Partially Recursive Acceptance Rejection

Mark Huber
Department of Mathematical Sciences
Claremont McKenna College

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Perfect Simulation

Monte Carlo Methods

For $w \geq 0$ over discrete space Ω:

Generate random variable X so that

$$\mathbb{P}(X = i) = \frac{w(i)}{\sum_{j \in \Omega} w(j)}$$

Use random draws of X to approximate

$$\sum_{j \in \Omega} w(j)$$

Monte Carlo Methods Continuous Version

For $f \geq 0$ over $\mathbb{R}^d$:

Generate random variable X so that

$$\mathbb{P}(X \in A) = \frac{\int_A f(x)\, dx}{\int_{\mathbb{R}^d} f(x)\, dx}$$

Use random draws of X to approximate

$$\int_{\mathbb{R}^d} f(x)\, dx$$

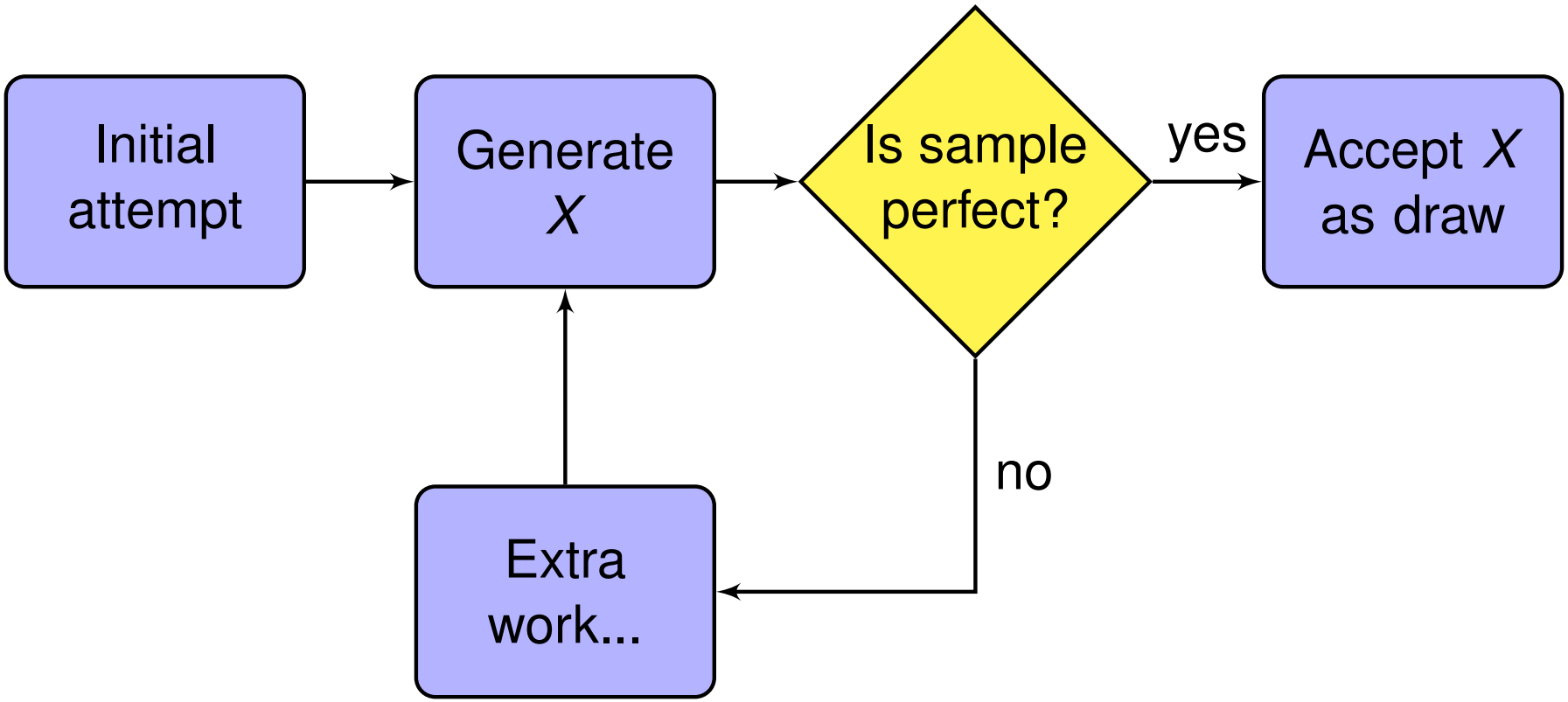
Applications

- Exact p values [Frequentist Statistics]
- Model selection [Bayesian Statistics]
- Phase Transitions [Statistical Physics]
- Approximation Algorithms for #P complete problems [Theoretical Computer Science]

Perfect simulation

Definition (Perfect simulation)

A *perfect simulation* algorithm draws variates exactly from a target distribution in a random number of steps.



Ways to design perfect simulation algorithms

Acceptance/Rejection [Buffon 1777, von Neumann 1933]
Works well for single dimension, not so good in high dimensions

Coupling from the past [Propp, Wilson 1996]
Uses a proxy Markov chain, works well in high dimensions

Popping [Wilson 1996]
Random spanning trees, sink free orientations

Retrospective Sampling [Beskos, Papspilopoulos, Roberts 2006]
Sampling stochastic differential equations perfectly

My work in perfect sampling

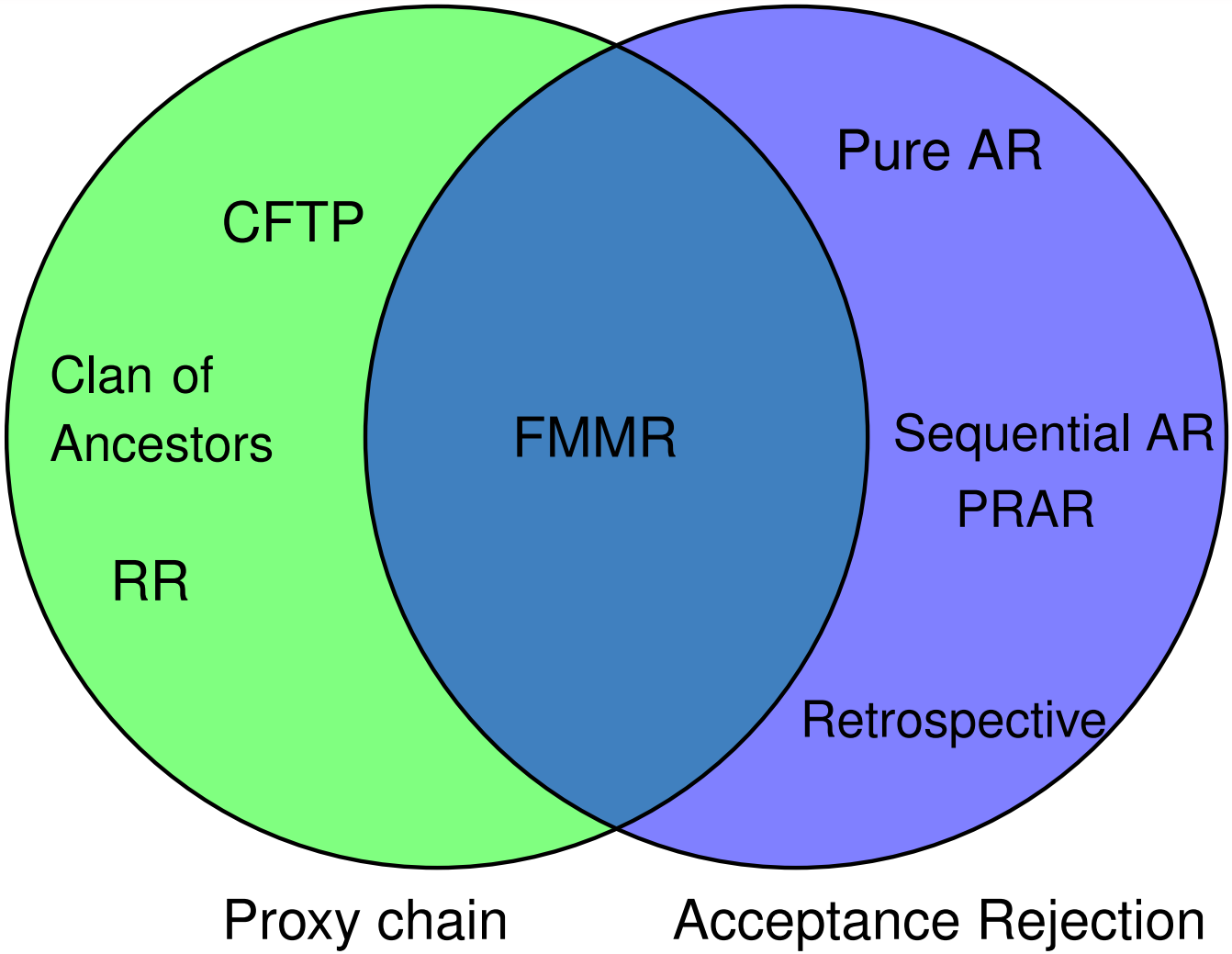
Bounding chains [H. 1999,2004]
Extending CFTP to a wider set of problems

Randomness Recycler [Fill, H. 2000]
Avoiding the need for a proxy Markov chain as in CFTP, FMMR

Scaling Sequential Acceptance Rejection [H. 2004]
Perfect sampling for matchings, permanent

Partially Recursive Acceptance Rejection [H. present]
Pure acceptance rejection for weakly coupled spin systems

Proxy Markov chains and Acceptance/Rejection



Acceptance Rejection

Basic Acceptance/Rejection

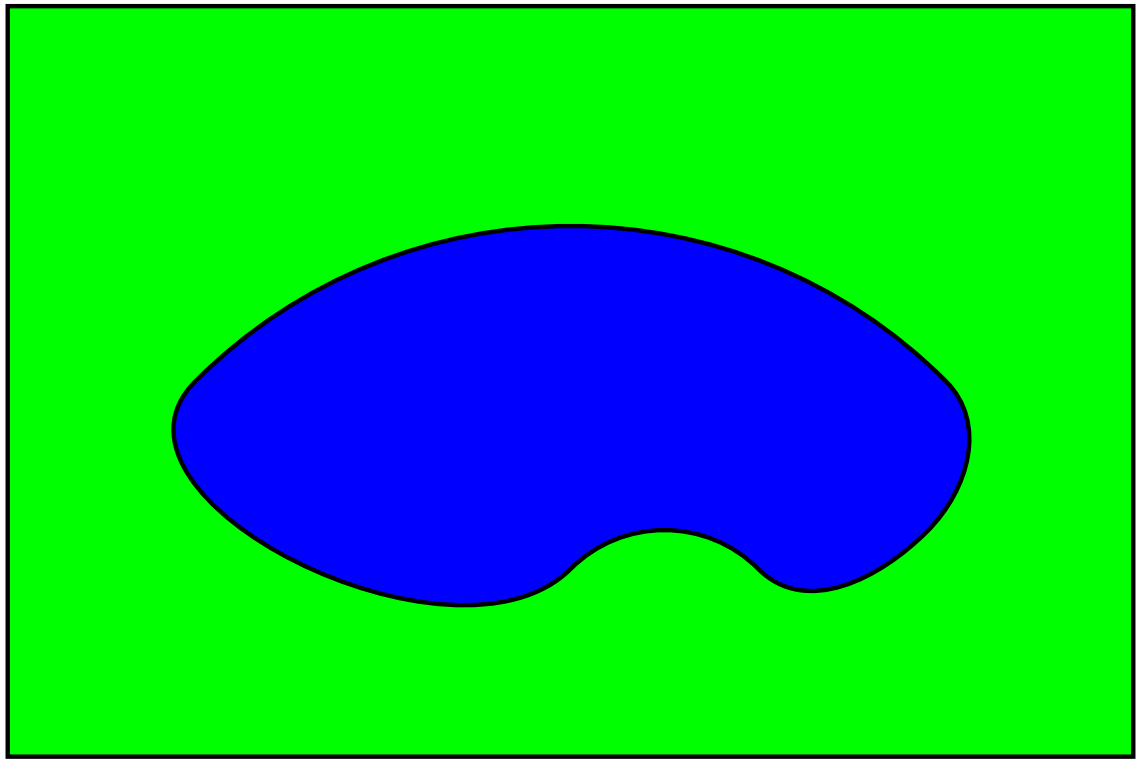
Before running the algorithm

- Goal: Generate X uniformly from B
- Find A that is easier to uniformly sample from where $B \subset A$

Basic acceptance rejection algorithm

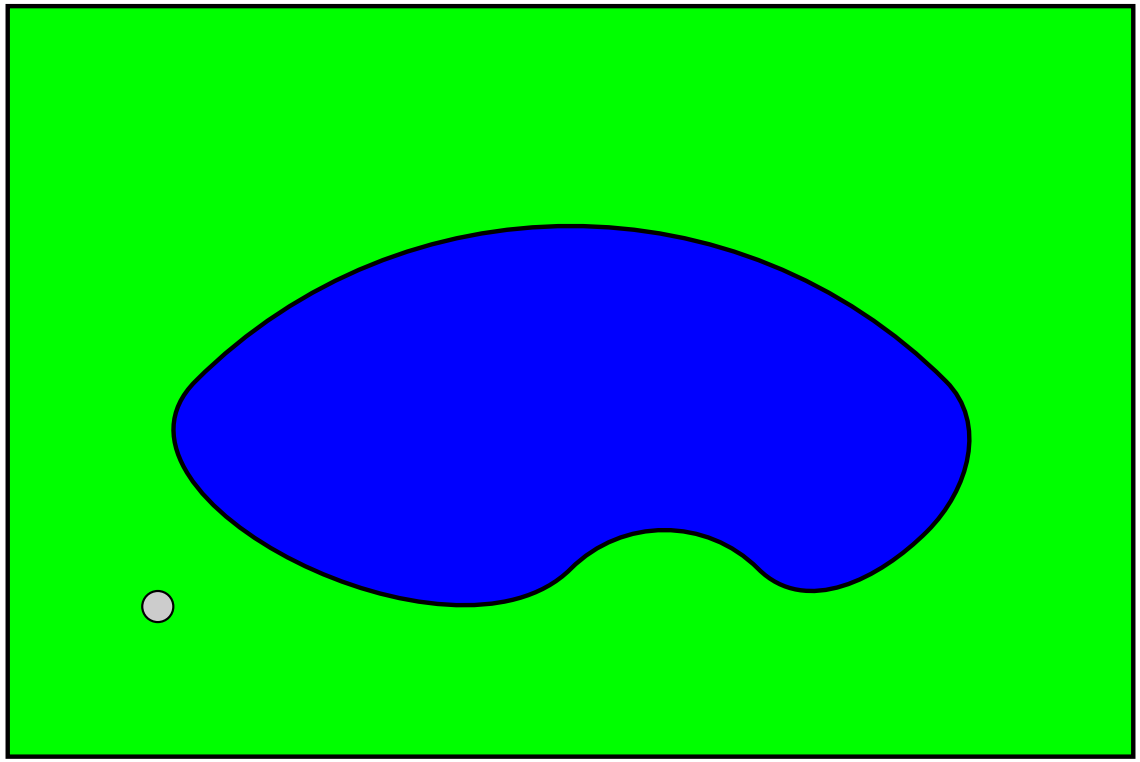
- Step 1: Sample X uniformly from A
- Step 2a: If X is in A output as uniform sample from B
- Step 2b: Else go to Step 1

Acceptance Rejection



Fire uniformly at green region
Until land in blue region

Acceptance Rejection



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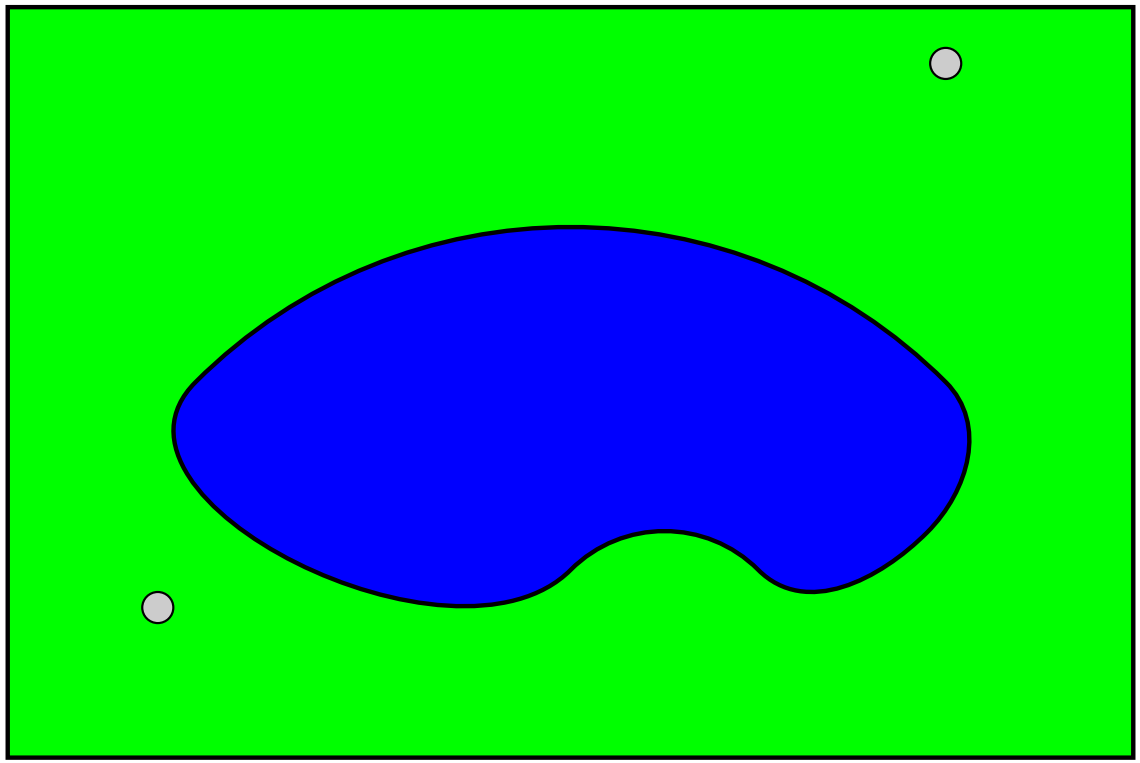
Acceptance Rejection



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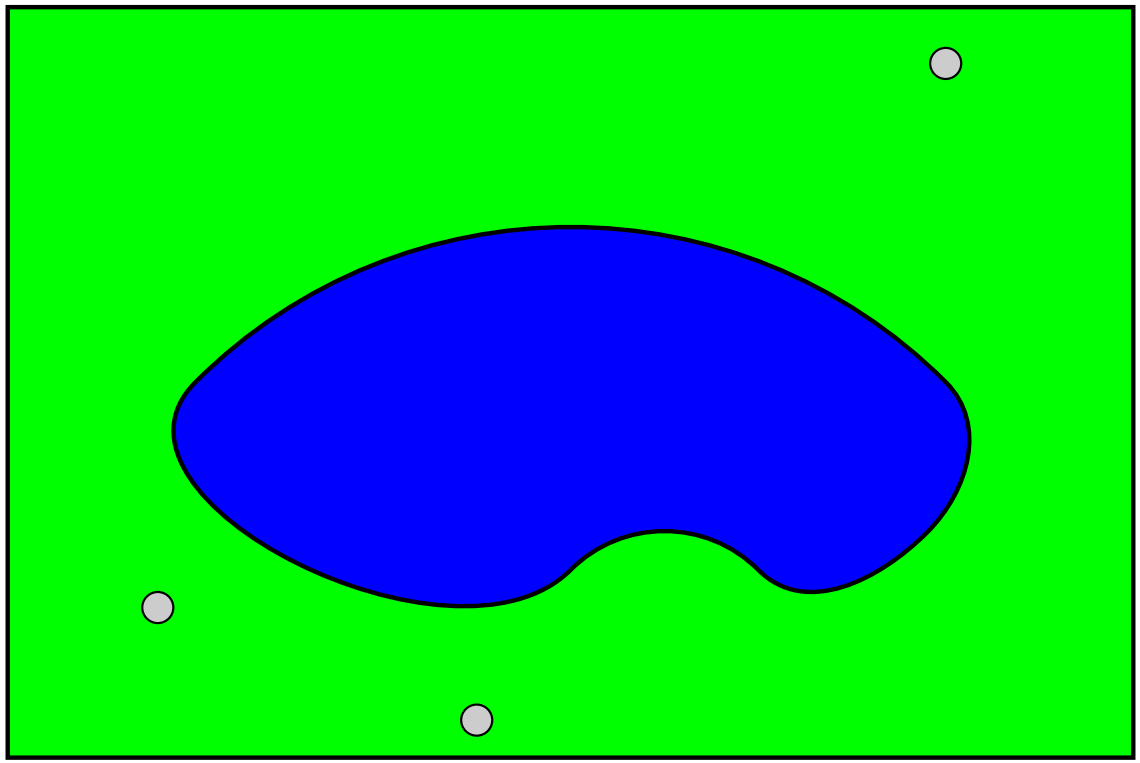
Acceptance Rejection



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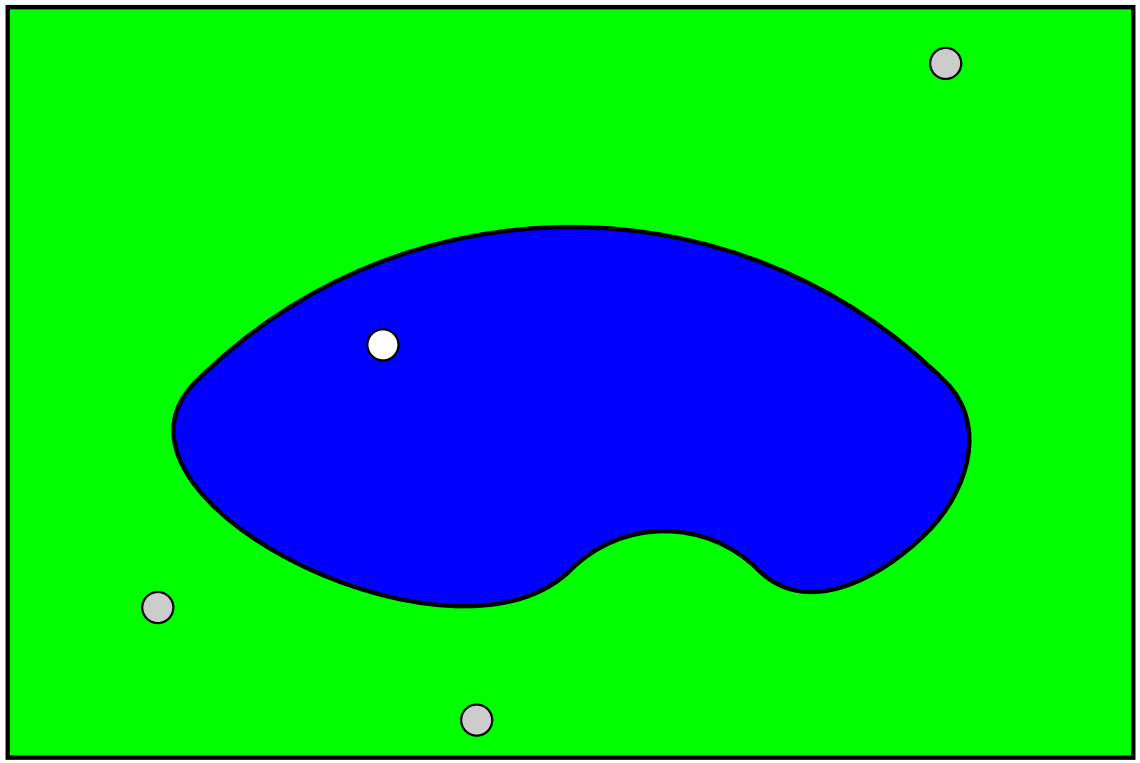
Acceptance Rejection



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A word about uniformity

Fundamental Theorem of Simulation

Can make any problem a uniform one by adding an auxiliary random variable.

Example: to draw a normal random variable

- To draw a standard normal random variable
- Draw (X, Y) uniformly from $\{(x, y) : 0 \leq y \leq (2\pi)^{-1/2} \exp(-x^2/2)\}$
- Keep X

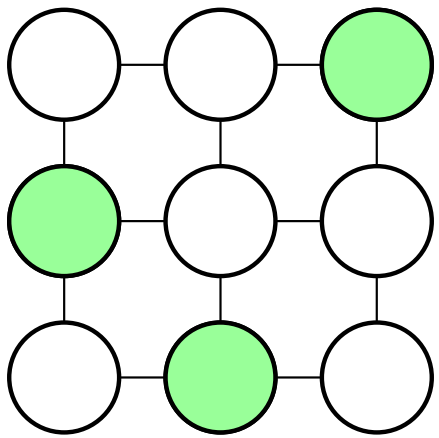
▸ Animation

Coloring nodes with AR

A representative problem

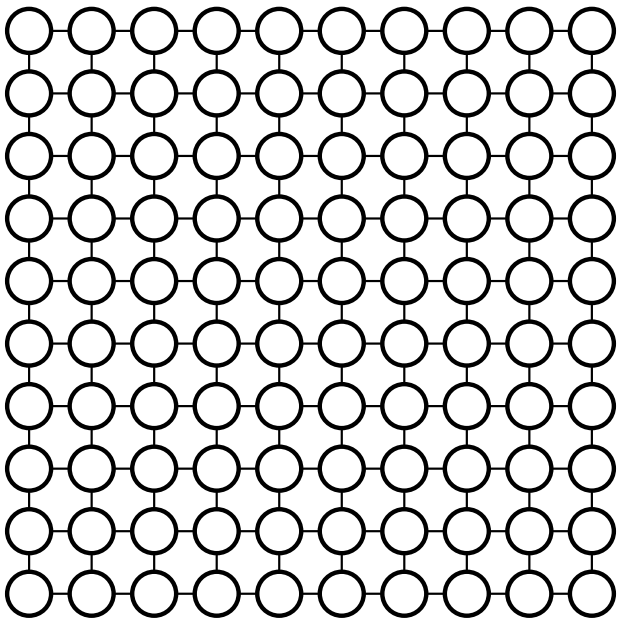
Definition

An *independent set* of a graph is a subset of nodes where no edge has both endpoints in the subset.



Basic AR for independent sets

- Draw X uniformly from subsets of nodes
- If X is not an independent set, go to first step

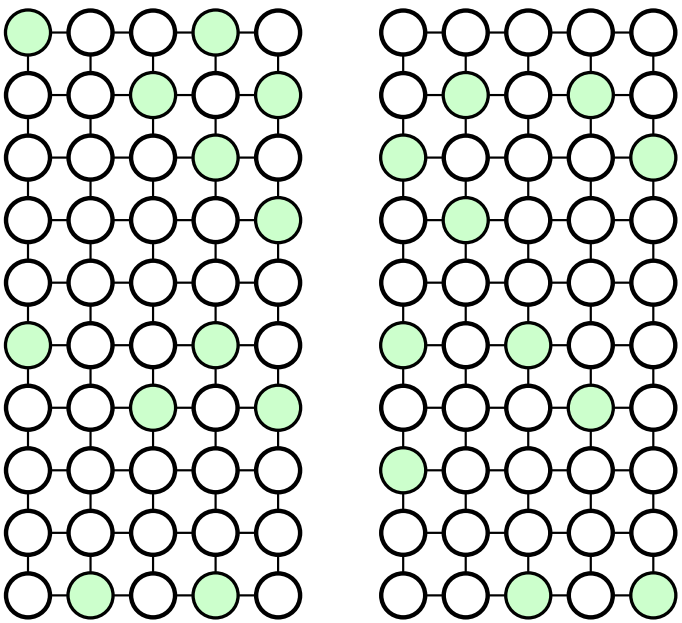


Chance of accepting for 10 by 10 grid $< 10^{-10}$.

Recursive AR on nodes

To sample from π_V over $\Omega = C^V$

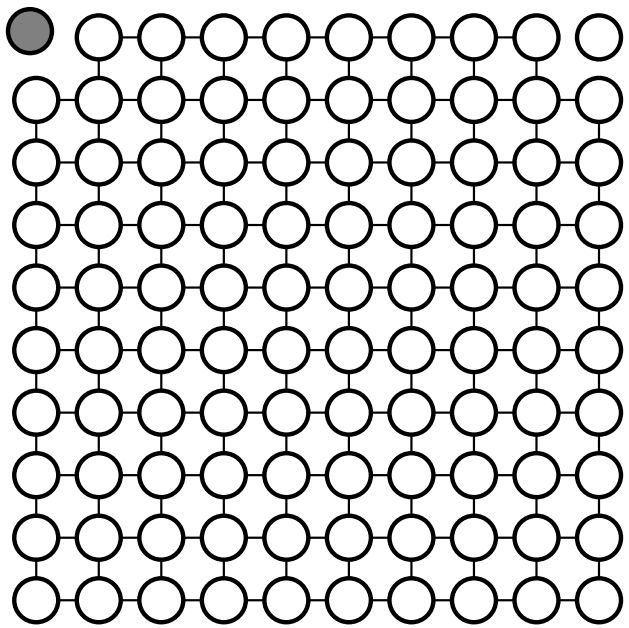
- Partition set of nodes V into V_1 and V_2
- Recursively generate X_1 from π_{V_1} and X_2 from π_{V_2}
- Find probability X_1 with X_2 form configuration on V
- Accept with that probability, otherwise start over



Better idea

Split set of nodes into $\{v\}$ and $V \setminus \{v\}$

- Easy to draw uniformly from independent sets on v
- With probability 1/2 v in set, otherwise it is out



Key observation

Standard recursive AR

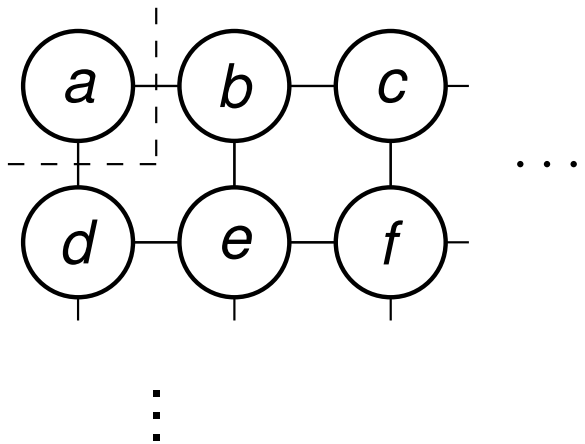
- Draw X_1 on v, X_2 on $V \setminus \{v\}$ first
- If combined form independent set, accept, otherwise reject

Mixing up the order

- Draw X_1 on v first
- If v not in independent set, always accept, don't need X_2!
- If v in ind. set, don't need all of X_2...
- ...only need to know about neighbors of v

One at a time

Build up the sample one node at a time



- First make a in set or out each with probability $1/2$;
- If a out, always accept
- Else find out if b and d are in set, that determines acceptance for a

Examples

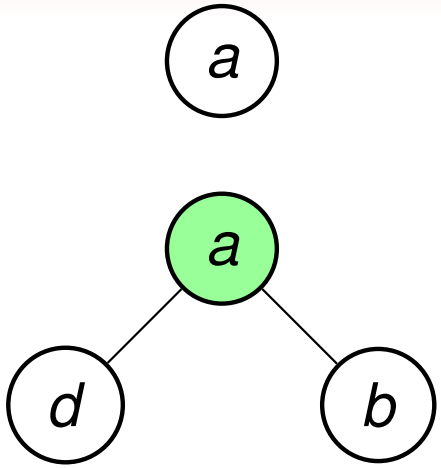
a out
Result: *a* is out of set

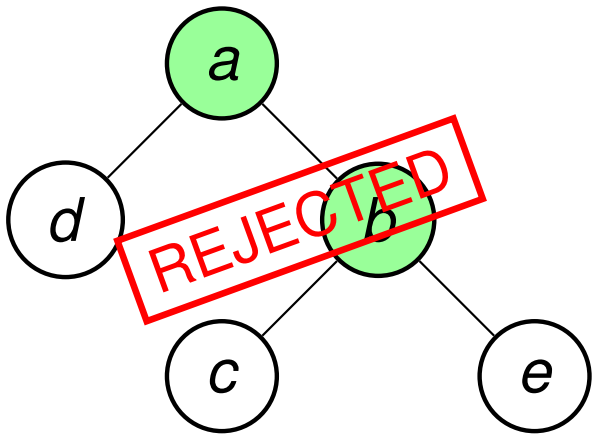
---

a in: put *b* and *d* on queue
b out
d out
Result: *a* is in, *b* is out, *d* is out

---

a in: put *b* and *d* on queue
b in: put *c* and *e* on queue
c out
e out
Result: with *c* and *e* out, *b* is also in, so reject *a* and everything removed, start over with *a*





The algorithm

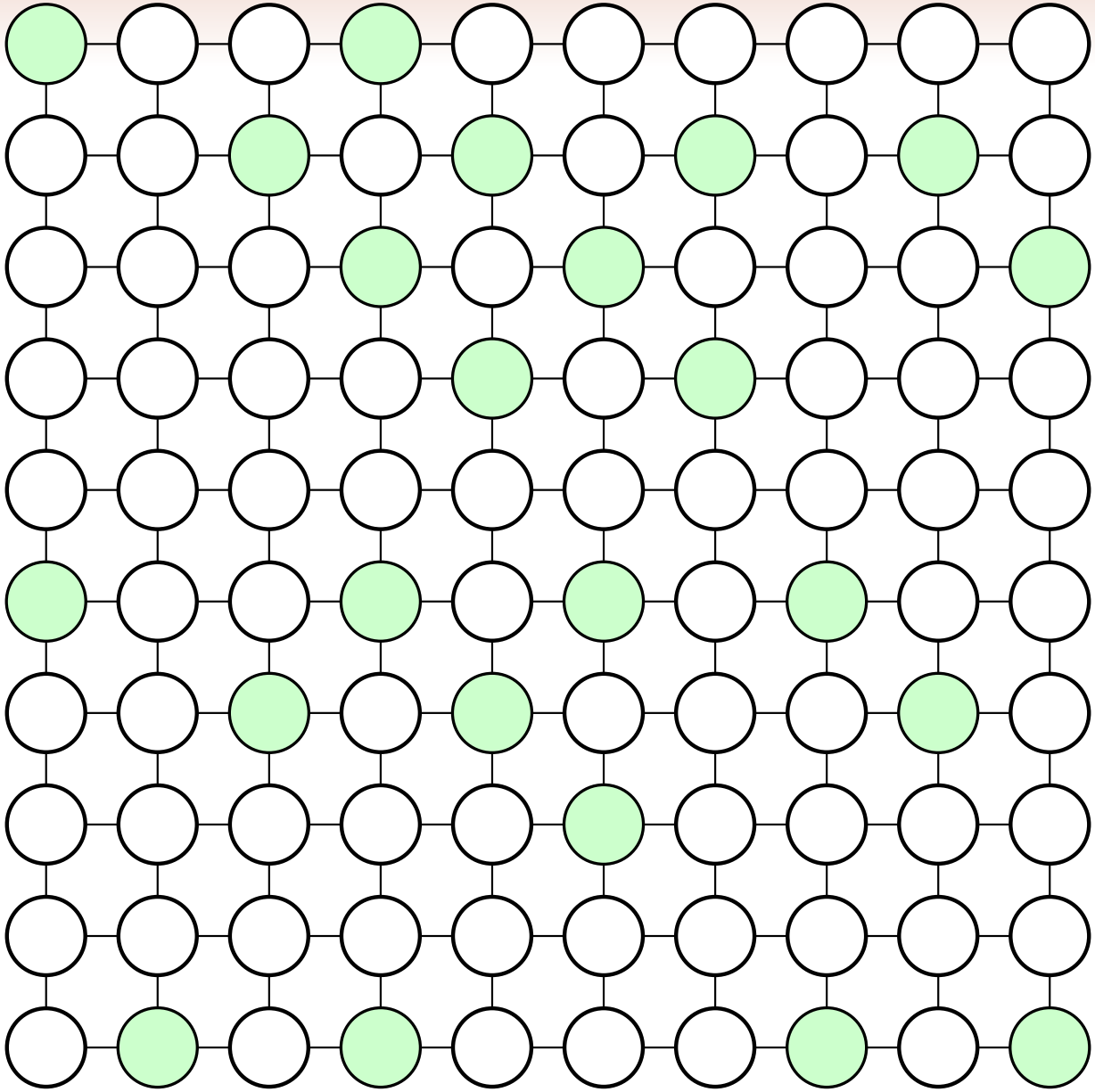
Begin with all nodes in list

- Get a node v off of list
- form its recursion tree
- Fix the values of all nodes in tree
- Continue until list empty

To form recursion tree

- With probability 1/2, node is out
- Otherwise node could be in: add neighbors to tree as children
- If all neighbors/children are out, then node is in...
- ...so reject and remove subtree formed by parent of node

A sample run on 10 by 10 grid



Analysis

Nodes that try to be “in” form node percolation process

- Since node in with probability 1/2, looks like at critical temperature
- But nodes that are “in” remove their siblings...
- ...which leads to subcritical behavior

More generally

- If interactions weak, tree shrinks in size on average
- Artificial phase transition

Method works for Markov random fields

Not just for independent sets...

$$\Omega = C^V, \quad f(x) = \left[\prod_{v \in V} a(x(v))\right] \left[\prod_{\{v,w\} \in E} b(x(v), x(w))\right]$$

This includes

- The Ising model
- Spin glasses
- Strauss model
- Kelly-Ripley interaction models
- Dimensions only interact locally

Strauss process

Like independent set, configuration is subset of nodes

- $x(v) = 1$ means in subset, $x(v) = 0$ means out
- $a(x(v)) = \lambda^{x(v)}$
- $b(x(v), x(w))$ is $\gamma < 1$ if $x(v) = x(w) = 1$
- Strauss density:

$$\lambda^{\#\text{ of occupied nodes}}\gamma^{\#\text{ of edges with both ends occupied}}$$

Using PRAR with Strauss

Changes to PRAR

- Initial value for v is 1 with probability $\lambda/(1+\lambda)$
- If $x(v) = 1$ proposed...
- ...only check neighbor with probability $1 - \gamma$

Running time polynomial

- Let Δ be the maximum degree of the graph
- Expected linear time algorithm if

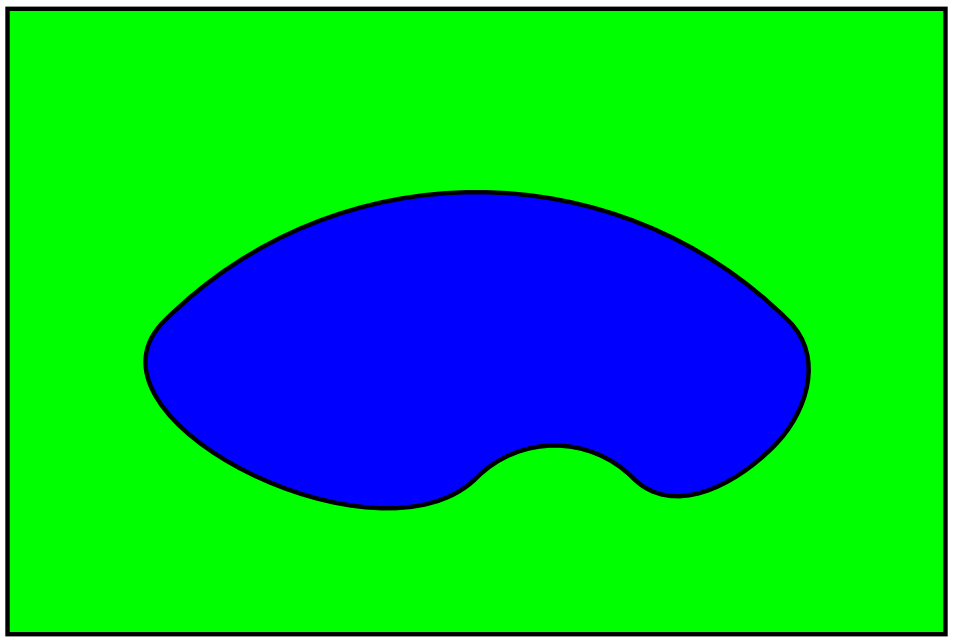
$$\frac{\Delta(1-\gamma)\lambda}{1+\lambda} < 1$$

Sequential Acceptance Rejection

Recursive Acceptance Rejection: Geometric view

Goal: sample from $B \subset A$

- Find disjoint $A_1, \ldots, A_n$ in A that cover B
- Let I be a random variable with $\mathbb{P}(I = i)$ to $\mu(A_i)/\mu(A)$ (otherwise $I = 0$)
- If $I = 0$ start over, else draw X recursively from A_I



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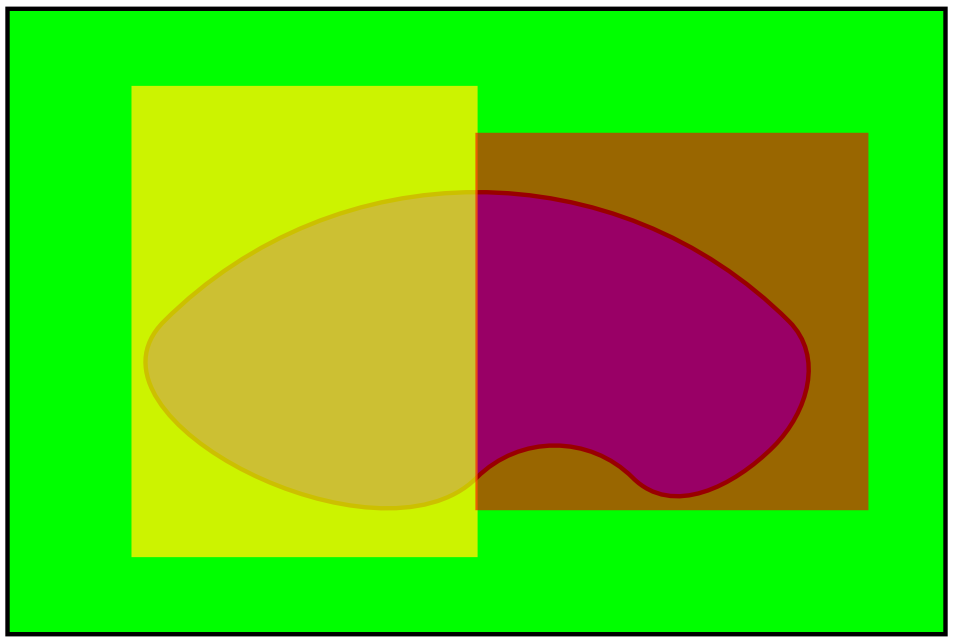


Acceptance Rejection without bounding sets

Do not need the sets A_i!

- Just need the *sizes* of A_i to find $\mathbb{P}(I = i)$
- Partition B into $B_1, \ldots, B_n$
- Enough to have an upper bound on size of B_i

For Sequential Acceptance Rejection

- Need partition $B_1, \ldots, B_n$ of B
- Upper bound function f such that $\mu(B) \leq f(B)$
- f must respect partition: $f(B_1) + f(B_2) + \cdots f(B_n) \leq f(B)$

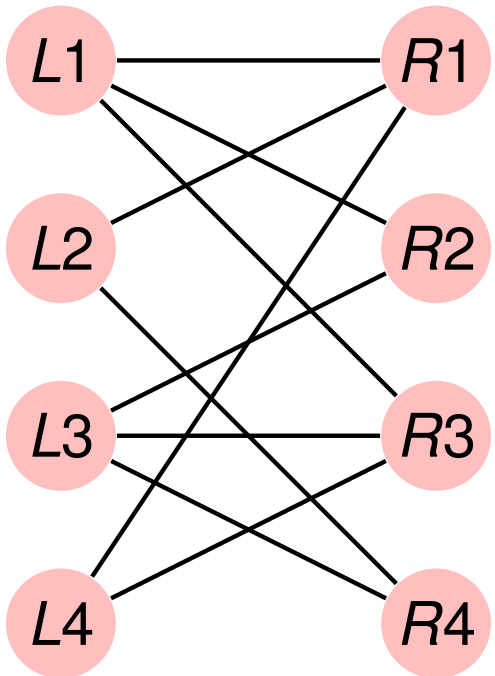
Result

Sequential Acceptance Rejection

- Gives method for class of problems where CFTP/RR/PRAR fail
- CFTP/RR/PRAR work well when Markov chain mixing provable by coupling
- Some Markov chains whose mixing time proved by conductance
- Example: Perfect matchings in graphs

Perfect Matchings

A perfect matching in a graph is a collection of edges such that every node is adjacent to exactly one edge



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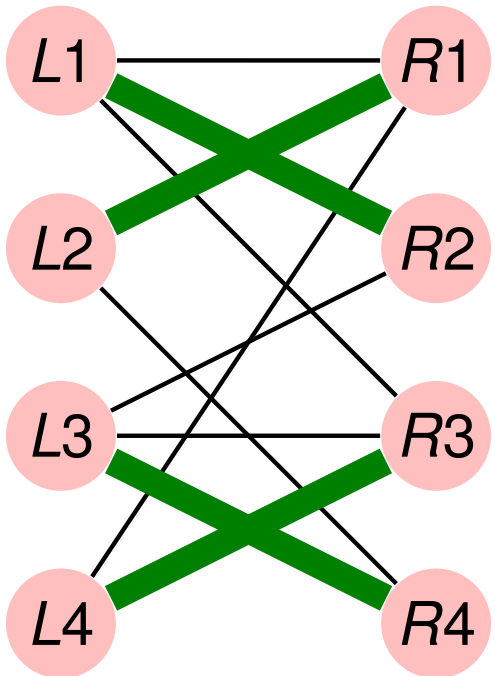
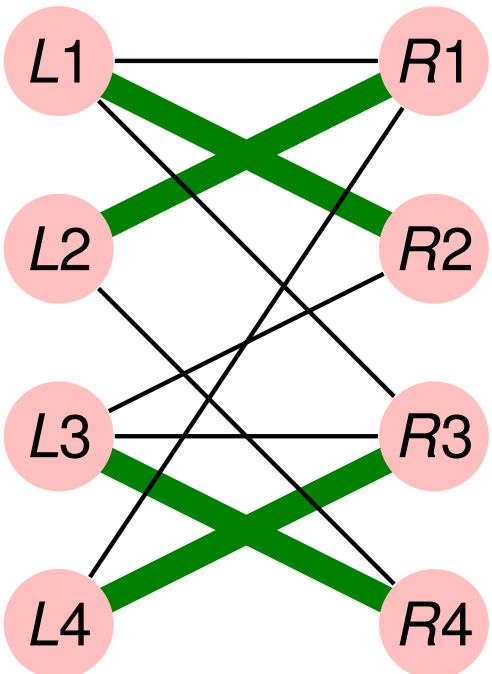


Encodings

More than one way to encode matching...

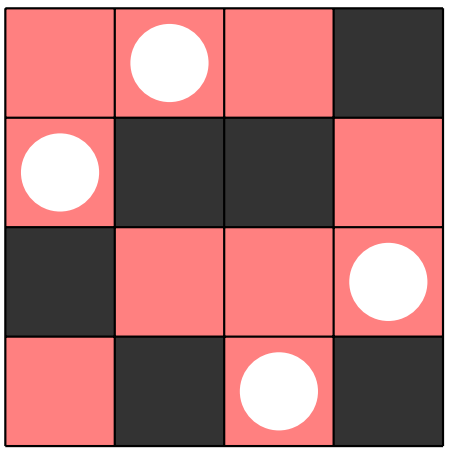
Perfect Matchings



Permutation

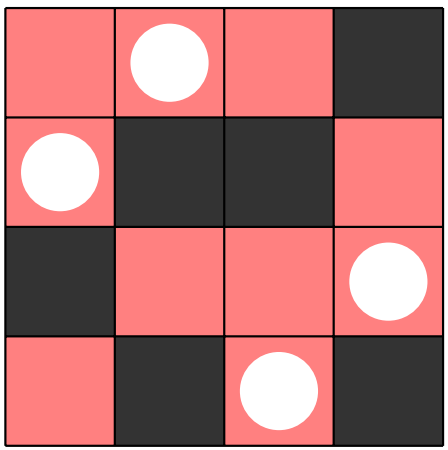
i	$\sigma(i)$
1	2
2	1
3	4
4	3

Rook Placement



More encodings....

Rook Placement



Matrix Encoding

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

Number of valid rook placements = permanent of matrix A

The Permanent

Definition (Permanent)

The permanent of a matrix $A = (A(i,j))_{i,j=1}^{n}$ is

$$\text{per}(A) = \sum_{\sigma \in S_n} \prod_{i=1}^{n} A(i, \sigma(i))$$

Similar in form to determinant, but much harder to compute!

Applications

The permanent of nonnegative matrix arises in...

- Nonparametric statistics (permutation statistical models)
- Contingency tables
- Graphs with given degree sequence
- One of first #P-complete problems

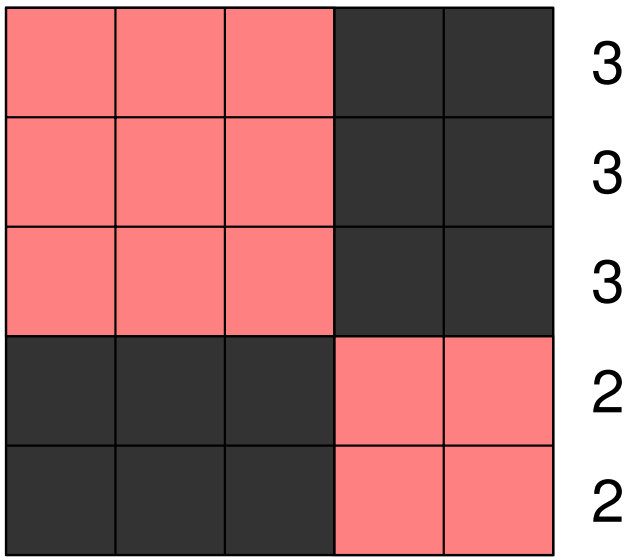
Goal

Basic Problem

- Count number of perfect matchings/restricted permutations/rook placements
- #P-complete problem, best can do is approximation
- Jerrum-Sinclair-Vigoda used Markov chain approach
- Even with improvements, still an $O(n^{10}(\log n)^4)$ algorithm
- With sequential AR get $O(n^4 \log n)$ but only for dense problems

To use SAR, need upper bounds on permanent

Consider the following example:



$$\text{per}(A) = 3!2!$$

Minc's Conjecture (1963)

For matrix A with fixed row sums $r(i)$ for i from one to n, this block structure maximizes the permanent

Of course, not all matrices in blocks

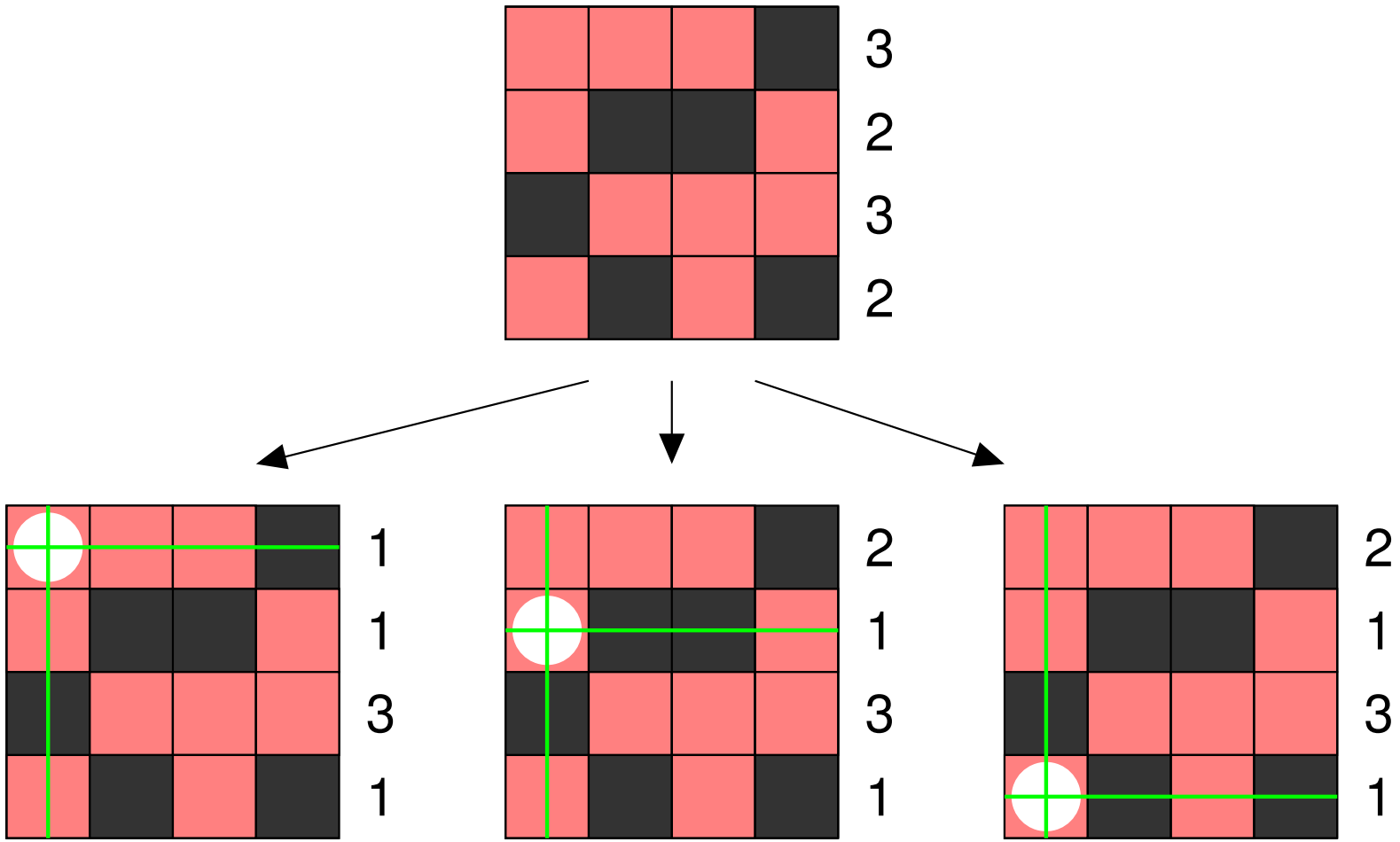
Bregman's Inequality (1973)

For matrices whose entries are 0 or 1:

$$\text{per}(A) \leq \prod_{i=1}^{n} [r(i)!]^{1/r(i)},$$

where $r(i)$ is the sum of row i of matrix A.

Problem: cannot prove via induction on minors



To work for upper bound...

Need

$$\text{bound}\begin{pmatrix}3\\2\\3\\2\end{pmatrix} \geq \text{bound}\begin{pmatrix}1\\1\\3\\1\end{pmatrix} + \text{bound}\begin{pmatrix}2\\1\\3\\1\end{pmatrix} + \text{bound}\begin{pmatrix}2\\1\\3\\1\end{pmatrix}$$

but for Minc/Bregman:

$$6.6038... \leq 1.81... + 2.57... + 2.57...$$

Understanding Minc's conjecture

Upper bound is:

$$f(r) = \prod_i g(r(i)), \text{ where } g(r) = (r!)^{1/r}$$

Use Stirling's inequality to understand $g(r)$:

$$g(r) \approx \frac{1}{e}\left[r + \frac{1}{2}\ln(r) + \frac{1}{2}\ln(2\pi)\right]$$

New upper bound

Theorem

For a matrix A with entries either 0 or 1 and row sums $r(i)$:

$$\mathrm{per}(A) \leq \prod_{i=1}^{n} h(r(i)),$$

where

$$h(r) = \frac{1}{e}\left[r + \frac{1}{2}\ln r + e - 1\right]$$

Moreover, this bound can be proved by induction on minors.

Example from earlier

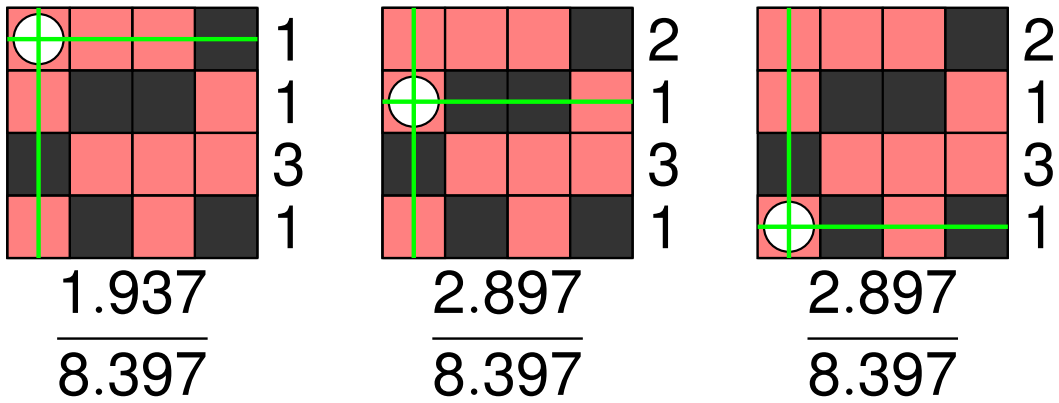
Need

$$\text{bound}\begin{pmatrix}3\\2\\3\\2\end{pmatrix} \geq \text{bound}\begin{pmatrix}1\\1\\3\\1\end{pmatrix} + \text{bound}\begin{pmatrix}2\\1\\3\\1\end{pmatrix} + \text{bound}\begin{pmatrix}2\\1\\3\\1\end{pmatrix}$$

and for new bound:

$$8.397... \geq 1.937... + 2.897... + 2.897 = 7.733...$$

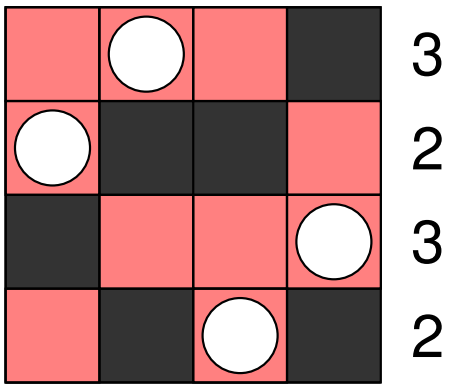
Sampling algorithm



Procedure

- Choose rook placement for first column...
- ...with probability bound of minor over original bound
- By Theorem, these ratios add to less than one
- If no placement chosen, reject and start over
- Otherwise continue until all rooks placed

Why does this work?



Probability of making this choice:

$$\frac{h(2,1,3,1)}{h(3,2,3,2)} \cdot \frac{h(1,1,2,1)}{h(2,1,3,1)} \cdot \frac{h(1,1,1,1)}{h(1,1,2,1)} \cdot \frac{h(1,1,1,1)}{h(1,1,1,1)} = \frac{1}{h(3,2,3,2)}$$

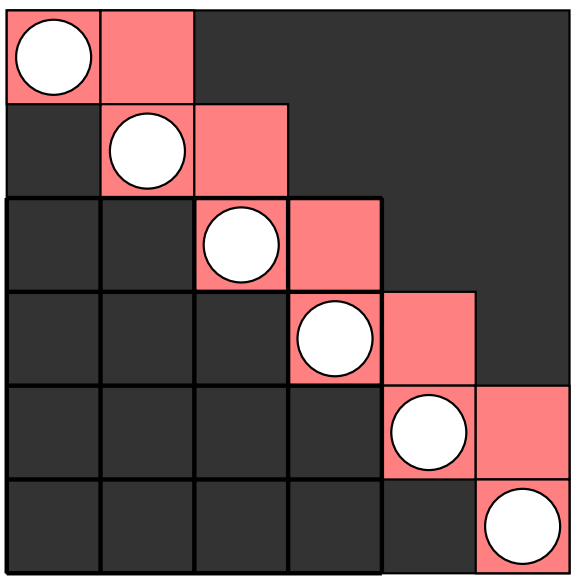
where $(3,2,3,2)$ are original row sums

How long does in take to run?

Average number of steps:

$$\frac{\text{bound}(\text{per}(A))}{\text{per}(A)}$$

Can be exponential in n
Example: A diagonal plus superdiagonal:



$$\text{per}(A) = 1$$

$$\text{bound}(\text{per}(A)) = (1.495\ldots)^{n-1}$$

Speeding things up

Upper and lower bounds

Regular graphs

- Minc: permanent large when 1's are clumped
- Van der Waerden: permanent small when entries spread out as much as possible

Lower bounding the permanent

Regular graphs

- Regular graphs have all degrees of all nodes are same
- Matrices all row and column sums are same, say r
- Van der Waerden lower bound for regular matrices

$$\operatorname{per}(A) \geq \operatorname{per} \begin{pmatrix} r/n & r/n & \cdots & r/n \\ r/n & r/n & \cdots & r/n \\ \vdots & \vdots & \cdots & \vdots \\ r/n & r/n & \cdots & r/n \end{pmatrix} = r^n \frac{n!}{n^n}$$

- Proved indep. by Egorychev (1981), Falikman (1981)

Use Stirling as before

For regular problems:

$$\sqrt{2\pi n}\left(\frac{r}{e}\right)^n \leq \text{per}(A) \leq \left(\frac{r+(1/2)\ln r + e - 1}{e}\right)^n$$

Looking at ratio of upper to lower bound:

$$\frac{\text{upper}}{\text{lower}} = \frac{1}{\sqrt{2\pi n}}\left(1 + \frac{1}{2r}\ln r + e - 1\right)^n \approx \frac{1}{\sqrt{2\pi n}} r^{n/2r}(e-1)^{n/r}$$

So if problem is dense:

$$r \geq \gamma n, \quad \gamma \in [0,1]$$

then runtime polynomial

Achieving regularity

Sinkhorn step

1. Divide each row by its row sum
2. Divide each column by its column sum

Repeat until nearly regular

- Row and col sums in $[1 - n^{-2}, 1 + n^{-2}]$ in $O(n^{4.5})$ steps
- Can be done in $O(n^4)$ using ellipsoid method

Sinkhorn in action

$$
\begin{array}{cccc|c}
1 & 1 & 1 & 0 & 3 \\
1 & 0 & 0 & 1 & 2 \\
0 & 1 & 1 & 1 & 3 \\
1 & 0 & 1 & 0 & 2 \\
\hline
3 & 2 & 3 & 2 &
\end{array}
\quad \rightarrow \quad
\begin{array}{cccc|c}
1/3 & 1/3 & 1/3 & 0 & 1 \\
1/2 & 0 & 0 & 1/2 & 1 \\
0 & 1/3 & 1/3 & 1/3 & 1 \\
1/2 & 0 & 1/2 & 0 & 1 \\
\hline
4/3 & 2/3 & 7/6 & 3/6 &
\end{array}
$$

$$
\rightarrow \quad
\begin{array}{cccc|c}
1/4 & 1/2 & 2/7 & 0 & 29/28 \\
3/8 & 0 & 0 & 3/5 & 39/40 \\
0 & 1/2 & 2/7 & 2/5 & 73/70 \\
3/8 & 0 & 3/4 & 0 & 45/56 \\
\hline
1 & 1 & 1 & 1 &
\end{array}
$$

After many Sinkhorn steps

.2069	.5450	.2479	0	≈ 1
.3381	0	0	.6618	≈ 1
0	.4549	.2069	.3381	≈ 1
.4549	0	.5450	0	≈ 1
1	1	1	1	

This has permanent about .1359

Making rows as large as possible

Last scaling of rows

- Want row sums as large as possible
- Divide each row through by its maximum entry
- All entries still in $[0, 1]$

.3797	1	.4549	0	1.8346
.5108	0	0	1	1.5108
0	1	.4549	.7432	2.1982
.8346	0	1	0	1.8346

The Theorem/Method

Theorem

For a matrix A with entries in $[0,1]$ *and row sums* $r(i)$*:*

$$\text{per}(A) \leq \prod_{i=1}^{n} h(r(i)),$$

where

$$h(r) = \begin{cases} e^{-1}[r + \frac{1}{2}\ln r + e - 1] & r > 1 \\ e^{-1}[1 + (e-1)r] & r \leq 1 \end{cases}$$

Moreover, this bound can be proved by induction on minors.

Summary: Speeding things up

What to do

- Regularize matrix using Sinkhorn steps or ellipsoid method
- Van der Waerden's inequality lower bounds permanent

Theorem (H.,Law 2008)

If original row sums at least γn *for* $\gamma \in (.5, 1]$*, then*

$$\frac{\text{bound}(\text{per}(A))}{\text{per}(A)} \leq n^{-.5+.5/(2\gamma-1)}.$$

Conclusions

Perfect simulation

- Many different protocols now exist for designing algorithms
- Partial Recursive Acceptance Rejection fast on graphs
- Sequential Acceptance Rejection fast for scalable problems

Open questions

- Is PRAR faster or slower than CFTP for, say, Ising?
- Can the permanent be reduced to dense problem?

References

M. Jerrum, L. Valiant, and V. Vazirani.
Random generation of combinatorial structures from a uniform distribution
Theoret. Comput. Sci., **43**, 169–188, 1986

M. Huber.
Exact Sampling from perfect matchings from dense regular bipartite graphs
Algorithmica, **44**, 183–193, 2006

M. Huber and J. Law.
Fast approximation of the permanent for very dense problems
Proc. of Syposium on Discrete Algorithms, 681–689, 2008

Standard normal random variables

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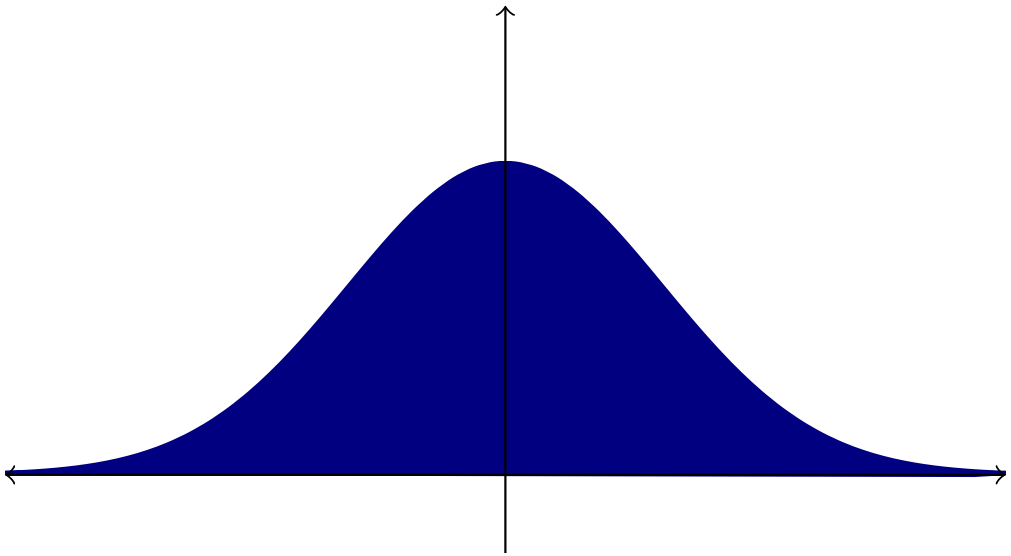

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Finish

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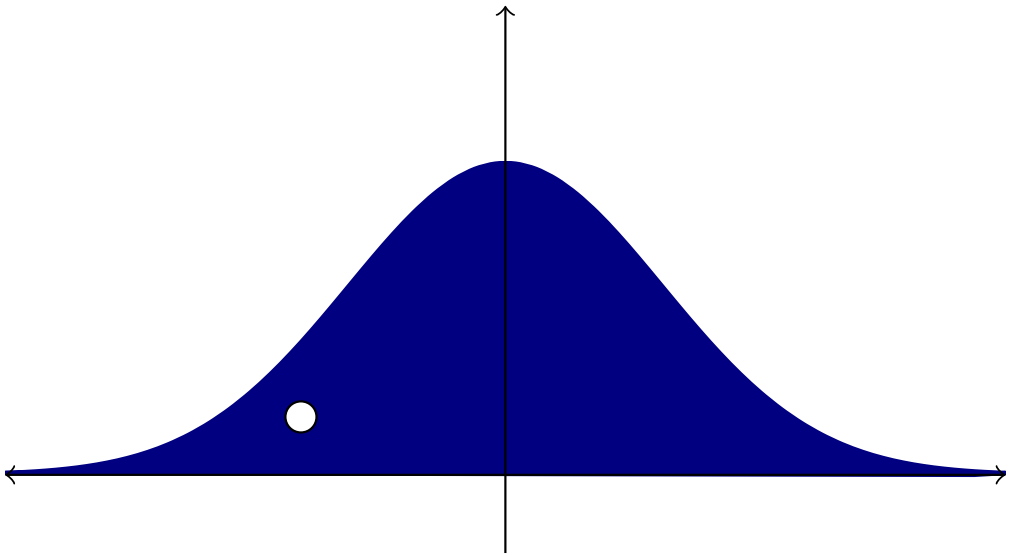

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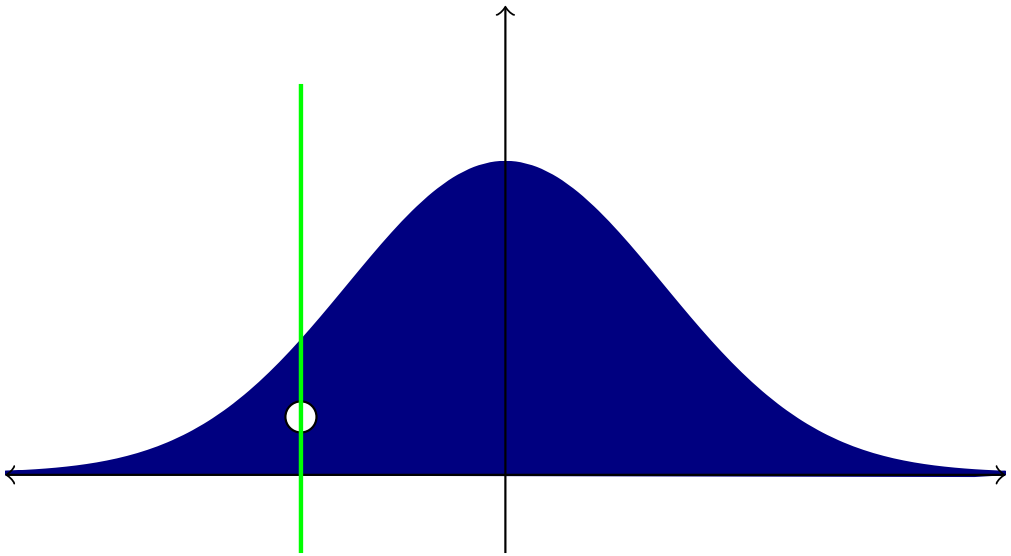

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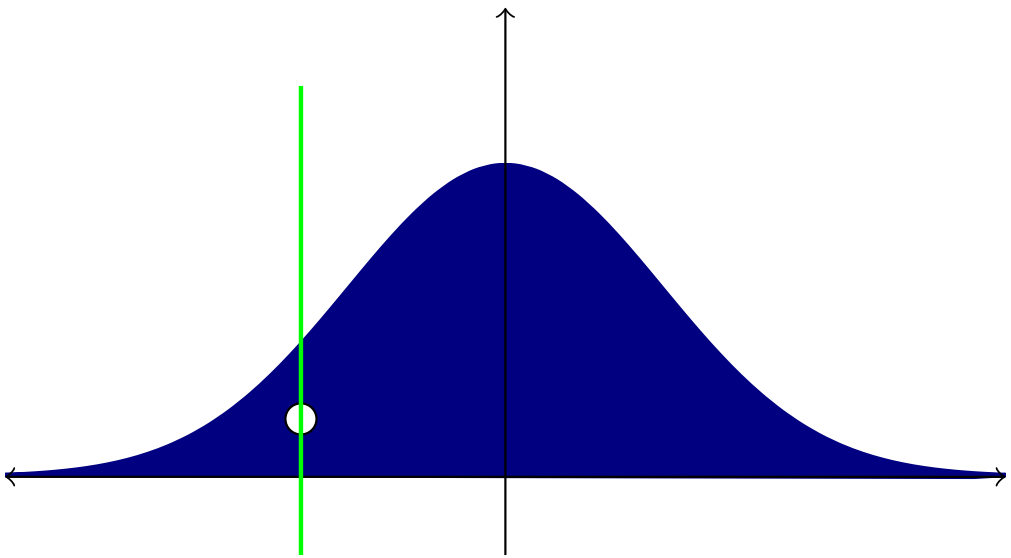

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▸ Restart

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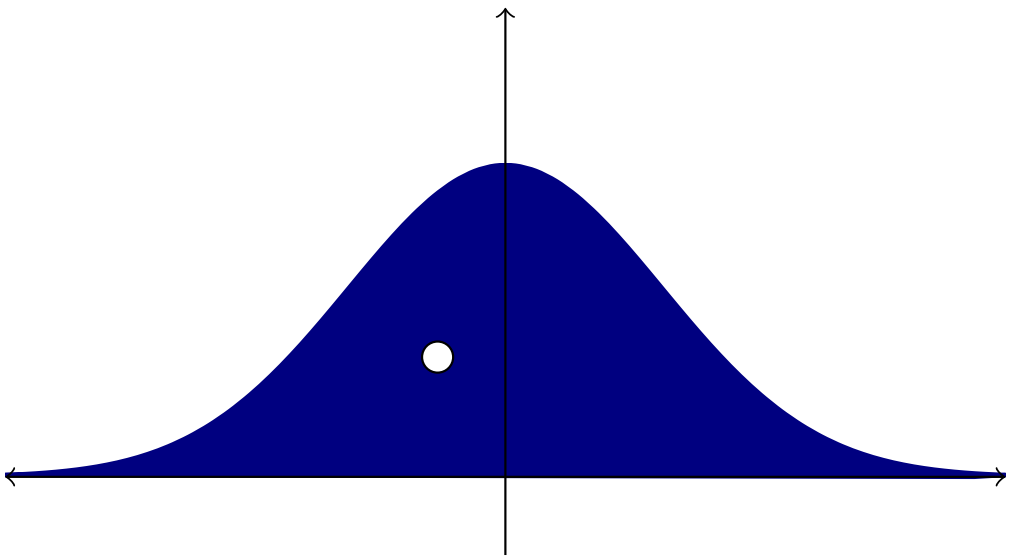

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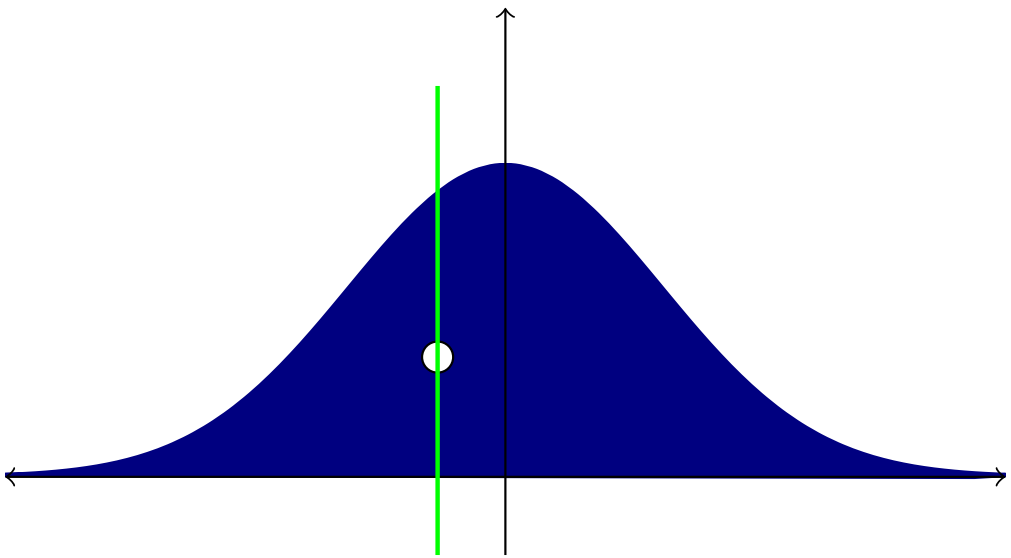

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▸ Restart

▸ Finish

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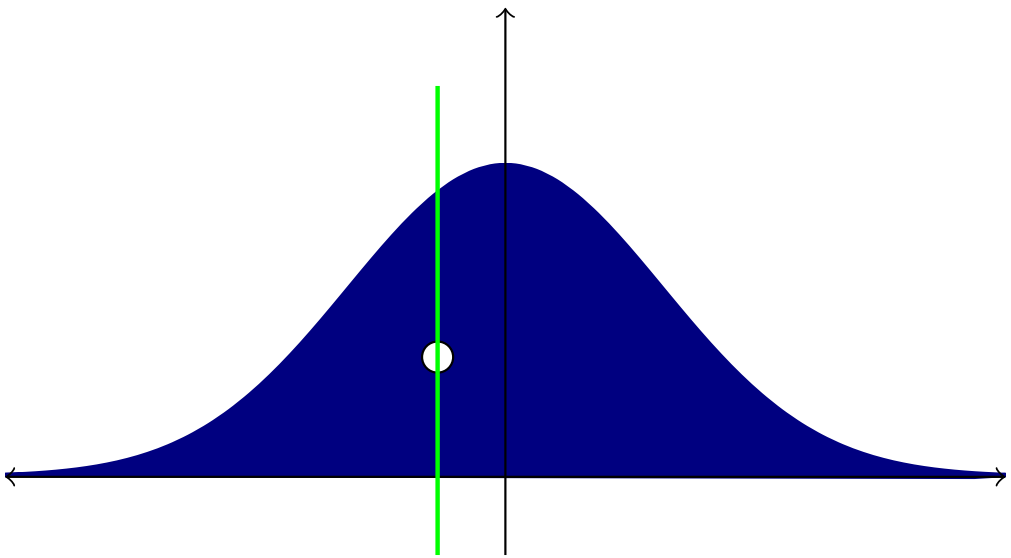

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-1.3077
-0.4336

▸ Restart

▸ Finish

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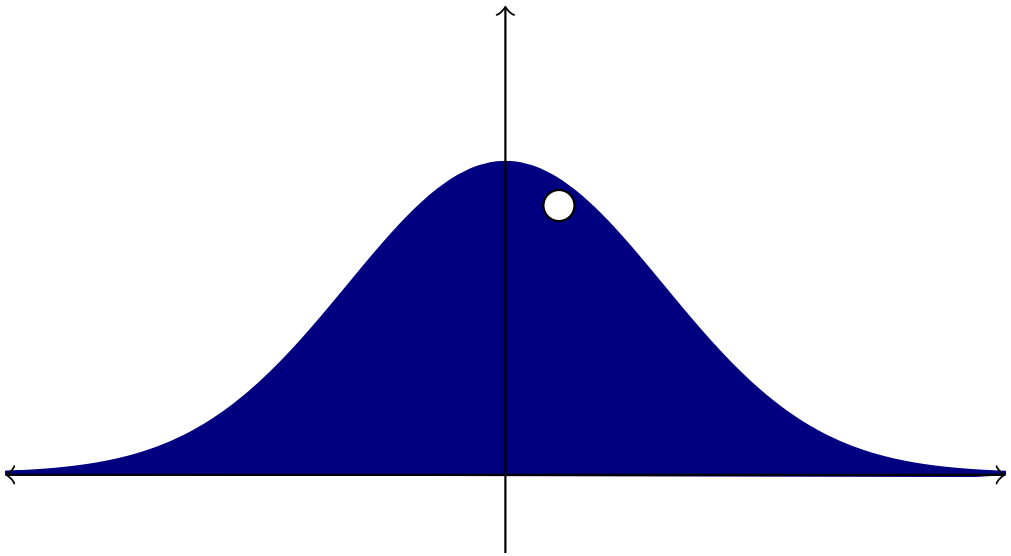

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▸ Restart

▸ Finish

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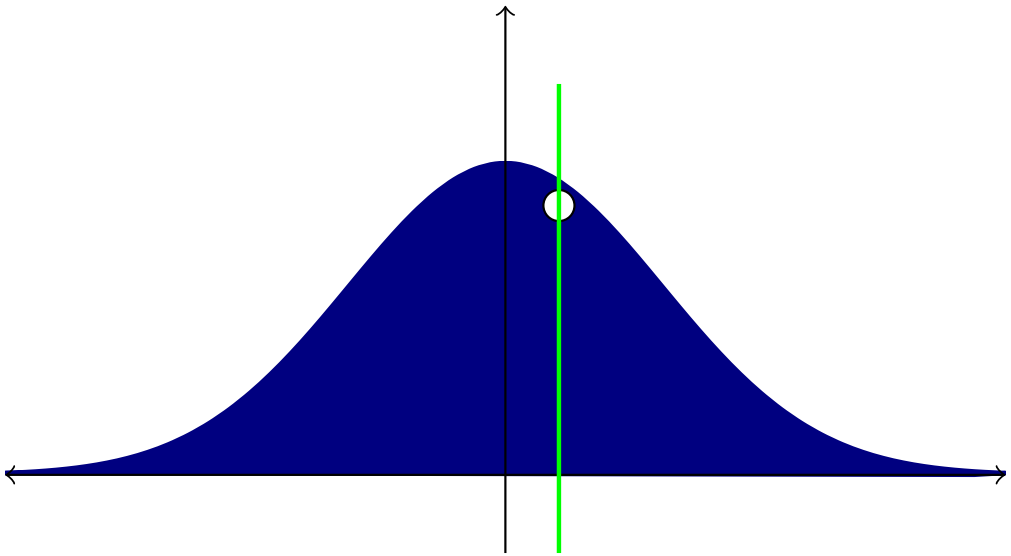

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-0.4336

▸ Restart

▸ Finish

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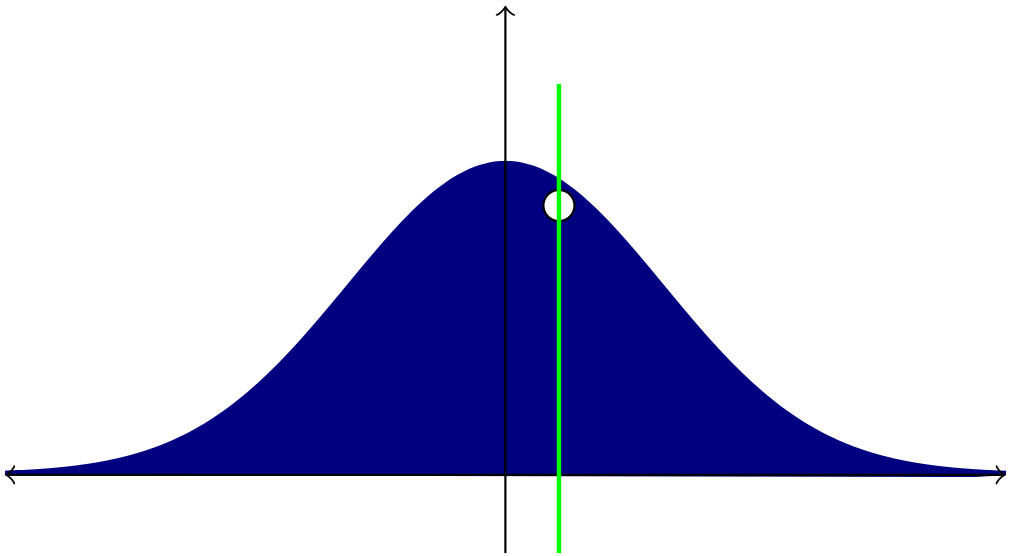

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0.3426

▸ Restart

▸ Finish

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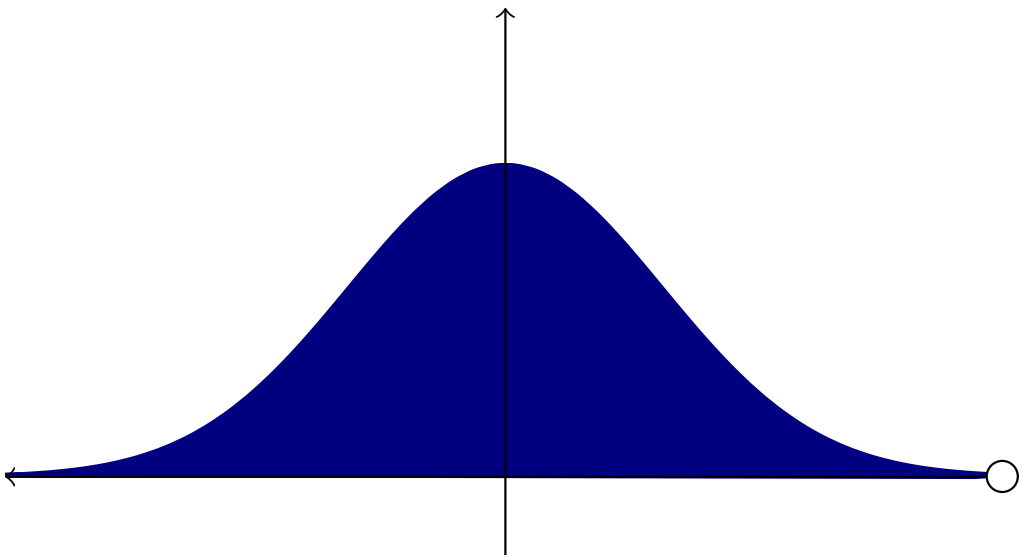

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0.3426

▸ Restart

▸ Finish

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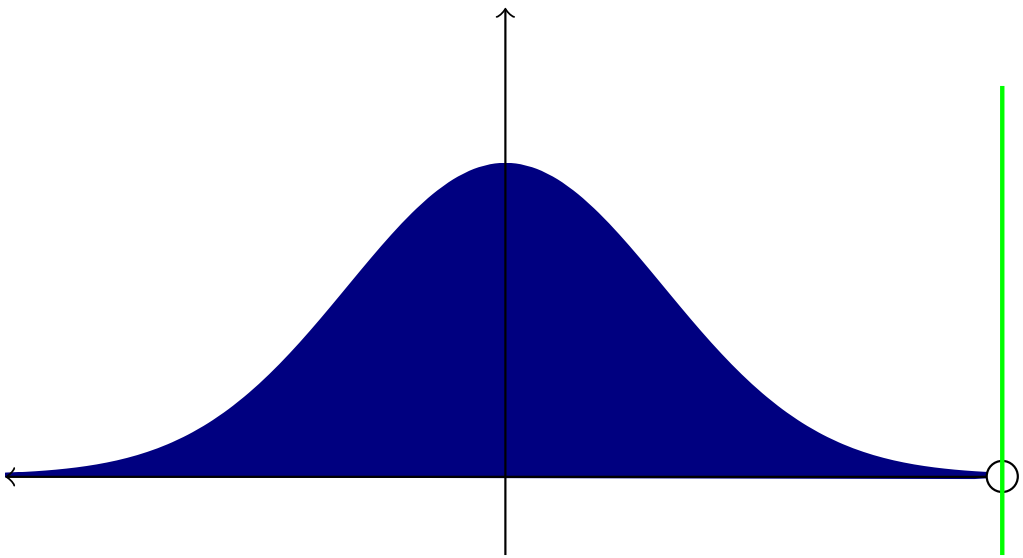

X
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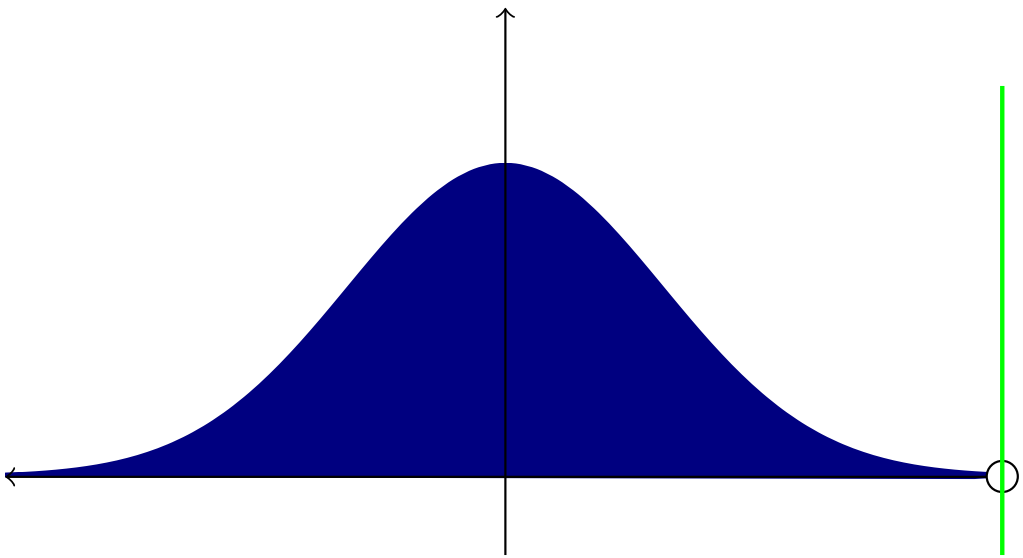
0.3426

▸ Restart

▸ Finish

Standard normal random variables



X
-1.3077
-0.4336
0.3426
3.1784

▸ Restart

▸ Finish

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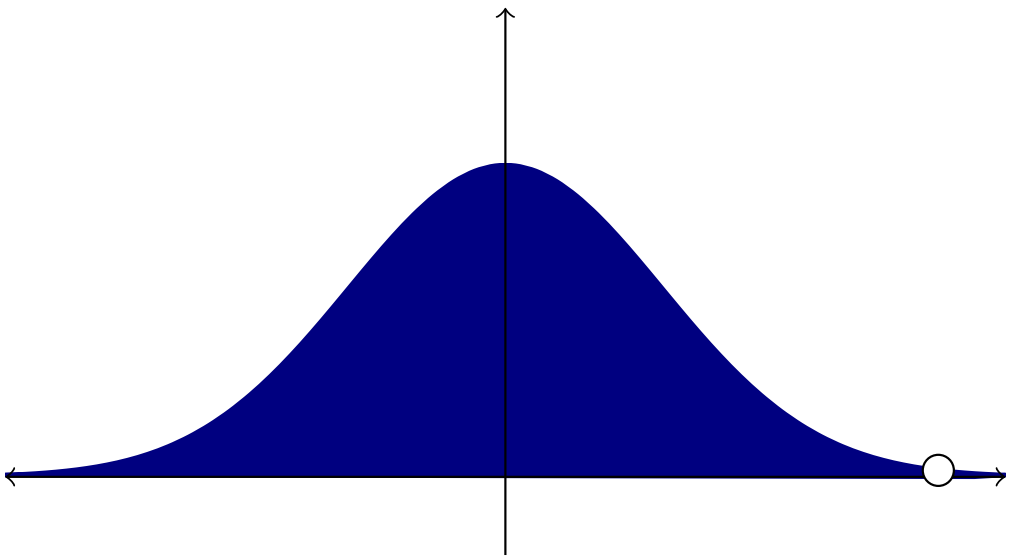

X
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-0.4336
0.3426
3.1784

▸ Restart

▸ Finish

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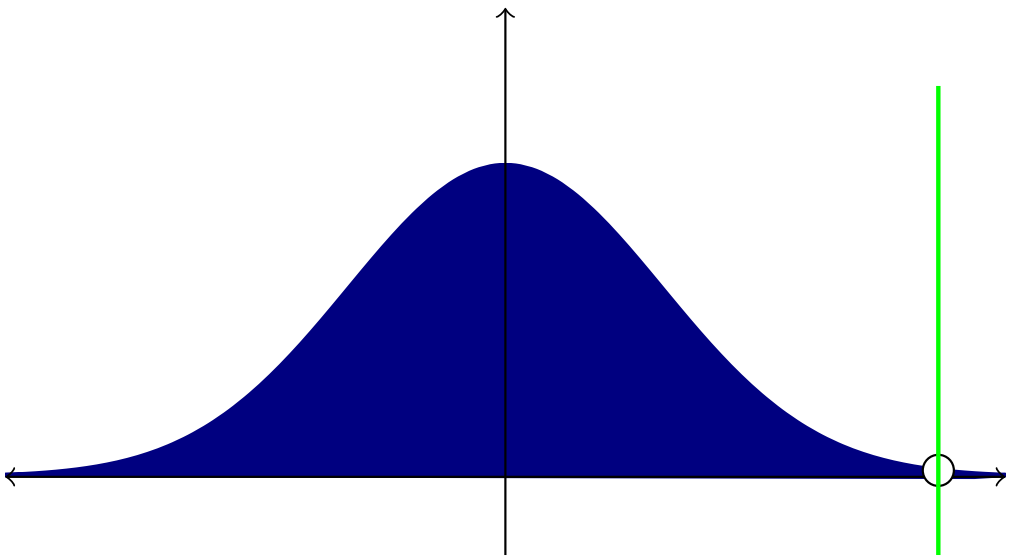

X
-1.3077
-0.4336
0.3426
3.1784

▸ Restart

▸ Finish

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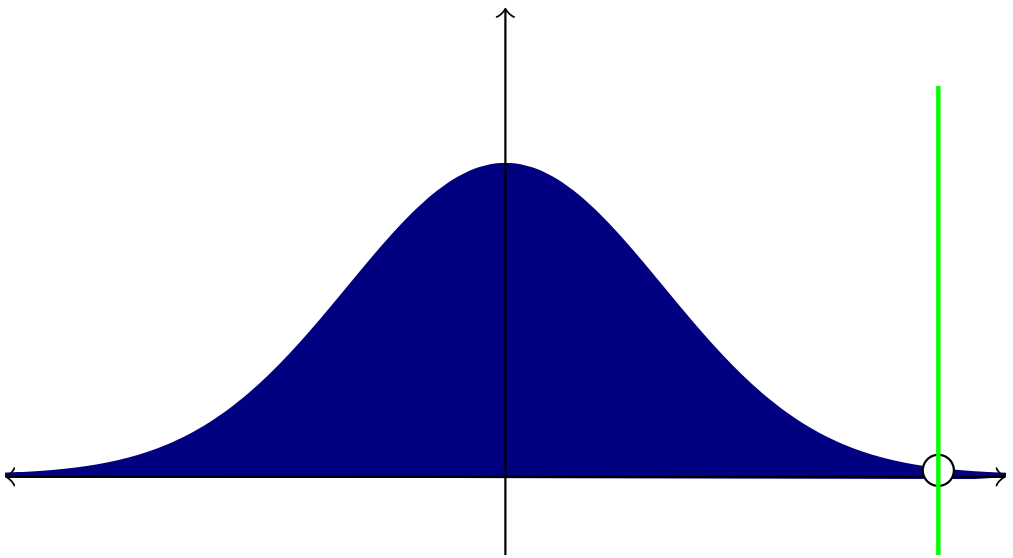

X
-1.3077
-0.4336
0.3426
3.1784
2.7794

Restart

Finish

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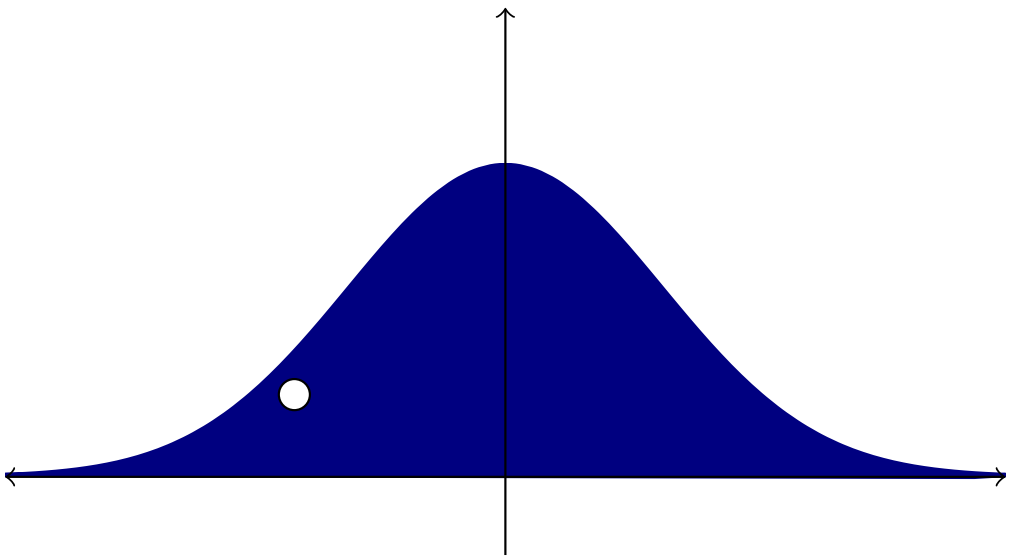

X
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0.3426
3.1784
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▸ Restart

▸ Finish

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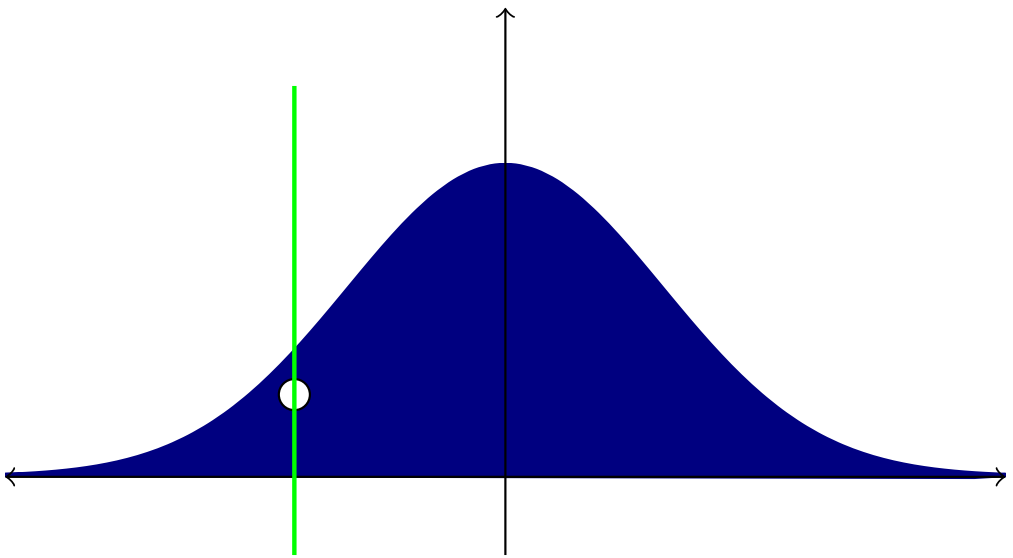

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3.1784
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Restart

Finish

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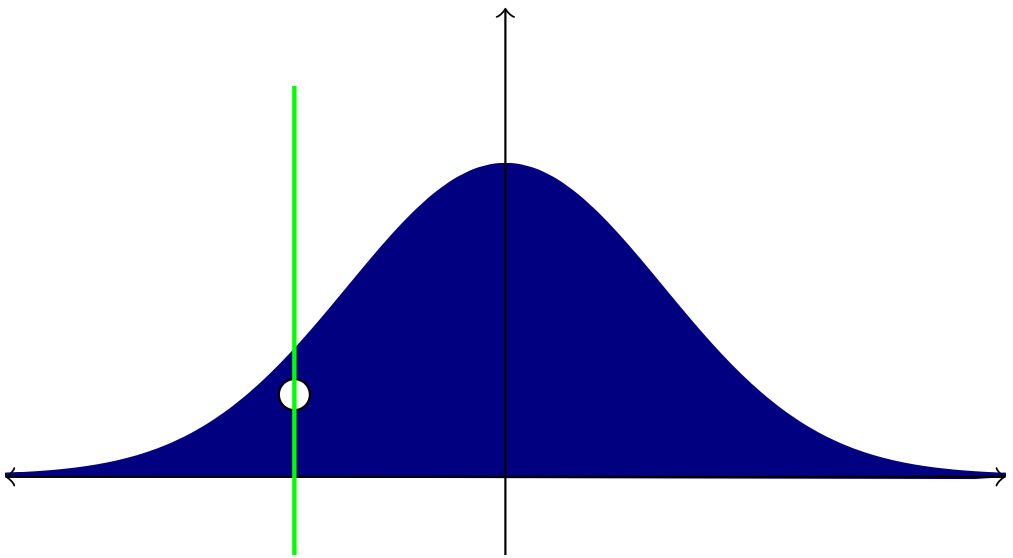

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Restart

Finish

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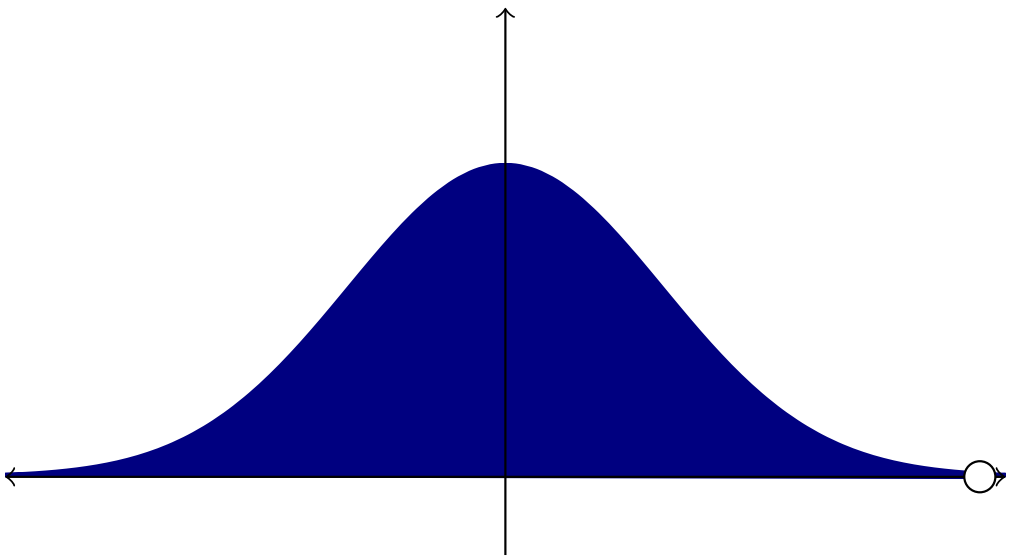

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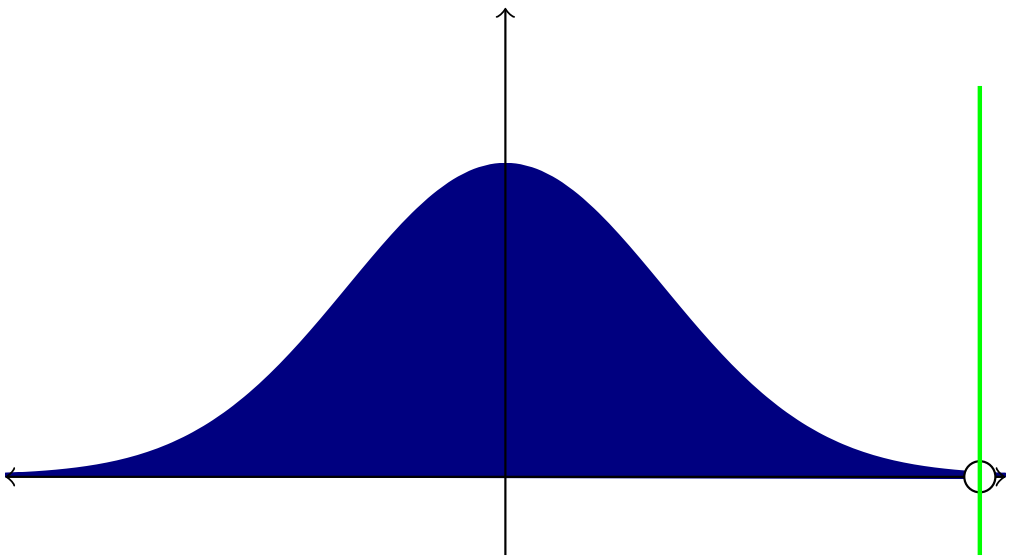
3.1784
2.7794
-1.3499

▸ Restart

▸ Finish

Standard normal random variables



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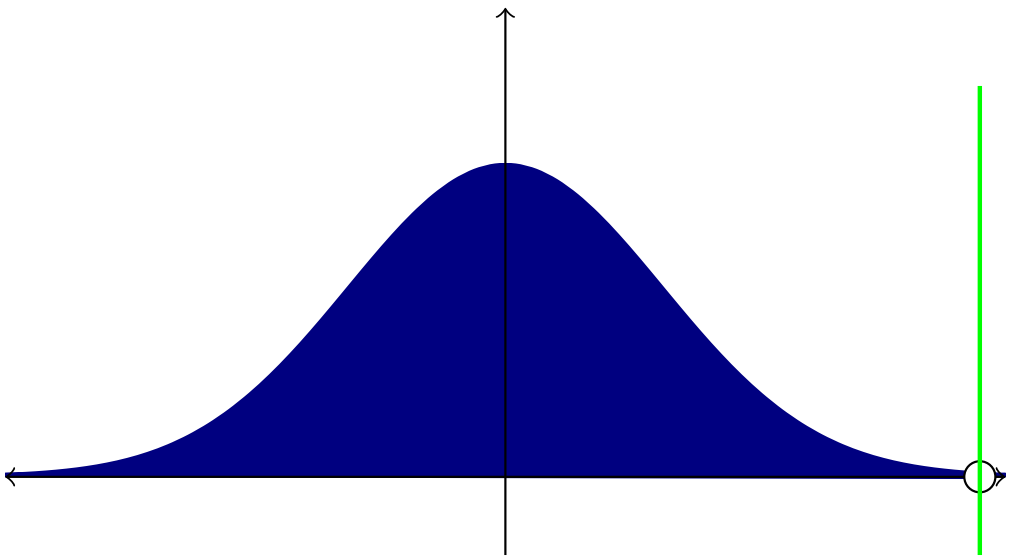
3.1784
2.7794
-1.3499

Restart

Finish

Standard normal random variables



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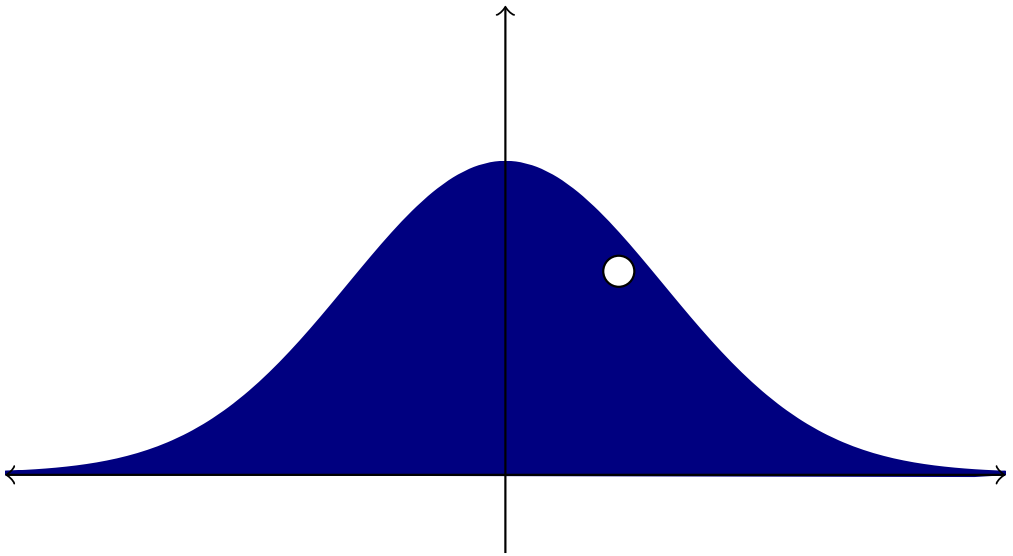

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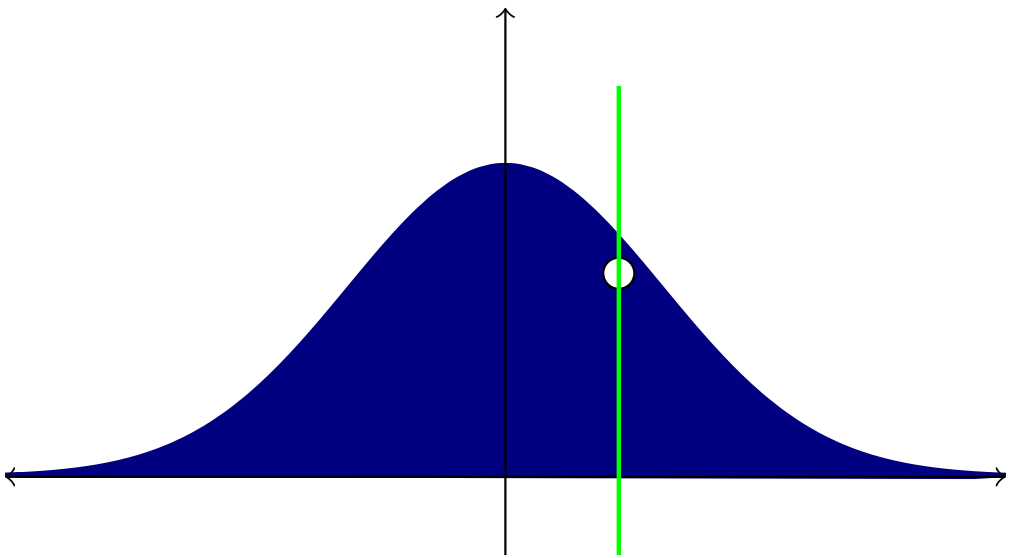

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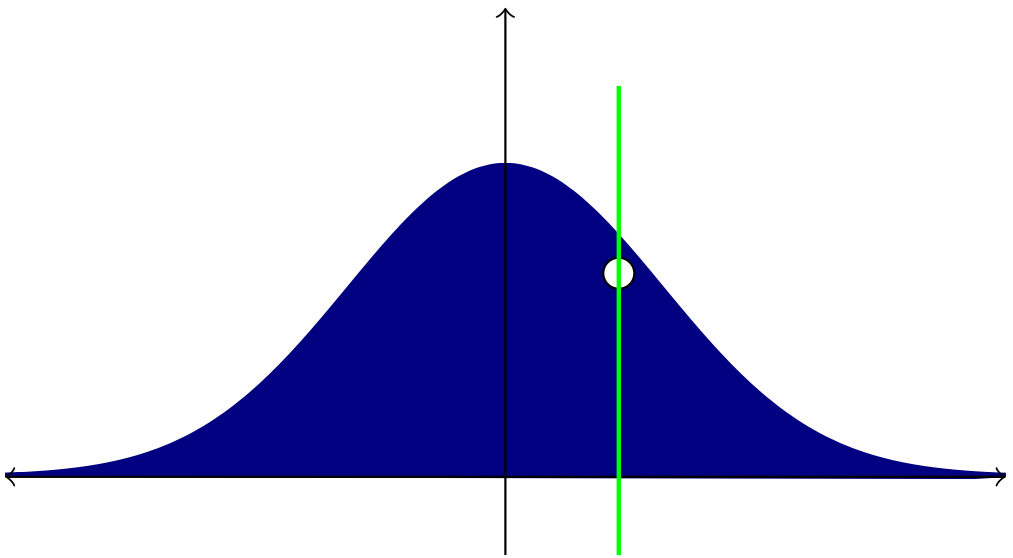

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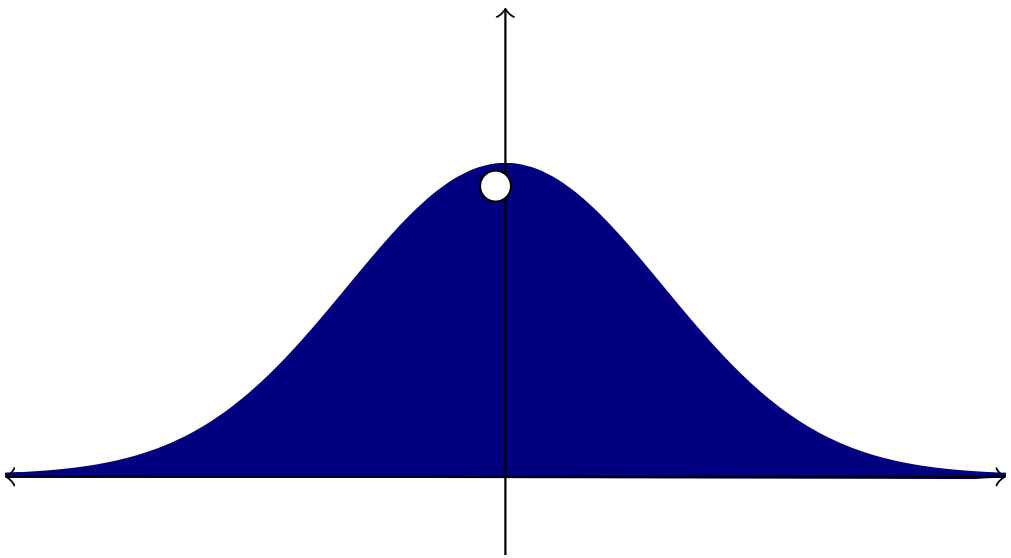
Standard normal random variables



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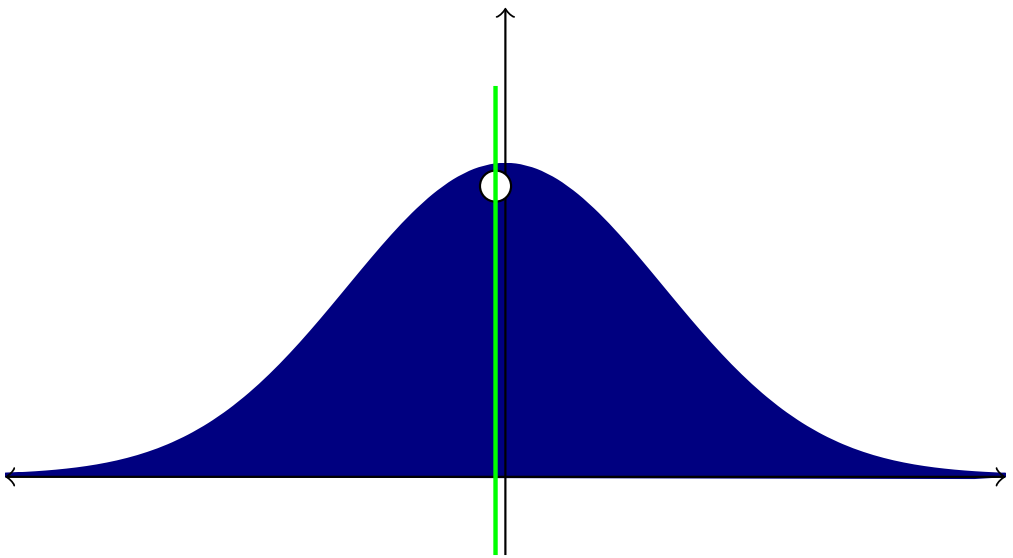
▸ Restart

▸ Finish

Standard normal random variables



X
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2.7794
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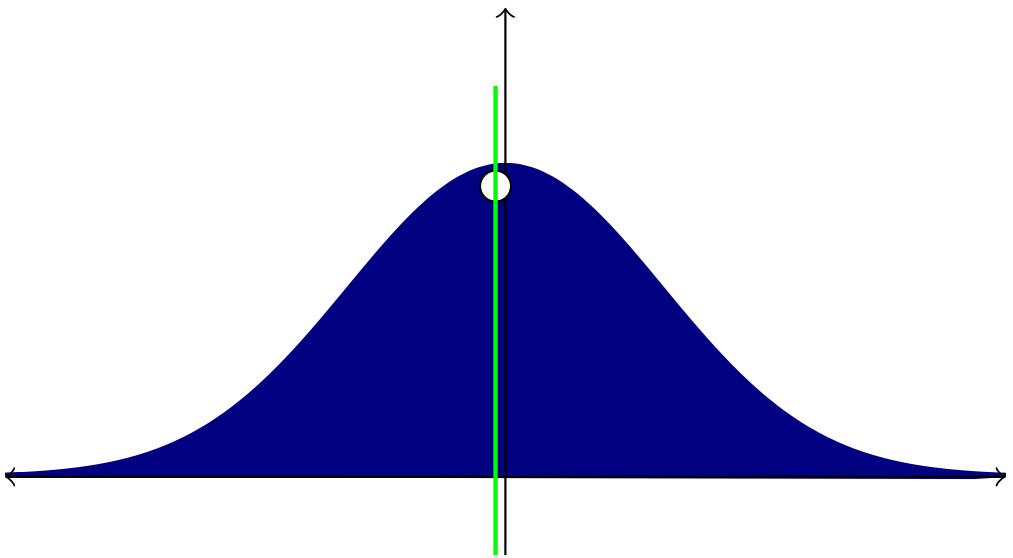
Restart

Finish

Standard normal random variables



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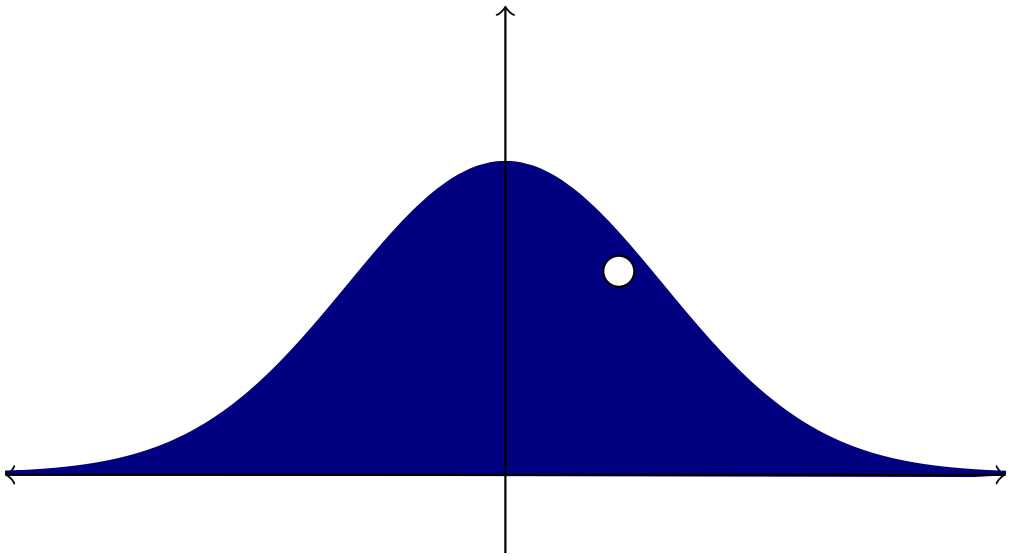
-0.0631

▸ Restart

▸ Finish

Standard normal random variables



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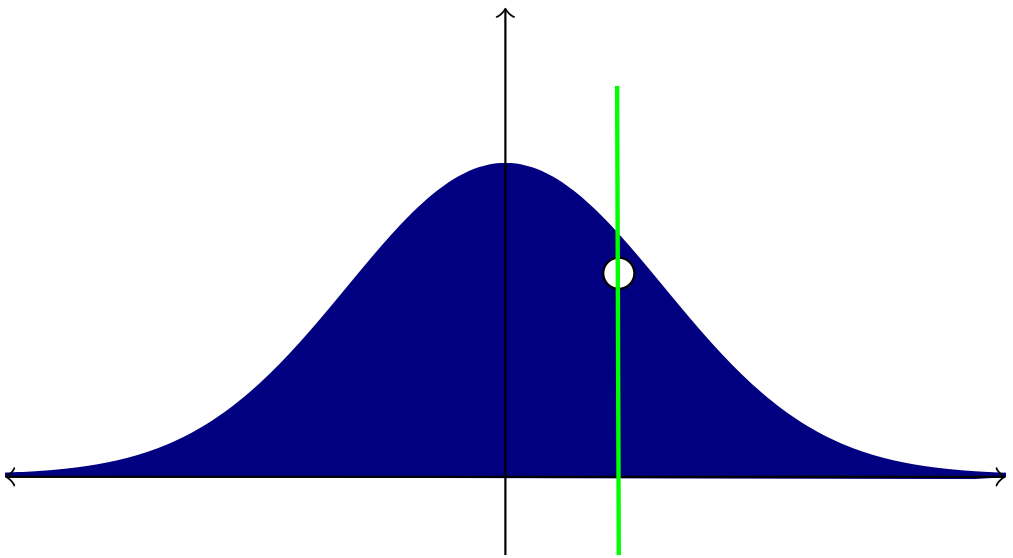

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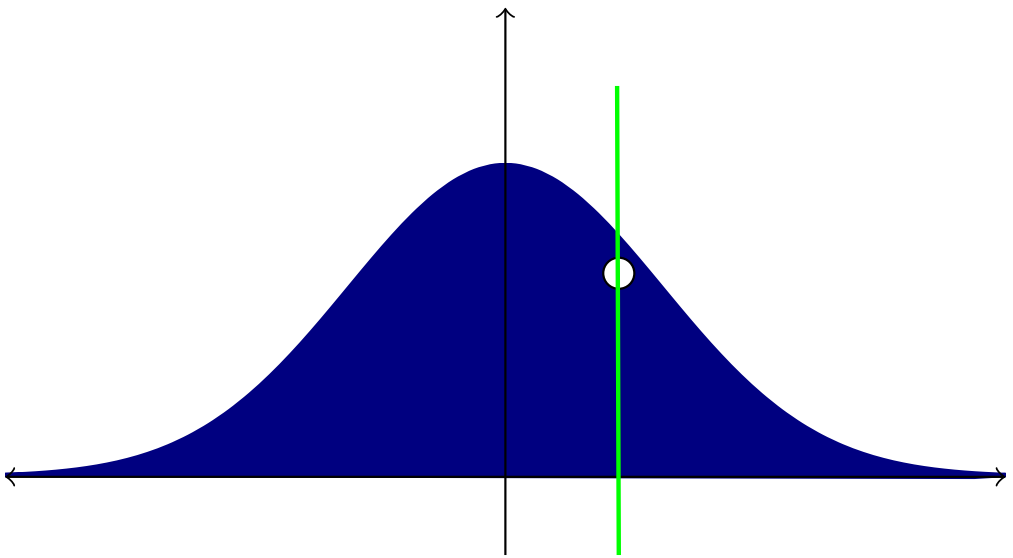

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Restart

Finish