

An estimate for the chance  $p$  of heads  
on a coin where the relative error does  
not depend on  $p$

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# The Problem

## *Flipping coins*



Heads



Tails

## *The question*

What is the probability the coin is heads?

## *Basic estimate*

Step 1: Numerically encode coins:

$$\text{Heads} = 1, \text{Tails} = 0$$

Step 2: Assign probability distribution:

$$C \sim \text{Bernoulli}(p) \Rightarrow \mathbb{P}(X = 1) = p, \mathbb{P}(X = 0) = 1 - p$$

Step 3: Basic estimate:

$$\hat{p}_n = \frac{C_1 + \dots + C_n}{n}, \quad C_i \stackrel{\text{iid}}{\sim} \text{Bern}(p)$$

*This has lead to some great mathematics*

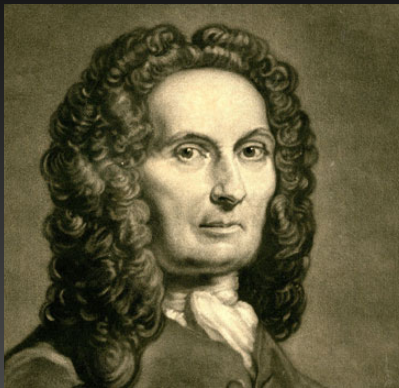
Jacob Bernoulli proved in 1713 an early version of the Strong Law of Large Numbers.



Strong Law of Large Numbers:

$$\lim_{n \rightarrow \infty} \hat{p}_n = p \text{ with probability } 1$$

*But how fast does it converge?*

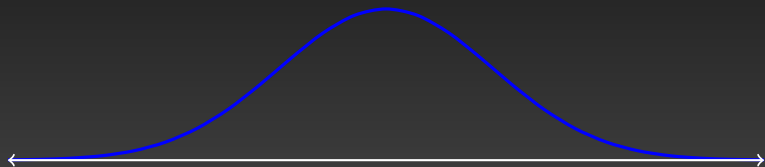


**Abraham de Moivre**

proved in 1733 an early version of the Central Limit Theorem in order to study how the simple estimate behaves

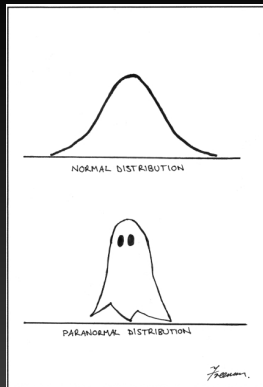
## *The Central Limit Theorem*

The CLT says that in the limit as you add independent, identically distributed random variables, the resulting density approaches a normal distribution:



Our coin flips are iid, so  $\hat{p}$  approximately normal...





M. Freeman, A visual comparison of normal and paranormal distributions, *J. of Epidemiology and Community Health*, 60(1), p. 6, 2006

## *Central Limit Theorem*

The CLT has some drawbacks for this problem

- ▶ Convergence to normal polynomial in  $n$
- ▶ Tails exponentially small in  $n$
- ▶ Not accurate out in the tails
- ▶ For confidence close to 1
- ▶ Bad for small  $p$
- ▶ Gives additive error, not relative error

## Relative Error

### Definition

The *relative error* of an estimate  $\hat{p}$  for  $p$  is

$$\frac{\hat{p}}{p} - 1 = \frac{\hat{p} - p}{p}.$$

**Example:** Actual answer: 20%  
Estimate: 23%  
Relative error:  $3\%/20\% = 15\%$

*Today*

I will present an unbiased estimate  $\hat{p}$  for  $p$   
where the relative error does not depend in any  
way on  $p$ .

## *Estimate properties*

### The new estimate

- ▶ Requires a random number of flips
- ▶ Unbiased
- ▶ Number of flips very close to optimal
- ▶ Relative error distribution known exactly
- ▶ Allows easy construction of exact confidence intervals

## *Relative error and basic estimate: An example*

For the basic estimate, relative error heavily depends on  $p$

Suppose  $n = 5$  and  $p = 0.25$ .

Then

$$\hat{p}_n \in \left\{ \frac{0}{5}, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, \frac{5}{5} \right\}.$$

and

$$\frac{\hat{p}_n}{p} \in \left\{ \frac{0}{5}, \frac{4}{5}, \frac{8}{5}, \frac{12}{5}, \frac{16}{5}, \frac{20}{5} \right\}.$$

The values that  $[\hat{p}_n/p] - 1$  takes on depends on  $p$ !

## *More generally*

More generally:

$$\frac{\hat{p}_n}{p} \in \left\{ \frac{0}{np}, \frac{1}{np}, \frac{2}{np}, \dots, \frac{n}{np} \right\}$$

### New estimate

- ▶ Distribution of  $\hat{p}/p - 1$  does not depend on  $p$
- ▶ Allows us to easily find exact confidence intervals

## *But is it fast?*

**Goal:** for  $\epsilon > 0$  and  $\delta > 0$ ,

$$\mathbb{P}(|(\hat{p}/p) - 1| > \epsilon) < \delta$$

Suppose we knew  $p$  ahead of time, what should  $n$  be exactly for

$$\epsilon = 10\% \text{ and } \delta = 5\%?$$

Can directly calculate tails of a binomial to get:

$p$	Exact $n$
1/20	7219
1/100	37546



## *New algorithm*

Let  $T_\rho$  be number of flips required by new estimate

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$\epsilon = 0.1, \delta = 0.05$			
$\rho$	Exact $n$	$\mathbb{E}[T_\rho]$	$\mathbb{E}[T_\rho]/n$
1/20	7 219	7 700	1.067
1/100	37 545	38 500	1.025

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$\epsilon = 0.01, \delta = 10^{-6}$			
$\rho$	Exact $n$	$\mathbb{E}[T_\rho]$	$\mathbb{E}[T_\rho]/n$
1/20	4 545 010	4 789 800	1.053
1/100	236 850 500	239 490 000	1.011

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## *Estimate properties*

### The new estimate

- ▶ Requires a random number of flips
- ▶ Unbiased
- ▶ Number of flips very close to optimal
- ▶ Relative error distribution known exactly
- ▶ Allows easy construction of exact confidence intervals

## *How did I get started on this problem?*

My work is in perfect simulation

- ▶ Drawing samples exactly from high dimensional models...
- ▶ ...usually using a random number of samples.

Examples

- ▶ Ising (and autonormal) model
- ▶ Strauss model
- ▶ Widom-Rowlinson
- ▶ Allele frequency tables
- ▶ Colorings of graphs
- ▶ Matérn type III process
- ▶ Weighted assignments

Numerous applications

# Applications

## *Application: Finding the permanent of a matrix*

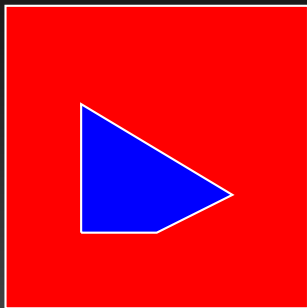
M. Huber and J. Law. Fast approximation of the permanent for very dense problem. In *Proc. of 19th ACM-SIAM Symp. on Discrete Alg.*, pp. 681–689, 2008

### *Definition*

Suppose  $n$  workers are to be assigned to jobs  $\{1, 2, \dots, n\}$ , but each worker is only qualified for a specified set of jobs. The number of such assignments is called the *permanent*.

## Acceptance/Rejection

HL 2008 was an example of an acceptance/rejection method...



**Goal:** Estimate size of blue

1. Draw  $X_1, \dots, X_n$  from red region
2. Let  $k$  be the number of  $X_i$  that fell into blue
3. Estimate is  $(k/n)$  times size of red region

## *This is just the coin problem!*

Probability of heads  $p$  is size of blue over size of red

- ▶ Want to minimize number of draws from red region...
- ▶ ...is the same as number of flips of a coin

In the paper, used a Chernoff bound to bound Binomial tails:

$$14p^{-1}\epsilon^{-2}\ln(2/\delta)$$

flips of the coin sufficed

## *Then I was asked to referee a paper...*

The authors had referenced the 2008 permanent paper...

- ▶ They used the 14 constant
- ▶ This constant is way too large
- ▶ So I started work to reduce this constant



## *How should number of samples vary with $p$ ?*

To get a rough idea of how many samples needed, consider  $\hat{p}_n$

$$\mathbb{E}[\hat{p}_n] = p, \quad \text{SD}(\hat{p}_n) = \sqrt{\frac{(p)(1-p)}{n}}$$

So to get  $\text{SD}(\hat{p}_n) \approx \epsilon p \dots$

$$n \approx \epsilon^{-2}(1-p)/p$$

Number of samples should be  $\Theta(1/p)$ , but we don't know  $p$

## DKLR

P. Dagum, R. Karp, M. Luby, and S. Ross. An optimal algorithm for Monte Carlo estimation. *Siam. J. Comput.*, 29(5):1484–1496, 2000.

They solved the  $1/p$  problem in the following clever way:

1. Keep flipping coins until get  $k$  heads
2. Estimate is  $k$  divided by number of flips

**Run time** On average, draw  $k/p$  samples

[Biased estimate, however]

Their theorem: to get  $\mathbb{P}(|(\hat{p}_{\text{DKLR}}/p) - 1| > \epsilon) < \delta$ ,

$$k \geq 1 + 4(e - 2)(1 + \epsilon) \ln(2/\delta) \epsilon^{-2}$$

Note  $4(e - 2) \approx 2.873 \dots$

## *Running time for DKLR*

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$\epsilon = 0.1, \delta = 0.05$			
$\rho$	Exact $n$	$\mathbb{E}[T_\rho]$	$\mathbb{E}[T_{\text{DKLR}}]$
1/20	7 219	7 700	23 340
1/100	37 545	38 500	116 700

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## *Application: Exact $p$ values*

M. Huber, Y. Chen, I. Dinwoodie, A. Dobra, and M. Nicholas, Monte Carlo algorithms for Hardy-Weinberg proportions, *Biometrics*, 62(1), pp. 49–53, 2006.

### *Definition*

A  $p$  value is the probability that a statistic applied to a draw from the null hypothesis model is more unusual than the statistic applied to the data.

Low  $p$ -value = evidence that null hypothesis is untrue

## *Estimating $p$ -values with perfect samples*

Want  $p$ -value for a statistic  $S(\cdot)$

A  $p$ -value is just

$$\mathbb{P}(S(X) \text{ is weirder than } S(\text{data}))$$

where  $X$  is a draw from statistical model

So if have algorithm for drawing  $X$  exactly from model...

This is again exactly the coin flipping problem!

## The Estimate

## *Uniform and exponential random variables*

Say  $U \sim \text{Unif}([0, 1])$  if for all  $0 < a < b < 1$ ,

$$\mathbb{P}(a < U < b) = b - a.$$

To get an exponential random variable (with rate 1):

$$U \sim \text{Unif}([0, 1]) \Rightarrow -\ln(U) \sim \text{Exp}(1)$$

## *The algorithm in words:*

Before you begin:

- ▶ Fix  $k$  a positive integer

The estimate:

1. Flip a coin
2. Draw an exponential random variable of rate 1
3. Add the exponential to a total of time
4. Keep doing 1 through 3 until you have  $k$  heads
5. The final estimate is  $k - 1$  divided by the sum of the exponentials



## *The algorithm in pseudocode*

### Gamma Bernoulli Approximation Scheme

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GBAS *Input:*  $k \geq 2$

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- 1)  $R \leftarrow 0, S \leftarrow 0$
  - 2) Repeat
  - 3)      $X \leftarrow \text{Bern}(p), A \leftarrow \text{Exp}(1)$
  - 4)      $S \leftarrow S + X, R \leftarrow R + A$
  - 5) Until  $S = k$
  - 6)  $\hat{p} \leftarrow (k - 1)/R$
-

## Poisson point process

### Definition

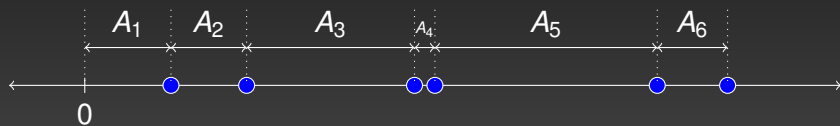
$P$  is a *Poisson point process* on a region  $A$  of rate  $\lambda$  if for any  $B \subseteq A$  of finite size, the mean number of points of  $P$  that fall in  $B$  is  $\lambda$  times the size of  $B$ . Also, the # of points in an interval is independent of the # of points in a disjoint interval.



Expected number in interval of length 2 is  $2\lambda$

## Equivalent Formulation

Distances between points are iid  
exponential random variables of rate  $\lambda$   
(take exp rate 1, divide by  $\lambda$ )

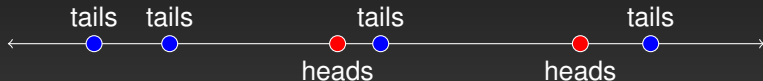


$$A_1, A_2, A_3, \dots \stackrel{\text{iid}}{\sim} \text{Exp}(\lambda)$$

## *Back to mean formulation...*

Suppose for each point flip  $\text{Bern}(p)$

Only keep points that get heads



Expected number in interval  $[a, b]$  is  $\lambda p(b - a)$

New effective rate:  $\lambda p$

Process called *thinning*

## *Estimate: Poisson formulation*

- ▶ Run Poisson process forward in time from 0
- ▶ Each point flip a coin—only keep heads
- ▶ Continue until have  $k$  heads
- ▶ Let  $P_k$  be time of the  $k$ th head
- ▶ Estimate is  $(k - 1)/P_k$



## *Gamma Bernoulli Approximation Scheme*

---

GBAS *Input:*  $k \geq 2$

---

- 1)  $R \leftarrow 0, S \leftarrow 0$
  - 2) Repeat
  - 3)      $X \leftarrow \text{Bern}(p), A \leftarrow \text{Exp}(1)$
  - 4)      $S \leftarrow S + X, R \leftarrow R + A$
  - 5) Until  $S = k$
  - 6)  $\hat{p} \leftarrow (k - 1)/R$
-

## *Gamma distributions*

Because  $P_i - P_{i-1} \sim \text{Exp}(p)$

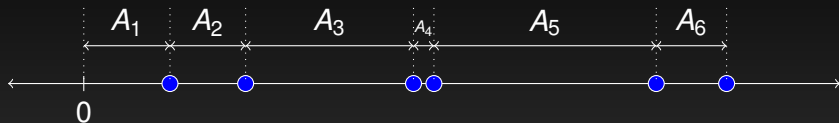
$P_k \sim \text{Gamma}(k, p)$  [sum of  $k$  exponentials]

So  $1/P_k \sim \text{InverseGamma}(k, p)$

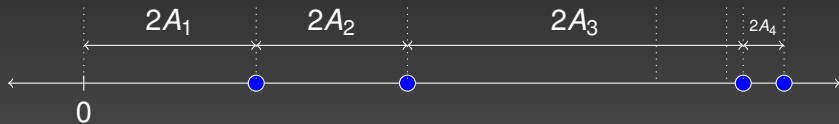
$$\mathbb{E} \left[ \frac{k-1}{P_k} \right] = (k-1) \mathbb{E}[P_k^{-1}] = (k-1) \frac{p}{k-1} = p$$

Estimate is unbiased!

## *Back to exponential formulation...*



Multiply all the  $A_i$  by 2:



New expected number in  $[0, t] =$  old expected in  $[0, t/2]$

So  $\lambda(t - 0)/2 \Rightarrow$  new rate is  $\lambda/2$



## Scaling exponentials

### Fact

If  $X \sim \text{Exp}(\lambda)$ , then  $cX \sim \text{Exp}(\lambda/c)$ .

### Fact

If  $X \sim \text{Gamma}(k, \lambda)$ , then  $X \sim \text{Gamma}(k, \lambda/c)$ .

That means

$$\frac{\hat{p}}{p} = \frac{k-1}{pP_k} = (k-1)A,$$

where  $A \sim \text{InverseGamma}(k, p/p) = \text{InverseGamma}(k, 1)$

## *Relative error independent of $p$*

### *Theorem*

*For  $\hat{p}$  given earlier,*

$$\mathbb{E}[\hat{p}] = p, \quad \frac{\hat{p}}{p} - 1 \sim (k-1)A - 1,$$

*where  $A \sim \text{InverseGamma}(k, 1)$ , making the relative error independent of  $p$ . The expected number of flips used by the estimate is  $k/p$ .*

## Filling in the table

Recall the table we had earlier...

$\epsilon = 0.1, \delta = 0.05$			
$p$	Exact $n$	$\mathbb{E}[T_p]$	$\mathbb{E}[T_p]/n$
1/20	7 219	7 700	1.067
1/100	37 545	38 500	1.025

How I filled in those entries:

$$\min_n \mathbb{P}(|(\text{Bin}(n, 1/20)/n)/(1/20) - 1| > 0.1) < 0.05 = 7219$$

$$\min_k \mathbb{P}(|(k-1)\text{InverseGamma}(k, 1) - 1| > 0.1) < 0.05 = 385,$$

and  $385/p = 385/(1/20) = 7700$ .

Comparison to

## *How many samples should be taken if CLT exact?*

What should the constant be?

For basic estimate  $\hat{p}_n$ :

$$\mathbb{E}[C_i] = p, \quad \text{SD}(C_i) = \sqrt{p(1-p)},$$

by CLT

$$\hat{p}_n = \frac{C_1 + \cdots + C_n}{n} \approx \text{N} \left( p, \frac{p(1-p)}{n} \right)$$

which means

$$\frac{\hat{p}_n}{p} \approx \text{N} \left( 1, \frac{1-p}{np} \right)$$

*So for relative error...*

Subtracting 1

$$\frac{\hat{p}_n}{p} - 1 \approx N\left(0, \frac{1-p}{np}\right)$$

Hence

$$\sqrt{\frac{np}{1-p}} \left(\frac{\hat{p}}{p} - 1\right) \approx N(0, 1)$$

## *Bounding the normal tail*

$Z \sim N(0, 1)$  with density  $\phi(x) = \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)$ ,

$$\left(\frac{1}{a} - \frac{1}{a^3}\right) \phi(a) \leq \mathbb{P}(Z \geq a) \leq \left(\frac{1}{a}\right) \phi(a)$$

## Combining these results

$$\begin{aligned}\mathbb{P}\left(\left|\frac{\hat{p}_n}{p} - 1\right| > \epsilon\right) &= \mathbb{P}\left(\sqrt{\frac{np}{1-p}} \left|\frac{\hat{p}_n}{p} - 1\right| > \epsilon\sqrt{\frac{np}{1-p}}\right) \\ &\approx \mathbb{P}\left(|Z| > \epsilon\sqrt{\frac{np}{1-p}}\right)\end{aligned}$$

Note

$$\phi\left(\sqrt{\frac{np}{1-p}}\epsilon\right) = \frac{1}{\sqrt{2\pi}} \exp(-np\epsilon^2/(1-p))$$



## *The result*

When CLT holds exactly

Let  $C_i \sim N(p, p(1 - p))$ , then

$$n = \left[ \frac{2(1-p)}{p} \epsilon^2 \right] \ln(2/\delta) + \text{lower order terms}$$

New estimate

Let  $C_i \sim \text{Bern}(p)$ , then

$$\mathbb{E}[T] = \left[ \frac{2}{p} \epsilon^2 \right] \ln(2/\delta) + \text{lower order terms}$$

Final thoughts

## *Some current projects*

### **Bernoulli Factory**

Given a  $p$  coin, can you flip a  $2p$  coin?

### **Concentration**

If you only bound standard deviation can you get concentration as if you had a normal random variable?

Current results: Assuming CLT need  $\epsilon^{-2}$ , new method  $64 + \epsilon^{-2}$

### **Partition functions**

How many samples are necessary to estimate the normalizing constant of a Gibbs distribution?

### **Simulation with fixed correlation**

Copulas are not the only method (with Nevena Marić)

# Summary

## Applications

- ▶ Numerical integration
- ▶ Finding exact  $p$  values

## The new estimate

- ▶ Unbiased
- ▶ Easy to build
- ▶ Nearly optimal number of samples (lose factor of  $1 - p$ )
- ▶ Relative error  $(\hat{p}/p) - 1$  independent of  $p$
- ▶ Easy to get exact confidence intervals