Computational statistical physics: The example of hard spheres

Lectures at the 16th Chris Engelbrecht Summer School in Theoretical Physics, Drakensberg, KwaZulu-Natal, South Africa

Fifth part: The A and Ω of Monte Carlo Algorithms

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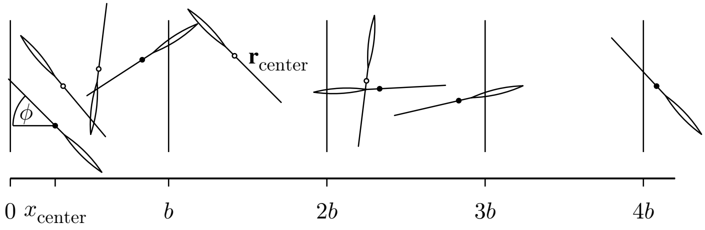
A

Buffon's needle problem (1777)

- Georges Louis Leclerc, Comte de Buffon (1707-1788)

Coordinates in Buffon's problem

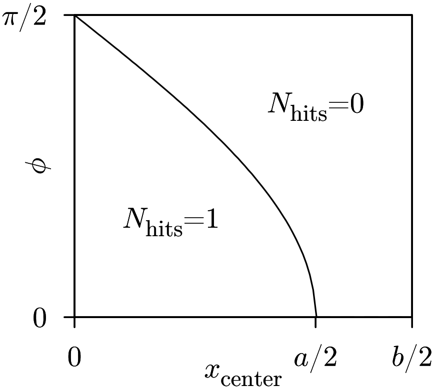


- use 'reduced pad'

$$0 < \phi < \frac{\pi}{2}$$

$$0 < x_{\text{center}} < \frac{b}{2}.$$

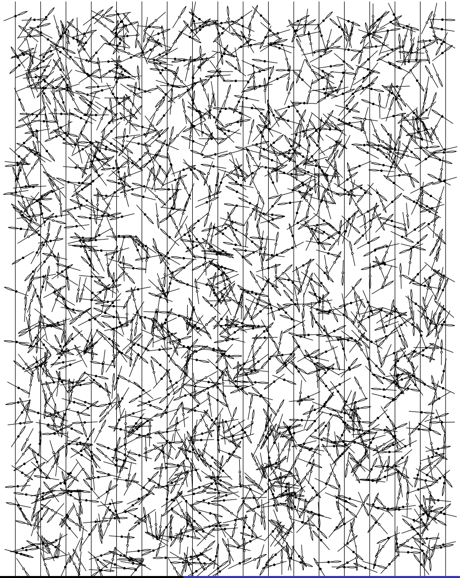
'Landing pad' in Buffon's problem



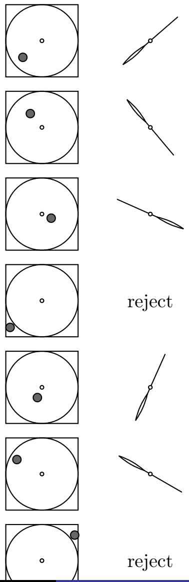
procedure `direct-needle`
$N_{\text{hits}} \leftarrow 0$
for $i = 1, \ldots, N$ **do**
$$\left\{ \begin{array}{l} x_{\text{center}} \leftarrow \texttt{ran}[0, \frac{b}{2}] \\ \phi \leftarrow \texttt{ran}[0, \frac{\pi}{2}] \\ x_{\text{tip}} \leftarrow x_{\text{center}} - \frac{a}{2} \texttt{cos}\ \phi \\ \textbf{if } (x_{\text{tip}} < 0)\ N_{\text{hits}} \leftarrow N_{\text{hits}} + 1 \end{array} \right.$$
output N_{hits}

- computes π.
- has a conceptual problem.

Buffon's problem (simulation)



pebble-needle trick



procedure `direct-needle[patch]`

$x_{\text{center}} \leftarrow \texttt{ran}[0, b/2]$

1 $\delta x \leftarrow \texttt{ran}[0, 1]$

$\delta y \leftarrow \texttt{ran}[0, 1]$

$|\mathbf{x}| \leftarrow \sqrt{\delta x^2 + \delta y^2}$

if $(|\mathbf{x}| > 1)$ **goto** 1

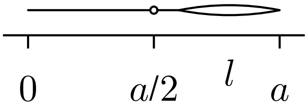
$x_{\text{tip}} \leftarrow x_{\text{center}} - \frac{1}{2} a \cdot \delta x / |\mathbf{x}|$

$N_{\text{hits}} \leftarrow 0$

if $(x_{\text{tip}} < 0)$ $N_{\text{hits}} \leftarrow 1$

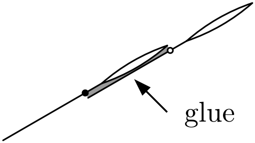
output N_{hits}

- Interior coordinate of a needle



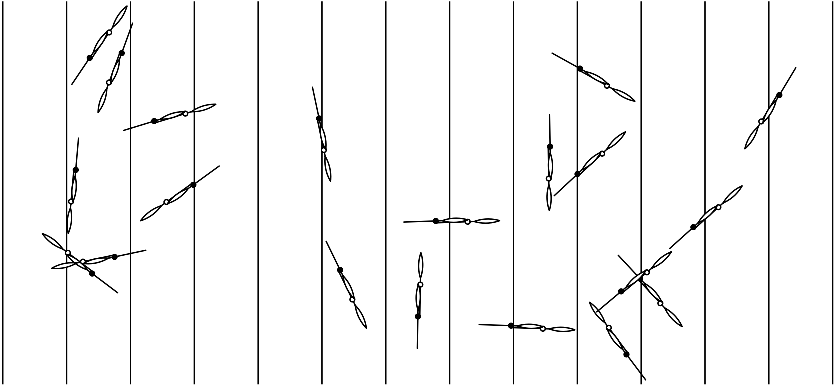
$$\left\{\begin{array}{c}\text{Are the needles more likely}\\ \text{to hit a crack}\\ \text{at their tip, center, or ear?}\end{array}\right\} \left\{\begin{array}{c}\text{tip}\\ \text{center}\\ \text{ear}\end{array}\right\} \text{(circle one).}$$

Gadget Nº 1



- made up of a black-centered and a white-centered needle

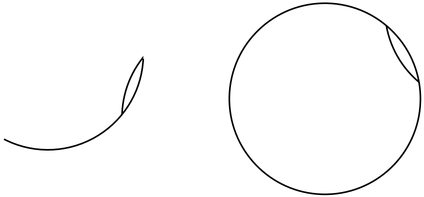
Buffon’s experiment with Gadget Nº 1



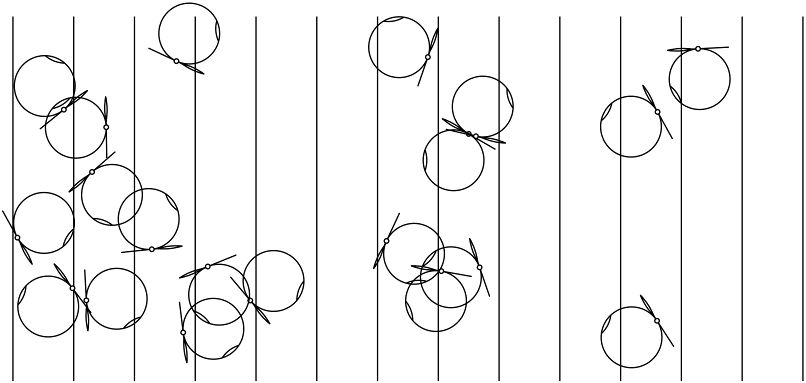
Conclusions (1)

$$\left\{\begin{matrix}\text{mean number}\\\text{of hits}\end{matrix}\right\} = \Upsilon \cdot \left\{\text{length of needle}\right\}$$

Cobbler's needles and crazy cobbler's needles



Buffon's experiment with Gadget Nº 2

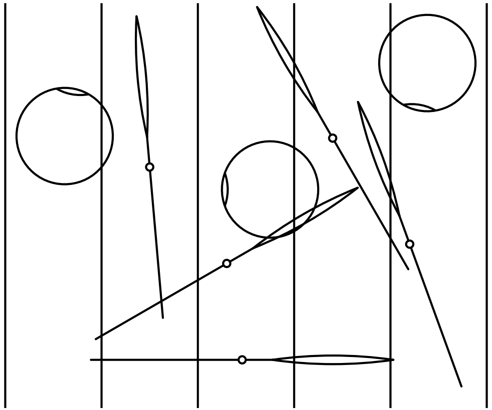


Conclusions (2)

$$\left\{\begin{matrix}\text{mean number}\\ \text{of hits}\end{matrix}\right\} = \Upsilon \cdot \left\{\begin{matrix}\text{length of needle}\\ \text{of any shape}\end{matrix}\right\}$$

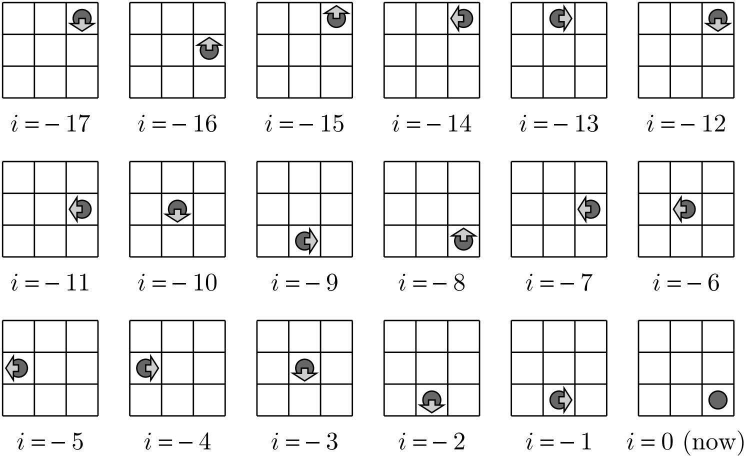
- We need to compute Υ

Straight and round needles

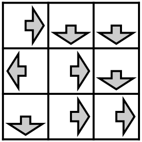


$$\Omega$$

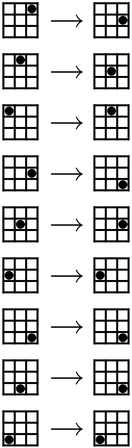
Discrete pebble game



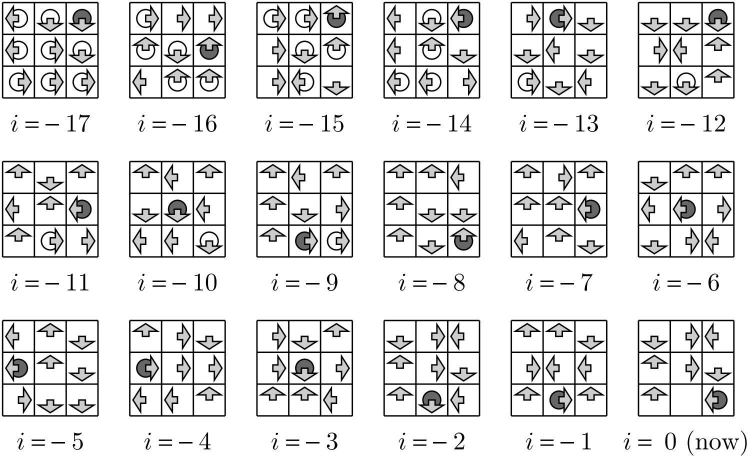
random map



i



Perfect sampling



scenic view of a simulation with random maps