Introduction to Monte Carlo Event Generators

Stefan Gieseke

Institut für Theoretische Physik
KIT

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Karlsruhe Institute of Technology

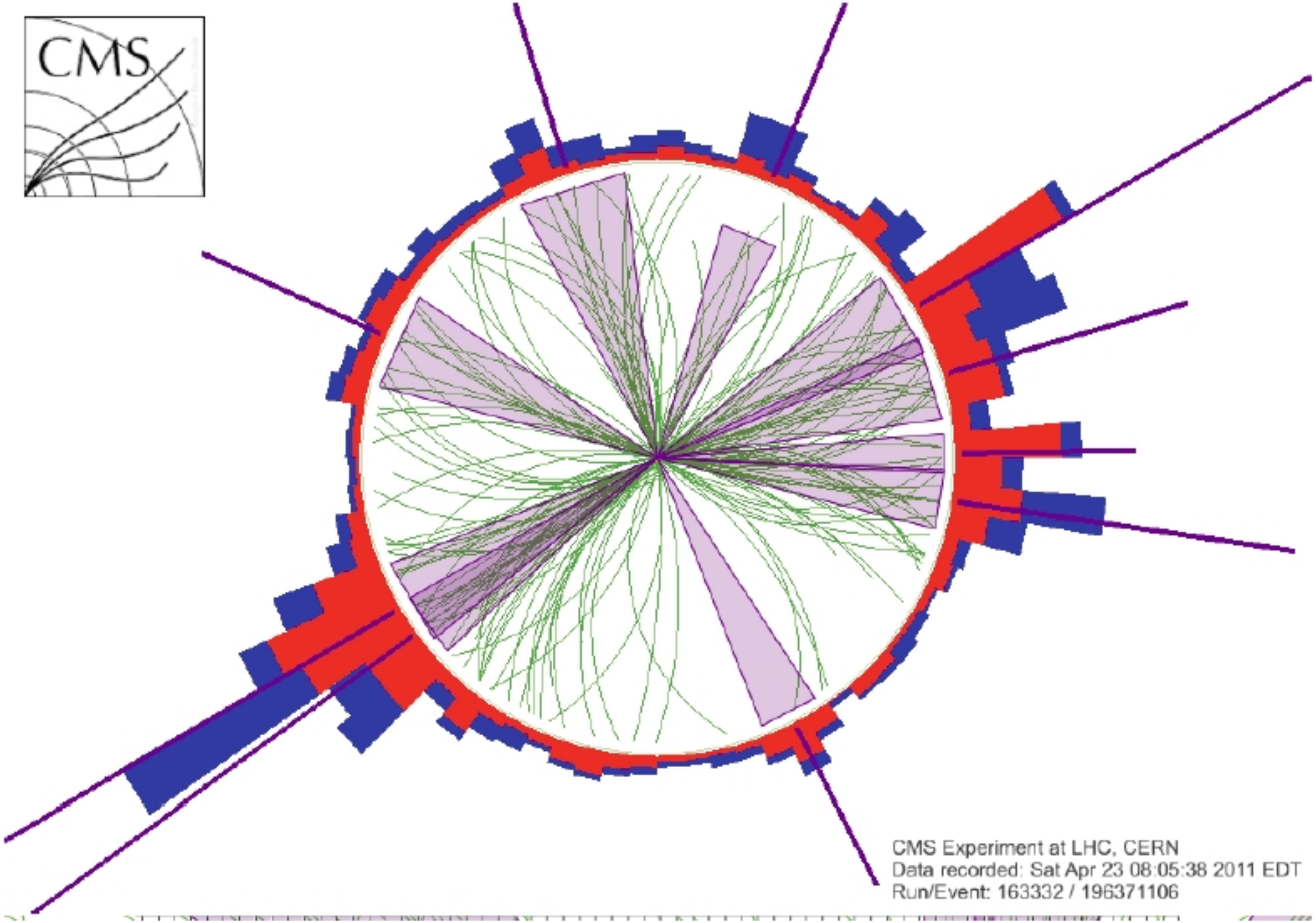
Bundesministerium
für Bildung
und Forschung

TRR 257 - Particle Physics Phenomenology
after the Higgs Discovery

Motivation: jets

[Google Images]

Motivation: jets (at LHC of course)



[CMS 2011]

Why Monte Carlos?

We want to understand

$$\mathscr{L}_{\rm int} \longleftrightarrow \text{Final states} \; .$$

Why Monte Carlos?

LHC experiments require
sound understanding of signals and *backgrounds*.

↑

Full detector simulation.

↑

Fully exclusive hadronic final state.

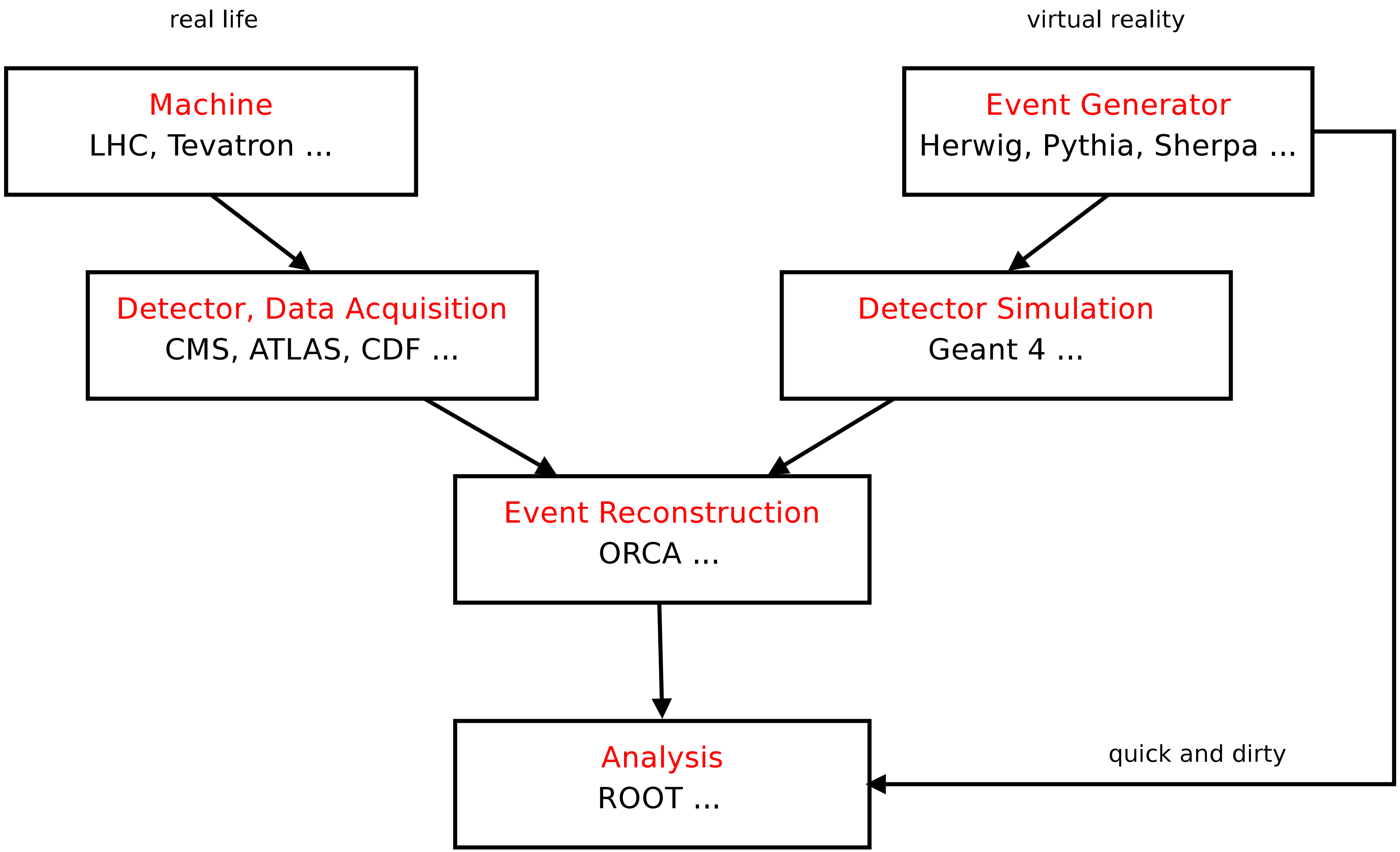
↑

Monte Carlo event generator with
parton shower, hadronization model, decays of unstable particles.

↑

Parton level computations.

Experiment and Simulation



Monte Carlo Event Generators

- Complex final states in full detail (jets).
- Arbitrary observables and cuts from final states.
- Studies of new physics models.

- Rates and topologies of final states.
- Background studies.
- Detector Design.
- Detector Performance Studies (Acceptance).

- *Obvious* for calculation of observables on the quantum level
$$|A|^2 \longrightarrow \text{Probability}.$$

pp Event Generator

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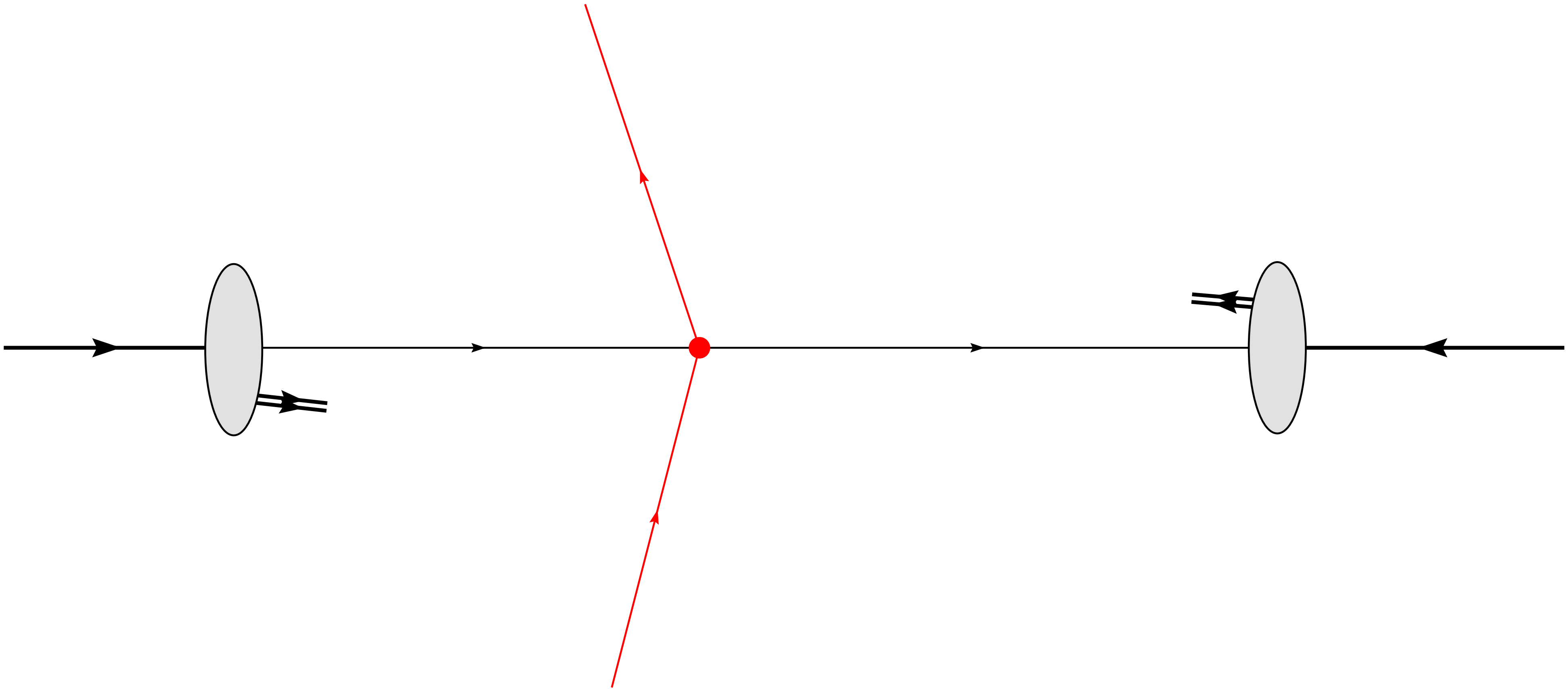

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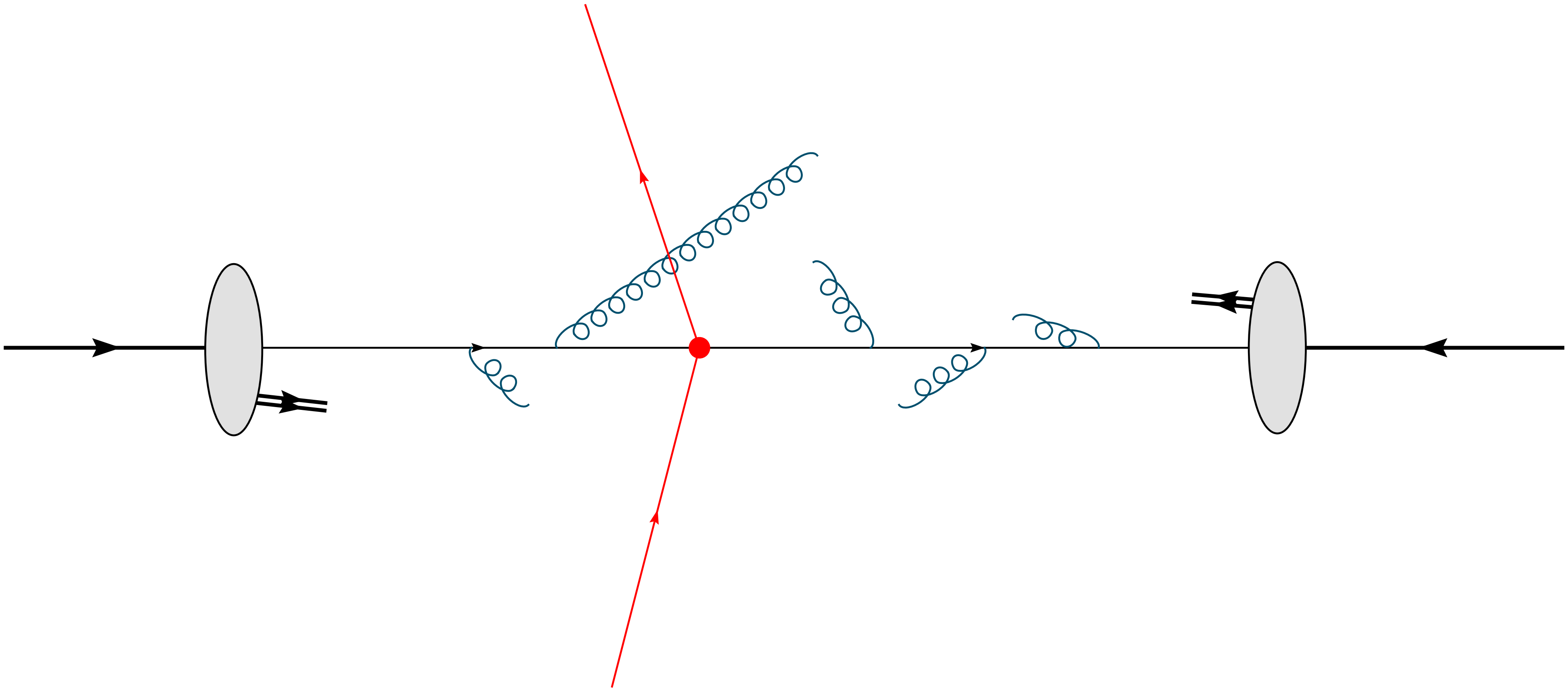

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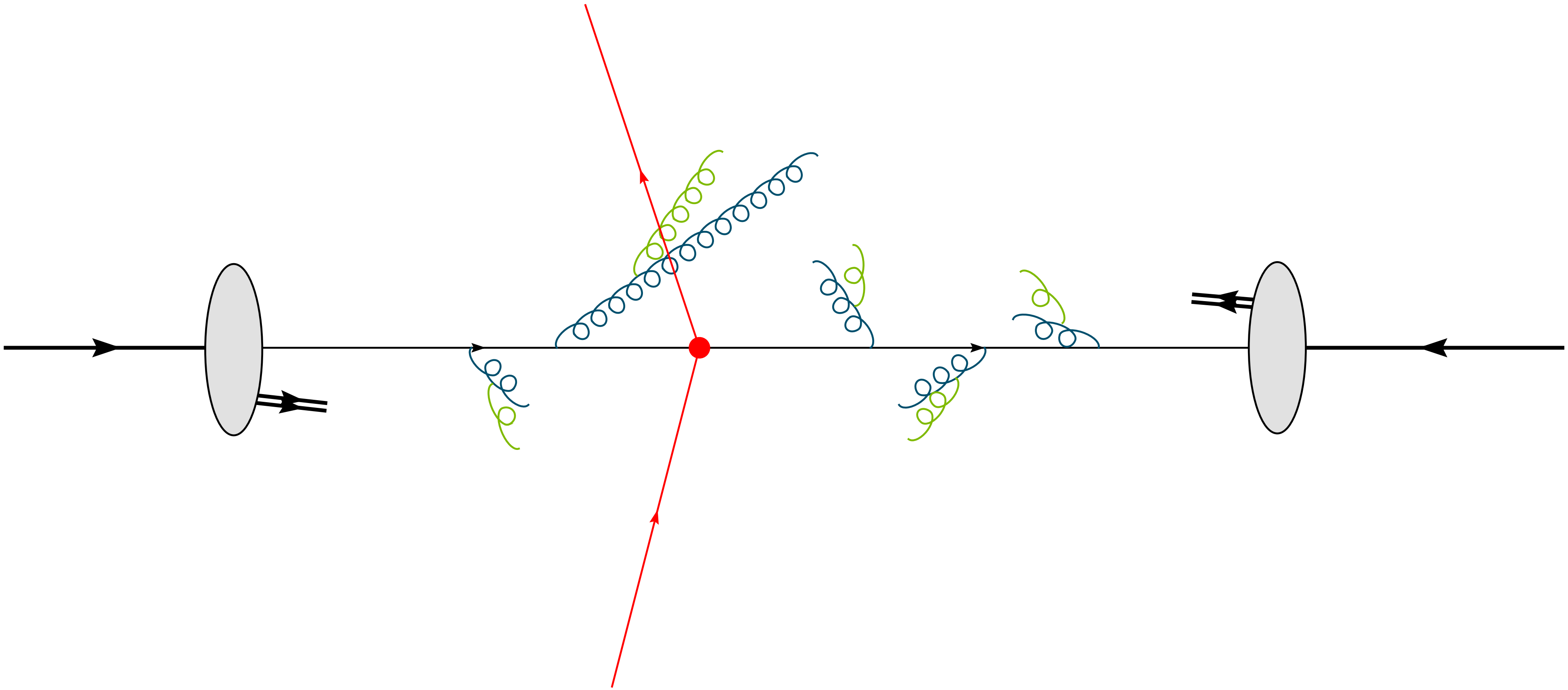

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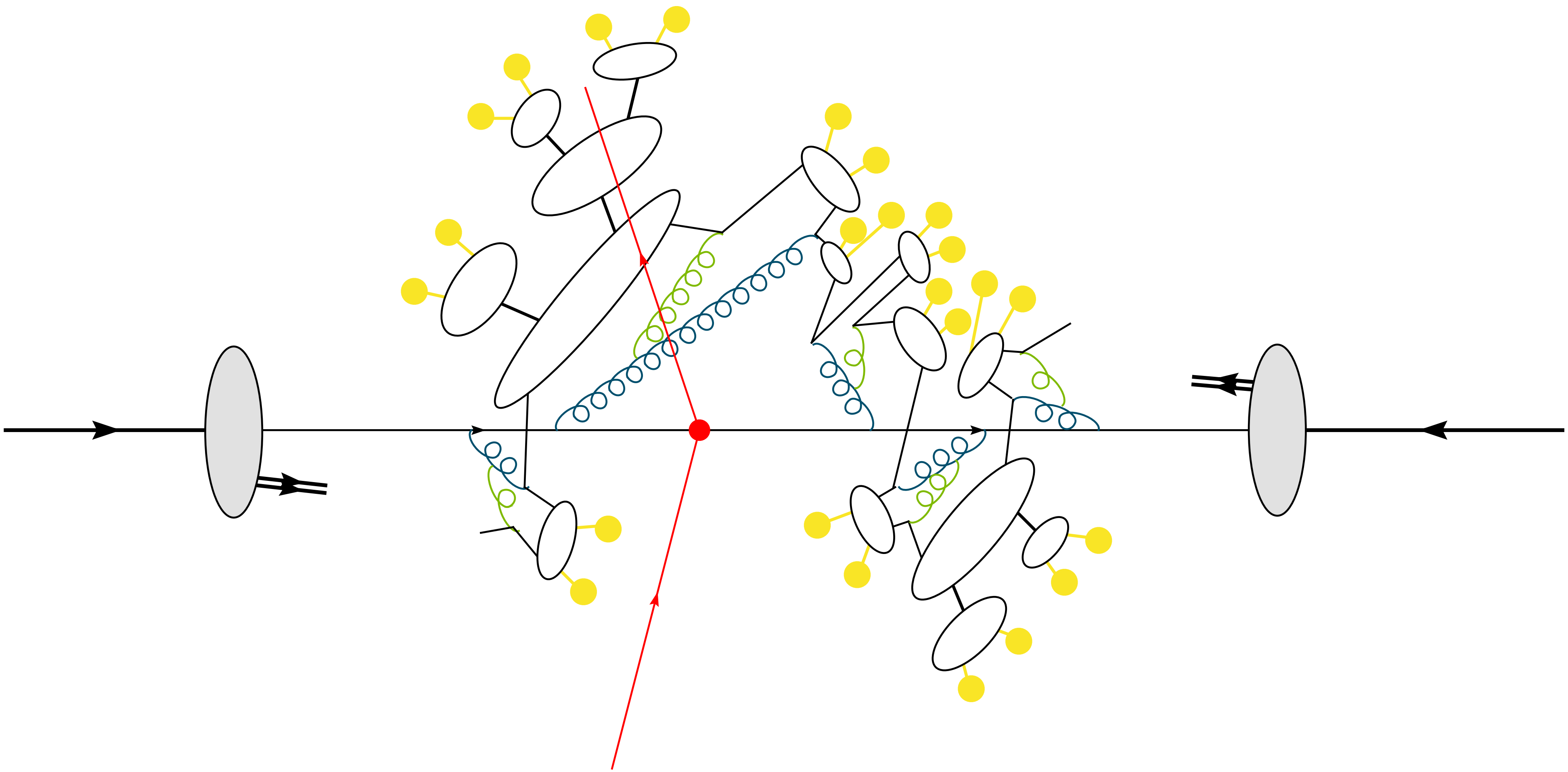

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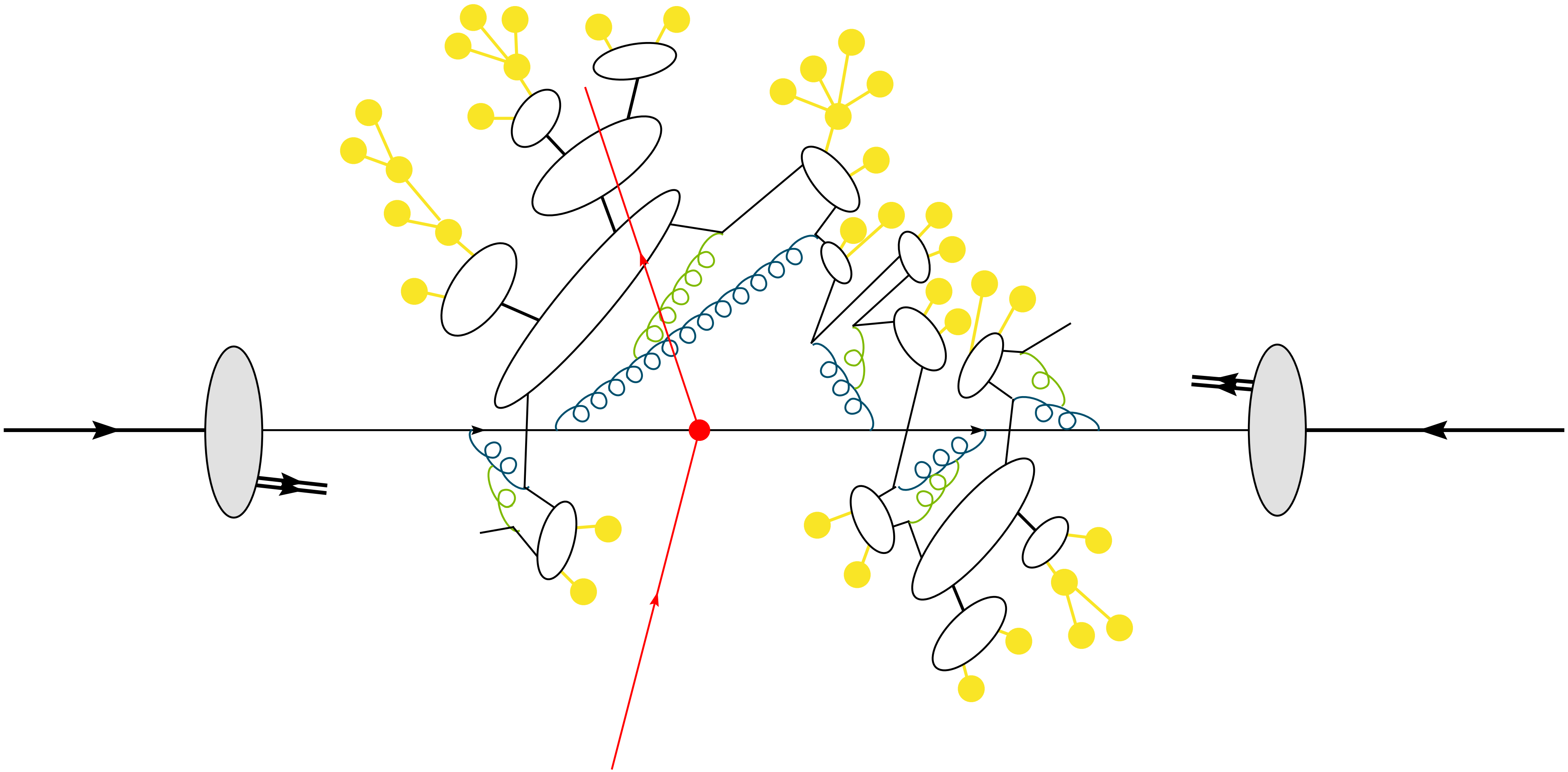

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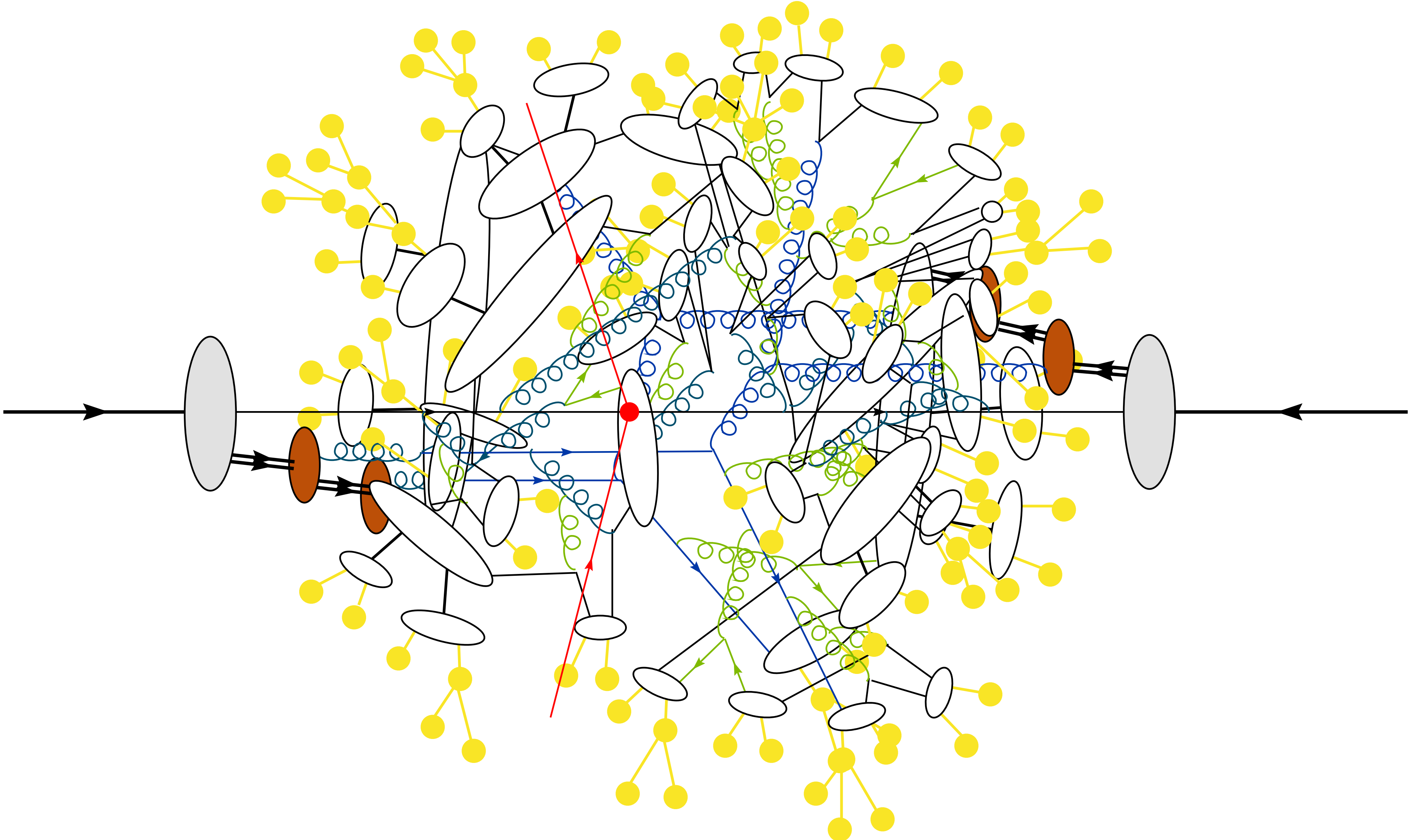


Divide and conquer

Partonic cross section from Feynman diagrams

$$\mathrm{d}\sigma = \mathrm{d}\sigma_{\mathrm{hard}}\mathrm{d}P(\text{partons} \to \text{hadrons})$$

$$\begin{aligned}
\mathrm{d}P(\text{partons} \to \text{hadrons}) = \;& \mathrm{d}P(\text{resonance decays}) && [\Gamma > Q_0] \\
& \times \mathrm{d}P(\text{parton shower}) && [\text{TeV} \to Q_0] \\
& \times \mathrm{d}P(\text{hadronisation}) && [\sim Q_0] \\
& \times \mathrm{d}P(\text{hadronic decays}) && [O(\text{MeV})]
\end{aligned}$$

Underlying event from multiple partonic interactions

$$\mathrm{d}\sigma \longleftarrow \mathrm{d}\sigma(\text{QCD } 2 \to 2)$$

Plan for these lectures

- Monte Carlo Methods
- Hard Scattering
- Parton Showers
- Hadronization and Hadronic Decays

  Underlying Event
- Multiple Parton Interactions (MPI) Modelling

Monte Carlo Methods

Monte Carlo Methods

Introduction to the most important MC sampling (= integration) techniques.

1. Hit and miss.
2. Simple MC integration.
3. (Some) methods of variance reduction.
4. Adaptive MC, VEGAS.
5. Multichannel.
6. Mini event generator in particle physics.

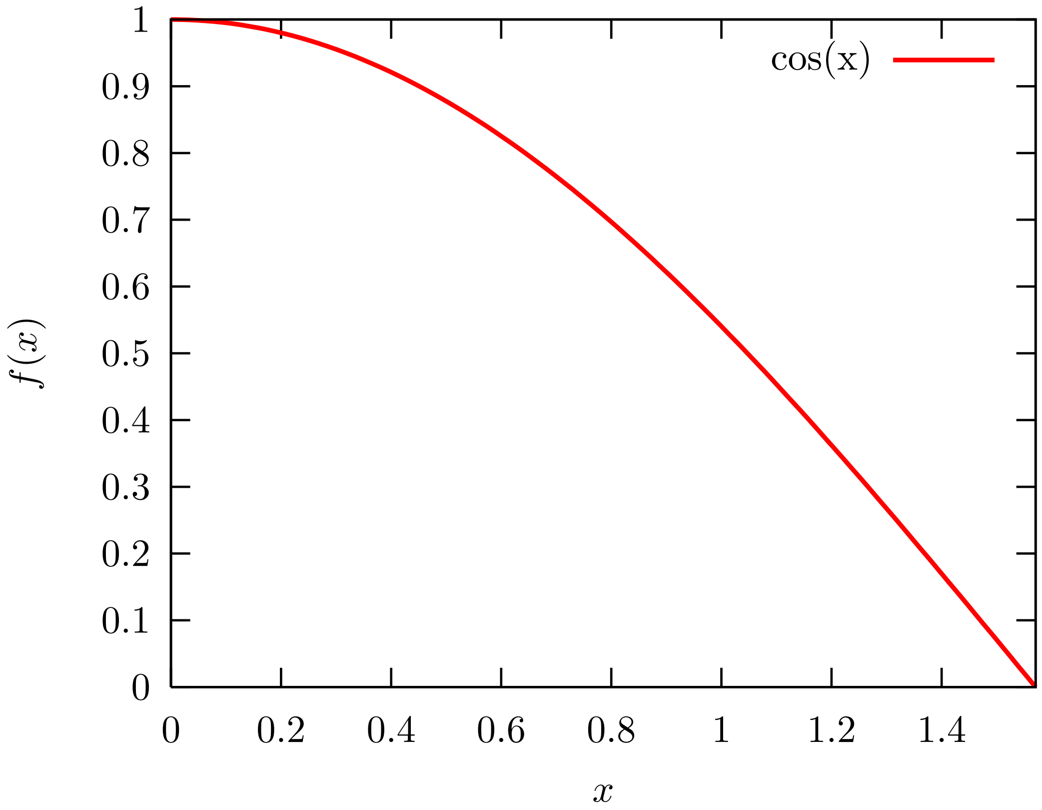
Probability

Example: $f(x) = \cos(x)$.

Probability density:

$$dP = f(x)\,dx$$

is probability to find value x.



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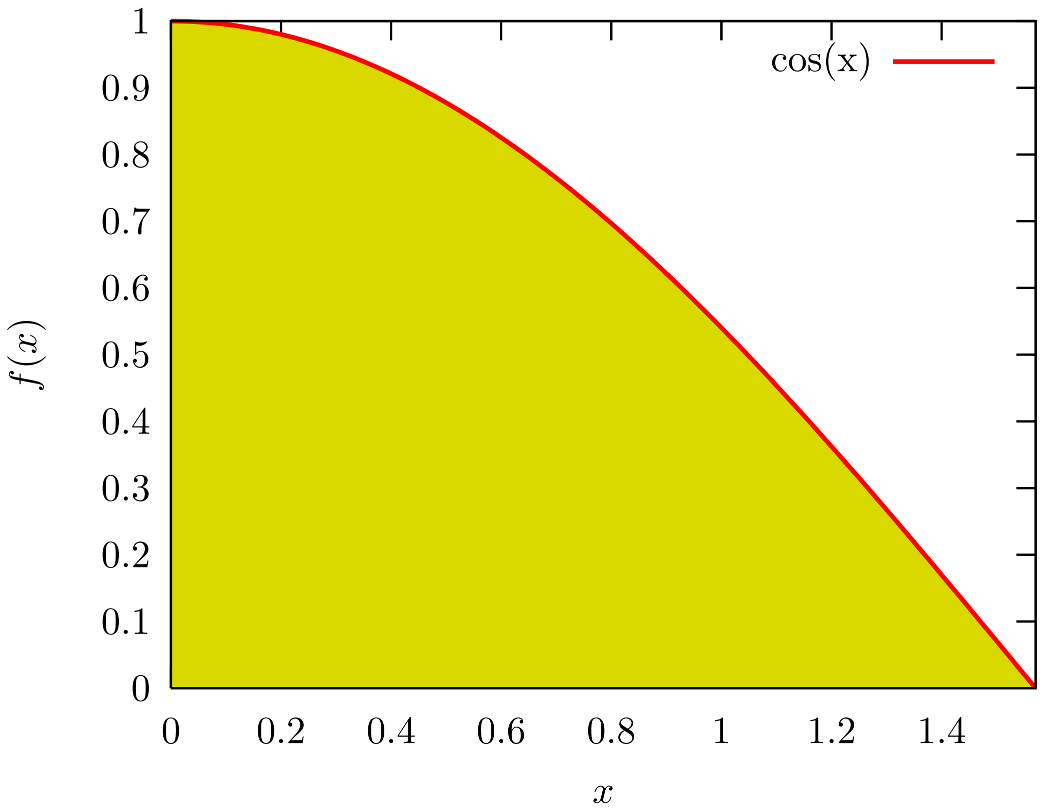
is called *probability distribution*.



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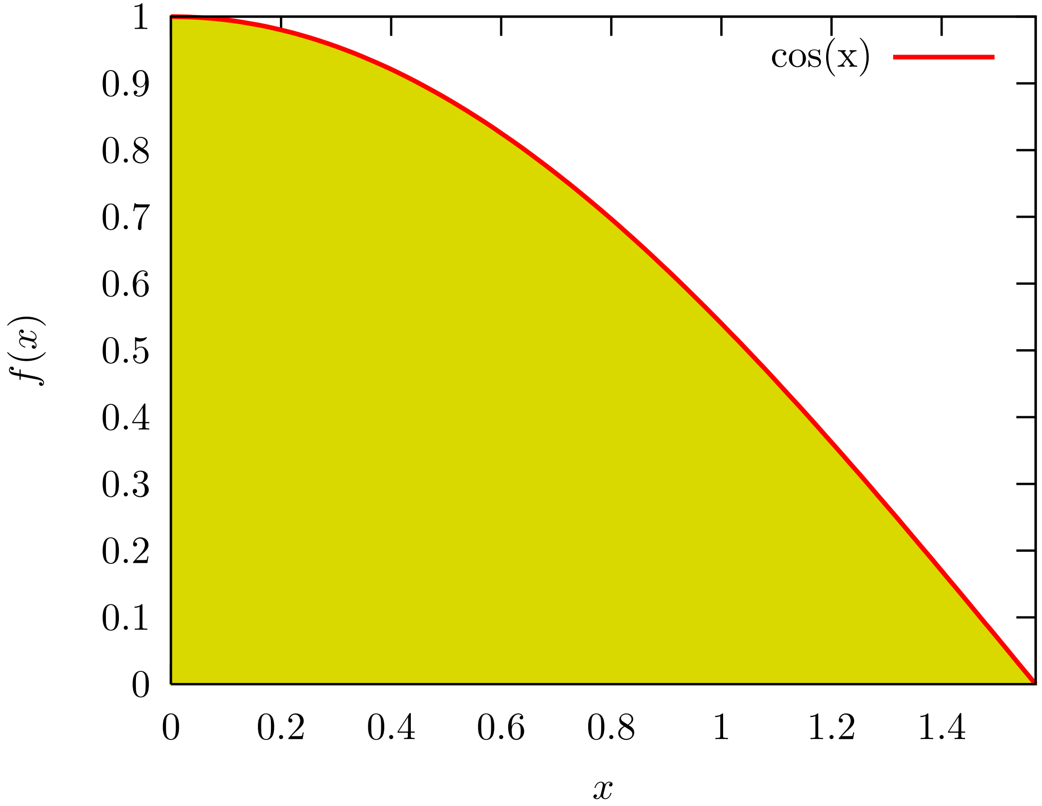

Probability $\sim$ *Area*

Hit and Miss

Hit and miss method:

- throw N random points (x, y) into region.
- Count hits N_{hit}, i.e. whenever $y < f(x)$.

Then

$$I \approx V \frac{N_{\text{hit}}}{N}.$$

approaches 1 again in our example.

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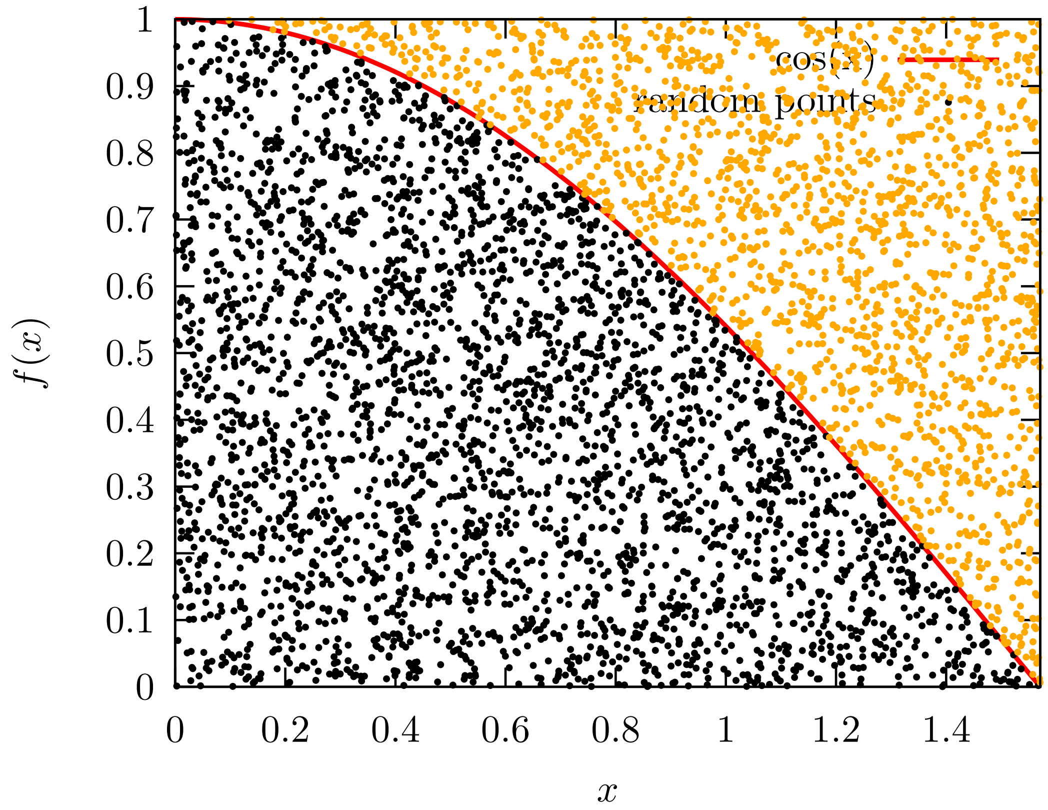

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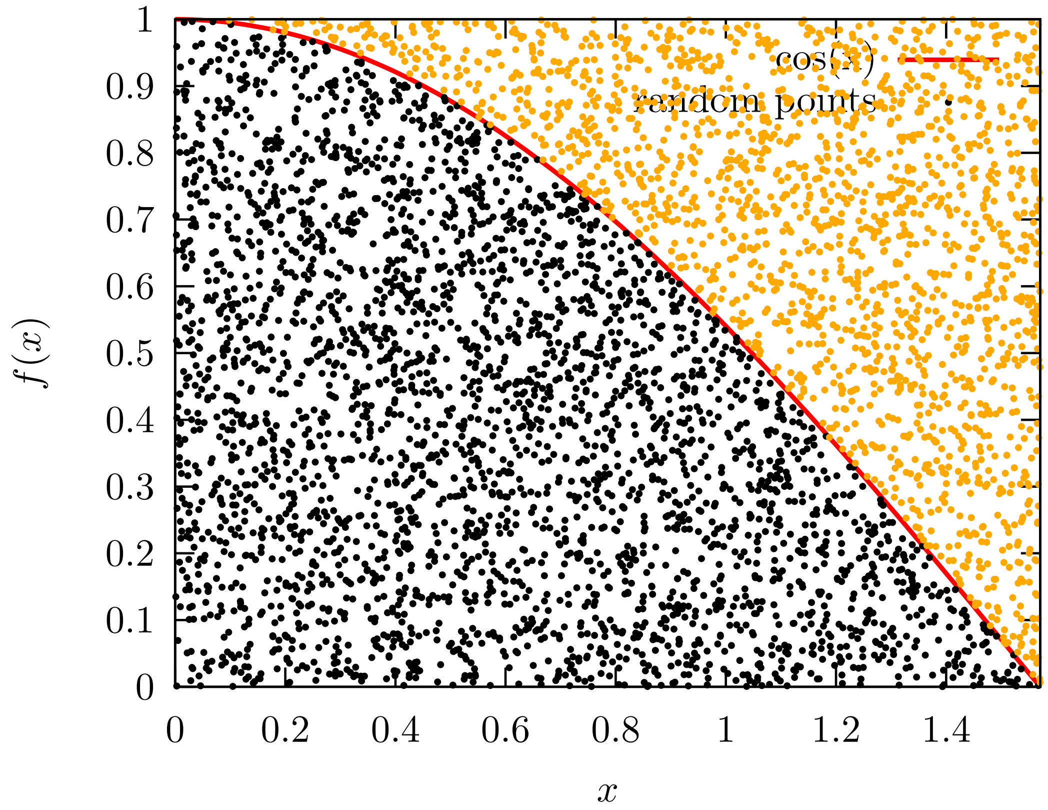
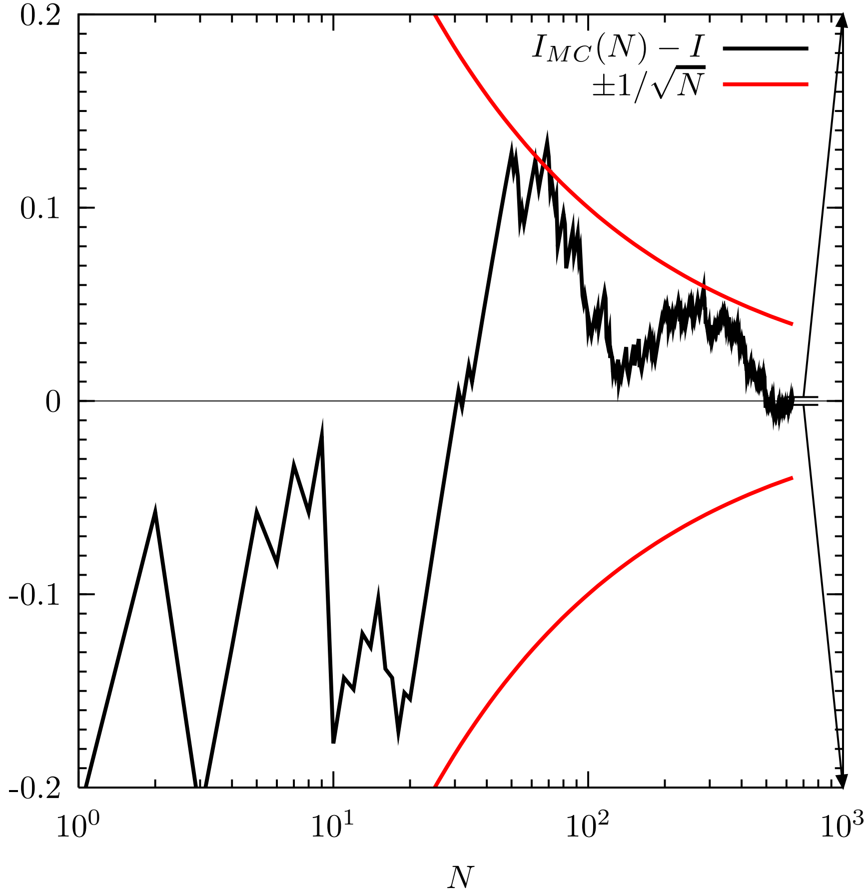


Every accepted value of x can be considered an event in this picture. As $f(x)$ is the 'histogram' of x, it seems obvious that the x values are distributed as $f(x)$ from this picture.

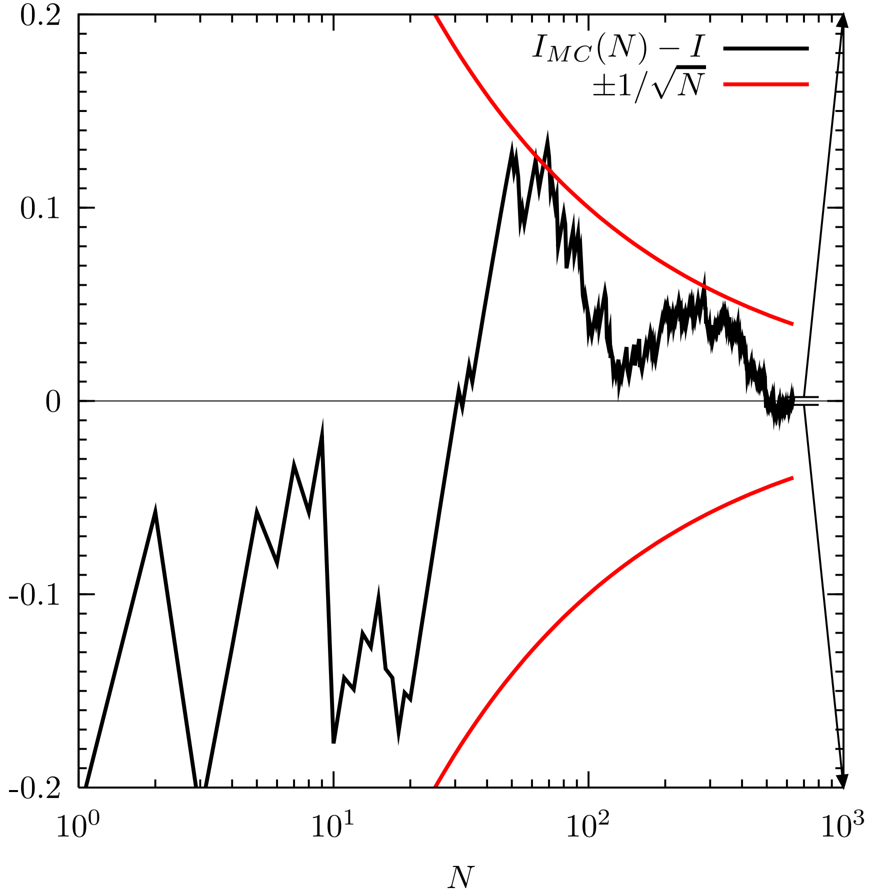
Hit and Miss



How well does it converge?

Error $1/\sqrt{N}$.

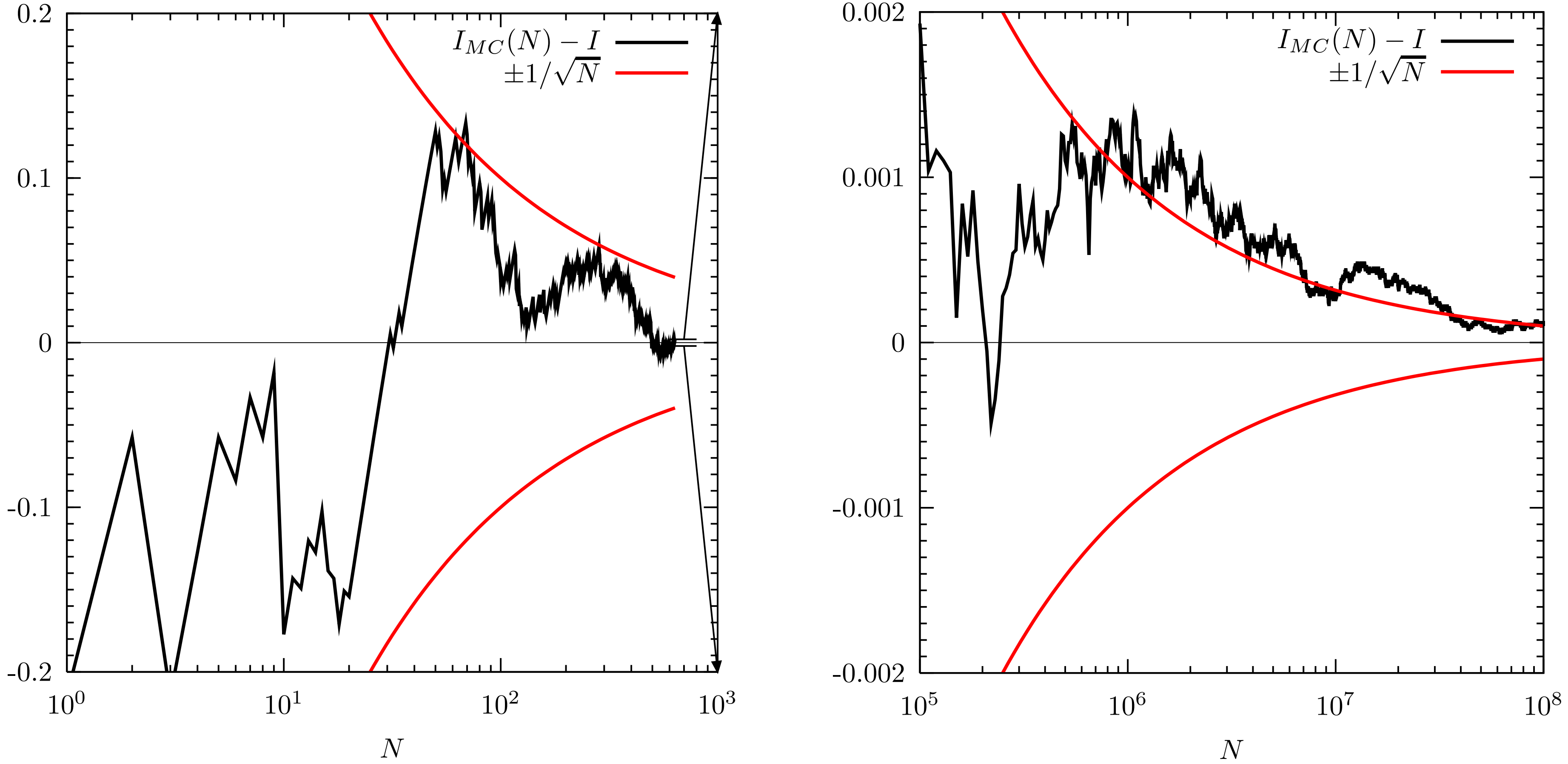
Hit and Miss



More points, zoom in…

Error $1/\sqrt{N}$.

Hit and Miss



Error $1/\sqrt{N}$.

Hit and Miss

This method is used in many event generators. However, it is not sufficient as such.

- Can handle any density $f(x)$,
  however wild and unknown it is.
- $f(x)$ should be bounded from above.
- Sampling will be very *inefficient* whenever $\mathrm{Var}(f)$ is large.

Improvements go under the name variance reduction as they improve the error of the crude MC at the same time.

Simple MC integration

Mean value theorem of integration:

$$\begin{aligned} I &= \int_{x_0}^{x_1} f(x)\,dx \\ &= (x_1 - x_0)\langle f(x)\rangle \end{aligned}$$

(Riemann integral).

Simple MC integration

Mean value theorem of integration:

$$
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&= (x_1 - x_0)\langle f(x)\rangle \\
&\approx (x_1 - x_0)\frac{1}{N}\sum_{i=1}^{N} f(x_i)
\end{aligned}
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(Riemann integral).

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Sum doesn't depend on ordering
$\longrightarrow$ randomize x_i.

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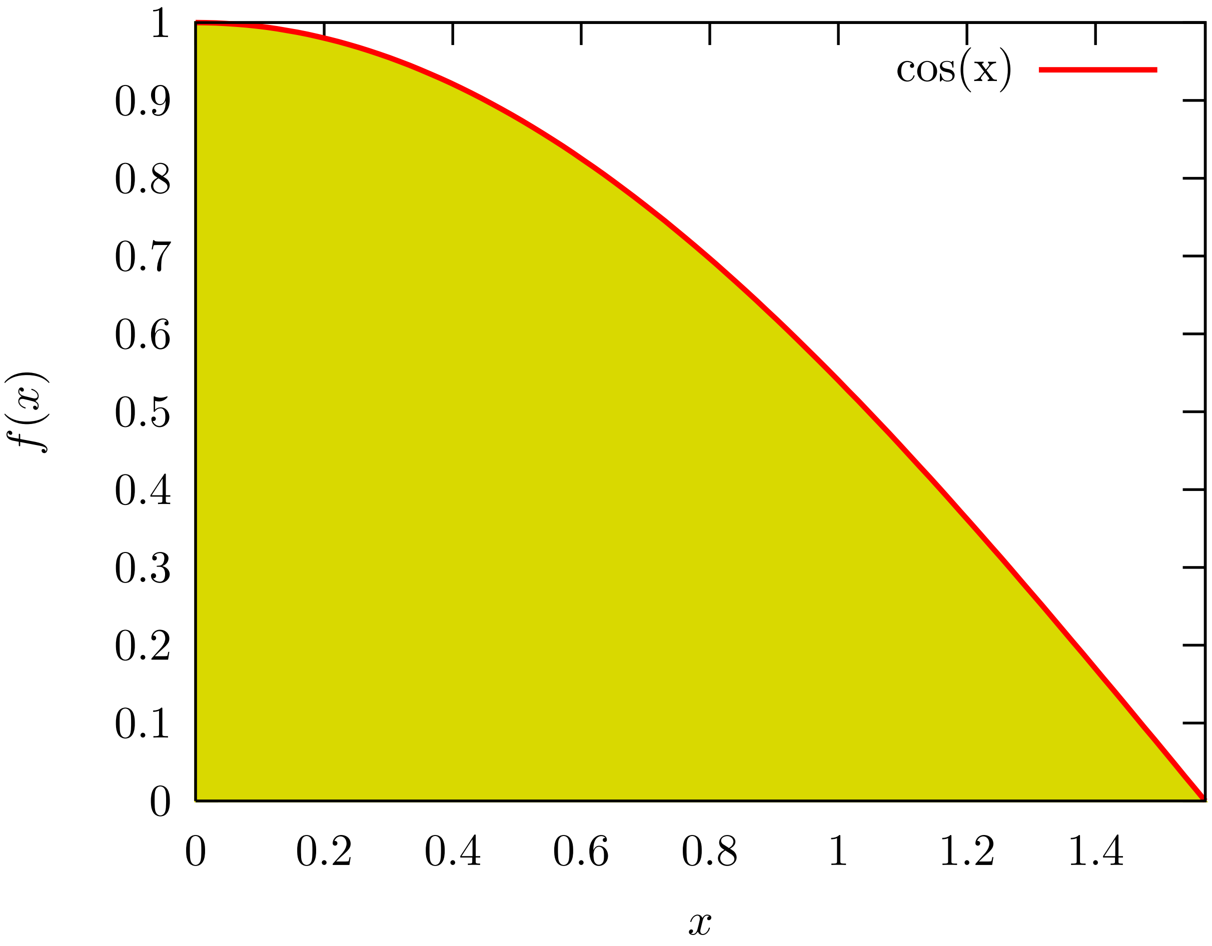
Sum doesn't depend on ordering
$\longrightarrow$ randomize x_i.

Yields a flat distribution of events x_i,
but weighted with *weight* $f(x_i)$ ($\rightarrow$ unweighting).

Simple MC integration

Pictorially:

$$I = \int_{x_0}^{x_1} f(x)\, dx$$
$$= (x_1 - x_0)\langle f(x)\rangle$$



Simple MC integration

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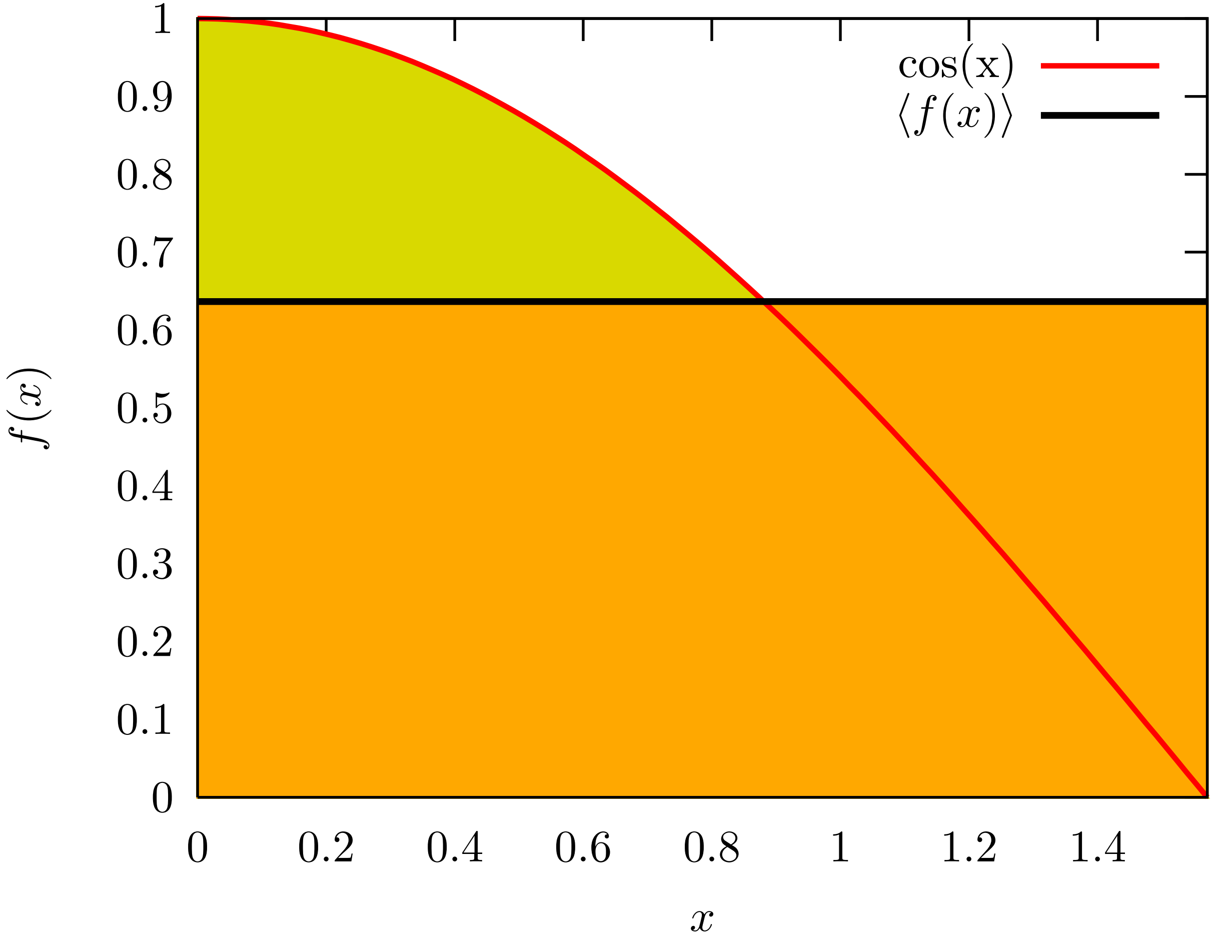
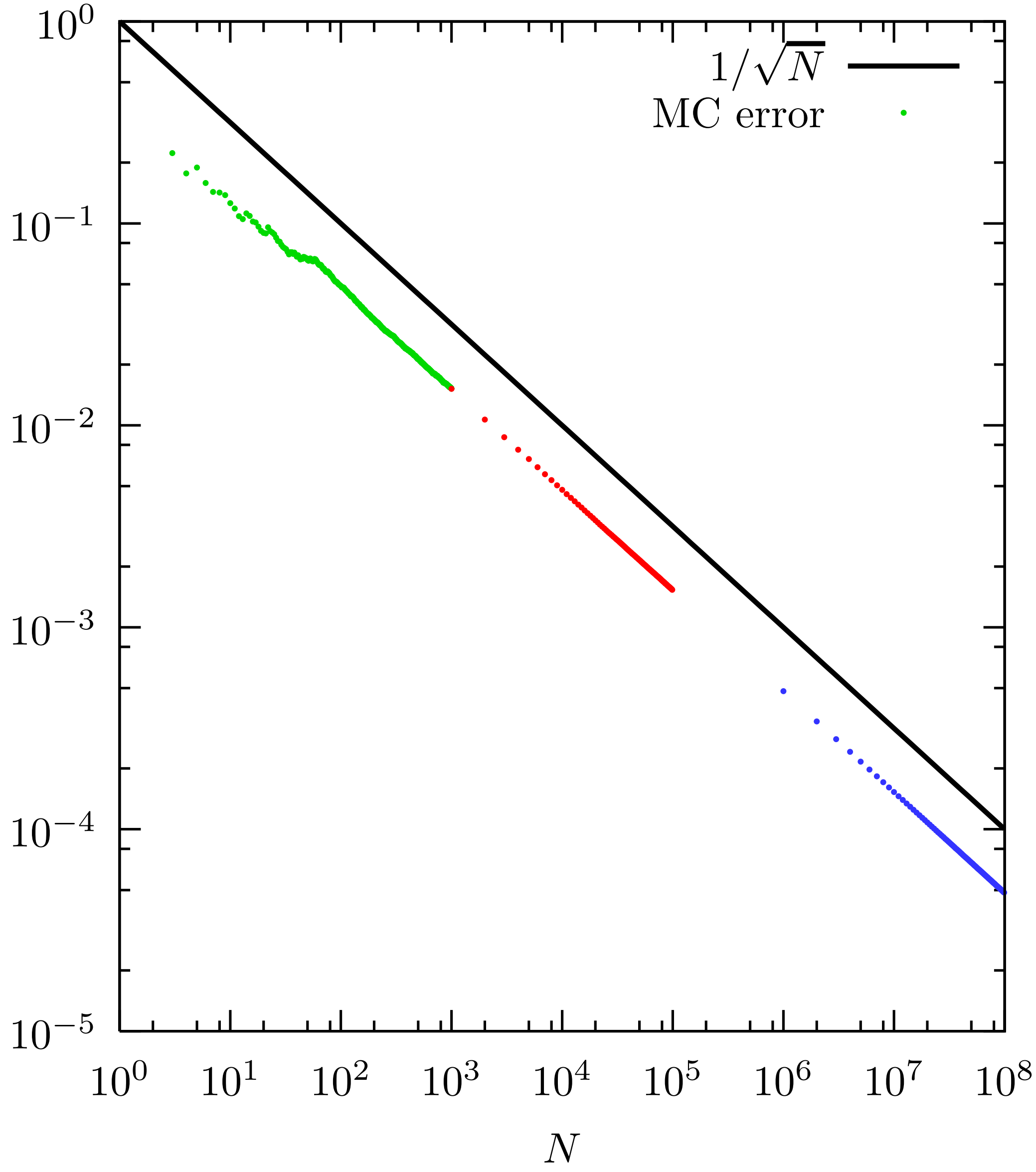


Simple MC integration

What's the error?



Again, looks like

$$\sigma \sim \frac{1}{\sqrt{N}}$$

Simple MC integration

What's the error?

We can calculate it (central limit theorem for the average):

In general: *Crude MC*

$$
\begin{aligned}
I &= \int f dV \\
&\approx V\langle f\rangle \pm V\sqrt{\frac{\langle f\rangle^2 - \langle f^2\rangle}{N}} \\
&\approx V\langle f\rangle \pm V\frac{\sigma}{\sqrt{N}}
\end{aligned}
$$

Simple MC integration

What's the error?

We can calculate it (central limit theorem for the average):

Our example: $\cos(x), 0 \leq x \leq \pi/2$,
compute σ_{MC} from

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

$$\langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} f^2(x_i).$$

Simple MC integration

What's the error?

We can calculate it (central limit theorem for the average):

Compute σ directly ($V = \pi/2$):

$$\langle f \rangle = \int_0^{\pi/2} \cos(x)\, dx = 1$$
$$\langle f^2 \rangle = \int_0^{\pi/2} \cos^2(x)\, dx = \frac{\pi}{4}$$

then

$$\sigma = \sqrt{1^2 - \frac{\pi}{4}} \approx 0.4633.$$

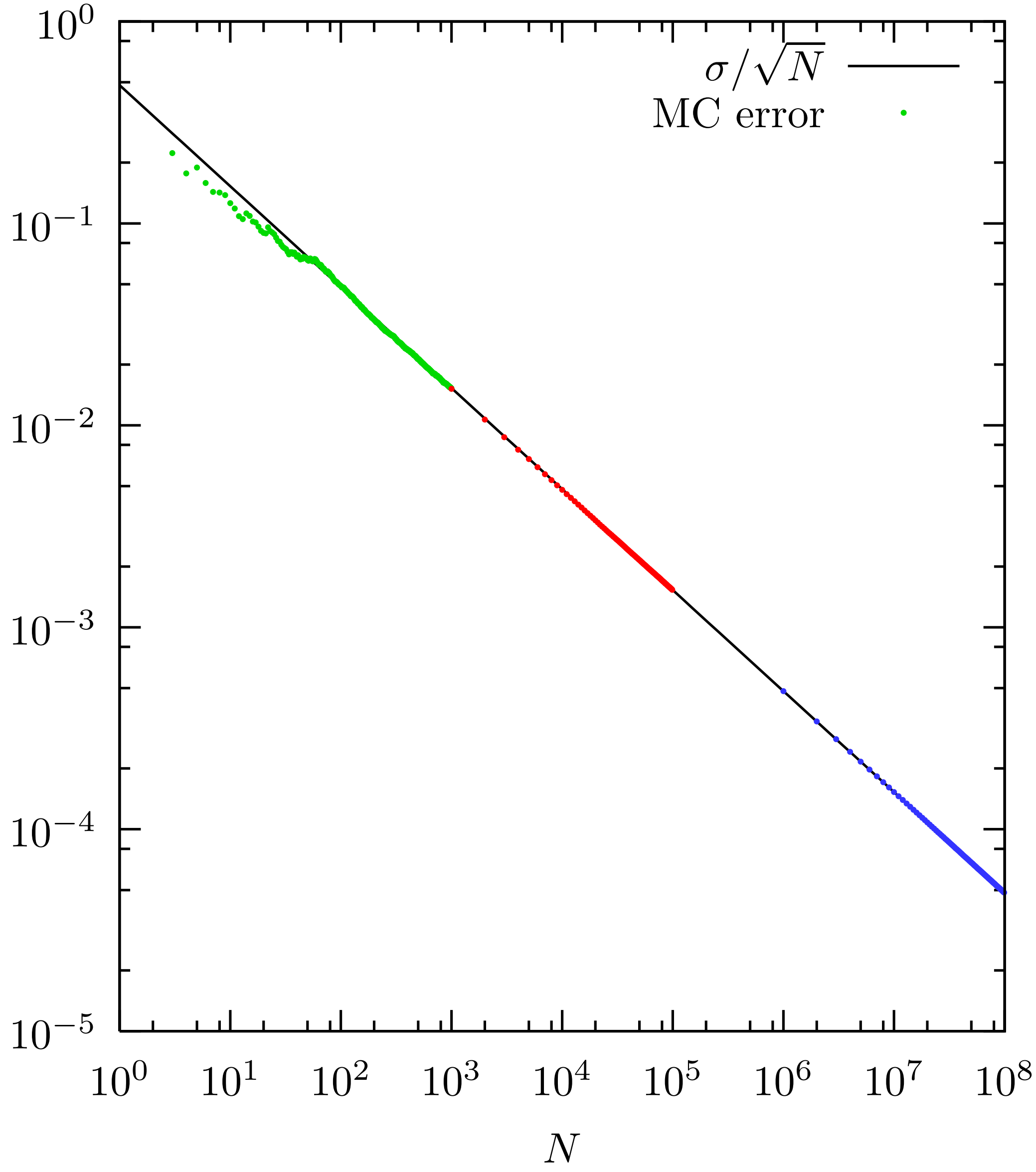
Simple MC integration

What's the error?

Now, compare

$$\sigma_{MC} = \frac{0.4633}{\sqrt{N}}$$

with error estimate from MC.



Simple MC integration

What's the error?

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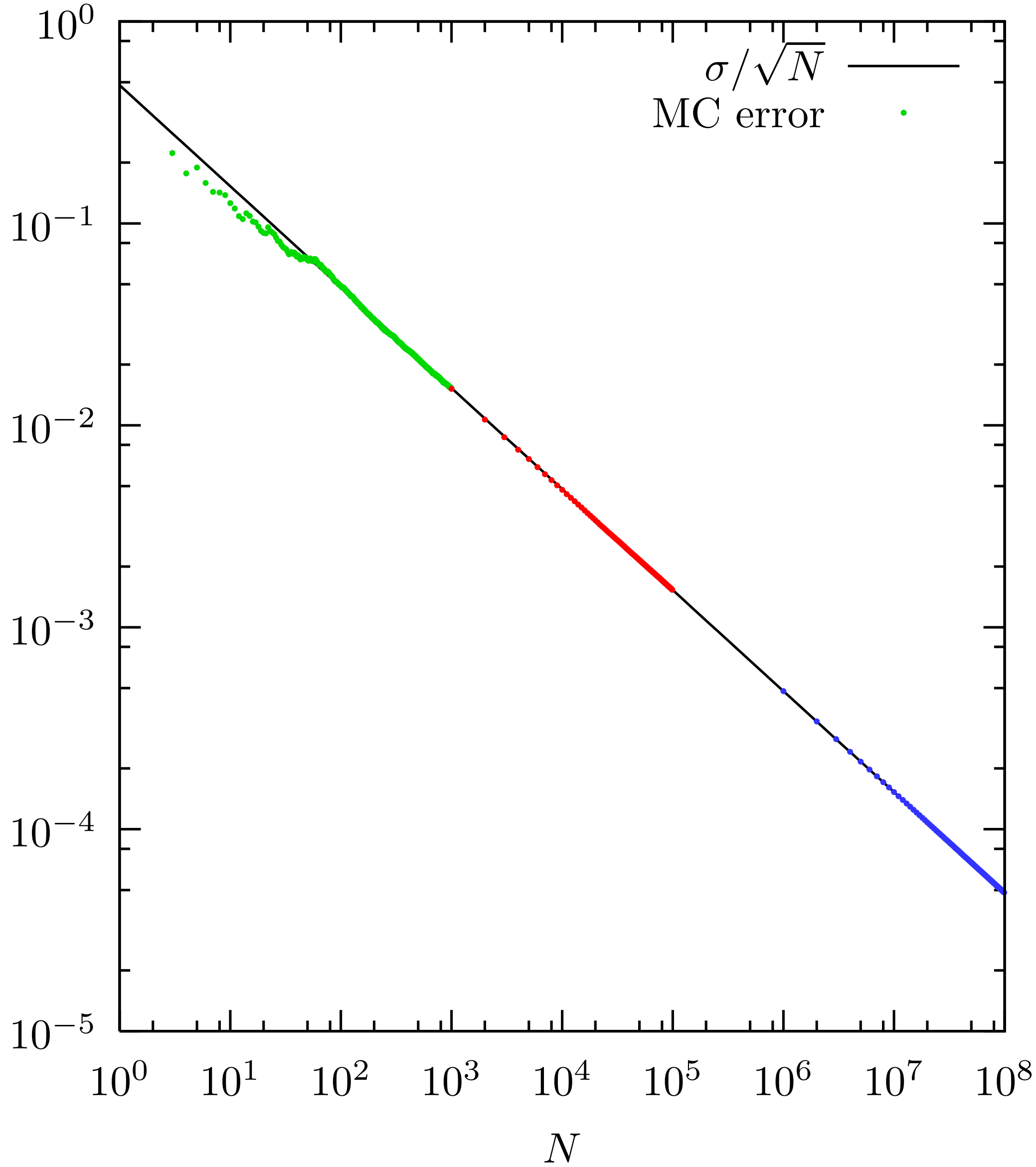
Spot on.



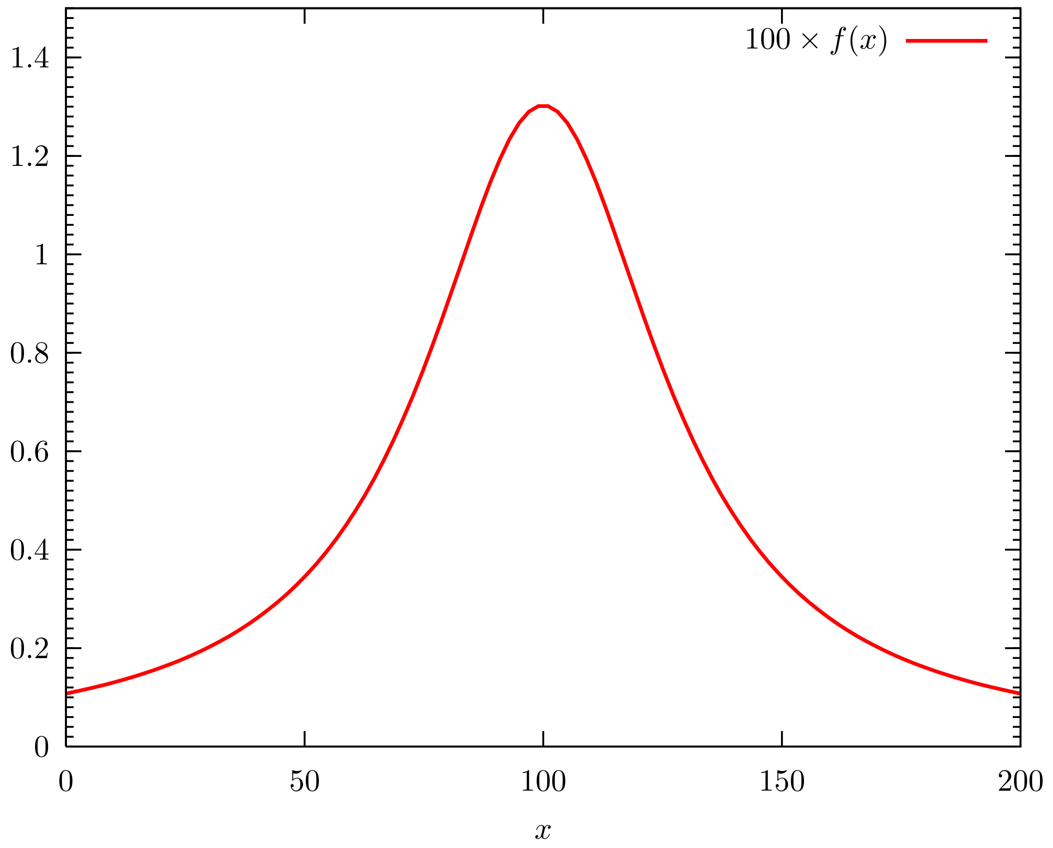
Inverting the Integral

Another basic MC method, based on the observation that

$$\textit{Probability} \sim \textit{Area}$$

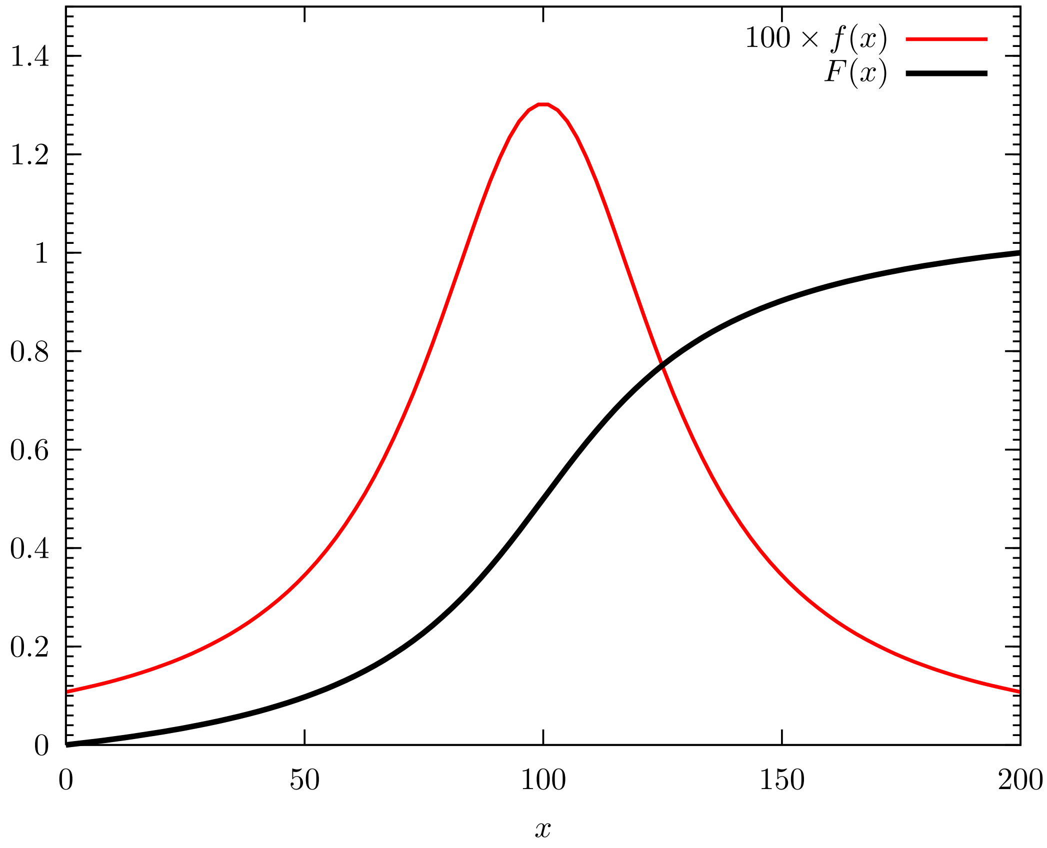
Inverting the Integral

- Probability density $f(x)$. Not necessarily normalized.



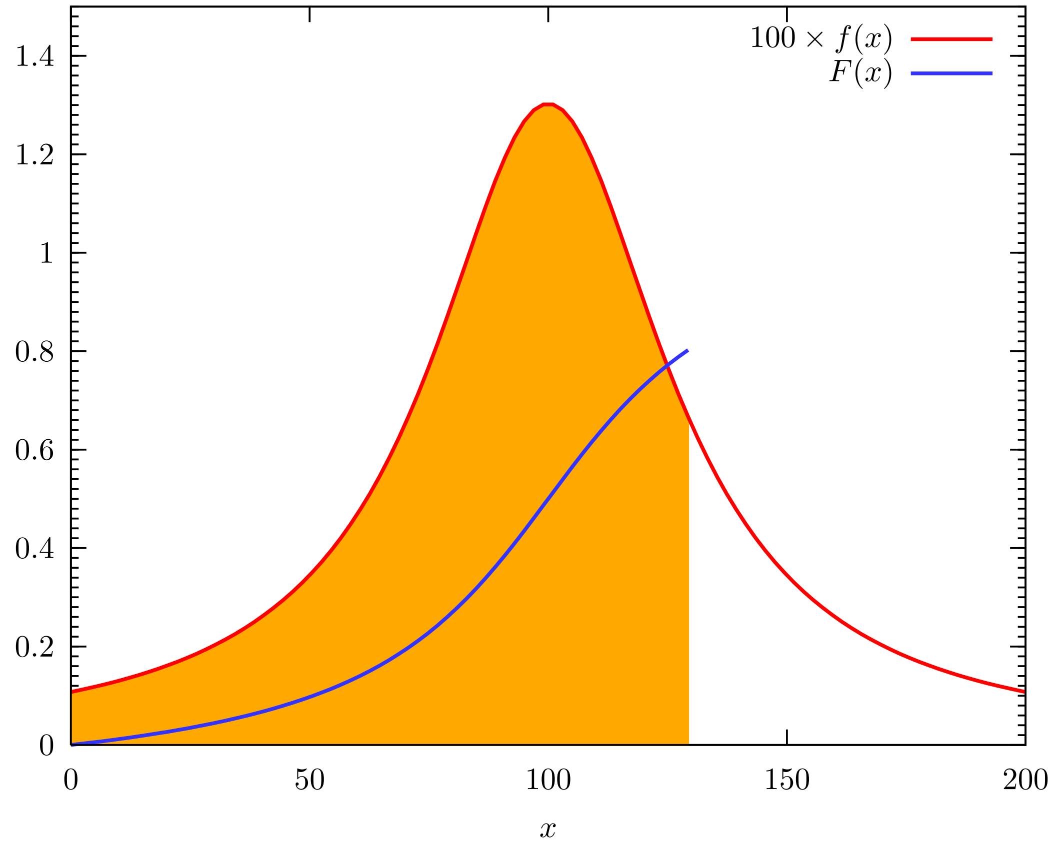
Inverting the Integral

- Probability density $f(x)$. Not necessarily normalized.
- Integral $F(x)$ known,



Inverting the Integral

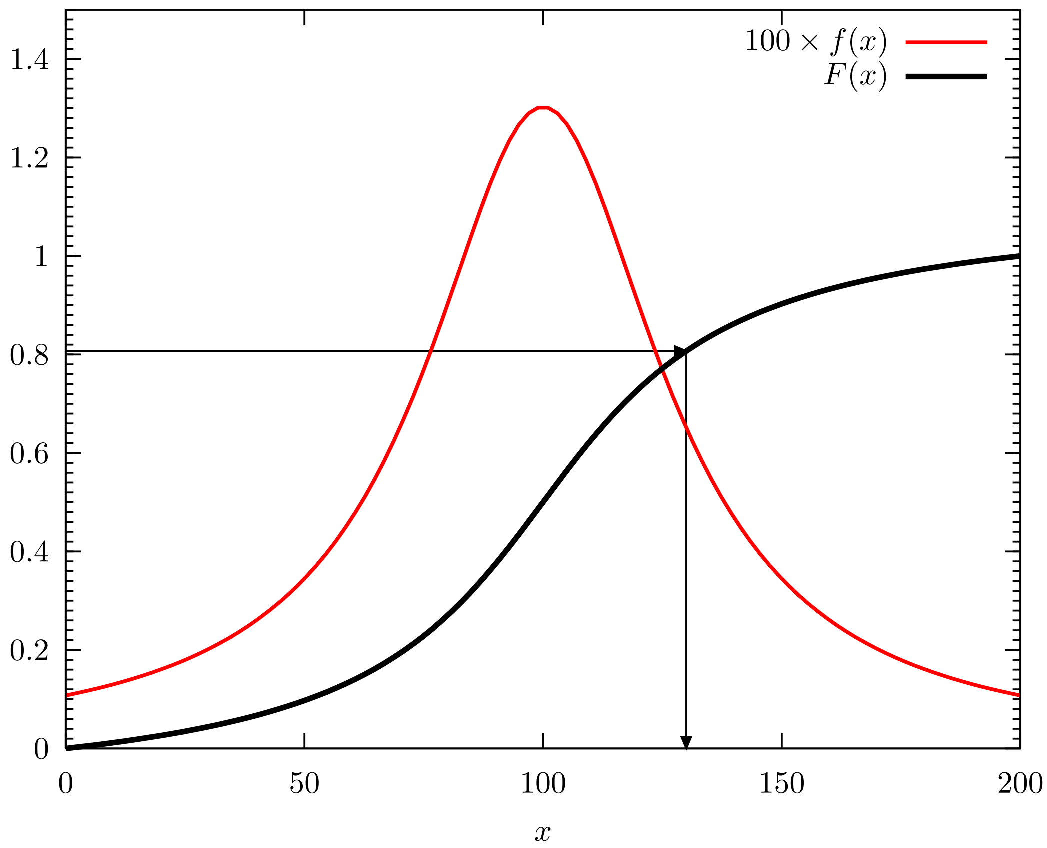
- Probability density $f(x)$. Not necessarily normalized.
- Integral $F(x)$ known,
- $P(x < x_s) = F(x_s)$.



Inverting the Integral

- Probability density $f(x)$. Not necessarily normalized.
- Integral $F(x)$ known,
- $P(x < x_s) = F(x_s)$.
- Probability = 'area', distributed evenly,

$$\int_{x_0}^{x} dP = r$$



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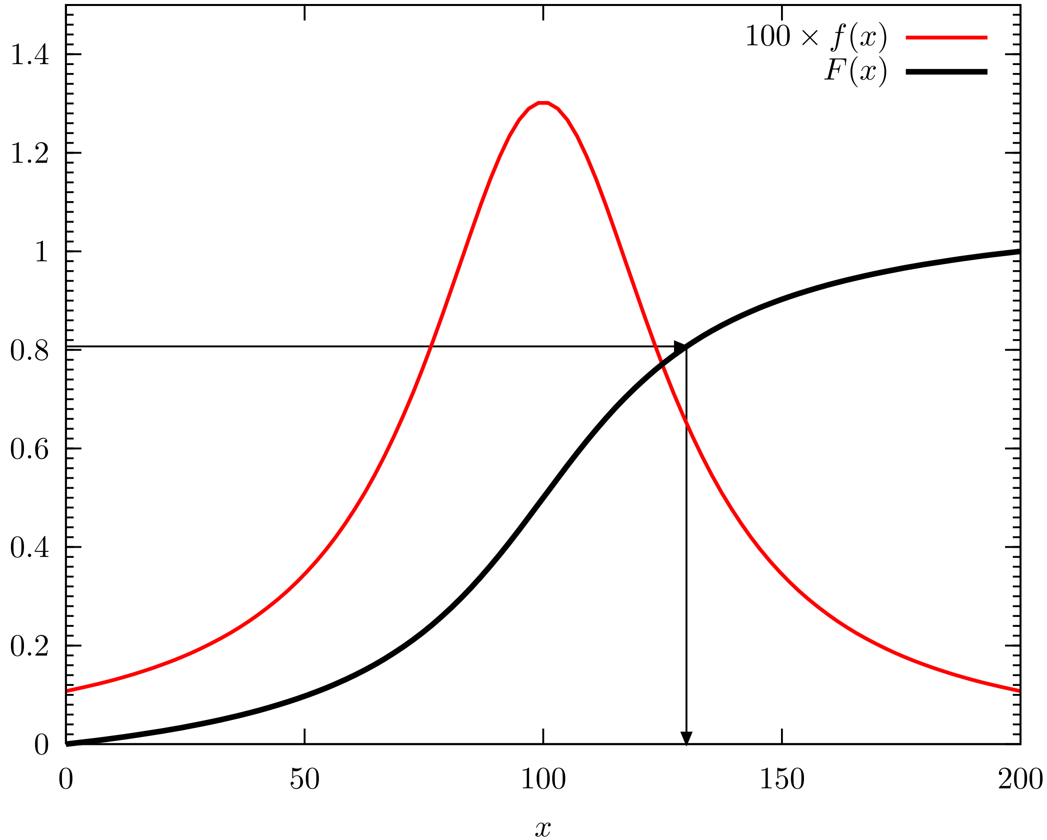


Sample x according to $f(x)$ with

$$x = F^{-1}\left[F(x_0) + r\big(F(x_1) - F(x_0)\big)\right] .$$

Inverting the Integral

Another basic MC method, based on the observation that

$$\textit{Probability} \sim \textit{Area}$$

Sample x according to $f(x)$ with

$$x = F^{-1}\Big[F(x_0) + r\big(F(x_1) - F(x_0)\big)\Big]\ .$$

Optimal method, but we need to know

- The integral $F(x) = \int f(x)\,\mathrm{d}x$,
- It's inverse $F^{-1}(y)$.

That's rarely the case for real problems.

But very powerful in combination with other techniques.

Importance sampling

Error on Crude MC $\sigma_{MC} = \sigma / \sqrt{N}$.
$\Longrightarrow$ Reduce error by reducing variance of integrand.

Importance sampling

Error on Crude MC $\sigma_{MC} = \sigma/\sqrt{N}$.
$\Longrightarrow$ Reduce error by reducing variance of integrand.

Idea: *Divide out the singular structure.*

$$I = \int f \, \mathrm{d}V = \int \frac{f}{p} p \mathrm{d}V \approx \left\langle \frac{f}{p} \right\rangle \pm \sqrt{\frac{\langle f^2/p^2 \rangle - \langle f/p \rangle^2}{N}} \,.$$

where we have chosen $\int p \, \mathrm{d}V = 1$ for convenience.

Note: need to sample flat in $p \, \mathrm{d}V$, so we better know $\int p \mathrm{d}V$ and it's inverse.

Importance sampling

Consider error term:

$$E = \left\langle \frac{f^2}{p^2} \right\rangle - \left\langle \frac{f}{p} \right\rangle^2 = \int \frac{f^2}{p^2} p \mathrm{d}V - \left[\int \frac{f}{p} p \mathrm{d}V \right]^2$$

$$= \int \frac{f^2}{p} \mathrm{d}V - \left[\int f \, \mathrm{d}V \right]^2 .$$

Importance sampling

Consider error term:

$$E = \int \frac{f^2}{p}\,\mathrm{d}V - \left[\int f\,\mathrm{d}V\right]^2 .$$

Best choice of p? Minimises E $\rightarrow$ functional variation of error term with (normalized) p:

$$0 = \delta E = \delta\left(\int \frac{f^2}{p}\,\mathrm{d}V - \left[\int f\,\mathrm{d}V\right]^2 + \lambda \int p\,\mathrm{d}V\right)$$

$$= \int \left(-\frac{f^2}{p^2} + \lambda\right)\mathrm{d}V\delta p \, ,$$

Importance sampling

Consider error term:

$$E = \int \frac{f^2}{p}\,\mathrm{d}V - \left[\int f\,\mathrm{d}V\right]^2 .$$

Best choice of p? Minimises E $\to$ functional variation of error term with (normalized) p:

$$0 = \delta E = \int \left(-\frac{f^2}{p^2} + \lambda\right) \mathrm{d}V\,\delta p ,$$

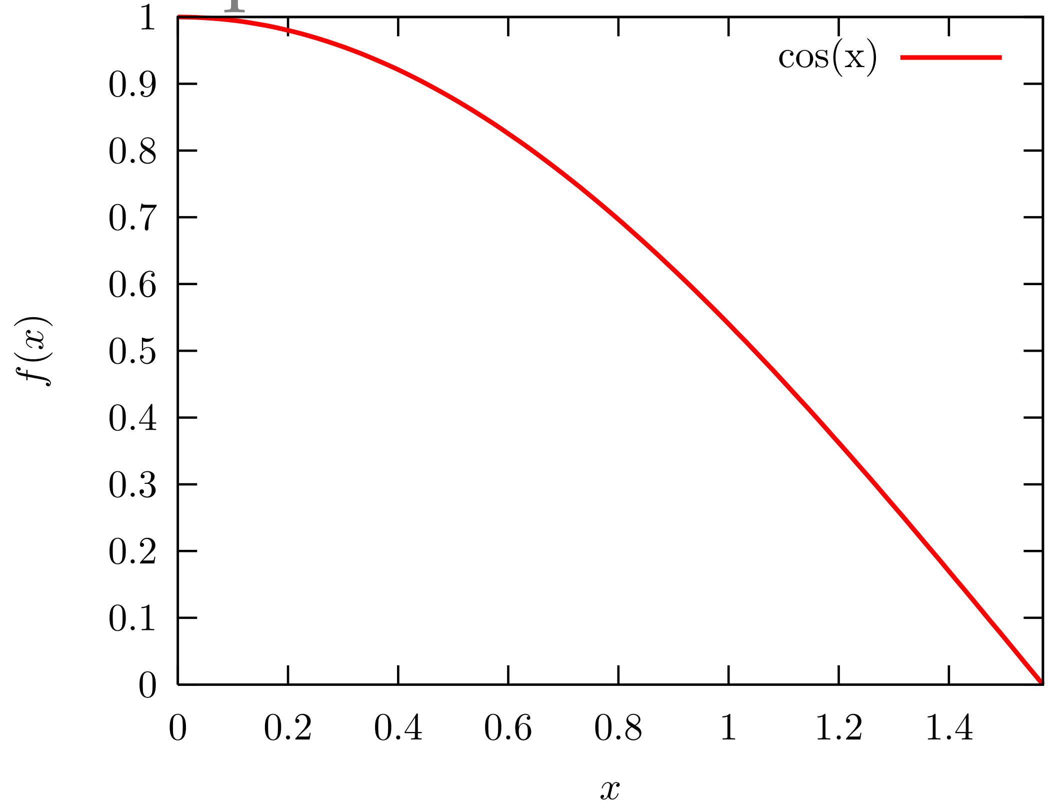
hence

$$p = \frac{|f|}{\sqrt{\lambda}} = \frac{|f|}{\int |f|\,\mathrm{d}V} .$$

Choose p as close to f as possible.

Importance sampling — example

Improving $\cos(x)$
sampling,



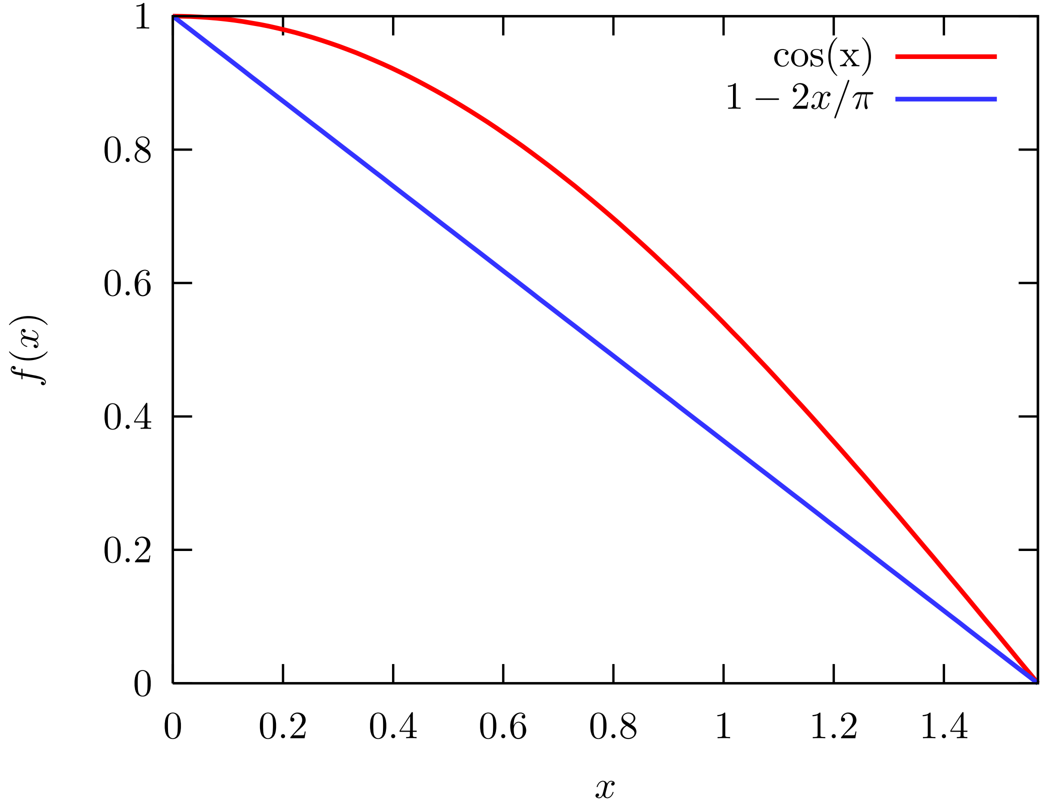
Importance sampling — example

Improving $\cos(x)$ sampling,

$$I = \int_0^{\pi/2} \cos(x)\, dx$$

$$= \int_0^{\pi/2} \frac{\cos(x)}{1 - \frac{2}{\pi}x} \left(1 - \frac{2}{\pi}x\right) dx$$

$$= \int_0^{1} \left.\frac{\cos(x)}{1 - \frac{2}{\pi}x}\right|_{x=x(\rho)} d\rho \ .$$



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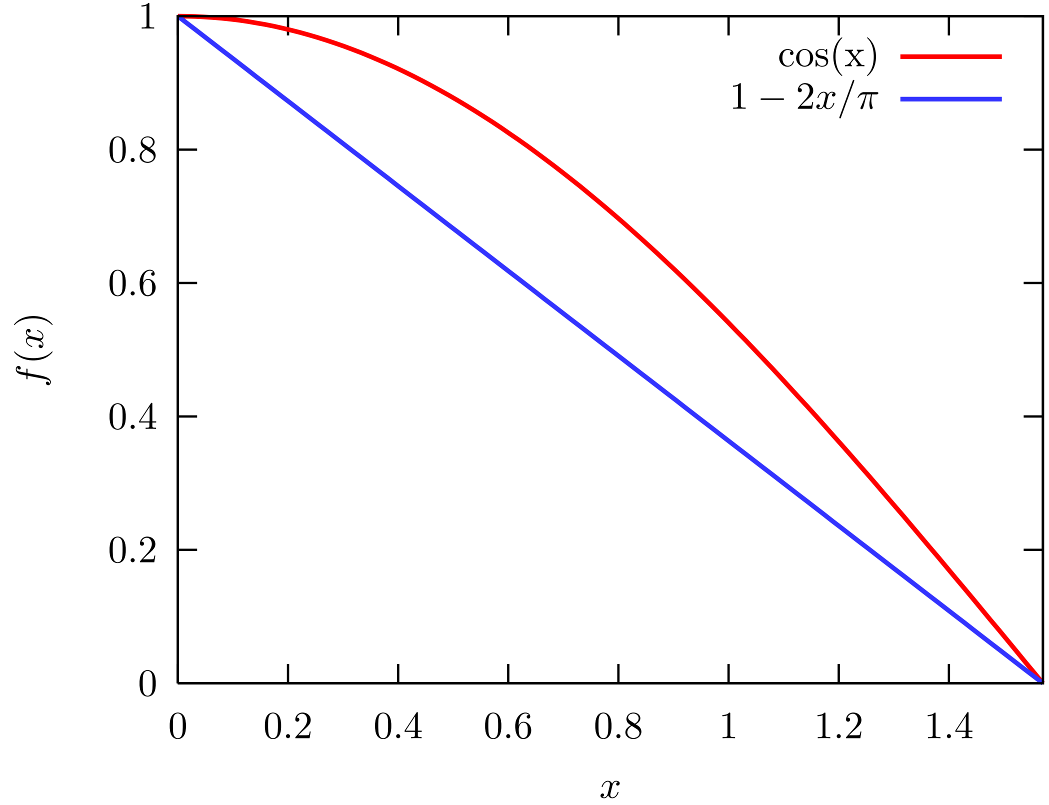


Sample x with *inverting the integral* technique (flat random number ρ),

$$x = \frac{\pi}{2}\left(1-\sqrt{1-\rho}\right) \hat{=} \frac{\pi}{2}\left(1-\sqrt{\rho}\right) \qquad \left(I = \int_0^1 \frac{\cos\left(\frac{\pi}{2}\left(1-\sqrt{\rho}\right)\right)}{\sqrt{\rho}}\, d\rho.\right)$$

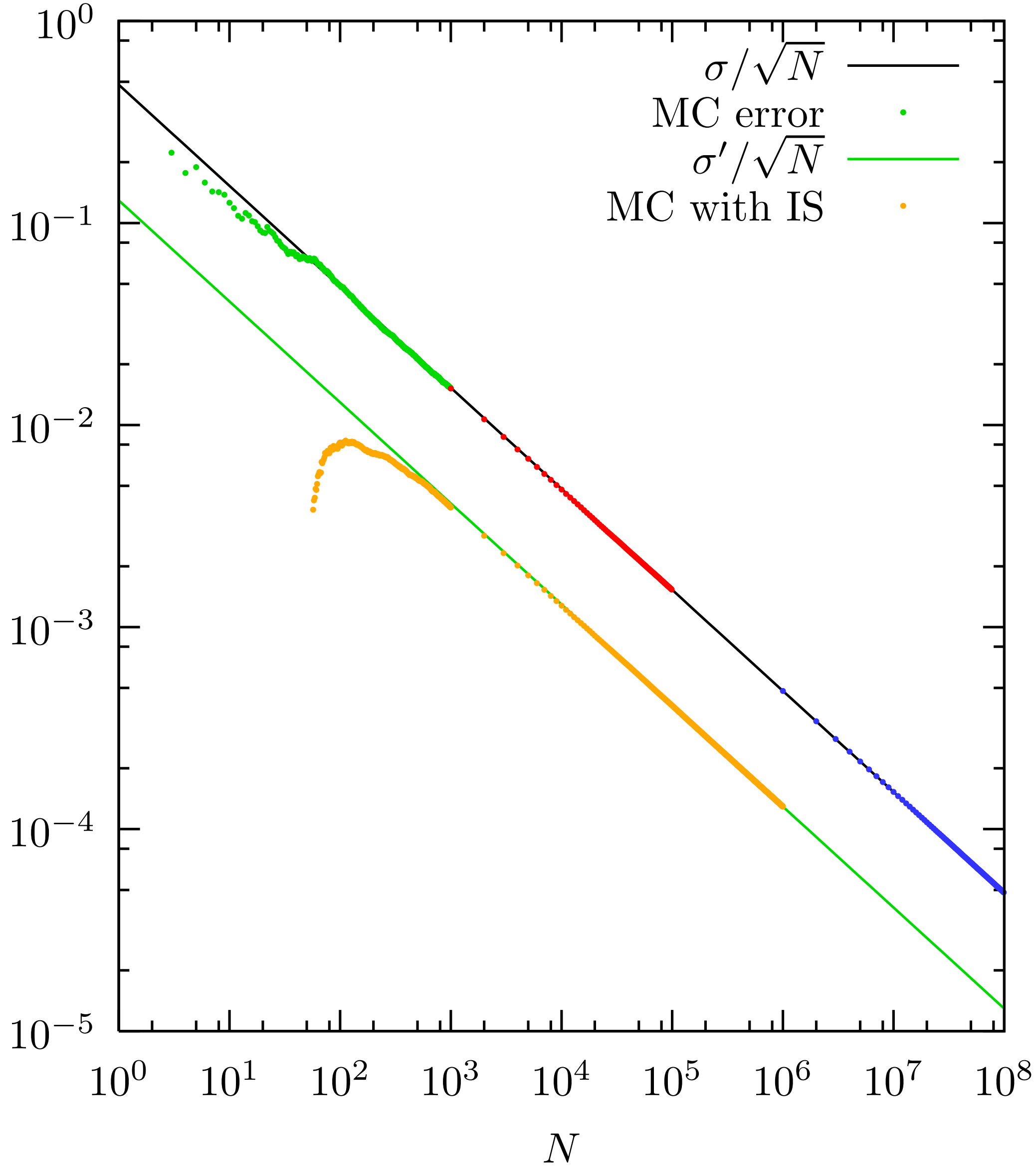
Importance sampling — example

Improving $\cos(x)$ sampling,

much better convergence,

about 80% "accepted events".

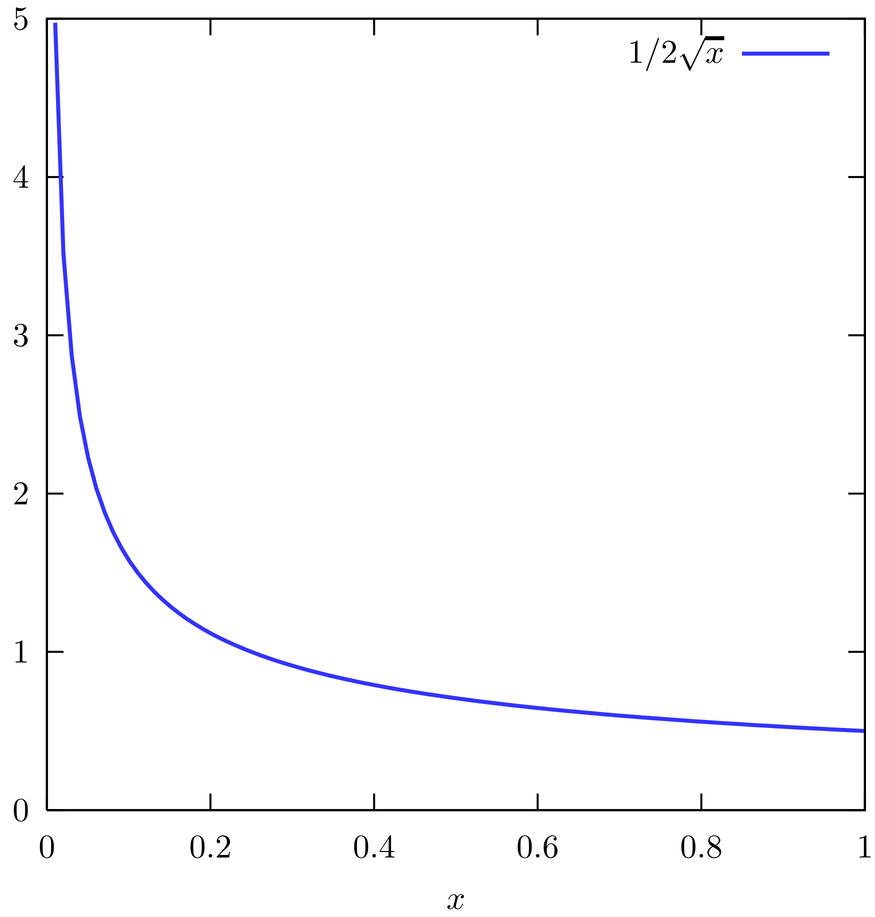
Reduced variance ($\sigma' = 0.027$) $\Rightarrow$ better efficiency.



Importance sampling — better example

More interesting for divergent integrands, eg

$$\frac{1}{2\sqrt{x}}\ ,$$



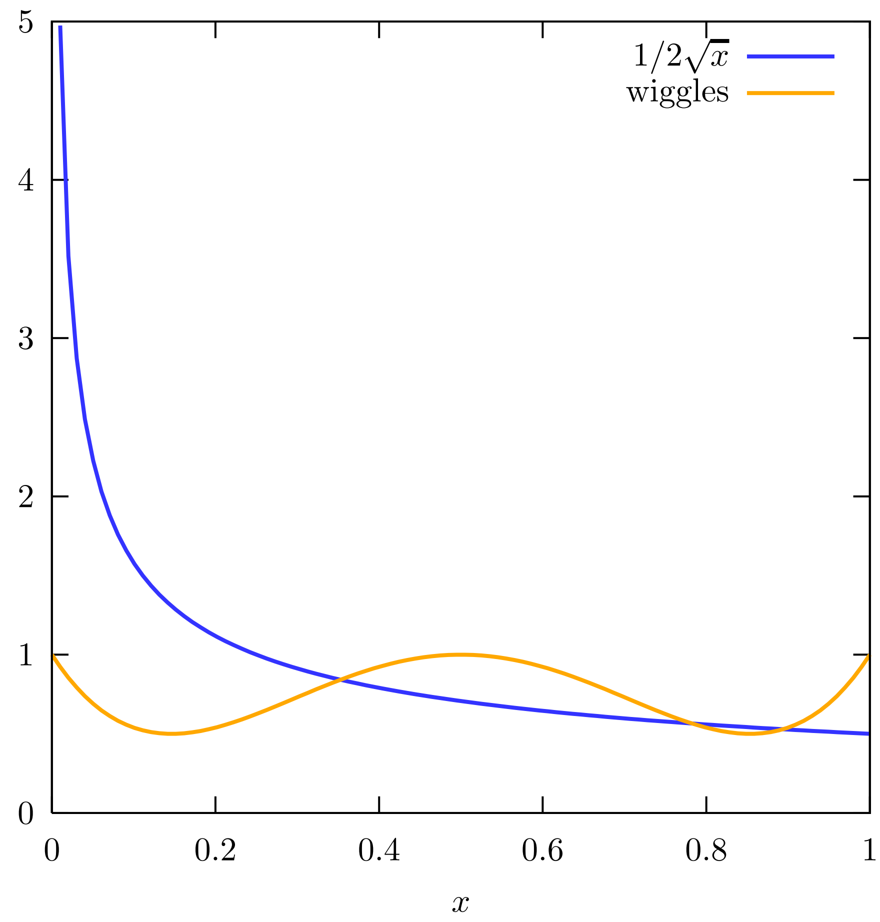
Importance sampling — better example

More interesting for divergent integrands, eg

$$\frac{1}{2\sqrt{x}} \, ,$$

with some wiggles,

$$p(x) = 1 - 8x + 40x^2 - 64x^3 + 32x^4 \, .$$



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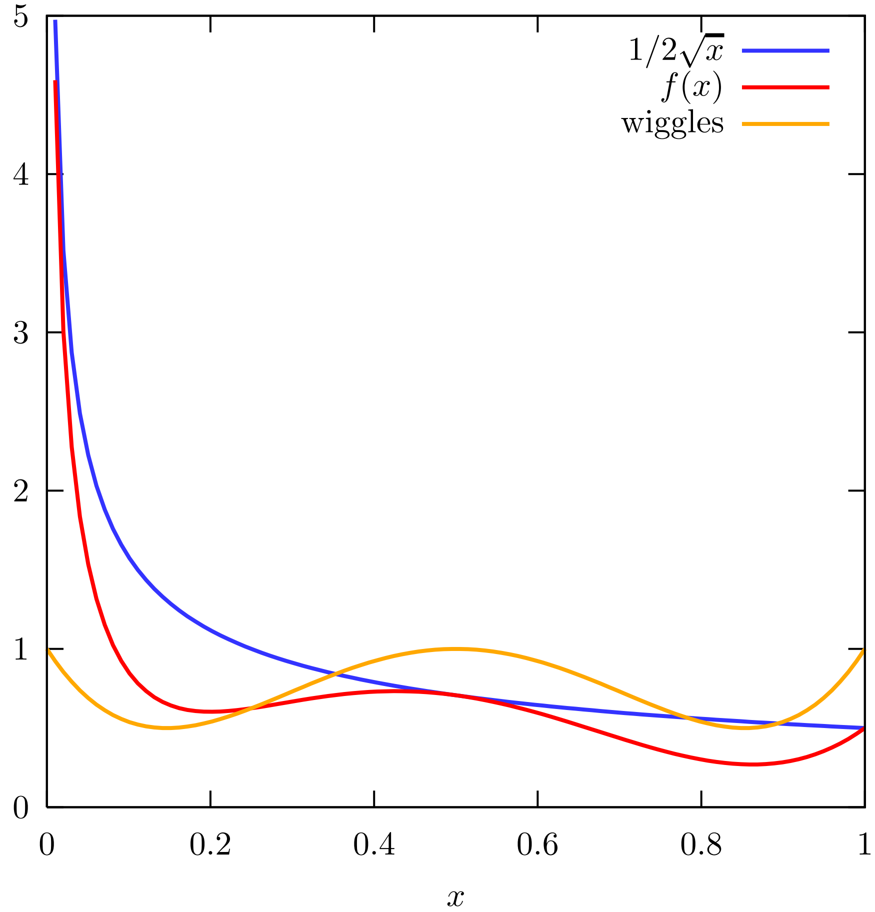
with some wiggles,

$$p(x) = 1 - 8x + 40x^2 - 64x^3 + 32x^4\,.$$

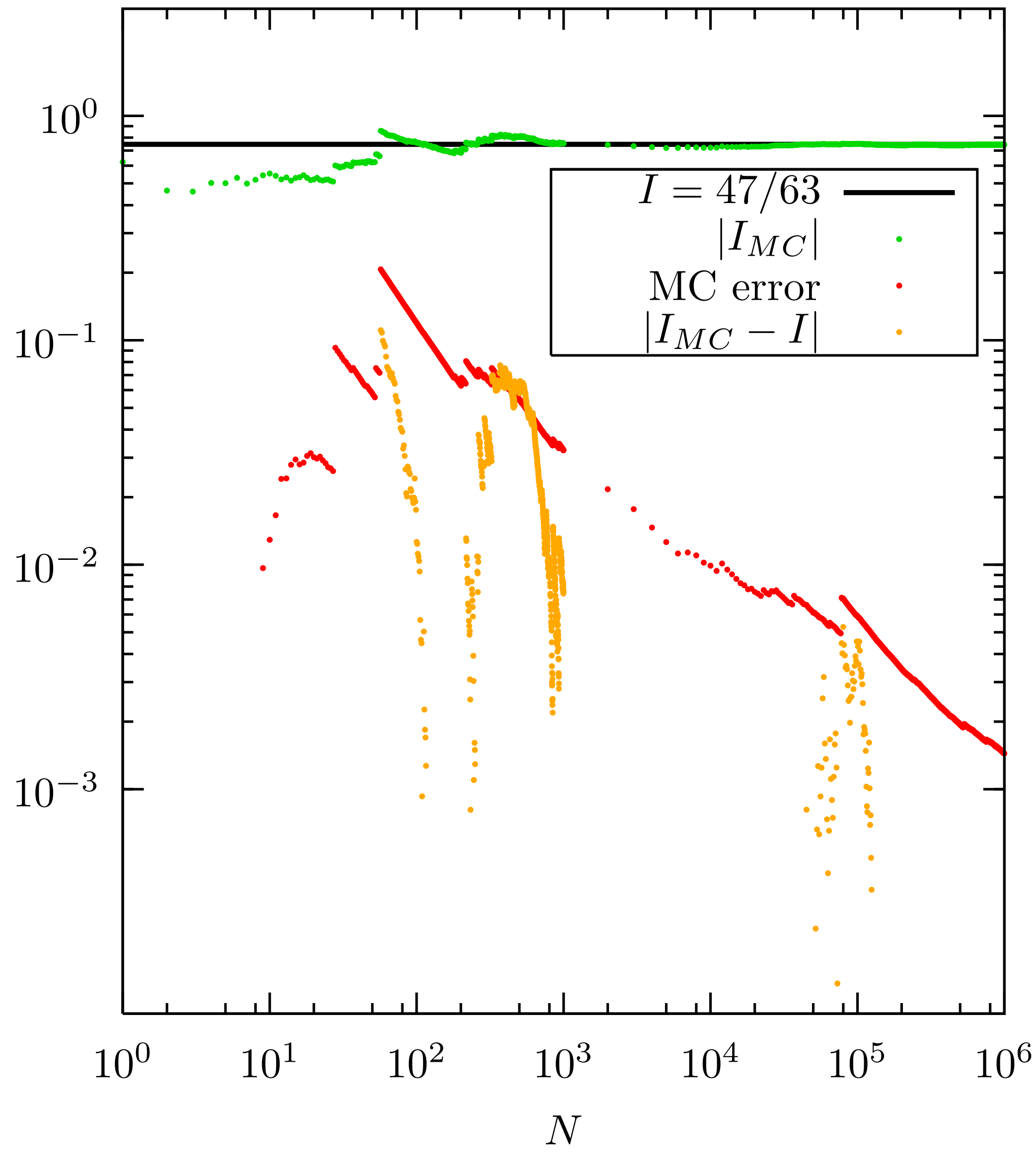
i.e. we want to integrate

$$f(x) = \frac{p(x)}{2\sqrt{x}}\,.$$



Importance sampling — better example

- Crude MC gives result in reasonable 'time'.
- Error a bit unstable.
- Event generation with maximum weight $w_{\max} = 20$. (that's arbitrary.)
- hit/miss/events with $(w > w_{\max}) =$ 36566/963434/617 with 1M generated events.

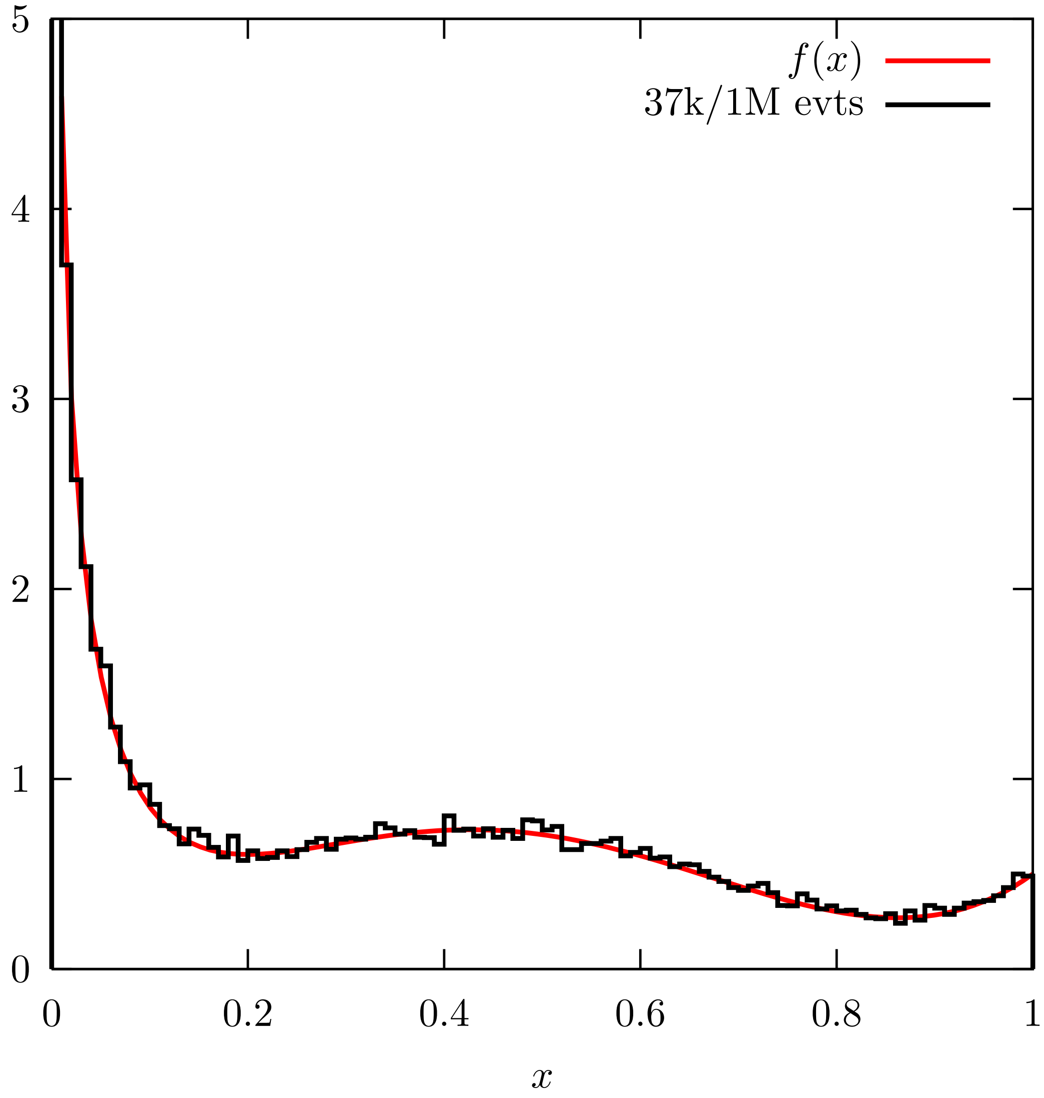


Importance sampling — better example

Want events:

use hit+mass variant here:

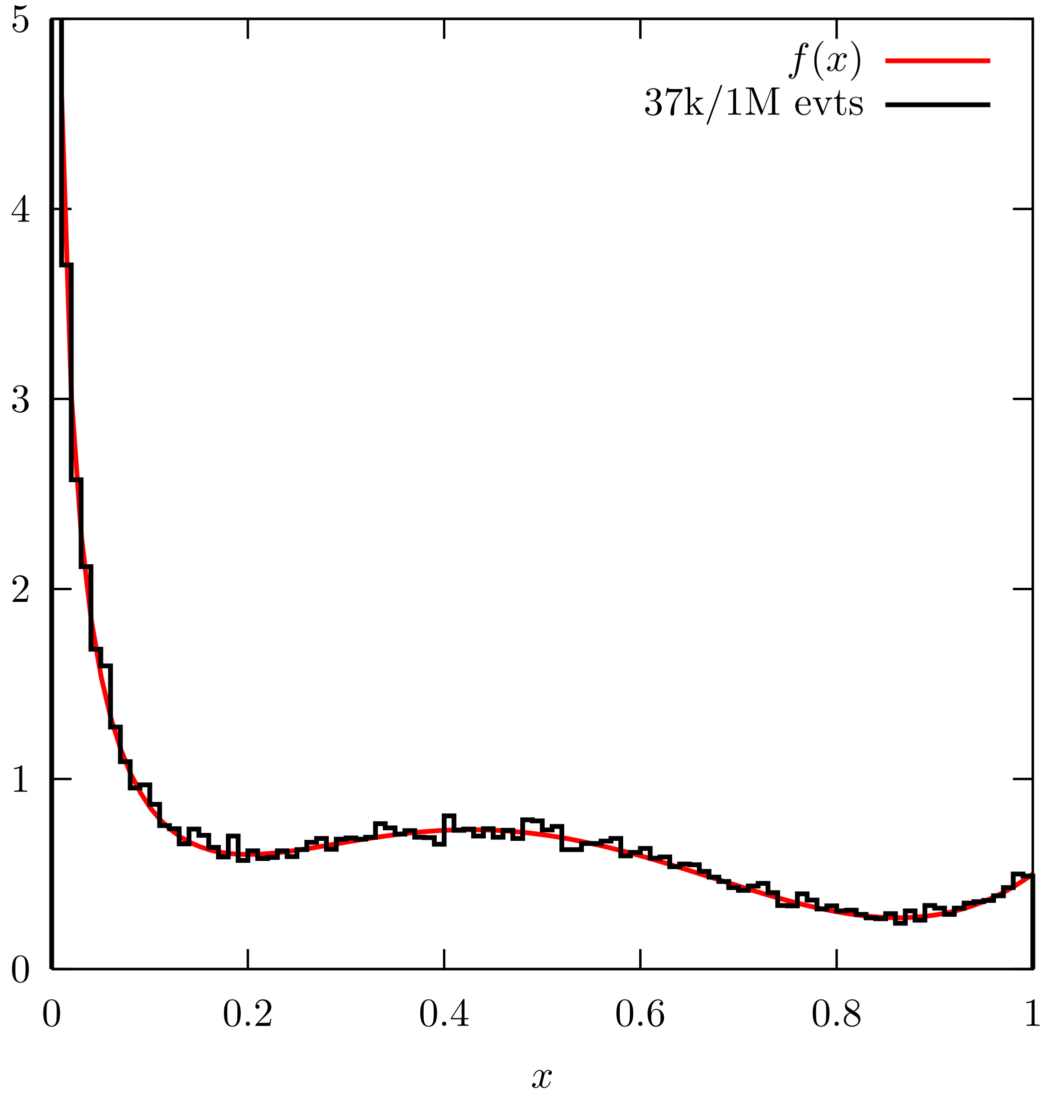
- Choose new random number r
- $w = f(x)$ in this case.
- if $r < w/w_{\max}$ then "hit".
- MC efficiency = hit$/N$.



Importance sampling — better example

Want events:
use hit+mass variant here:

- Choose new random number r
- $w = f(x)$ in this case.
- if $r < w/w_{\max}$ then "hit".
- MC efficiency = hit$/N$.
- Efficiency for MC events only 3.7%.
- Note the wiggly histogram.



Importance sampling — better example

Now importance sampling, i.e. divide out $1/2\sqrt{x}$.

$$\int_0^1 \frac{p(x)}{2\sqrt{x}}\,dx = \int_0^1 \left(\frac{p(x)}{2\sqrt{x}}\bigg/\frac{1}{2\sqrt{x}}\right)\frac{dx}{2\sqrt{x}}$$
$$= \int_0^1 p(x)\,d\sqrt{x}$$
$$= \int_0^1 p(x(\rho))\,d\rho$$
$$= \int_0^1 1 - 8\rho^2 + 40\rho^4 - 64\rho^6 + 32\rho^8\,d\rho$$

so,

$$\rho = \sqrt{x}, \qquad d\rho = \frac{dx}{2\sqrt{x}}$$

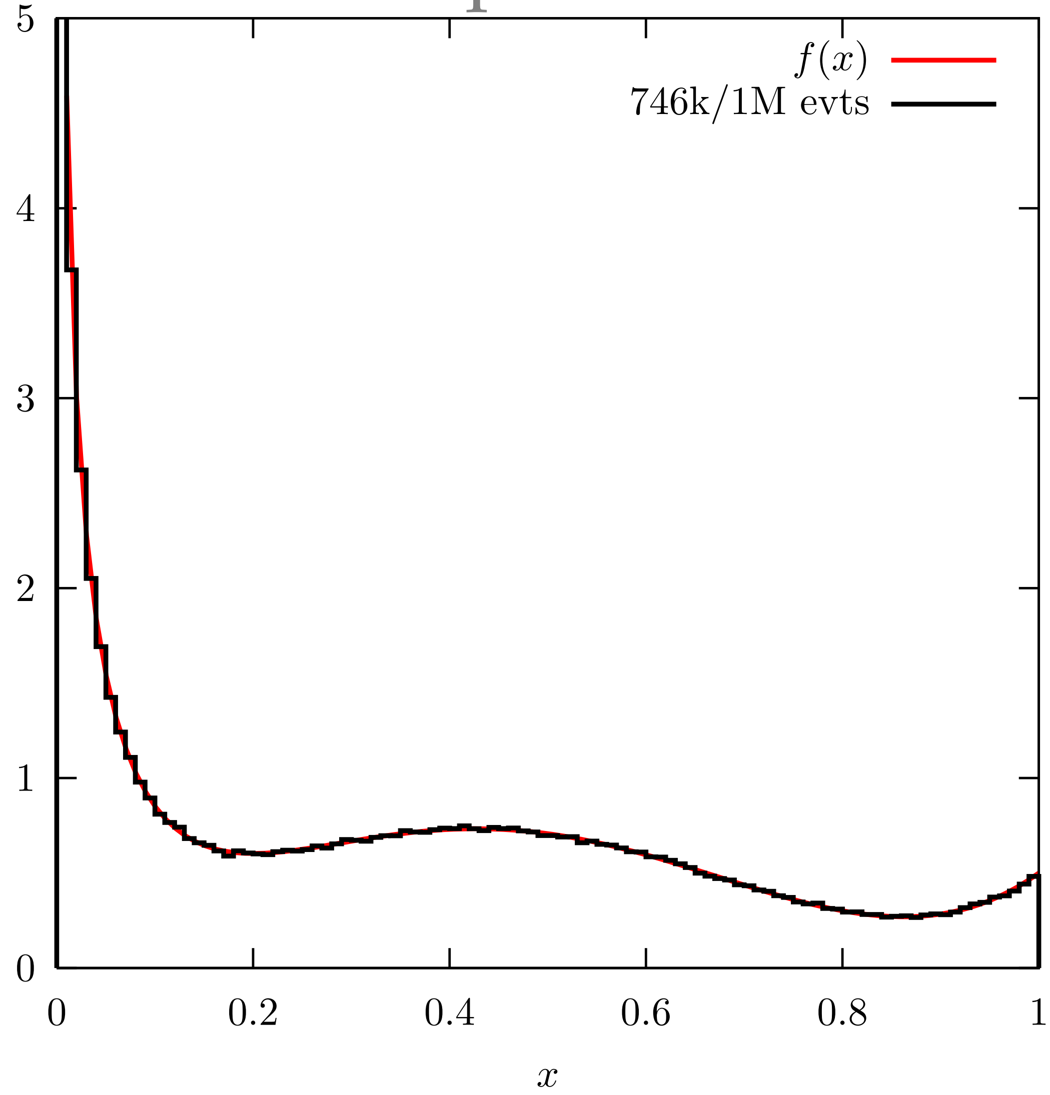
x sampled with *inverting the integral* from flat random numbers ρ, $x = \rho^2$.

Importance sampling — better example

$$\int_0^1 \frac{p(x)}{2\sqrt{x}}\,dx = \int_0^1 p(x(\rho))\,d\rho$$

with

$$\rho = \sqrt{x}, \qquad d\rho = \frac{dx}{2\sqrt{x}}$$



Events generated with $w_{\max} = 1$, as $p(x) \leq 1$, no guesswork needed here! Now, we get 74.6% MC efficiency.

Importance sampling — better example

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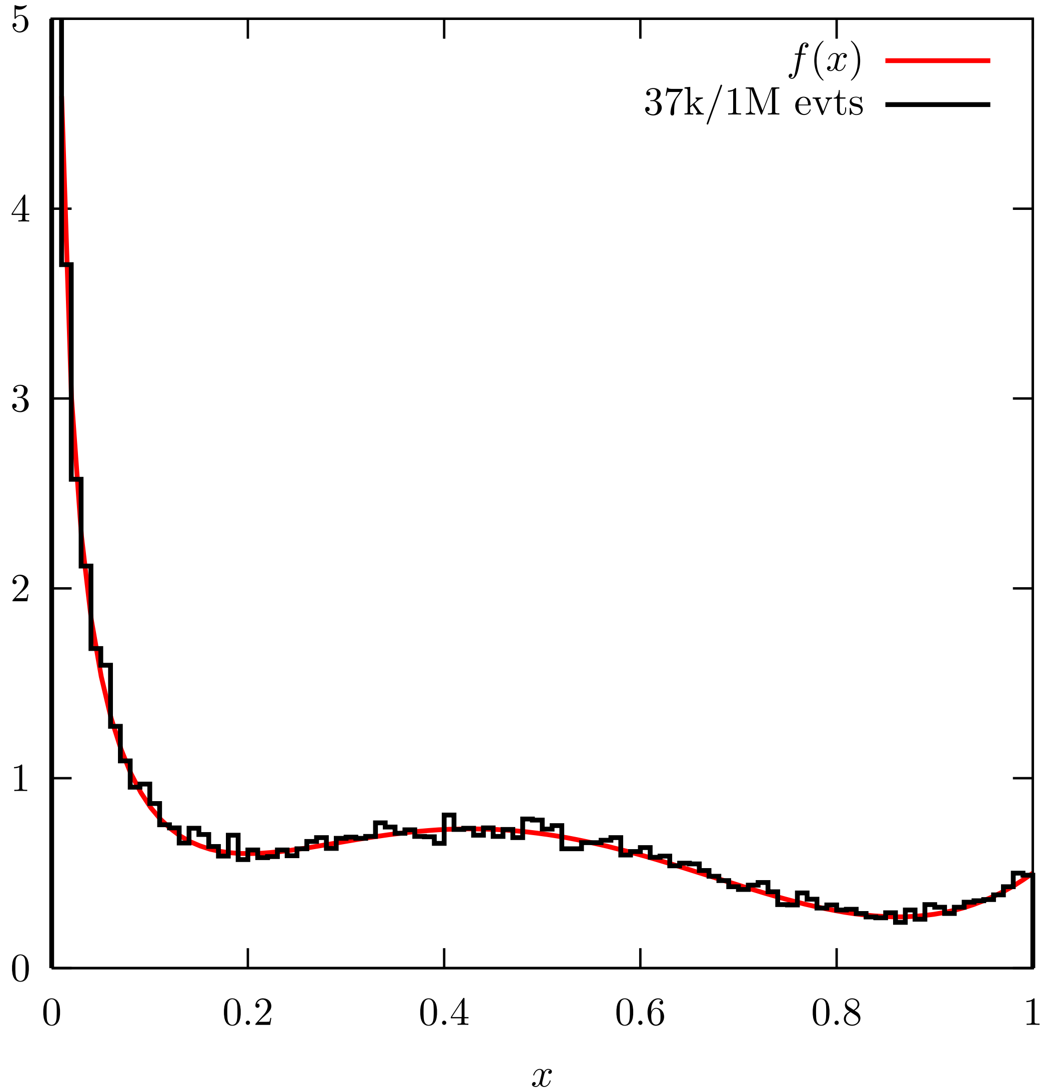
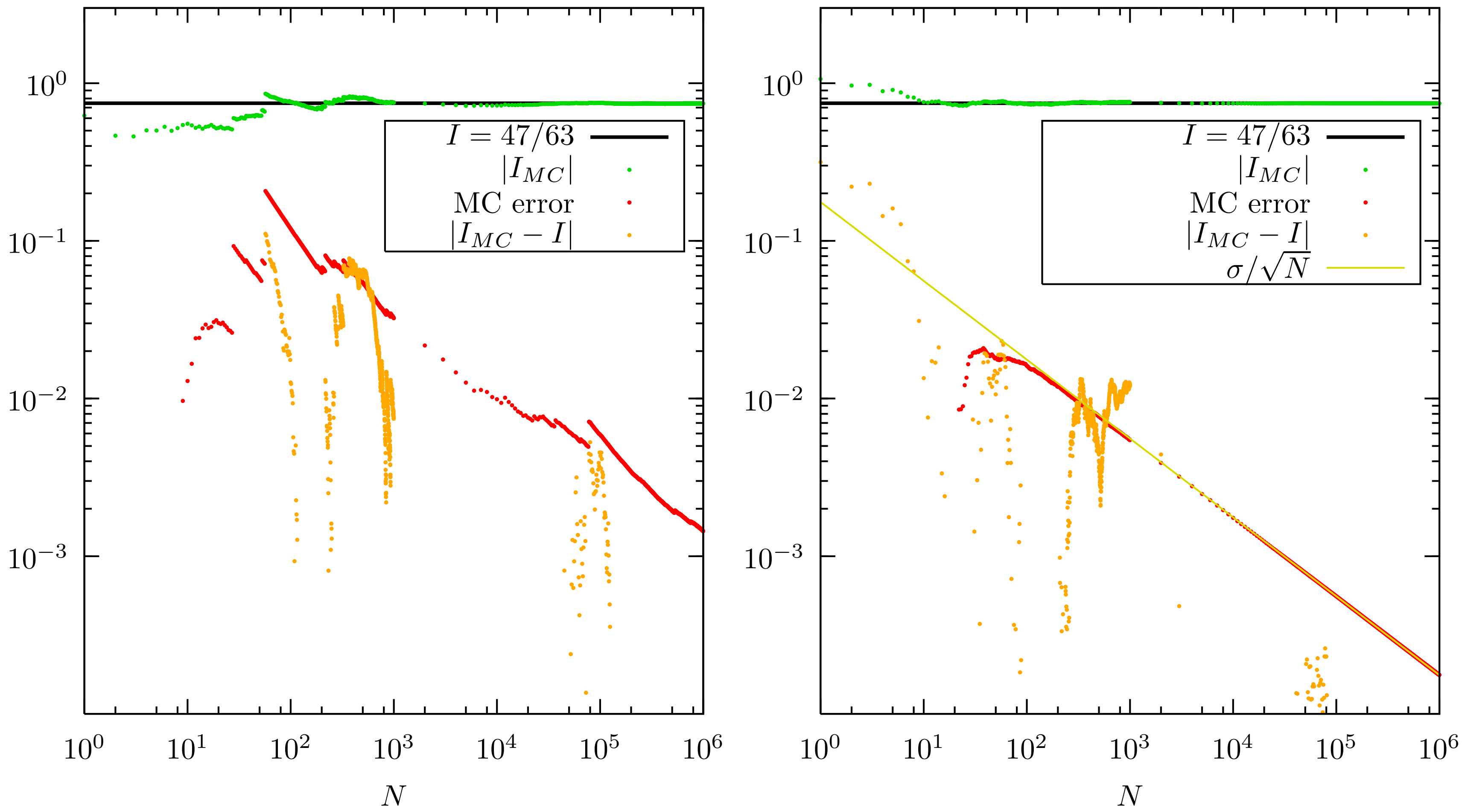


Events generated with $w_{\max} = 1$, as $p(x) \leq 1$, no guesswork needed here! Now, we get 74.6% MC efficiency.
. . . as opposed to 3.7%.

Importance sampling — better example

Crude MC vs Importance sampling.



100× more events needed to reach same accuracy.

Importance sampling — another useful example

Breit–Wigner peaks appear in many realistic MEs for cross sections and decays.

$$I = \int_{s_0}^{s_1} \frac{ds}{(s-m^2)^2 + m^2\Gamma^2}$$

Importance sampling — another useful example

Breit–Wigner peaks appear in many realistic MEs for cross sections and decays.

$$I = \int_{s_0}^{s_1} \frac{ds}{(s-m^2)^2 + m^2\Gamma^2} = \frac{1}{m\Gamma} \int_{y_0}^{y_1} \frac{dy}{y^2+1} \qquad (y = \frac{s-m^2}{m\Gamma})$$

$$= \frac{1}{m\Gamma} \arctan \frac{s-m^2}{m\Gamma} \bigg|_{s_0}^{s_1}$$

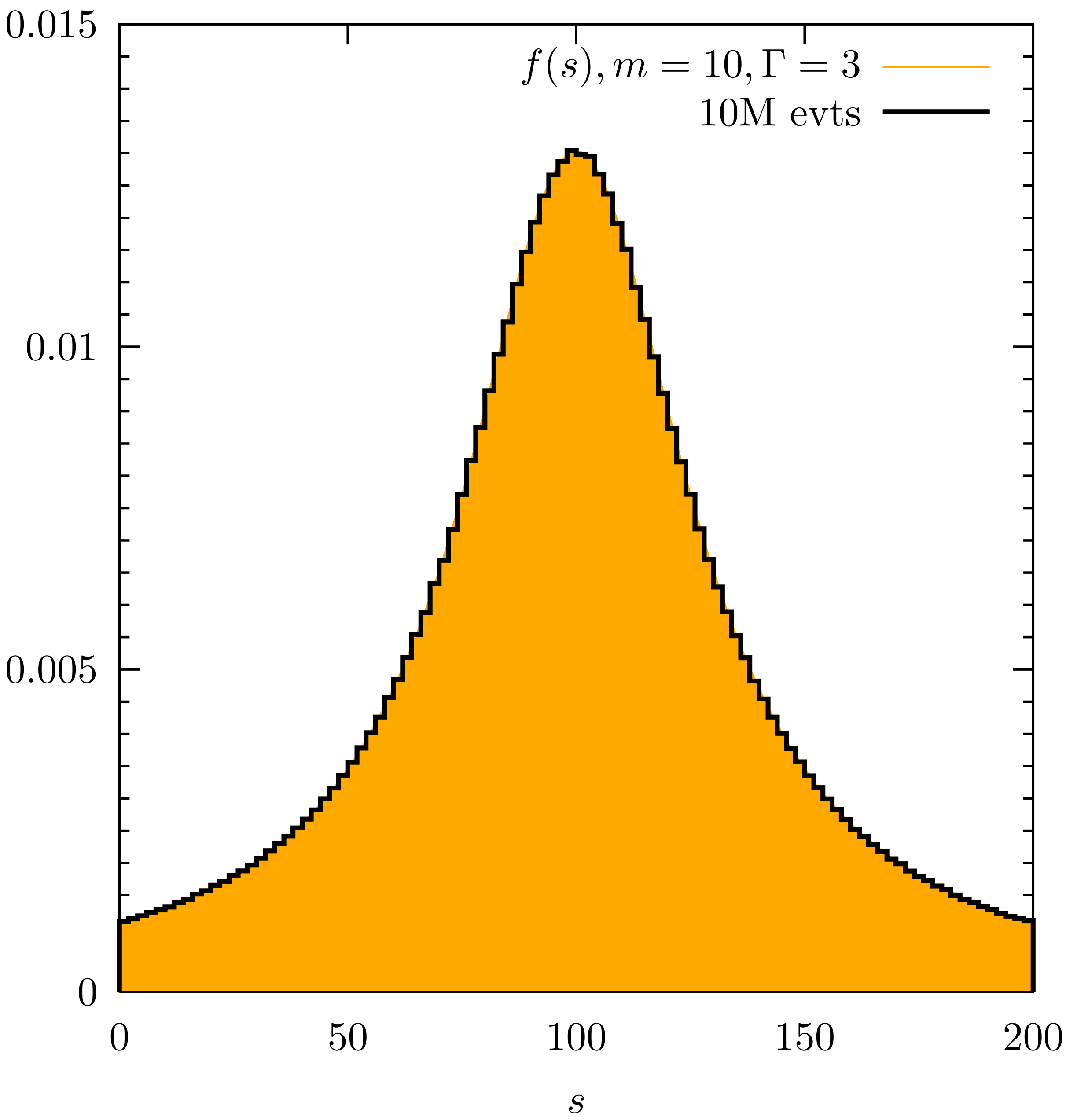
Inverting the integral gives (“tan mapping”).

$$f(s) = \frac{m\Gamma}{(s-m^2)^2 + m^2\Gamma^2} \ ,$$

$$F(s) = \arctan \frac{s-m^2}{m\Gamma} = \rho \ ,$$

$$F^{-1}(\rho) = m^2 + m\Gamma \tan \rho \ .$$

Importance sampling — another useful example



VEGAS

- Classic algorithm.
- Automatic impotance sampling.
- Adopt grid size.
- Often used for multidimensional integration.
- Very robust.

VEGAS

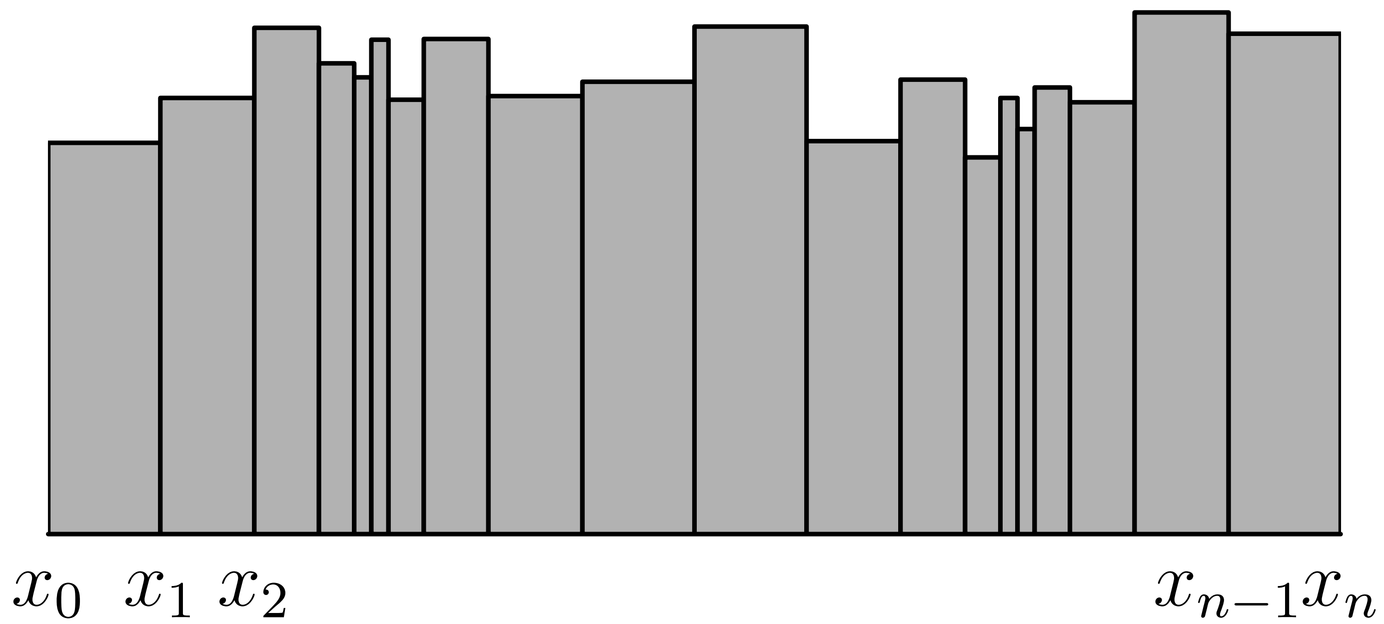
- start with equidistant grid $x_0, x_1, \ldots, x_N$.
- Sample a number of points $\big(x_{s,i}, f(x_{s,i})\big)$, compute first estimate of integral as $\langle f \rangle$.
- Resize grid:
  choose x_i' such that contribution from partial areas inside $x_i < x < x_{i+1}$ to integral is $\langle f \rangle / N$.
- Remember, optimal $p(x) \sim |f(x)|$.
- Sample again with same number of points into every bin $x_i < x < x_{i+1}$. Results in step weight function with steps

$$p_i = \frac{1}{N(x_i - x_{i-1})}\,, \qquad x_i < x < x_{i+1}\,.$$

- $\Rightarrow$ Sample often where density is high.

VEGAS

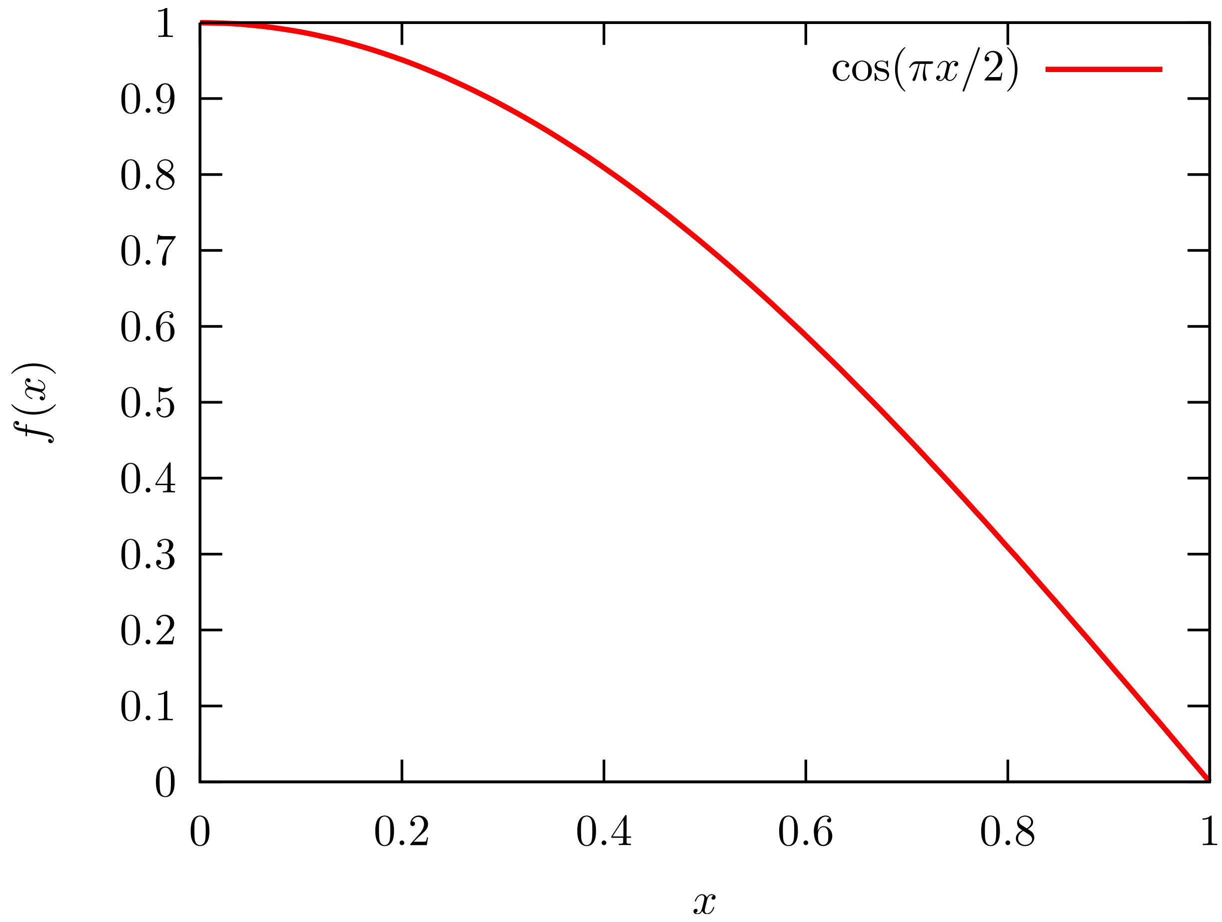
Rebinning:



[from T. Ohl, VAMP]

VEGAS

Example: $\cos(\frac{\pi x}{2})$
$N_{\text{grid}} = 20, 100$
Convergence improved.



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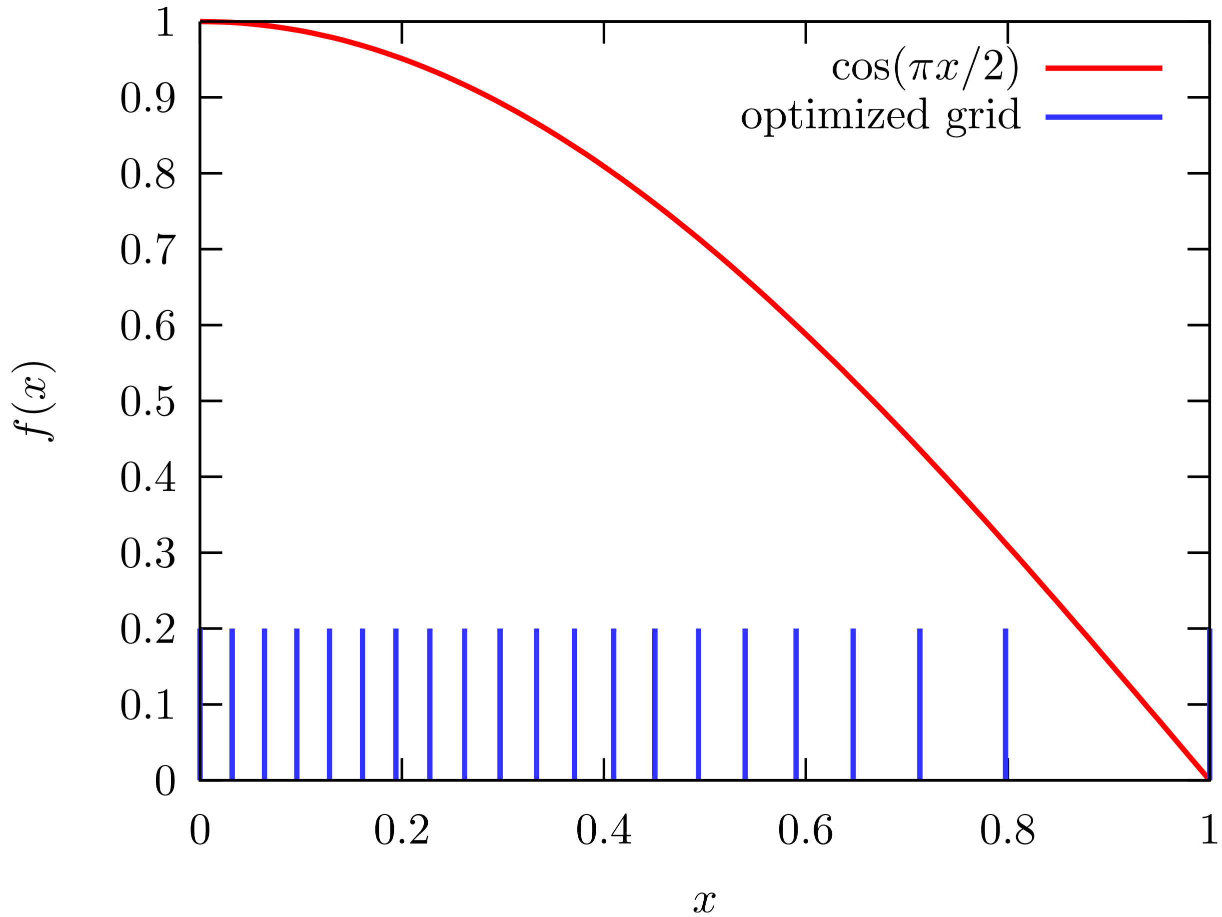

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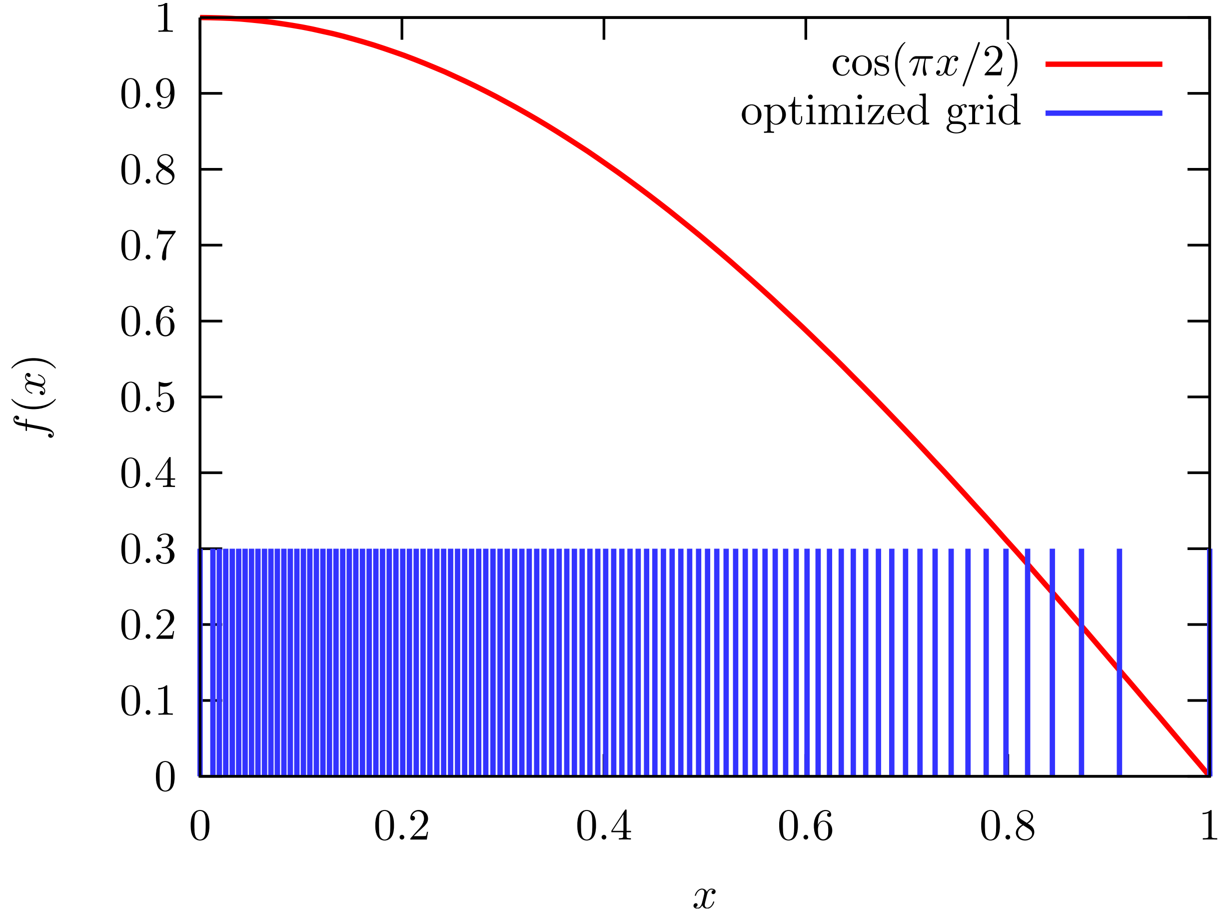

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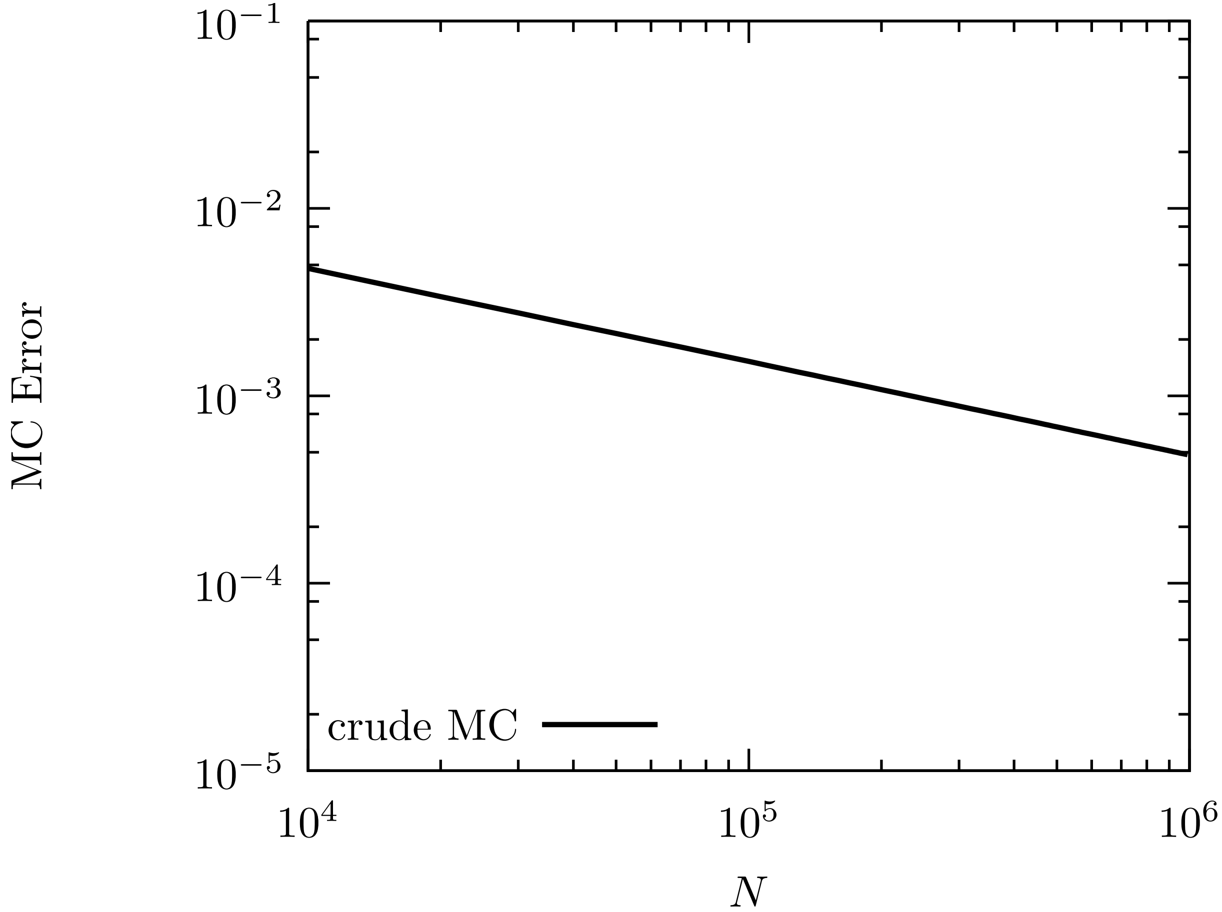

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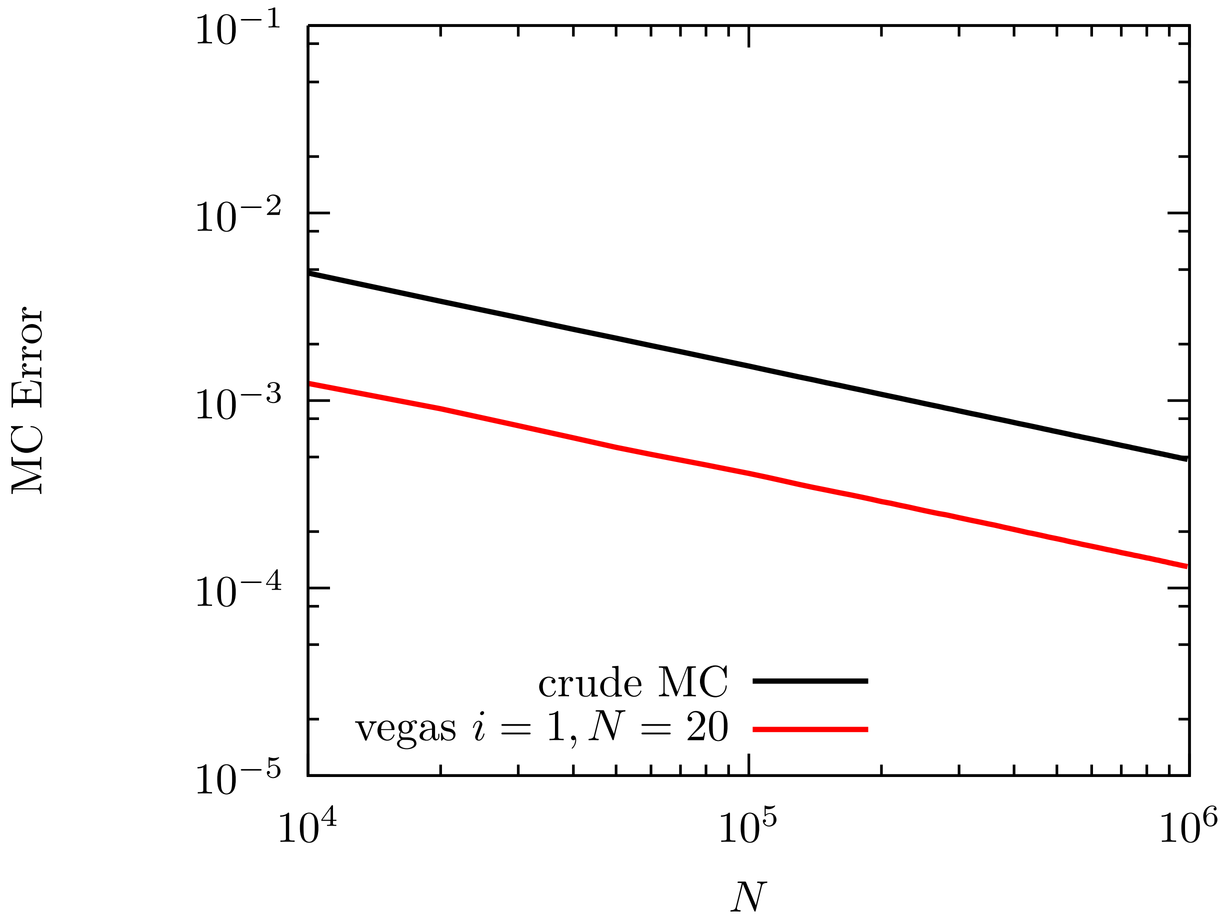

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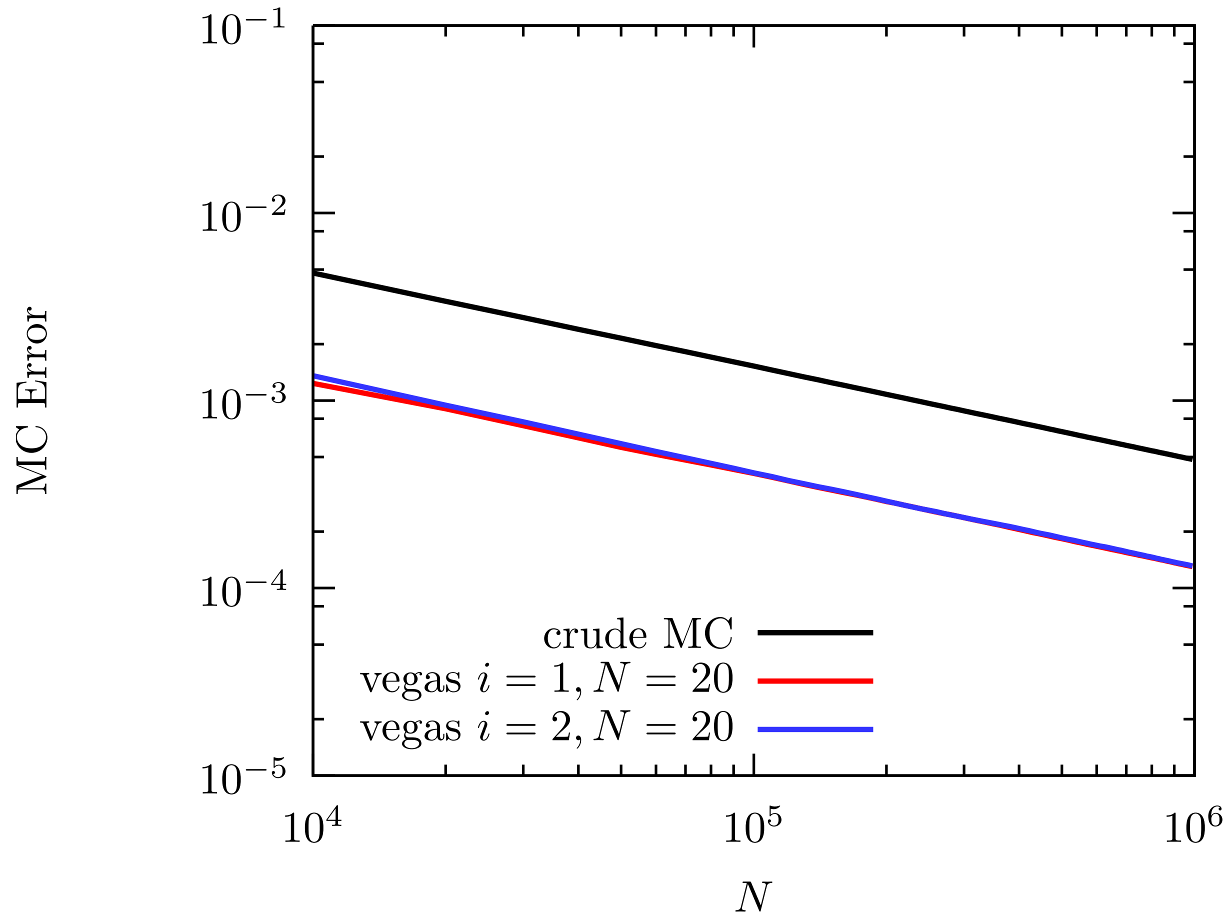

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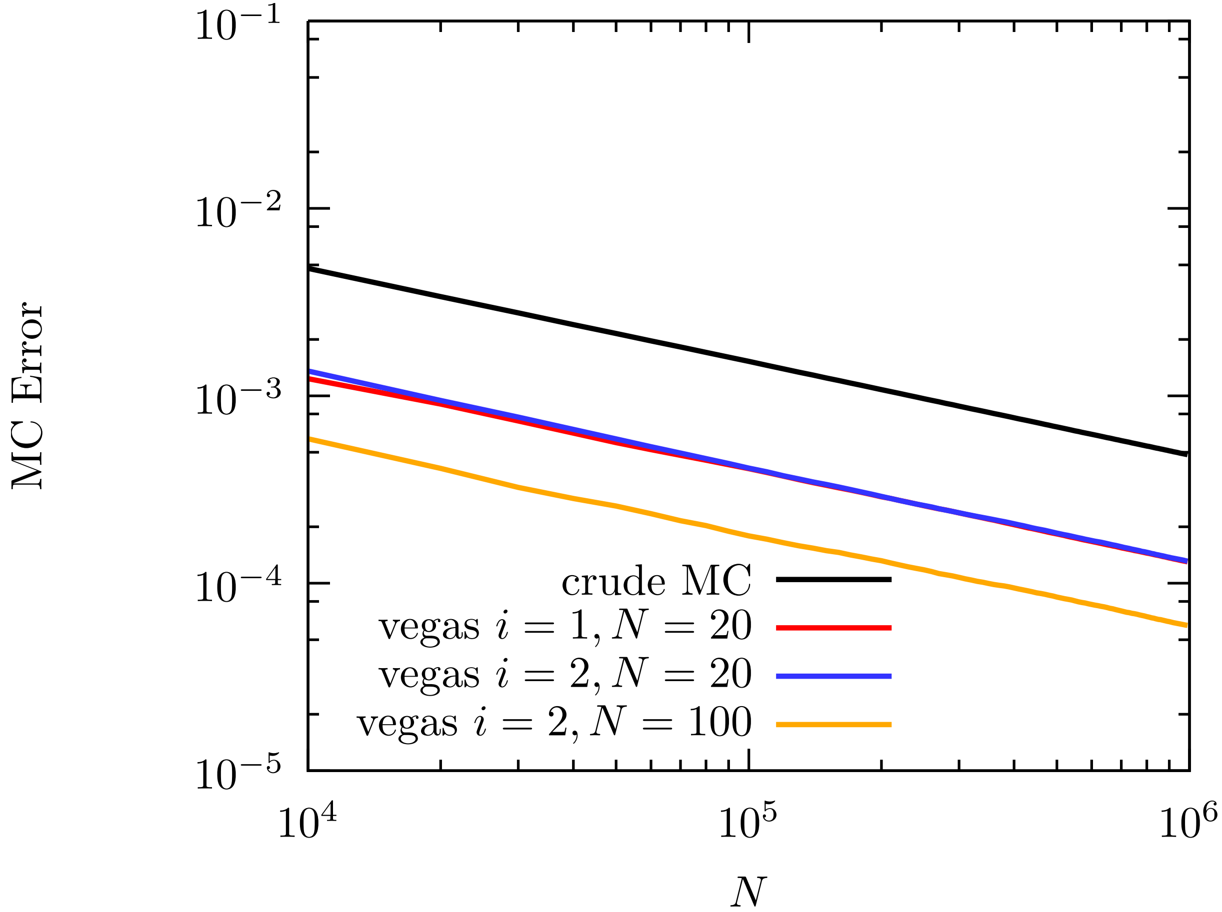

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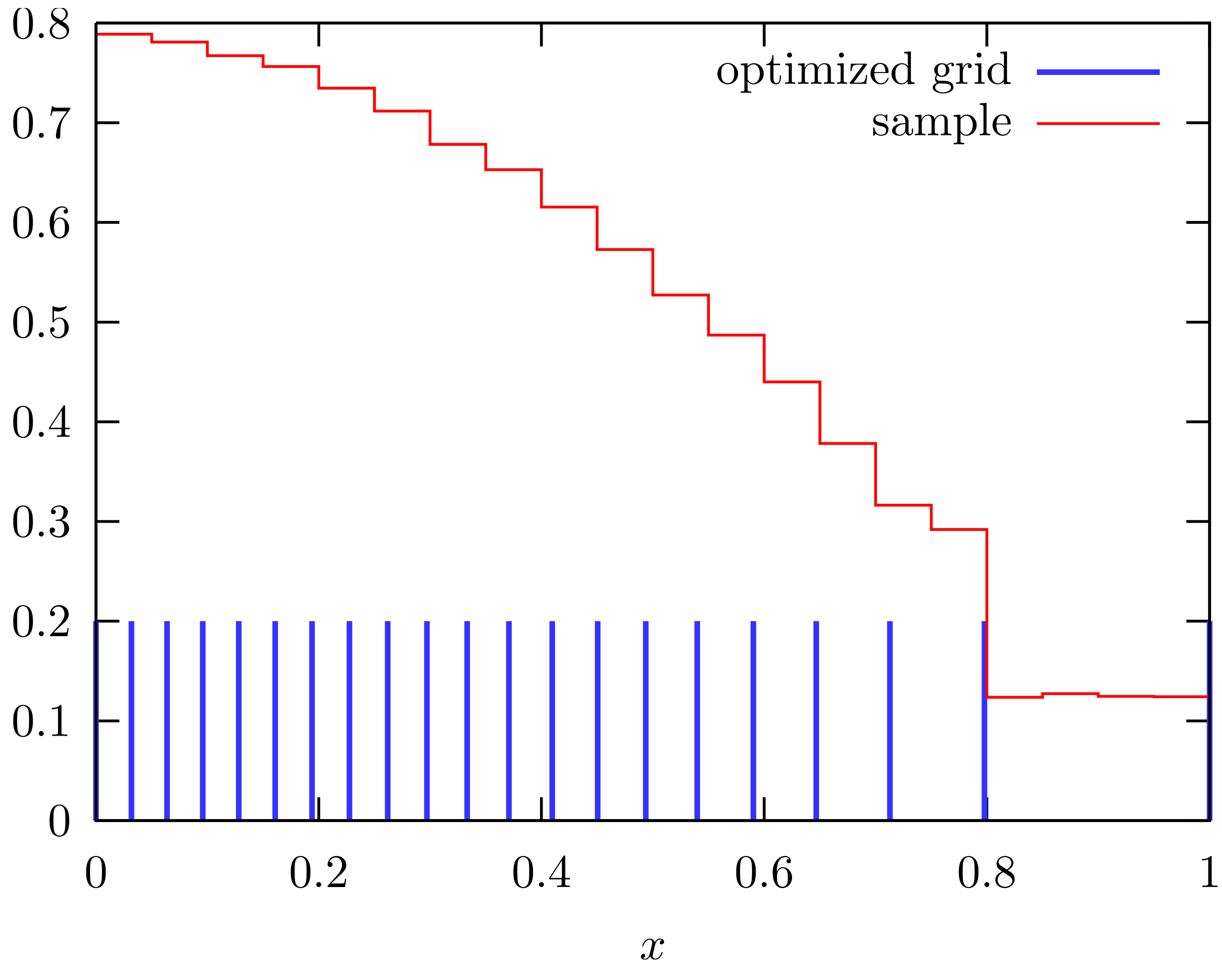

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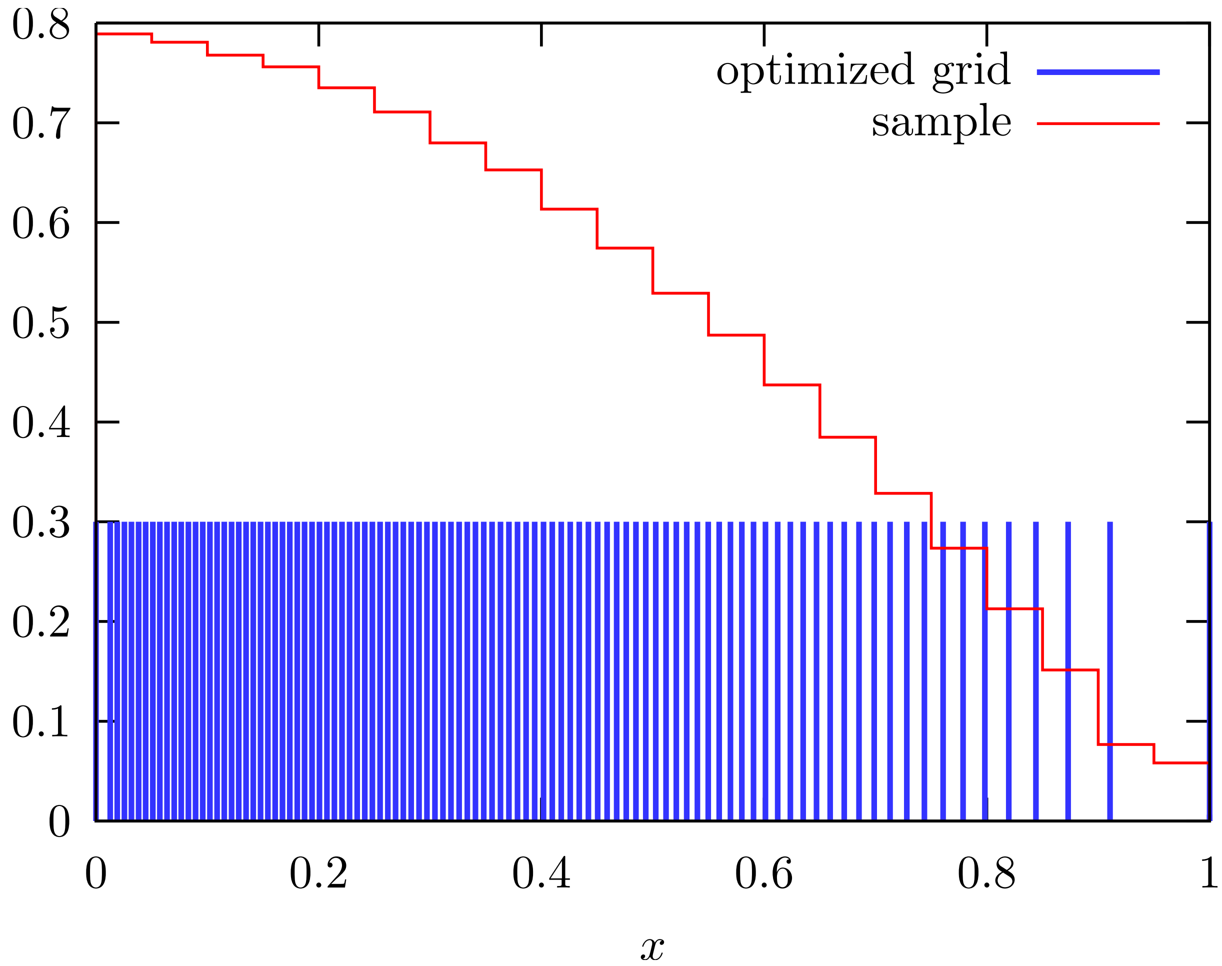

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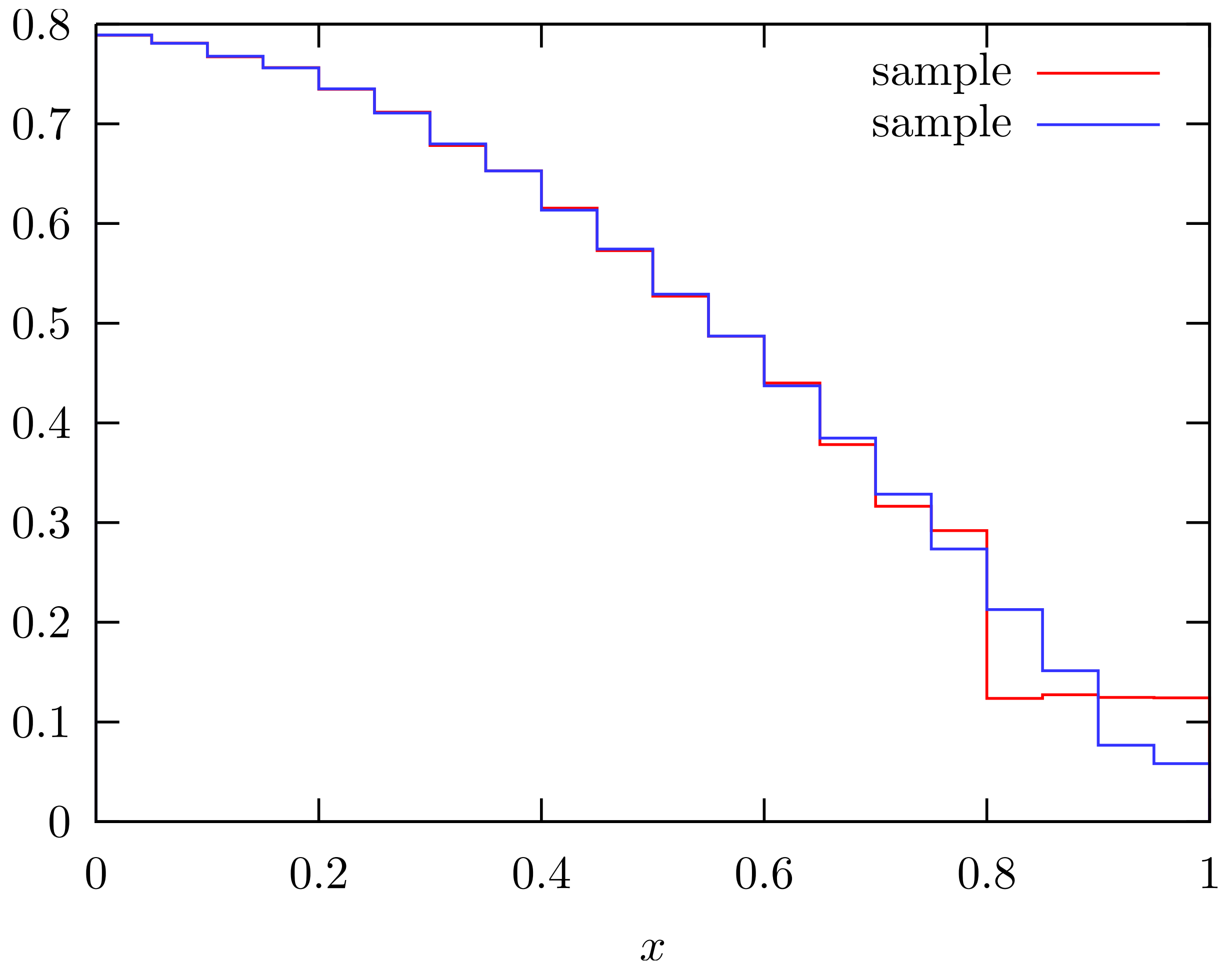
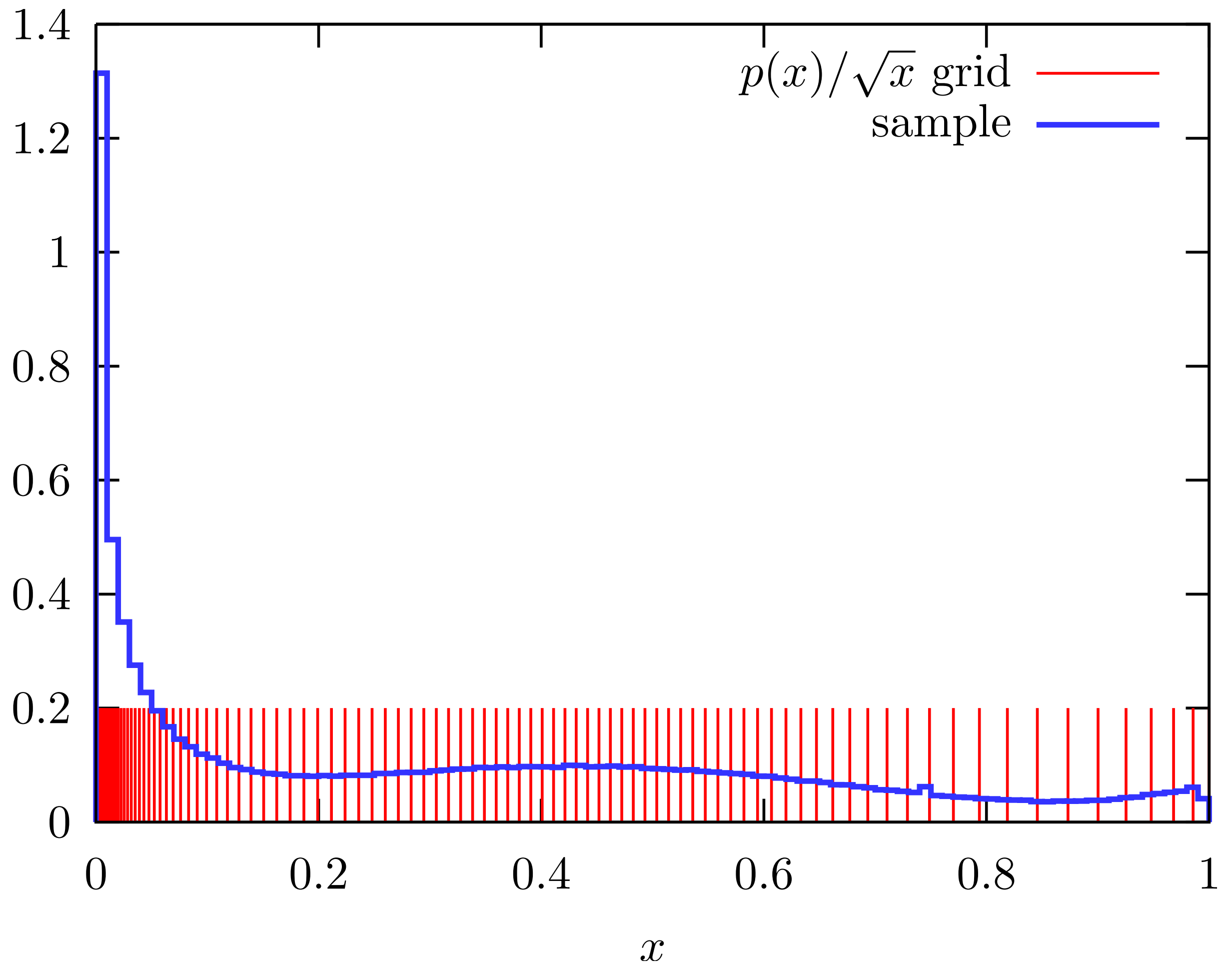


VEGAS

Second example:
$p(x)/\sqrt{x}$
(divergence with wiggles)



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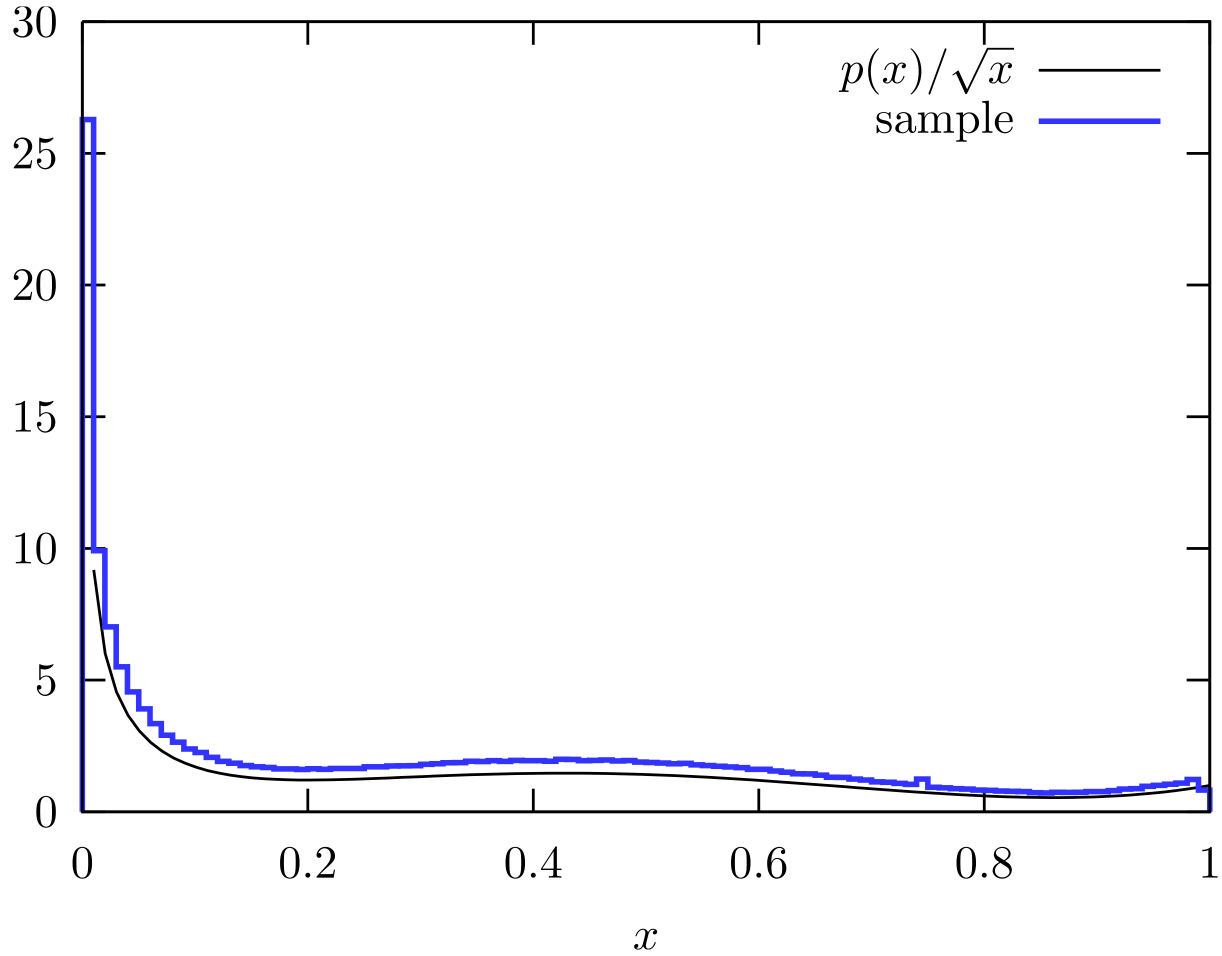

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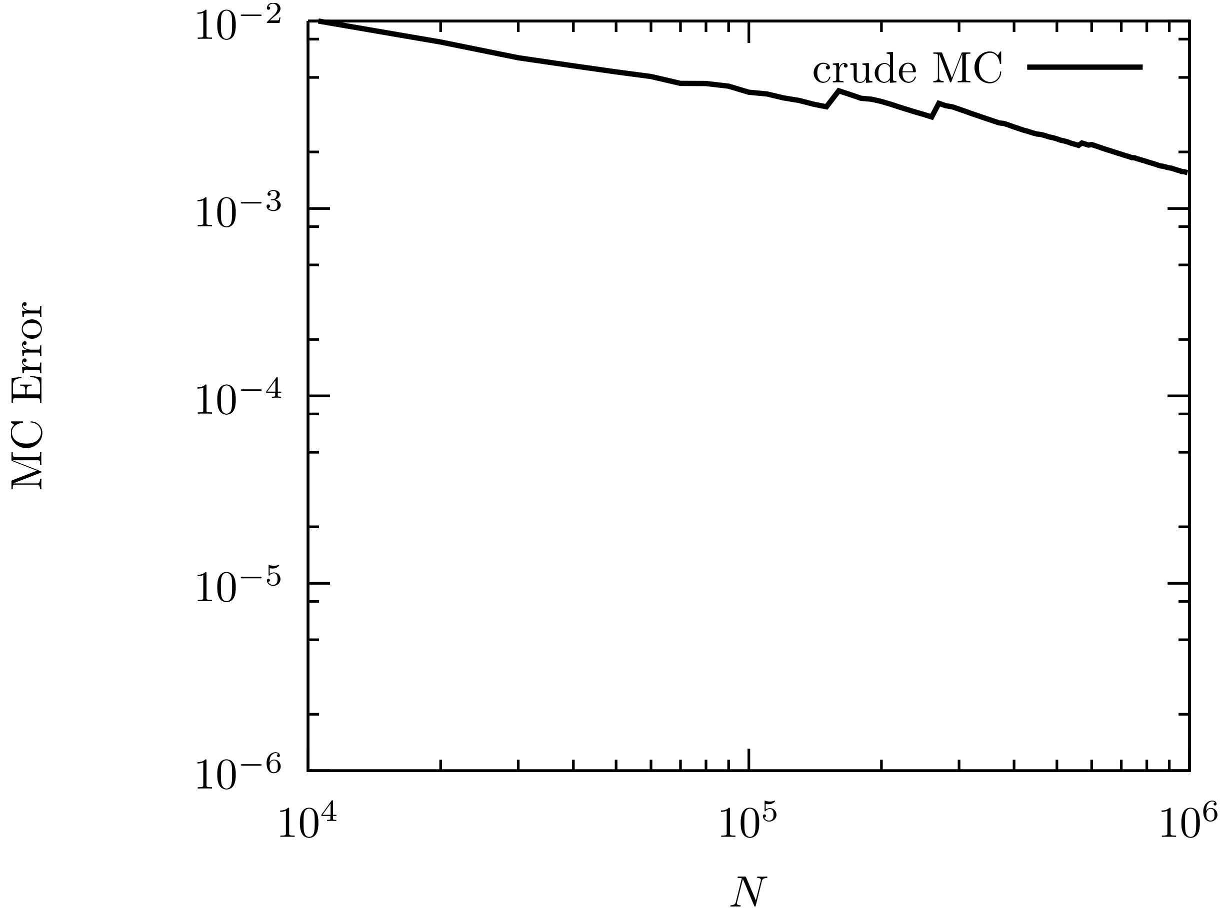

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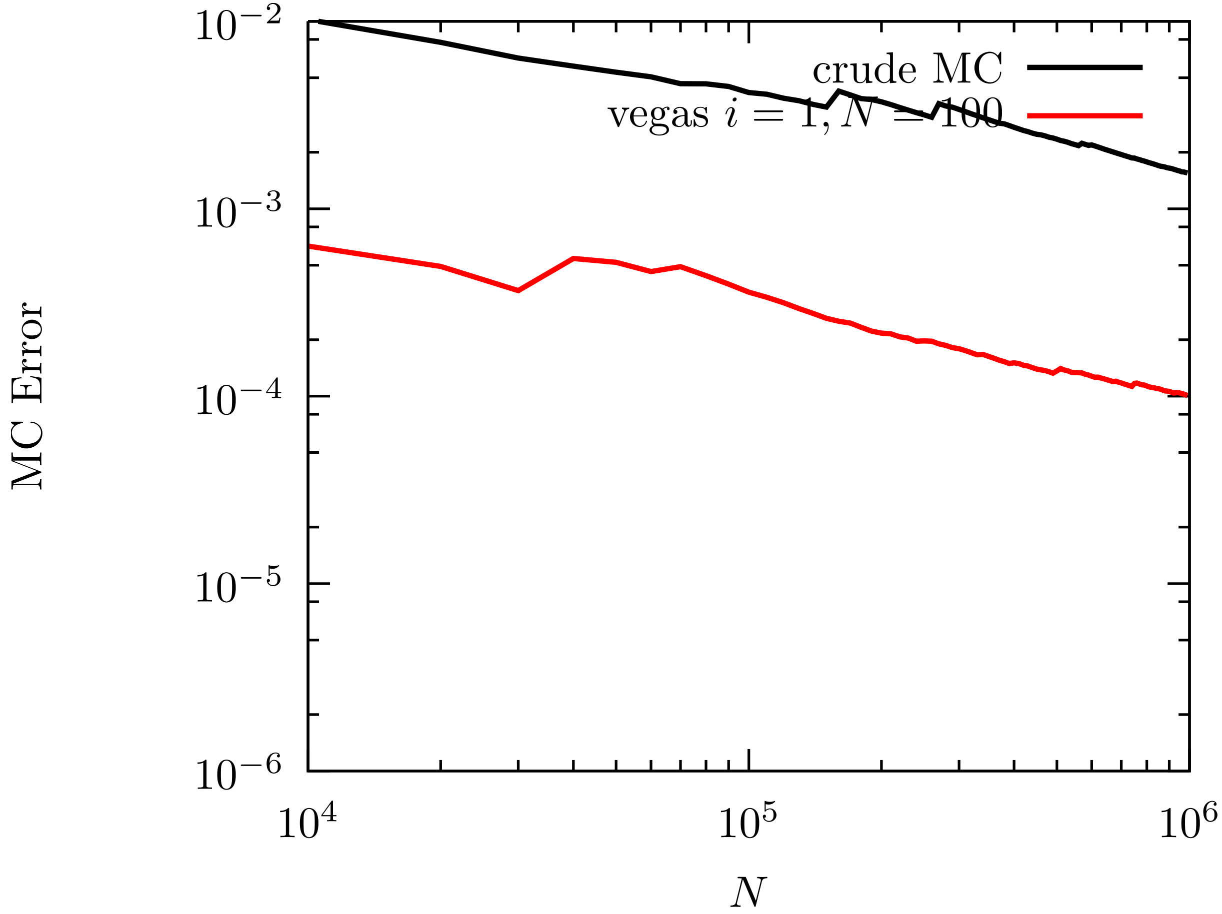

Acc 10^{-4} after $N = 10^6$ comparable with 'inverting the integral'.

VEGAS

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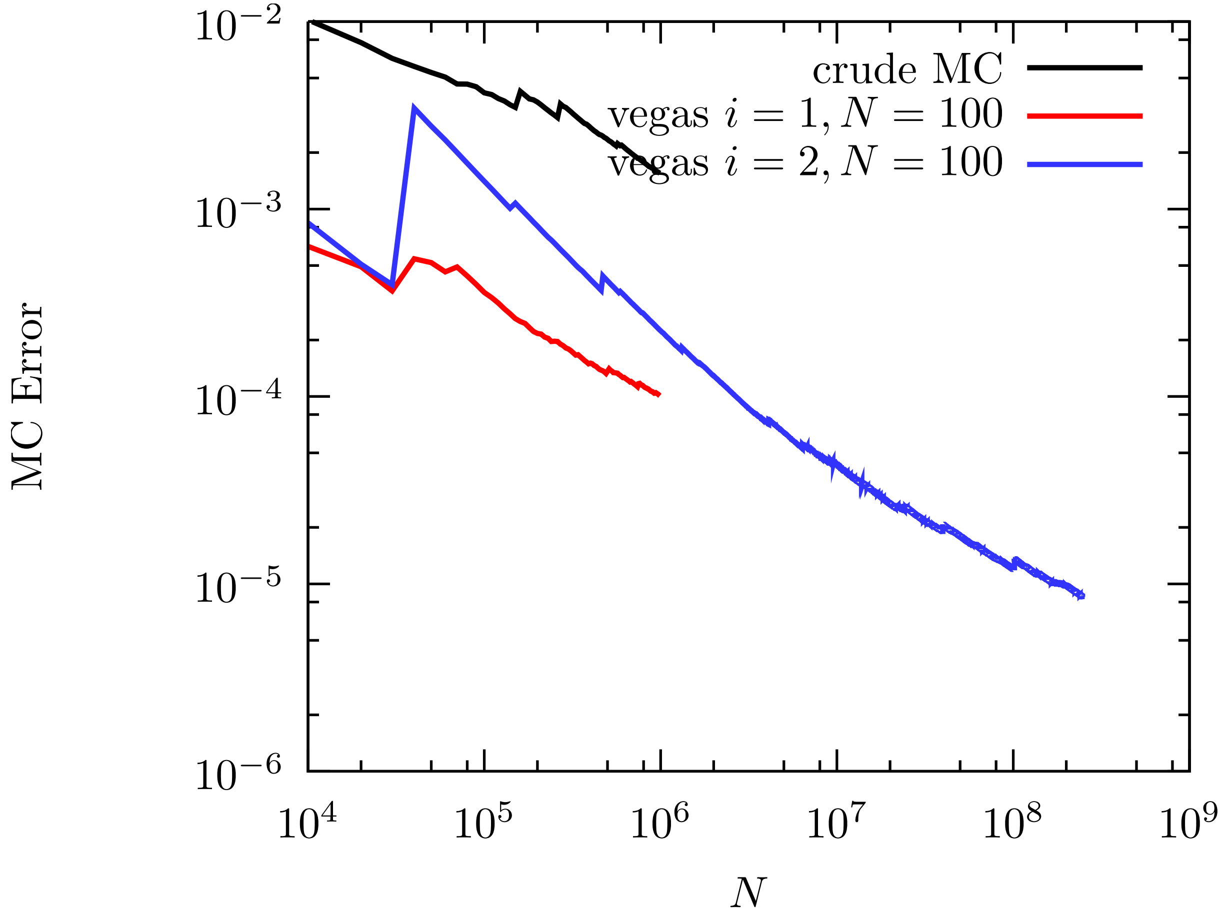
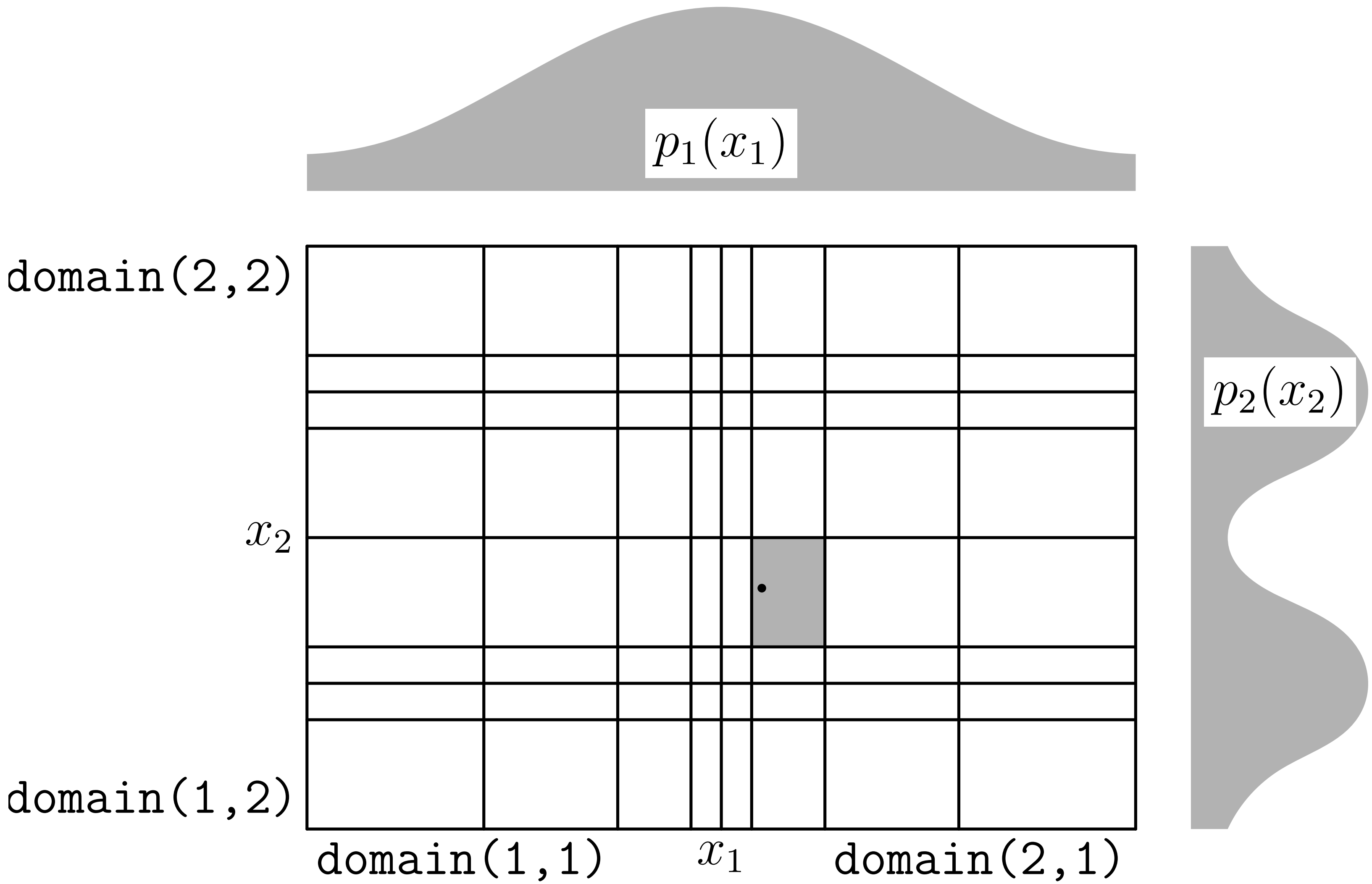


VEGAS

Problem to adapt in multiple dimensions:

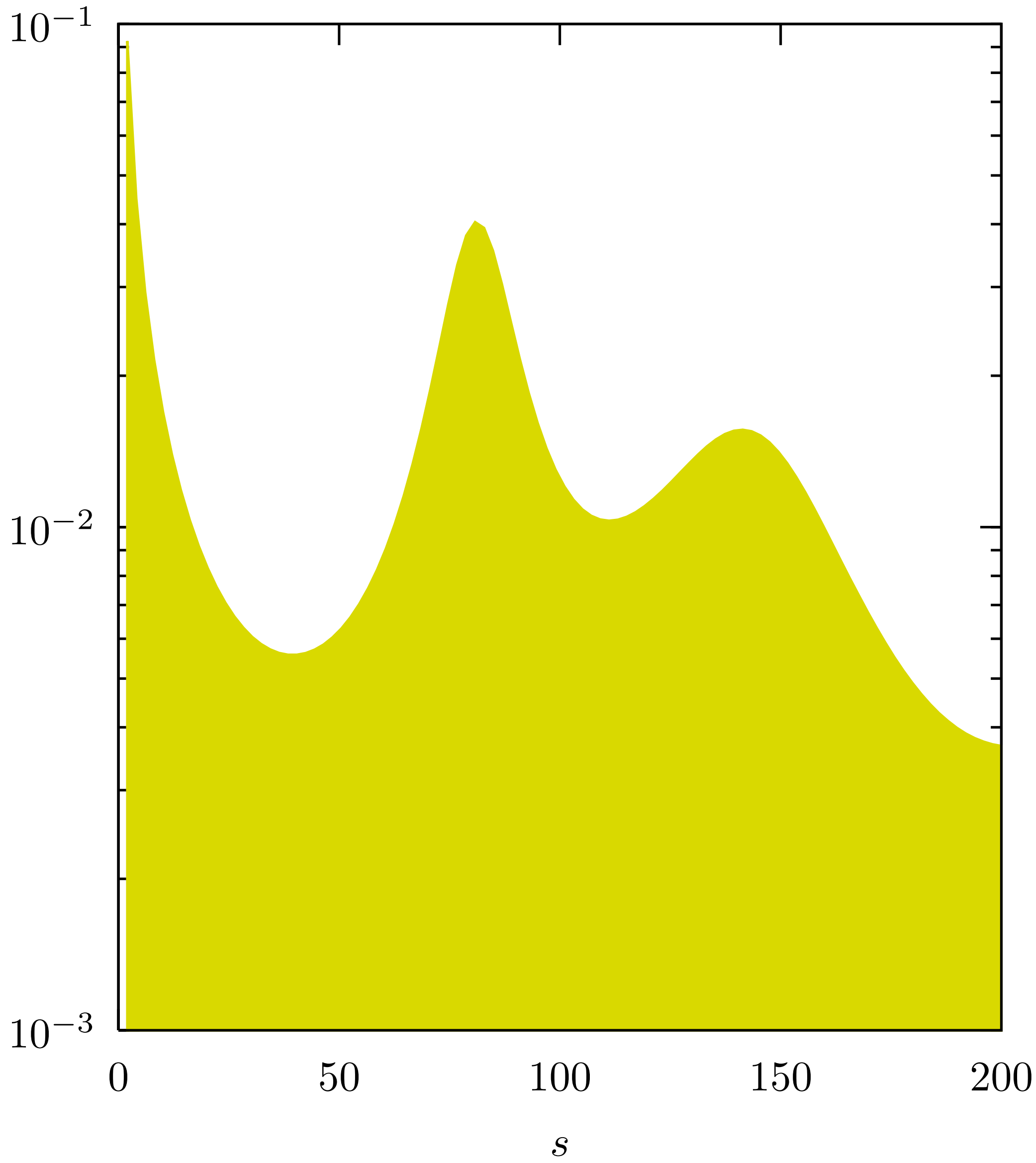


[from T. Ohl, VAMP]

Multichannel MC

Typical problem:

- $f(s)$ has multiple peaks ($\times$ wiggles from ME).



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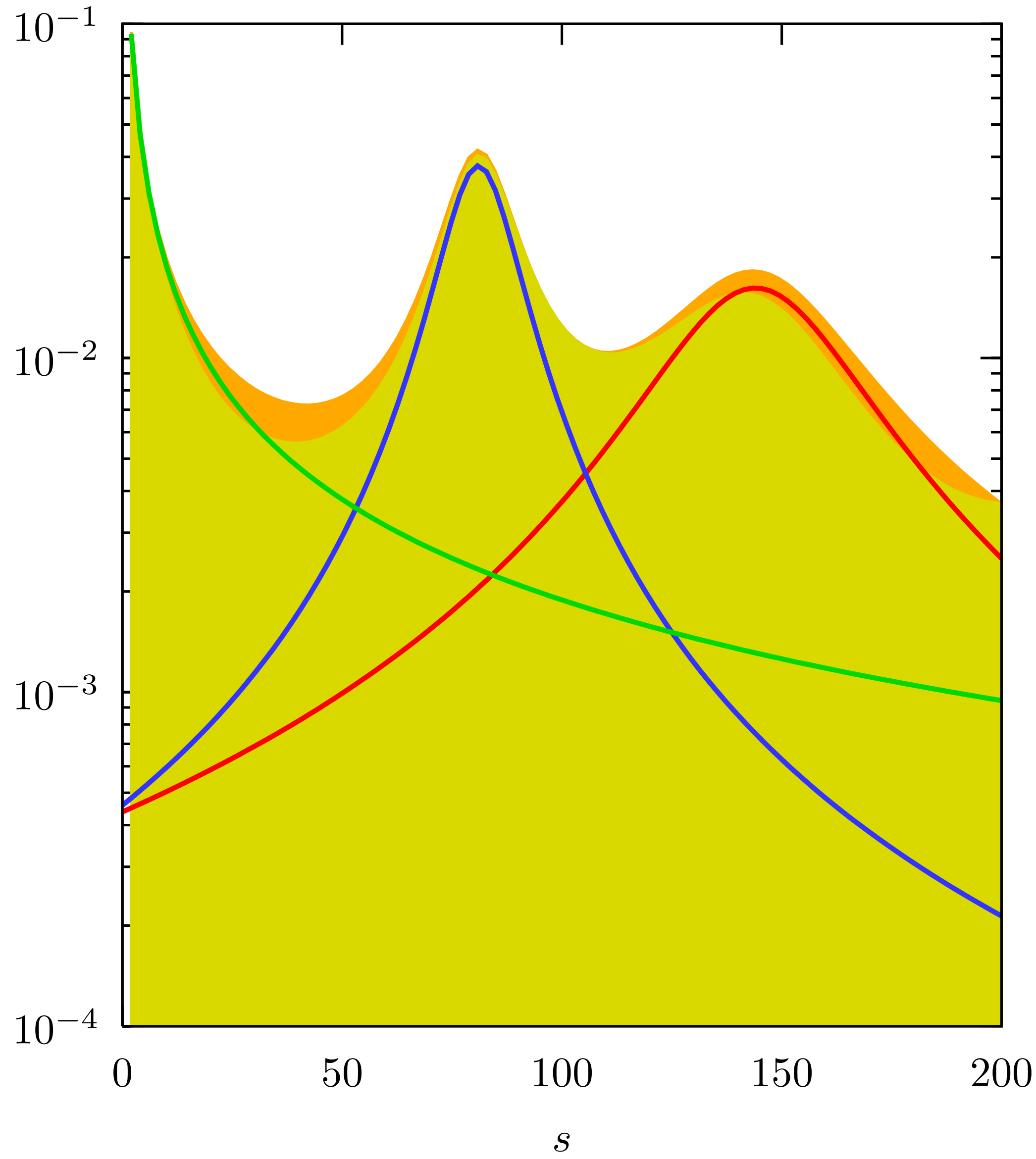
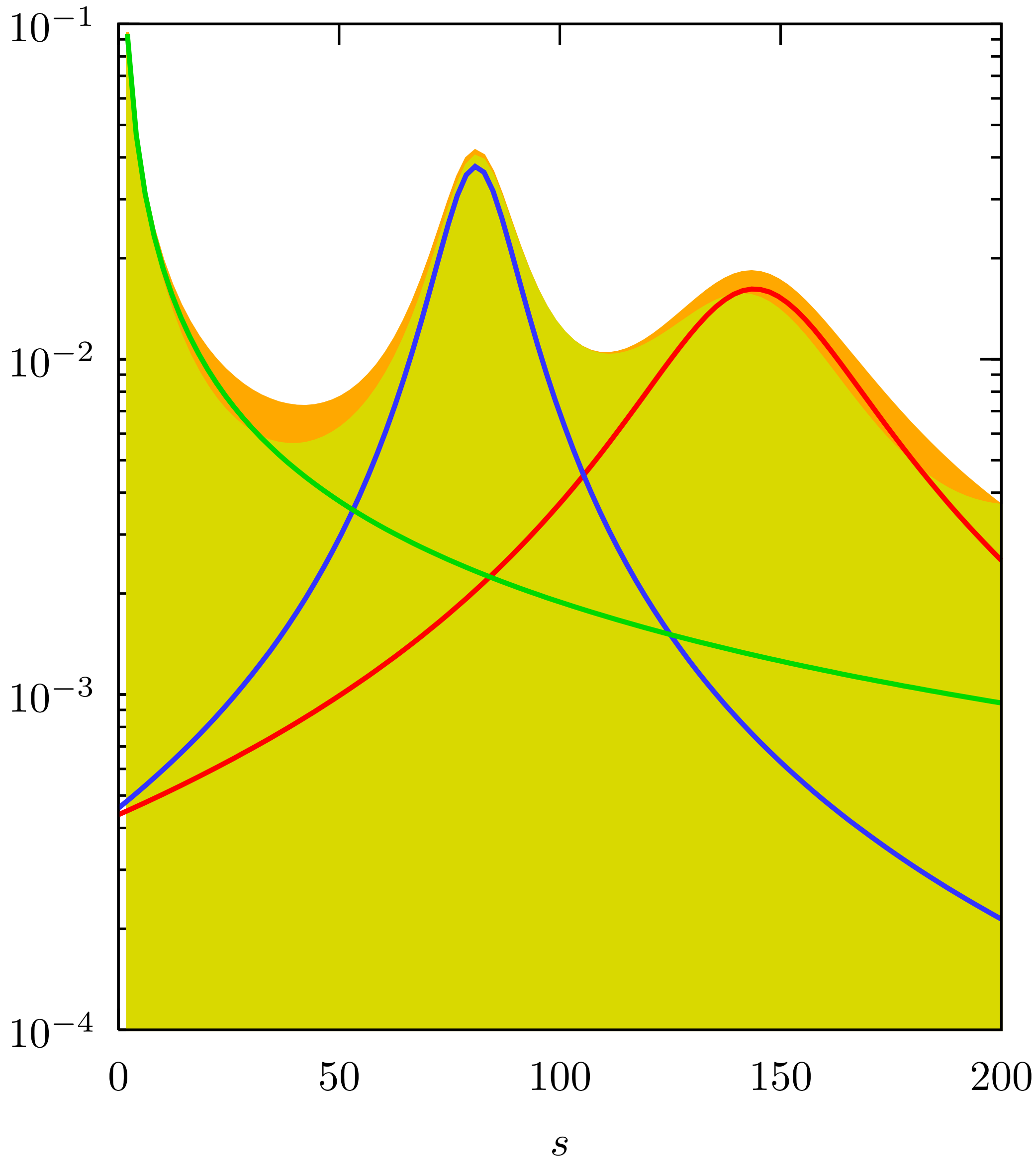


Multichannel MC

Typical problem:

- $f(s)$ has multiple peaks ($\times$ wiggles from ME).
- Usually have some idea of the peak structure.
- Encode this in sum of sample functions $g_i(s)$ with weights $\alpha_i, \sum_i \alpha_i = 1$.

$$g(s) = \sum_i \alpha_i g_i(s) \ .$$



Multichannel MC

Now rewrite

$$\int_{s_0}^{s_1} f(s)\,ds = \int_{s_0}^{s_1} \frac{f(s)}{g(s)} g(s)\,ds$$
$$= \int_{s_0}^{s_1} \frac{f(s)}{g(s)} \sum_i \alpha_i g_i(s)\,ds$$
$$= \sum_i \alpha_i \int_{s_0}^{s_1} \frac{f(s)}{g(s)} g_i(s)\,ds$$

Now $g_i(s)\,ds = d\rho_i$ (inverting the integral).

Multichannel MC

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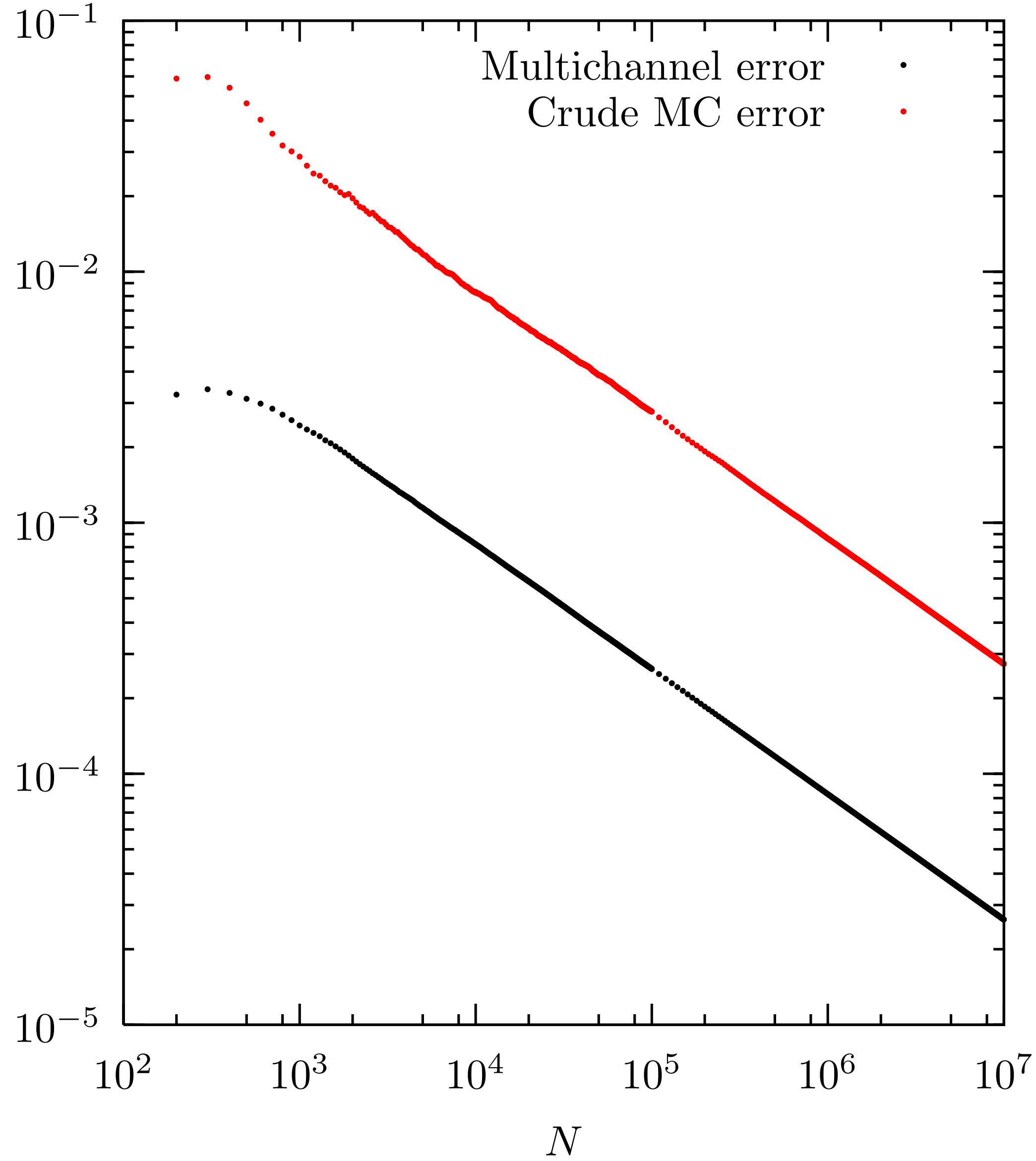
Now $g_i(s)\,ds = d\rho_i$ (inverting the integral).

Select the distribution $g_i(s)$ you'd like to sample next event from acc to weights α_i.

α_i can be optimized after a number of trials.

Multichannel MC

Works quite well:



Hard Scattering

Hard scattering

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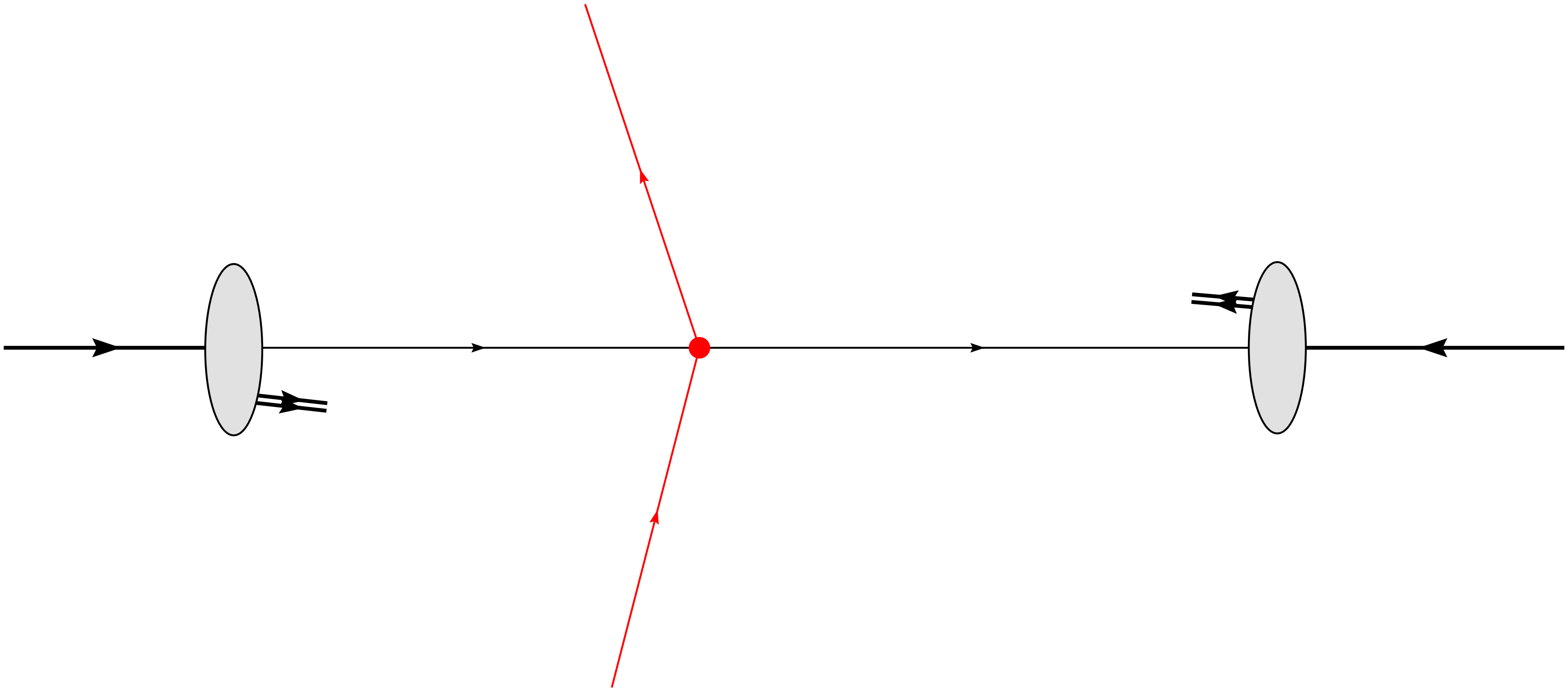
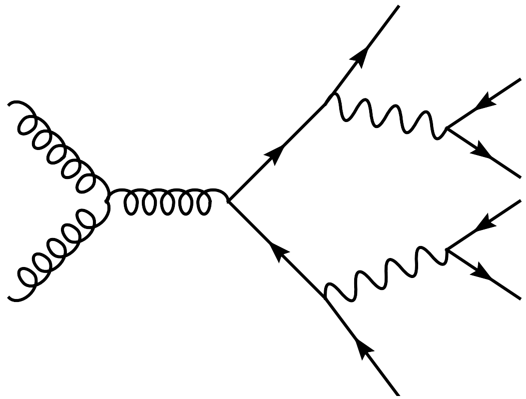


Matrix elements

- Perturbation theory/Feynman diagrams give us (fairly accurate) final states for a few number of legs ($\mathcal{O}(1)$).



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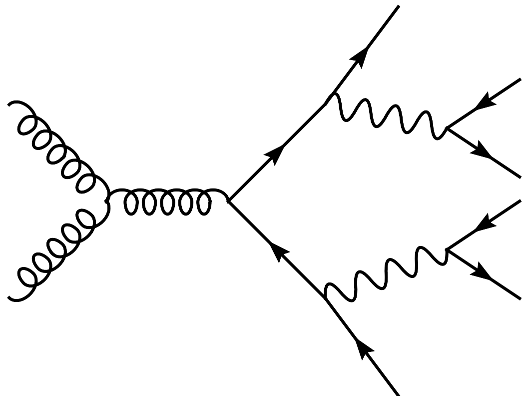

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- Starting point for further simulation.
- Want exclusive final state at the LHC ($O(100)$).

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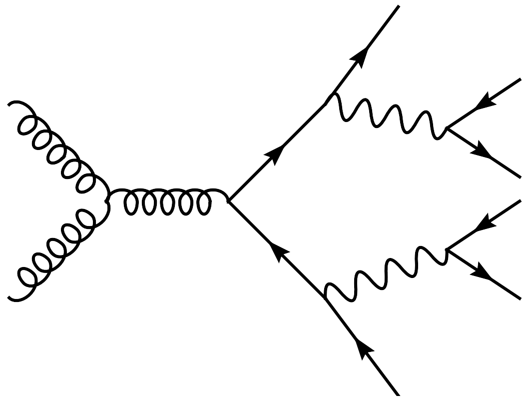

- OK for very inclusive observables.
- Starting point for further simulation.
- Want exclusive final state at the LHC ($O(100)$).
- Want arbitrary cuts.
- $\rightarrow$ use Monte Carlo methods.

Matrix elements

Where do we get (LO) $|M|^2$ from?

- Most/important simple processes (SM and BSM) are 'built in'.
- Calculate yourself (≤ 3 particles in final state).
- Matrix element generators:
  - MadGraph/MadEvent.
  - Comix/AMEGIC (part of Sherpa).
  - HELAC/PHEGAS.
  - Whizard.
  - CalcHEP/CompHEP.

  generate code or event files that can be further processed.
- $\rightarrow$ FeynRules interface to ME generators.

Also NLO mostly automatically available.
See "Matching and Merging".

Cross section formula

From Matrix element, we calculate

$$\sigma = \int f_i(x_1, \mu^2) f_j(x_2, \mu^2) \frac{1}{F} \overline{\sum} |M|^2 \qquad \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}\Phi_n \ ,$$

Cross section formula

From Matrix element, we calculate

$$\sigma = \int f_i(x_1,\mu^2) f_j(x_2,\mu^2) \frac{1}{F} \overline{\sum} |M|^2 \, \Theta(\text{cuts}) \, \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}\Phi_n \ ,$$

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now,

$$\frac{1}{F} \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}\Phi_n = J(\vec{x}) \prod_{i=1}^{3n-2} \mathrm{d}x_i \qquad \left(\mathrm{d}\Phi_n = (2\pi)^4 \delta^{(4)}(\ldots) \prod_{i=1}^{n} \frac{\mathrm{d}^3\vec{p}}{(2\pi)^3 2E_i} \right)$$

such that

$$\sigma = \int g(\vec{x}) \, \mathrm{d}^{3n-2}\vec{x} \ , \qquad \left(g(\vec{x}) = J(\vec{x}) f_i f_j \overline{\sum} |M|^2 \Theta(\text{cuts}) \right)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \frac{g(\vec{x}_i)}{p(\vec{x}_i)} = \frac{1}{N} \sum_{i=1}^{N} w_i \ .$$

Cross section formula

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We generate events $\vec{x}_i$ with weights w_i.

Mini event generator

- We generate pairs $(\vec{x}_i, w_i)$.

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$$P_i = \frac{w_i}{w_{\max}} \; .$$

Generate events with same frequency as in nature!

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- Use immediately to book weighted histogram of arbitrary observable (possibly with additional cuts!)
- Keep event $\vec{x}_i$ with probability

$$P_i = \frac{w_i}{w_{\max}} \ ,$$

where $w_{\max}$ has to be chosen sensibly.
$\to$ reweighting, when $\max(w_i) = \bar{w}_{\max} > w_{\max}$, as

$$P_i = \frac{w_i}{\bar{w}_{\max}} = \frac{w_i}{w_{\max}} \cdot \frac{w_{\max}}{\bar{w}_{\max}} \ ,$$

i.e. reject events with probability $(w_{\max}/\bar{w}_{\max})$ afterwards.

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- Use immediately to book weighted histogram of arbitrary observable (possibly with additional cuts!)
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Generate events with same frequency as in nature!

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Some comments:

- Use common Monte Carlo techniques to generate events efficiently. Goal: small variance in w_i distribution!

Matrix elements

Some comments:

- Use common Monte Carlo techniques to generate events efficiently. Goal: small variance in w_i distribution!
- Efficient generation closely tied to knowledge of $f(\vec{x}_i)$, *i.e.* the matrix element's propagator structure.
  $\rightarrow$ build phase space generator already while generating ME's automatically.