Monte Carlo techniques

Application to QCD

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CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE

CDCS
CENTER FOR DATA AND COMPUTING
IN NATURAL SCIENCES

Bundesministerium
für Bildung
und Forschung

Introduction

Introduction

Quotation

« **Monte Carlo** refers to any type of techniques that makes use of **random numbers**, probabilities and statistics **to solve** a problem numerically. »

Hannes Jung

Introduction

Motivation

- MC techniques are widely used in physics:
  - deal with high-dimensional problems;
  - often easy to interpret at event level.
- Today we will introduce them
  - first with pedagogical examples,
  - then in the context of Quantum Chromodynamics (QCD).
- We will alternate slides and hands-on sessions.

Main source: QCD and MC lectures, by Hannes JUNG

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Goal

Calculate the following integral:

$$I = \int_{\Omega} f(u) \; \mathrm{d}u \tag{1}$$

for any (more or less smooth) function f.

Introduction

Exercises

- Either in plain C++ or in Python with Jupyter notebooks
- Just follow the instructions on the GitHub repository.

Advice: work in pairs

- Formulate your choices loudly.
- Review one another.
- Exchange ideas.

Red block

Question!

Grey block

Hands on!

Basics

Probability density function (p.d.f.)

The random variable X has p.d.f. g (non-negative, integrable, and normalised to unity) if:

$$\mathbb{P}\left[a \leq X \leq b\right] = \int_a^b g(x) \, \mathrm{d}x \tag{2}$$

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Expectation value and variance

Given f a function of a random variable X following a p.d.f. g:

expectation value $$\mathbb{E}\left[f\right] = \int_{-\infty}^{+\infty} f(x) g(x) \; \mathrm{d}x \tag{3}$$

variance $$\mathbb{V}\left[f\right] = \mathbb{E}\left[\left(f - \mathbb{E}\left[f\right]\right)^2\right] \tag{4}$$

General form

Given realisations x_i of the random variable X, for $N \to \infty$:

$$\mu \equiv \frac{1}{N} \sum_{i=1}^{N} f(x_i) \longrightarrow \mathbb{E}\left[f\right] \tag{5}$$

Basics

Law of Large Numbers

General form

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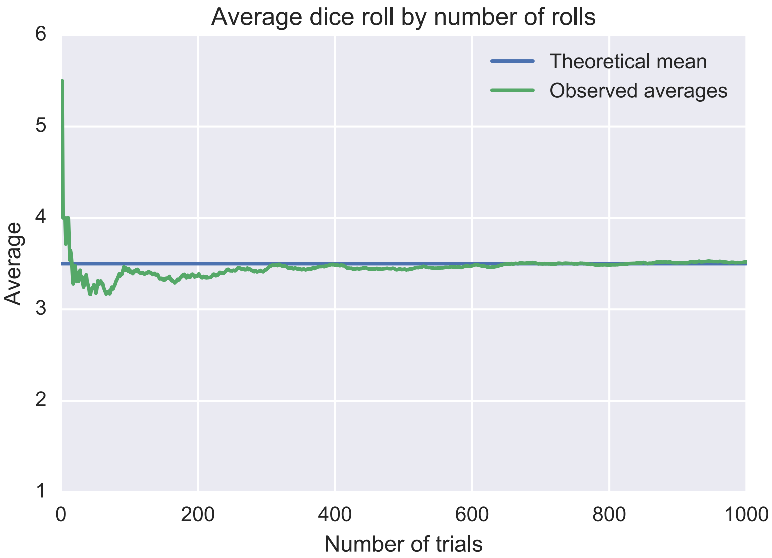
Simple form

If $x_i \equiv u_i \sim \mathcal{U}[a, b]$, for $N \to \infty$:

$$\frac{1}{N} \sum_{i=1}^{N} f(u_i) \longrightarrow \frac{1}{b-a} \int_a^b f(u) \, \mathrm{d}u \tag{6}$$

Basics

Law of Large Numbers



Apply simple form of LLN

$$I \approx I_{\text{MC}} = \frac{b-a}{N} \sum_{i=1}^{N} f(u_i) \tag{7}$$

$$\sigma_{\text{MC}}^2 = \mathbb{V}\left[I_{\text{MC}}\right] = \frac{(b-a)^2}{N} \mathbb{V}\left[f\right] \tag{8}$$

$$= \frac{(b-a)^2}{N^2} \sum_{i=1}^{N} \left(f(u_i)\right)^2 - \frac{1}{N} I_{\text{MC}}^2 \tag{9}$$

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$$= \frac{(b-a)^2}{N^2} \sum_{i=1}^{N} \left(f(u_i)\right)^2 - \frac{1}{N} I^2_{\mathrm{MC}} \tag{9}$$

Question

How to generate random numbers?

Pseudo random generator for a uniform distribution

- Linear congruential generator (e.g. `std::rand()`) to generate integer numbers in $[0, m[$.

$$I_{i+1} \equiv aI_i + c \pmod{m} \tag{10}$$

I_0	**seed**	c	increment
a	multiplier	m	modulus

- `RANLUX`, which may be seen as a linear congruential generator with a smart choice of a, c, m, implemented in `TRandom1`.
- The **Mersenne Twister** generator, as implemented in `TRandom3` or `std::mt19937_64`.
- ...

Basics

Random number generator

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Question

What would be the desired properties for a good pseudo random generator?

Basics

Random number generator

Exercise #1

Check the correlations of numbers generated with the linear congruential generator and with one of the `TRandom` classes in ROOT.

Basics

Random number generator

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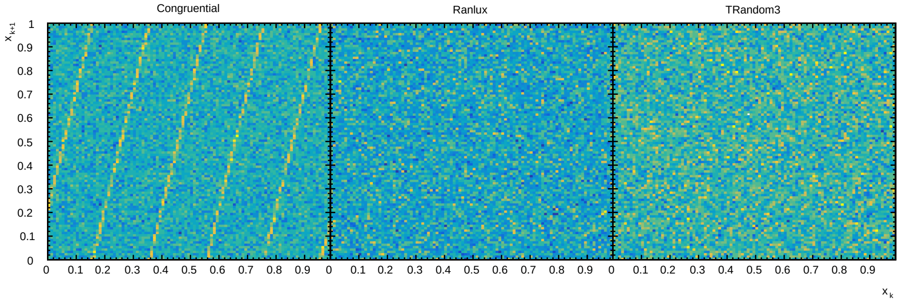

Exercise #3

Calculate the following integral with the help of MC generators:

$$\int_0^1 3x^2 \, \mathrm{d}x \tag{11}$$

and its uncertainty for different values of N.

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Result

$$N = 10^3: \quad I_{\mathsf{MC}} = 1.02013 \pm 0.0274001 \tag{12}$$

$$N = 10^6: \quad I_{\mathsf{MC}} = 0.99945 \pm 0.0008942 \tag{13}$$

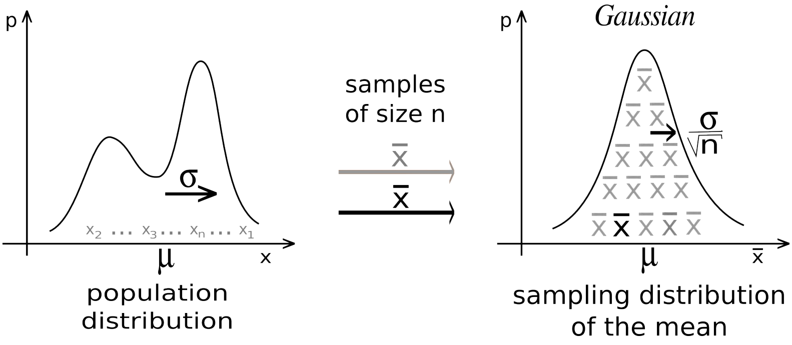
Basics

Gaussian generator

Central limit theorem (CLT)

Given N i.i.d. random variables X_i with expected value μ and variance σ^2, then for $N \to \infty$, the average random variable $\bar{X}_N$ tends to follow a normal distribution:

$$\bar{X}_N \equiv \frac{1}{N} \sum_{i=1}^{N} X_i \sim \mathcal{N}(\mu, \sigma^2) \tag{14}$$



UHH

Basics

Gaussian generator

Exercise #2

Construct a Gaussian random number generator with the help of the CLT and of one of the uniform pseudo random number generators.

Reminder

For $u_i \sim \mathcal{U}[0,1]$, $\mu = N/2$ and $\sigma^2 = N/12$.

Basics

Gaussian generator

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Reminder

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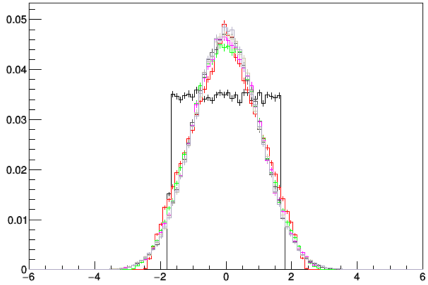

Question

What if f covers different orders of magnitude? or has a divergency? (e.g. $1/x$)

Basics

Importance sampling

Question

What if f covers different orders of magnitude? or has a divergency? (e.g. $1/x$)

Using the general form of LLN

Consider a p.d.f. g such that the x_is populate more the region(s) of interest:

$$I = \int_a^b f(u)\ \mathrm{d}u = \int_a^b \frac{f(x)}{g(x)} g(x)\ \mathrm{d}x = \mathbb{E}\left[\frac{f}{g}\right] \quad (15)$$

$$\Rightarrow I \approx I_{\mathrm{MC}} = \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{g(x_i)} \quad (16)$$

$$\sigma^2_{\mathrm{MC}} = \frac{1}{N^2} \sum_{i=1}^{N} \left(\frac{f(x_i)}{g(x_i)}\right)^2 - \frac{1}{N} I^2_{\mathrm{MC}} \quad (17)$$

Generation of non-uniformly distributed random numbers

Given $u_i \sim \mathcal{U}[0,1]$, the sample x_i are described by the p.d.f. g if:

$$\int_{-\infty}^{x_i} g(x) \, \mathrm{d}x = u_i \int_{-\infty}^{+\infty} g(x) \, \mathrm{d}x \tag{18}$$

Basics

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Exercise #5

- Calculate the following integral (and its uncertainty) using uniformly distributed random numbers (i.e. without importance sampling):

$$\int_{0.0001}^{1} \frac{(1-x)^5}{x}\ \mathrm{d}x \tag{19}$$

- Then, given Eq. 18, show how to draw random numbers with $g(x) \sim \frac{1}{x}$, and repeat this integral with importance sampling.
- Compare with the exact result using the incomplete Beta function.

Basics

Importance sampling

Result from exercise #5

- With linear sampling:

$$N = 10^3: \quad I_{\mathsf{MC}} = 4.85467 \pm 1.23751 \tag{20}$$

$$N = 10^6: \quad I_{\mathsf{MC}} = 6.90493 \pm 0.098539 \tag{21}$$

$$N = 10^9: \quad I_{\mathsf{MC}} = 6.92964 \pm 0.00314253 \tag{22}$$

- To draw random numbers:

$$x_i = x_{\mathsf{min}} \left(\frac{x_{\mathsf{max}}}{x_{\mathsf{min}}} \right)^{u_i} \tag{23}$$

Then with importance sampling:

$$N = 10^5: \quad 6.93396 \pm 0.00992476 \tag{24}$$

- Exact value: 6.92747479226

MC integration

Utilise elements of probability theory to calculate integrals.

MC integration

Utilise elements of probability theory to calculate integrals.

Other methods

- Stratified sampling

$$\int_a^b f(x)\ \mathrm{d}x = \int_a^c f(x)\ \mathrm{d}x + \int_c^b f(x)\ \mathrm{d}x \tag{25}$$

- Subtraction method

$$\int_a^b f(x)\ \mathrm{d}x = \int_a^b g(x)\ \mathrm{d}x + \int_a^b (f(x) - g(x))\ \mathrm{d}x \tag{26}$$

- Hit & Miss (a.k.a. brute force method)
- ...

Application

Application
Introduction

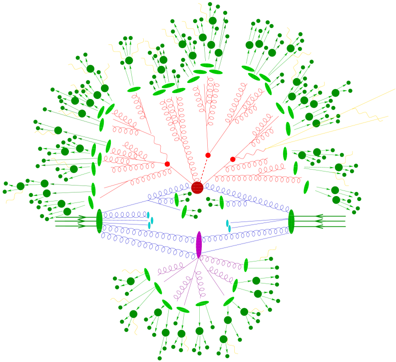
Factorisation

$$\overbrace{\sigma_{pp\to \text{jet}+X}}^{\text{hadronic cross section}} = \sum_{ij\in gq\bar{q}} \overbrace{f_i(x_i,\mu_F^2)\otimes f_j(x_j,\mu_F^2)}^{\text{PDFs}}$$

$$\underbrace{\otimes\, \hat{\sigma}_{ij\to \text{jet}+X}\left(x_i, x_j, \frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2}, \alpha_S(\mu_R^2)\right)}_{\text{partonic cross section}}$$

Phenomenology of MC event generators

interaction = Parton Distribution Function (PDF)
$\otimes$ Matrix Element (ME)
$\otimes$ Parton Shower (PS)
$\otimes$ underlying event (UL)
$\otimes$ hadronisation
$\otimes$ photon radiation



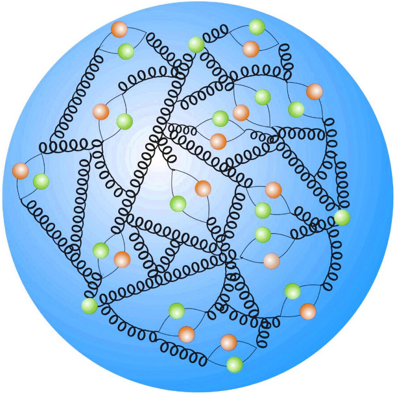
Physics case

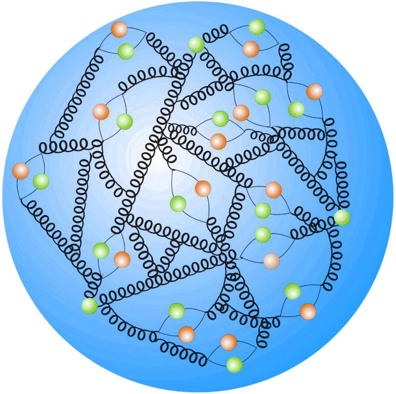
- First, we will try to better understand the PDFs and their evolution:
  - We will assume a simplistic PDF $f(x, t_0 = m_p) = 3\frac{(1-x)^5}{x}$.
  - We will use MC integration to calculate this PDF at harder scales t.
- Then, we will consider $gg \to hX$ and investigate the kinematics of h:
  - First we will neglect the PDF evolution and consider partons directly taken from our simplistic PDF.
  - Then we will combine the PDF evolution for each of the incoming partons and see the impact on the kinematics.

NB: We calculate everything at the lowest order in perturbation theory.

Application

PDF evolution



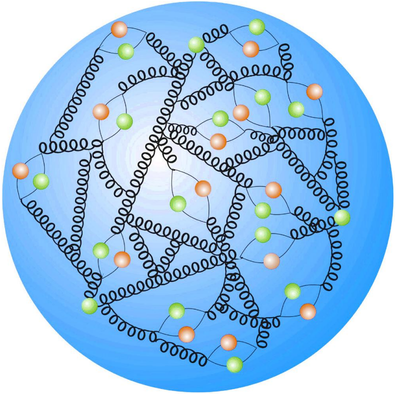


Application

PDF evolution

Nature of PDFs

- Complex objects describing the non-perturbative content of the hadron.
- Also contain a perturbative part, whose (collinear) evolution is described by DGLAP equations.
- Parameterised with a non-physical variable, the scale.
- More-or-less universal, to be constrained with real data.



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DGLAP equations

$$\frac{\mathrm{d} f_a(x,\mu_F^2)}{\mathrm{d}\ln\mu_F^2} = \sum_{b\in\{q,g\}} \int_x^1 \frac{\mathrm{d}z}{z} \frac{\alpha_S(\mu_F^2)}{2\pi} f_b\left(\frac{x}{z},\mu_F^2\right) P_{ba}(z) \quad (27)$$

f_a	PDF for parton $a \in \{q,g\}$	μ_F^2	factorisation scale
x	momentum fraction	α_S	strong coupling (running)
		P_{ba}	splitting function

Application

PDF evolution

Iterative expression

From scale t_0 to scale t:

$$f(x,t) = \underbrace{f(x,t_0)\Delta_s(x,t_0,t)}_{\text{evolution without radiation}} + \underbrace{\int \frac{\mathrm{d}z}{z} \int \frac{\mathrm{d}t'}{t'} \Delta_s(x,t',t) P(z) f\left(\frac{x}{z}, t'\right)}_{\text{parton splitting}} \tag{28}$$

with the Sudakov form factor (probability of non-branching):

$$\Delta_s(x,t_0,t) = \exp\left(-\int_x^{z_\mathrm{M}} \mathrm{d}z \int_{t_0}^{t} \frac{\mathrm{d}t''}{t''} \frac{\alpha_S(t'')}{2\pi} P(z)\right) \tag{29}$$

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PDF evolution

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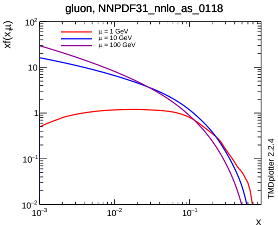


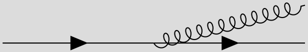
Properties

- Factorisation property is only proven rigorously for a few processes but holds for many others.
- Usually constrained with real data, regularly updated with newer data appearing on the market.

Application
PDF evolution

Splitting functions

$$P_{qq}^{\mathrm{LO}}(z) = \frac{4}{3}\frac{1+z^2}{1-z} \tag{30}$$



$$P_{gq}^{\mathrm{LO}}(z) = \frac{3}{2}\left(z^2 + (1-z)^2\right) \tag{31}$$

$$P_{qg}^{\mathrm{LO}}(z) = \frac{4}{3}\frac{1+(1-z)^2}{z} \tag{32}$$

$$P_{gg}^{\mathrm{LO}}(z) = 3\left(\frac{z}{1-z} + \frac{1-z}{z} + z\,(1-z)\right) \tag{33}$$

Splitting functions

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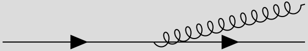

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Exercise #6

Calculate Δ_s to describe the PDF evolution without branching from a starting scale of $t_0 = m_p^2 \approx 1~\mathrm{GeV}^2$ to a scale of $10, 100, 500~\mathrm{GeV}^2$.

- For the integral in Δ_S, use $0.01 < z < 0.99$.
- Consider the running of the strong coupling α_S.
- Try first P_{qq}, then P_{gg}.

Exercise #7

Evolve a PDF $f(x,t_0) = 3\frac{(1-x)^5}{x}$ from a starting scale of $t_0 = m_p^2 \approx 1\ \mathrm{GeV}^2$ to a hard scale of $t = 100\ \mathrm{GeV}^2$ (alternate evolution and branching until the scale is reached).

- Consider $\alpha_S = 0.1$ for simplification.
- To simplify the calculation, you may use $P_{gg}(z) \approx 6\left(\frac{1}{z} + \frac{1}{1-z}\right)$ for the splitting, and only $P_{gg}(z) \approx 6\frac{1}{1-z}$ for Δ_s.
- In addition, the partons start with an intrinsic $k_\mathrm{T} \sim \mathcal{N}(0, 0.7^2)$.

Plot $xf(x)$ and k_T at the starting and hard scales.

Application

Cross section calculation

Exercise #8

Calculate the hadronic cross section of Higgs production via gluon fusion at the lowest order, with the same starting distributions for x and k_{T} as previously, but neglecting the evolution for the moment.

- Assume $\sqrt{s} = 7\ \mathrm{TeV}$.
- Require $120 < m_h < 130\ \mathrm{GeV}$.
- The partonic cross section is given by $\hat{\sigma} = \alpha_S^2 \frac{\sqrt{2}}{\pi} \frac{G_F}{576}$ with $G_F = 1.166 \cdot 10^{-5}\ \mathrm{GeV}^{-1}$.
- The Higgs production follows a Breit-Wigner distribution:

$$P(m) = \frac{1}{2\pi} \frac{\Gamma_h}{(m - m_h)^2 + \Gamma_h^2/4} \tag{34}$$

Plot the kinematics of the partons and of the Higgs $(p_{\mathrm{T}}, \eta, m)$.

Application

Cross section calculation

Exercise #9

Calculate the hadronic cross section of Higgs production via gluon fusion at the lowest order, with the same starting distributions for x and k_T as previously, considering in addition the evolution from a starting scale at the proton mass to a hard scale at the Higgs mass.

- Consider only P_{gg} in the evolution.
- Make the same assumptions as in exercise #8.

Plot the kinematics of the partons at the starting and hard scales, as well as the kinematics of the Higgs (p_T, η, m).

Summary

Summary

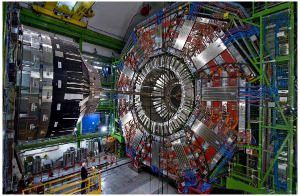
We have

- introduced MC integration;
- applied the basic techniques in purely pedagogical examples;
- then in a more realistic (though simplified) concrete example, based on QCD evolution.

Thank you for your attention!

Back-up

→



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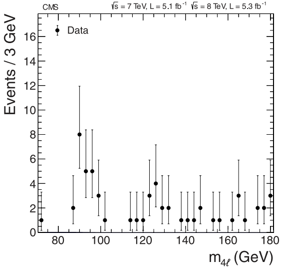
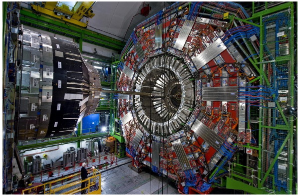
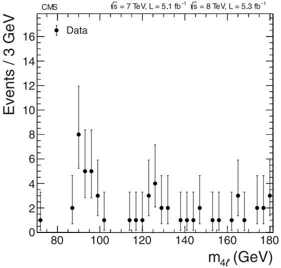

CMS
$\sqrt{s}$ = 7 TeV, L = 5.1 fb^{-1} $\sqrt{s}$ = 8 TeV, L = 5.3 fb^{-1}
Data
Events / 3 GeV
$m_{4\ell}$ (GeV)
0
2
4
6
8
10
12
14
16
80
100
120
140
160
180

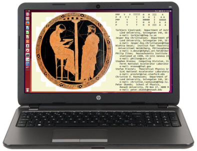
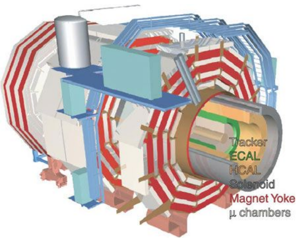
PCD

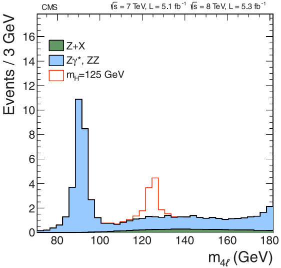
P. Connor

Acronyms

Visiting card

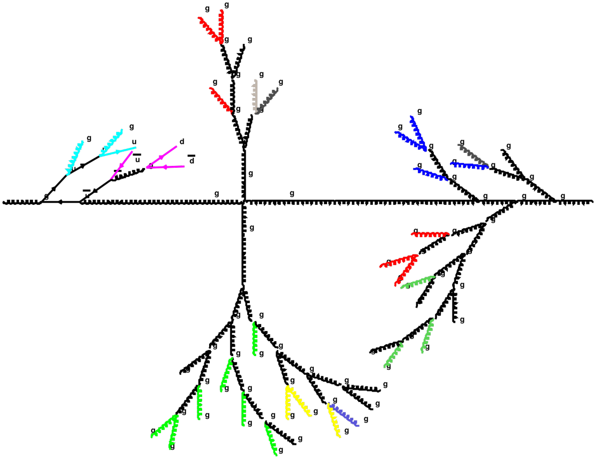
 →  →  → 

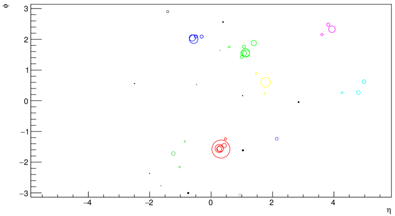
 → 

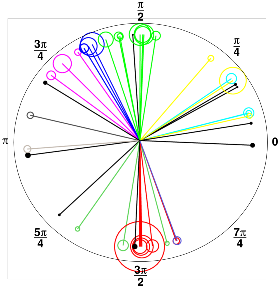
→  → 

Description

Visualisation of parton shower generated by PYTHIA 8 + partons merged by anti-k_T jet algorithm







Acronyms I

CLT Central limit theorem. 21–23

DGLAP after the five physicists Dokshitzer, Gribov, Lipatov, Altarelli and Parisi. 34–36

i.i.d. independent and identically distributed. 21

LLN Law of Large Numbers. 13, 14, 24, 25

MC Monte Carlo. 4, 5, 19, 20, 32, 33, 45

ME Matrix Element. 32

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