Monte Carlo Methods

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DESY Theory Group

Outline and Disclaimer

What the lecture will cover:

- Monte Carlo methods: What and how.
- From integrals to integrands and back: integration and sampling.
- Some more advanced topics, modulo time constraints.

What the lecture certainly not covers:

- The art of (pseudo-) random number generation.
- Technical details of available methods/codes.
- MC methods outside HEP, in particular in statistical physics.

A Travel Guide to Monte Carlo

If there are any questions, don't hesitate to interrupt me.

A Travel Guide to Monte Carlo

Getting started:

- Why go to Monte Carlo at all?

A first tour:

- Sampling by inversion.
- Dealing with many variables: hit-and-miss.
- From hits to weights and integrals.

For experienced visitors:

- Loading the dice: variance reduction.
- A first glimpse on VEGAS.

Additional tours for longer stays:

- MC methods for NLO & parton showers.

Expectations to the Journey.

The Task, Physics Wise.

Given some cross section differential in all momentum components ...

- Calculate the total cross section σ.
- With arbitrary acceptance criteria ('cuts').
- Produce a sample of events $(p_1, ..., p_n)$ with probability density

$$\frac{1}{\sigma}\mathrm{d}\sigma(p_1, ..., p_n) \ .$$

- Book histograms for arbitrary observables, and compare to data

The Task, Technically.

Given a function $p(x_1, ..., x_n)$,
and a volume $V = \{(x_1, ..., x_n) \in \mathbb{R}^n | v(x_1, ..., x_n) = 0\}$ ...

- Calculate
$$N(p, V) = \int_V p(x_1, ..., x_n) \mathrm{d}^n x \ .$$
- Produce a sample of events $(x_1, ..., x_n) \in V$ with probability density
$$\frac{1}{N(p, V)} p(x_1, ..., x_n) \mathrm{d}^n x \ .$$
- Book histograms for arbitrary functions $O(x_1, ..., x_n)$.

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Well, we could just do numerical integrations,

$$N(p, V) = \int_V^{\text{Gauss},\ldots} p(x_1, \ldots, x_n)\mathrm{d}^n x \ .$$

Don't even need 'events', nor histograms, but calculate

$$\frac{\mathrm{d}p}{\mathrm{d}O} = \int_V p(x_1, \ldots, x_n)\delta(O - O(x_1, \ldots, x_n))\mathrm{d}^n x$$

the same way, and just plot into measured histograms.

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So what?

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There are $n = 3k - 4$ variables for k outgoing particles.

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MC methods are the only feasible way to achieve the task.

We'll see how ...

Getting into Touch with MC Methods.

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We'll start off with drawing random variates in a single variable.

May seem unrelated to the problems we want to solve, yet:

- Gives a first feeling for what is going on.
- Often needed as helper for more efficient algorithms.

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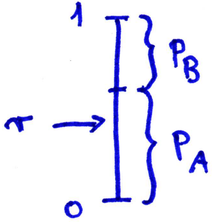
Choose between two outcomes A and B with probabilities $P_{A,B}$.
How to implement an algorithm selecting either one according to $P_{A,B}$?

Have **rnd**() to return equally distributed random numbers $r \in [0, 1]$.

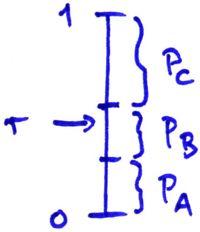
$r \leftarrow$ **rnd**()
if $r < P_A$ **then**
  return A
else
  return B
end if



How to do things with some probability?

Choose between three outcomes A, B and C with probabilities $P_{A,B,C}$.

$r \leftarrow$ **rnd**()
if $r < P_A$ **then**
  return A
else if $r < P_A + P_B$ **then**
  return B
else
  return C
end if



Etc.

Sampling by Inversion.

Suppose we got $p(x) \geq 0$ and $V = [a, b]$ to define a probability density

$$P(x)\mathrm{d}x = \theta(b-x)\theta(x-a)\frac{p(x)\mathrm{d}x}{\int_a^b p(z)\mathrm{d}z}$$

from which we are to draw random variates.

We'll assume that p is sufficiently simple such that

- we can calculate the integral of p, and
- we can solve

$$\int_a^x p(z)\mathrm{d}z = r \int_a^b p(z)\mathrm{d}z$$

for x as a function of $r \in [0, 1]$.

Sampling by Inversion.

The algorithm generating events according to $P(x)$ is simple:

$r \leftarrow$ **rnd**()
$x \leftarrow$ solution of
$\int_a^x p(z)\mathrm{d}z = r \;\; \int_a^b p(z)\mathrm{d}z$
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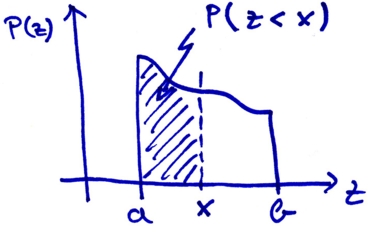

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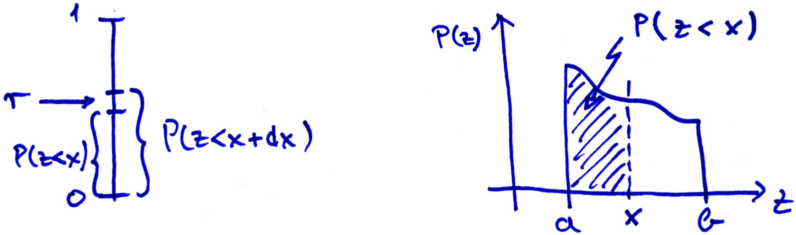

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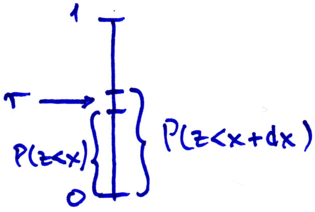

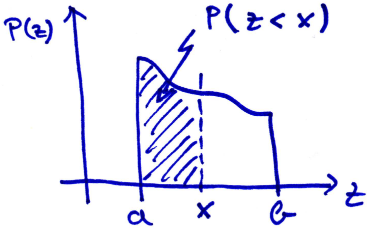

$$\mathrm{d}r = P(z)\mathrm{d}z$$

We only solved a change of variables.

Sampling by Inversion: Example.

Suppose we have $p(x) = x$ on $[0, 1]$. Then solve $\frac{x^2}{2} = r\ \frac{1}{2}$.

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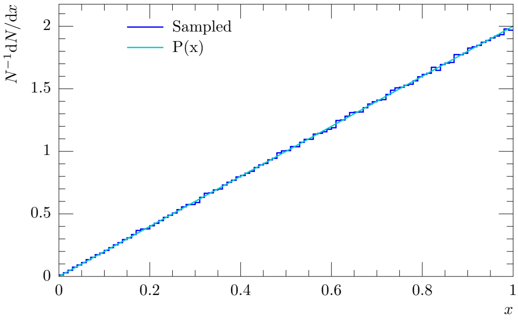

Dealing with Many Variables: Hit-and-Miss.

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```
loop
  r ← rnd()
  x ← a + r(b − a)
  r′ ← rnd()
  if r′ < p(x)/c then
    return x
  end if
end loop
```

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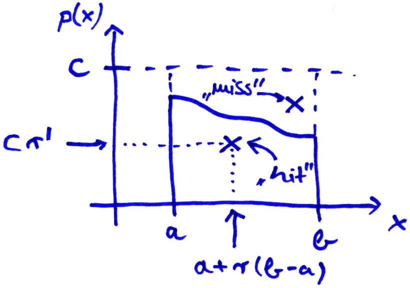

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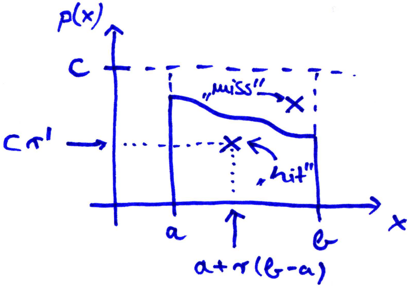

The frequency of hits in $[x, x + \mathrm{d}x]$ is directly proportional to $p(x)$.

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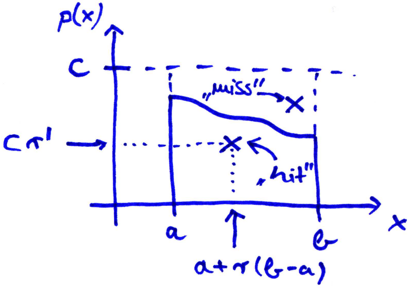

Note that we did not have to know the normalization!

Dealing with Many Variables: Hit-and-Miss.

Given a function $p(x_1, ..., x_n)$,
and a volume $V = \{(x_1, ..., x_n) \in \mathbb{R}^n | v(x_1, ..., x_n) = 0\}$ ...

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And a hypercube $I = [a_1, b_1] \times \cdots \times [a_n, b_n]$ with $V \subset I$.

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Define

$$p_V(x_1, ..., x_n) = \begin{cases} p(x_1, ..., x_n) & : \quad v(x_1, ..., x_n) = 0 \\ 0 & : \quad \text{otherwise} \end{cases} \quad .$$

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loop
  for $i = 1..n$ **do**
    $r \leftarrow$ **rnd**()
    $x_i \leftarrow a_i + r(b_i - a_i)$
  end for
  $r' \leftarrow$ **rnd**()
  if $r' < p_V(x_1, ..., x_n)/c$ **then**
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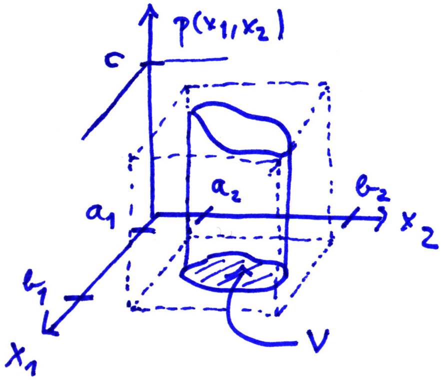

Remark.

Unless stated otherwise: Back to one variable.

Generalizations should be obvious now.

If not: Please ask!

From Hits to Weights and Integrals.

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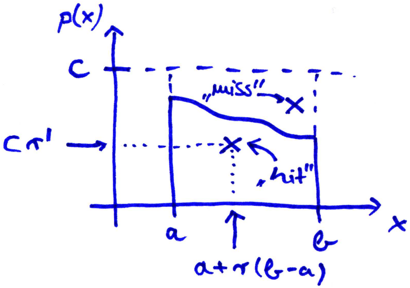

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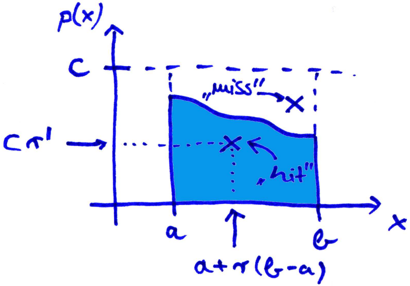
From Hits to Weights and Integrals.

We actually *estimated* the normalization, if we were counting hits:

$$\int_a^b p(x)\mathrm{d}x \approx \frac{\#\text{hits}}{\#\text{hits} + \#\text{misses}} \times c(a-b)\ .$$



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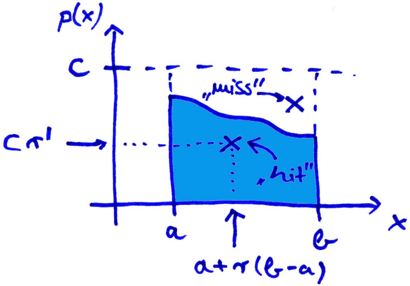

In other words: We have just (approximately) calculated an integral!

Weights, Averages, and Variances.

Let's put the estimate onto a more waterproof ground.

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Averaging p over $[a, b]$ is connected to its integral,

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$$\langle p \rangle = \frac{1}{b-a} \int_a^b p(x) \, \mathrm{d}x \; .$$

Now estimate the average by

- recording p's value at random points x_i,
- for a total of N points:

$$\langle p \rangle_{\text{estimate}} = \frac{1}{N} \sum_{i=1}^{N} p(x_i) \; .$$

Weights, Averages, and Variances.

We'll call $w_i = p(x_i)$ the *weight* of an event x_i.
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The variance of $\langle p \rangle_{\text{estimate}}$ is

$$\sigma^2 \left[\langle p \rangle_{\text{estimate}}\right] = \frac{1}{N}\left(\frac{1}{N}\sum_{i=1}^{N} w_i^2 - \left(\frac{1}{N}\sum_{i=1}^{N} w_i\right)^2\right) .$$

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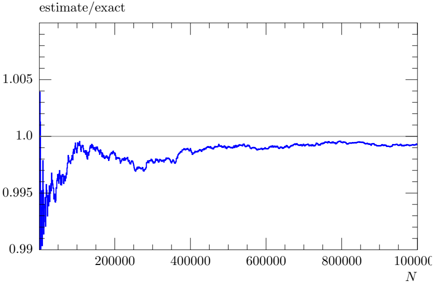
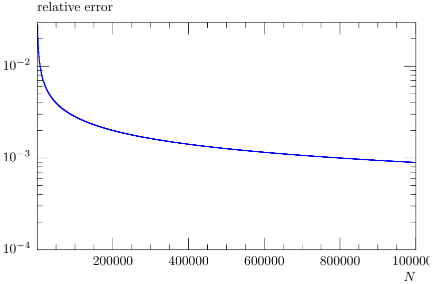
$$\boxed{\int_a^b p(x)\,\mathrm{d}x = (b-a)\langle p\rangle_{\text{estimate}} \pm (b-a)\sigma\left[\langle p\rangle_{\text{estimate}}\right]}$$

Monte Carlo Integrals: Example.

Integrate $p(x) = x^2$ on $[0, 1]$.





Uncertainty drops as $1/\sqrt{N}$. Mind the independent measurements.

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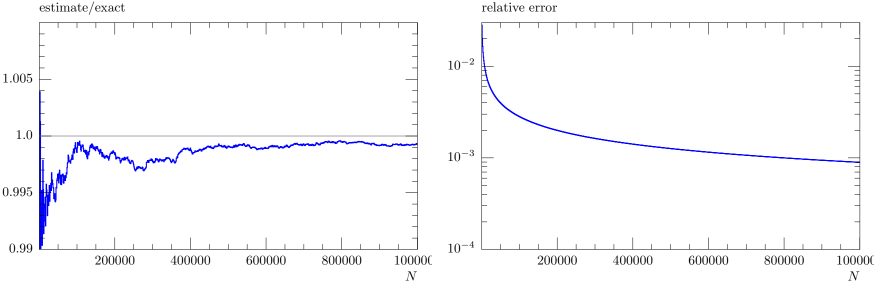

Doesn't really converge to the true value, right?

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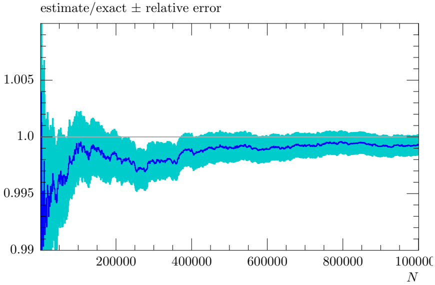

Even worse: Error band just scratches true value for large N.

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Never, ever use things like:

`rnd(), drand48() ...`

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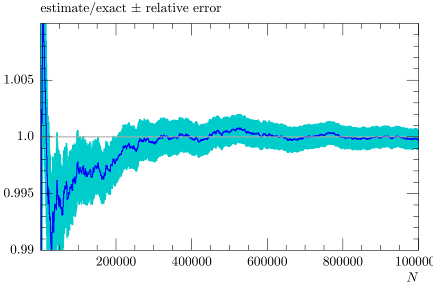

Same thing, better random number generator.

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Assign weights

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Then

$$\int_a^b p(x)\mathrm{d}x \approx \frac{\#\text{hits}}{\#\text{hits} + \#\text{misses}} \times c(a-b)$$

as conjectured.

But now we know how accurate this estimate is.

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Just a scaling of variables:

$$\int_a^b p(x)\mathrm{d}x = c \int_a^b \frac{p(x)}{c}\mathrm{d}x$$

True *changes* of variables when trying to cheat in the casino ...

A Travel Guide to Monte Carlo

Time for questions.

Uncertainties, continued.

Mind the integral's uncertainty,

$$\sigma^2 \left[\langle p \rangle_{\text{estimate}} \right] = \langle \sigma^2 \left[p \right] \rangle_{\text{estimate}} \ .$$

If p has large variance, need a very large N for a reasonable uncertainty.

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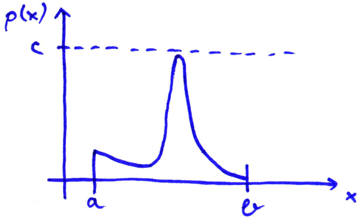
If p has large variance, need a very large N for a reasonable uncertainty.

Connected to this is an inacceptable efficiency of hit-and-miss,

$$\epsilon = \frac{\#\text{hits}}{\#\text{hits} + \#\text{misses}} \ll 1 \ .$$



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First set some notation,

$$\langle p \rangle \to \langle p \rangle_1 \ ,$$

where in general

$$\langle p \rangle_r = \int_a^b p(x) r(x) \mathrm{d}x \ .$$

Loading the Dice: Variance Reduction.

The basic ingredients to variance reduction:

- A constant function has zero variance.
- And we always have

$$\langle p \rangle_1 = \left\langle \frac{p}{r} \right\rangle_r \quad .$$

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- A constant function has zero variance.
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$$\langle p \rangle_1 = \left\langle \frac{p}{r} \right\rangle_r \ .$$

So, ideally

$$\langle p \rangle_1 = \langle 1 \rangle_p$$

with zero variance ???

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What does $\left\langle \frac{p}{r} \right\rangle_r$ actually mean?

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What does $\left\langle \frac{p}{r} \right\rangle_r$ actually mean?

– A change of variables,

$$p(x)\mathrm{d}x = p(x(R))\frac{\mathrm{d}x(R)}{\mathrm{d}R}\mathrm{d}R$$

with $r(x)\mathrm{d}x = \mathrm{d}R$.
Record p/r at points inside the transformed volume.

Loading the Dice: Variance Reduction.

What does $\left\langle \frac{p}{r} \right\rangle_r$ actually mean?

- A change of variables,

$$p(x)\mathrm{d}x = p(x(R))\frac{\mathrm{d}x(R)}{\mathrm{d}R}\mathrm{d}R$$

  with $r(x)\mathrm{d}x = \mathrm{d}R$.
  Record p/r at points inside the transformed volume.
- If $r(x)$ is normalized to define a probability density:
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To arrive at $\langle 1 \rangle_p$ we would actually have to know the integral.
Then the uncertainty is – of course – zero.

Loading the Dice: Variance Reduction.

The best we can hope for is finding a r, which is very similar to p,

$$\frac{p(x)}{r(x)} \approx \text{constant} \ .$$

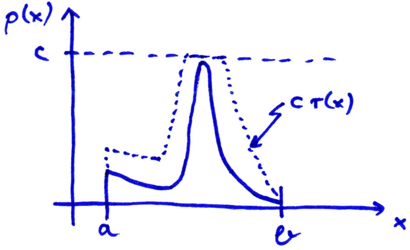
And sufficiently simple, such that we can distribute points with a probability density defined by r.

Loading the Dice: Variance Reduction.

This also helps with the hit-and-miss efficiency:

If we know c such that $c\ r(x) \geq p(x)$, we can

- Propose points with density defined by r, and
- accept a hit x with probability $\frac{p(x)}{c\ r(x)}$.



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Bottom line:

- Generate more points where p has large fluctuations.
- Generate less points where p is essentially constant.
- Divide out the bias introduced thereby.

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A bit of terminology:

What we got to know here is known as **'importance sampling'**.

Loading the Dice: Variance Reduction.

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There is also **‘stratified sampling’**.

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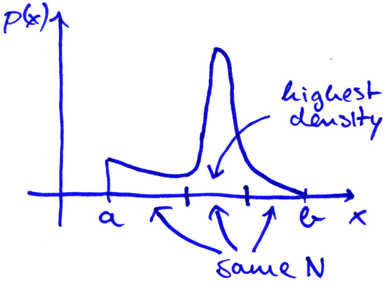

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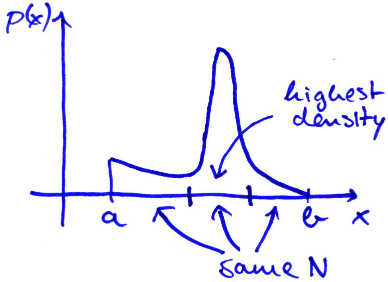
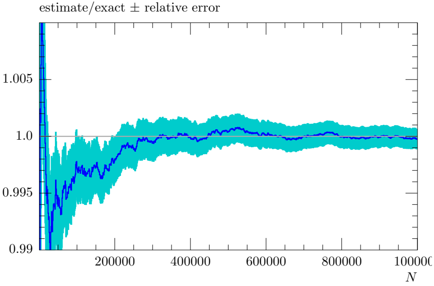
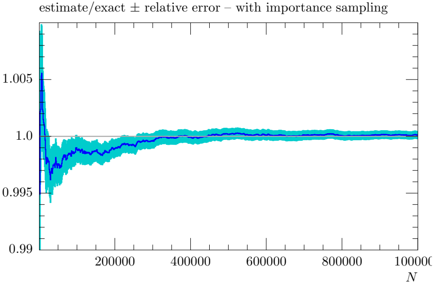


This is just another way of implementing a $r(x)$ made up of step functions.

Variance Reduction: Example.

Integrate $p(x) = x^2$ on $[0, 1]$. Importance sampling with $r(x) = x$.





Detour: From Integrals and Weights to Hits.

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From MC integration we obtain a sample of *weighted* events, (x_i, w_i).

For event generation, we are interested in *unweighted* events, (x_i, c).
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To get to unweighted events,

- find the maximum weight w_{max},
- keep each weighted event (x_i, w_i) with probability w_i/w_{max}, and
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NB: For a proper variance reduction, the weight's variance is small compared to the average weight: efficient 'unweighting'.

A First Glimpse on VEGAS.

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- An algorithm for stratified sampling.
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- Adaptive: Adjust $r(x)$ in each *iteration* to get smaller variance.

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Implementations: Lepage's listing, MONACO, GSL, dVegas, ...

A First Glimpse on VEGAS.

The troubles with many variables.

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Suppose we want to make up $r(x_1, ..., x_n)$ of step functions.
Divide each variable range $[a_i, b_i]$ into k intervals

$$[a_i = x_{i,0}, x_{i,1}], [x_{i,1}, x_{i,2}], ..., [x_{i,k-1}, b_i = x_{i,k}] \ ,$$

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and let

$$r(x_1, \ldots, x_n) =$$
$$\sum_{i_1, \ldots, i_n = 1}^{k} r_{i_1, \ldots, i_n} \theta(x_{1,i_1} - x_1)\theta(x_1 - x_{1,i_1-1}) \cdots \theta(x_{n,i_n} - x_n)\theta(x_n - x_{n,i_n-1}) \ .$$

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A `double` is 64 $\mathrm{Bits} = 8\ \mathrm{Bytes}$:

$$4^{10} \times 8\ \mathrm{Bytes} = 8\ \mathrm{GBytes}$$

Not an option.

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$n \times k$ values to store instead of k^n.
Now need 320 Bytes instead of 8 GBytes!

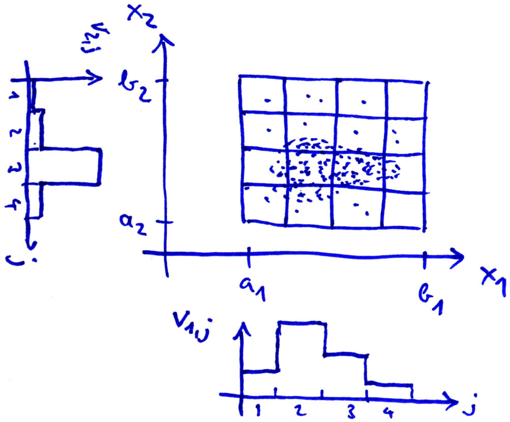
A First Glimpse on VEGAS.

Keep number of points per interval fixed.
Trade of $r_{i,j}$ to keep track of

$$v_{i,j} = \frac{1}{(b_1 - a_1)\cdots(x_{i,j} - x_{i,j-1})\cdots(b_n - a_n)} \times \int_{a_1}^{b_1} \mathrm{d}x_1 \cdots \int_{x_{i,j-1}}^{x_{i,j}} \mathrm{d}x_i \cdots \int_{a_n}^{b_n} \mathrm{d}x_n \; p(x_1, ..., x_n) \; ,$$

i.e. the average weight in $[x_{i,j-1}, x_{i,j}]$ *projected* onto variable i.

A First Glimpse on VEGAS.

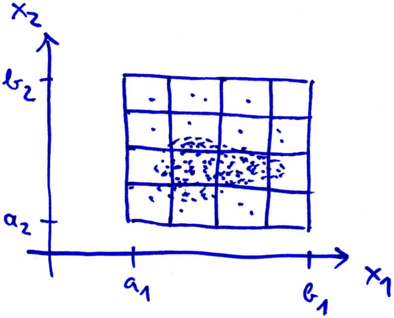


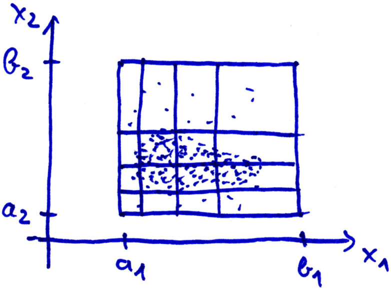
A First Glimpse on VEGAS.

The adaptive algorithm:

- Make a first run ('iteration') with N points.
- Adjust the $x_{i,j}$ such as to have higher density, where $v_{i,j}$ are large.
- Repeat for M iterations.

A First Glimpse on VEGAS.





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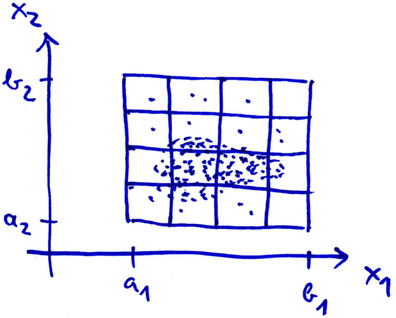

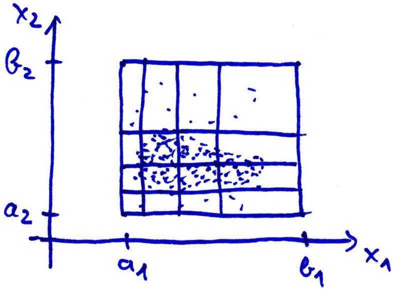

- Adjust the $x_{i,j}$ such as to have higher density, where $v_{i,j}$ are large.

This criterion is actually not unique, and rather complicated.

A Travel Guide to Monte Carlo

Time for questions.

MC Methods for NLO & Parton Showers.

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Negative 'probability densities':

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Negative ‘probability densities’:

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Markov processes:

- next parton shower emission.

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Parts of a NLO differential cross section can be negative.

Can we still make sense of this in terms of MC methods?

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If we just want to calculate an integral, there’s no problem.
We just have that some of the weights w_i are negative.

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Parts of a NLO differential cross section can be negative.

Can we still make sense of this in terms of MC methods?

If we just want to calculate an integral, there’s no problem.
We just have that some of the weights w_i are negative.

But what about ‘events’?

Negative ‘Probability Densities’

There’s a very simple way out of this:

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There's a very simple way out of this:

If $p(x)$ goes negative for some values of x ...

- Generate events according to $|p(x)|$.
- For x with $p(x) > 0$ add an event to histogram bin.
- For x with $p(x) < 0$ subtract an event from histogram bin.

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In other words:

Unweight from w_i to $c \times \mathrm{sign}(w_i)$ with
acceptance probability $|w_i|/\max|w_i|$.

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Draw events from a probability density

$$\frac{\mathrm{d}S_p(\mu, q|Q)}{\mathrm{d}q} = \Delta_p(\mu|Q)\delta(q-\mu) + p(q)\Delta_p(q|Q)\theta(Q-q)\theta(q-\mu)$$

where

$$\Delta_p(q|Q) = \exp\left(-\int_q^Q P(t)\mathrm{d}t\right) \ .$$

Markov Processes.

How to achieve this?

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First note, that we're truly facing a probability density,

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We just use sampling by inversion, solving for q in

$$\int_{\mu}^{q} \frac{\mathrm{d}S_p(\mu, t|Q)}{\mathrm{d}t} \mathrm{d}t = \Delta_p(q|Q) = \mathbf{rnd}() \ .$$

Markov Processes.

There's a caveat:

$$\Delta_p(q|Q) = \mathbf{rnd}()$$

has no solution if **rnd**() returned a value smaller than $\Delta_p(\mu|Q)$.

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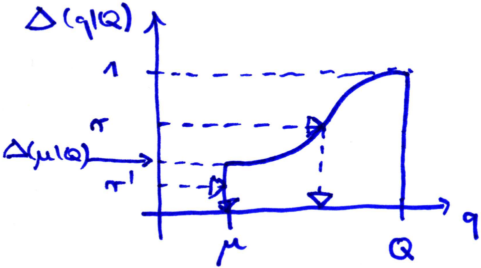
This is precisely giving us the contribution multiplying the δ-function.



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What if we can't solve $\Delta_p(q|Q) = \mathbf{rnd}()$ for q?

Markov Processes.

What if we can't solve $\Delta_p(q|Q) = \mathbf{rnd}()$ for q?

There's something like a hit-and-miss algorithm,
known as the 'Sudakov veto algorithm'.

Unfortunately, we'll have to leave Monte Carlo now ...

Memories from Monte Carlo

differential cross sections

events

probability densities

hits and misses

weights

total cross sections

integrals

Hands on a MC Event Generator

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Everything outlined in the lecture more or less feeds into a Monte Carlo event generator.

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We'll now get to know one of these: Herwig++.

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(After coffee...)