Independent Trials and Trial Size

Computational Physics Exercise 1

source code: `https://github.com/rojinaks/ComputationalPhysics`

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In this paper a stochastic method for computing π is introduced and analyzed. The Idea is that the area of the unit circle is given by $\pi \approx 3.1416$ and the area of a square with a width of 2 is 4. Using this it is possible to calculate π by generating P two-dimensional points (from a uniform distribution) inside the square and counting how many of them also are located inside the unit circle.

The points are labeled $\vec{r}_p = (x_p, y_p)$ with $\vec{r}_p \in [-1, 1] \times [-1, 1]$. By using the Iverson Bracket

$$[X] = \begin{cases} 1 & \text{if X is true} \\ 0 & \text{otherwise} \end{cases}$$

We can write the formula for π_x, where the x stands for the experiment, as

$$\pi_x = \mathrm{E}[4[X^2 + Y^2 \leq 1]] = \frac{4}{P} \sum_{p=1}^{P} [x_p^2 + y_p^2 \leq 1]. \tag{1}$$

The experiment can be repeated X times, so that we get a final answer

$$\pi_\mathrm{f} = \frac{1}{X} \sum_{x=1}^{X} \pi_x \qquad \Delta\pi_\mathrm{f} = \sqrt{\frac{1}{X-1} \sum_{x=1}^{X} (\pi_\mathrm{f} - \pi_x)^2}. \tag{2}$$

1 One big experiment

Let $P = 10\,000$ and $X = 1$. Since only one experiment is done, eq. (2) cannot be used to calculate the uncertainty. Because of that the uncertainty is defined as

$$\Delta\pi_x = \sqrt{\mathrm{Var}(4[X^2 + Y^2 \leq 1])} \tag{3}$$

with $\mathrm{Var}(X)$ being the variance of the random variable X. Letting the experiment run results in a value of

$$\pi_x = 3.1 \pm 1.7, \tag{4}$$

which is considering the uncertainty of approximately 53 % close to the real value.

When doing just one experiment, the distribution of the generated points is of interest. For this the histogram of the radii $R = \sqrt{X^2 + Y^2}$ and the squared radii are plotted in figs. 2a and 2b. For the radii we can see a linear rising distribution with a maximum at $r = 1$, after which the distribution drops. The linear rise is explainable with the following argumentation:
The points generated inside the square are distributed uniformly, but since the circumference of a circle is proportional to the radius, the point density $n(r)$ also has to be $n(r) \sim r$. The drop after $r = 1$ occurs because a circle with radius 1 is the biggest that fits inside a 2×2 square, so there will be fewer points that can be generated with that radius and thus the distribution for $r > 1$ can be written as $n(r) \sim r(1 - f(r))$ where the function $f(r)$. Let us think about a circle with a radius bigger than 1 and concentrate on and eighth of the circle. This is shown in fig. 1. The part of the circle between the marked 0 and $\phi_{\max}$ are outside the square. The value for ϕ in terms of the radius r and the coordinate x is

$$\phi(r, x) = \arctan\left(\frac{\sqrt{r^2 - x^2}}{x}\right).$$

We see that $\phi(r, r) = 0$ and $\phi_{\max} = \phi(r, 1) = \arctan\left(\sqrt{r^2 - 1}\right)$ for a square with a width of 2. Since we have 8 such parts outside the square, the normalized distribution can be written as

$$n(r) = \frac{\pi}{2} r(1 - f(r))$$

with

$$f(r) = \begin{cases} 0 & r \leq 1 \\ \frac{4}{\pi} \arctan\left(\sqrt{r^2 - 1}\right) & 1 < r \leq \sqrt{2} \\ 1 & r > \sqrt{2} \end{cases}$$

because $n(r)$ has to be zero for $r > \sqrt{2}$. In fig. 2a the generated with the expected distribution are shown. Clearly they look very similar to each other.

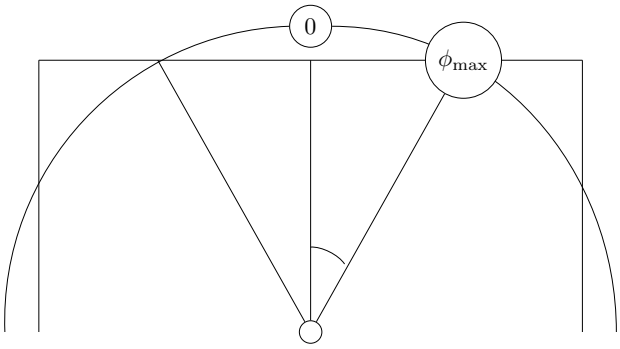


Figure 1: A circle that is partly inside and partly outside a square.

The R^2 distribution can be calculated from the R distribution. For two random variables X, Y and a function $V : X \to Y$ and given distribution $n(x)$, the distribution of Y can be calculated with the dirac delta $\delta(x)$ by

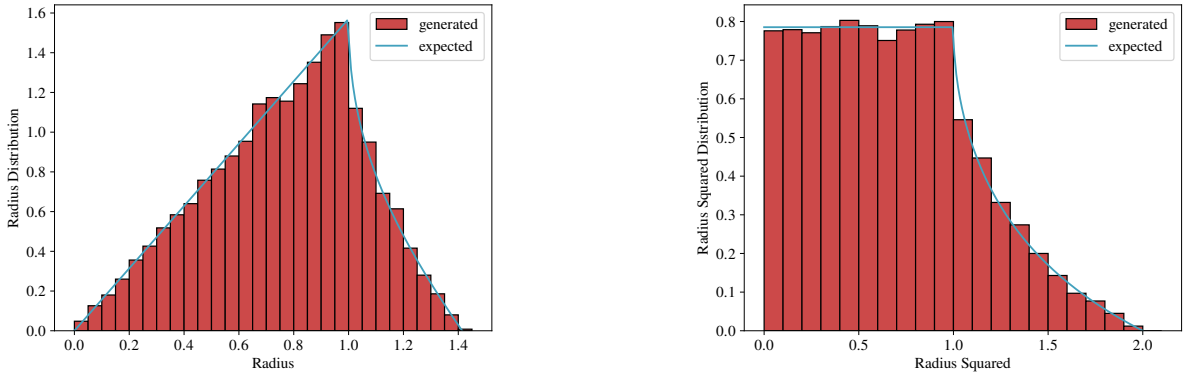
$$p(y) = \int_X dx\, n(x)\delta(y - V(x)).$$

For the variable $\rho = r^2$ we get

$$\begin{aligned} p(\rho) &= \frac{\pi}{2} \int_0^\infty dr\, r(1 - f(r))\delta(r^2 - \rho) \\ &= \frac{\pi}{4} - \begin{cases} 0 & \rho \leq 1 \\ \arctan\left(\sqrt{\rho - 1}\right) & 1 < \rho \leq 2 \\ \frac{\pi}{4} & \rho > 2 \end{cases} \end{aligned}$$

In fig. 2b it is shown that the data satisfies the expectation.

The distribution of the indicator variable $[X^2 + Y^2 \leq 1]$ is shown in fig. 3.



(a) Radii of generated points.

(b) Squared radii of generated points.

Figure 2: Normalized histograms of generated data with $P = 10\,000$ and $X = 1$ compared to expected distributions.

2 Rearranging Calculations

The number of calculations is now split into $P = 100$ and $X = 100$. In this case we get a value of

$$\pi_\mathrm{f} = 3.15 \pm 0.16. \tag{5}$$

This value has a much smaller error (5.1 %) compared to section 1. A histogram for the distribution of π_x is shown in fig. 4. In that case the π_x histogram resembles a gaussian distribution.

With $P = 1$ and $X = 10\,000$ we get a value of

$$\pi_\mathrm{f} = 3.2 \pm 1.7, \tag{6}$$

which is identical to the calculation from section 1. In fact, they have to be the same because they are mathematically the same. In the special case where $X = 1$, the final π value is given by

$$\pi_\mathrm{f} = \frac{4}{P} \sum_{p=1}^{P} [r_p^2 \leq 1] \qquad \Delta\pi_\mathrm{f} = \sqrt{\frac{1}{P-1} \sum_{p=1}^{P} (4[r_p^2 \leq 1] - \pi_\mathrm{f})^2}$$

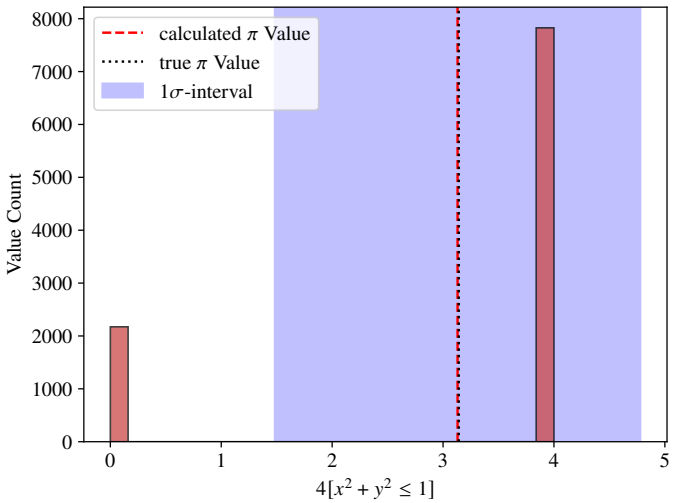


Figure 3: Histogram of the indicator variable $[X^2 + Y^2 \leq 1]$ for an experiment with $P = 10\,000$.

with using the definition of the variance from above. For the special case of $P = 1$ and the uncertainty from eq. (2) we get

$$\pi_\mathrm{f} = \frac{4}{X}\sum_{x=1}^{X}[r_x^2 \leq 1] \qquad \Delta\pi_\mathrm{f} = \sqrt{\frac{1}{X-1}\sum_{x=1}^{X}(4[r_x^2 \leq 1] - \pi_\mathrm{f})^2}.$$

For $X = P$ it is clear that they are the same, so similar results are expected. Since we can compare the results for both extreme cases, one can make the assumption that the definition of eq. (3) for $X = 1$ is as good as the definition in 2 for the general case.

Rearranging how we spent the random numbers makes a difference, because with using fewer experiments the uncertainty should get higher because there are fewer values that contribute to the uncertainty, but on the other hand the opposite will happen because the fewer π_x values that we calculate will be more precise because they were calculated with a bigger number of generated points. This will be shown in section 3.

3 Uncertainty Dependency of X and P

Now we focus on how the uncertainty changes as a function of X and P. The π values were calculated for 16 different combinations of point- and experiment count. The results are shown in table 1 with the corresponding histograms for the π_x distributions. It is easy to see that for a constant P the uncertainty does not change with higher X which is surprising, because it means that for a given number of generated points the π value cannot be made more precise with higher experiment count. The uncertainties for every P are shown in fig. 7 where no particular correlation can be seen. In fig. 7 a correlation between the uncertainty and P for constant X is clearly visible. For the log-log plot in fig. 8 a linear function would be a good approximation, thus we can write

$$\log \mathrm{err}(P) = -n \log P + b$$

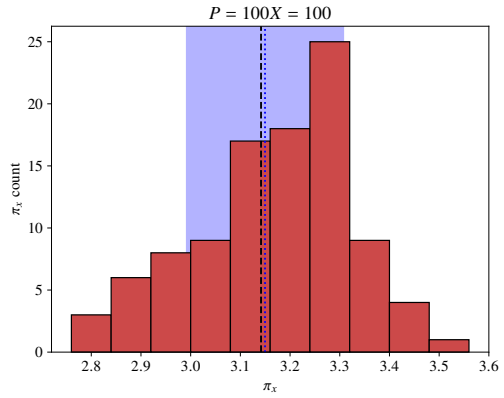


Figure 4: Histogram of calculated π values with $P = 100$ and $X = 100$.

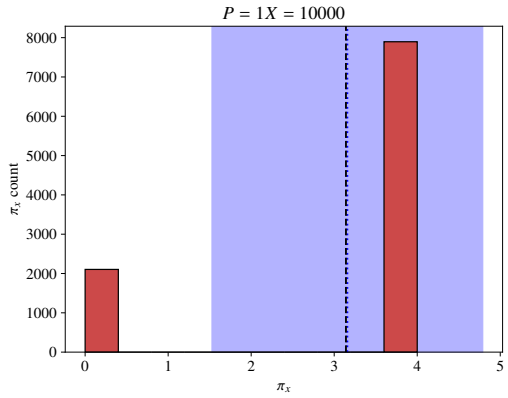


Figure 5: Histogram of calculated π values with $P = 1$ and $X = 10\,000$.

Table 1: Calcuated π values for different P and X.

$X \backslash P$	10	100	1000	10000
10	3.20 ± 0.62	3.104 ± 0.136	3.109 ± 0.047	3.143 ± 0.016
100	3.072 ± 0.518	3.171 ± 0.171	3.140 ± 0.053	3.144 ± 0.017
1000	3.125 ± 0.529	3.136 ± 0.164	3.141 ± 0.052	3.141 ± 0.017
10000	3.144 ± 0.521	3.142 ± 0.164	3.142 ± 0.052	3.142 ± 0.016

with $b, n > 0$. This results in the relation

$$\mathrm{err}(P) = \frac{\mathrm{e}^b}{P^n}$$

for the uncertainty. This function will not be fitted to the data but from visual inspection it is clear that the same relation with same parameters b and n will hold for every X.

With this information we can conclude that the most efficient way to calculate π with a given PX is to maximize P and keep X small, although From section 1 it is known that X has to be atleast bigger than 1.

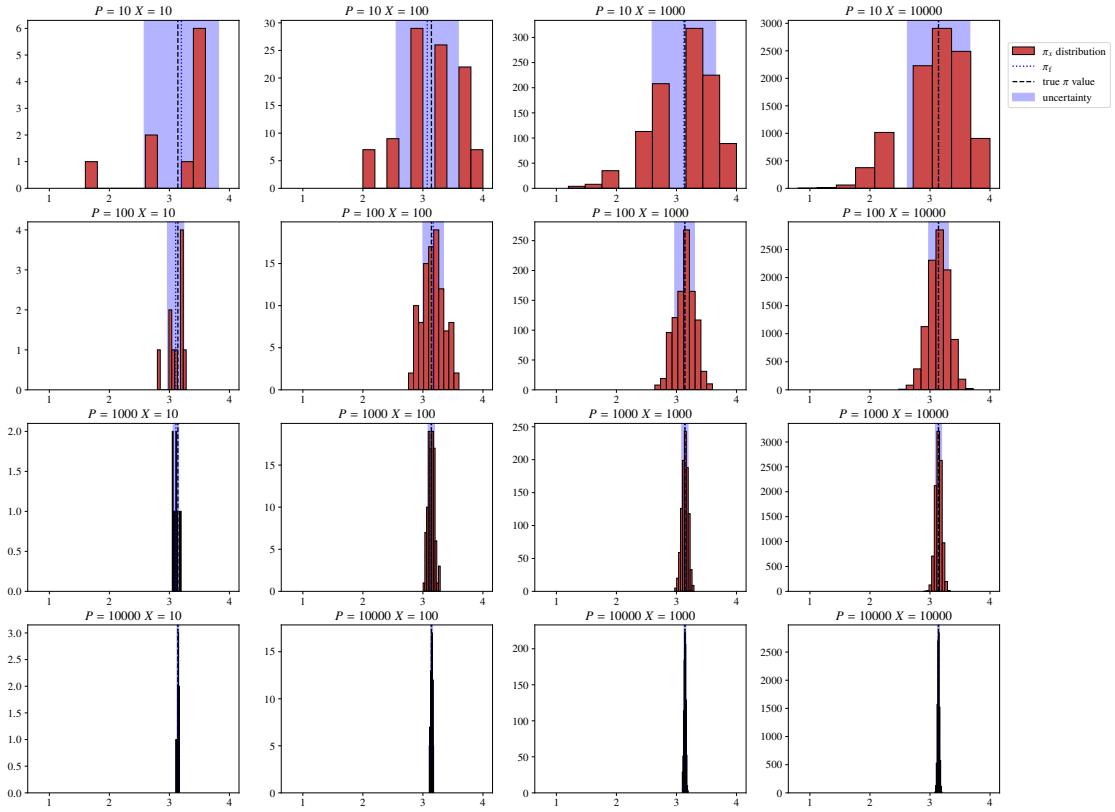


Figure 6: π_x distributions for different combinations of P and X.

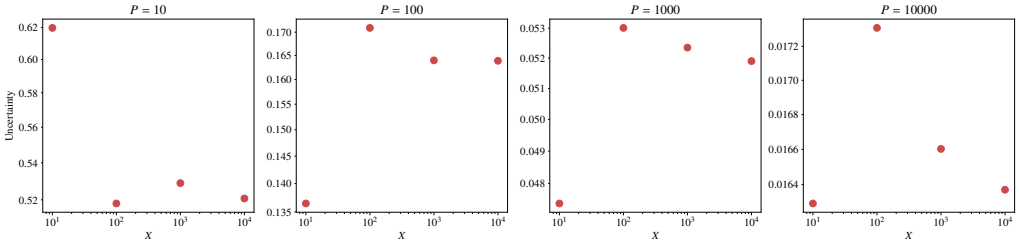


Figure 7: Uncertainty as a function of X for different P values.

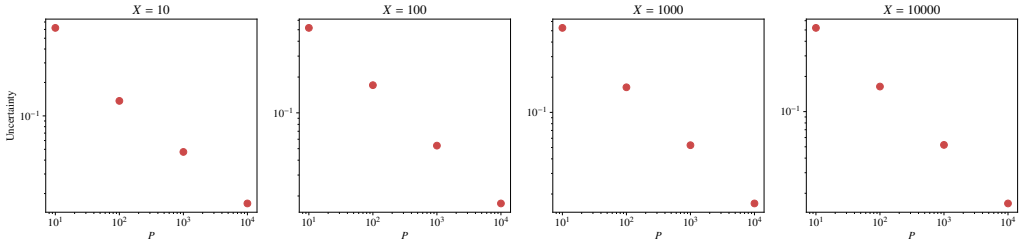


Figure 8: Uncertainty as a function of P for different X values.