Computational Physics
Problem Set 7

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November 8, 2021

1 Monte Carlo Integration

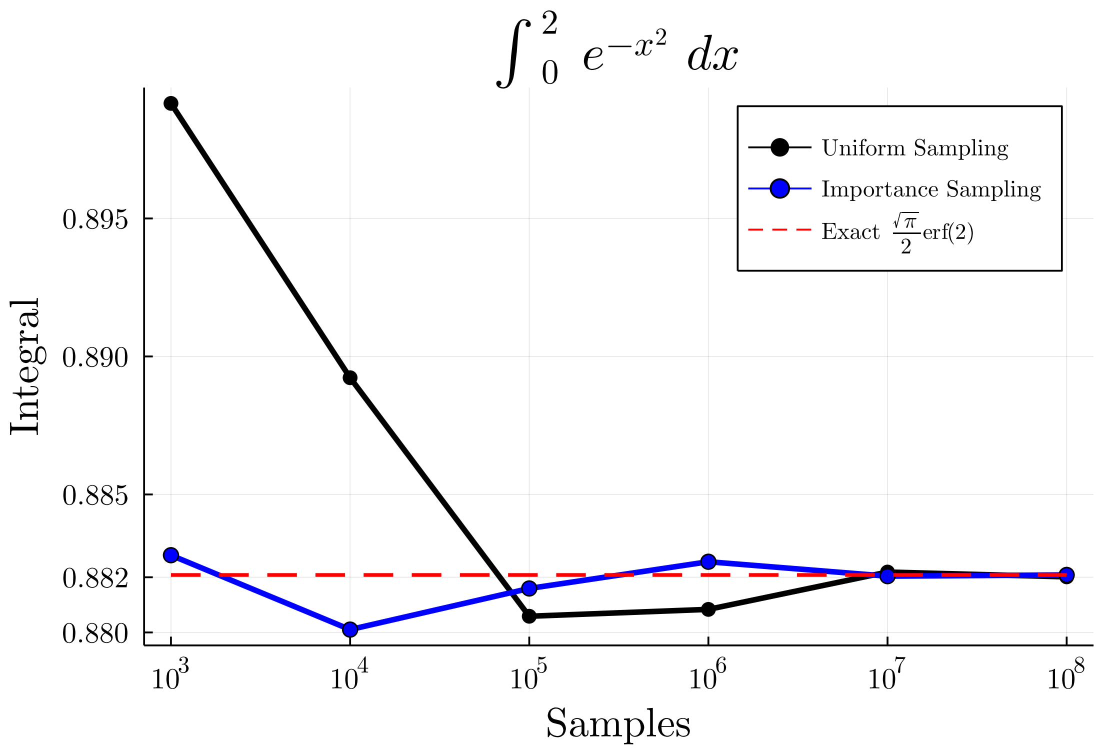
1.1 Uniform Sampling vs. Importance Sampling: $\frac{\sqrt{\pi}}{2}\operatorname{erf}(2) = \int_0^2 e^{-x^2}\,dx$

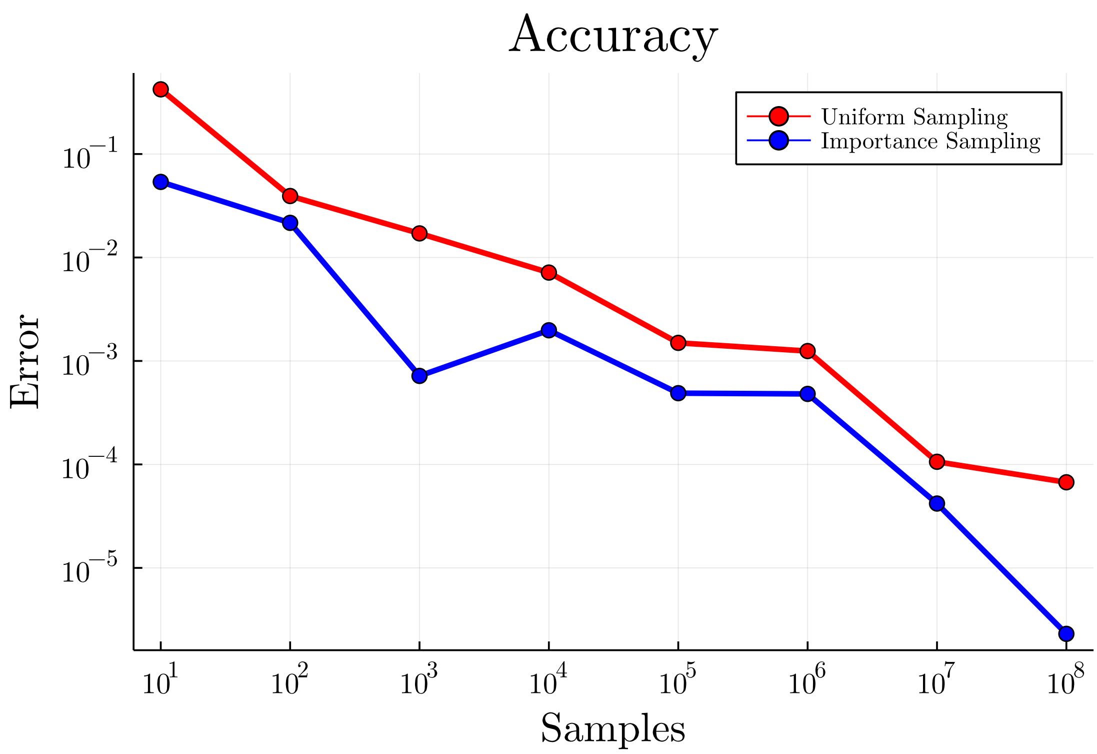
Table 1: The exact value of the integral $\frac{\sqrt{\pi}}{2}\operatorname{erf}(2) = \int_0^2 e^{-x^2}\,dx$ up to the 6th decimal is 0.882081. The runtimes are from an AMD Ryzen 7 5800H @3.2GHz (up to 4.4GHz)

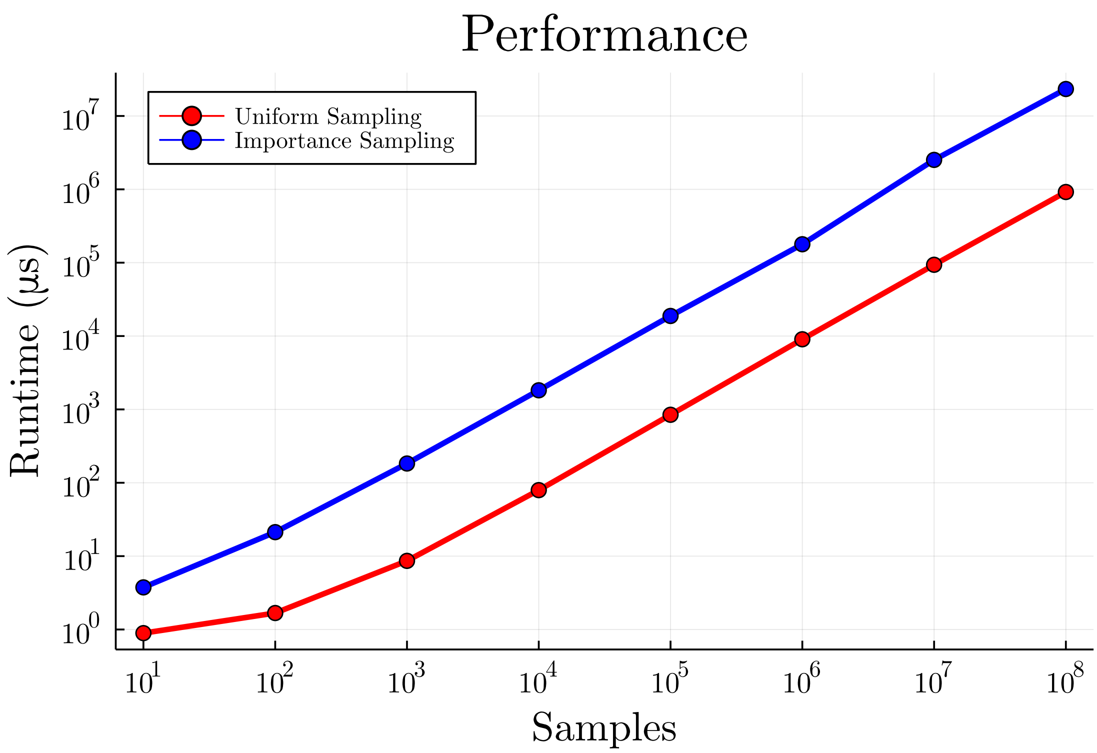
Number of Samples	Calculated Integral		Runtime	
	Uniform Sampling	Importance Sampling	Uniform Sampling	Importance Sampling
10	0.460596	0.93583	0.891 513 µs	3.748 94 µs
100	0.921345	0.903689	1.6772 µs	21.2343 µs
1000	0.899169	0.882798	8.6187 µs	183.041 µs
10000	0.889229	0.880103	79.3509 µs	1.822 76 ms
100000	0.880586	0.881593	844.887 µs	18.7801 ms
1000000	0.880835	0.882562	9.040 39 ms	178.5040 ms
10^7	0.882187	0.88204	93.6652 ms	2.519 25 s
10^8	0.882014	0.882084	0.919 785 s	23.3132 s

Table 2: Errors of each method. The "actual" error is the deviation of the calculation from $\frac{\pi}{2}\,\mathrm{erf}(2)$.

Number of Samples	Calculated Standard Error		Actual Error	
	Uniform Sampling	Importance Sampling	Uniform Sampling	Importance Sampling
10	0.211308	0.094789	0.421485	0.0537491
100	0.0699633	0.0242373	0.0392635	0.021608
1000	0.0220645	0.00838951	0.0170874	0.000716757
10000	0.00685873	0.0026753	0.00714762	0.00197877
100000	0.00217824	0.000843176	0.00149538	0.000488134
1000000	0.000688905	0.000265692	0.00124646	0.000480197
10^7	0.000217995	$8.413\,55 \times 10^{-5}$	0.000106063	4.187×10^{-5}
10^8	$6.893\,27 \times 10^{-5}$	$2.660\,06 \times 10^{-5}$	$6.720\,89 \times 10^{-5}$	$2.303\,87 \times 10^{-6}$




Accuracy
Uniform Sampling
Importance Sampling
Error
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
Samples


Performance
Uniform Sampling
Importance Sampling
Runtime (μs)
10^{7}
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7} 10^{8}
Samples

1.2 Center of Mass of Sphere with Linearly Increasing Density in One Direction

A sphere with radius R has a density that linearly increases in the z direction, such that the density at $z = 2R$ is twice the density at $z = 0$. To calculate the position of the center of mass, we must evaluate the integral

$$\mathbf{r}_{cm} = \frac{\int_{\text{sphere}} \rho(\mathbf{r})\mathbf{r}\, dV}{\int_{\text{sphere}} \rho(\mathbf{r})\, dV}. \tag{1}$$

Since the sphere is symmetric in the x and y directions, the center of mass is at $x = 0$ and $y = 0$. It remains to find the z position of the center of mass. In polar coordinates

$$\rho(z = 2R) = 2\rho(z = 0) \implies \rho(r = R, \theta = 0) = 2\rho(r = R, \theta = \pi) \tag{2}$$

$$\xRightarrow{\rho(z) is linear} \rho(r, \theta) = \rho_0\Big(3 + \frac{r}{R}\cos\theta\Big) \implies \tag{3}$$

$$z_{cm} = \frac{\displaystyle\int_{\text{sphere}} z\rho\, dV}{\displaystyle\int_{\text{sphere}} \rho\, dV} = \frac{\displaystyle\int_0^R \int_0^\pi \int_0^{2\pi} \rho_0\Big(3 + \frac{r}{R}\cos\theta\Big) r^3 \sin\theta\cos\theta\, d\varphi\, d\theta\, dr}{\displaystyle\int_0^R \int_0^\pi \int_0^{2\pi} \rho_0\Big(3 + \frac{r}{R}\cos\theta\Big) r^2 \sin\theta\, d\varphi\, d\theta\, dr} \tag{4}$$

$$z_{cm} = \frac{\displaystyle\int_0^R \int_0^\pi \Big(3 + \frac{r}{R}\cos\theta\Big) r^3 \sin\theta\cos\theta\, d\theta\, dr}{\displaystyle\int_0^R \int_0^\pi \Big(3 + \frac{r}{R}\cos\theta\Big) r^2 \sin\theta\, d\theta\, dr} \tag{5}$$

We can use the Monte Carlo integration method to calculate (5) and find the center of mass. These integrals can also be calculated analytically to check the accuracy of the numerical results:

$$z_{cm} = \frac{R^4 \displaystyle\int_0^\pi \left(\frac{3}{4} + \frac{\cos\theta}{5}\right) \sin\theta\cos\theta\, d\theta}{R^3 \displaystyle\int_0^\pi \left(1 + \frac{\cos\theta}{4}\right) \sin\theta\, d\theta} \tag{6}$$

$$= \frac{\frac{3}{8}\displaystyle\int_0^\pi \sin(2\theta)\, d\theta + \frac{1}{5}\int_{-1}^{+1} \cos^2\theta\, d(\cos\theta)}{\displaystyle\int_0^\pi \left(\sin\theta + \frac{\sin(2\theta)}{2}\right) d\theta} R \tag{7}$$

$$= \frac{-\frac{3}{16}\cos(2\theta)\Big|_0^\pi + \frac{x^3}{15}\Big|_{-1}^{+1}}{-\cos\theta\Big|_0^\pi - \frac{\cos(2\theta)}{4}\Big|_0^\pi} \tag{8}$$

$$\boxed{z_{cm} = \frac{R}{15}} \tag{9}$$

Numerically evaluating the two integrals in (5) by the Monte Carlo Integration method, uniformly sampling 40 million points, we get

$$z_{cm} = (0.06667 \pm 0.00009)R, \tag{10}$$

which is exactly equal to $R/15$ up to the 5th decimal place.

2 Metropolis Algorithm

Table 3: For 10^8 samples

Step Size *Delta*	Acceptance Rate a_r	Correlation Length ξ
15.8846	0.1004	7.23 ± 0.03
7.969	0.19996	3.53 ± 0.03
5.3048	0.300005	2.3 ± 0.03
3.888	0.4003	1.84 ± 0.01
2.9486	0.4991	2.06 ± 0.02
2.2094	0.5992	2.72 ± 0.02
1.578	0.7007	4.11 ± 0.02
1.0236	0.8002	7.89 ± 0.02
0.5	0.9008	27.76 ± 0.01

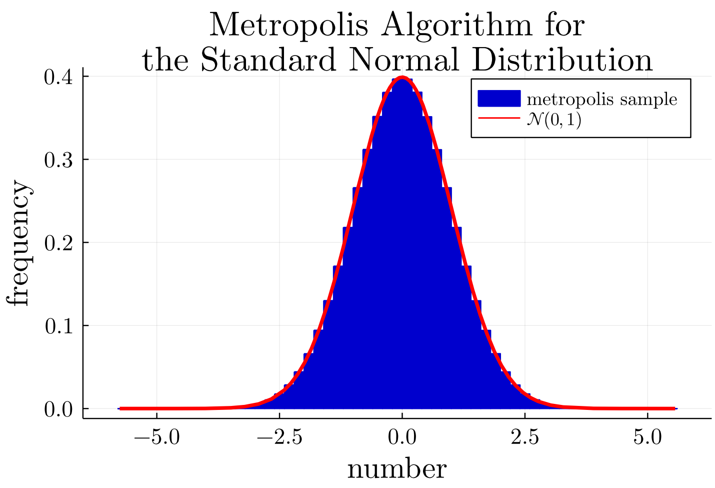
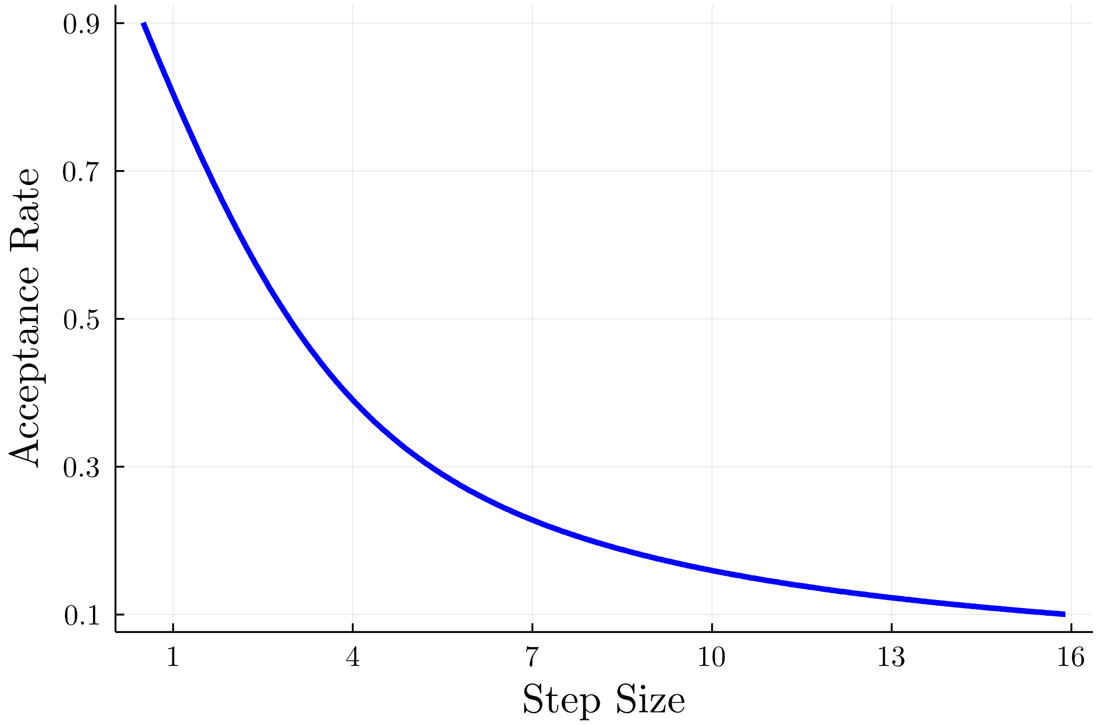
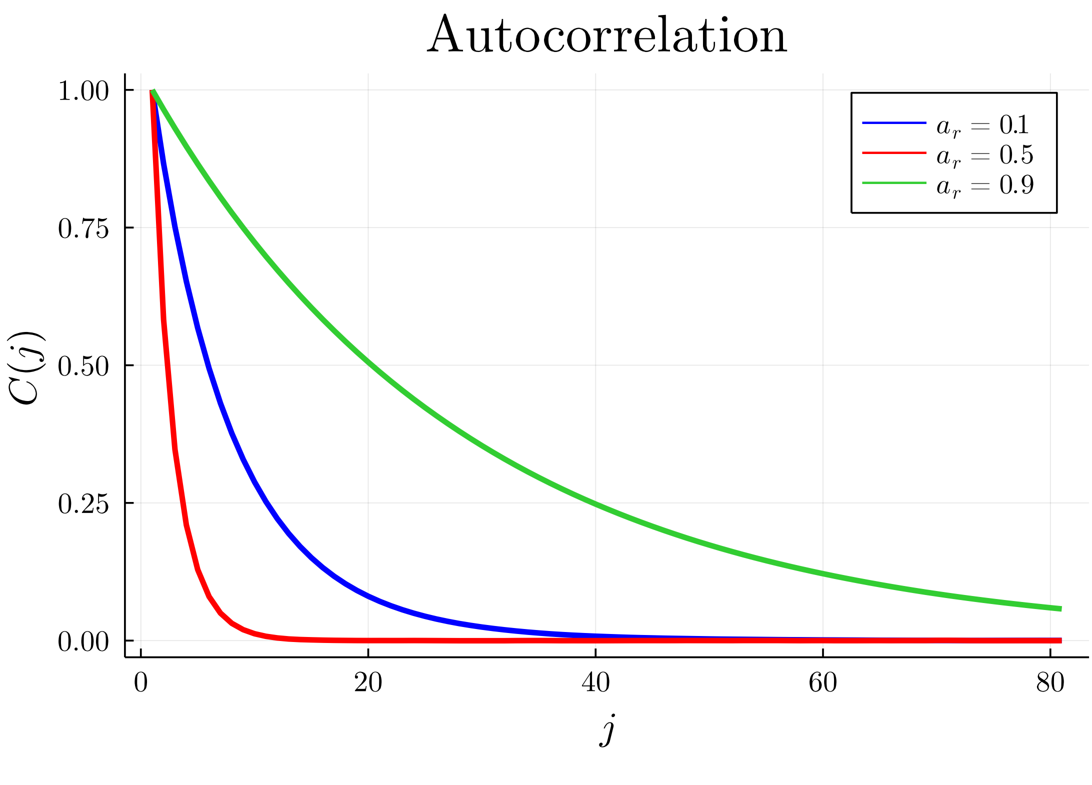


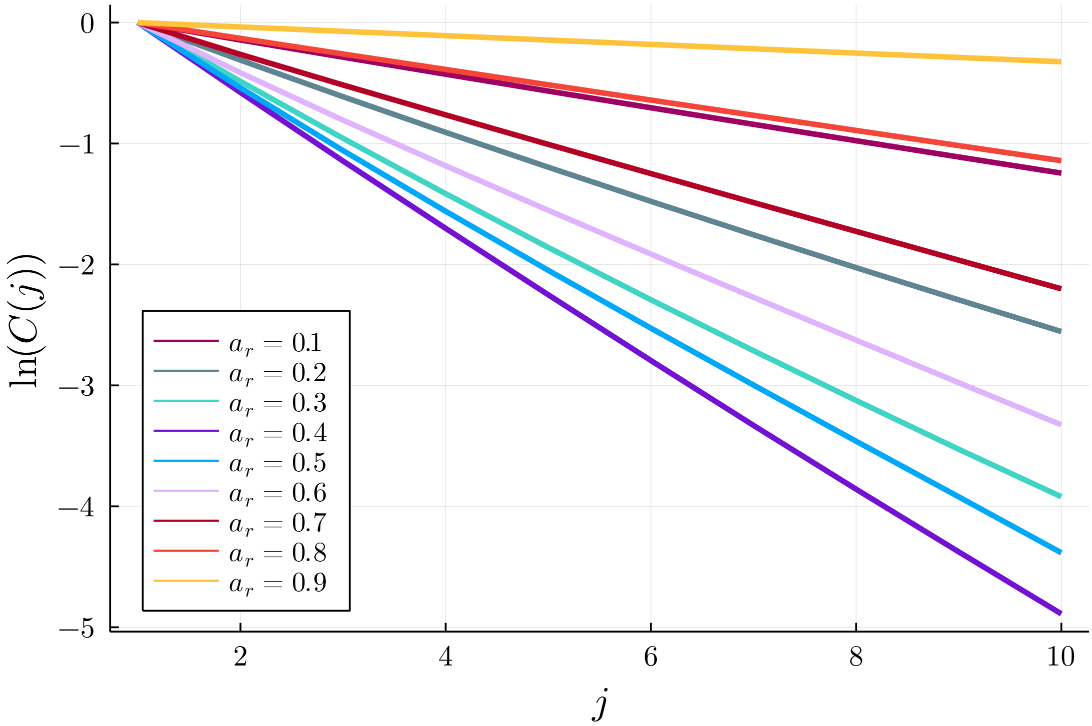
Figure 1: For 10^8 samples, step size 3 and acceptance rate 0.49



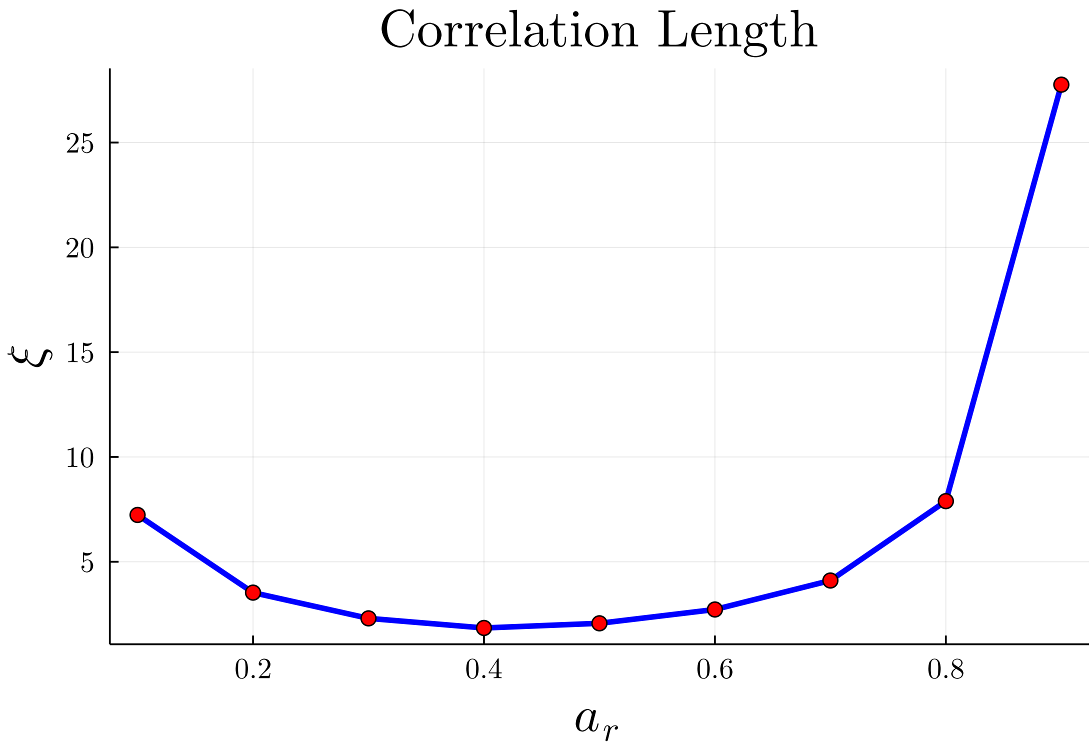
0.9
0.7
0.5
0.3
0.1
Acceptance Rate
1
4
7
10
13
16
Step Size



Autocorrelation
1.00
0.75
0.50
0.25
0.00
$C(j)$
0
20
40
60
80
j
$a_r = 0.1$
$a_r = 0.5$
$a_r = 0.9$



$\ln(C(j))$
j
$a_r = 0.1$
$a_r = 0.2$
$a_r = 0.3$
$a_r = 0.4$
$a_r = 0.5$
$a_r = 0.6$
$a_r = 0.7$
$a_r = 0.8$
$a_r = 0.9$



Correlation Length
ξ
a_r