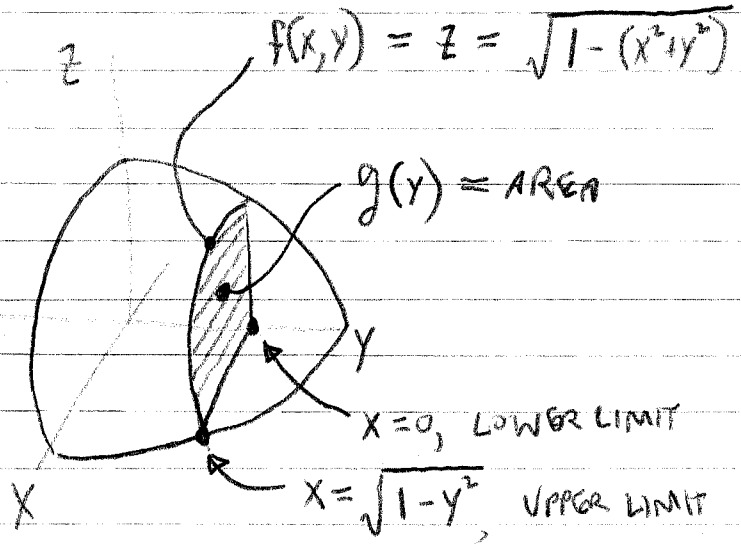


EXAMPLE 2

RECALL OUR CONVERGENCE TESTS WITH THE QUARTER-CIRCLE INTEGRATION. WE COULD CONSTRUCT AN INTEGRATION OF A SPHERE OVER ONE OCTANT BY NESTING THESE.



$$\text{SPHERE VOLUME} = 8 \int_{y=0}^1 dy \underbrace{\int_{x=0}^{\sqrt{1-y^2}} \sqrt{1-(x^2+y^2)} dx}_{g(y)}$$

BASED ON OUR PRIOR EXPERIENCE, CONVERGENCE OF THE QUARTER-CIRCLE INTEGRAL IS

$$O(N^{-3/2}) \text{ --- REGARDLESS OF THE NOMINAL "ORDER" OF THE QUADRATURE.}$$

SO OUR DOUBLE INTEGRAL WOULD CONVERGE LIKE

$$O(N^{-3/4}).$$

E.G. ACCURACY OF 10^{-3} REQUIRES $N = 10^4$. →

7

EXAMPLE, CONT.

SUPPOSE WE ARE INTEGRATING THE V-DIMENSIONAL
HYPERSPHERE TO FIND ITS VOLUME.

$$M = v - 1$$

CONVERGENCE:

$$O(N^{-3/2M}) = O(N^{\frac{-3}{2(v-1)}}$$

NOTE HOW BAD THINGS HAVE BECOME WITH A MODERATELY "NASTY" INTEGRAND!

E.G. $v = 4$ -D HYPERSPHERE $\rightarrow O(N^{-1/2})$
 $v = 7$ -D HYPERSPHERE $\rightarrow O(N^{-1/4})$

Q: IF I THROW 100 DARTS AT A v -DIMENSIONAL DART BOARD AND 25 HIT THE BULLSEY, WHAT IS THE PROBABILITY THAT MY NEXT THROW WILL HIT, AND WHAT IS THE UNCERTAINTY?

$$P = \int_{\text{BULLSEY}} d^v x P(\vec{x}) = ? \pm ?$$

A: $p \approx \frac{25 \pm 5}{100} = 0.25 \pm 0.05$

\swarrow $5 = \sqrt{25} \approx \sqrt{100p} = \sqrt{Np}$

Q: HOW WOULD p CONVERGE AS I INCREASE N FROM 100 TO 1,000,000? HOW DOES THIS DEPEND ON v ?

A: $O(N^{-1/2})$, INDEPENDENT OF v !

THE DART BOARD IDEA IS CALLED MONTE CARLO INTEGRATION. (8)

LET'S BE MORE PRECISE.

- LOOK AT hypersphere 1. m & DISCUSS.

THE ALGORITHM: $(\vec{x}^1, \vec{x}^2, \dots, \vec{x}^N)$

① CHOOSE N POINTS WITHIN THE HYPERCUBE, WHERE
 $0 < x_n^i < 1$, $n = 1, 2, \dots, V$, FROM UNIFORM DISTRIBUTION.

② EVALUATE HOW MANY POINTS ARE WITHIN THE
HYPERSPHERE, N' .

$$\langle N' \rangle = N p$$

WHERE $p =$ CHANCE OF HITTING THE BULLSEYE (HYPERSPHERE)

$$p = \frac{\text{VOLUME OF HYPERSPHERE}}{\text{VOLUME OF HYPERCUBE}}$$

$$\text{③ VOLUME OF HYPERSPHERE} = p \cdot 2^V \approx \frac{N'}{N} 2^V$$

WE EXPECT CONVERGENCE OF $\mathcal{O}(N^{-1/2})$.

MORE CAREFUL CALCULATION OF MONTE CARLO UNCERTAINTY... THIS COMES DOWN TO ESTIMATING p :

THE DISTRIBUTION OF \mathcal{N}' , $P(\mathcal{N}' | \mathcal{N}, p)$ IS A BINOMIAL DISTRIBUTION.

A SINGLE TRIAL IS EITHER 0 OR 1 COUNT, WITH A MEAN OF p AND VARIANCE

$$\sigma_1^2 \equiv \sum_x P(x) (x-p)^2 = p(1-p)^2 + (1-p)(0-p)^2 = p(1-p)$$

TO OBTAIN THE VARIANCE FOR \mathcal{N} TRIALS, WE ADD IN QUADRATURE:

$$\sigma_{\mathcal{N}}^2 = \mathcal{N} \sigma_1^2 = \mathcal{N} p(1-p).$$

THUS, WHEN WE MEASURE \mathcal{N}' , WE GET

$$\mathcal{N}' \approx \mathcal{N} p \pm \sqrt{\mathcal{N} p(1-p)}$$

$$\Rightarrow p \approx \frac{\mathcal{N}'}{\mathcal{N}} \pm \sqrt{\frac{p(1-p)}{\mathcal{N}}}$$

FRACTIONAL UNCERTAINTY IN p , AND THUS IN THE VOLUME OF THE HYPERSPHERE, IS

$$\frac{\Delta V}{V} = \frac{\Delta p}{p} = \sqrt{\frac{(1-p)}{\mathcal{N} p}}$$

AS EXPECTED,
 $\mathcal{O}(\mathcal{N}^{-1/2})$

THIS IS THE GENERAL FORM OF THE UNCERTAINTY FOR ANY SIMPLE MONTE CARLO CALCULATION (NOT JUST THE HYPERSPHERE VOLUME — THOSE DETAILS DID NOT ENTER IN TO OUR CALCULATION).

RANDOM NUMBER GENERATION — NR CH.7

RNG IS ESSENTIAL TO MONTE-CARLO. OCTAVE HAS A PRETTY GOOD RNG BUILT INTO THE RAND FUNCTION. YOU CAN USE IT BLINDLY, BUT IT'S WORTH KNOWING WHAT IS GOING ON UNDER THE HOOD.

IMPORTANT CONCEPTS:

① COMPUTERS ARE DETERMINISTIC MACHINES. RNG ALGORITHMS RELY ON "PSEUDO-RANDOM SEQUENCES" — SEQUENCES OF BIG INTEGERS* THAT APPEAR TO BE STATISTICALLY INDEPENDENT.

② ALL PSEUDO-RANDOM SEQUENCES ARE ACTUALLY PERIODIC.

FOR EXAMPLE, OCTAVE'S RAND REPEATS AFTER $2^{19937} - 1$ CYCLES. (THAT'S $\sim 10^{6000}$...!)

③ THE "STATE" OF THE RNG IS THE BIG INTEGER, WHICH WILL BE PERMUTED AND MUNGED IN SOME STANDARD WAY TO MANUFACTURE THE NEXT INTEGER IN THE SEQUENCE.

THE ENTIRE STATE OF THE RNG SHOULD NEVER BE USED AS A "RANDOM" NUMBER. USE A FRACTION OF IT, STARTING FROM THE LSB. MORE SIGNIFICANT BITS WILL EVOLVE ACCORDING TO A MORE OBVIOUS PATTERN.

④ WHERE TO START THE PSEUDO-RANDOM SEQUENCE? IT IS COMMONLY INITIALIZED FROM THE SYSTEM ENTROPY CACHE (`/dev/urandom`), CPU CLOCK, ETC.



* OR EQUIVALENTLY, VECTORS OF SMALLER INTEGERS

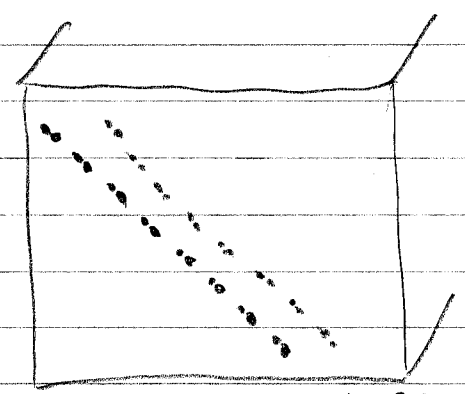
RNG, CONT.

⑤ A SEED (STATE VECTOR, OR PART THEREOF) MAY BE SAVED FOR FUTURE REFERENCE, OR USED TO RE-INITIALIZE THE RNG.

• THIS IS A HELPFUL WAY TO REPEAT EXACTLY THE SAME STRING OF PSEUDO-RANDOM NUMBERS AGAIN IN THE FUTURE. THIS REPEATABLE RANDOMNESS IS OFTEN HELPFUL FOR CODE DEVELOPMENT, DEBUGGING, OR MAKING YOUR SCIENTIFIC RESULTS STRICTLY REPEATABLE.

• BY SAVING THE SEED AFTER A STRING OF RANDOM CALCULATIONS, YOU CAN PICK UP LATER WHERE YOU LEFT OFF. THIS IS HELPFUL ON SYSTEMS THAT AREN'T SO GOOD AT INITIALIZING THE RNG.

⑥ PERIODICITIES IN THE RNG ARE MOST EASILY SPOTTED BY FILLING A MANY-DIMENSIONAL CUBE WITH POINTS, AND LOOKING FOR CLUSTERING IN PLANES.



IN OTHER WORDS, RNG FLAWS BECOME APPARENT SOMETIMES IN HIGH-DIMENSIONAL MONTE CARLO WORK!

CAN WE DO BETTER THAN $1/\sqrt{N}$?

(11)

THERE ARE MANY APPROACHES TO SPEEDING CONVERGENCE FOR MONTE CARLO METHODS.

SEE http://www-graphics.stanford.edu/papers/veach_thesis

- ONE CLASS OF METHODS REDUCES THE VARIANCE BY DISTRIBUTING THE POINTS SOMEWHAT MORE UNIFORMLY IN THE VOLUME.
 - QUASI-RANDOM NUMBER SEQUENCES
E.G. SOBOL NUMBERS
 - STRATIFIED SAMPLING

Q: IF MORE UNIFORMITY HELPS, WHY NOT USE A REGULAR GRID, AND FORGET THE RANDOM STUFF?

A: THAT PUTS US BACK AT THE TRAPEZOID OR MIDPOINT RULE, $\mathcal{O}(N^{-2/m})$ OR WORSE!

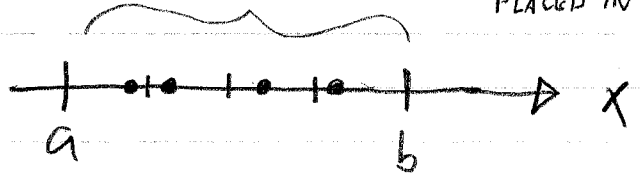
.... THEN HOW MIGHT SOME DEGREE OF UNIFORMITY HELP, AND WHAT MIGHT WE MEAN BY THAT?

STRATIFIED SAMPLING

- THE IDEA IS TO DIVIDE THE DOMAIN INTO SUBAREAS, AND GET THE VOLUME OF EACH BY REGULAR M-C.
- WORKS BEST IF THE INTEGRAND IS RELATIVELY CONSTANT WITHIN EACH SUBAREA.
- WE CAN COME CLOSE TO THE IDEAL BY DIVIDING INTO N EQUAL SUBAREAS:

1D EXAMPLE:

$N=4$, 4 SUBAREAS, 1 POINT RANDOMLY PLACED IN EACH.



$$h = (b-a)/N$$

$$x = a + h(0:N-1) + h * \text{rand}(N)$$

STARTING VALUE

$[0, h, 2h, \dots, b-h]$

N UNIFORMLY DISTRIBUTED RANDOM DEVIATES BETWEEN 0 AND h .

KEY POINTS

- AS WITH PLAIN MONTE CARLO, EVERY x IS EQUALLY PROBABLE.
- POINTS DO NOT CLUSTER TOGETHER.
- MOST SUBAREAS ARE VERY UNIFORM, BECAUSE WE'VE MADE THEM AS SMALL AS POSSIBLE.

HOW & WHY DOES STRATIFIED SAMPLING HELP?

CONSIDER THE V -SPHERE, WITH A 3D GRID OF N POINTS, SPACING h APART, PERTURBED RANDOMLY WITHIN THEIR h^V -VOLUME SUBDOMAINS.

THERE ARE 3 KINDS OF SUBDOMAINS:

- ① THOSE FULLY INSIDE THE HYPERSPHERE. EACH CONTRIBUTES h^V OF VOLUME, WHICH IS EXACTLY CORRECT. THERE ARE NEARLY pN OF THESE.
- ② THOSE FULLY OUTSIDE THE HYPERSPHERE, WHICH DON'T CONTRIBUTE ANYTHING.

ALL THE RANDOM ERROR COMES FROM THE LAST CATEGORY:

- ③ THOSE STRADDLING THE SURFACE OF THE HYPERSPHERE, SINCE THE SURFACE HAS $V-1$ DIMENSIONS, THE NUMBER OF STRADDLING SUBDOMAINS SCALES AS $N^{(V-1)/V}$. THE FRACTIONAL ERROR IN THE SURFACE CONTRIBUTION TO THE VOLUME IS

$$\frac{\Delta V_{\text{SURF}}}{V_{\text{SURF}}} = \frac{1}{\sqrt{N^{(V-1)/V}}} = N^{-(V-1)/2V}$$

THIS IS ONLY A FRACTION OF THE TOTAL VOLUME:

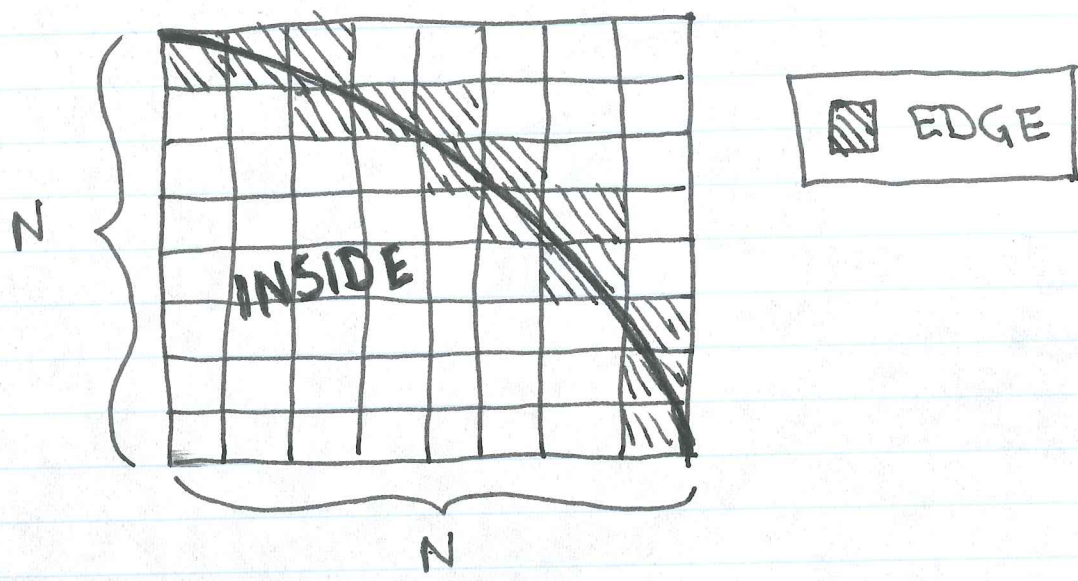
$$\frac{V_{\text{SURF}}}{V_{\text{TOT}}} = \frac{N^{(V-1)/V}}{N} = N^{-1/V}$$

SO THE RANDOM ERROR IN THE TOTAL VOLUME IS:

$$\frac{\Delta V_{\text{TOT}}}{V_{\text{TOT}}} = \frac{\Delta V_{\text{SURF}}}{V_{\text{TOT}}} = \frac{\Delta V_{\text{SURF}}}{V_{\text{SURF}}} \frac{V_{\text{SURF}}}{V_{\text{TOT}}} = N^{-(V+1)/2V}$$

$$\boxed{\frac{\Delta V}{V} = N^{-\left(\frac{1}{2} + \frac{1}{2V}\right)}} \quad \text{HELPS MOST FOR SMALL } V!$$

PICTORIAL JUSTIFICATION OF POINT ③



2D

$$\mathcal{N} = N^2$$

$$\mathcal{N}_{IN} \approx \rho N^2 \propto N^2$$

$$\mathcal{N}_{EDGE} \propto N$$

3D

$$\mathcal{N} = N^3$$

$$\mathcal{N}_{IN} \propto N^3$$

$$\mathcal{N}_{EDGE} \propto N^2$$

V-DIMENSIONS

$$\mathcal{N} = N^v$$

$$\mathcal{N}_{IN} \propto N^v$$

$$\mathcal{N}_{EDGE} \propto N^{v-1}$$

$$\therefore \mathcal{N}_{EDGE} \propto N^{v-1} = \left(\mathcal{N}^{\frac{1}{v}}\right)^{v-1} = \mathcal{N}^{(v-1)/v}$$

FRACTIONAL ERROR

$$\frac{\Delta V_{SURF}}{V_{SURF}} \approx \frac{1}{\sqrt{\mathcal{N}_{EDGE}}} \propto \mathcal{N}^{-(v-1)/2v}$$

$$\frac{\Delta V_{TOT}}{V_{TOT}} = \frac{\Delta V_{SURF}}{V_{TOT}}$$

$$\propto \frac{\Delta V_{SURF}}{V_{SURF}} \cdot \frac{V_{SURF}}{V_{TOT}} \propto \mathcal{N}^{-(\frac{1}{2} + \frac{1}{2v})}$$

$$\frac{V_{SURF}}{V_{TOT}} = \frac{\mathcal{N}_{SURF}}{\mathcal{N}} \propto \frac{\mathcal{N}}{\mathcal{N}} = \mathcal{N}^{-1/v}$$