# Simulating QCD Jet Production in $e^+e^-$ annihilation

– concepts of Monte Carlo event generators for collider experiments –

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Intro Lecture – part I

07/06/24

# Scope of the project

**Methods & Physics of Monte-Carlo event generators for the simulation of high-energy scattering events**

## Particle Physics at High-Energy Colliders

- investigate nature of short-range phenomena by scattering experiments
- bring high-energetic particle beams to collision, e.g. $e^+e^-$, $ep$, or $pp$
- measure & analyse the resulting final states

$\leadsto$ experimental challenge: identify & measure all particles emerging from individual beam clashes, reconstruct energies & momenta, specific detector components for $\gamma$, $e^\pm$, $\mu^\pm$, $n$, $p$, ..., $\not{E}_T$

$\leadsto$ theoretical challenge: confront measurements with hypotheses for the underlying physics

# The HEP trinity

**Theory**

**QFT in Lagrangian formulation**
of quantum nature, non-deterministic
**benchmark Standard Model $\mathcal{L}_{\mathrm{SM}}$**
hypothetical New Physics $\mathcal{L}_{\mathrm{BSM}}$

**Experiment**

**complex multi-component detector**
ATLAS, CMS, LHCb, ...
**reconstruction of individual events**
degrading, upgrades, improvements

**Simulation: linking theory & experiment**

**multi-purpose Monte Carlo generators**

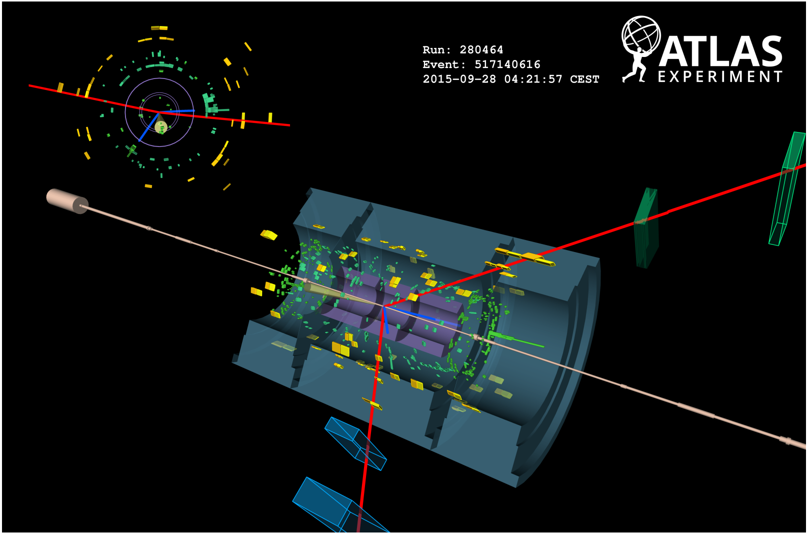
- stochastic simulation of particle-level events
- Herwig, Pythia, Sherpa, ...

**detector simulation codes**

- detailed models for all detector components
- Geant4 based, Neural Network approaches, ...

**provide fully-simulated event samples**

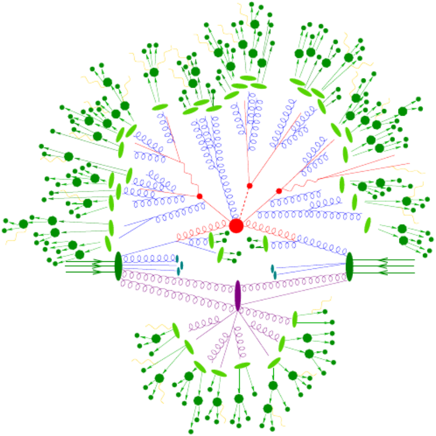
# Particle detectors & Real collider data




ATLAS event display: $pp \to H \to ZZ^* \to 2e2\mu + X$ event

# Monte Carlo Event Generators: the global picture

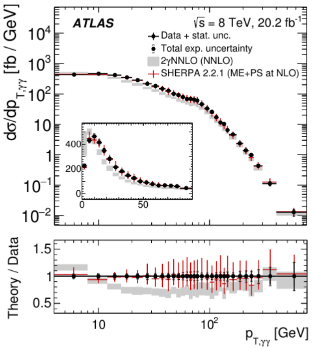
- perturbative methods
  - **Hard interaction**
    exact matrix elements $|\mathcal{M}|^2$
    LO,NLO,NNLO – QCD, NLO – EW
  - **Radiative corrections**
    parton showers in the initial and final state
    resummation of soft-collinear logs: LL, NLL
- non-perturbative models
  - **Multiple Interactions**
    beyond factorization: modelling
  - **Hadronization**
    parton–hadron transition
  - **Hadron Decays**
    phase space or effective theories



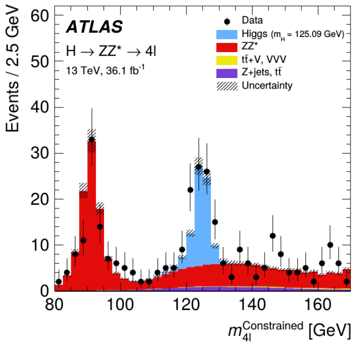
$\hookrightarrow$ predict fully exclusive final states
$\hookrightarrow$ factorize short & long range physics
$\hookrightarrow$ subject to approximations/compromises
$\hookrightarrow$ variety of specialized methods & tools

# Real-world LHC applications

**Di-Photon production**




**Higgs-Boson production**

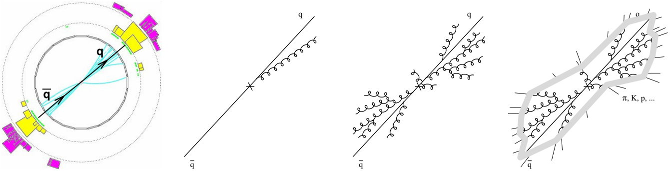



- confronting experiment with Standard Model theory predictions
- precision Standard Model measurements and searches for New Physics

# Outline of the project

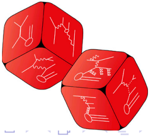
## physics issues related to the modelling of high-energy collisions

- **Part I:** hard process generation, here $e^+e^- \to q\bar{q}$ at lowest order
  - integrate cross section for $e^+e^- \to q\bar{q}$
  - generate corresponding scattering events fully differentially
- **Part II:** final-state parton showering, *i.e.* soft- & collinear gluon emissions
  - simulate $q\bar{q}$-initiated final-state parton cascade
  - analyse QCD jet observables, compare to reference data

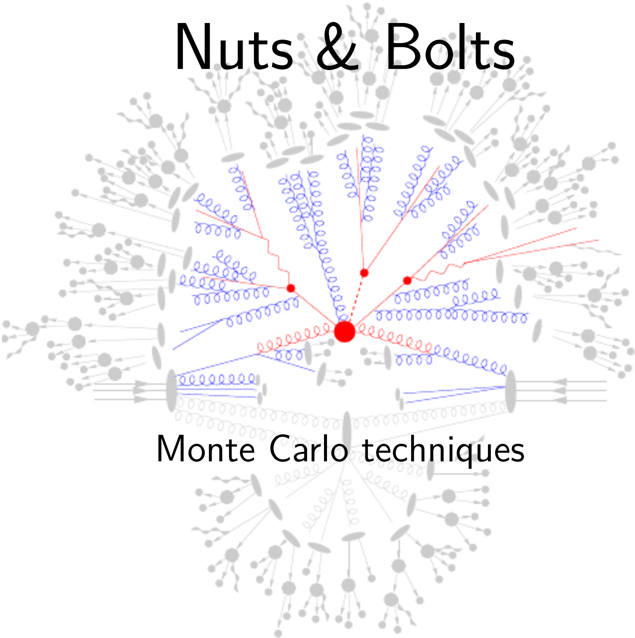



## aspects of numerical methods/solutions used to tackle these

- Monte Carlo Importance Sampling
- Markov Chain parton-branching simulation
- sequential jet reconstruction algorithms



# Nuts & Bolts



Monte Carlo techniques

# Monte-Carlo techniques

## "Spatial" problems: without memory

- What is the volume of a given body?

  Pick a point at random, use uniform probability in this area.
- What is the integrated cross section of a given process?

  Pick an event at random, according to the differential cross section.

## "Temporal" problems: have memory

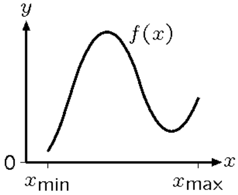
- Financial systems: What is the probability for a stock to have price $X$ at time $t$, given the price $Y$ at $t_0$?
- Parton shower: What is the probability for a parton to branch at a scale $Q$, given that it was created at a scale $Q_0$?

## In particle physics often combined problems

What is the probability for a parton to branch at $Q$, with the daughters sharing the mother momentum in some specific way?

# Monte-Carlo techniques: “Spatial” problems

Assume function $f(x)$ in range $x_{\mathrm{min}} \leq x \leq x_{\mathrm{max}}$,
where $f(x) \geq 0$ everywhere
(in practise $x$ is multi-dimensional)




## Two standard tasks

1. Calculate definite integral (approximatively)

$$I = \int_{x_{\mathrm{min}}}^{x_{\mathrm{max}}} f(x')dx' = (x_{\mathrm{max}} - x_{\mathrm{min}})\langle f(x) \rangle$$

random points $\in [x_{\mathrm{min}}, x_{\mathrm{max}}]$

$$\simeq I_N = (x_{\mathrm{max}} - x_{\mathrm{min}}) \frac{1}{N} \sum_{i=1}^{N} f(x_i) \pm (x_{\mathrm{max}} - x_{\mathrm{min}}) \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}}$$

$\rightsquigarrow$ error scales with $1/\sqrt{N}$, independent of $d$

$\rightsquigarrow$ estimate improves by adding single point to the current estimate

2. Select $x$ at random according to $f(x)$

# Monte-Carlo techniques: Basics

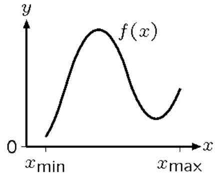
## Select $x$ according to $f(x)$

as $P(x) \sim f(x) = \int\limits_0^{f(x)} dy$

equivalent to uniform selection of $(x, y)$ in area

$x_{\min} \le x \le x_{\max}$ & $0 \le y \le f(x)$

$\rightsquigarrow \int\limits_{x_{\min}}^{x} f(x')dx' = \# \int\limits_{x_{\min}}^{x_{\max}} f(x')dx'$

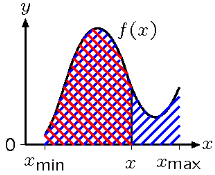



## Analytical solution: inverse transform

known primitive function $F(x)$ and inverse $F^{-1}$

$F(x) - F(x_{\min}) = \#(F(x_{\max}) - F(x_{\min})) = \#A_{\text{tot}}$

$\rightsquigarrow x = F^{-1}(F(x_{\min}) + \#A_{\text{tot}})$




## Example: $f(x) = e^{-x}$ for $x \ge 0$

$F(x) = 1 - e^{-x}$

$1 - e^{-x} = \#1 \rightsquigarrow x = -\ln(\#)$

# Monte-Carlo techniques: Variance Reduction

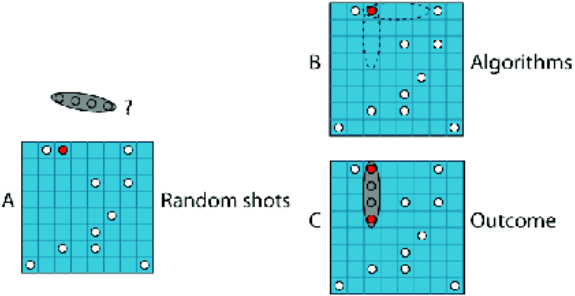
## Variance reduction techniques: Motivation

- MC error estimate scales as $1/\sqrt{N}$, independent of dimension
- second limiting factor, the intrinsic variance of the integrand, i.e. $V_N$

  $\rightsquigarrow$ devise techniques to reduce variance, thus enhancing MC convergence: **stratified sampling, control variates, importance sampling**

## Example: Battleships

Use of (cleverly chosen) random points.



# Monte-Carlo techniques: Variance Reduction

## Importance Sampling

- large variation of $f(x)$ leads to large uncertainty on MC estimate
- MC most efficient when each point $x_i$ has nearly same weight $f(x_i)$
- arrange by choosing large number of points where function is largest
- compensate for overpopulation by reducing function value accordingly
- mathematically, IS corresponds to change of integration variable

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

with $g(x) = \frac{dG}{dx} = \frac{\partial^d}{\partial x_1 \ldots \partial x_d} G(x)$

$\rightsquigarrow$ points chosen according to $G(x)$ instead of uniformly

$\rightsquigarrow$ $f$ weighted inversely by $g(x) = dG/dx$

$\rightsquigarrow$ relevant variance is $V(f/g)$, small if $g(x)$ & $f(x)$ similar in shape

# Monte-Carlo techniques: Variance Reduction

## Importance Sampling cont'd

**conditions on the mapping function $g(x)$**

(i) $g(x)$ is probability density: $g(x) \geq 0$ and $\int g(x')dx' = 1$

(ii) $G(x)$, the integral of $g(x)$, is known analytically
(integrated distribution, increasing monotonically with $x$)

(iii) either function $G(x)$ can be inverted (solved) for $x$ analytically or, alternatively, a $g$-distributed random-number generator is available

(iv) the ratio $f(x)/g(x)$ is ideally nearly constant
$\leadsto$ variance $V(f/g)$ will be small compared to $V(f)$

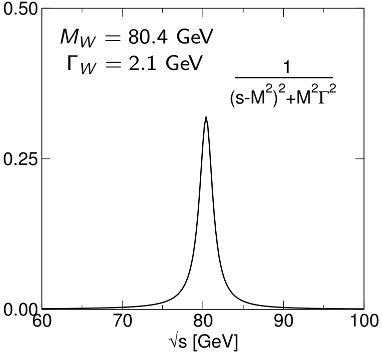
$$E_N = \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{g(x_i)}\,, \qquad V_N\left(\frac{f}{g}\right) = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{f(x_i)}{g(x_i)}\right)^2 - E_N^2$$

## Importance Sampling: disadvantages

dangerous if function $g(x)$ approaches zero where $f$ is non-vanishing, then $V(f/g)$ becomes infinite and usual techniques to estimate the variance from sample points may not detect this, if region of $g = 0$ is small

## Breit–Wigner propagator – particle with mass $M$ and decay width $\Gamma$

$$\boxed{I = \int_{s_{\min}}^{s_{\max}} \frac{\mathrm{d}s}{(s-M^2)^2 + M^2\Gamma^2}}$$




use mapping (variable transform)

$$\begin{aligned} s &= M\Gamma \tan\rho + M^2 \\ \rightsquigarrow \mathrm{d}s &= M\Gamma \sec^2\rho \, \mathrm{d}\rho \end{aligned}$$

such that

$$\begin{aligned} I &= \int_{\rho_{\min}}^{\rho_{\max}} \frac{M\Gamma \sec^2\rho \, \mathrm{d}\rho}{M^2\Gamma^2 \tan^2\rho + M^2\Gamma^2} \\ &= \frac{1}{M\Gamma} \int_{\rho_{\min}}^{\rho_{\max}} \mathrm{d}\rho \quad \rightsquigarrow \quad \delta I = 0 \end{aligned}$$

$\rightsquigarrow$ pick $\rho$ uniformly from

$$\begin{aligned} \rho &= \rho_{\min} + \#(\rho_{\max} - \rho_{\min}) \\ \rho_{\min/\max} &= \arctan\left(\frac{s_{\min/\max} - M^2}{M\Gamma}\right) \end{aligned}$$

# Monte-Carlo techniques: Hit-or-Miss method

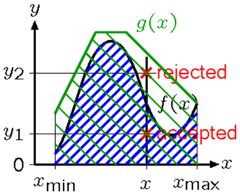
## Sampling according to $f(x)$

known $g(x)$ as local overestimate for target $f(x)$:

$g(x) \geq f(x)$ in $x_{\mathrm{min}} \leq x \leq x_{\mathrm{max}}$

and $G(x) = \int_{\mathrm{x_{min}}}^{x} g(x')dx'$ & $G^{-1}(y)$ are simple

1. select $x =$ according to distribution $g(x)$
2. select $y = \#g(x)$
3. if $y \leq f(x)$ accept point $[N_{\mathrm{acc}}{++},\ N_{\mathrm{try}}{++}]$
   if $y > f(x)$ reject point $[N_{\mathrm{fail}}{++},\ N_{\mathrm{try}}{++}]$



# Monte-Carlo techniques: Hit-or-Miss method

**Example: $f(x) = xe^{-x}$ and $g(x) = Ne^{-x/2}$**

ensure that $g(x)$ is local overestimate:

$$\frac{f(x)}{g(x)} = \frac{xe^{-x/2}}{N} \overset{!}{\leq} 1 \to \text{find maximum}$$

$$\frac{d}{dx}\left(\frac{f(x)}{g(x)}\right) = \frac{1}{N}\left(1 - \frac{x}{2}\right) e^{-x/2} \overset{!}{=} 0 \rightsquigarrow x = 2$$

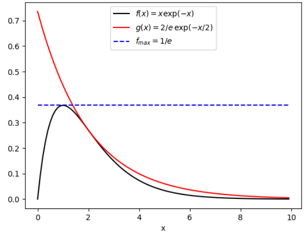
normalize such that $g(2) = f(2) \rightsquigarrow N = 2/e$

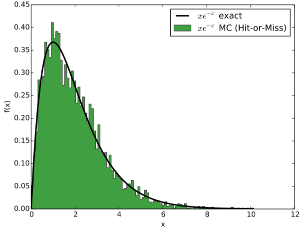
from $G(x) \sim 1 - e^{-x/2} = \#_1$

$\rightsquigarrow x = -2\ln(\#_1),\ y = \#_2 g(x) = \#_2 2e^{-(1+x/2)}$

$\rightsquigarrow$ efficiency IS: $N_{\mathrm{acc}}/N_{\mathrm{try}} = 68.4\%$

$\rightsquigarrow$ efficiency $f_{\mathrm{max}} = e^{-1}$: $N_{\mathrm{acc}}/N_{\mathrm{try}} = 13.5\%$



# Monte-Carlo techniques: “Temporal” Problems

## The radioactive decay problem

- known probability $f(t) \geq 0$ that *something will happen* at time $t$
  [nucleus decays, parton branches, transistor fails]
- *something happens* at $t$ **only** if it didn’t happen at $t' < t$

# Monte-Carlo techniques: "Temporal" Problems

## The radioactive decay problem

- known probability $f(t) \geq 0$ that *something will happen* at time $t$

  [nucleus decays, parton branches, transistor fails]
- *something happens* at $t$ **only** if it didn't happen at $t' < t$

Define: $N(t)$: probability that *nothing* happend until $t$ $[N(0) = 1]$

$P(t) = -dN(t)/dt = f(t)N(t)$: probability for decay at time $t$

# Monte-Carlo techniques: "Temporal" Problems

**The radioactive decay problem**

- known probability $f(t) \geq 0$ that *something will happen* at time $t$
  [nucleus decays, parton branches, transistor fails]
- *something happens* at $t$ **only** if it didn't happen at $t' < t$

Define: $N(t)$: probability that *nothing* happend until $t$ [$N(0) = 1$]

$$P(t) = -dN(t)/dt = f(t)N(t): \text{ probability for decay at time } t$$

Solution:

$$\begin{aligned} N(t) &= \exp\left\{-\int_0^t f(t')dt'\right\} \qquad [f(t) = \lambda \text{ simple radioactive decay}] \\ P(t) &= f(t)\exp\left\{-\int_0^t f(t')dt'\right\} \end{aligned}$$

- naïve answer $P(t) = f(t)$ modified by exponential suppression
  [$P(t) \approx f(t)$ at small $t$ only, otherwise damping]
- in parton-shower picture, $N(t)$ is called the Sudakov form factor

# Monte-Carlo techniques: "Temporal" Problems

## The radioactive decay problem: solution

- assume $f(t)$ has primitive function $F(t)$ with known inverse $F^{-1}$
- standard solution to find "decay" time $t$:

$$\int\limits_0^t P(t')dt' = N(0) - N(t) = 1 - \exp\{-(F(t) - F(0))\} = 1 - \#$$

$$\exp\{-(F(t) - F(0))\} = \#$$

$$\rightsquigarrow \quad t = F^{-1}(F(0) - \ln(\#))$$

- simple radioactive decay, i.e. $f(t) = \lambda$

$$F(t) = \lambda t = -\ln(\#) \quad \rightsquigarrow \quad t = -\ln(\#)/\lambda$$

- if $f(t)$ not sufficiently "nice", use importance sampling & Hit-or-Miss
- however, simple condition $f(t) \leq g(t) \;\; \forall \;\; t \geq 0$ is not sufficient

$$\rightsquigarrow \quad \hat{P}(t) = g(t)\exp\left\{-\int\limits_0^t g(t')dt'\right\}$$

$\rightsquigarrow$ does not yield proper exponential factor

# Monte-Carlo techniques: “Temporal” Problems

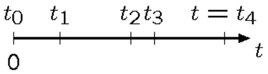
## The Veto Algorithm [Seymour 1995]

if $f(t)$ has no simple $F(t)$ or $F^{-1}$: use “nice” $g(t) \geq f(t)$

1. start with $i = 0$ and $t_0 = 0$
2. increment $i$ and select $t_i = G^{-1}(G(t_{i-1}) - \ln(\#_1))$
   [according to $g(t)$, but with constraint $t_i > t_{i-1}$]
3. if $f(t_i)/g(t_i) \leq \#_2$ go back to step 2
   otherwise, keep $t_i$ as “decay” time

$\rightsquigarrow$ next step only depends on the very previous one

$\rightsquigarrow$ Markovian process



# Monte-Carlo techniques: The Veto Algorithm

## Iterative Proof

**consider the various ways in which a specific time $t$ can be selected**

- probability that first try is accepted, i.e. $t = t_1$, such that no intermediate $t$ values need to be rejected

$$P_0^g(t) \;=\; \underbrace{\exp\left\{-\int_0^t g(t')dt'\right\} g(t)}_{P^g(t)} \;\times\; \underbrace{\frac{f(t)}{g(t)}}_{\text{prob. to accept } t}$$

- consider case, where one intermediate step, $t_1$, got rejected, only second step, $t = t_2$, is accepted, i.e. $0 \le t_1 \le t_2 = t$

$$P_1^g(t) = \underbrace{\int_0^t \exp\left\{-\int_0^{t_1} g(t')dt'\right\} g(t_1)}_{\text{prob. to select } t_1 \,<\, t} \underbrace{\left(1 - \frac{f(t_1)}{g(t_1)}\right)}_{\text{prob. to reject } t_1} \underbrace{\times \exp\left\{-\int_{t_1}^t g(t'')dt''\right\} g(t)\frac{f(t)}{g(t)}}_{\text{prob. to select \& accept } t \,=\, t_2 \,>\, t_1} dt_1$$

$$\leadsto \quad P_1^g(t) = P_0^g(t)\int_0^t \left(g(t_1) - f(t_1)\right) dt_1$$

# Monte-Carlo techniques: The Veto Algorithm

## Iterative Proof cont'd

- considering arbitrary intermediate steps the probability to accept $t$ yields

$$
\begin{aligned}
P^g(t) &= \sum_{i=0}^{\infty} P_i^g(t) \\
&= P_0^g(t) \sum_{i=0}^{\infty} \frac{1}{i!} \left( \int_0^t \left(g(t') - f(t')\right) dt' \right)^i \\
&= f(t) \exp\left\{ - \int_0^t g(t') dt' \right\} \exp\left\{ \int_0^t \left(g(t') - f(t')\right) dt' \right\} \\
&= f(t) \exp\left\{ - \int_0^t f(t') dt' \right\} \\
&= P(t) \quad \text{q.e.d.}
\end{aligned}
$$

# Monte-Carlo techniques: The Veto Algorithm

## Discussion

- Veto Algorithm standard tool in event generation, e.g. QCD parton showers
- numerical implementation of true Markovian decay/emission process
- process can be stopped at any intermediate scale/time $t_{\max}$
- usually $f(t)$ function of additional variables $x$, however, easy to generalise
  - find suitable $g(t,x)$ with $f(t,x) \leq g(t,x)$, the $g(t)$ used in the veto algorithm is then simply given by the integral

$$g(t) = \int g(t,x')dx'$$

  - each time a value $t_i$ is selected also the $x_i$ need to be picked, following density $g(t_i,x)dx$
  - the point $(t_i,x_i)$ gets accepted with probability $f(t_i,x_i)/g(t_i,x_i)$

# Monte-Carlo techniques

## Summary

- use Monte Carlo methods to perform integrals and sample distributions
  - need only few points to estimate $\int f(x')dx'$
  - each additional point increases accuracy
- techniques generalise to many dimensions
  - typical LHC phase space $\sim d^3\vec{p} \times 100$'s particles
  - error scales as $1/\sqrt{N}$ vs. $1/N^{2/d}$ or $1/N^{4/d}$ (Trapezoidal or Simpson's Rule)
- suitable for complicated integration regions
  - kinematic cuts or detector cracks
- can sample distributions where exact solutions cannot be found
- use of adaptive techniques to reduce variances
- Veto Algorithm applicable for parton-shower simulations

# Questions/Self-Tests

- Implement the above discussed variance reduction example, *i.e.* $f(x) = xe^{-x}$ with $g(x) = 2e^{(-1+x/2)}$
- How to sample points $x \in [\epsilon, 1-\epsilon]$ according to $f(x) = \frac{(1-x)}{x}$?
- Plot the Breit–Wigner distribution for the SM Higgs-boson propagator ($M_H = 125.1$ GeV, $\Gamma_H = 4.2$ MeV)
- Repeat the proof of the Veto Algorithm, see also backup

# Literature/Further Reading

- Buckley et al. "General-purpose event generators for LHC physics"
  Phys. Rept. **504** (2011), 145-233
  arXiv:1101.2599 [hep-ph]

- Salam "Elements of QCD for hadron colliders"
  CERN Yellow Rep. School Proc. **5** (2020), 1-56
  arXiv:1011.5131 [hep-ph]

- Ellis, Stirling, Webber "QCD and collider physics"
  Camb. Monogr. Part. Phys. Nucl. Phys. Cosmol. **8** (1996), 1-435

# Backup slides

## Breit–Wigner propagator – Jacobian

consider $\displaystyle\int_{s_{\min}}^{s_{\max}} ds\, f(s) \rightarrow \int_0^1 d\# \frac{1}{g_{\text{prop}}(s(\#))} f(s(\#))$

1. Breit–Wigner mapping

$$\int_{s_{\min}}^{s_{\max}} ds = \int_{\rho_{\min}}^{\rho_{\max}} M\Gamma \sec^2\rho\, d\rho$$

$$\text{with} \quad \rho(\#) = \rho_{\min} + \#(\rho_{\max} - \rho_{\min})$$

$$\frac{d\rho}{d\#} = \rho_{\max} - \rho_{\min}$$

$$\int_{s_{\min}}^{s_{\max}} ds = \int_0^1 d\# \frac{(s_\# - M^2)^2 + M^2\Gamma^2}{M\Gamma}(\rho_{\max} - \rho_{\min})$$

$$\text{where} \quad s_\# = s(\rho(\#)) = M\Gamma \tan(\rho(\#)) + M^2$$

# Monte-Carlo techniques: The Veto Algorithm

## Iterative Proof cont'd

- for $P_2^g(t)$ need to consider two intermediate times, i.e. $0 \leq t_1 \leq t_2 \leq t_3 = t$

$$
\begin{aligned}
P_2^g(t) &= P_0^g(t) \underbrace{\int_0^t dt_1 \,(g(t_1) - f(t_1)) \int_{t_1}^t dt_2 \,(g(t_2) - f(t_2))}_{\text{nested integrals}} \\
&= P_0^g(t) \frac{1}{2} \left( \int_0^t \left(g(t') - f(t)'\right) dt' \right)^2
\end{aligned}
$$

# Monte-Carlo techniques: The Veto Algorithm

## Iterative Proof cont'd

- for $P_2^g(t)$ need to consider two intermediate times, i.e. $0 \leq t_1 \leq t_2 \leq t_3 = t$

$$
\begin{aligned}
P_2^g(t) &= P_0^g(t) \underbrace{\int_0^t dt_1 \left(g(t_1) - f(t_1)\right) \int_{t_1}^t dt_2 \left(g(t_2) - f(t_2)\right)}_{\text{nested integrals}} \\
&= P_0^g(t) \frac{1}{2} \left( \int_0^t \left(g(t') - f(t)'\right) dt' \right)^2
\end{aligned}
$$

## Proof – nested integrals

to prove the last equality consider inclusion of the region where $t_2 < t_1$

$$
\int_0^t dt_1 \left(g(t_1) - f(t_1)\right) \int_{t_1}^t dt_2 \left(g(t_2) - f(t_2)\right) + \int_0^t dt_2 \left(g(t_2) - f(t_2)\right) \int_{t_2}^t dt_1 \left(g(t_1) - f(t_1)\right)
$$

$$
= \int_0^t dt' \left(g(t') - f(t')\right) \left[ 2 \int_{t'}^t dt'' \left(g(t'') - f(t'')\right) \right] = \left( \int_0^t dt' \left(g(t') - f(t')\right) \right)^2
$$

# Monte-Carlo techniques: The Veto Algorithm

## Iterative Proof cont'd

- for $P_2^g(t)$ need to consider two intermediate times, i.e. $0 \leq t_1 \leq t_2 \leq t_3 = t$

$$P_2^g(t) = P_0^g(t) \underbrace{\int_0^t dt_1 \left(g(t_1) - f(t_1)\right) \int_{t_1}^t dt_2 \left(g(t_2) - f(t_2)\right)}_{\text{nested integrals}}$$

$$= P_0^g(t) \frac{1}{2} \left( \int_0^t \left(g(t') - f(t)'\right) dt' \right)^2$$

## Proof – nested integrals

generalisation to $n$ factors

$$\frac{1}{n!} \int_0^t \left( \int_{t''}^t f(t') dt' \right)^n f(t'') dt'' = \frac{1}{(n+1)!} \left( \int_0^t f(t) dt \right)^{n+1}$$