

# Monte Carlo Method



# Motivation

Evaluation of cross sections leads to

$$\sigma = \int dx_1 dx_2 \sum_{\text{subp}} f_{a_1/p}(x_1) f_{a_2/\bar{p}}(x_2)$$

$$\frac{1}{2\hat{s}(2\pi)^{3n-4}} \int d\Phi_n(x_1 P_A + x_2 P_B; \ p_1 \dots p_n) \Theta(\text{cuts}) \overline{\sum} |\mathcal{M}|^2 (a_1 a_2 \to b_1 \dots b_n)$$

there are 3n-2 integrals. We also need to simulate the detector!

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We need effective techniques to perform the calculations!

### Shortcomings of traditional numerical methods

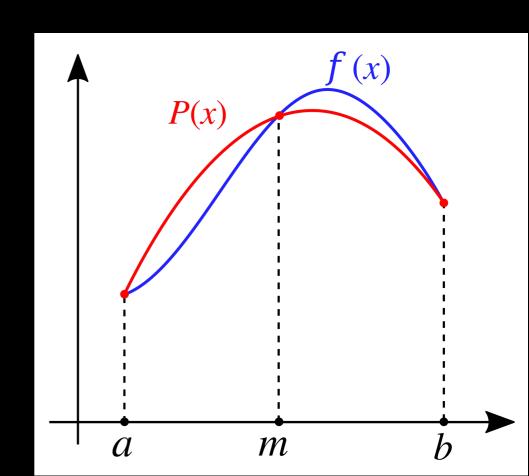
• Traditional methods work well for low dimensional integrals:

#### Simpson's rule:

$$\int_{x_0}^{x_2} dx \ f(x) = \frac{\Delta x}{3} \left[ f(x_0) + 4f(x_1) + f(x_2) \right] + \frac{(\Delta x)^5}{90} f^{(4)}(\xi)$$

Notice 
$$\Delta x \propto \frac{1}{N}$$

This can be improved



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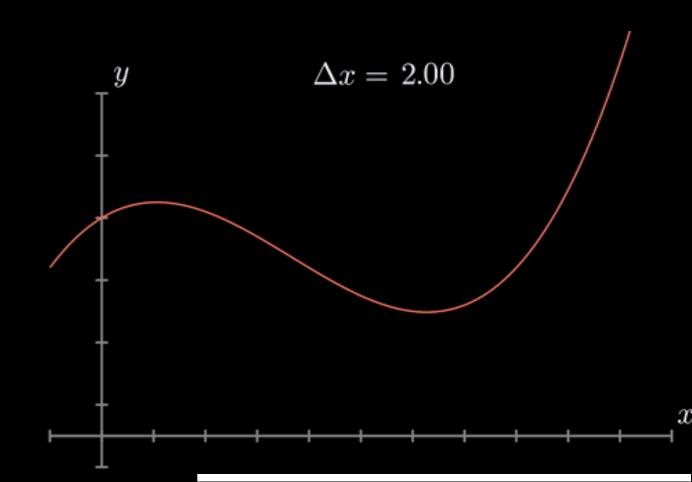
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• Traditional methods work well for low dimensional integrals:

method/uncertainty	1 dimension	d dimensions
Trapedoidal rule	$\frac{1}{n^2}$	$\frac{1}{n^{2/d}}$
Simpson's rule	$\frac{1}{n^4}$	$\frac{1}{n^{4/d}}$
Gauss rule	$\frac{1}{n^{2m-1}}$	$\frac{1}{n^{(2m-1)/d}}$
Monte Carlo	$\frac{1}{\sqrt{n}}$	$\frac{1}{\sqrt{n}}$

• I/d factor renders the methods inefficient

#### Example

$$I = \int_0^1 dx \, \cos\left(\frac{\pi}{2}x\right) = \frac{2}{\pi} \simeq 0.63661977$$

evaluations	Simpson	MC
3	0.638	0.3
5	0.6367	0.8
20	0.63662	0.6
100	0.636619	0.65
1000	0.636619	0.636

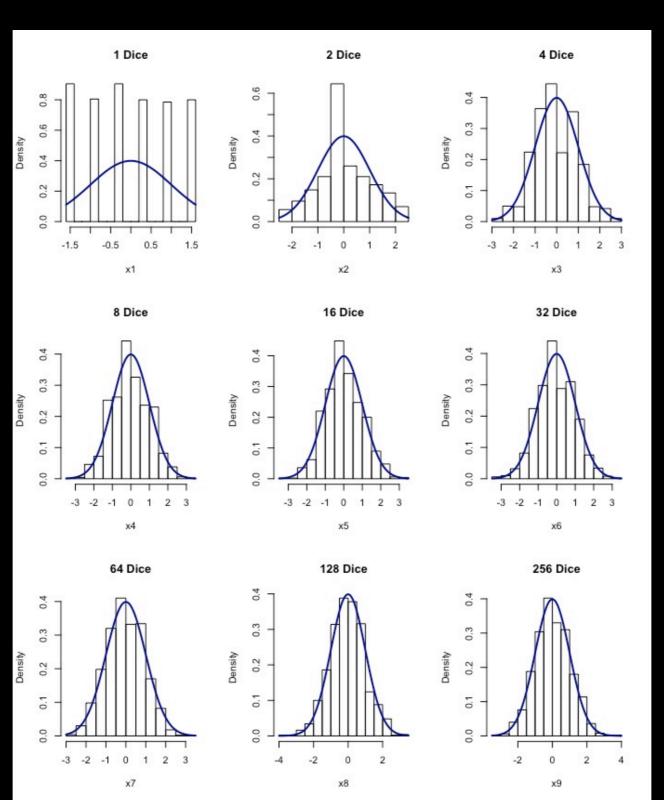
## Introduction

- MC transforms the problem into a stochastic one.
- MC provides approximate solutions using statistical sampling experiments.
- MC has a wide range of applications from economics to physics
- MC is a statistical method used in simulation of data
- MC uses a sequence of random numbers as data
- MC can be applied to problems with no probabilistic content

# Central Limit Theorem

The sum of a "large number" of random variables is always normally

distributed



### Basic idea

- MC is the most efficient way to perform multi-dimensional integrals.
- The simplest idea: integrand is a function of a random variable

$$x \in [0,1]$$
 and  $\langle f \rangle = \int_0^1 dx f(x) \simeq \frac{1}{N} \sum_{j=1}^N f(x_j)$ 

x is uniformly distributed [crude MC]

- f(x) is a crude estimator of  $\langle f \rangle$
- f(x) is a random variable with variance

$$\sigma_1^2 = \int_0^1 dx \ (f - \langle f \rangle)^2 \quad \Longrightarrow \quad \sigma_N = \frac{\sigma_1}{\sqrt{N}}$$

• We can estimate the probability of the result being correct:

$$\lim_{N \to \infty} \text{Prob} \left( -a \frac{\sigma_1}{\sqrt{N}} \le \frac{1}{N} \sum_{j=1}^{N} f(x_j) - I \le b \frac{\sigma_1}{\sqrt{N}} \right) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{b} dt \ e^{-\frac{t^2}{2}}$$

• we can estimate the error from the MC simulation

$$s^{2} = \frac{1}{n-1} \sum_{j=1}^{n} (f(x_{j}) - \langle f \rangle)^{2}$$

### Initial remarks

- I. MC is exact for f constant. The flatter the better!
- 2. We should avoid near-singular integrands, e.g.,

$$\int \frac{ds}{(s-M)^2 + M^2 \Gamma^2} = \frac{d\theta}{M\Gamma} \quad \text{with} \quad s - M^2 = M\Gamma \tan \theta$$

- 3. Avoid discontinuities of f if possible.
- 4. MC is a direct simulation of what happens physically.
- 5. We can also generate events weighted by f(x)
- 6. The dependence on N is fixed
- 7. We can improve the method reducing  $\sigma_1$

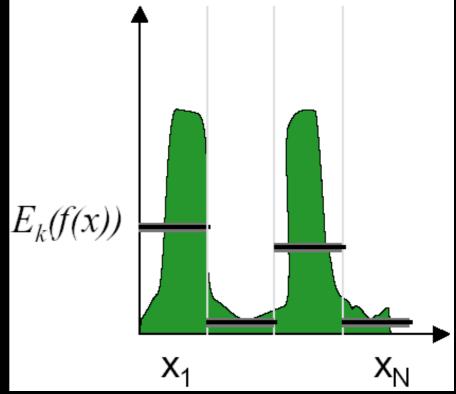
$$\sigma_1^2 = \int_0^1 dx \ (f - \langle f \rangle)^2 \quad \Longrightarrow \quad \sigma_N = \frac{\sigma_1}{\sqrt{N}}$$

## Stratified sampling

• just break the range of integration

$$0 = \alpha_0 < \alpha_1 \cdots < \alpha_k = 1$$

apply crude MC to each interval

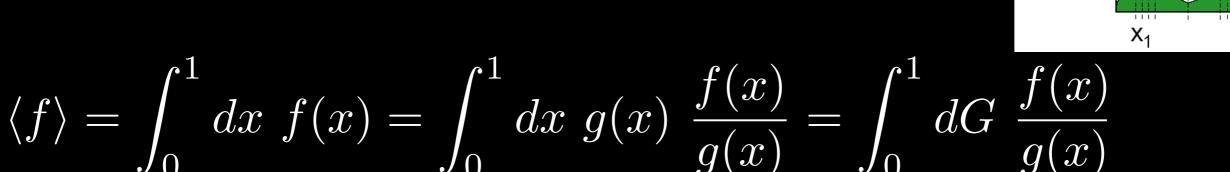


$$\langle f \rangle \simeq \sum_{j=1}^{k} (\alpha_j - \alpha_{j-1}) \frac{1}{n_j} \sum_{i=1}^{n_j} f(\alpha_{j-1} + (\alpha_j - \alpha_{j-1}) x_{ij})$$

variance is reduce for same number of calls of f.

### Importance sampling

- use more points where the function is larger
- implementation using g(x) pdf:



 $X_N$ 

where 
$$G(x) = \int_0^x dy \ g(y)$$

Generating random numbers according g(x):

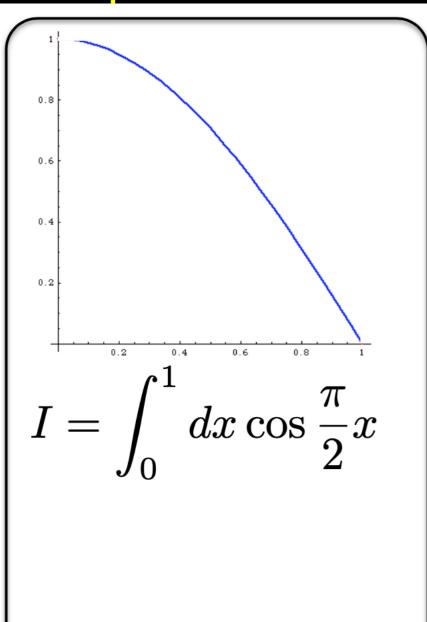
$$\langle f \rangle = \frac{1}{N} \sum_{j=1}^{N} \frac{f(x_j)}{g(x_j)}$$

• choosing g(x) we can reduce the variance.

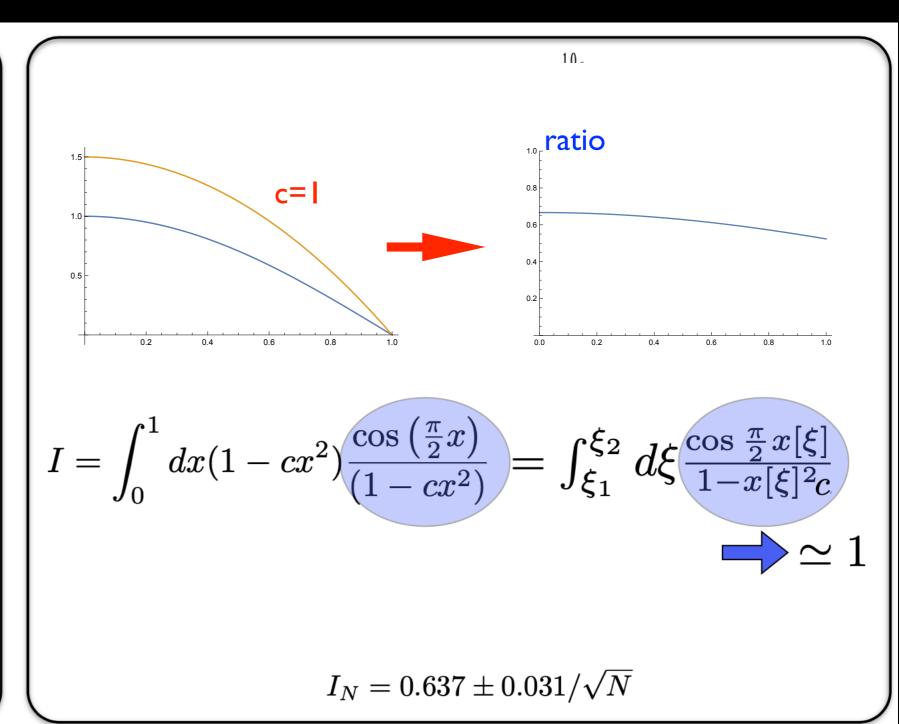
• the variance is 
$$\sigma_{f/g}^2 = \int_0^1 dG \, \left( \frac{f(x)}{g(x)} - \langle f \rangle \right)^2$$

- g should be simple to obtain G explicitly
- if g=cf the variance vanishes
- choose a good function g similar to f
- g(x) approaching zero might jeopardize the variance gain

#### Example



$$I_N = 0.637 \pm 0.307/\sqrt{N}$$



The change reduces the number of evaluations by 100

- Main features of the method:
- I. Random variable distribution should be close to the integrated function
- 2. Basically this is a change of variable to render the integrand flatter
- 3. Requires the knowledge of the approximate function
- 4. Requires knowing the integrated function main features

### Control Variates

Use g(x) with a known integral as

$$\int dx \ f(x) = \int dx \ (f(x) - g(x)) + \int dx \ g(x)$$

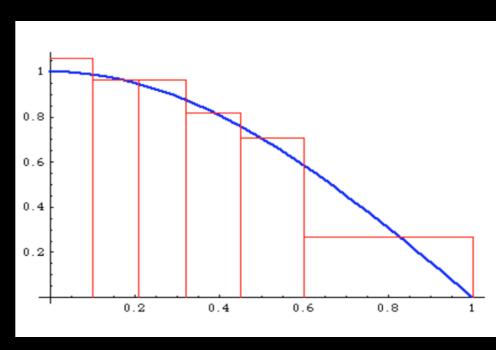
to reduce the variance

### Adaptative Monte Carlo

- Basic idea: to create the approximation function on the flight
- VEGAS algorithm combines stratified and importance samplings
- VEGAS creates an approximated version of the ideal function

$$g(x) = \frac{|f(x)|}{\int dx |f(x)|}$$

- I. start with equal bins
- 2. rebin to each bin have similar contribution
- 3. redo the integration with importance sampling and return to 2



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- At each iteration j

$$E_j = \frac{1}{N_j} \sum_{k=1}^{N_j} \frac{f(x_k)}{g(x_k)}$$
 with estimated variance  $S_j = \frac{1}{N_j} \sum_{k=1}^{N_j} \left(\frac{f(x_k)}{g(x_k)}\right)^2 - E_j^2$ 

the cumulative estimate after m iterations is

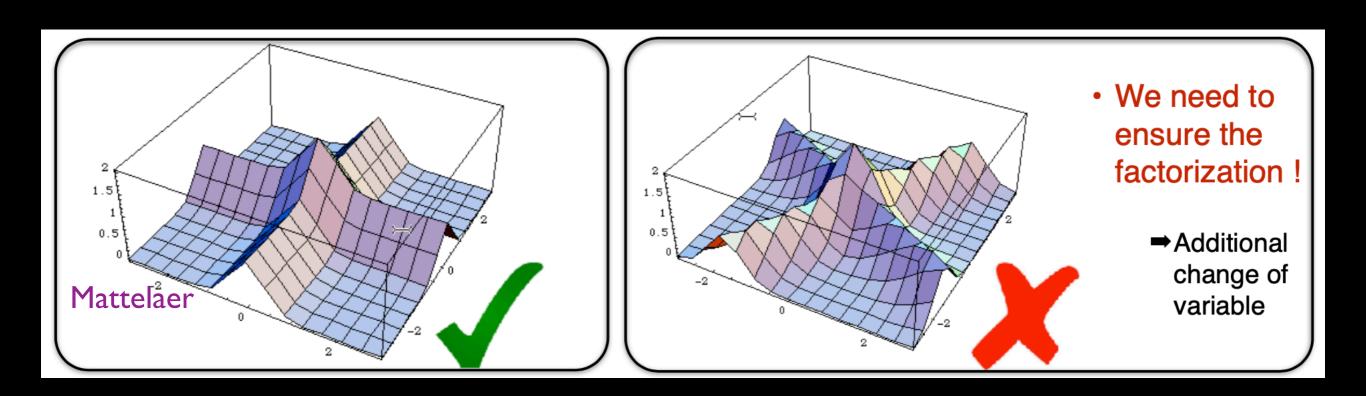
$$E = \left(\sum_{j=1}^{m} \frac{N_j}{S_j^2}\right)^{-1} \sum_{j=1}^{m} \frac{N_j E_j}{S_j^2}$$

and the estimated chi squared 
$$\frac{\chi^2}{dof} = \frac{1}{m-1} \sum_{j=1}^m \frac{(E-E_j)^2}{S_j^2}$$

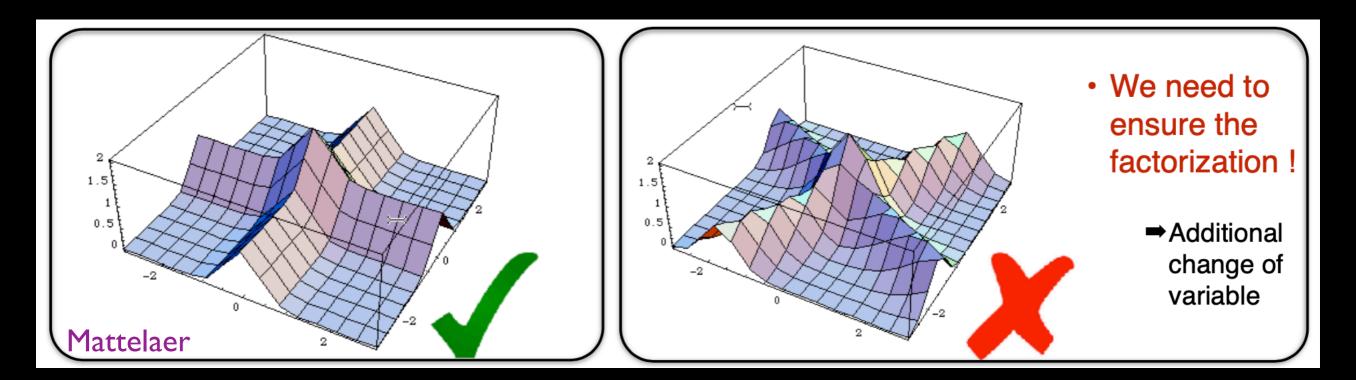
• In more than one dimension, we use a separable probability g(x)

$$g(x) = g_{x_1}(x_1)g_{x_2}(x_2)\dots g_{x_D}(x_D)$$

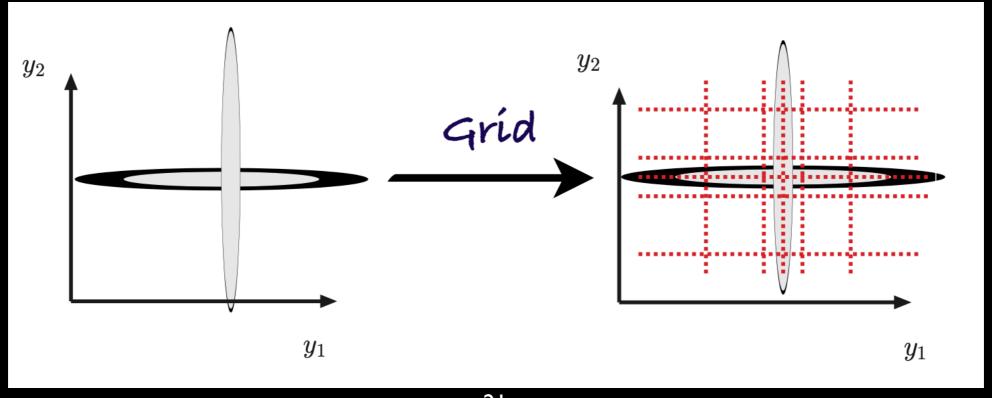
• there are potential problems



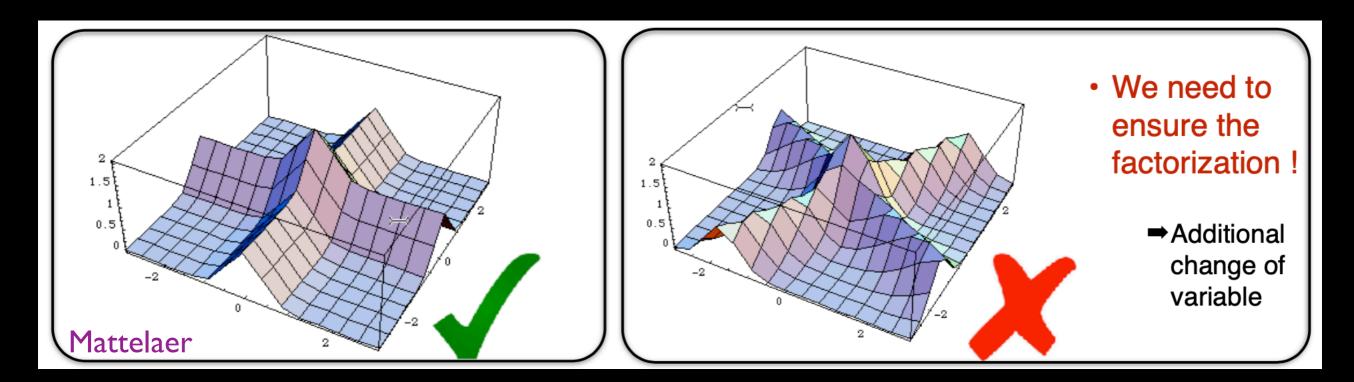
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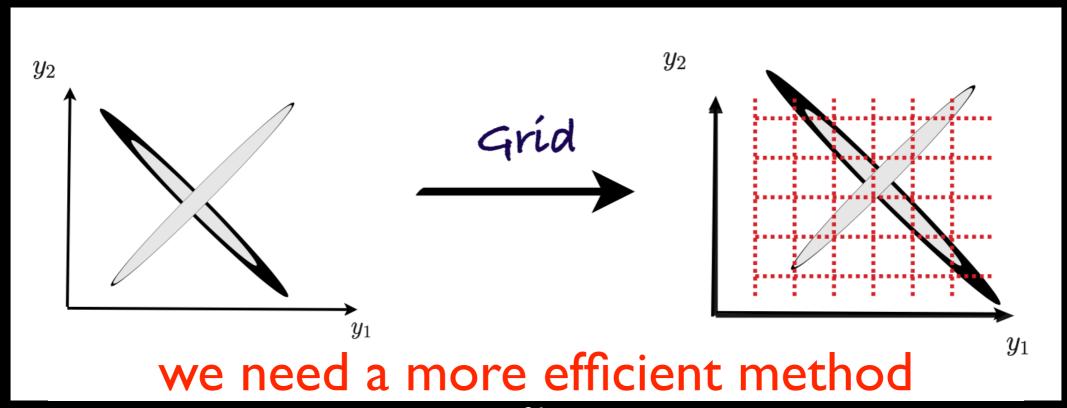
#### • There can be impact in the efficiency



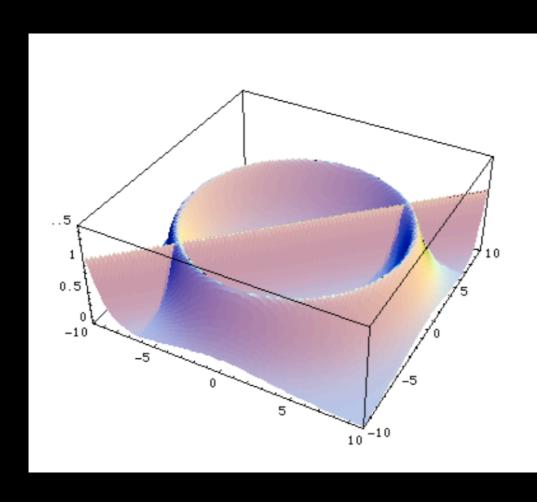
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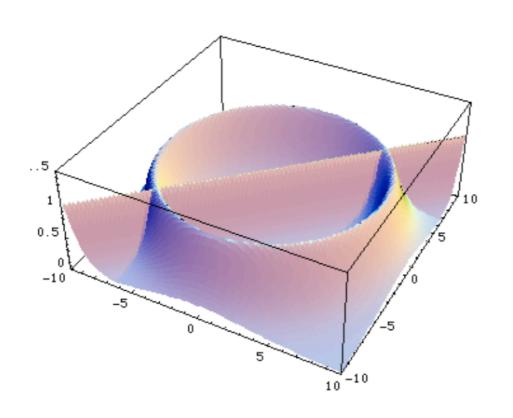


### Multi-channel Monte Carlo



What do we do if there is no transformation that aligns all integrand peaks to the chosen axes? Vegas is bound to fail!

[extracted from O. Mattelaer, MC Lecture at IFT Madrid, 2015]



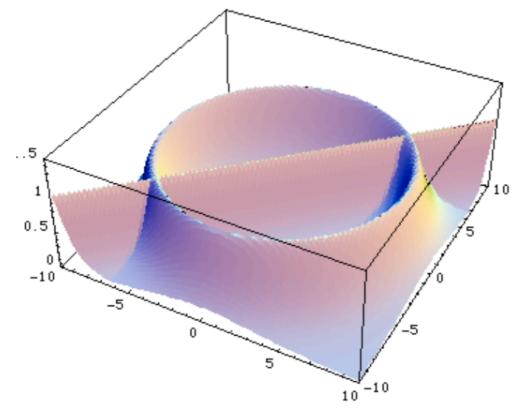
What do we do if there is no transformation that aligns all integrand peaks to the chosen axes? Vegas is bound to fail!

Solution: use different transformations = channels

$$p(x) = \sum_{i=1}^n \alpha_i p_i(x)$$
 with  $\sum_{i=1}^n \alpha_i = 1$ 

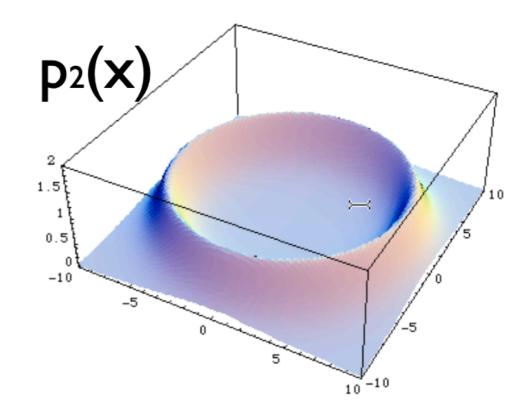
with each  $p_i(x)$  taking care of one "peak" at the time

Catch: we need to know the integrand! Know thy problem:-)



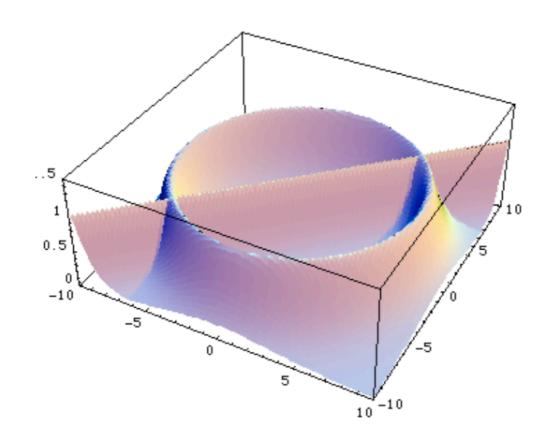
$$p(x) = \sum_{i=1}^{n} \alpha_i p_i(x)$$

with  $\sum_{i=1}^n \alpha_i = 1$ 



Mattelaer Olivier

Monte-Carlo Lecture: IFT 2015



$$p(x) = \sum_{i=1}^{n} \alpha_i p_i(x)$$

with

$$\sum_{i=1}^{n} \alpha_i = 1$$

Then,

$$I = \int f(x)dx = \sum_{i=1}^{n} \alpha_i \int \frac{f(x)}{p(x)} p_i(x)dx$$

$$\approx 1$$

## Weighted to Unweighted Events

- How do we generate x according to the pdf p(x)?
- First method: inverse transform method
- Consider the cumulative distribution function

$$P(x) = \int_{-\infty}^{x} dt \ p(t) \Longrightarrow P(x) \in [0, 1]$$

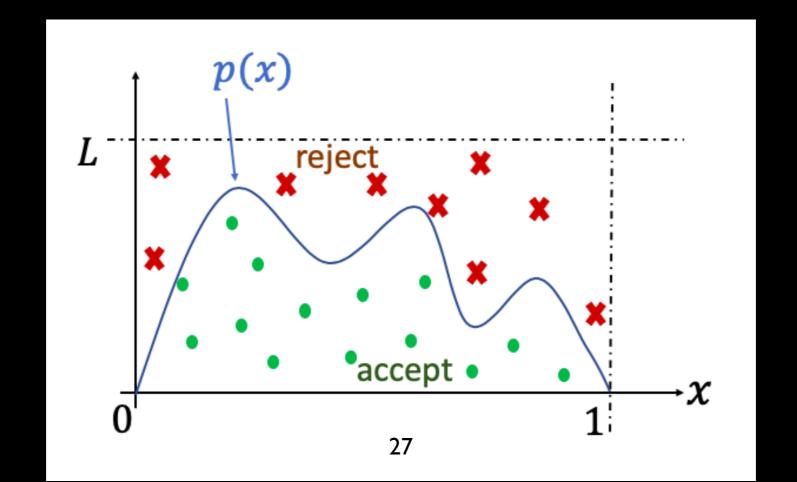
Now consider a random variable u uniformly distributed in [0,1]

$$x = P^{-1}(u) \Longrightarrow p(x)dx = du$$

• This requires knowing analytically the inverse of P

### Acceptance-rejection method

- Consider x a random variable uniformly distributed between [0,1]
- Draw a first value of the  $x(x_1)$
- Draw a second value of x (x<sub>2</sub>)
- Accept x<sub>1</sub> if  $p(x_1) \ge x_2 L$
- the resulting distribution of accepted points follow p(x)



• Let's return to the cross section evaluation

$$\sigma = \int dx_1 dx_2 \sum_{\text{subp}} f_{a_1/p}(x_1) f_{a_2/\bar{p}}(x_2)$$

$$\frac{1}{2\hat{s}(2\pi)^{3n-4}} \int d\Phi_n(x_1 P_A + x_2 P_B; \ p_1 \dots p_n) \Theta(\text{cuts}) \overline{\sum} |\mathcal{M}|^2 (a_1 a_2 \to b_1 \dots b_n)$$

that requires a suitable choice of the integration variables

• Initially we map the integration region into a 3n-2 hypercube

$$dx_1 dx_2 d\Phi_n = J \prod_{i=1}^{3n-2} dr_i$$

- It is easy to reconstruct the momenta and implement the cuts
- This procedure generate weighted events with weight

$$\mathbf{w} = \sum_{\{\mathbf{r_i}\}} \; \frac{J}{2\hat{s}(2\pi)^{3n-4}} \; \sum_{\substack{\text{subprocesses}}} \; f(\mathbf{x_1}) f(\mathbf{x_2}) \overline{\sum} |\mathcal{M}|^2 \; \Theta(\text{cuts}) \; ,$$

- Now it is possible to generate distributions
- Unweighted events can also be obtained

**\*** Example:  $e^+e^- \rightarrow 2$  particles in the final state

$$d\Phi_2 = \frac{1}{4} \, \frac{|\vec{p}_1^{cm}|}{\sqrt{s}} \, d\cos\theta_1 d\phi_1 = \frac{1}{4} \, \frac{|\vec{p}_1^{cm}|}{\sqrt{s}} \, \times 4\pi \times dr_1 dr_2$$

with  $\cos \theta_1 = -1 + 2r_1$  and  $\phi_1 = 2\pi r_2$ . More, I can construct the (massless) momentum with this

$$p_1 = \frac{\sqrt{s}}{2} (1, \sin \theta_1 \cos \phi_1, \sin \theta_1 \sin \phi_1, \cos \theta_1)$$

$$p_2 = \frac{\sqrt{s}}{2} (1, -\sin \theta_1 \cos \phi_1, -\sin \theta_1 \sin \phi_1, -\cos \theta_1)$$



## References

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- Barger & Phillips, chapter 11
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- O. Mattelaer <a href="https://cp3.irmp.ucl.ac.be/projects/madgraph/attachment/wiki/">https://cp3.irmp.ucl.ac.be/projects/</a>
   madgraph/attachment/wiki/
   Madrid2015\_2%20MC/
   15\_09\_07\_Madrid\_MC.pdf