Slide 1

A Monte Carlo Primer

Slide 2

How Many Words Do I Know ?

- Well, I could count them
- Systematically, using a dictionary
- What about using only a few pages (good, but how many ?)

Slide 3

Do I Really Know How to Communicate ?

- Many words are useless – sort of, unless you are into the poetry stuff
- A good usage (vs prescriptive) dictionary should rate how common/useful the words are
- Now, I need a lot of pages before getting any accuracy
- What about biasing my random sampling (e.g. using the Boston Globe) ?

Slide 4

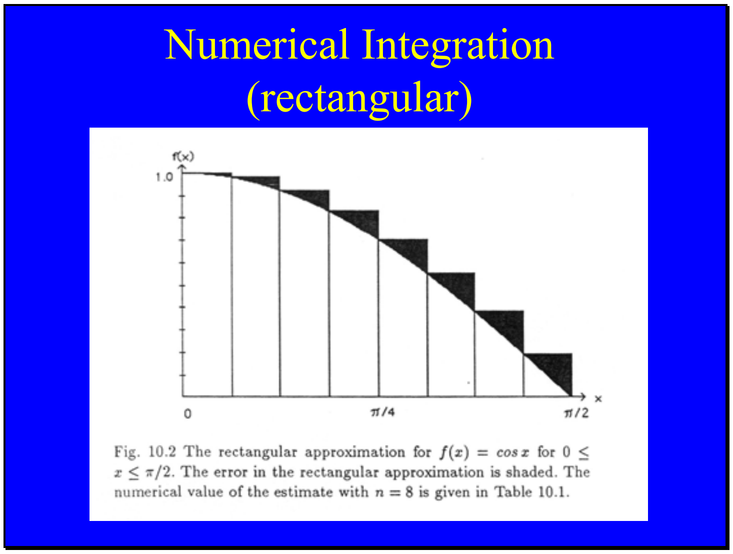

Fig. 10.2 The rectangular approximation for $f(x) = \cos x$ for $0 \leq x \leq \pi/2$. The error in the rectangular approximation is shaded. The numerical value of the estimate with $n = 8$ is given in Table 10.1.

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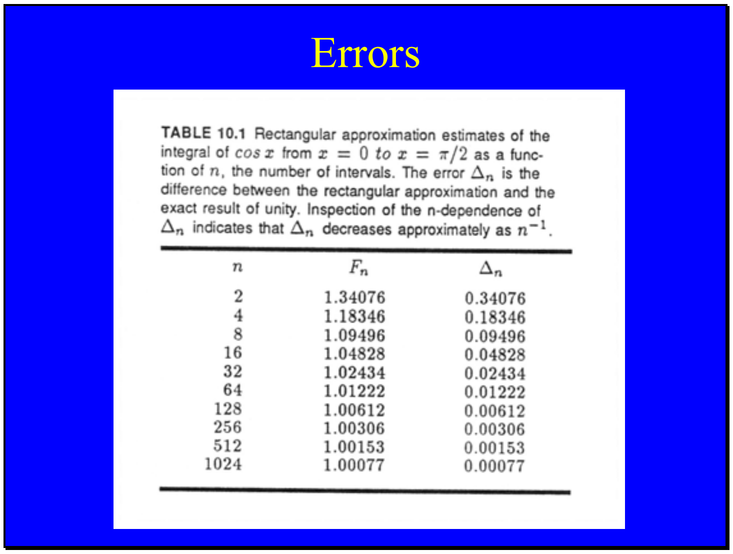

TABLE 10.1 Rectangular approximation estimates of the integral of $\cos x$ from $x = 0$ to $x = \pi/2$ as a function of n, the number of intervals. The error Δ_n is the difference between the rectangular approximation and the exact result of unity. Inspection of the n-dependence of Δ_n indicates that Δ_n decreases approximately as n^{-1}.

n	F_n	Δ_n
2	1.34076	0.34076
4	1.18346	0.18346
8	1.09496	0.09496
16	1.04828	0.04828
32	1.02434	0.02434
64	1.01222	0.01222
128	1.00612	0.00612
256	1.00306	0.00306
512	1.00153	0.00153
1024	1.00077	0.00077

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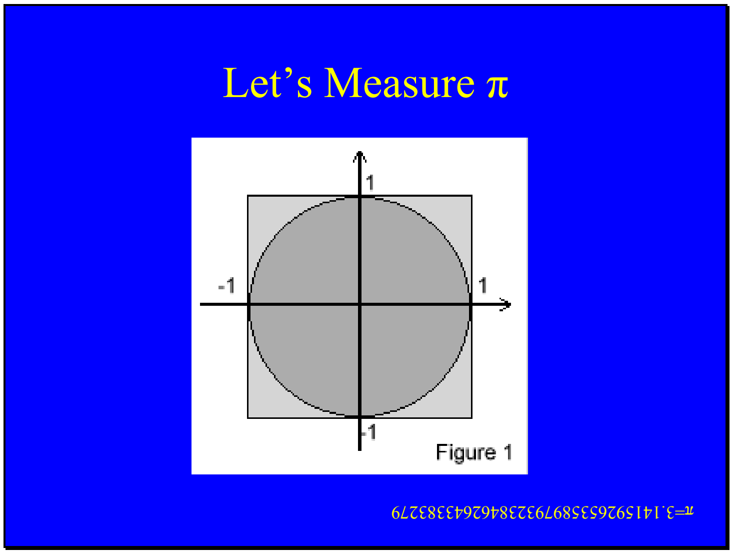
Let's Measure π
1
-1
1
-1
Figure 1
π=3.14159265358979323846264338327 9

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Srinivasa Ramanujan

$$\frac{1}{\pi} = \frac{\sqrt{8}}{9801}\sum_{n=0}^{\infty}\frac{(4n)!(1103+26390n)}{(n!)^4 396^{4n}}$$

(roughly 8 decimal places for each term…)

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Let’s take a Zen attitude

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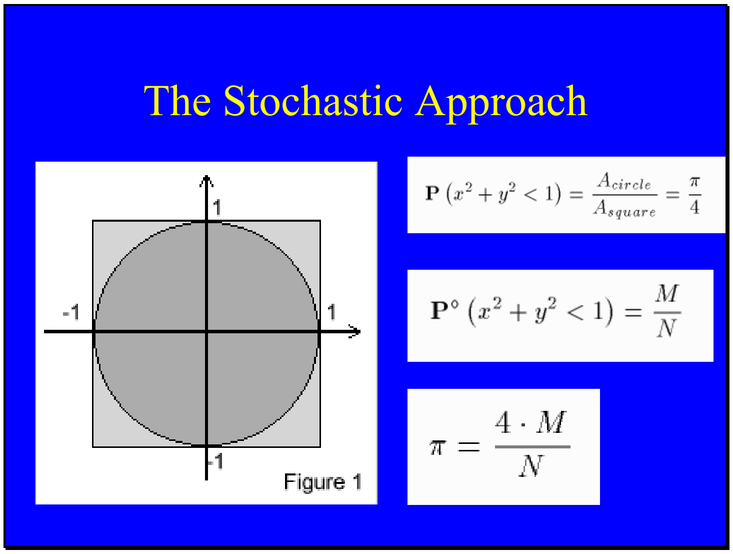
The Stochastic Approach
1
-1
1
-1
Figure 1
$\mathbf{P}\left(x^2 + y^2 < 1\right) = \frac{A_{circle}}{A_{square}} = \frac{\pi}{4}$
$\mathbf{P}^{\circ}\left(x^2 + y^2 < 1\right) = \frac{M}{N}$
$\pi = \frac{4 \cdot M}{N}$

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Let's Try…

http://www.daimi.aau.dk/~u951581/pi/MonteCarlo/

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Buffon's Needle

http://www.angelfire.com/wa/hurben/images

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Why Bother ?

- Multidimensional integrals
- Try calculating the volume of an hypersphere in 20 dimensions…
- Systems with a large number of degrees of freedom
  - Many atoms in a gas, liquid, solid (partition function)
  - Many electrons in an atom (wavefunctions)

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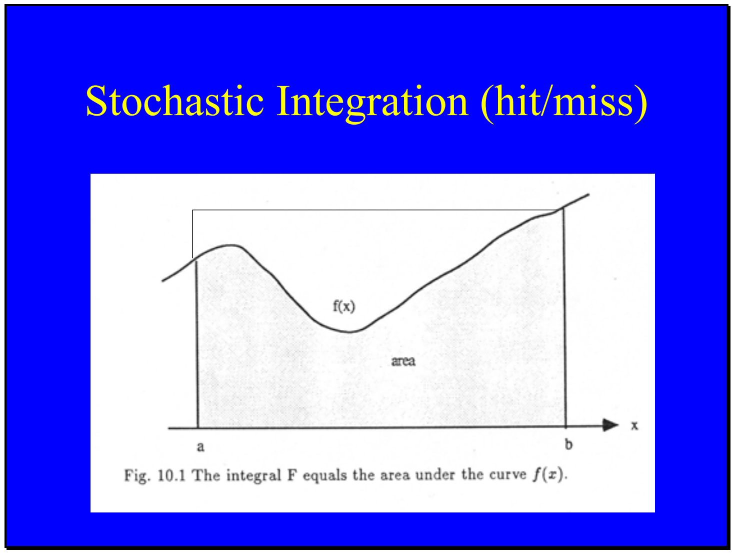
Stochastic Integration (hit/miss)
f(x)
area
x
a
b
Fig. 10.1 The integral F equals the area under the curve f(x).

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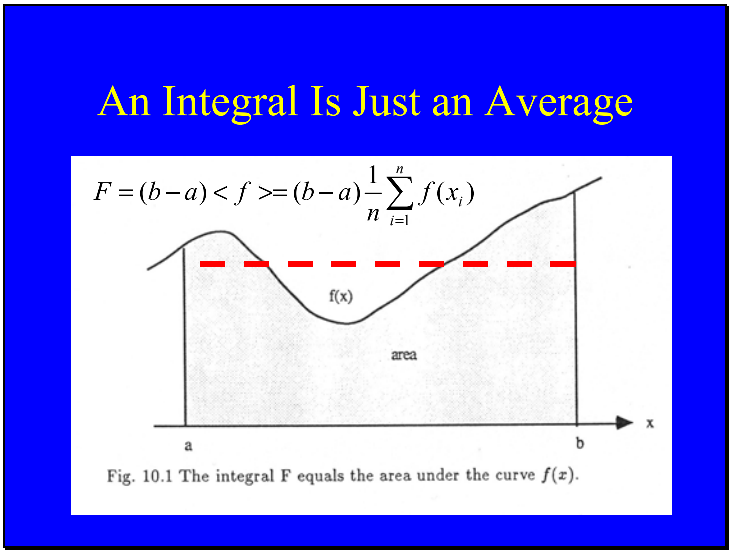
An Integral Is Just an Average
$F = (b-a) < f >= (b-a)\frac{1}{n}\sum_{i=1}^{n} f(x_i)$
f(x)
area
a
b
x
Fig. 10.1 The integral F equals the area under the curve $f(x)$.

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Central Limit Theorem

$$I = \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

We can consider $f_i=f(x_i)$ as a random variable – then, for large *n*, we have that the variance of *I* is 1/N the variance of *f*

$$\sigma_I^2 = \frac{1}{n}\sigma_f^2 = \frac{1}{n}\left[\frac{1}{n}\sum_{i=1}^{n} f^2(x_i) - \left(\frac{1}{n}\sum_{i=1}^{n} f(x_i)\right)^2\right]$$

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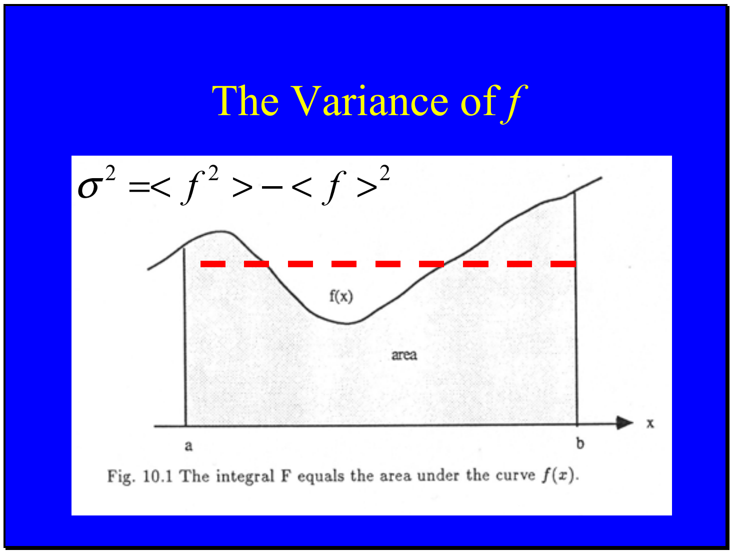

The Variance of f
σ² =< f² > − < f >²
f(x)
area
x
a
b
Fig. 10.1 The integral F equals the area under the curve f(x).

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$$\sigma^2 = < \left(f - < f > \right)^2 >$$

$$\sigma^2 = < f^2 - 2f < f > + < f >^2 >$$

$$\sigma^2 = < f^2 > - < f >^2$$

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Excellent Scaling Properties !

•The uncertainty in the estimate of the integral scales as

$$\sigma_I = \frac{1}{\sqrt{n}}$$

•For numerical integration, the error is

$$\sigma_I = \frac{1}{n^{\frac{k}{D}}}$$

Where D is the dimensionality, and k is related to the algorithm (Simpson, trapezoidal…)

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Importance Sampling

- If the variance of the function that we have to integrate is 0, the variance on our integral is 0
- Try to integrate functions with reduced variance

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Importance Sampling

$$F = \int_a^b f(x)dx = (b-a)\frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

$$\int_a^b p(x)d(x) = 1 \qquad F = \int_a^b \left[\frac{f(x)}{p(x)}\right] p(x)dx$$

If x is not uniformly distributed, but distributed as *p(x)*, then

$$F = (b-a)\frac{1}{n}\sum_{i=1}^{n}\frac{f(x_i)}{p(x_i)}$$

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Example

$$F = \int_0^1 \exp\left(-x^2\right) dx$$

TABLE 10.4 Monte Carlo estimates of the integral (10.48) using the uniform probability density $p(x) = 1$ and non-uniform probability density $p(x) = Ae^{-x}$. The normalization constant A is chosen such that $p(x)$ is normalized on the unit interval. The exact value of the integral is approximately 0.7468. The estimates F_n, standard deviation σ, and the probable error $\sigma/n^{1/2}$ are shown. The CPU time (seconds) is shown for comparison only and was found on a Macintosh computer running True BASIC.

	$p(x) = 1$	$p(x) = Ae^{-x}$
n (trials)	20000	1000
F_n	0.7452	0.7482
σ	0.2009	0.0544
$\sigma/n^{1/2}$	0.0016	0.0017
CPU time per trial (sec)	0.0077	0.0280
Total CPU time (secs)	154	28

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Good enough for Mathematica…

In order to integrate a function over a complicated domain D, Monte Carlo integration picks random points over some simple domain which is a superset of D, checks whether each point is within D, and estimates the area of D (volume, n-D content, etc.) as the area of D’multiplied by the fraction of points falling within D’. Monte Carlo integration is implemented in Mathematica as Nintegrate[f,…,Method->MonteCarlo].

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References

- http://www.npac.syr.edu/users/paulc/lectures/montecarlo/
- Koonin, *Computational Physics*
- Press, Teukolsky, Vetterling, Flannery, *Numerical Recipes*