Monte Carlo Methods in High Energy Physics

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Lecture 4: Markovian Monte Carlo.

- **Motivation.**
- **Basics of Markov chains.**
- **One-dimensional Markovian Monte Carlo algorithm.**
- **Non-singlet structure function evolution.**
- **Multicomponent Markovian algorithm.**

$\Longrightarrow$ http://cern.ch/placzek

Motivation

- In HEP there are some problems which can be formulated in terms of integral or differential-integral equations (or systems of such equations).
- A well-known problem of this type is QCD evolution of parton distributions inside a proton which can be described by the Gribov-Lipatov-Altarelli-Parisi (GLAP) equations.
- Although there exist various numerical-analysis methods for solving such equations, using Monte Carlo techniques has certain advantages: it allows not only for solving the equations but also for generating events in terms of particle flavours and four-momenta, which is particularly useful for experimental applications.
- Monte Carlo algorithms for solving the GLAP equations are based on simulating Markov chains (random walks).
- Particularly useful are the so-called parton-shower algorithms which are the basis of popular Monte Carlo event generators for the QCD processes, such as PYTHIA, HERWIG, etc.

Basics of Markov chains

Let a system have a finite or countable set of possible states $S_1, S_2, \ldots$, and X_t be the state that it is at time t. Let's consider discrete times labelled consicutively with $1, 2, \ldots$.

▷ X_t is a random variable and we may define the conditional probabilities:

$$\mathcal{P}(X_t = S_j | X_{t_1} = S_{i_1}, X_{t_2} = S_{i_2}, \ldots , X_{t_n} = S_{i_n}).$$

► The system is a **Markov chain** if the distribution of X_t is independent of all previous states except for its immediate predecessor X_{t-1}, i.e.

$$\mathcal{P}(X_t = S_j | X_{t-1} = S_{i_{t-1}}, \ldots , X_2 = S_{i_2}, X_1 = S_{i_1}) = \mathcal{P}(X_t = S_j | X_{t-1} = S_{i_{t-1}}).$$

▷ This can easily be extented to system with continuous states by replacing probabilities with density functions.

- **Examples of Markov chains (random walks):**

  Brownian motions, diffusion in gases, "a walk of a drunk sailor", etc.

▷ Mathematically, Monte Carlo methods based on Markov chains can be applied to solving systems of linear equations, integral equations, partial differential equations, eigenvalue problems, computing the inverse matrix, etc.

One-dimensional Markovian MC algorithm

1-dimensional forward Markovian walk

▶ Let the probability of a single **forward Markovian step** be given by:

$$p(t|t_n) = \phi(t)\Theta(t-t_n)\exp\left(-\int_{t_n}^{t}\phi(t')dt'\right),$$
$$\int_{tn}^{\infty} p(t|t_n)dt = 1, \qquad p(t|0) \equiv p(t).$$

▷ Changing the evolution variable $t \longrightarrow T(t)$:

$$T(t) = \Phi(t) = \int_0^t \phi(t)dt, \qquad \phi(t) = \frac{d\Phi(t)}{dt},$$

simplifies greatly the transition probability:

$$P(T|T_n) = \Theta(T-T_n)\exp(T_n - T), \qquad \int_{T_n}^{\infty} P(T|T_n)\,dT = 1.$$

NB. The above is ”the old Monte Carlo recipe” for the *Poissonian distribution*.

1-dimensional Markovian algorithm step-by-step

$[\mathbf{1}]$ Generate t_1 according to $p(t_1) = p(t_1|t_0 = 0)$

(a) $t_1 > t_{\max}$: $P_0 = \int_{t_{\max}}^{\infty} p(t_1|t_0) = e^{-T_{\max}}$; **Retain** $N = 0$; **Trash** t_1. **EXIT**.

(b) $t_1 < t_{\max}$: $P_{N\geq 1} = \int_0^{t_{\max}} dt_1\, p(t_1|t_0)$. **Retain** t_1. **Go to** $[\mathbf{2}]$

$[\mathbf{2}]$ Generate t_2 according to $p(t_2|t_1)$

(a) $t_2 > t_{\max}$: $P_1 = \int_{t_{\max}}^{\infty} p(t_2|t_1)$. **Retain** $N = 1$, t_1; **Trash** t_2. **EXIT**.

(b) $t_2 < t_{\max}$: $P_{N\geq 2} = \int_{t_1}^{t_{\max}} dt_2\, p(t_2|t_1)$. **Retain** (t_1, t_2). **Go to** $[\mathbf{3}]$.

$\ldots$

$[\mathbf{n+1}]$ Generate t_{n+1} according to $p(t_{n+1}|t_n)$.

(a) $t_{n+1} > t_{\max}$: $P_{N\geq n+1} = \int_{t_{n+1}}^{t_{\max}} dt_{n+1}\, p(t_{n+1}|t_n)$.

Retain $N = n$, $(t_0, t_1, \ldots, t_n)$; **Trash** t_{n+1}. **EXIT**.

(b) $t_{n+1} < t_{\max}$: $P_{N\geq n+1} = \int_{t_{n+1}}^{t_{\max}} dt_{n+1}\, p(t_{n+1}|t_n)$.

Retain t_{n+1} and **Go to** $[\mathbf{n+2}]$.

$[\mathbf{n+2}]$ ... ... and so on until a successful **EXIT**.

$$P_N = \int_0^{t_{\max}} dt_1 p(t_1|t_0) \int_{t_1}^{t_{\max}} dt_2 p(t_2|t_1) \ldots \int_{t_{n-1}}^{t_{\max}} dt_n p(t_N|t_{N-1}) \int_{t_{\max}}^{\infty} dt_{N+1} p(t_{N+1}|t_N),$$

$$= \frac{1}{N!} (T_{\max})^N e^{-T_{\max}} \quad \leftarrow \textit{Poissonian distribution} \;\; P(T_{\max})$$

The 1-dimensional Markovian algorithm

▶ The fully differential distribution:

$$p_N(t_1,t_2,\ldots,t_N) = e^{-\int_0^{t_{\max}}\phi(t)dt}\Theta(t_{\max}-t_N)\prod_{n=1}^{N}\phi(t_n)\,\Theta(t_n-t_{n-1}),$$

$$P_N(T_1,T_2,\ldots,T_N) = e^{-T_{\max}}\,\Theta(T_{\max}-T_N)\prod_{n=1}^{N}\Theta(T_n-T_{n-1}).$$

is easily extracted from the integral:

$$P_N = e^{-T_{\max}}\int_0^{T_{\max}} dT_1 \int_{T_1}^{T_{\max}} dT_2 \cdots \int_{T_{N-1}}^{T_{\max}} dT_N$$
$$= e^{-\int_0^{t_{\max}}\phi(t)dt}\int_0^{t_{\max}}\phi(t_1)dt_1\int_{t_1}^{t_{\max}}\phi(t_2)dt_2\cdots\int_{t_{N-1}}^{t_{\max}}\phi(t_N)dt_N\,.$$

▷ One could generate randomly N according to P_N, and $(t_1,t_2,\ldots,t_N)$ according to $p_N(t_1,t_2,\ldots,t_N)$ without the use of the Markovian algorithm.

$\Rightarrow$ However, Markovian has some advantages, both for physics and Monte Carlo.

Non-singlet structure function evolution

A $\mathbf{2}$-dimensional Markovian process for the QED/QCD structure function evolution can be derived from the non-singlet GLAP evolution equation:

$$\frac{\partial}{\partial \ln Q} D(x,Q) = \int_x^1 \frac{dz}{z} P(z) \frac{\alpha(Q,z)}{\pi} D(x/z,Q),$$

where $P(z)$ is the Altarelli-Parisi splitting function, usually regulated with some IR regulator $\epsilon \ll 1$:

$$\begin{aligned} P(z) &= C_F \left[\frac{1+z^2}{(1-z)_+} + \frac{3}{2}\delta(1-z) \right] \\ &= C_F \left[\frac{1+z^2}{1-z}\Theta(1-z-\epsilon) + \delta(1-z)\left(\frac{3}{2} + 2\ln\epsilon\right) \right] . \end{aligned}$$

► In a more compact notation the evolution equation reads:

$$\frac{\partial}{\partial \ln Q} D(x,Q) = \frac{\alpha(Q,\cdot)}{\pi} P(\cdot) \otimes D(\cdot,Q)(x),$$

where

$$f_1(\cdot) \otimes f_2(\cdot)(z) = \int dz_1 dz_2 \delta(z - z_1 z_2) f_1(z_1) f_2(z_2) \,,$$

$$f_1(\cdot) \otimes f_2(\cdot) \otimes \cdots \otimes f_n(\cdot)(z) = \int dz_1 dz_2 \ldots dz_n \delta(z - z_1 z_2 \ldots z_n) f_1(z_1) f_2(z_2) \ldots f_n(z_n).$$

Integral representation

Introducing the following notation:

$$t = \ln Q, \quad \phi(t) = \int_0^1 dz\, \frac{\alpha(Q,z)}{\pi}\, P_\epsilon(z), \quad \Phi(t) = \int_{t_0}^{t} \phi(t')dt'\,,$$

where

$$P_\epsilon(z) = \frac{1+z^2}{1-z}\,\Theta(1-\epsilon-z)\,,$$

we get

$$\frac{\partial}{\partial t} D(x,t) + D(x,t)\frac{\partial\Phi(t)}{\partial t} = \frac{\alpha(t,\cdot)}{\pi} P_\epsilon(\cdot) \otimes D(\cdot,t)(x).$$

Substituting

$$D(x,t) = \bar{D}(x,t)e^{-\Phi(t)}$$

we eliminate the non-homogenous term $\partial\Phi(t)/\partial t$ and turn to the integral representation

$$\bar{D}(x,t) = \bar{D}(x,t_0) + \int_{t_0}^{t} dt_1 \frac{\alpha(t_1)}{\pi} P_\epsilon(\cdot) \otimes \bar{D}(\cdot,t_1)(x),$$

which can be solved iteratively.

▷ We have now the explicit Sudakov exponential formfactor for a given IR cut-off ϵ!

Iterative solution

- An iterative solution to the integral evolution equation can be expressed in terms of a series of $\mathbf{2n}$-dimensional integrals:

$$
\begin{aligned}
\bar{D}(x,t) &= \bar{D}(x,t_0) \\
&+ \int_{t_0}^{t} dt_1 \frac{\alpha(t_1)}{\pi} P_\epsilon(\cdot) \otimes \bar{D}(\cdot,t_0)(x) \\
&+ \int_{t_0}^{t} dt_1 \frac{\alpha(t_1)}{\pi} P_\epsilon(\cdot) \otimes \int_{t_0}^{t_1} dt_2 \frac{\alpha(t_1)}{\pi} P_\epsilon(\cdot) \otimes \bar{D}(\cdot,t_0)(x) \\
&+ \int_{t_0}^{t} dt_1 \frac{\alpha(t_1)}{\pi} P_\epsilon(\cdot) \otimes \int_{t_0}^{t_1} dt_2 \frac{\alpha(t_1)}{\pi} P_\epsilon(\cdot) \otimes \ldots \int_{t_0}^{t_{n-1}} dt_n \frac{\alpha(t_n)}{\pi} P_\epsilon(\cdot) \otimes \bar{D}(\cdot,t_0)(x) \\
&+ \ldots \\
&= \bar{D}(x,t_0) \\
&+ \sum_{n=1}^{\infty} \int_{t_0}^{t} \prod_{i=1}^{n} dt_i \; \Theta(t_i - t_{i-1}) \int_0^1 \prod_{i=1}^{n} dz_i \; \frac{\alpha(t_i)}{\pi} P_\epsilon(z_i) \int_0^1 dz_0 \; \bar{D}(z_0,t_0) \; \delta(x - \prod_{i=0}^{n} z_i).
\end{aligned}
$$

- In real life $\bar{D}(x,t)$ comes in the convolution with some hard cross section $H(x)$, hence the $\delta(x - \prod_i z_i)$ constraint is absent.

Master Formula for structure function evolution

Usually $\bar{D}(x,t)$ is convoluted with the hard cross section $H(x)$, hence NO $\delta(x - \prod_i z_i)$:

$$\int dx \bar{D}(x,t) H(x) = \int dz_0 \bar{D}(z_0, t_0)$$

$$\times \left\{ 1 + \sum_{n=1}^{\infty} \int_{t_0}^{t} \prod_{i=1}^{n} dt_i \, \Theta(t_i - t_{i-1}) \int_0^1 \prod_{i=1}^{n} dz_i \, \frac{\alpha(t_i)}{\pi} P_\epsilon(z_i) \right\} H\Big(\prod_{i=0}^{n} z_i \Big)$$

► **Various paths are possible for the MC implementation:**

- "Forward Markovian evolution": Assumes that $H(x) = 1$ or very mild, applies to final state radiation (FSR) in QED and QCD; see PYTHIA and HERWIG.
- "Backward Markovian evolution" of Sjöstrand: requires prior knowledge of $D(x,t)$, most popular in QCD MC, e.g. PYTHIA, HERWIG.
- "Constrained Markovian evolution": forward evolution but with a constraint imposed by $H(x)$, does not require prior knowledge of $D(x,t)$; S. Jadach et al., in progress.
- "Non-Markovian algorithm": the evolution equation (raw splitting kernels) used as the only source for constructing D-distributions; S. Jadach et al., in progress.

Derivation of the 2-dimensional Markovian algorithm

Define a normalized differential conditional probability for a single Markovian forward step:

$$dP_{n\geq i}(t_i, z_i|t_{i-1}) = p(t_i, z_i|t_{i-1})dt_i dz_i, \quad \int dP_{n\geq i}(t_i, z_i|t_{i-1}) = 1.$$

It is identified easily as:

$$p(t_i, z_i|t_{i-1})dt_i dz_i = \Theta(t_i - t_{i-1})\, e^{-\Phi(t_i)+\Phi(t_{i-1})} dt_i\, \frac{\alpha(t_i)}{\pi} P_\epsilon(z_i) dz_i$$
$$= \Theta(T_i - T_{i-1})\, e^{-T_i + T_{i-1}}\, dT_i\, \frac{\frac{\alpha(t_i)}{\pi} P_\epsilon(z_i)}{\int \frac{\alpha(t_i)}{\pi} P_\epsilon(z) dz}\, dz_i.$$

► Markovian interpretation requires adding one extra integration variable $\mathbf{t_{n+1}}$, representing a “trashed variable”, i.e. falling beyond the limit $t_{\max}$.

▷ It is “fabricated” using the identity:

$$e^T \int_t^\infty dt' \int_0^1 dz\, p(t', z|t_n) \equiv e^T \int_T^\infty dT'\, e^{-T'+T_n} = e^{T_n} = e^{\Phi_n}\, .$$

Master Formula for 2-dimensional Markovian parton-shower algorithm

"Markovianization" done by adding the "artificial" extra integration over t_{n+1} leads us to:

$$D(x,t) = \int dz_0 D(z_0,t_0) \Bigg\{ \int\limits_{t_1>0} dt_1 dz_1 \; p(t_1,z_1|0)\,\delta(x-z_0)$$

$$+ \sum_{n=1}^{\infty} \int\limits_{t<t_n} \prod_{i=1}^{n} p(t_i,z_i|t_{i-1}) dt_i dz_i \int\limits_{t_{n+1}>t} dt_{n+1} dz_1 \; p(t_{n+1},z_{n+1}|t_n)\,\delta\Big(x - \prod_{i=0}^{n} z_i\Big)\Bigg\}$$

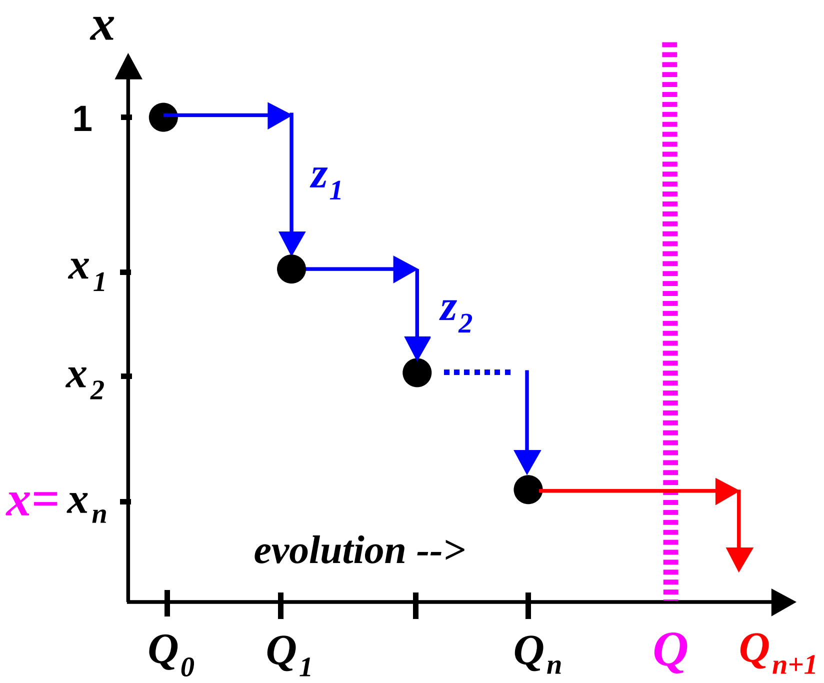
which is now **directly applicable in the Markovian algorithm**.

In the 2-dimensional Markovian Monte Carlo algorithm:

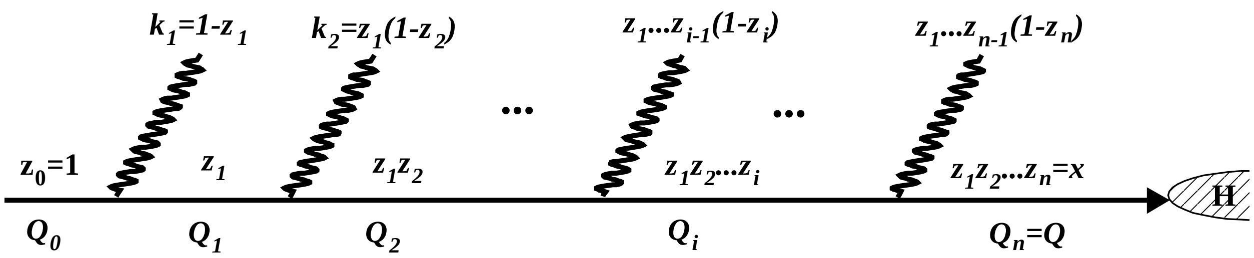
- At each step a new pair (t_i, z_i) is generated according to the conditional probability density $p(t_i,z_i|t_{i-1})dt_i dz_i$.
- The process continues until the "overflow" $t_{n+1} > t_{\max} = t$ happens for $n+1 = i$.
- The accepted MC event is $[n,\ (t_1,z_1),(t_2,z_2),\ldots,(t_n,z_n)]$.
  The pair (t_{n+1}, z_{n+1}) is trashed!
- In case of the "overflow" at the first step: $n=0$ and $x=z_0$.

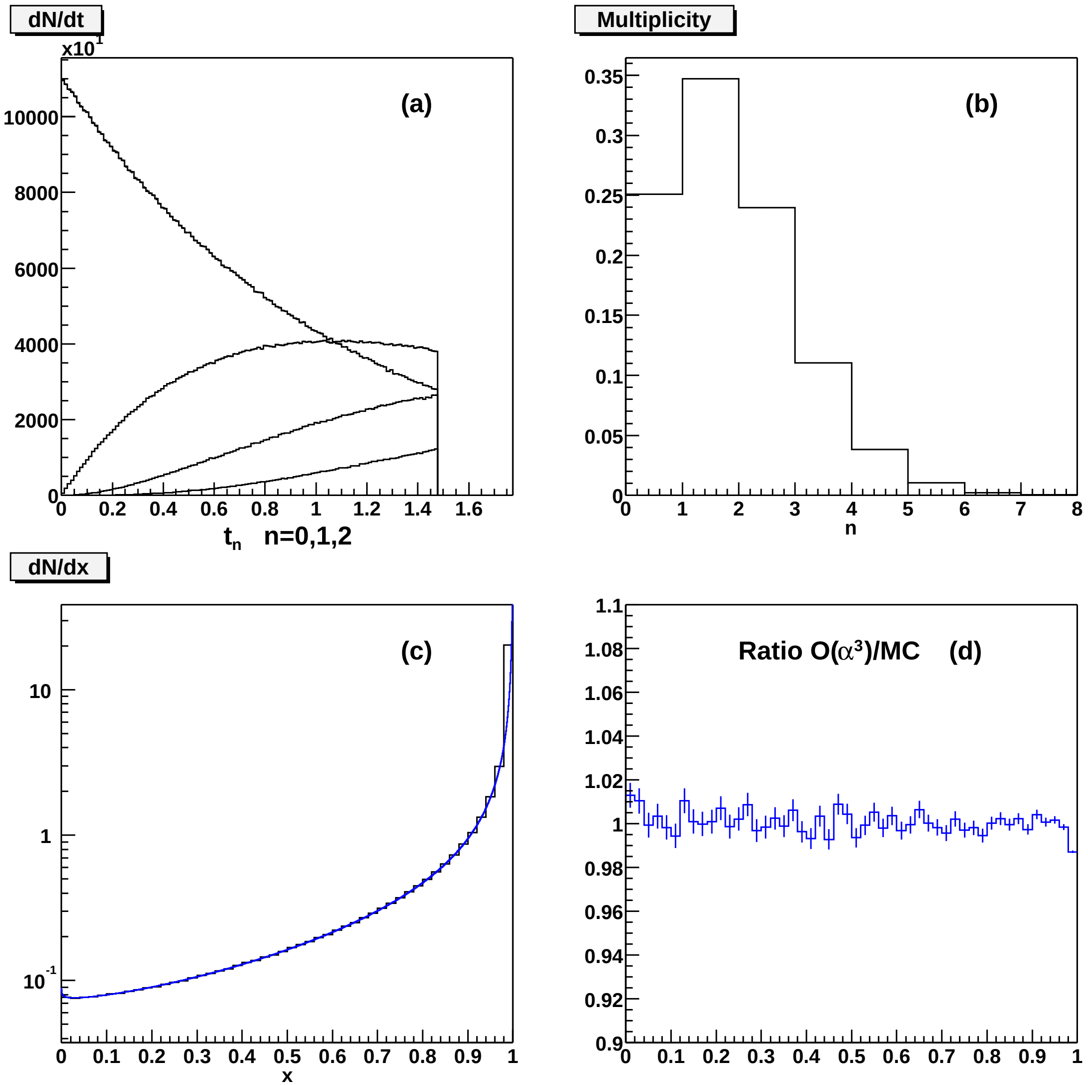
► The claim is that this $x = \prod_{i=0}^{n} z_i$ will be distributed **exactly** (up to a Monte Carlo statistical error) according to the desired distribution $D(x,t)$.

Markovian path for ISR



The Markovian path in the (x, Q) phase space related to the calculation of $D(x, Q)$ (upper plot) and the ISR-type kinematic tree (lower plot).





The beauty of this MC is that the Altarelli-Parisi kernel is the only input!

This MC solution is the EXACT infinite order LL solution for the non-singlet electron QED structure function.

Numerical results for the QED ISR parton shower at 1TeV: (a) distributions of the evolution variables $t_i, i = 0, 1, 2, 3$; (b) photon multiplicity distribution; (c) distribution $D(x, Q)$ of electron, histogram is MC, smooth curve is analytical results from the literature. (d) The ratio of the analytical and MC.

Multicomponent Markovian algorithm

- For the singlet structure functions we have a system of coupled evolution equations:

$$\frac{\partial}{\partial t} D_k(t,x) = \sum_j \int_x^1 \frac{dz}{z} P_{kj}(z) \frac{\alpha_S(t,z)}{\pi} D_j\left(t, \frac{x}{z}\right)$$
$$= \sum_j \frac{\alpha_S(t,\cdot)}{\pi} P_{kj}(\cdot) \otimes D_j(t,\cdot) = \sum_j \mathcal{P}_{kj}(t,\cdot) \otimes D_j(t,\cdot)\,.$$

where $t = \ln Q$ and the indices j,k runs over all partons.

▷ The generalized Altarelli-Parisi kernel can be written as:

$$\mathcal{P}_{kj}(t,z) = -\mathcal{P}^{\delta}_{kk}(\epsilon)\, \delta_{kj}\, \delta(1-z) + \mathcal{P}^{\Theta}_{kj}(t,z)\, \Theta(1-z-\epsilon)\,.$$

- The iterative solution now reads

$$D_k(t,x) = e^{-\Phi_k(t,t_0)} D_k(t_0,x) + \sum_{n=1}^{\infty} \sum_{k_0,\dots,k_{n-1}} \prod_{i=1}^{n} \left[\int_{t_0}^{t} dt_i\ \Theta(t_i - t_{i-1}) \int_0^1 dz_i \right]$$
$$\times\, e^{-\Phi_k(t,t_n)} \int_0^1 dx_0\ \prod_{i=1}^{n} \left[\mathcal{P}^{\Theta}_{k_i k_{i-1}}(t_i,z_i) e^{-\Phi_{k_{i-1}}(t_i,t_{i-1})} \right] D_{k_0}(t_0,x_0) \delta(x - x_0 \prod_{i=1}^{n} z_i)\,,$$

where the Sudakov form-factor exponent: $\Phi_k(t,t_0) = \int_{t_0}^{t} dt'\ \mathcal{P}^{\delta}_{kk}(\epsilon)\,.$

Weighted Markovian algorithm

- The properly normalized Markovian transition probability is now:

$$\omega(t_i, x_i, k_i | t_{i-1}, x_{i-1}, k_{i-1}) \equiv \Theta(t_i - t_{i-1})\, \mathcal{P}^{\Theta}_{k_i k_{i-1}}(t_i, x_i/x_{i-1})\, e^{-T_{k_{i-1}}(t_i, t_{i-1})},$$

$$\int_{t_{i-1}}^{\infty} dt_i \int_0^1 dz_i \sum_{k_i} \omega(t_i, x_i, k_i | t_{i-1}, x_{i-1}, k_{i-1}) \equiv 1,$$

where

$$T_k(t, t_0) = \int_{t_0}^{t} dt' \int_{\epsilon'}^{1-\epsilon} dz \sum_j \mathcal{P}^{\Theta}_{jk}(t', z)\,.$$

▷ However, since in general $T_k(t, t_0) \neq \Phi_k(t, t_0)$, using the above transition probability in the Makovian algorithm does not reproduce our iterative formula!

$\longrightarrow$ This can be corrected by weighting each event with the factor:

$$w = e^{\Delta_{k_n}(t, t_n)} \prod_{i=1}^{n} e^{\Delta_{k_{i-1}}(t_i, t_{i-1})}\,,$$

where

$$\Delta_k(t, t_0) = T_k(t, t_0) - \Phi_k(t, t_0) = \int_{t_0}^{t} dt' \int_{\epsilon'}^{1} dz \sum_j \mathcal{P}_{jk}(t', z)\,.$$

$\Longrightarrow$ **Weighted Markovian algorithm**

Master Formula for multicomponent Markovian algorithm

- In order to complete construction of the Markovian solution we have to add $(n+1)$th "spill-over" variables. This can be accomplished by using the following identity:

$$
e^{-\Phi_{k_n}(t,t_n)} = e^{\Delta_{k_n}(t,t_n)} \int_t^{\infty} dt_{n+1} \int_0^1 dz_{n+1} \sum_{k_{n+1}} \omega(t_{n+1}, x_{n+1}, k_{n+1} | t_n, x_n, k_n) \, .
$$

- Finally, we obtain the iterative formula for the multicomponent Markovian algorithm:

$$
\begin{aligned}
D_k(t,x) = {} & e^{\Delta_k(t,t_0)} \int\limits_{t_1>t} dt_1 dz_1 \sum_{k_1} \omega(t_1, x_1, k_1 | t_0, x_0, k) \;\; D_k(t_0, x) \\
& + \sum_{n=1}^{\infty} \int_0^1 dx_0 \int\limits_{t_{n+1}>t} dt_{n+1} dz_{n+1} \sum_{k_{n+1}} \sum_{k_0,\dots,k_{n-1}} \prod_{i=1}^{n} \int_{t_i<t}^{t} dt_i dz_i \\
& \times e^{\Delta_{k_n}(t,t_n)} \omega(t_{n+1}, x_{n+1}, k_{n+1} | t_n, x_n, k_n) \\
& \times \prod_{i=1}^{n} e^{\Delta_{k_{i-1}}(t_i,t_{i-1})} \omega(t_i, x_i, k_i | t_{i-1}, x_{i-1}, k_{i-1}) \\
& \times \delta\Big(x - x_0 \prod_{i=1}^{n} z_i\Big) \; D_{k_0}(t_0, x_0).
\end{aligned}
$$

Generation of a single Markovian step

▶ A single step forward $(t_0, x_0, k_0) \to (t_1, z_1 x_0, k_1)$ in the primary Markovian algorithm is generated according to the probability density:

$$d\omega(t_1, z_1 x_0, k_1 | t_0, x_0, k_0) = \Theta(t_1 - t_0)\, \mathcal{P}^{\Theta}_{k_1 k_0}(t_1, z_1)\, e^{-T_{k_0}(t_1,t_0)} dt_1 dz_1 \,.$$

▷ Methods of generation of the above 3-dimensional distribution can be found from:

$$
\begin{aligned}
1 &\equiv \int_{t_0}^{\infty} dt_1 \sum_{k_1} \int_0^1 dz_1\, \omega(t_1, z_1 x_0, k_1 | t_0, x_0, k_0) \\
&= \int_1^0 d\big(e^{-T_{k_0}(t_1,t_0)}\big) \sum_{k_1} \frac{\int dz'\, \mathcal{P}^{\Theta}_{k_1 k_0}(t_1, z')}{\sum_j \int dz'\, \mathcal{P}^{\Theta}_{j k_0}(t_1, z')} \int_0^1 dz_1\, \frac{\mathcal{P}^{\Theta}_{k_1 k_0}(t_1, z_1)}{\int dz'\, \mathcal{P}^{\Theta}_{k_1 k_0}(t_1, z')} \\
&= \int_0^1 dr(t_1) \sum_{k_1} p(k_1|t_1) \int_0^1 dz_1\, \rho(z_1|k_1, t_1) \,.
\end{aligned}
$$

Generation scheme:

- First, generate t according to the density $r(t)$ (e.g. using the inverse transform method).
- For the chosen value of t, generate the parton type k according to $p(k|t)$.
- Finally, having the values of t and k, generate the variable z according to $\rho(z|k,t)$.

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