MATH 380

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Simulation Modeling

Modeling a 'situation'/'phenomenon' by simulating its behavior, when we don't have the underlying data & cannot experiment or observe the 'situation' easily (too expensive w.r.t. time/money; too disruptive; doesn't exist; ...)

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→ scaled physical models in engineering

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→ scaled physical models in engineering

→ randomly generated experiments/data that fit the situation

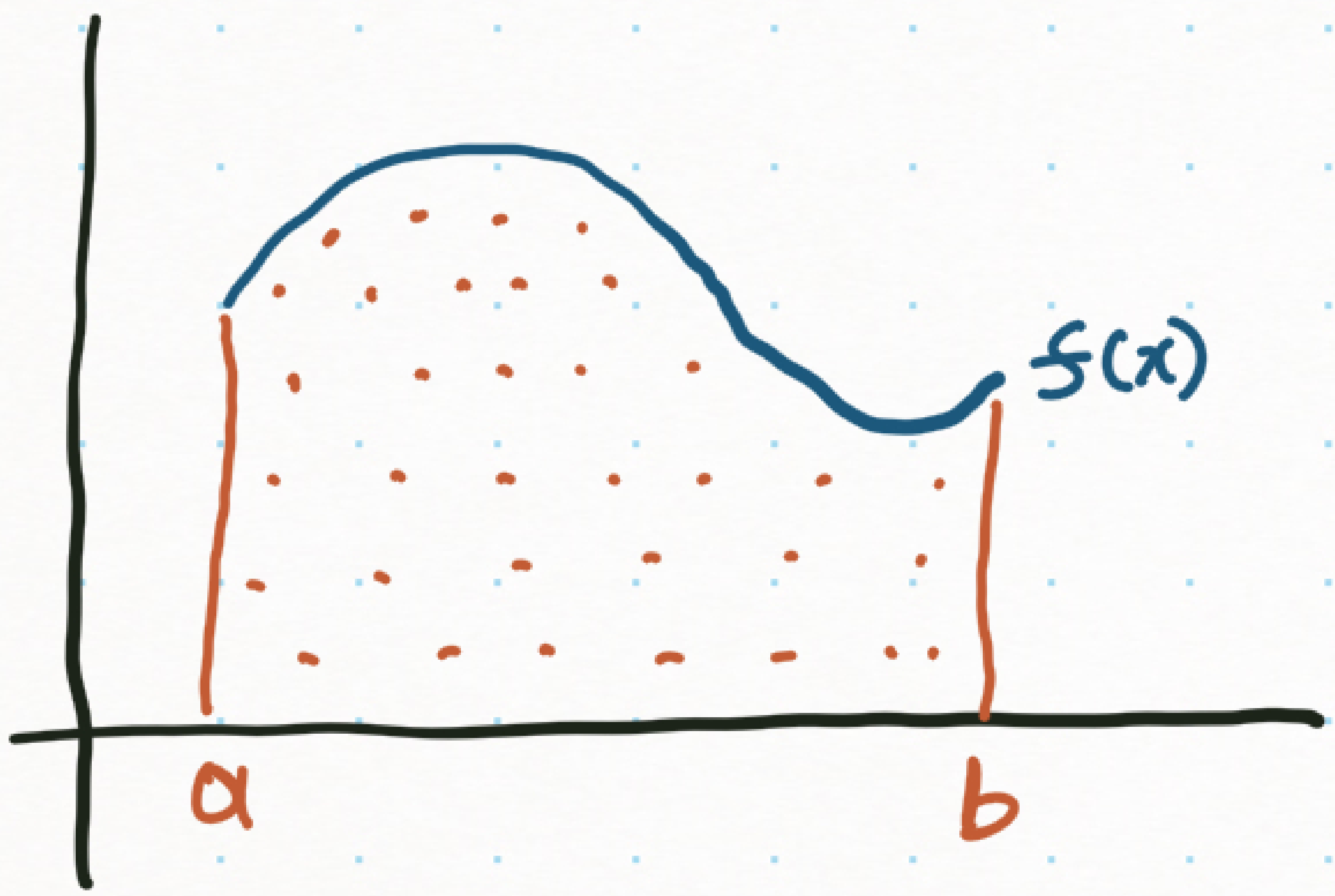
Monte Carlo simulation

e.g. Investigate strategies for improving rush hour service of CTA buses
- we need to simulate the arrival/departure of buses
- & demand of the passengers for different routes.
- ....

Simulating Deterministic Behavior

Estimating a definite integral (area under a curve)

$$\int_a^b f(x)\,dx$$



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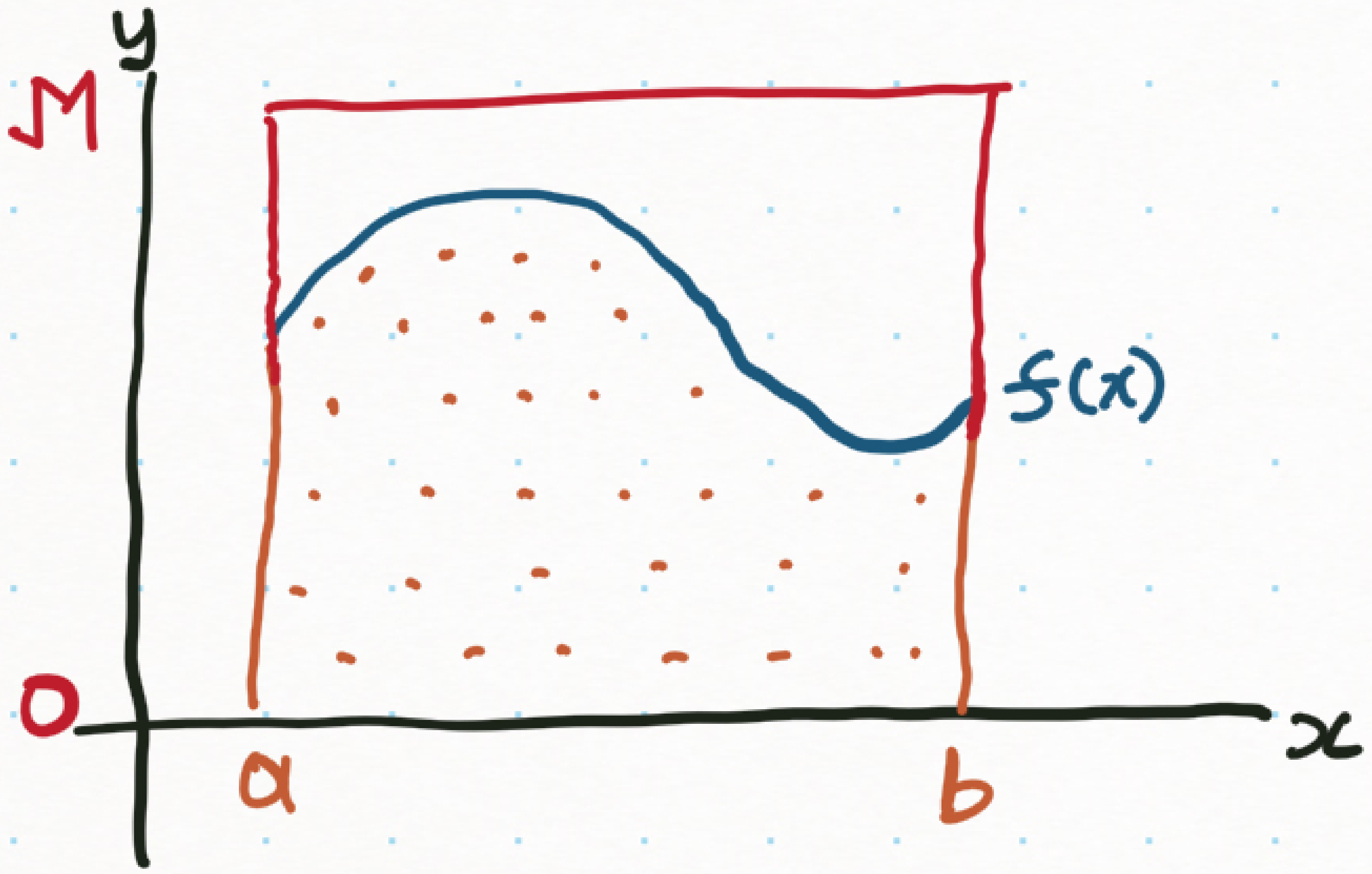

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Randomly pick points (x,y) in the "Bounding Box" $[a,b] \times [0,M]$ and check how many of the points are below the curve $y = f(x)$.

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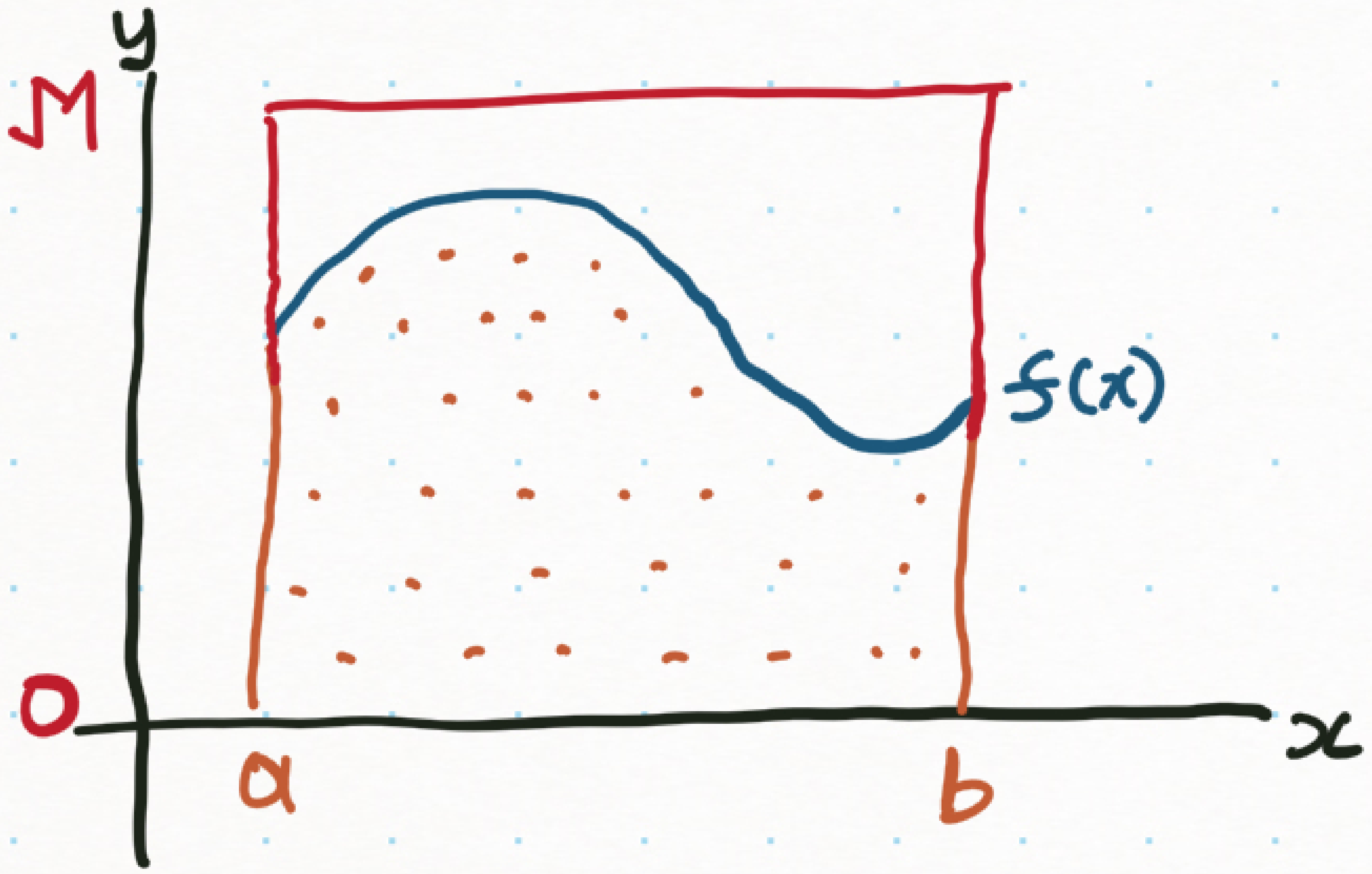

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We expect

$$\frac{\#\text{points below the curve}}{\#\text{points in total}} \approx \frac{\text{area under the curve}}{\text{Total area of bounding box}}$$

$$\int_a^b f(x)\,dx = \text{area under the curve} \approx \left(\frac{\#\text{points below the curve}}{\#\text{points in total}}\right) \times \left(\text{Total area of b-box}\right)$$

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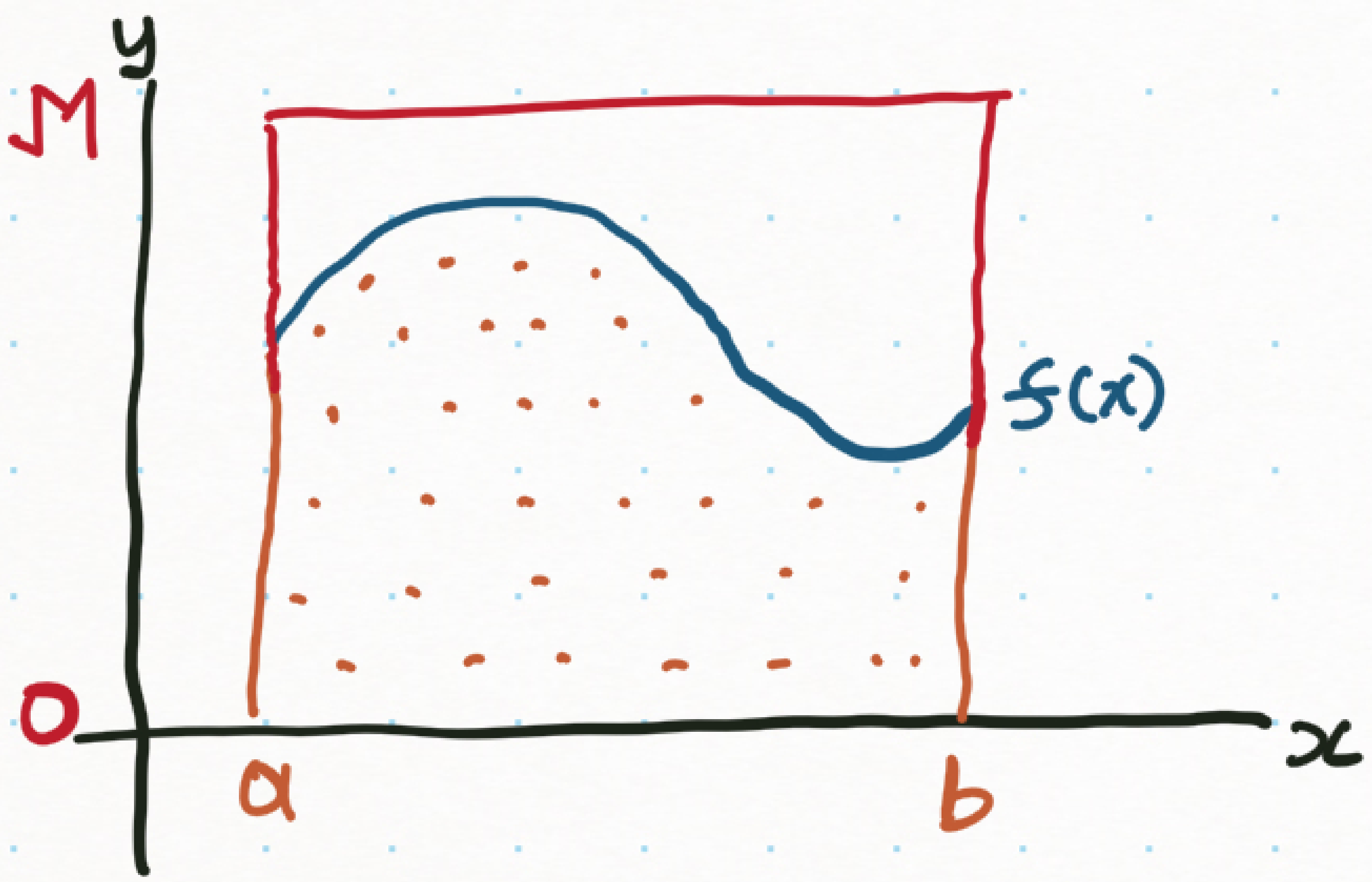

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→ How to find the bounding box?

→ How to generate random points in the box?

Simulating Deterministic Behavior

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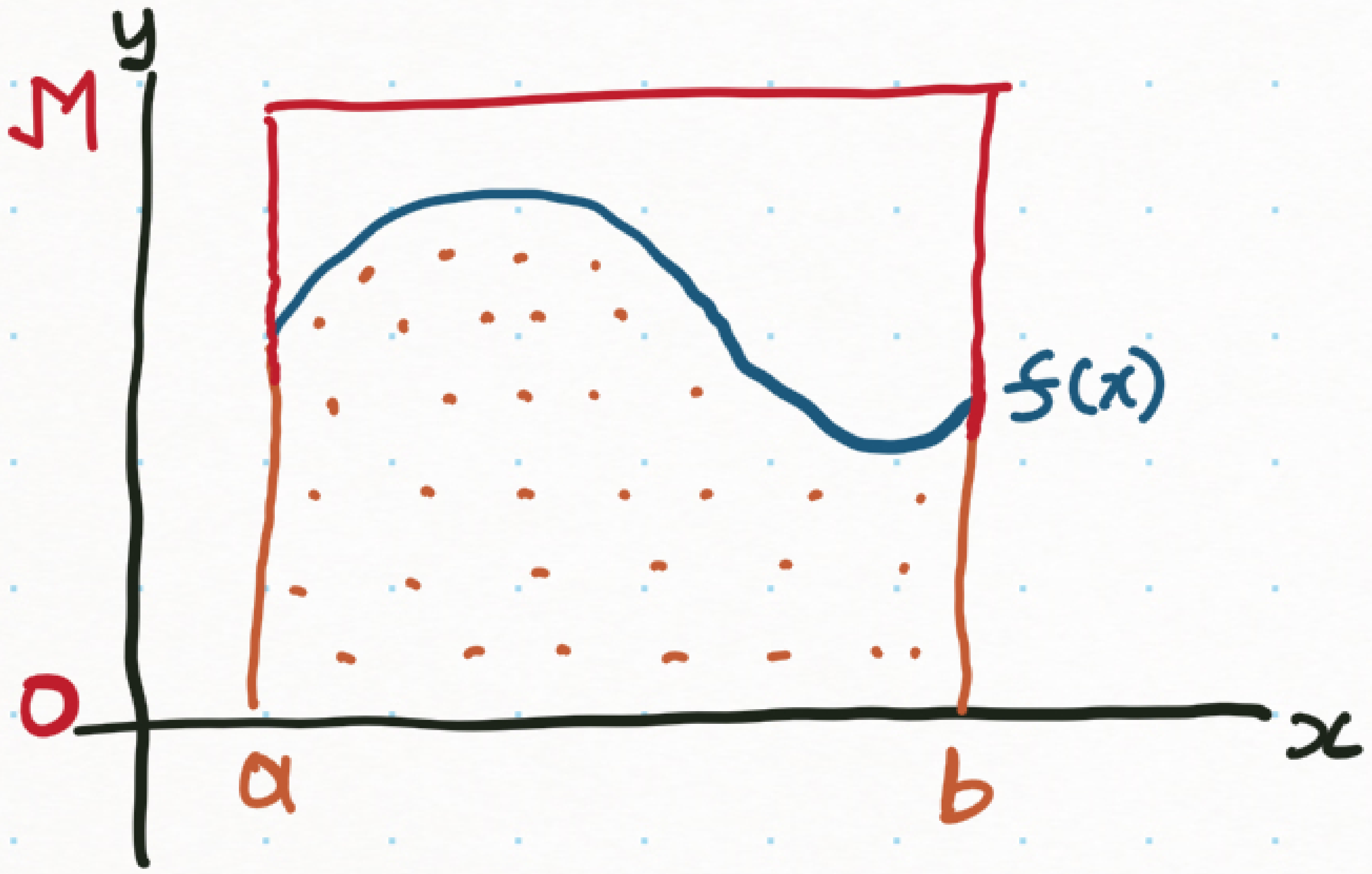

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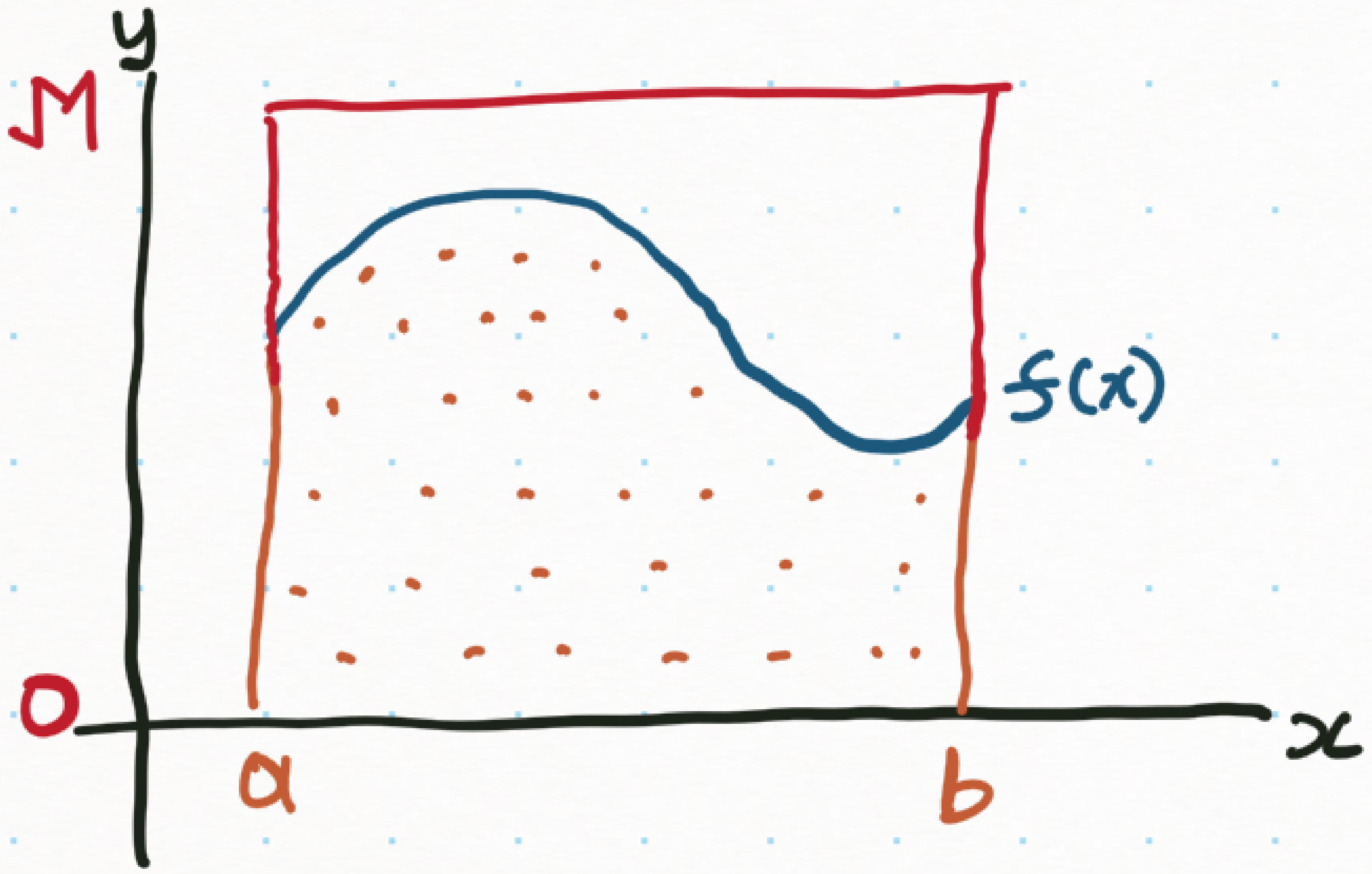

Bounding Box

Find bounds on the values each variable can take.

we know $x \in [a, b]$

& we can find M as $\max\limits_{x \in [a,b]} f(x) \leq M$.

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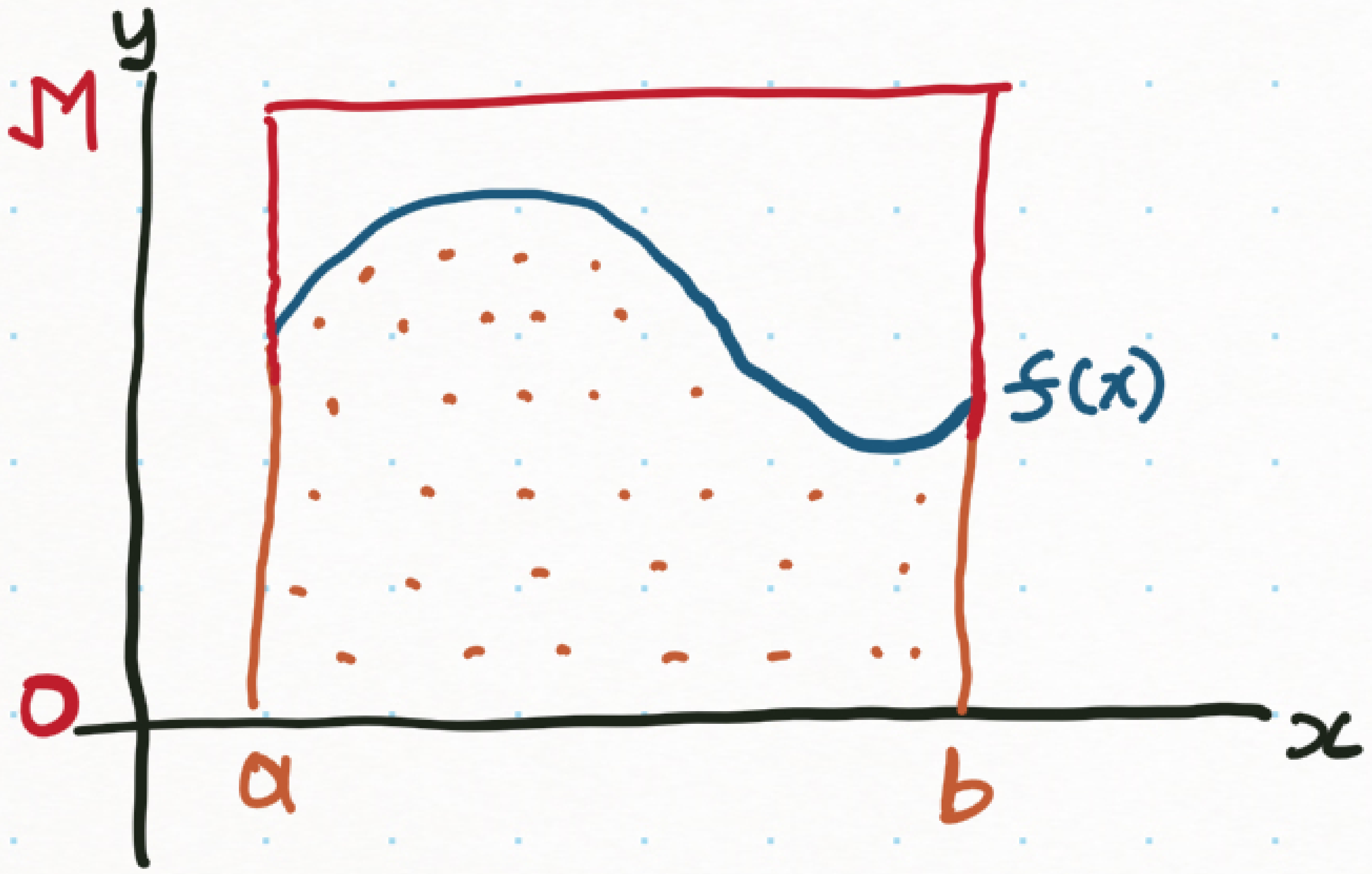

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To generate random points in the Bounding Box

Generate each coordinate randomly using a built-in random number generator in your programming language.

e.g. The function rand in MATLAB returns a uniformly distributed numbers from $[0, 1]$

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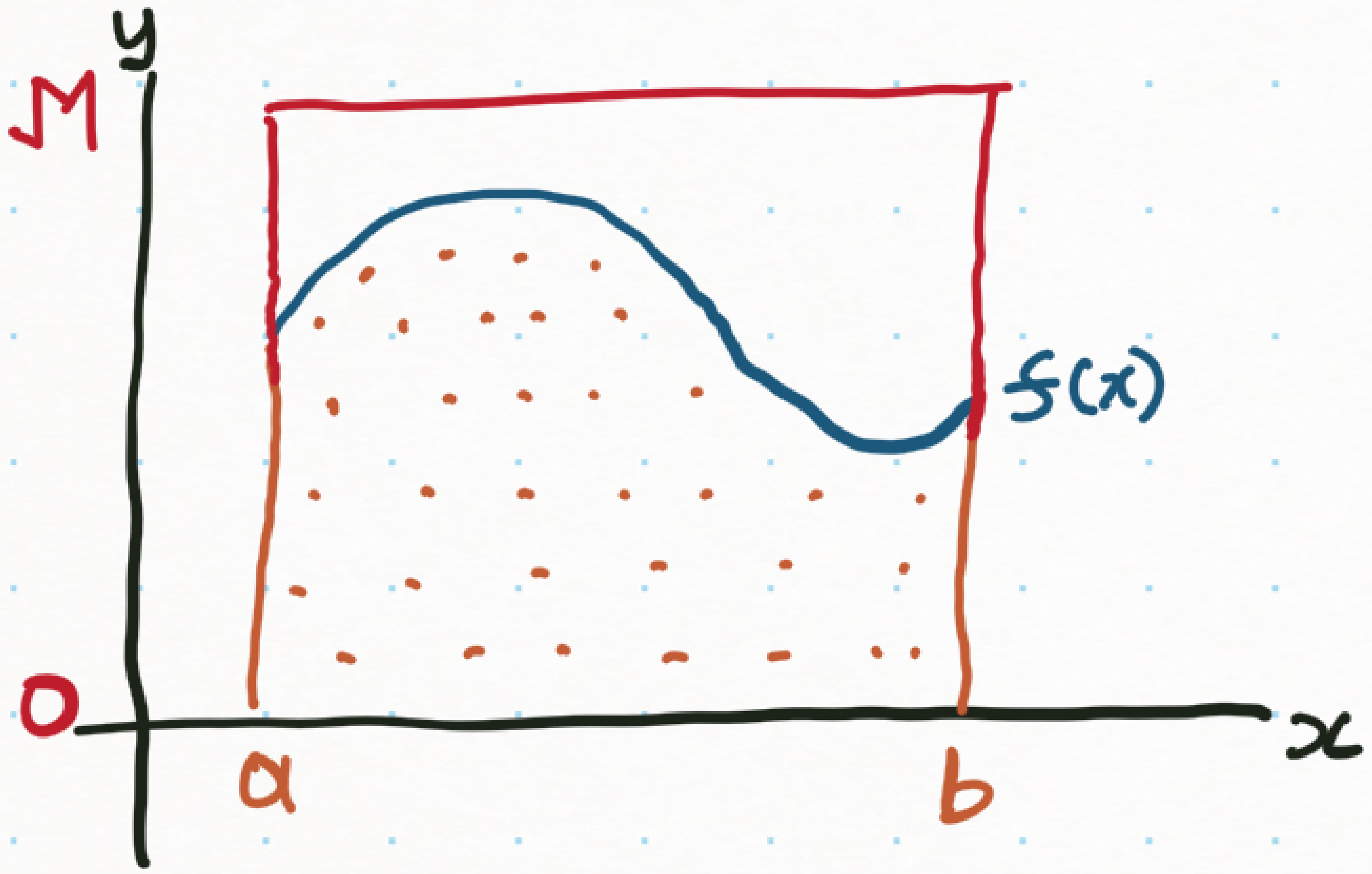

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e.g. The function rand in MATLAB returns a uniformly distributed numbers from $[0, 1]$

$r = \text{rand}$
$x = (b-a)r + a$

$s = \text{rand}$
$y = (M)s$

so, $x \in [a, b]$ independently
$y \in [0, M]$ randomly generated

Monte Carlo Area Algorithm

Given $f(x)$, $a \leq x \leq b$, find a bounding box $[a,b] \times [0,M]$ that encloses the area under $y = f(x)$.

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OUTPUT A = approximate area under $y=f(x)$, $a \leq x \leq b$

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Step 1 Set $C=0$

Step 2 For $i=1,2,\ldots,n$, Do steps 2a & 2b.

Step 2a Generate random (x_i, y_i) s.t. $x_i \in [a,b]$ & $y_i \in [0,M]$

$r = \text{rand}$, $s = \text{rand}$, let $x_i = (b-a)*r + a$ & let $y_i = M*s$

Step 2b Check if $y_i \le f(x_i)$.

If $y_i \le f(x_i)$ then $C \leftarrow C+1$, else $C \leftarrow C$.

Step 3 Compute $A =$

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Step 3 Compute $A = \underbrace{M\,(b-a)}_{\text{area of b-box}} * \dfrac{C}{n}$

#successful trials

#total trials

How to apply this Monte Carlo simulation for volume under a surface?

e.g. Volume of the sphere that lies in the first octant?

Volume under $x^2+y^2+z^2 \leq 1$ when $x \geq 0,\ y \geq 0,\ z \geq 0$.

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Some principles ① Find a bounding box $[a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$
i.e., $a_1 \leq x \leq b_1$, $a_2 \leq y \leq b_2$, $a_3 \leq z \leq b_3$
that encloses the volume we are interested in.

e.g.: $[0,1] \times [0,1] \times [0,1]$ in the example above

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② Generate n random points (x_i, y_i, z_i) in this bounding-box and check how many of them lie under the surface

e.g. $x_i^2 + y_i^2 + z_i^2 \leq 1$ in the example above.

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③ Estimate the volume using the principle

$$\text{Volume under surface} \approx (\text{volume of b-box}) * \left(\frac{\#\text{ points below the surface}}{\#\text{ total points}} \right)$$

Monte Carlo Volume Algorithm

Given $f(x,y)$, ——— find a bounding box $[a_1,b_1]\times[a_2,b_2]\times[a_3,b_3]$ that encloses the volume under $z=f(x,y)$

INPUT $n = \#$ random points to be generated

OUTPUT V = approximate volume under $z=f(x,y)$, ———

Step 1 Set $C=0$

Step 2 For $i=1,2,\ldots,n$, Do steps 2a & 2b.

Step 2a Generate random (x_i, y_i, z_i) s.t. $x_i\in[a_1,b_1]$ & $y_i\in[a_2,b_2]$ & $z_i\in[a_3,b_3]$

→ show the transformation from rand

Step 2b Check if $z_i\le f(x_i,y_i)$

If $z_i\le f(x_i,y_i)$ then $C\leftarrow C+1$, else $C\leftarrow C$.

Step 3 Compute $V = \underbrace{(b_1-a_1)(b_2-a_2)(b_3-a_3)}_{\text{volume of b-box}} * \frac{C}{n}$

#successful trials

#total trials

Monte-Carlo Integration

- error in estimate, but errors can be made smaller (though not "smoothly") with larger numbers of points generated.

- How to do this in high dimensions?
  - → a simple bounding-box like ours will give very high rate of failure
  - → simple uniform sampling of random points will give high rate of failure

Better / powerful techniques have been developed....

Markov chain Monte Carlo

Monte Carlo simulation when working in non-numerical applications..

Generating Random Numbers

Middle-Square Method

[Von Neumann, Ulam & Metropolis at LAL in 1946, to simulate neutron collisons]

1. Start with a 4-digit number x_0 (seed)
2. Square it to a 8-digit number (add leading 0 if needed)
3. Take the middle 4 digits as the next random number.

& so on

n	0	1	2	3	4	...
x_n	2041	1656	7423	1009	0180	...

$(2041)^2 = 04\underline{1656}81$ & so on.

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Nothing special about "4".

Generating Random Numbers

Linear Congruence Method [Lehmer 1951]

→ Basis for many modern pseudorandom number generators

0. Pick 3 integers a, b, c.
1. Get a seed x_0 (hopefully random, may output of "middle-square")
2. Generate a sequence $x_{n+1} = (a x_n + b) \pmod{c}$, $n = 0, 1, 2, \ldots$

↑ remainder when $a x_n + b$ is divided by c

So, each $x_n \in \{0, 1, \ldots, c-1\}$

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- Typically c is very big. e.g. $c = 2^{31}$ in many computer systems.

  e.g. For a random number in $[0, 1]$ with 8 digits we want $c > 10^8$

  Use scaling to convert a number into any range.

- Cycling! (To avoid short cycles, choose a, b, c well).

Simulating Probabilistic Behavior

Probability ≡ chance of a random / uncertain event occuring is a way of understanding non-deterministic events.

For our purpose, we think of

$$\text{Probability of an event occuring (over the long-term)} = \frac{\#\text{ favorable outcomes}}{\#\text{ total outcomes.}}$$

How can we simulate

→ Flipping a coin

→ Rolling a die

→ & so on

?

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A Fair Coin

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So we want to simulate the output of a function

$$f(x) = \begin{cases} \text{"Head"}, & \sim 50\% \text{ of the time} \\ \text{"Tail"}, & \sim 50\% \text{ of the time} \end{cases}$$

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$$f(x) = \begin{cases} \text{"Head"}, & 0 \le x \le 0.5 \\ \text{"Tail"}, & 0.5 < x \le 1 \end{cases}$$

where $f(x) : [0,1] \to \{\text{"Head"}, \text{"Tail"}\}$

Monte Carlo Fair Coin (Input n = # coin flips)

Step 1. Initialize $H = 0$

Step 2. For $i = 1, \dots, n$, DO Steps 2a and 2b.

Step 2a. Generate a random number $x_i \in [0,1]$

Step 2b.

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If $x_i \in (0.5, 1]$ then OUTPUT "Tail" and $H \leftarrow H$.

Step 3. OUTPUT $p = ?$ "Probability of Heads in this experiment".

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In the long-term, we expect the outcome of repeatedly flipping a fair coin to be Heads about 50% of the time, Tails about 50% of the time.

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An Unfair Coin

In the long-term, we expect the outcome of repeatedly flipping a fair coin to be Heads about 75% of the time
Tails about 25% of the time.

So we want to simulate the output of a function

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Step 2a. Generate a random number $x_i \in [0,1]$

Step 2b. If $x_i \in [\;?\;]$ then OUTPUT "Head" and $H \leftarrow H+1$.
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Tails about 25% of the time.

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$$f(x) = \begin{cases} \text{"Head"}, & 0 \le x \le 0.75 \\ \text{"Tail"}, & 0.75 < x \le 1 \end{cases}$$

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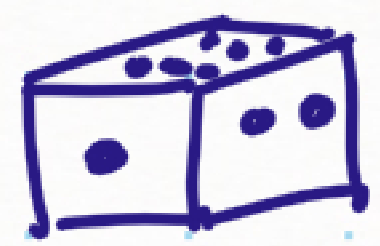
A Fair Die



Six outcomes $\{1,2,3,4,5,6\}$
all equally likely ($1/6^{th}$ chance).

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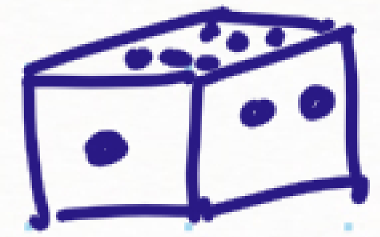

Six outcomes $\{1,2,3,4,5,6\}$
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Monte Carlo Fair Die

(Input n = # rolls of the die)

Step 1. Initialize $S1=0$, $S2=0$, $S3=0$, $S4=0$, $S5=0$, $S6=0$.

Step 2. For $i=1,\dots,n$, DO steps 2a and 2b.

Step 2a. Generate a random number $x_i \in [0,1]$

Step 2b. If ?______ then OUTPUT "Rolled 1" and $S1 \leftarrow S1+1$

If ______ then OUTPUT "Rolled 2" and $S2 \leftarrow S2+1$

If ______ then OUTPUT "Rolled 3" and $S3 \leftarrow S3+1$

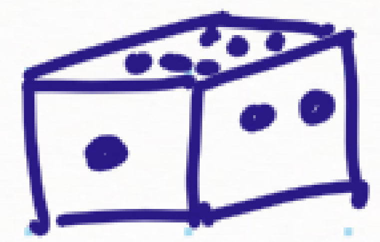
⋮

If ______ then OUTPUT "Rolled 6" and $S6 \leftarrow S6+1$

Step 3. For each $i=1,2,3,4,5,6$

OUTPUT ? "Probability of rolling i in this experiment".

A Fair Die



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Step 2. For $i=1,\dots,n$, DO steps 2a and 2b.

Step 2a. Generate a random number $x_i \in [0,1]$

Step 2b. If $x_i \in [0, 1/6]$ then OUTPUT "Rolled 1" and $S1 \leftarrow S1+1$

If $x_i \in (1/6, 2/6]$ then OUTPUT "Rolled 2" and $S2 \leftarrow S2+1$

If $x_i \in (2/6, 3/6]$ then OUTPUT "Rolled 3" and $S3 \leftarrow S3+1$

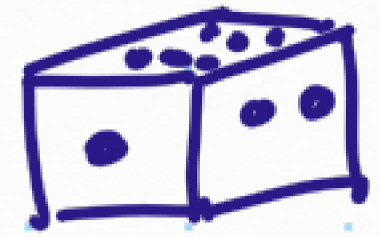
⋮

If $x_i \in (5/6, 1]$ then OUTPUT "Rolled 6" and $S6 \leftarrow S6+1$

Step 3. For each $i=1,2,3,4,5,6$

OUTPUT $\dfrac{S_i}{n}$ "Probability of rolling i in this experiment".

An Unfair Die



Six outcomes $\{1,2,3,4,5,6\}$ with chances $\{20\%, 30\%, 10\%, 10\%, 10\%, 20\%\}$ respectively.

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Step 2b. If $x_i \in [\ ?\ ]$ then OUTPUT "Rolled 1" and $S1 \leftarrow S1+1$

If $x_i \in (\ ?\ ]$ then OUTPUT "Rolled 2" and $S2 \leftarrow S2+1$

If $x_i \in (\ ?\ ]$ then OUTPUT "Rolled 3" and $S3 \leftarrow S3+1$

⋮

If $x_i \in (\ ?\ ]$ then OUTPUT "Rolled 6" and $S6 \leftarrow S6+1$

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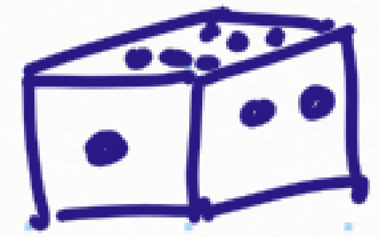

Six outcomes $\{1,2,3,4,5,6\}$ with chances $\{20\%, 30\%, 10\%, 10\%, 10\%, 20\%\}$ respectively.

Monte Carlo Unfair Die (Input n = # rolls of the die)

Step 1. Initialize $S1=0,\ S2=0,\ S3=0,\ S4=0,\ S5=0,\ S6=0$.

Step 2. For $i=1,\dots,n$, DO steps 2a and 2b.

Step 2a. Generate a random number $x_i \in [0,1]$

Step 2b. If $x_i \in [0, 0.2]$ then OUTPUT "Rolled 1" and $S1 \leftarrow S1+1$

If $x_i \in (0.2, 0.5]$ then OUTPUT "Rolled 2" and $S2 \leftarrow S2+1$

If $x_i \in (0.5, 0.6]$ then OUTPUT "Rolled 3" and $S3 \leftarrow S3+1$

$\vdots$

If $x_i \in (0.8, 1]$ then OUTPUT "Rolled 6" and $S6 \leftarrow S6+1$

Step 3. For each $i=1,2,3,4,5,6$

OUTPUT $\frac{S_i}{n}$ "Probability of rolling i in this experiment".

Arriving on your vacation, you are dismayed to learn that the local weather service forecasts $p \in [0,1]$ (say, $p = 60\%$) chance of rain each day this week. What will your "rain experience" during the vacation be like? What are the chances of at least 3 consecutive rainy days?

Arriving on your vacation, you are dismayed to learn that the local weather service forecasts $p \in [0,1]$ (say, $p = 60\%$) chance of rain each day this week. What will your "rain experience" during the vacation be like? What are the chances of at least 3 consecutive rainy days?

Variables: $X_t = \begin{cases} 0 & \text{if no rain on day } t \\ 1 & \text{if rain on day } t \end{cases}, \; t = 1, 2, 3, \ldots, 7.$

Assumptions: Rain on one day has no influence on rain on other days.
i.e., X_t's are independent.

$\mathbb{P}[X_t = 0] = \underset{= 0.6}{p}$ and $\mathbb{P}[X_t = 1] = \underset{= 0.4}{1 - p}$.

Objective: Simulate daily occurrence of rain for a week and determine the probability that $X_t = X_{t+1} = X_{t+2} = 1$ for some $t = 1, 2, 3, 4, 5$

Rainy Days Simulation

Step 1. Initialize $R=0$ and $TR=0$

Step 2. For $t=1$ to 7, DO Steps 2a, 2b, 2c, & 2d.

Step 2a. Generate a random number $x(t) \in [0,1]$

Step 2b. If $x(t) \in [\ ?\ ]$ then $X(t)=1$

If $x(t) \in (\ ?\ ]$ then $X(t)=0$

Rainy Days Simulation

Step 1. Initialize $R = 0$ and $TR = 0$

Step 2. For $t = 1$ to 7, DO Steps 2a, 2b, 2c, & 2d.

Step 2a. Generate a random number $x(t) \in [0, 1]$

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t) = 1$

If $x(t) \in (0.6, 1]$ then $X(t) = 0$

Step 2c. If $X(t) = 1$ then $R \leftarrow R+1$ & OUTPUT "Rain on day t"

If $X(t) = 0$ then $R \leftarrow 0$ & OUTPUT "No Rain on day t".

Why?

Step 2d. If $R \geq 3$ then $TR \leftarrow TR+1$

Step 3. OUTPUT TR ?

We can estimate probability of 3 consecutive rainy days using TR:

probability $= TR/?$

Rainy Days Simulation

Step 1. Initialize $R=0$ and $TR=0$

Step 2. For $t=1$ to 7, DO steps 2a, 2b, 2c, & 2d.

Step 2a. Generate a random number $x(t) \in [0,1]$

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t)=1$

If $x(t) \in (0.6, 1]$ then $X(t)=0$

Step 2c. If $X(t)=1$ then $R \leftarrow R+1$ & OUTPUT "Rain on day t"

If $X(t)=0$ then $R \leftarrow 0$ & OUTPUT "No Rain on day t".

Step 2d. If $R \geq 3$ then $TR \leftarrow TR+1$

Step 3. OUTPUT TR "Number of 3 consecutive rainy days"

We can estimate probability of 3 consecutive rainy days using TR:

probability $= TR/?$

Rainy Week Simulation

"Rainy Week" ≡ 4 or more days of rain

Step 1.

Step 2.

Step 3.

Rainy Week Simulation

"Rainy Week" ≡ 4 or more days of rain

Step 1. Initialize $R = 0$

Step 2. For $t = 1$ To 7, DO Steps 2a, 2b & 2c.

Step 2a. Generate a random number $x(t) \in [0,1]$

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t) = 1$
If $x(t) \in (0.6, 1]$ then $X(t) = 0$

Step 2c. If $X(t) = 1$ then $R \leftarrow R+1$ & OUTPUT "Rain on day t"
If $X(t) = 0$ then $R \leftarrow$? & OUTPUT "No Rain on day t".

Step 3. If $R \geq 4$ then OUTPUT "Rainy Week" with R raindays

Rainy Week Simulation

"Rainy Week" ≡ 4 or more days of rain

Step 1. Initialize $R = 0$

Step 2. For $t = 1$ To 7, DO Steps 2a, 2b & 2c.

Step 2a. Generate a random number $x(t) \in [0,1]$

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t) = 1$

If $x(t) \in (0.6, 1]$ then $X(t) = 0$

Step 2c. If $X(t) = 1$ then $R \leftarrow R+1$ & OUTPUT "Rain on day t"

If $X(t) = 0$ then $R \leftarrow R$ & OUTPUT "No Rain on day t".

Step 3. If $R \geq 4$ then OUTPUT "Rainy Week" with R raindays

What if we also know the probability of having high winds on each day (say $q \in [0,1]$, e.g. $q = 0.7$) and want to simulate how many days in the coming week have neither rain nor high winds?

"Nice week" $\equiv$ at least 4 days with neither rain nor high winds

Nice Week Simulation

Step 1. Initialize NRW $= 0$

Step 2. For $t = 1$ To 7, DO steps 2a, 2b & 2c.

Step 2a. Generate a random number $x(t)$.

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t) = 1$

If $x(t) \in (0.6, 1]$ then $X(t) = 0$

Step 2c.

Step 3.

Nice Week Simulation

Step 1. Initialize $NRW = 0$

Step 2. For $t = 1$ To 7, DO Steps 2a, 2b & 2c.

Step 2a. Generate a random numbers $x(t), y(t) \in [0, 1]$

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t) = 1$

If $x(t) \in (0.6, 1]$ then $X(t) = 0$

If $y(t) \in [0, 0.7]$ then $Y(t) = 1$

If $y(t) \in (0.7, 1]$ then $Y(t) = 0$

Step 2c.

Step 3.

Nice Week Simulation

Step 1. Initialize NRW = 0

Step 2. For $t = 1$ To 7, DO Steps 2a, 2b & 2c.

Step 2a. Generate a random numbers $x(t), y(t) \in [0, 1]$

Step 2b. If $x(t) \in [0, 0.6]$ then $X(t) = 1$

If $x(t) \in (0.6, 1]$ then $X(t) = 0$

If $y(t) \in [0, 0.7]$ then $Y(t) = 1$

If $y(t) \in (0.7, 1]$ then $Y(t) = 0$

Step 2c. If $X(t) = 1$ and $Y(t) = 1$ then $NRW \leftarrow NRW$

If $X(t) = 1$ and $Y(t) = 0$ then $NRW \leftarrow NRW$

If $X(t) = 0$ and $Y(t) = 1$ then $NRW \leftarrow NRW$

If $X(t) = 0$ and $Y(t) = 0$ then $NRW \leftarrow NRW + 1$

Step 3. If $NRW \geq 4$ then OUTPUT "Nice Week" with NRW days of no rain & winds what assumptions underly our previous simulation models?

How can we improve these models?