&0\\0&1&1\\1&0&0\\1&0&0\end{matrix}\qquad\begin{matrix}1&0&1\\1&1&0\\1&0&0\\0&1&0\end{matrix}\qquad\begin{matrix}1&0&1\\1&1&0\\0&1&0\\1&0&0\end{matrix}\qquad\begin{matrix}0&1&1\\1&1&0\\1&0&0\\1&0&0\end{matrix}$$

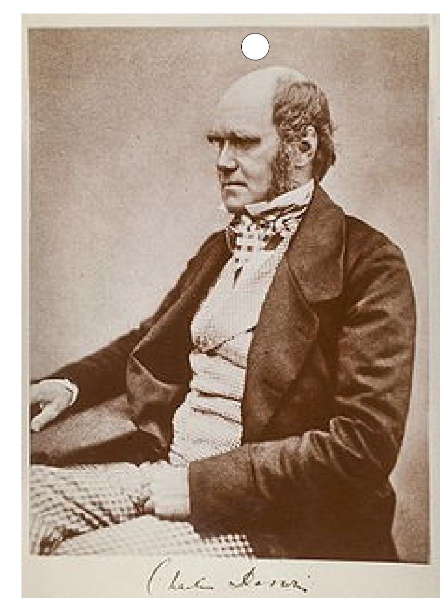
$$\begin{matrix}1&1&0\\1&1&0\\1&0&0\\0&0&1\end{matrix}\qquad\begin{matrix}1&1&0\\1&1&0\\0&0&1\\1&0&0\end{matrix}\qquad\begin{matrix}1&1&0\\1&0&1\\1&0&0\\0&1&0\end{matrix}\qquad\begin{matrix}1&1&0\\1&0&1\\0&1&0\\1&0&0\end{matrix}$$



Background

- This example is typical in ecology.
- Existing sampling methods:
  - Heuristic approximations
  - Markov chain Monte Carlo (MCMC)
  - Sequential Importance Sampling (SIS)
- Issue: Existing theory does not provide adequate guarantees on convergence rates.
- **We offer an exact algorithm that is tractable in many cases.**





Previous Work

- Heuristic approximations

  Connor and Simberloff (1979), Patterson and Atmar (1986), Gilpin and Diamond (1982), Coleman et al. (1982)

- Markov chain Monte Carlo (MCMC)

  Brualdi (1980), Roberts and Stone (1990), Manly (1995), Chen, Diaconis, Holmes, and Liu (2005), (*and many more!*)

- Sequential Importance Sampling (SIS)

  Chen, Diaconis, Holmes, and Liu (2005), Harrison (to appear)

Theory

- There exists a **recursion** that efficiently counts the number of binary matrices with given margins (when the column sums are not too large).
- Main idea: **exploit symmetries**

Theorem

$$\bar{N}(\mathbf{p},\mathbf{r}) = \sum_{\mathbf{s}\in C^{\mathbf{r}}(p_1)} \binom{\mathbf{r}}{\mathbf{s}} \bar{N}(L\mathbf{p},\mathbf{r}\backslash\mathbf{s})$$

- O($mn^b(\log n)^3$) time for *m* x *n* matrices, assuming bounded margins and $b \geq$ max column sum.
- After counting, **sampling** is *easy and fast*.

Example #1: Darwin's finches

We compare results with

Chen, Diaconis, Holmes, and Liu (JASA 2005).

Results for Darwin's Finch Data, using $\bar{S}^2$

Method	# samples	p-value	Sampling time
Exact	1,000,000	$(4.67 \pm .22) \times 10^{-4}$	31 minutes
SIS	1,000,000	$(3.96 \pm .36) \times 10^{-4}$	18 minutes
MCMC	15,000,000	$(3.56 \pm .68) \times 10^{-4}$	18 minutes

Exact 95% Confidence Interval: (4.26, 5.11) x 10^{-4}

Number of matrices with margins as observed:

- Exact number: 67,149,106,137,567,626 (1.4 sec)
- Chen's estimate: 6.7150×10^{16}

Example #1: Darwin's finches

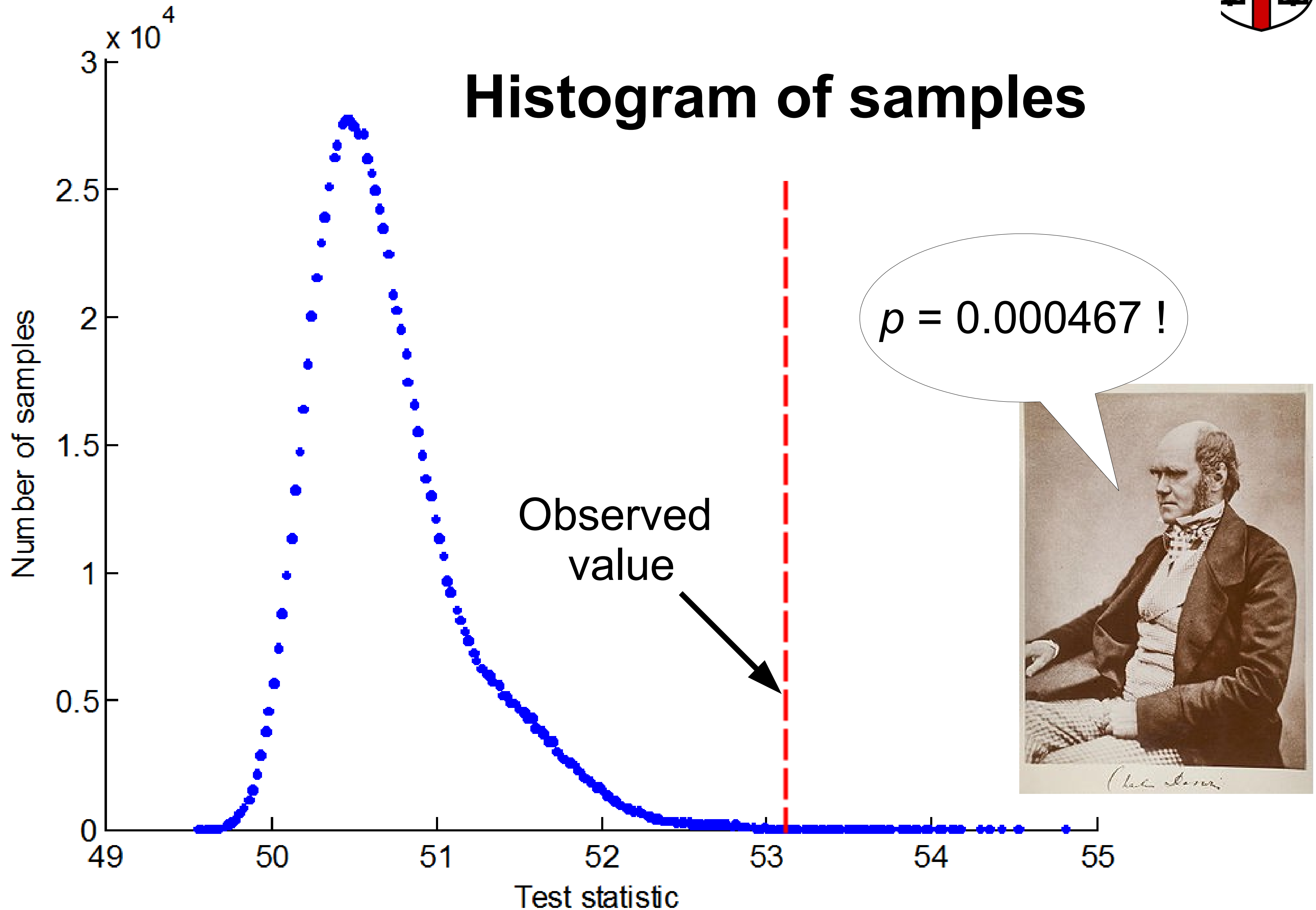


Table 1: 26 Mammalian Species in 28 Mountain Ranges in the American Southwest

	Range																											
Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
A	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0
B	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0
C	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	1	1
D	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	1	1	1	1	1	0	1	0	0	0	0
E	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	0	1	0	0	0	0
F	1	1	1	1	1	0	0	0	1	1	1	1	1	0	1	1	0	1	1	1	1	0	1	0	1	0	0	0
G	1	1	1	1	1	1	1	0	1	1	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
H	1	1	1	1	1	1	0	1	1	0	1	0	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0
I	1	1	1	1	1	1	1	1	0	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
J	1	1	1	1	1	1	1	1	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
L	1	1	1	1	1	0	0	1	1	0	0	0	1	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0
M	1	1	1	1	1	0	0	0	0	0	0	1	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
N	1	1	1	1	0	1	1	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
P	1	1	0	1	1	1	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Q	1	1	1	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
R	1	1	1	1	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
T	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
U	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
V	1	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
W	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
X	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Y	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Z	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Patterson and Atmar, 1986

Example #2: Montane mammals

We compare results with Patterson and Atmar, 1986.

Results for Montane Mammal Data, using S_n

Method	# samples	p-value	mean of S_n	std. dev.	min	max
Exact	1,000,000	$0.0322 \pm .00018$	80.71	9.697	44	132
Heuristic	1,000	9×10^{-20}	227.9	18.135	180	287

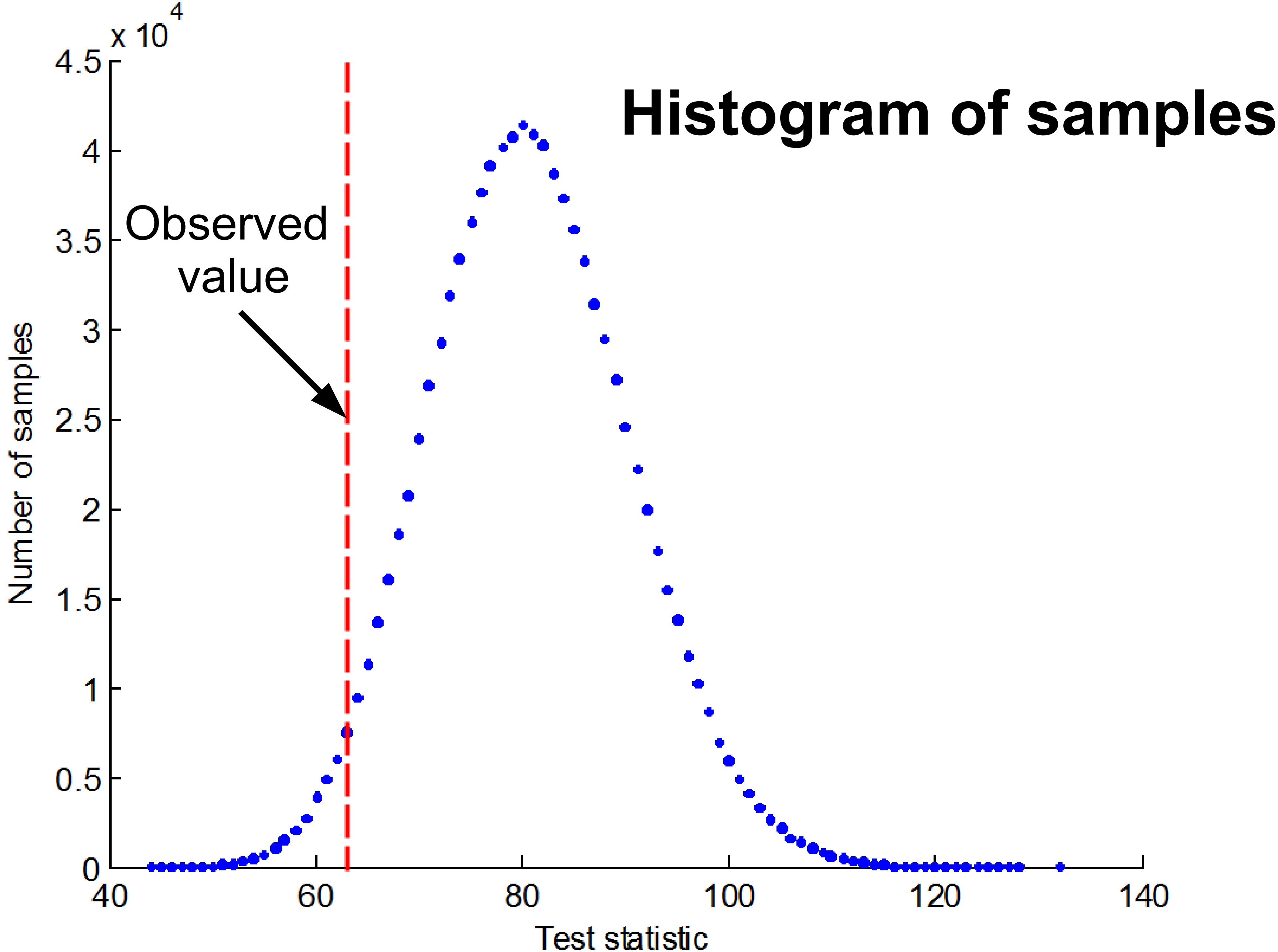
Test statistic S_n = "nested subset statistic" (Observed value: 63)

Number of matrices with margins as observed:

2,663,296,694,330,271,332,856,672,902,543,209,853,700

~ 2.6×10^{39} (computed in 32 minutes)

Example #2: Montane mammals



20 Lizard Species on 25 Islands in the Gulf of California

	Island																								
Lizard	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1	1	0	1	0	0	0	0	0	0	0	0	0	0	1	1	0	1	0	0	0	0	1	0	1	0
2	1	1	1	1	1	1	1	1	1	1	0	1	0	1	1	1	1	1	1	1	1	1	1	1	1
3	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	0	1	1	0	0
4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	1	0	1	0
5	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	1	0	1	1	1	0	1	1	1	1	1	1	0	1	1	1	1	0	1	0	0	1	1	1	0
7	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	1	0	0	0	1	1	1	1
8	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0	1	1	1	0
9	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	1	1	1	0
11	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0
13	1	0	1	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	1	1	1	1
14	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	1	1	1	1	0	0	0	1	1	1	0	0	0	1	1	1	1	1	1	1	1	1	1	1	0
17	0	0	1	0	0	0	0	0	0	0	0	0	0	1	1	1	0	1	1	0	0	1	0	1	1
18	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1
20	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Manly, 1995

Example #3: Island lizards

We compare results with Manly, 1995.

Results for Island Lizards, using S_d

Method	# samples	p-value
Exact	1,000,000	$(1.34 \pm .12) \times 10^{-4}$
MCMC	1,000,000	$(5.0 \pm .4) \times 10^{-4}$

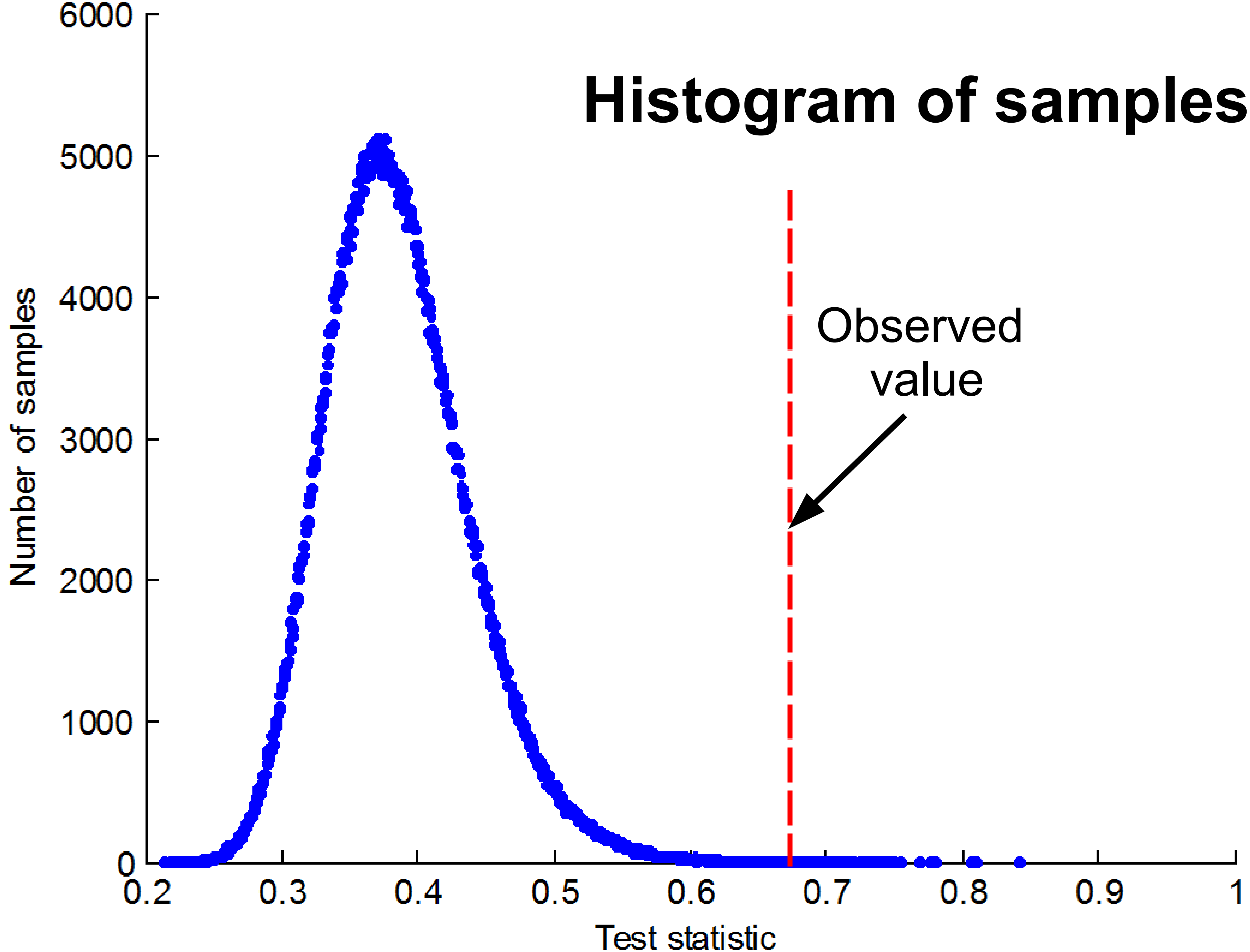
Test statistic S_d = “deviation from expected co-occurrences”

Number of matrices with margins as observed:

55,838,420,515,731,001,979,319,625,577,023,858,901,579,264

~ 5.5×10^{43} (computed in 11 minutes)

Example #3: Island lizards



Summary

- Uniform distribution on binary matrices with given row/column sums
- Existing theory does not provide adequate guarantees on convergence rates.
- **We offer an exact algorithm that is tractable in many cases.**

Contact info:

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Thank you for listening!