Uniform sampling from an n-sphere

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Abstract

In this paper we discuss the problem of generating uniformly distributed points inside or on the surface of an n-dimensional unit sphere. We propose two methods: the first is a transformation to n-spherical coordinates and uses a Gaussian covering distribution and acceptance/rejection sampling. The second generates an n-dimensional Gaussian distribution, whose isotropic n-vectors are projected onto the surface. The acceptance/rejection method samples hyperspherical angles with $sin^k(\phi)$ distributions. The isotropic method is by far the simplest and gives a result directly in cartesian n-space coordinates.

1 Introduction

It is well known that inscribing a unit ball inside an n dimensional cube of side $d = 2$ (twice the unit radius) is a very ineffective procedure as an acceptance/rejection method for generating a uniformly distributed sample inside the ball. Indeed, the acceptance ratio is given by the ratio of the volume of the unit ball to the volume 2^n of the inscribing cube. In two dimensions, this ratio [1] is $\pi/4$, in three dimensions $\pi/6$. When n is large, however, this ratio gets very small. The volume of an n dimensional unit sphere can be computed by using Gauss's expression $\int e^{-x^2} dx = \sqrt{\pi}$, so

$$\pi^{n/2} = \int_{r=0}^{\infty} e^{-r^2} r^{n-1} dr \int d\Omega_n \tag{1}$$

where $d\Omega_n$ is the increment of n-dimensional solid angle. The r integral is easy, we get

$$\Omega_n = \int d\Omega_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}. \tag{2}$$

Using this value for the solid angle, the ratio of the unit n-sphere volume to the volume of the $d = 2$ sided n-cube is

$$\begin{aligned}
\frac{\text{vol. of unit } n\text{-sphere}}{\text{vol. } n\text{-cube}} &= \frac{\Omega_n \int_0^1 dr r^{n-1}}{2^n} \\
&= \frac{\pi^{n/2}}{n2^{n-1}\Gamma(n/2)} \\
&\sim \sqrt{\frac{2}{\pi}}\,\frac{1}{n}\,(\frac{\sqrt{\pi e}}{2})^n\,(\frac{n}{2})^{-\frac{n-1}{2}} \quad \text{for large } n.
\end{aligned} \tag{3}$$

For example, for $n = 20$, this ratio (3) is approximately $\frac{1}{4} \times 10^{-7}$. In the following, we give two more effective methods. The first gives the point coordinates as hyperspherical angles, then we show a procedure which gives the points directly in n-space cartesian coordinates.

2 n-Spherical coordinates

We first construct an $n-1$ dimensional system of angular coordinates suitable for an n-sphere with radius r. Similar analysis can be found in [2], for example. The $n-1$ angles ϕ_p, $p = 1...n-1$, $(0 \leq \phi_{n-1} \leq 2 \cdot \pi$, otherwise $0 \leq \phi_p \leq \pi$, for $p = 1..n-2)$ give cartesian coordinates

$$\begin{aligned}
x_1 &= r\ cos(\phi_1) \\
x_2 &= r\ sin(\phi_1)cos(\phi_2) \\
x_3 &= r\ sin(\phi_1)sin(\phi_2)cos(\phi_3) \\
x_4 &= r\ sin(\phi_1)sin(\phi_2)sin(\phi_3)cos(\phi_4) \\
&... \\
x_{n-1} &= r\ sin(\phi_1)sin(\phi_2)sin(\phi_3)...sin(\phi_{n-2})cos(\phi_{n-1}) \\
x_n &= r\ sin(\phi_1)sin(\phi_2)sin(\phi_3)...sin(\phi_{n-2})sin(\phi_{n-1})
\end{aligned} \tag{4}$$

or, more concisely

$$\begin{aligned}
x_k &= r\ cos(\phi_k) \prod_{l=1}^{k-1} sin(\phi_l) \quad \text{for } k = 1...n-1, \\
x_n &= r \prod_{l=1}^{n-1} sin(\phi_l)
\end{aligned} \tag{5}$$

The inverse transformation is

$$\begin{aligned}
\phi_k &= \cos^{-1}\left(\frac{x_k}{\sqrt{r^2-\sum_{i=1}^{k-1} x_i^2}}\right), \quad \text{for } k = 1...n-2, \text{ and} \\
\phi_{n-1} &= \tan^{-1}\left(\frac{x_n}{x_{n-1}}\right).
\end{aligned} \tag{6}$$

We will also need the Jacobian of this transformation

$$J(x,\{r,\phi\}) = \begin{vmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_1}{\partial \phi_1} & \cdots & \frac{\partial x_1}{\partial \phi_{n-1}} \\ \frac{\partial x_2}{\partial r} & \frac{\partial x_2}{\partial \phi_1} & \cdots & \frac{\partial x_2}{\partial \phi_{n-1}} \\ & \cdots & & \\ \frac{\partial x_n}{\partial r} & \frac{\partial x_n}{\partial \phi_1} & \cdots & \frac{\partial x_n}{\partial \phi_{n-1}} \end{vmatrix}$$

It is straightforward to write this as

$$J = \prod_{p=1}^{n-1}((\prod_{q=1}^{p} sin(\phi_q))cos(\phi_p))\times$$

$$\begin{vmatrix} 1 & -r\ tan(\phi_1) & & & \bigcirc \\ 1 & r\ cot(\phi_1) & -r\ tan(\phi_2) & & \\ 1 & r\ cot(\phi_1) & r\ cot(\phi_2) & -r\ tan(\phi_3) & \\ ... & & & & \\ 1 & r\ cot(\phi_1) & r\ cot(\phi_2) & ... & -r\ tan(\phi_{n-2}) \\ 1 & r\ cot(\phi_1) & r\ cot(\phi_2) & ... & r\ cot(\phi_{n-1}) \end{vmatrix}$$

Which after pulling out some factors gives

$$J = r^{n-1}\prod_{p=1}^{n-1}(cos^2(\phi_p)\prod_{q=1}^{p-1} sin(\phi_q)) \times$$

$$\begin{vmatrix} 1 & -(tan(\phi_1))^2 & & & \bigcirc \\ 1 & 1 & -(tan(\phi_2))^2 & & \\ 1 & 1 & 1 & -(tan(\phi_3))^2 & \\ & ... & & & \\ 1 & 1 & 1 & ... & -(tan(\phi_{n-1}))^2 \\ 1 & 1 & 1 & ... & 1 \end{vmatrix}$$

Cramer's rule for the determinant puts the reduction in successive sub-blocks from upper left to lower right and yields

$$
\begin{aligned}
J &= r^{n-1}\prod_{p=1}^{n-1}(\prod_{q=1}^{p-1} sin(\phi_q)) \\
&= r^{n-1}\prod_{p=1}^{n-1}(sin(\phi_p))^{n-p-1}. \qquad (7)
\end{aligned}
$$

Given the cartesian coordinate transformation (4) and the Jacobian (7), we now proceed to derive an algorithm for sampling uniformly on the surface of the n-sphere. Since the r coordinate can be sampled using direct inversion: $r = r_0 u^{1/n}$, where $u \in (0,1)$ uniformly and r_0 is the n-sphere radius (e.g. $r_0 = 1$), an algorithm for uniform sampling on the surface of the unit n-ball suffices for both interior and surface problems for arbitrary radii.

3 A Gaussian covering

The following inequality shows the truncated Gaussian $e^{-k\,(\phi-\pi/2)^2/2}$, for $0 \le \phi \le \pi$, will serve as a covering for the $(sin(\phi))^k$ distributions of each independent angle ϕ_p $(k = n-p-1)$ which appears in (7)

$$sin(\phi) \le e^{-(\phi-\pi/2)^2/2}.$$

This inequality is obvious from a graph (see Figure 1), but is easily proved. By symmetry, it suffices to show for $0 \le x \le \pi/2$ that

$$
\begin{aligned}
e^{-x^2/2} - cos(x) &= \sum_{j=1}^{\infty}\frac{1-\frac{1}{(4j)!!}}{2^{2j}(2j)!}x^{4j} - \sum_{j=1}^{\infty}\frac{1-\frac{1}{(4j+2)!!}}{2^{2j+1}(2j+1)!}x^{4j+2} \\
&\ge \sum_{j=1}^{\infty}\frac{1}{2^{2j}(2j)!}\frac{7}{8}x^{4j} - \sum_{j=1}^{\infty}\frac{1}{2^{2j+1}(2j+1)!}x^{4j+2} \\
&\ge (\frac{7}{8}-\frac{\pi^2}{24})\sum_{j=1}^{\infty}\frac{1}{2^{2j}(2j)!}x^{4j} \\
&\ge 0.
\end{aligned}
$$

Here we use the standard notation (e.g. [3]) $k!! \equiv k\cdot(k-2)\cdot(k-4)...(1)$, if k is odd, and $k!! \equiv k\cdot(k-2)\cdot(k-4)...(2)$, if k is even.

Figure 1 shows the covering of $(sin(\phi))^k$ for $k = 1, 5$ and 20. For each $\phi = \phi_p$ in (7), we need to sample from the (unnormalized) distribution function $e^{-k\,(\phi-\pi/2)^2/2}$ (here $k = n-p-1$) and apply the acceptance-rejection criteria [5][6] shown in Figure 2.

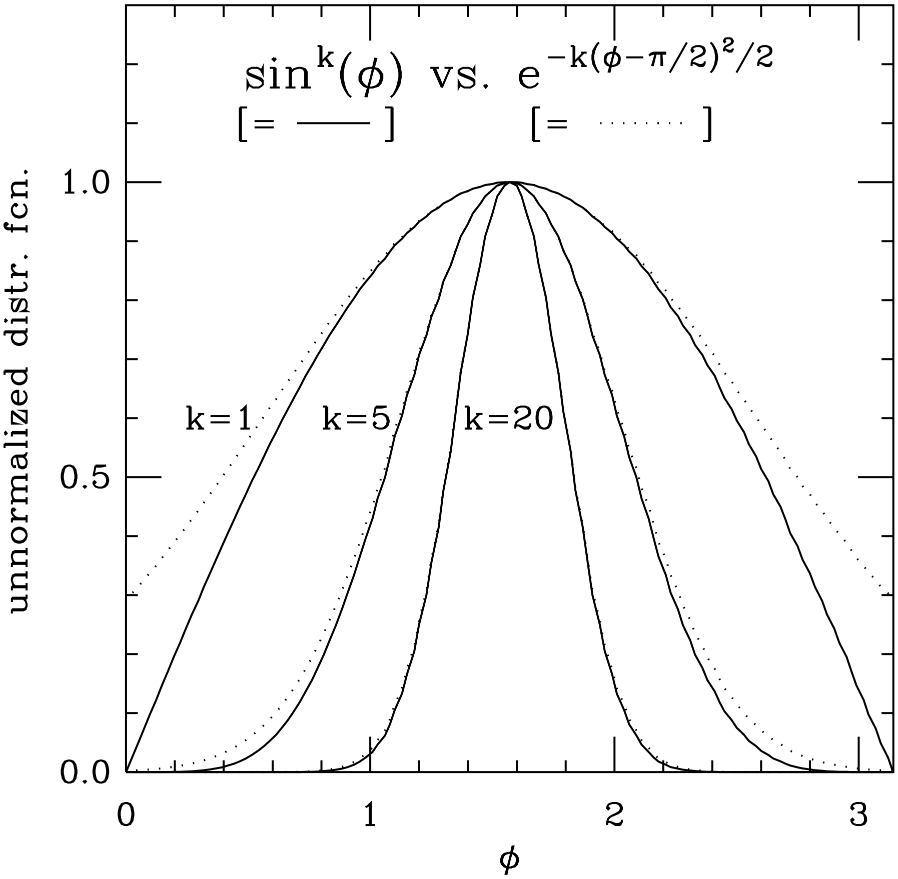

Figure 1: $sin^k(\phi)$ **vs.** $e^{-k\,(\phi-\pi/2)^2/2}$

We must now compute the acceptance ratio for each $k = n - p - 1$ angle in (7). As a practical matter we do not sample from the truncated Gaussian distribution $(0 \leq \phi \leq \pi)$, but rather use (say) the Box-Muller method [7] and reject those test ϕ values which fall outside this finite interval. The acceptance ratio is given by the ratio of the areas under the $(sin(\phi))^k$ for $0 \leq \phi \leq \pi$ curve divided by the area under the covering distribution $e^{-\frac{k}{2}(\phi-\pi/2)^2}$ for $-\infty < \phi < \infty$:

$$\begin{aligned}
\mathcal{A}_k &= P(0 \leq \phi \leq \pi) \cdot \frac{\int_0^\pi (sin(\phi))^k d\phi}{\int_0^\pi e^{-\frac{k}{2}(\phi-\frac{\pi}{2})^2} d\phi} \\
&= \frac{\int_0^\pi (sin(\phi))^k d\phi}{\int_{-\infty}^\infty e^{-\frac{k}{2}\,(\phi-\pi/2)^2} d\phi} = \sqrt{\frac{k}{2\pi}}\ \int_0^\pi (sin(\phi))^k d\phi \qquad (8)
\end{aligned}$$

The integral on the right hand side is given in [4],

```
AR1: v ← BOX-MULLER              # pick univariant normal [7][8]
     φ ← v/√k + π/2              # possible φ
     if(φ < 0 or φ > π)
       goto AR1                  # truncated distribution
     endif

     pick u ∈ (0,1)
     if((sin(φ))^k ≥ u · e^{-(k/2)(φ-π/2)^2})
       accept φ
     else
       goto AR1                  # pick another normal
     endif
```

Figure 2: **Pseudo-code for the Gaussian covering method**

$$\int_0^{\pi} (sin(\phi))^k d\phi = \frac{\sqrt{\pi}\Gamma(\frac{k}{2}+\frac{1}{2})}{\Gamma(\frac{k}{2}+1)}. \tag{9}$$

Since each angle ϕ_p is independent, each may be sampled in turn until a satisfactory $n-1$-vector $\vec{\phi}$ is obtained. This is not the case for the inscribing procedure mentioned in the Introduction §1. There, a possible point $\vec{x}$ is generated and if $|\vec{x}| \leq 1$, $\vec{x}$ is accepted. In order to assess the efficiency of this acceptance/rejection method, the average acceptance ratio for $k = 1...n-2$ in (7) is needed. Note that $\phi_{n-1} \in (0, 2\pi)$ is uniformly distributed, thus A/R is not used for this angle. Additionally, $\phi_{n-2} \in (0,\pi)$ has distribution function $sin(\phi_{n-2})$ (unnormalized), so may be sampled by direct inversion. For simplicity, the A/R analysis below includes ϕ_{n-2}, so the estimate (11) below is pessimistic.

$$< \mathcal{A} > = \frac{1}{n-2}\sum_{k=1}^{n-2} \mathcal{A}_k, \tag{10}$$

for large values of n. This value $< \mathcal{A} >$ when multiplied by $n-2$ and the work required to execute one step of the algorithm in Figure 2 will be the work required to generate one n-point on the unit n-sphere. For large k, the acceptance ratio for one angle has the asymptotic expansion

$$\mathcal{A}_k \sim 1 - \frac{1}{4}\frac{1}{k} + \frac{1}{32}\frac{1}{k^2} + O(\frac{1}{k^3}).$$

In fact, by numerical evaluation we have for $k \geq 1$, $\mathcal{A}_k \geq 1 - \frac{1}{4}\frac{1}{k}$, so

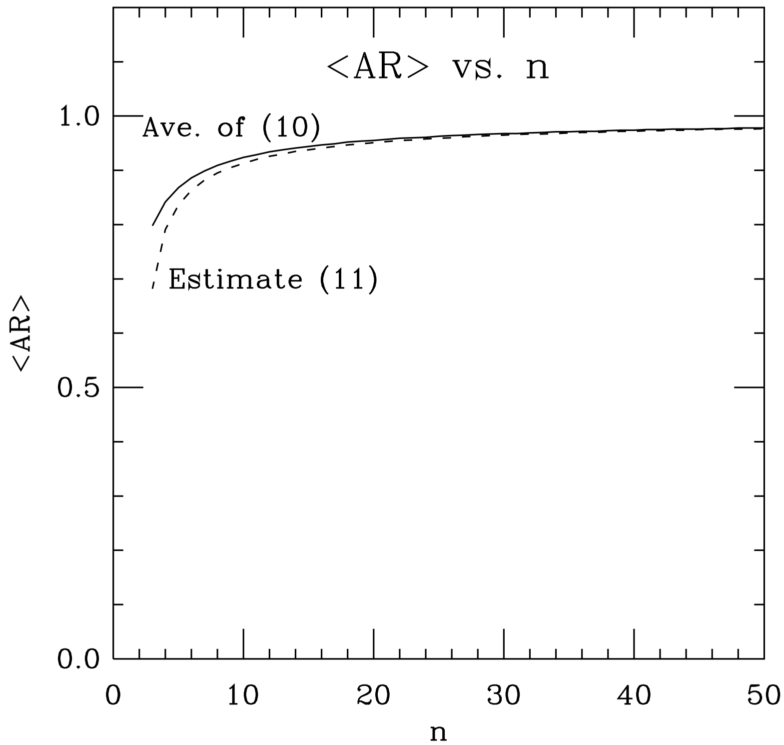

Figure 3: **Estimate (11) vs. numerical ave. of (10) for average acceptance ratio**

$$
\begin{aligned}
< \mathcal{A} > &\geq \frac{1}{n-2}\sum_{k=1}^{n-2}(1-\frac{1}{4k}) \\
&= 1-\frac{1}{4(n-2)}\sum_{k=1}^{n-2}\frac{1}{k} \\
&= 1-\frac{1}{4(n-2)}(C+\log(n-1)-\frac{1}{2(n-2)}+O(\frac{1}{(n-2)^2})),
\end{aligned}
$$

where the coefficient of the $O(\frac{1}{(n-2)^2})$ term is positive and C is Euler's constant. Thus, there exists an $0 < \alpha < \frac{1}{2}$ such that

$$\sum_{k=1}^{n-2}\frac{1}{k} \leq C+\log(n-1)-\frac{\alpha}{n-2},$$

so

$$-\sum_{k=1}^{n-2}\frac{1}{k} \geq -C-\log(n-1).$$

Finally,

$$< \mathcal{A} > \; \geq \; 1 - \frac{C}{4(n-2)} - \frac{\log{(n-1)}}{4(n-2)}. \qquad (11)$$

Figure 3 shows a comparison of the estimate (11) to a numerical computation of (10).

```
for i =1...n {
    z_i ← BOX-MULLER       # univariant normals
}
r ← sqrt(Σ_{i=1}^n z_i^2)
for i = 1...n {
    x_i ← z_i/r            # project onto surface
}
if (interior points) then
    r ← r_0 u^{1/n}        # u ∈ (0,1) uniformly
    for i = 1...n {
        x_i ← r x_i
    }
endif
```

Figure 4: **Pseudo-code for the isotropic method**

4 An isotropic Gaussian method

This procedure relies on the observation that products of independent Gaussian distributions are also Gaussian. That is, if coordinates z_i ($i = 1...n$) are each generated as zero mean, unit variance Gaussians, the resulting measure

$$\begin{aligned} d\mu(z) &= \frac{1}{(2\pi)^{n/2}}\, d^n z \prod_{i=1}^{n} exp(-\frac{z_i^2}{2}) \\ &= \frac{1}{(2\pi)^{n/2}}\, d\Omega_n \; dr r^{n-1} exp(-\frac{r^2}{2}), \end{aligned}$$

is isotropic. If R is a constant n-dimensional orthogonal "rotation" matrix, the distribution function for $z' = Rz$ will have the same form as z because ${r'}^2 = z^T(R^T R)z = z^T z = r^2$, and the volume element $d^n z' = |R| d^n z = d^n z$, since R is unimodular. Therefore, the $\vec{z}$ vectors are distributed isotropically. Vectors $\vec{x}$

$$\vec{x} = \vec{z}/r,$$

where $r = |\vec{z}|$, will also be isotropically distributed, but $|\vec{x}| = 1$ by construction. These $\vec{x}$ vectors are what we desire: uniformly distributed points on the unit n-sphere. Figure 4 shows explicitly the procedure.

5 Timing results and statistics

We have done several statistical tests, including moment analysis and χ^2 confidence level tests on the proposed n-sphere sampling methods. For example, since the sampling procedure using acceptance/rejection generates hyperspherical angles, it seemed of interest to check the quality of the x-space (cartesian coordinate) distributions given by (4). A straightforward calculation gives the distribution functions, which are, of course, not independent. The n-dimensional x-space uniform measure for the unit ball is

$$d\mu(\vec{x}) = \frac{n}{\Omega_n}\, d^n x$$

where Ω_n is the n-dimensional solid angle (2), and $|\vec{x}| \le 1$. Writing $\vec{x} = (x_1, \vec{y})$, that is separating one coordinate x_1 from the remaining $n-1$, the probability measure for this coordinate is

$$d\mu(x_1) = dx_1 \frac{n}{\Omega_n} \int_{|\vec{y}|^2 \le 1 - |x_1|^2} d^{n-1} y$$

which is easily evaluated by rescaling the y coordinates by $y_j = z_j \sqrt{1 - |x_1|^2}$, for $j = 2...n$. We get

$$\begin{aligned} d\mu(x_1) &= dx_1\, \frac{n}{\Omega_n}(1 - |x_1|^2)^{\frac{n-1}{2}} \int_{|\vec{z}|^2 \le 1} d^{n-1} z \\ &= dx_1\, \frac{n\,\Omega_{n-1}}{(n-1)\,\Omega_n}(1 - |x_1|^2)^{\frac{n-1}{2}}. \end{aligned} \tag{12}$$

Each x_i will have this distribution, which depends on all the others. We can, however, simply histogram each x_i coordinate from say a sample of N n-dimensional vectors, and compare these histograms to the distributions (12). Figures 5 and 6 show the results for a $n = 20$ dimensional space. The sample data were generated using the **zufall** random number package [8], the A/R method in Figure 2, and the transformation (4). Figure 5 shows the histogram comparisons to $d\mu(x_i)/dx_i$ (x_i

taken at the middle of the bins) multiplied by N and the bin width for x_1, x_5, x_{10}, x_{17} coordinates. In Figure 6 are shown the χ^2 confidence levels [9] (in percent). These confidence levels were computed using a more accurate procedure than the illustrated histograms. Instead of the crude mid-point function evaluations (curved lines) shown in the histograms (Figure 5), the χ^2 tests in Figure 6 used per bin numerical integration of (12) via **qag** [10] compared to the histogramed samples of the x_i's. The confidence levels are upper tail probabilities of the χ^2 distribution evaluated using the Pratt-Peizer method [11] multiplied by 100 (results in %).

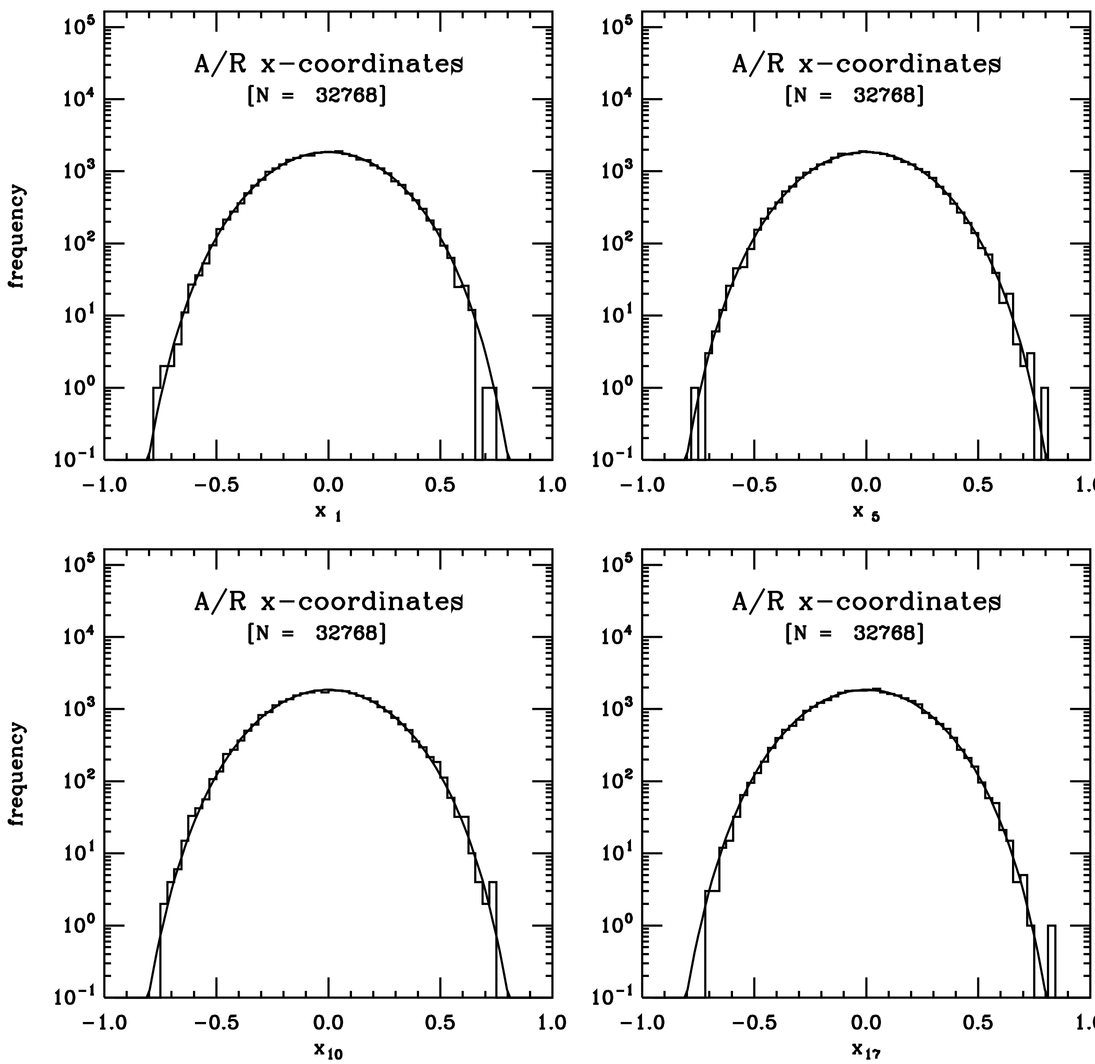

Figure 5: x**-coordinate histograms from A/R method:** n**=20**

In Figure 7 and Figure 8 are shown statistical performance results for the isotropic

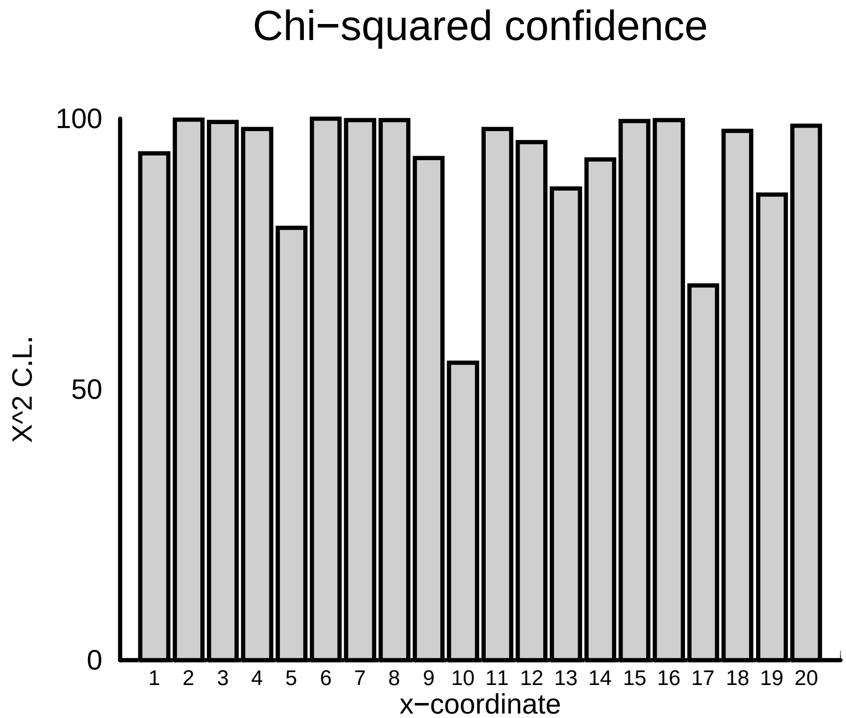

Figure 6: χ^2 **confidence levels (in %) for x coordinates generated by transformed A/R method: n=20, sample=32768, 64 bins**

method of §4. Again, the sample data used [8], but now algorithm Figure 4 and the inverse transformation (6). Confidence levels and χ^2 values were computed as in Figures 5 and 6 discussed above.

Histograms of the hyper-spherical angles $(\phi_1, \phi_7, \phi_{14}, \phi_{19})$ are shown in Figure 7, computed from (6). The curved lines show mid-bin evaluations of $\sin^{n-p-1}(\phi_p)$ multiplied by the inverse of normalization (9), by N and the histogram bin width. These curves are only for eyeball comparison of the distributions. In Figure 8 are shown the χ^2 confidence levels for histograms compared to the normalized $\sin^{n-p-1}(\phi_p)$ distributions, again using **qag** [10] integrations/bin.

Finally, in Figure 9 are shown timing data for the various methods: the unit n-sphere inscribed in an side=2 n-cube described in §1, the Gaussian covering method described in §3, and the isotropic method described in §4. For $n > 16$, timings for the inscribing method of §1 are extrapolations using (3) since for even modestly large values of n, this method is impractical. Timings for the Gaussian covering method Figure 2, and the isotropic method Figure 4, in both cartesian and hyperspherical angle representations ((4) and (6), respectively) are plotted. These timing data are results from the NEC SX-4 machine at CSCS, Manno, Switzerland.

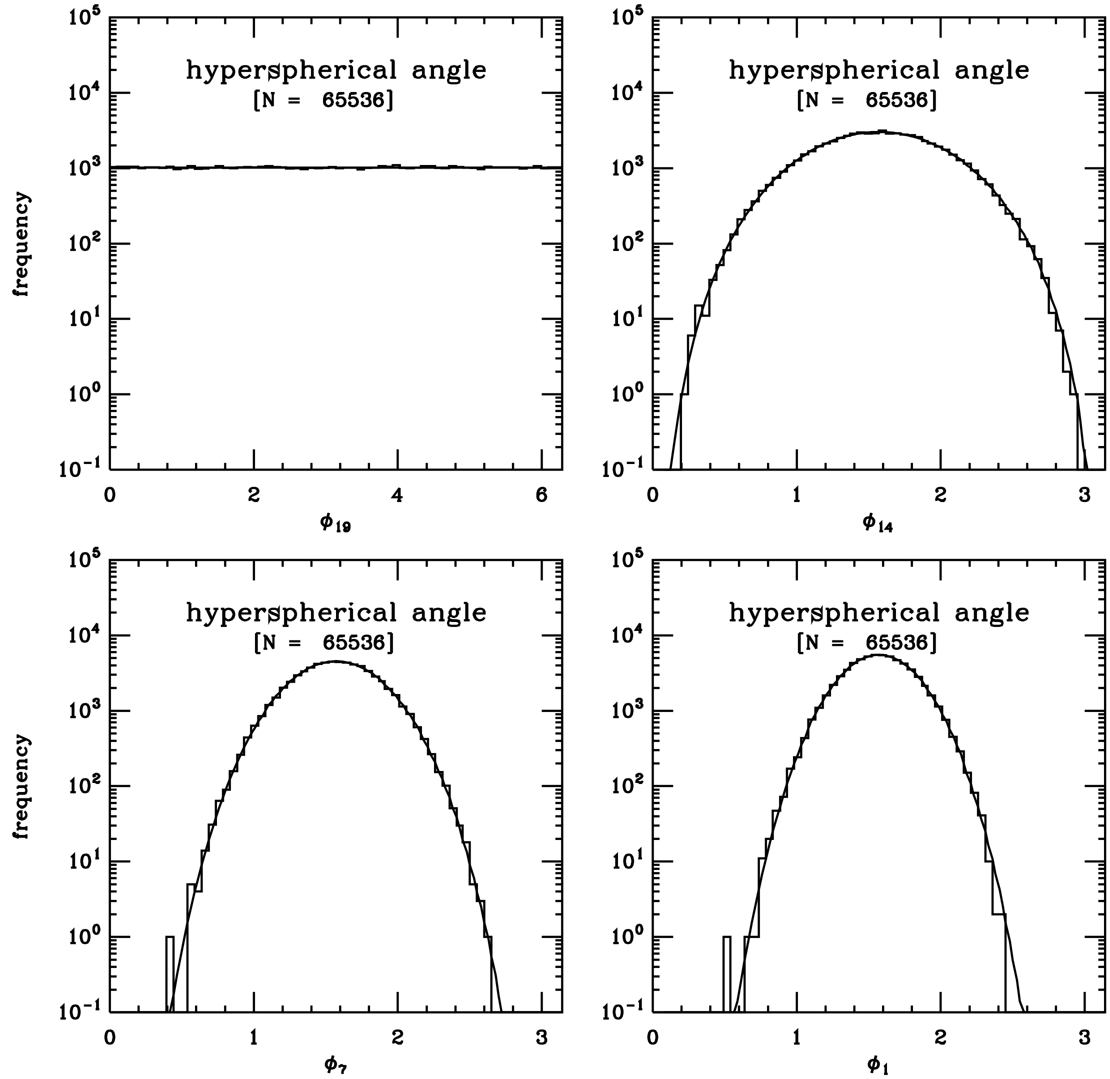

Figure 7: **Hyperspherical angle histograms from isotropic method: n=20**

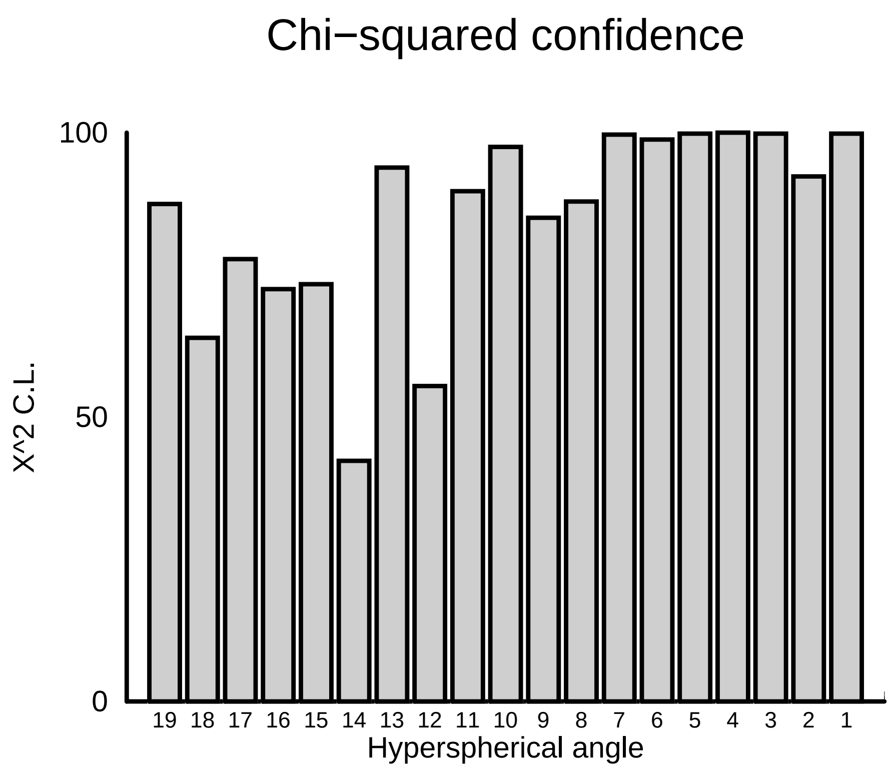

Figure 8: χ^2 **confidence levels (in %) for hyperspherical angles generated by isotropic method Figure 2:** n**=20, sample=65536, 64 bins**

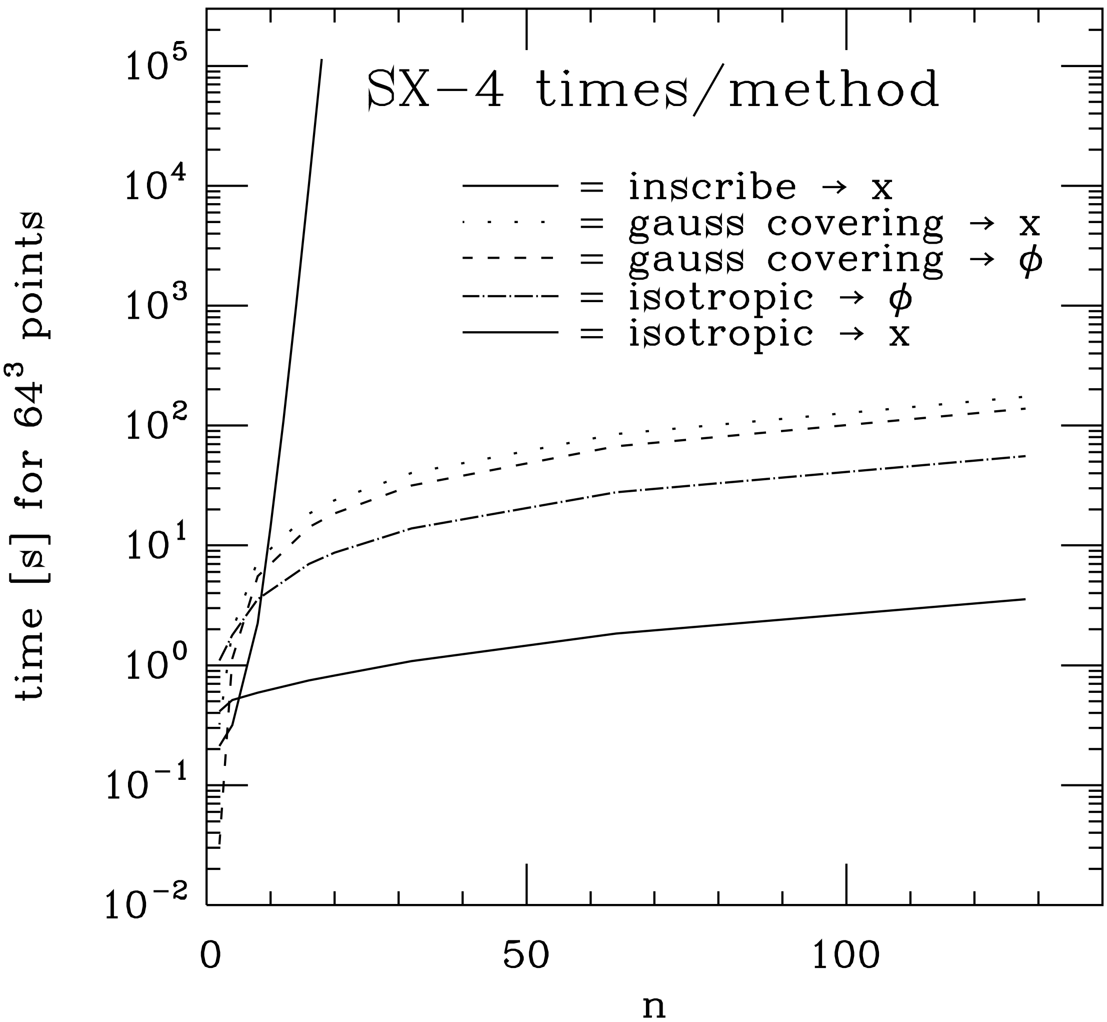

Figure 9: **Timings (in seconds) for various methods:** 64^3 n**-dimensional points on NEC SX-4 machine and zufall random number generator [8]**

6 Acknowledgements

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