An introduction to Feynman-Kac particle methods in statistical learning and rare event simulation

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Sydney University, March 28th 2014.

Some hyper-refs

- **Mean field simulation for Monte Carlo integration**. Chapman & Hall - Maths & Stats (2013).
- **Feynman-Kac formulae**, Genealogical & Interacting Particle Systems with appl., Springer (2004)
- **More references on the websitehttp://web.maths.unsw.edu.au/∼peterdel-moral/** [+ Links]

Summary

Equivalent branching/interacting particle algorithms

Sequential Monte Carlo	Sampling	Resampling
Particle Filters	Prediction	Updating
Genetic Algorithms	Mutation	Selection
Evolutionary Population	Exploration	Branching-selection
Diffusion Monte Carlo	Free evolutions	Absorption
Quantum Monte Carlo	Walkers motions	Reconfiguration
Sampling Algorithms	Transition prop.	Accept-reject-recycle
Stochastic model	**Markov chain** X_n **transitions** M_n	**Potential funct.** $G_n(X_n)$ **fitness/branch/...**

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More lively buzzwords:

Bootstrapping, spawning, cloning, pruning, replenish, splitting, condensation, resampled Monte Carlo, enrichment, go with the winner, subset simulation, rejection and weighting, look-a-head sampling, pilot exploration, weighted dynamics, quantum teleportation, ...

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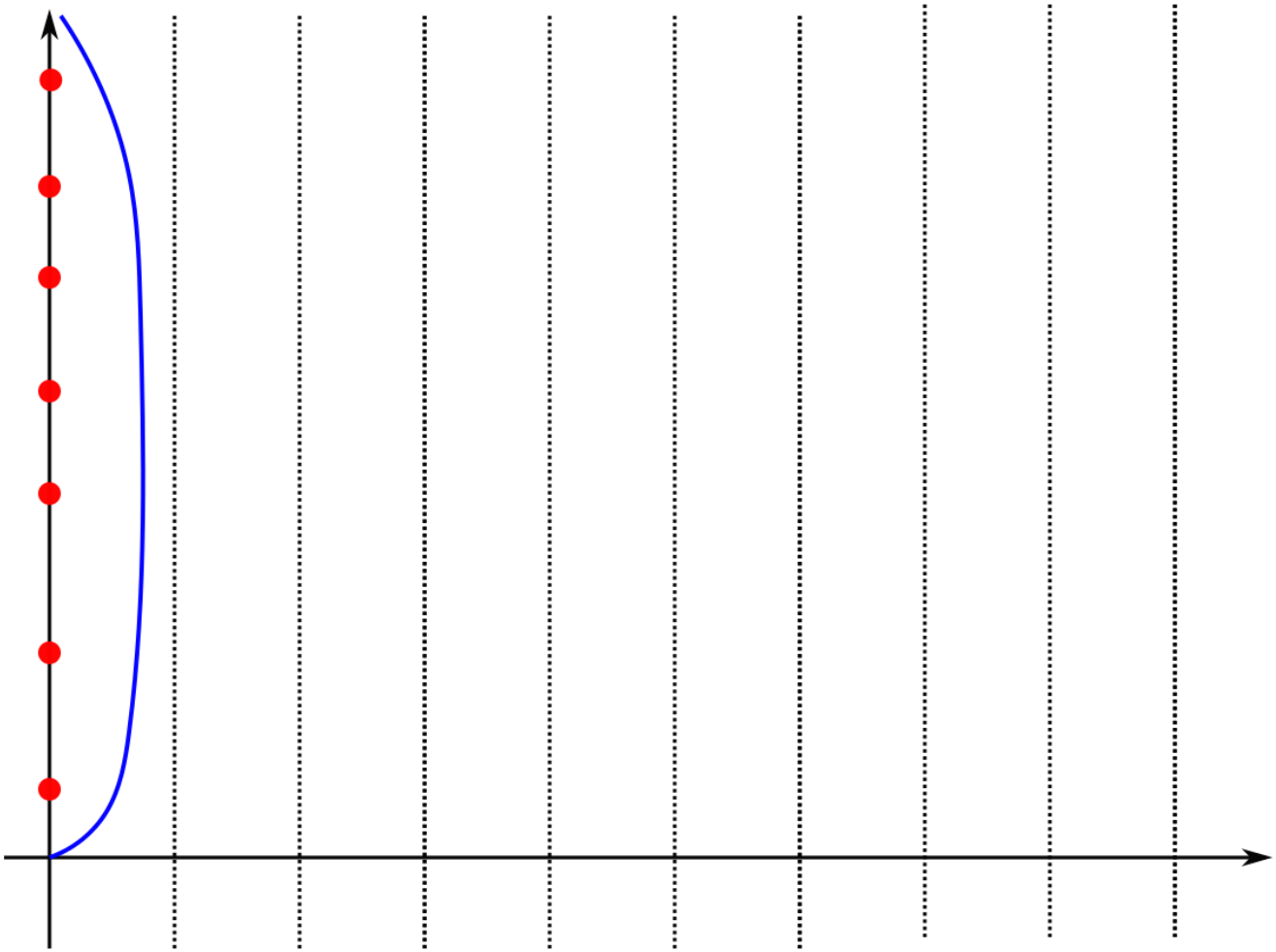
$1950 \leq$ **[(Meta)Heuristics]** $\leq 1996 =$ **Feynman-Kac particle model**

Graphical illustration : $\eta_n^N := \frac{1}{N}\sum_{1\leq i\leq N}\delta_{\xi_n^i} \simeq_{N\uparrow\infty} \eta_n$



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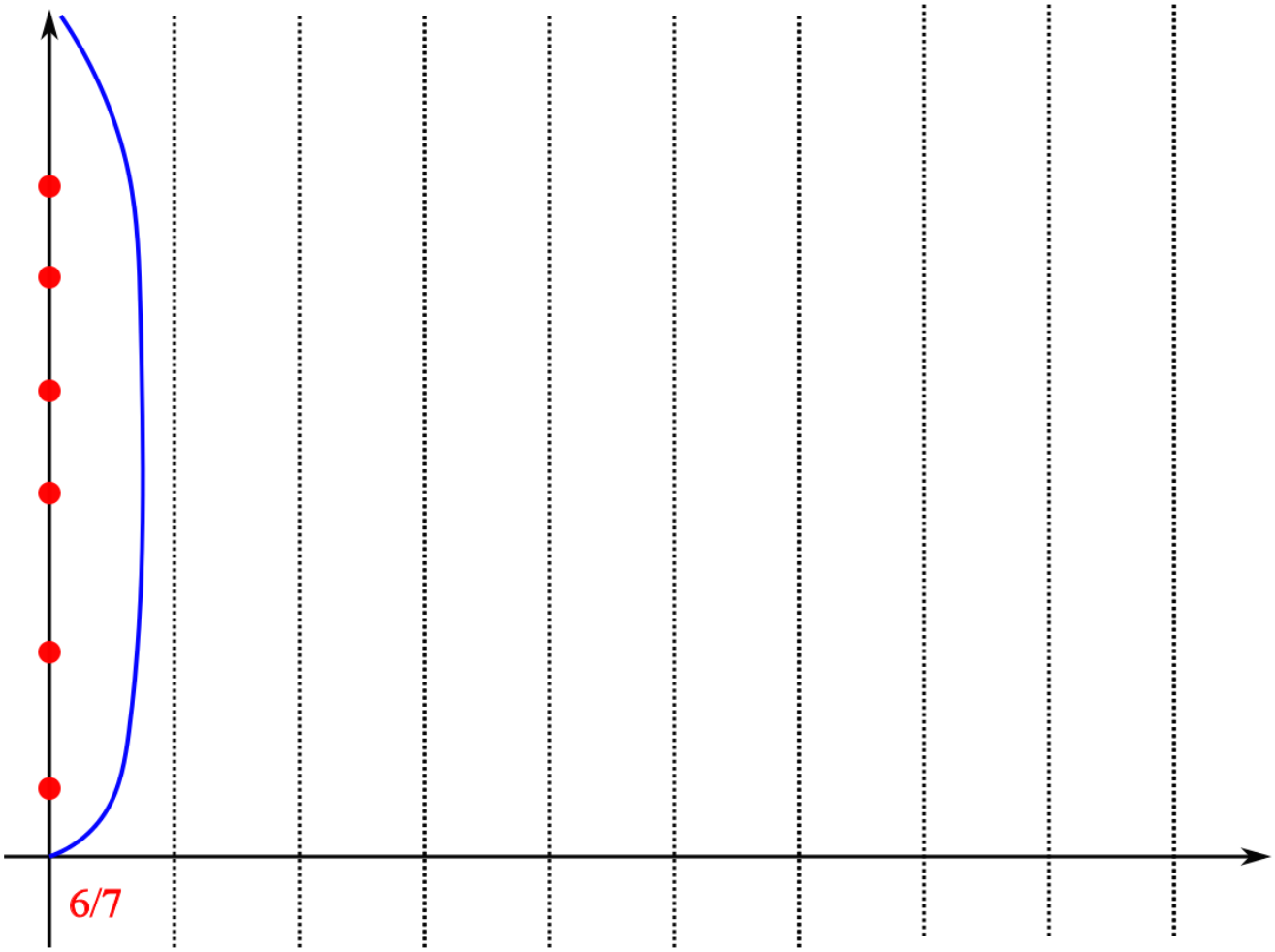

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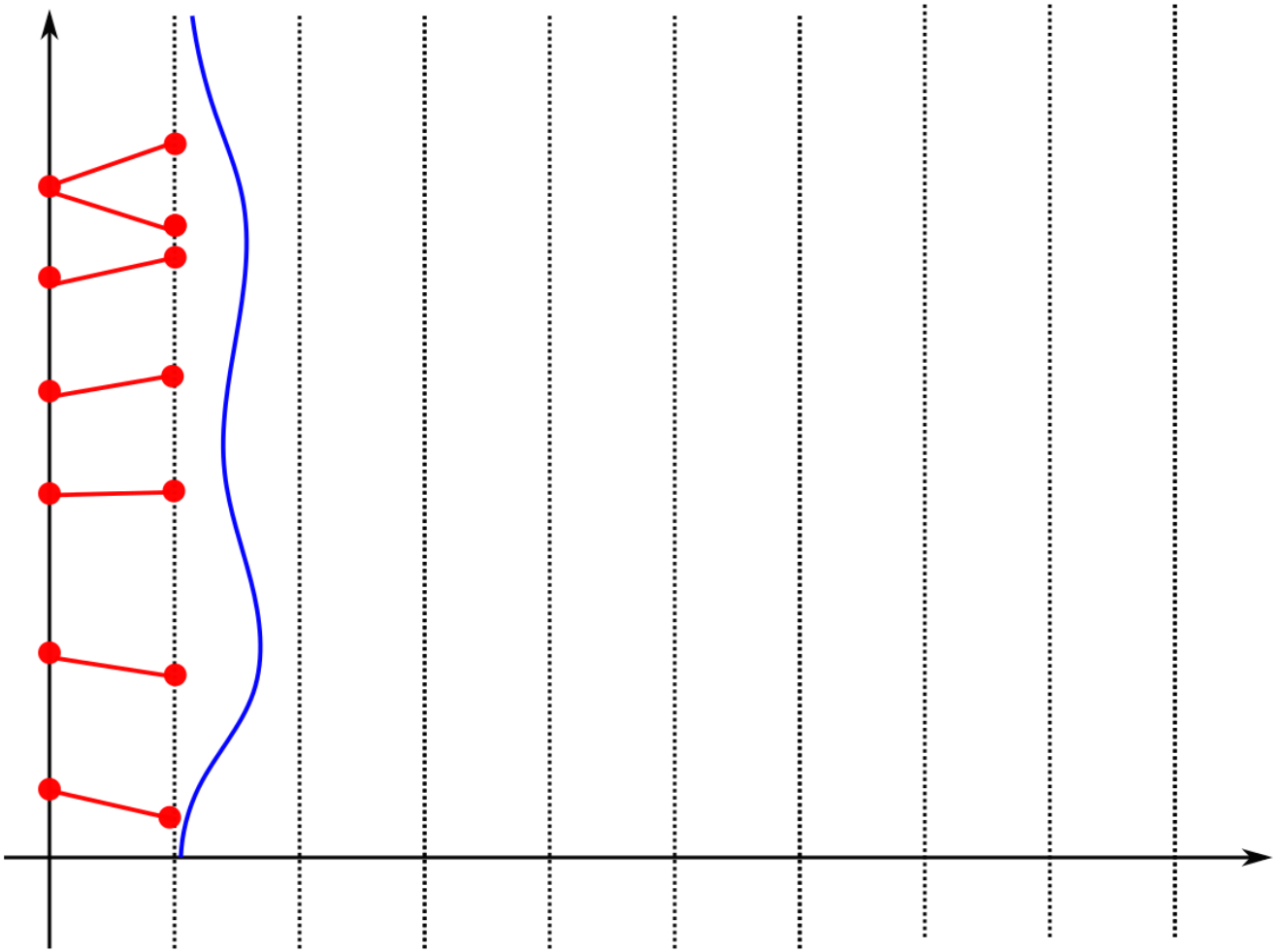

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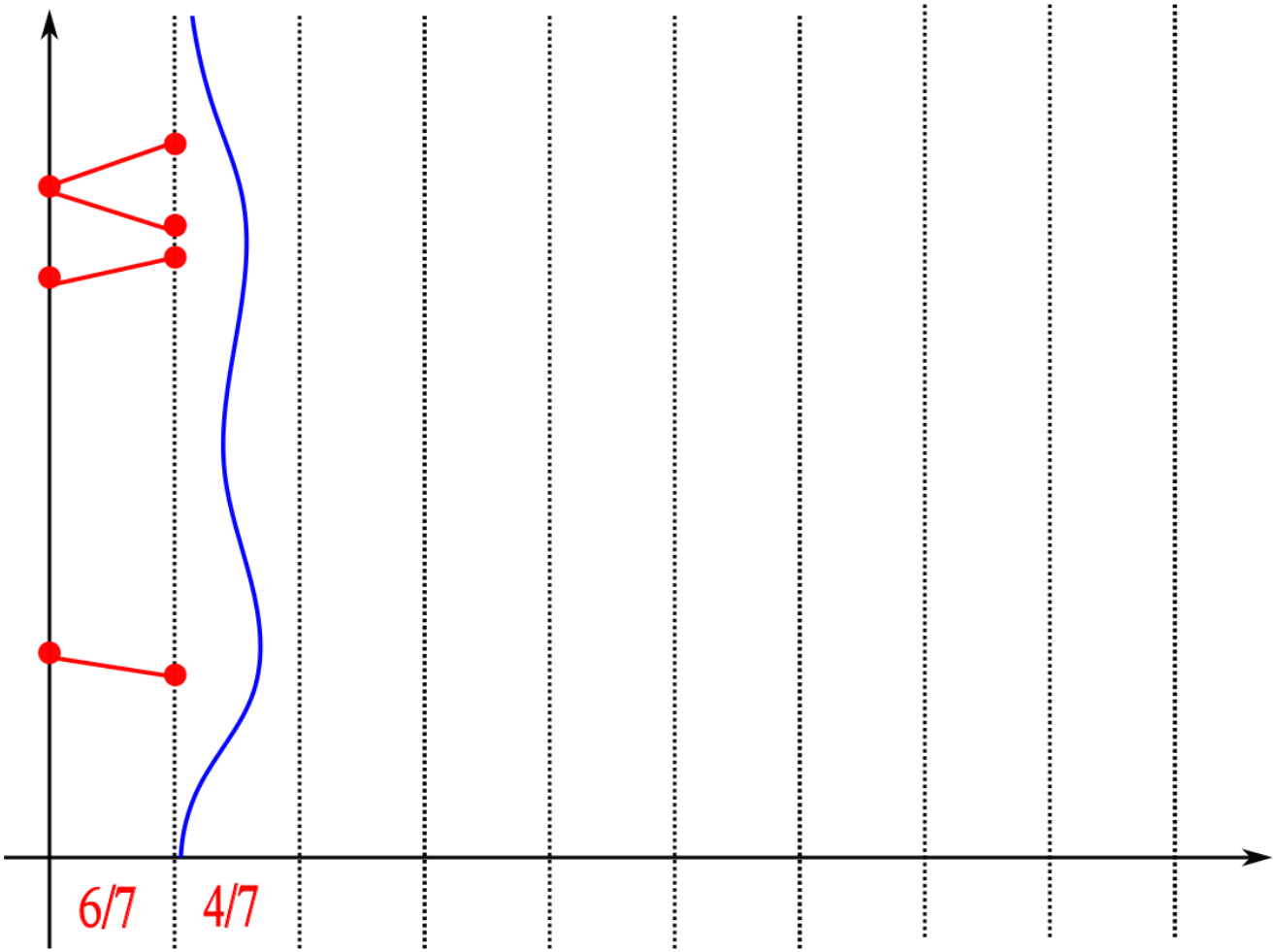

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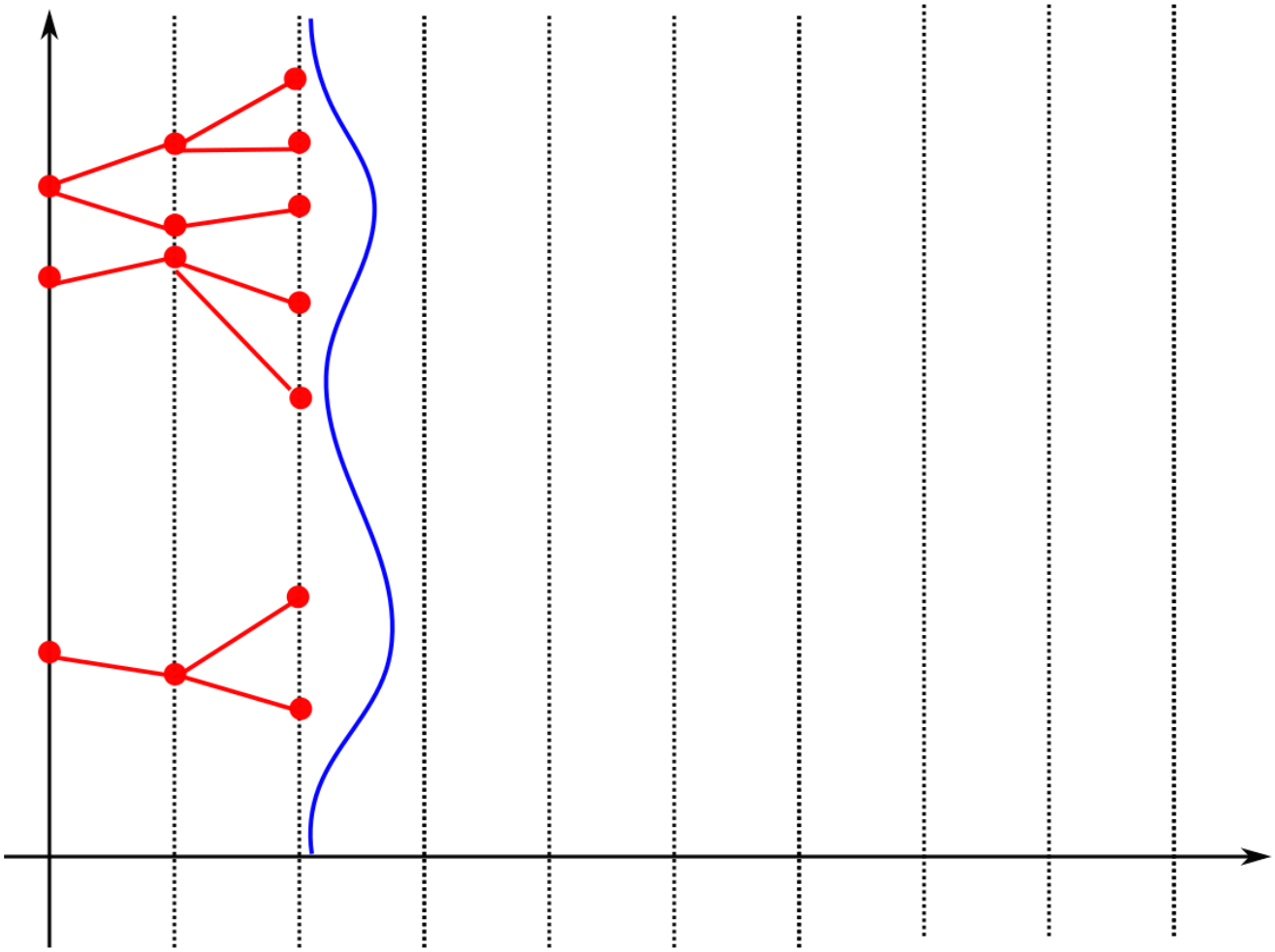

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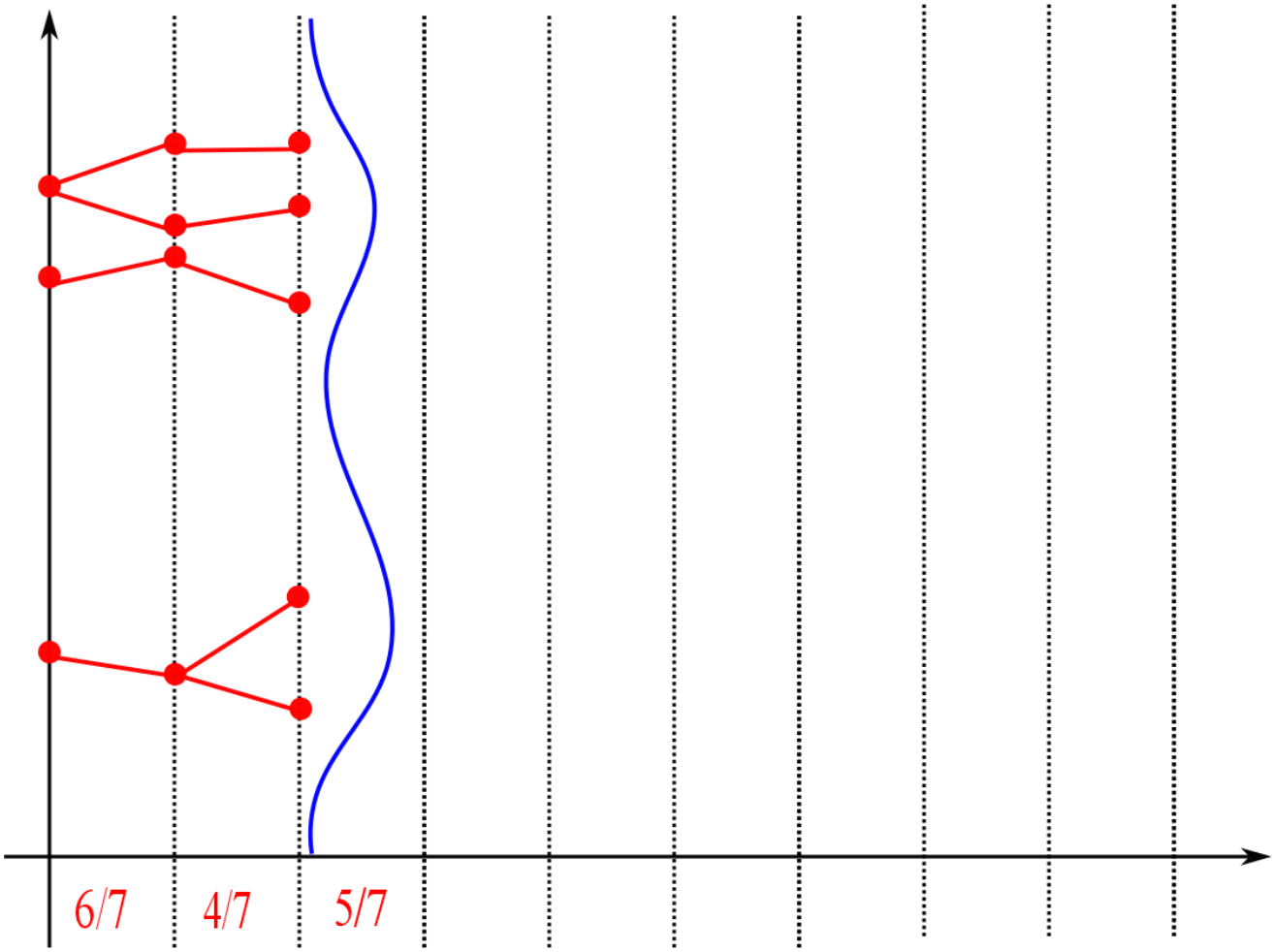

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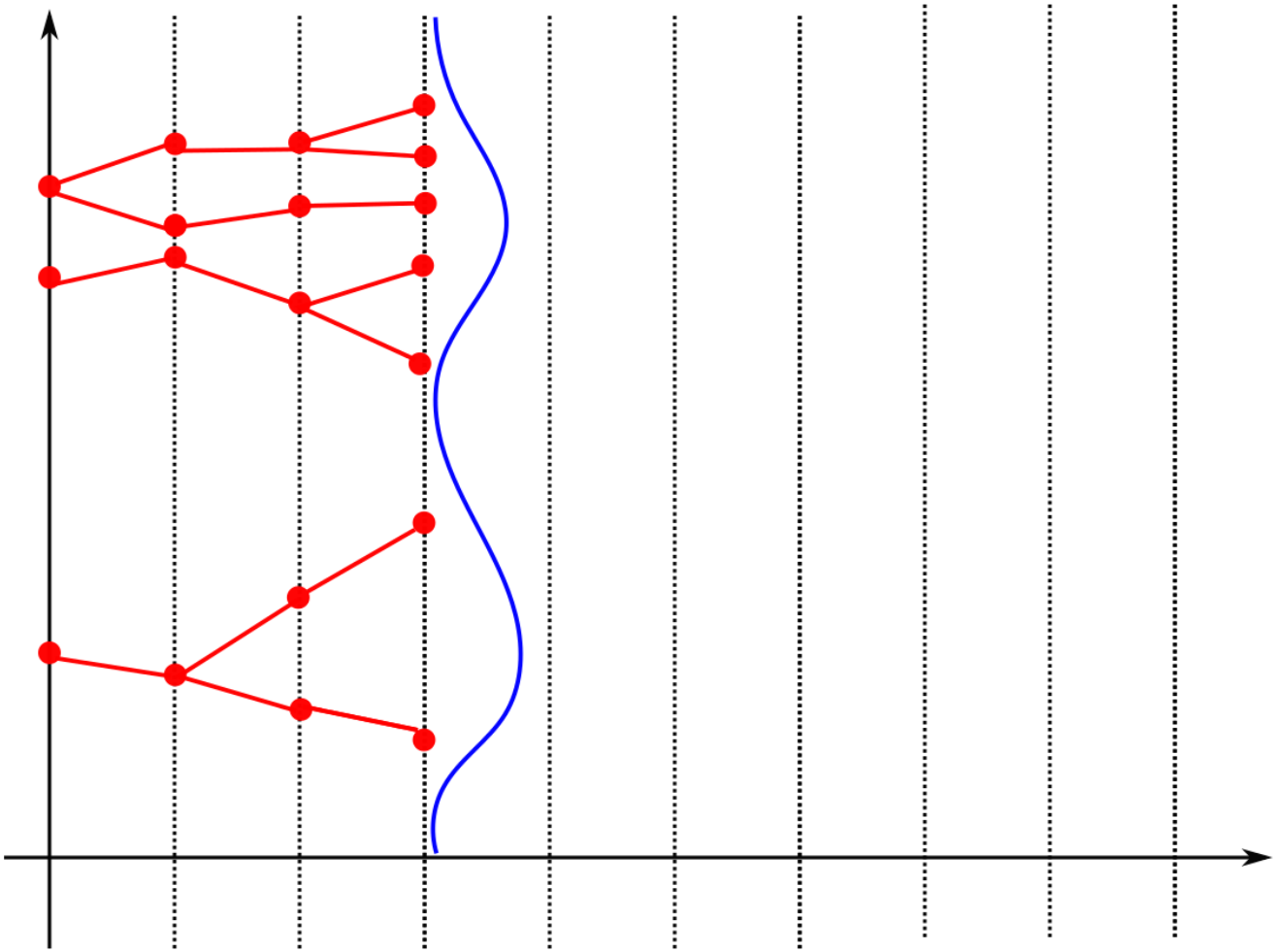

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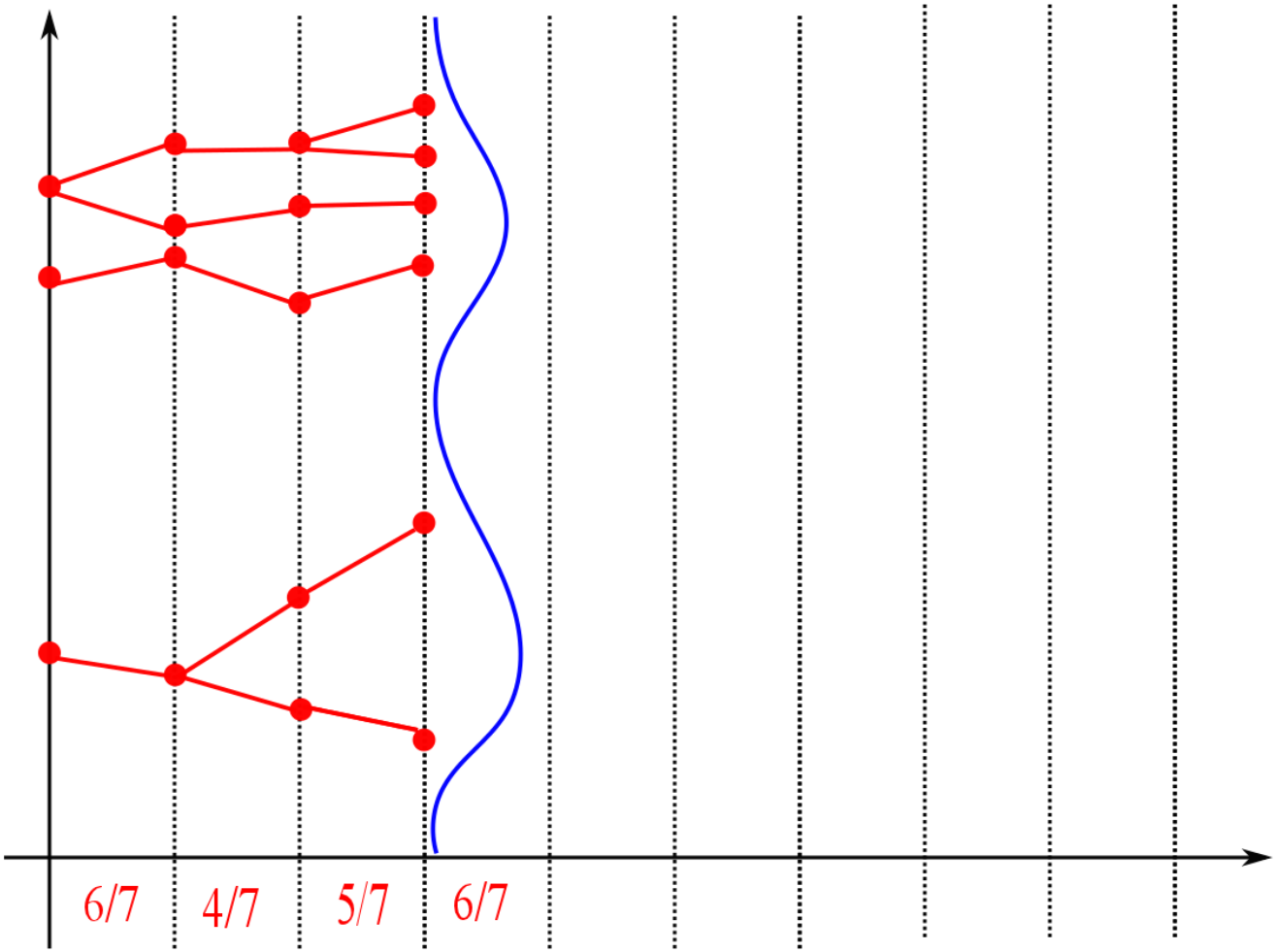

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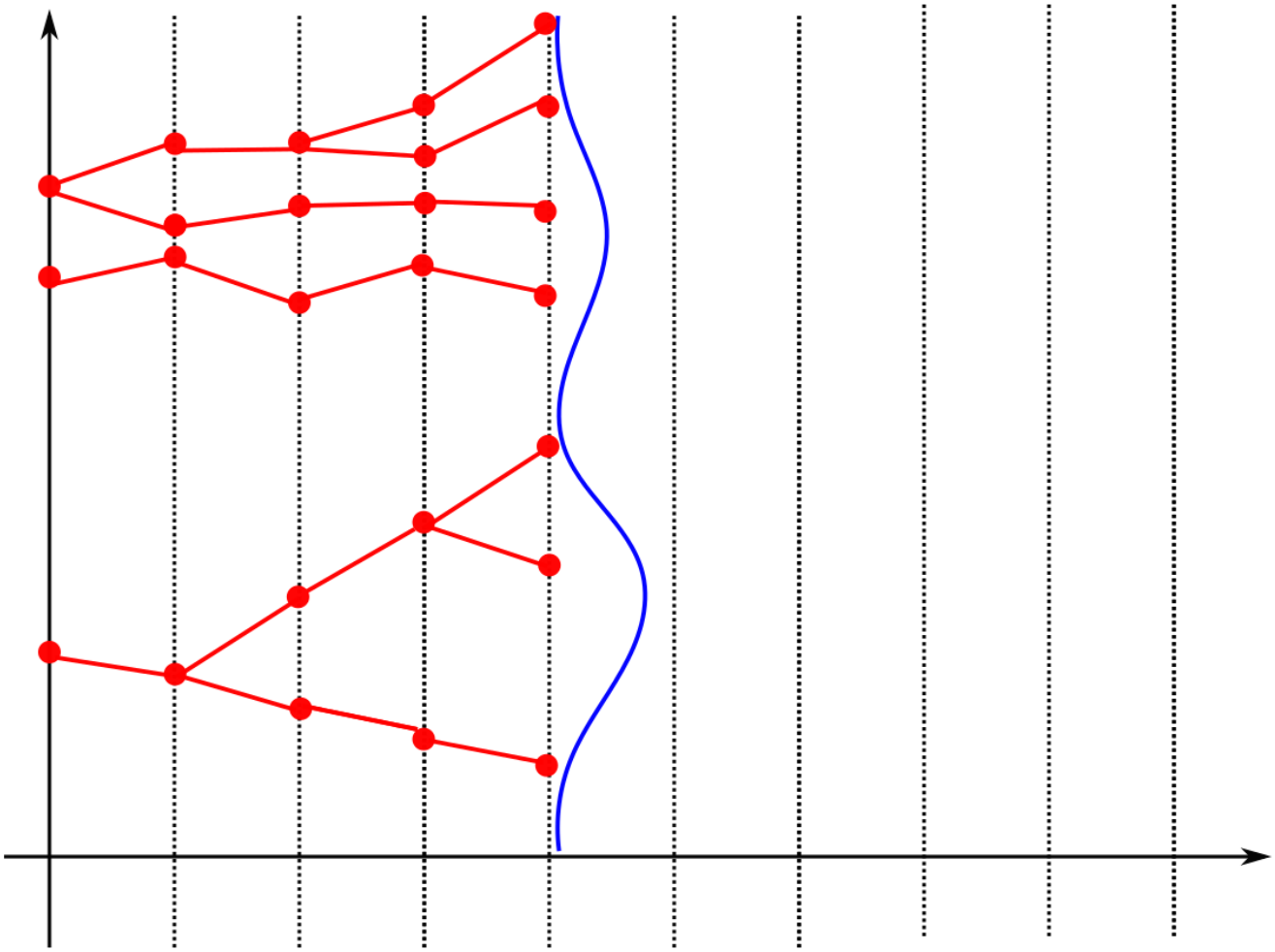

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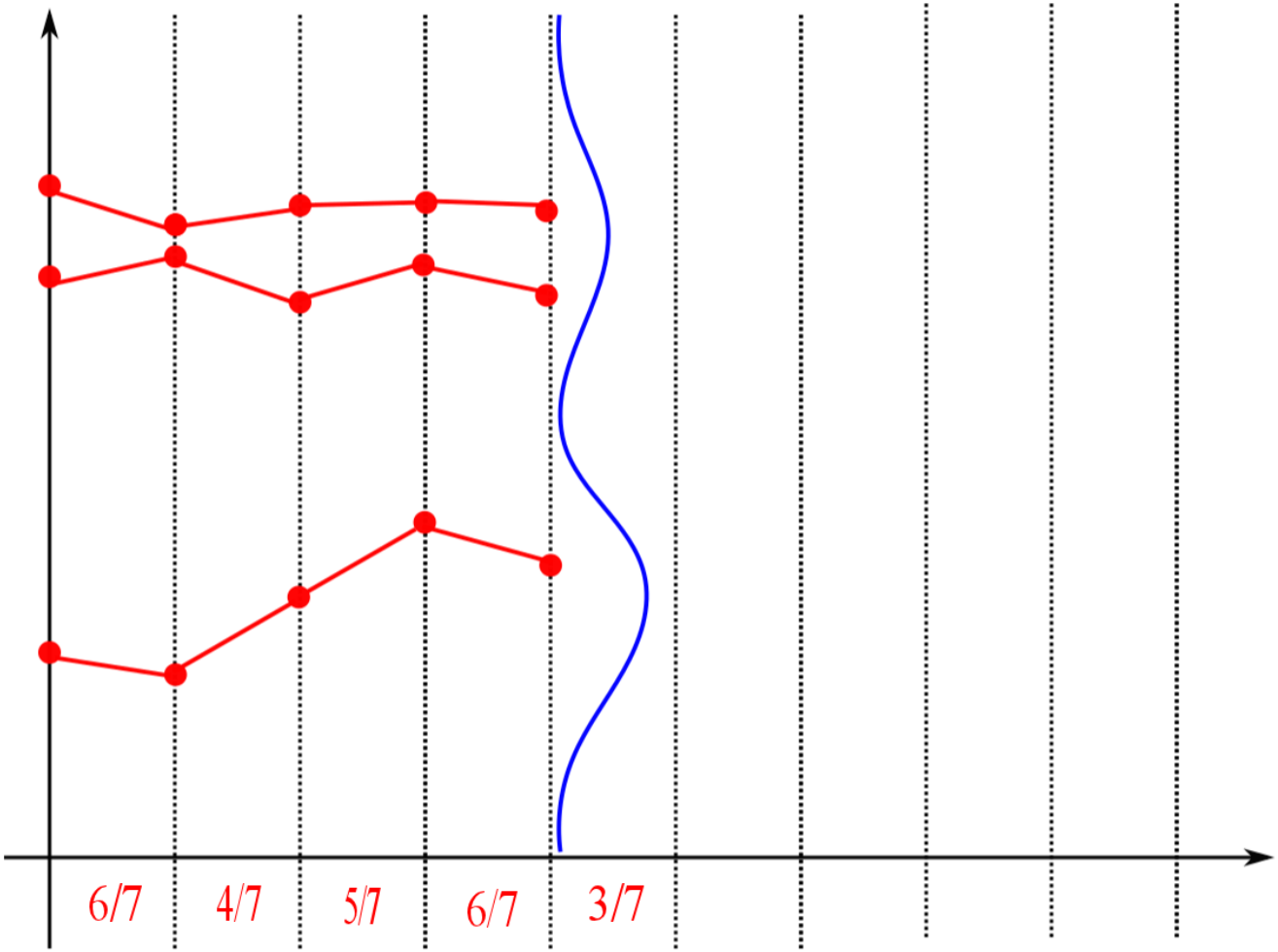

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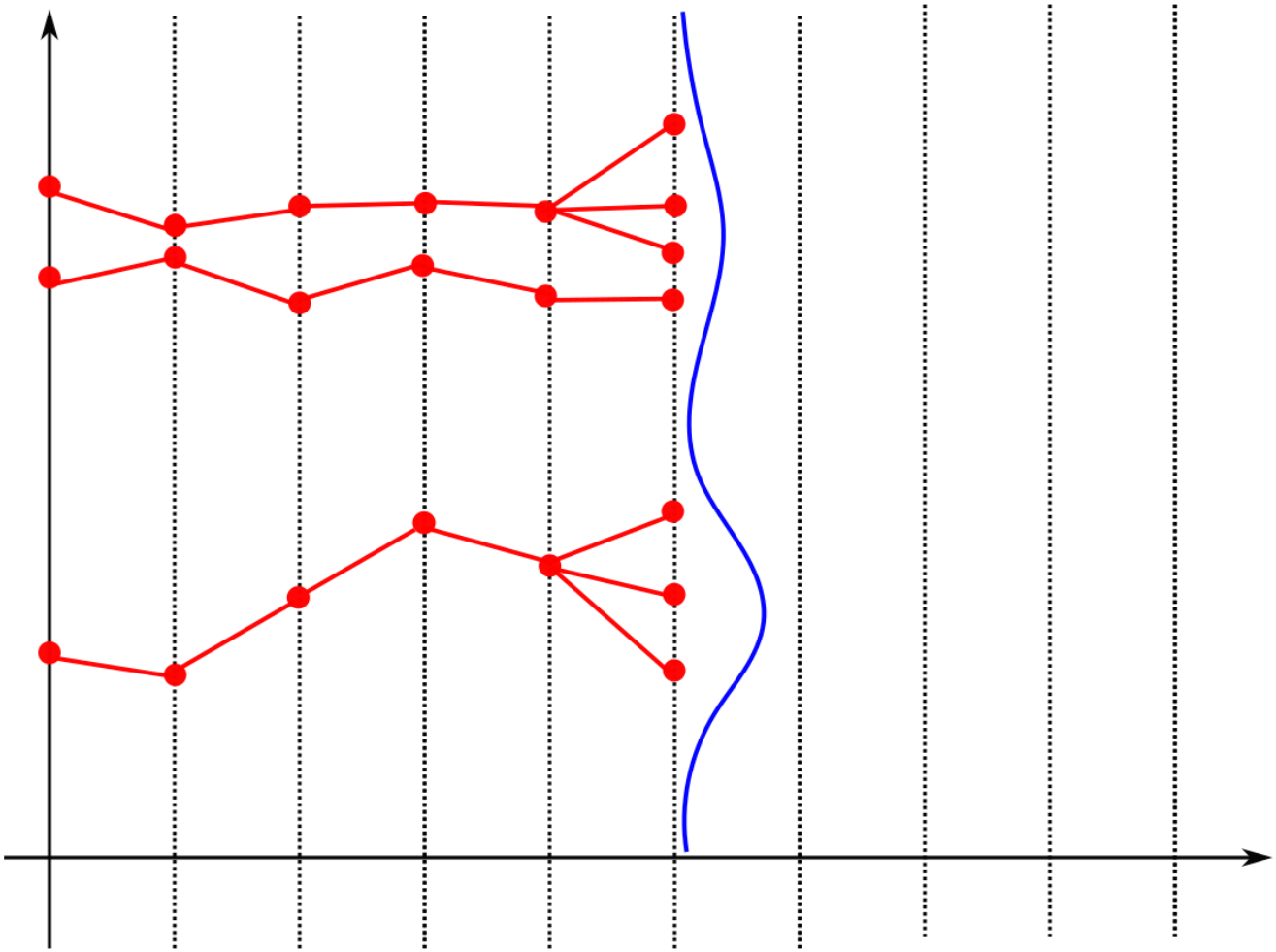

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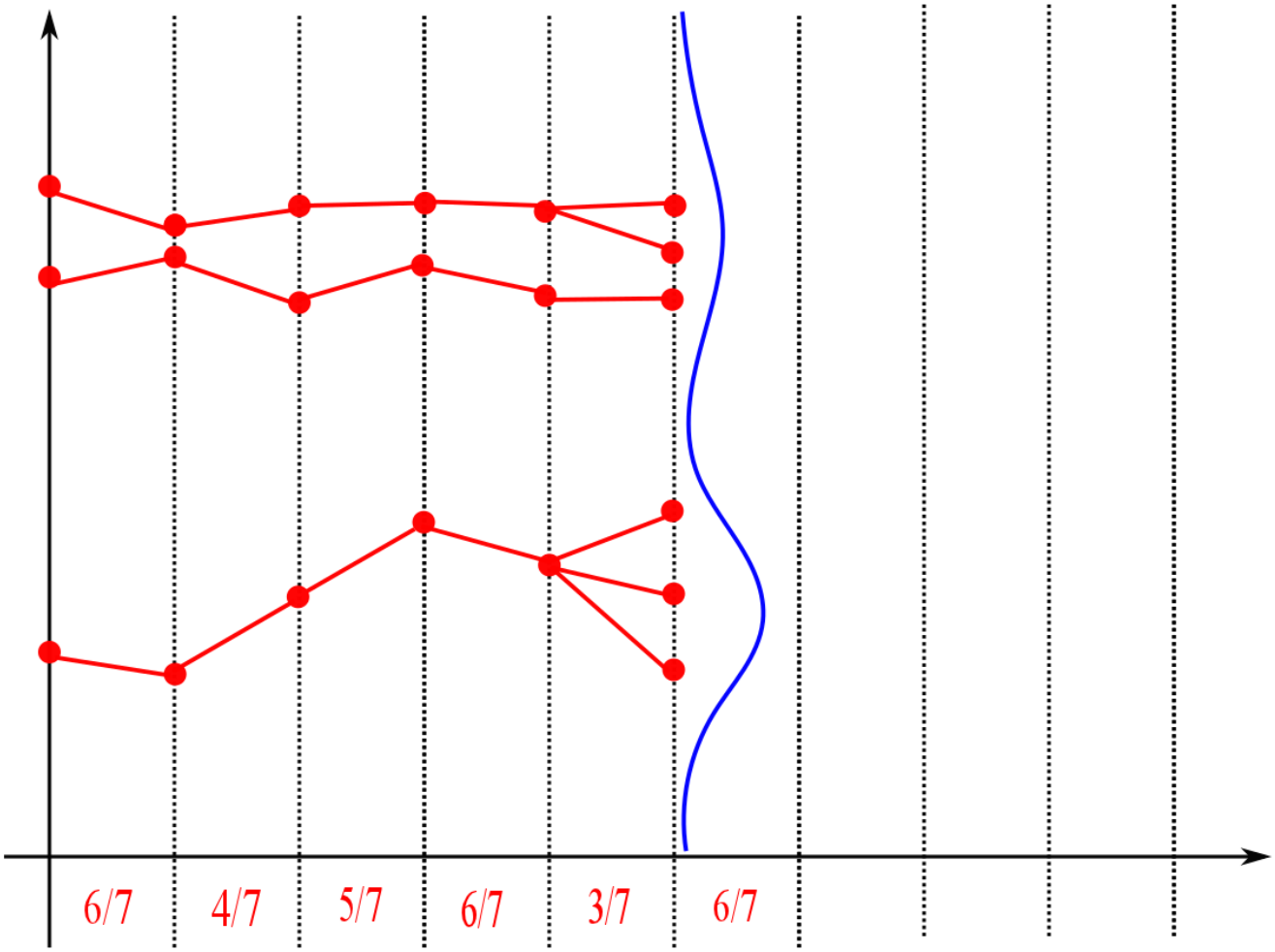

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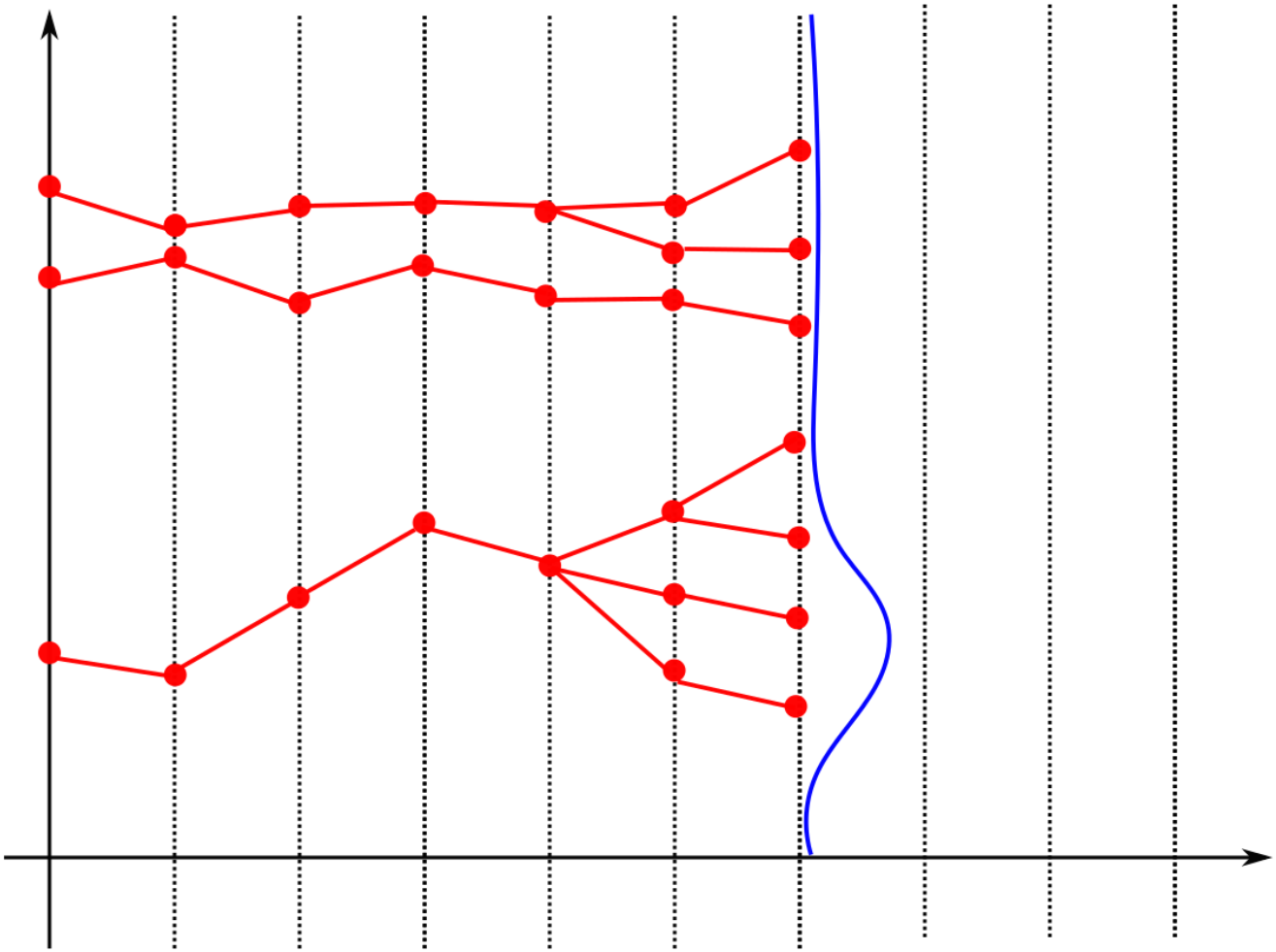

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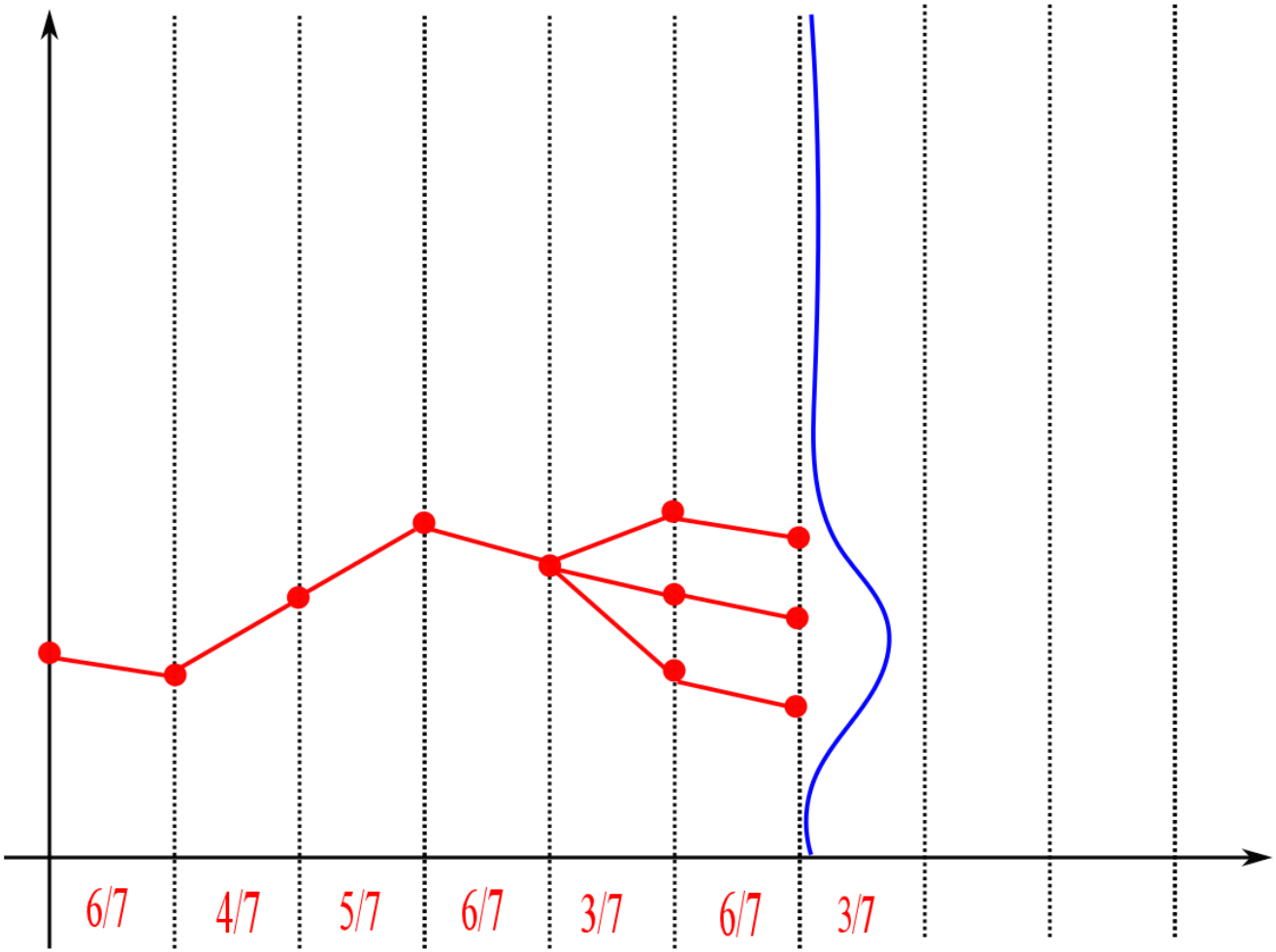

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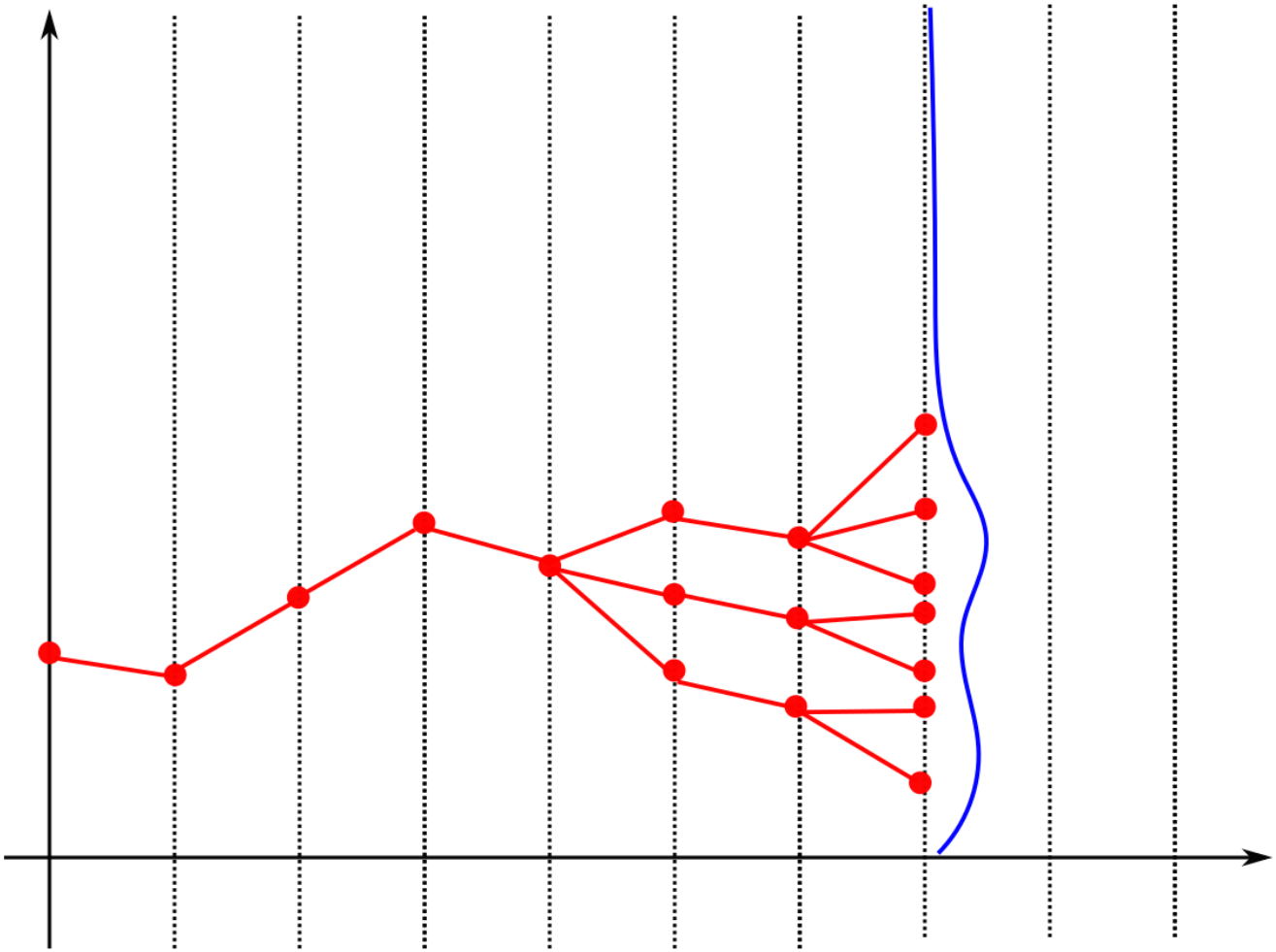

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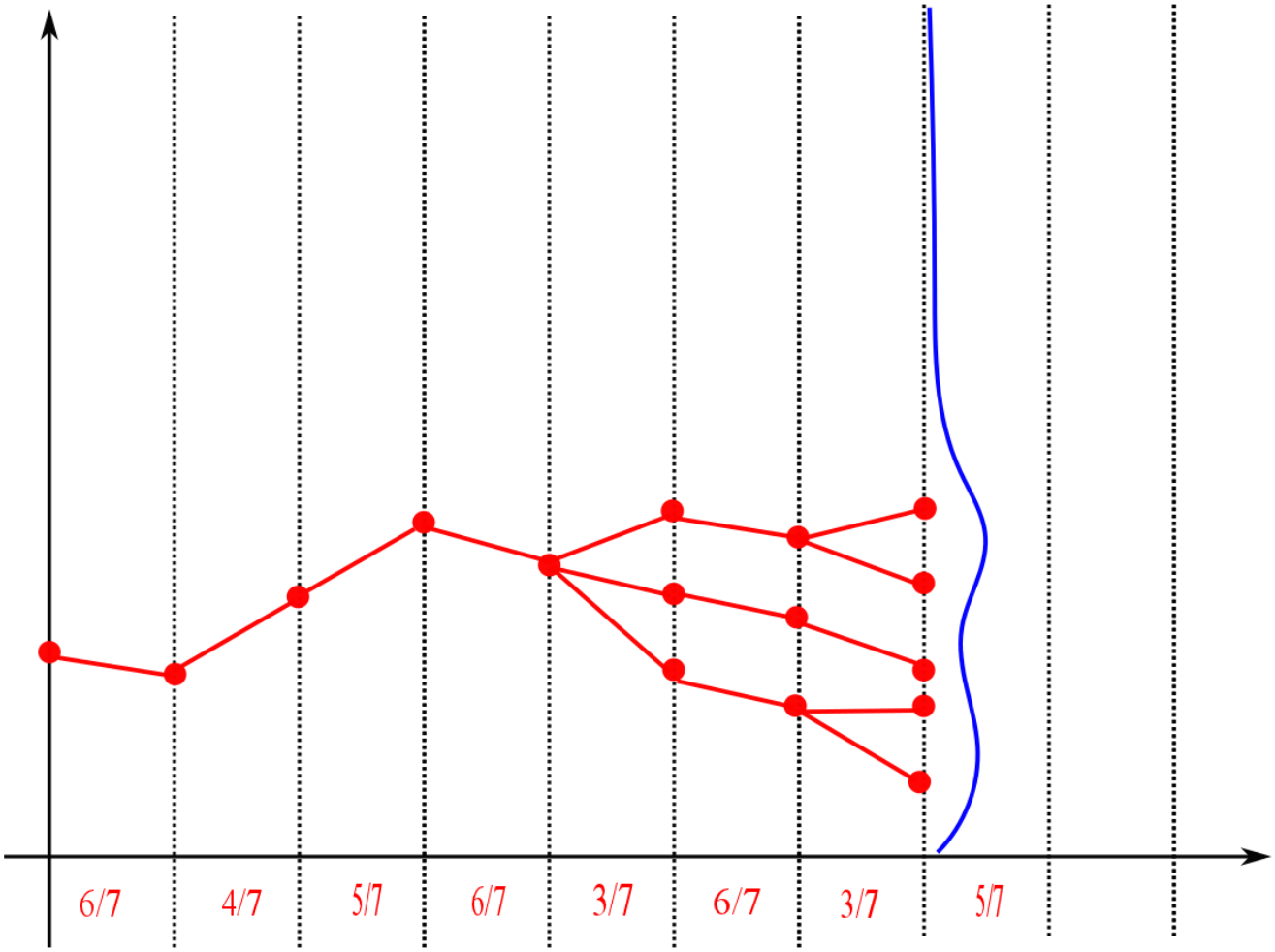

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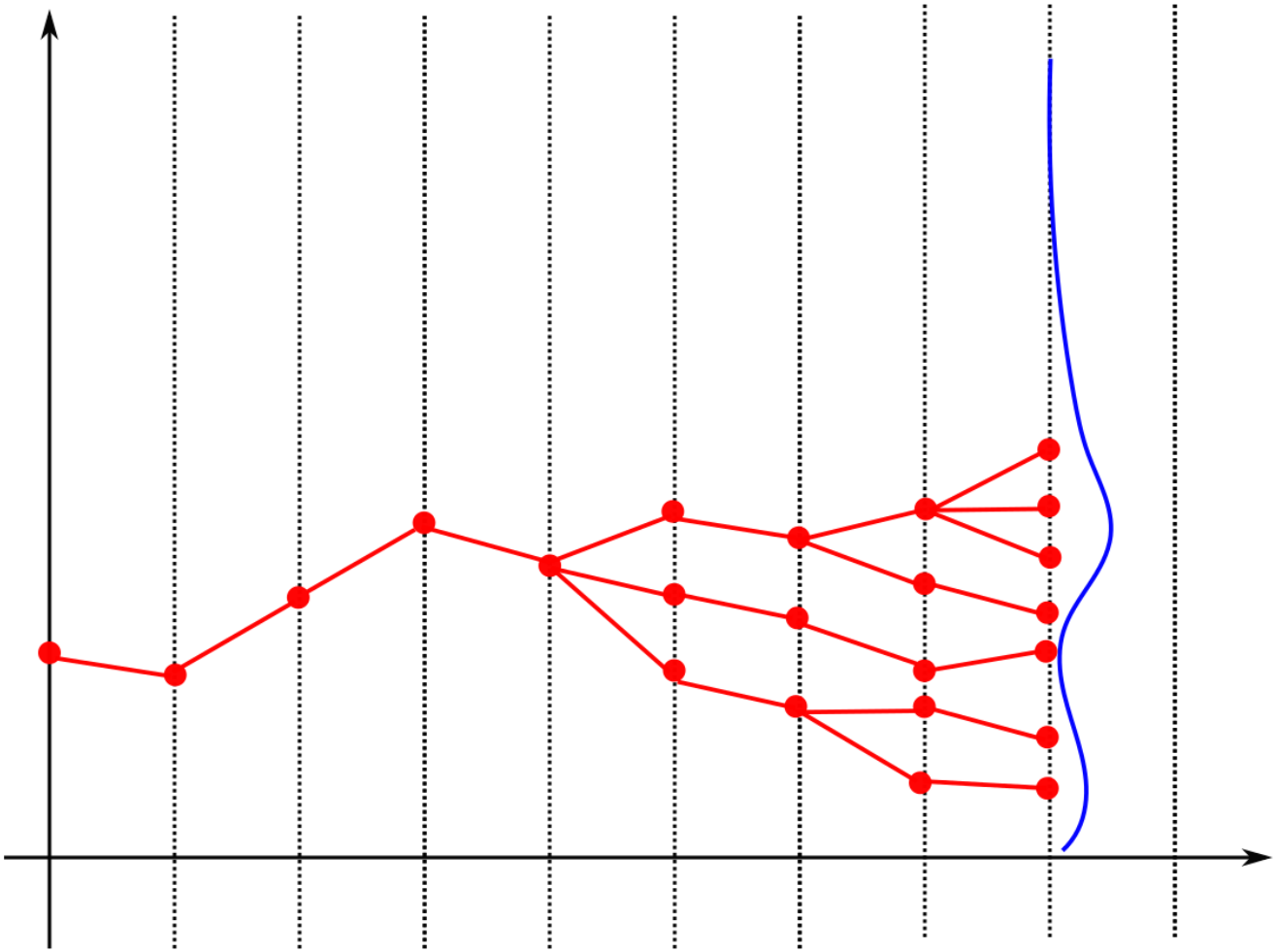

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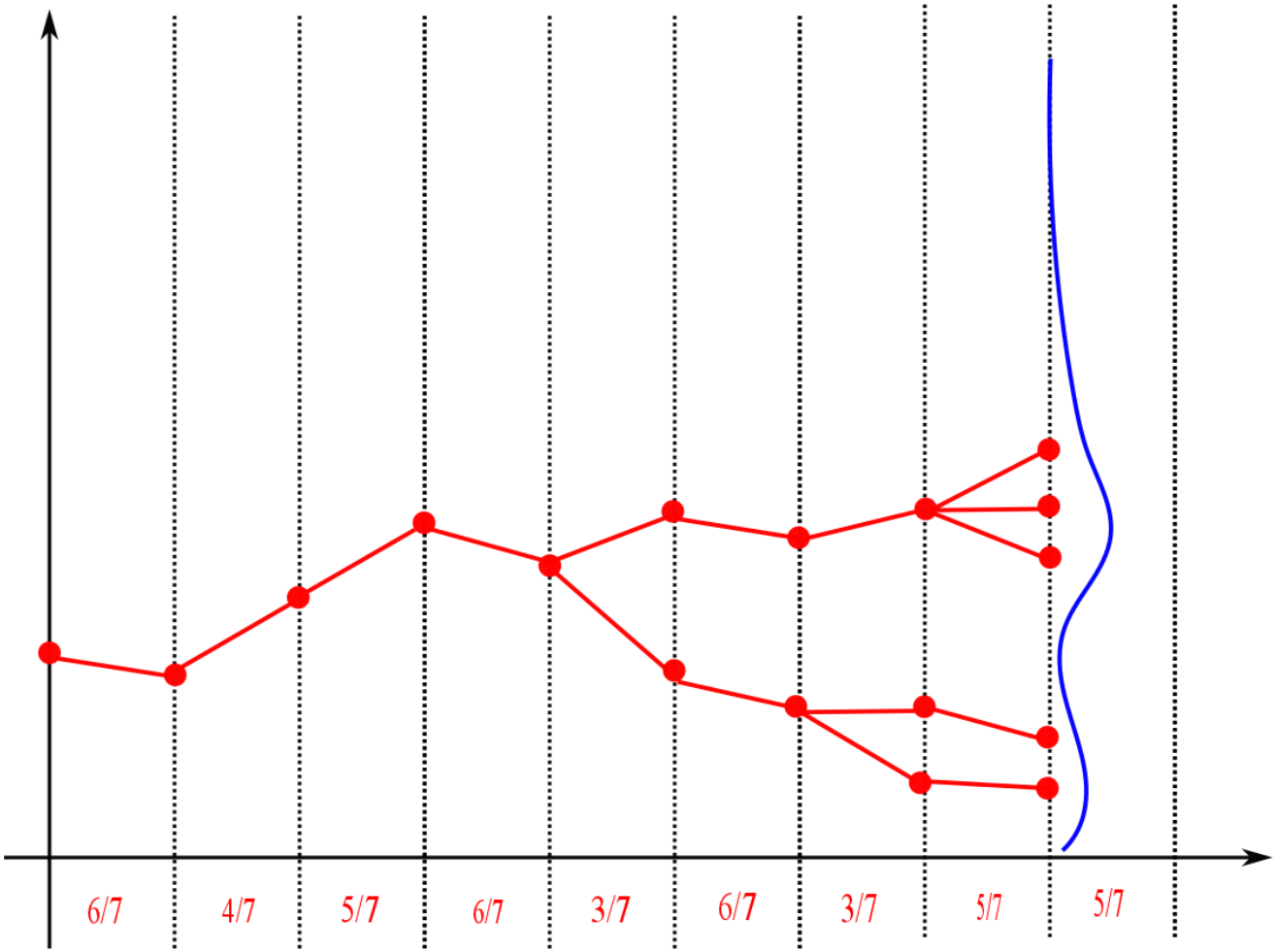

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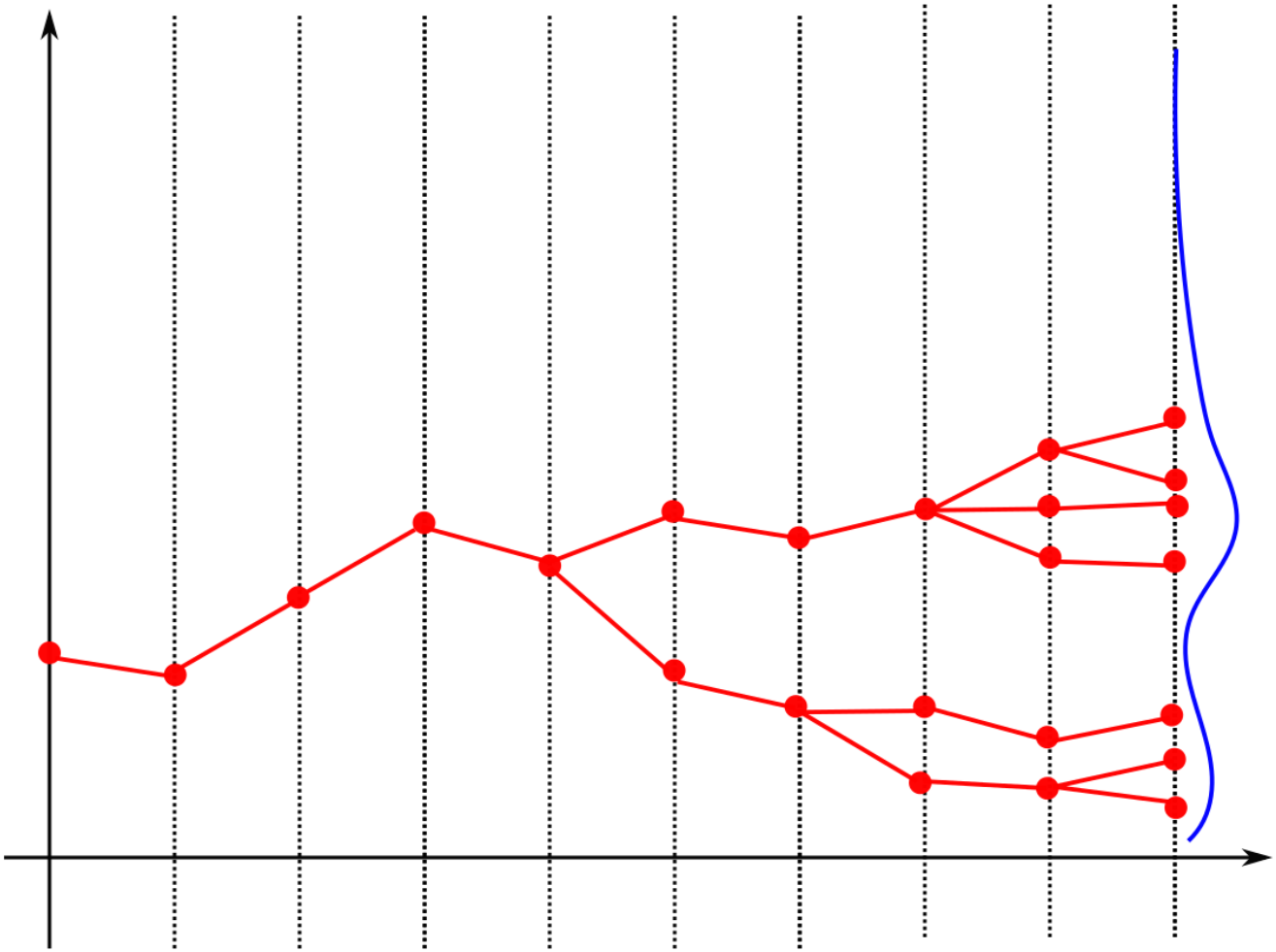
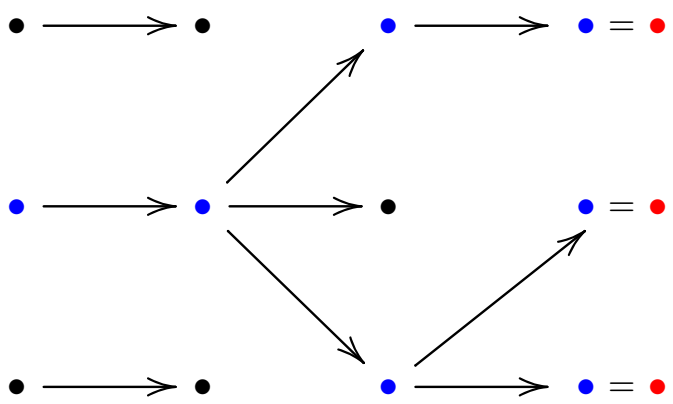


Interaction/branch. process $\hookrightarrow$ Genealogical trees ($N = 3$)



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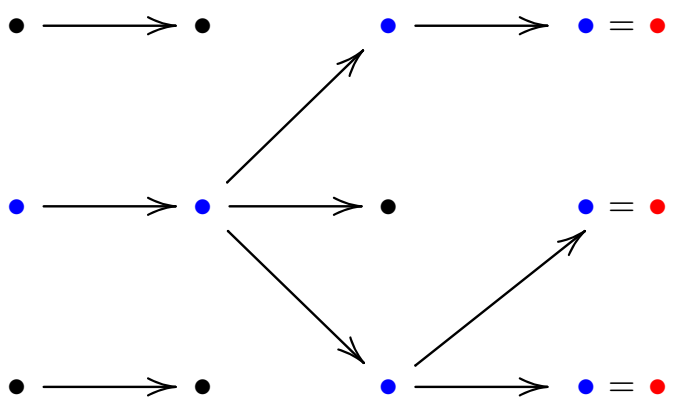

Limiting objects when $N \uparrow \infty$:

- **Current population** $\hookrightarrow \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} \delta_{\xi_n^i \leftarrow i\text{-th individual at time } n} \simeq \eta_n$

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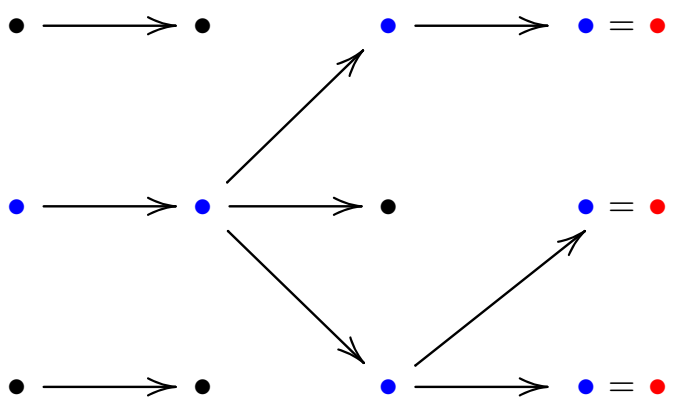

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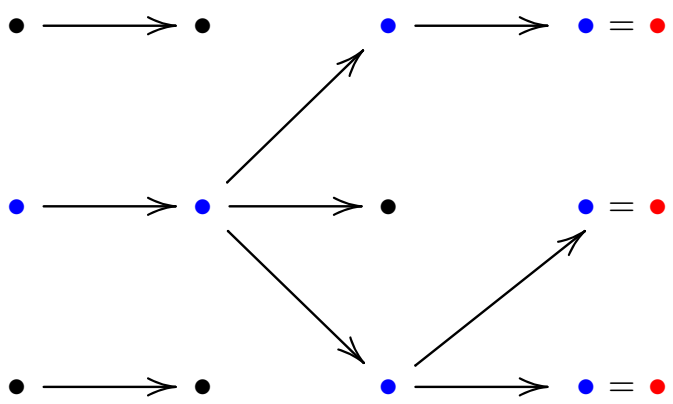

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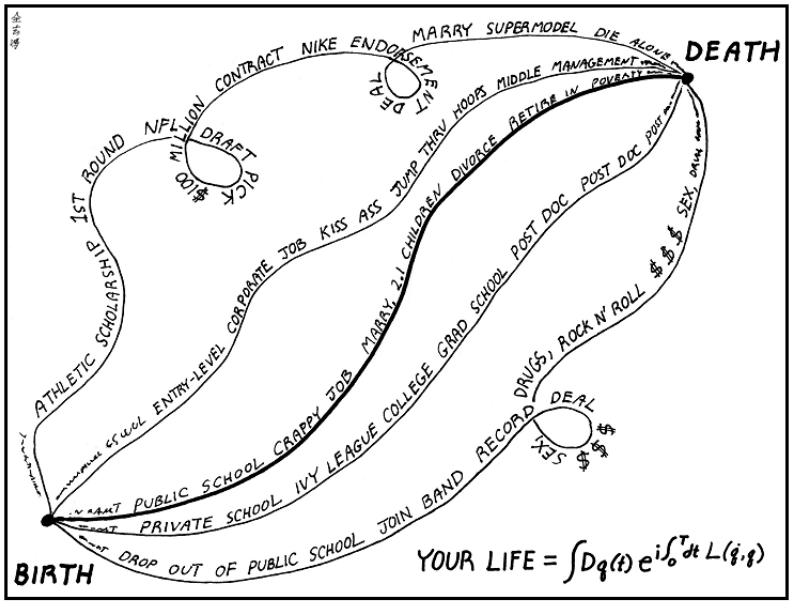
- **Normalizing constants of η_n and $\mathbb{Q}_n$** *[Unbias* MPRF 96*]*

$$\mathcal{Z}_n^N := \prod_{0 \leq p < n} \underbrace{\frac{1}{N} \sum_{1 \leq i \leq N} G_p(\xi_p^i)}_{\text{or proportions of successes}} \simeq \mathcal{Z}_n$$

A single limiting stochastic model $(\eta_n, \mathbb{Q}_n, \mathcal{Z}_n)$

Particle interpretation of Feynman-Kac path integrals



The Path Integral Formulation of Your Life

Summary

Feynman-Kac models ($\mathbb{P}\left(X_{n+1} \in dx \mid X_n\right) = M_{n+1}(X_n, dx)$)

$$d\mathbb{Q}_n := \frac{1}{\mathcal{Z}_n} \underbrace{\left\{ \prod_{0 \leq p < n} G_p(X_p) \right\}}_{\text{Weighted paths}} d\mathbb{P}_n \quad \text{with} \quad \mathbb{P}_n = \underbrace{\mathrm{Law}(X_0, \ldots, X_n)}_{\text{Free path evolution}}$$

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Sequential Monte Carlo reformulation

Target distributions :

$$\underbrace{\mathbb{Q}_{n+1}(d(x_0,\ldots,x_{n+1}))}_{\text{Target at time (n+1)}} \propto \underbrace{\mathbb{Q}_n(d(x_0,\ldots,x_n))}_{\text{Target at time (n)}} \times \underbrace{Q_{n+1}(x_n, dx_{n+1})}_{\geq 0 \text{ integral oper.}}$$

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Feynman-Kac model

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(Simple) Mean field interpretation

Nonlinear evolution equation

$$\eta_n = \Phi_n(\eta_{n-1}) \quad \text{for some mapping} \quad \Phi_n \ : \ \mathit{Proba} \rightsquigarrow \mathit{Proba}$$

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For Feynman-Kac models $=$ G_n**-Selection** & M_n**-Exploration**

Summary

The filtering problem $\subset$ Bayesian statistics

- X_t:=**Signal=Stochastic process (or r.v./parameter)**
  - Non cooperative targets (defense : missile, boat, plane,...).
  - Physics (Fluids : twisters, cyclones, ocean models, pressure/temperature/diffusion coefficients,...).
  - Finance (assets, portfolios, volatilities, default indexes,...).
  - Signal (speech, codes, informations transmissions, waves,...).
- Y_t=**Partial and Noisy observations of the signal X_t :**
  - Engineering : Radar, Sonar, GPS, ...
  - Physics (sensors : pressure/temperature/...).
  - Finance (assets, portfolios,...).
  - Statistics (real data: medecine, pharmacology, politics, economics, web data...).

The filtering problem $\subset$ Bayesian statistics

- X_t:=**Signal=Stochastic process (or r.v./parameter)**
  - Non cooperative targets (defense : missile, boat, plane,...).
  - Physics (Fluids : twisters, cyclones, ocean models, pressure/temperature/diffusion coefficients,...).
  - Finance (assets, portfolios, volatilities, default indexes,...).
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Obj.: Compute/Sample/Estimate **inductively** the flow of measures

$$t \in \mathbb{R}_+ \quad \text{or} \quad t = n \in \mathbb{N} \longrightarrow \eta_t = \mathrm{Law}(X_t \mid Y_0, \ldots, Y_t)$$

Path space models = Smoothing

$$X_t = (X'_0, \ldots, X'_t) \in E_t$$

$$\Updownarrow \textbf{[State space enlargement]}$$

$$\eta_t = \mathrm{Law}(X_t \mid Y_0, \ldots, Y_t) = \mathrm{Law}((X'_0, \ldots, X'_t) \mid (Y_0, \ldots, Y_t))$$

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Equivalent terminologies :

- Data Assimilation (forecasting, fluids/ocean models).
- Hidden Markov Chains Models (HMM).
- Posterior=Law($X|Y$) (Prior=$\mathrm{Law}(X)$).

Feynman-Kac representations

$$Q_{n+1}(x_n, dx_{n+1}) = G_n(x_n) \times M_{n+1}(x_n, dx_{n+1}) = p(y_n|x_n) \times p(x_{n+1}|x_n)\ dx_{n+1}$$

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or

$$\begin{aligned}
Q_{n+1}(x_n, dx_{n+1}) &= \underbrace{\widehat{G}_n(x_n)}_{\|} \times \underbrace{\widehat{M}_{n+1}(x_n, dx_{n+1})}_{\|} \\
&:= \underbrace{M_{n+1}(G_{n+1})(x_n)}_{\|} \times \underbrace{\frac{M_{n+1}(x_n, dx_{n+1})\, G_{n+1}(x_{n+1})}{M_{n+1}(G_{n+1})(x_n)}}_{\|} \\
&= p(y_{n+1}|x_n) \times p(x_{n+1}|x_n, y_{n+1})\ dx_{n+1}
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or any change of measure

$$\begin{aligned} Q_{n+1}(x_n, dx_{n+1}) &= \underbrace{\frac{dQ_{n+1}(x_n, \cdot)}{dM'_{n+1}(x_n, \cdot)}(x_{n+1})}_{\|} \times M'_{n+1}(x_n, dx_{n+1}) \\ &= G_n(x_n, x_{n+1}) \times M'_{n+1}(x_n, dx_{n+1}) \end{aligned}$$

Particle filters $= N$ "individuals"/particles" s.t. at **any time**

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \delta_{\widehat{\xi_t^i}} = \mathrm{Law}(X_t \mid (Y_0, \ldots, Y_t))$$

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Adaptive learning/filtering scheme :

1. Prediction/Exploration $\rightsquigarrow$ Sampling N local transitions M_n.
2. Updating/Correction $\rightsquigarrow$ birth and death process = branching particle algo (fixed size N).
   - Kill/stop individuals/proposal with poor G_n-likelihood value.
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$\rightsquigarrow$ Path space models : $X_t = (X'_0,\ldots,X'_t)$
$\Rightarrow$ **Genealogical tree based learning algorithm :**

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \delta_{\text{i-th ancestral line(t)}} = \mathrm{Law}((X'_0,\ldots,X'_t) \mid (Y_0,\ldots,Y_t))$$

Rare event analysis

Typical problem :

$$\text{Probability}\,(\text{Critical event}) << 10^{-6}$$

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More interestingly :

1. *Static model :* Law(Variable | Critical event)
2. *Kinetic model :* Law(Random process | Critical event)

Examples :
High energy level crossing, physical/chemical gateways, critical excursions, black-box, inputs leading to critical outputs, calibration/regulation w.r.t. reference outputs, extreme values,. . .

Feynman-Kac representations

- **Physical/biological/economical stochastic process X_n :** atomic/molecular configurations fluctuations, queueing evolutions, communication network, portfolio and financial assets, ...
- **Potential function G_n :** Event restrictions, Energy/Hamiltonian potential functions, overflows levels, critical thresholds, epidemic propagations, radiation dispersion, ruin levels.

$$\text{The critical event} = \underbrace{\text{Cascade of (less rare) events}}_{\rightsquigarrow \text{ product of potential functions}}$$

$$\Downarrow$$

Feynman-Kac model

$$\mathcal{Z}_n = \mathbb{P}\left(\text{Cascade of } n \text{ intermediate events}\right)$$

$$\mathbb{Q}_n = \text{Law}(\text{r.v. or trajectory} \mid n \text{ intermediate events})$$

Rare event particle algorithm - Genetic algo with N individuals

- X_n-**Exploration** of the set of all randomness of the system (transitions, internal fluctuations, model errors/defects)
- G_n-**Branching-Selection-Duplication** of the simulated "individuals" leading the system evolving in a critical regime.

  Branching on "more likely" gateways to critical regimes.

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Unbias probability estimate :

$$\mathbb{P}(n \text{ successive events})$$

$$= \mathbb{P}(n\text{-th} \mid (n-1) \text{ preceding}) \times \ldots \times \mathbb{P}(\text{2nd} \mid \text{the first}) \times \mathbb{P}(\text{the first})$$

$$\simeq_{N\uparrow\infty} P_n^N := [\% \text{ success } (n-1) \rightsquigarrow n\ ] \times \ldots \times [\% \text{ success } 1 \rightsquigarrow 2\ ] \times [\% \text{ in } 1\ ]$$

Default tree = Particle genealogical trees

$$\text{Law(alea, states, trajectories} \mid n \text{ events)}$$
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Open questions :

Statistical analysis, correlations/"Sobol type" indexes, defaults trees analysis, control problems, prediction analysis, ...

Restrictions/confinements models

- **Non intersecting simple random walks on $\mathbb{Z}^d$**

$$\mathcal{Z}_n = \mathbb{P}\left(\forall p < q < n,\ X_p \neq X_q\right) = \frac{\#\{\text{not} \cap \text{walks length n}\}}{(2d)^n} \simeq \exp\left(c\ n\right)$$

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Particle models :

$\rightsquigarrow$ Accept-Reject interacting X-motions w.r.t. conditioning events

Terminal levels conditioning and excursion models

1. **Terminal level set conditioning :**

$$\mathbb{P}(V_n(X_n) \geq a) \quad \& \quad \mathrm{Law}((X_0, \ldots, X_n) \mid V_n(X_n) \geq a)$$

2. **Fixed terminal value :** $\mathrm{Law}_{\pi,K}((X_0, \ldots, X_n) \mid X_n = x_n)$.

3. **Critical excursion behavior :**
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Particle models :

1. Interacting X-transitions increasing the potential V_n.
2. Interacting M-transitions increasing the Metropolis type potential ratio $\frac{\pi(dx_2)K(x_2,dx_1)}{\pi(dx_1)M(x_1,dx_2)}$
3. Interacting X-excursions on gateways levels $\rightsquigarrow B$.

Some target Boltzmann-Gibbs measures

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Some key advantages

- "No burning, no need to study the stability of MCMC models".
- Stochastic adaptive grid approximation
- Nonlinear system $\rightsquigarrow$ positive - beneficial interactions.
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with **[Theorem:]** $V_n^N \simeq V_n$ **independent** centered Gaussian fields .

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- Local conditional iid samples $\oplus$ Stability of nonlinear sg
$\rightsquigarrow$ **New theory on Interacting/Mean field empirical processes**

Summary

Example : Black box type models

$$\begin{array}{rcl} X & = & \text{Inputs} \\ & = & \text{Random variables} \end{array} \longrightarrow$$

$$\longrightarrow \begin{array}{rcl} Y & = & \text{Outputs} \\ & = & f(X) \end{array}$$

- **Black boxes :**

  Numerical codes, or analytical mathematical models related to some physical/chemical/biological/... quantities

  $\hookleftarrow$ *queueing, telecommunication networks, fluid mechanical codes, hydro-dynamical codes, sismic models, netronics, population dynamic models, . . .*

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- **Inputs :** environmental (temperatures, wave characteristics, pressure variations, wind models, client arrivals), unknown parameters (material resistance characteristics, defaults), formalized model errors (incomplete models, environment interactions), control driving sequences in an optimal control loop (configurations, kinetic parameters).

- **Outputs :** default functions/measures (fissures, energy distributions, increase rates, critical level crossings), optimality criteria values (regulation loops, max. likelihood functions).

IFREMER Code : hydro. + mechanical

(contract ALEA INRIA-IFREMER 2010)

- **Inputs :** wave spectrums, forecasting data, temperature profiles, model uncertainties.

  (ex. of formalisation : a trajectory/profile is represented by a 2000-line Gaussian vector)

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Multiple level particle branching algorithm:

- MCMC Exploration (shaker) on energy level s_n
- Selection configurations with the s_{n+1} level ($\oplus$ adaptive choice)

Security and reliability of nuclear plants

(Contract CIFRE, ALEA-EDF R&D Industrial risks)

- **Inputs :** material defaults, injection temperature, model parameters. (ex. = vectors of 20 Gaussian variables)
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Multiple level branching/particle algorithm $s_n \downarrow$
$\oplus$ **Sensitivity analysis (input variable correlations)**

Watermarking & Digital fingerprinting

(ANR Nebbiano 06-09, INRIA ALEA-ASPI-TEMICS)

- **Random variables :** hidden message (fingerprint)
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Multiple level branching/particle algorithm with $s_n \downarrow$

Optic fiber communication networks

- DM + J. Garnier. Simulations of rare events in fiber optics by interacting particle systems. Optics Communications (2006).
- DM + J. Garnier. Genealogical particle analysis of rare events. Ann. Appl. Probab. (2005).

Stochastic model :

- **Elementary pulses X_k on the k-th segment of the optic fiber (fictitious) :** Soliton type pulse profiles.
- **Aleas :** ω_k = random perturbations in each sections.

  (speed mode dispersion fluctuations)

$$X_k = \underbrace{F_k(X_{k-1}, \omega_k)}_{\text{Nonlinear Schrödinger equation}}$$

Rare event: Energy type function $V(X_T)$ too large (pulse amplitude, modal dispersion , $\downarrow$ power).

$$\mathbb{P}\left(V(X_T) \geq a\right) \quad \& \quad \textbf{Law}\left((X_t)_{0 \leq t \leq T} \mid V(X_T) \geq a\ \right)$$

Optic fiber communication networks

Particle algorithm = Genetic type model with N individuals

- Free exploration : $X_{t-1} \rightsquigarrow X_t = F_t(X_{t-1}, \omega_t)$.
- Selection of $\uparrow$ transition levels (criteria $(V(X_t) - V(X_{t-1}))$)

Food risk & Epidemic propagations

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Kinetic/Compartmental models $\sim$ unknown parameters Θ (exchange rates, kinetic constants) :

$$X_k = F_k(X_{k-1}, \omega_k, \Theta)$$

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- Calibration : partial and noisy observations (web/statistical data)

  $\rightsquigarrow$ **Particle filters, Sequential Monte Carlo methods.**

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$$X_k = F_k(X_{k-1}, \omega_k, \Theta)$$

- Calibration : partial and noisy observations (web/statistical data)
  $\rightsquigarrow$ **Particle filters, Sequential Monte Carlo methods.**
- Risk analysis: High level characteristic function $V(X) > a$, excursions in critical regimes,...
  $\rightsquigarrow$ **Same type of particle algorithms (branching, selection)**