Particle Monte Carlo methods in statistical learning and rare event simulation

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Some hyper-refs

- Feynman-Kac formulae, Genealogical & Interacting Particle Systems with appl., Springer (2004)
- Sequential Monte Carlo Samplers JRSS B. (2006). (joint work with Doucet & Jasra)
- On the concentration of interacting processes. Foundations & Trends in Machine Learning (2012). (joint work with Hu & Wu) [+ Refs]
- More references on the website http://www.math.u-bordeaux1.fr/~delmoral/index.html [+ Links]

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Stochastic particle sampling methods

Interacting jumps models Genetic type interacting particle models Particle Feynman-Kac models The 4 particle estimates Island particle models (⊂ Parallel Computing)

Bayesian statistical learning

Nonlinear filtering models Fixed parameter estimation in HMM models Particle stochastic gradient models Approximate Bayesian Computation Interacting Kalman-Filters Uncertainty propagations in numerical codes

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Concentration inequalities

Current population models Particle free energy Genealogical tree models Backward particle models

Stochastic particle sampling methods

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Bayesian statistical learning

Concentration inequalities

Introduction

Stochastic particle methods = Universal adaptive sampling technique

2 types of stochastic interacting particle models:

- Diffusive particle models with mean field drifts [McKean-Vlasov style]
- Interacting jump particle models
 [Boltzmann & Feynman-Kac style]

Lectures \subset Interacting jumps models

- Interacting jumps = Recycling transitions =
- ► Discrete time models (⇔ geometric rejection/jump times)





Genetic type interacting particle models

- Mutation-Proposals w.r.t. Markov transitions $X_{n-1} \rightsquigarrow X_n \in E_n$.
- ► Selection-Rejection-Recycling w.r.t. potential/fitness function G_n.





Equivalent 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 proposals	Accept-reject-recycle

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More botanical names:

bootstrapping, spawning, cloning, pruning, replenish, multi-level splitting, enrichment, go with the winner, ...

1950 \leq Meta-Heuristic style stochastic algorithms \leq 1996

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A single stochastic model

Particle interpretation of Feynman-Kac path integrals





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Genealogical tree evolution (Population size, Time horizon)=(N, n) = (3, 3)





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$$\mathbb{Q}_n := rac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \le p < n} G_p(X_p) \right\} \quad \mathbb{P}_n \quad \text{with} \quad \mathbb{P}_n := \operatorname{Law}(X_0, \dots, X_n)$$

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Example

$$G_n = 1_{A_n} \to \mathbb{Q}_n = \operatorname{Law}((X_0, \dots, X_n) \mid X_p \in A_p, \ p < n)$$

More formally

 $(\xi_{0,n}^{i}, \xi_{1,n}^{i}, \dots, \xi_{n,n}^{i}) := i$ -th ancetral line of the *i*-th current individual $= \xi_{n}^{i}$

$$\downarrow \\ \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\left(\xi_{0,n}^{i},\xi_{1,n}^{i},\ldots,\xi_{n,n}^{i}\right)} \longrightarrow_{N \to \infty} \mathbb{Q}_{n}$$

More formally

 $\begin{aligned} & \left(\xi_{0,n}^{i},\xi_{1,n}^{i},\ldots,\xi_{n,n}^{i}\right) := i\text{-th ancetral line of the }i\text{-th current individual} = \xi_{n}^{i} \\ & \downarrow \\ & \frac{1}{N}\sum_{1\leq i\leq N}\delta_{\left(\xi_{0,n}^{i},\xi_{1,n}^{i},\ldots,\xi_{n,n}^{i}\right)} \longrightarrow_{N\to\infty} \mathbb{Q}_{n} \end{aligned}$

 \oplus Current population models

$$\eta_n^N := \frac{1}{N} \sum_{1 \le i \le N} \delta_{\xi_n^i} \longrightarrow_{N \to \infty} \eta_n = n \text{-th time marginal of } \mathbb{Q}_n$$

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More formally

 $\begin{pmatrix} \xi_{0,n}^{i}, \xi_{1,n}^{i}, \dots, \xi_{n,n}^{i} \end{pmatrix} := i\text{-th ancetral line of the } i\text{-th current individual} = \xi_{n}^{i}$ \downarrow $\frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\left(\xi_{0,n}^{i}, \xi_{1,n}^{i}, \dots, \xi_{n,n}^{i}\right)} \longrightarrow_{N \to \infty} \mathbb{Q}_{n}$

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 \oplus Unbiased particle approximation

$$\mathcal{Z}_n^{N} = \prod_{0 \le p < n} \eta_p^{N}(G_p) \longrightarrow_{N \to \infty} \mathcal{Z}_n = \mathbb{E}\left(\prod_{0 \le p < n} G_p(X_p)\right) = \prod_{0 \le p < n} \eta_p(G_p)$$

More formally

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Ex.: $G_n = 1_{A_n} \rightsquigarrow \mathcal{Z}_n^N = \prod \text{ proportion of success} \longrightarrow \mathbb{P}(X_p \in A_p, p < n)$



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Complete ancestral tree when $M_n(x, dy) = H_n(x, y) \lambda(dy)$

Backward Markov chain model

$$\mathbb{Q}_n^{\mathcal{N}}(d(x_0,\ldots,x_n)) := \eta_n^{\mathcal{N}}(dx_n) \mathbb{M}_{n,\eta_{n-1}^{\mathcal{N}}}(x_n,dx_{n-1})\ldots \mathbb{M}_{1,\eta_0^{\mathcal{N}}}(x_1,dx_0)$$

with the random particle matrices:

 $\mathbb{M}_{n+1,\eta_n^{\mathsf{N}}}(x_{n+1},dx_n) \propto \eta_n^{\mathsf{N}}(dx_n) \ G_n(x_n) \ H_{n+1}(x_n,x_{n+1})$

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Example: Normalized additive functionals

$$\mathbf{f_n}(x_0, \dots, x_n) = \frac{1}{n+1} \sum_{0 \le p \le n} f_p(x_p)$$
$$\bigcup_n^{\mathbf{N}} (\mathbf{f_n}) := \frac{1}{n+1} \sum_{0 \le p \le n} \eta_n^{\mathbf{N}} \underbrace{\mathbb{M}_{n,\eta_{n-1}^{\mathbf{N}}} \dots \mathbb{M}_{p+1,\eta_p^{\mathbf{N}}}(f_p)}_{\text{matrix operations}}$$



with the Island evolution Markov chain model

$$\mathcal{X}_n := \eta_n^N$$
 and $\mathcal{G}_n(\mathcal{X}_n) = \eta_n^N(\mathbf{G}_n) = \mathcal{X}_n(\mathbf{G}_n)$
 \Downarrow

particle model with $(\mathcal{X}_n, \mathcal{G}_n(\mathcal{X}_n)) =$ Interacting Island particle model

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Bayesian statistical learning

Nonlinear filtering models Fixed parameter estimation in HMM models Particle stochastic gradient models Approximate Bayesian Computation Interacting Kalman-Filters Uncertainty propagations in numerical codes

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Concentration inequalities

Bayesian statistical learning



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Signal processing & filtering models

Law (Markov process $X \mid$ Noisy & Partial observations Y)



- Signal X : target evolution (missile, plane, robot, vehicle, image contours), forecasting models, assets volatility, speech signals, ...
- Observation Y : Radar/Sonar/Gps sensors, financial assets prices, image processing, audio receivers, statistical data measurements, ...

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⊂ Multiple objects tracking models (highly more complex pb)

- On the Stability and the Approximation of Branching Distribution Flows, with Applications to Nonlinear Multiple Target Filtering. Francois Caron, Pierre Del Moral, Michele Pace, and B.-N. Vo (HAL-INRIA RR-7376) [50p]. Stoch. Analysis and Applications Volume 29, Issue 6, 2011.
- Comparison of implementations of Gaussian mixture PHD filters. M. Pace, P. Del Moral, Fr. Caron 13th International Conference on Information. FUSION, EICC, Edinburgh, UK, 26-29 July (2010)

$$\operatorname{Law}\left(X = \sum_{1 \leq i \leq N_{t}^{X}} \delta_{X_{t}^{i}} \quad \middle| \quad Y = \sum_{1 \leq i \leq N_{t}^{Y}} \delta_{Y_{t}^{i}}\right)$$

Filtering (prediction \oplus smoothing)

$$p((x_0,...,x_n) | (y_0,...,y_n)) \& p(y_0,...,y_n) ?$$

Bayes' rule

$$p((x_0,\ldots,x_n) \mid (y_0,\ldots,y_n)) \propto \underbrace{p((y_0,\ldots,y_n) \mid (x_0,\ldots,x_n))}_{\prod_{0 \leq k \leq n} p(y_k \mid x_k) \leftarrow \text{likelihood functions } G_k} \times p(x_0,\ldots,x_n)$$

Filtering (prediction \oplus **smoothing)**

$$p((x_0,...,x_n) | (y_0,...,y_n)) \& p(y_0,...,y_n)$$
?

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Feynman-Kac models : $G_n(x_n) := p(y_n|x_n) \& \mathbb{P}_n := \operatorname{Law}(X_0, \dots, X_n)$

↓

$$\operatorname{Law}\left(\left(X_{0},\ldots,X_{n}\right) \mid Y_{p} = y_{p}, \ p < n\right) = \frac{1}{\mathcal{Z}_{n}} \left\{\prod_{0 \leq p < n} G_{p}(X_{p})\right\} \mathbb{P}_{n}$$

Filtering (prediction \oplus smoothing)

$$p((x_0,...,x_n) | (y_0,...,y_n)) \& p(y_0,...,y_n) ?$$

Bayes' rule

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Not unique stochastic model!

Hidden Markov chains problems

 $\Theta \rightsquigarrow \text{Signal} \ X^\Theta \rightsquigarrow \text{observations} \ Y^\Theta$



Law (fixed parameter $\Theta \mid$ Noisy & Partial observations Y^{Θ})

- ► Parameter ⊖ : kinetic model unknown parameters, statistical parameters (signal/sensors), hypothesis testing, ...
- ► Signal X^Θ: Single or multiple targets evolution, forecasting models, financial assets volatility, speech signals, video images, ...
- ► Observation Y^Θ: Radar/Sonar/Gps sensors, financial assets prices, image processing, statistical data measurements, ...

Posterior density

with

 $h_n(\theta) := p(y_n|\theta, (y_0, \dots, y_{n-1})) \quad \& \quad \lambda := \operatorname{Law}(\Theta)$

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First key observation

$$p((y_0,\ldots,y_n)|\theta) = \prod_{0\leq p\leq n} h_p(\theta) = \mathcal{Z}_n(\theta)$$

with the normalizing constant $Z_n(\theta)$ of the conditional distribution

$$p((x_0,...,x_n)|(y_0,...,y_n),\theta) = \frac{1}{p((y_0,...,y_n)|\theta)} p((y_0,...,y_n)|(x_0,...,x_n),\theta) p((x_0,...,x_n)|\theta)$$

Second key observation

 $h_n(\theta)$ and $\mathcal{Z}_n(\theta)$ easy to compute for linear/gaussian models

Third key observation : Any target measure of the form

$$\eta_n(d heta) = rac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \leq p \leq n} h_p(heta) \right\} imes \lambda(d heta)$$

is the *n*-th time marginal of the Feynman-Kac measure

$$\mathbb{Q}_n := \frac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \le p < n} G_p(\Theta_p) \right\} \quad \mathbb{P}_n$$

with

$$G_n = h_{n+1}$$
 and $\mathbb{P}_n := \operatorname{Law}(\Theta_0, \dots, \Theta_n)$

where

 $\Theta_{p-1} \rightsquigarrow \Theta_p$ as an MCMC move with target measure η_p

Particle auxiliary variables $\theta \rightsquigarrow \xi^{\theta} \sim P(\theta, d\xi)$

$$\overline{\eta}_n(d\overline{\theta}) \propto \left\{ \prod_{0 \le p \le n} \overline{h}_p(\overline{\theta}) \right\} \underbrace{\overline{\lambda}(d\overline{\theta})}_{=\lambda(d\theta) \times P(\theta, d\xi)}$$

with $\overline{\theta} = (\theta, \xi)$ and

$$\overline{h}_n(\overline{\theta}) := \frac{1}{N} \sum_{i=1}^N p(y_n \mid \xi_n^{\theta,i}) \simeq_{N\uparrow\infty} p(y_n \mid \theta, (y_0, \dots, y_{n-1})) = h_p(\theta)$$

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But by the unbiased property the θ -marginal of $\overline{\eta}_n$ coincides with

$$\operatorname{Law}\left(\Theta \mid (y_0, \ldots, y_n)\right) \propto \left\{\prod_{0 \leq p \leq n} h_p(\theta)\right\} \quad \lambda(d\theta)$$

Feynman-Kac formulation :

Ref. Markov chain $\overline{\Theta}_k = (\Theta_k, \xi^{(k)})$ MCMC with target $\overline{\eta}_n$ and $G_n = \overline{h}_{n+1}$

Particle steepest descent gradient models

$$\mathcal{Z}_n(\theta) = p((y_0, \dots, y_{n-1}) \mid \theta) = \mathbb{E}\left(\prod_{0 \le q < n} p(y_q \mid \theta, X_q^{\theta})\right)$$



Just after learning the frequest bescent needs in optimization optiss...

 $\nabla \log \mathcal{Z}_n(\theta) = \mathbb{Q}_n^{(\theta)}(\Lambda_n)$

with the Feynman-Kac measure $\mathbb{Q}_n^{(\theta)}$ on path space associated with

$$(X_n^{\theta}, G_n^{\theta}(x_n)) = (X_n^{\theta}, p(y_q \mid \theta, x_n))$$

and with the additive functional

$$\Lambda_n(x_0,\ldots,x_n) = \sum_{0 \le p < n} \nabla \log \left(p(x_{q+1}|\theta,x_q) p(y_q \mid \theta,x_q) \right)$$

Particle steepest descent gradient models

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Just after learning the Frequest basent netter in optimization chess ...

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~~ Particle gradient algorithm

$$\Theta_n = \Theta_{n-1} + \tau_n \, \mathbb{Q}_n^{(\theta)}(\Lambda_n) \simeq \Theta_{n-1} + \tau_n \, \mathbb{Q}_n^{(\theta), N}(\Lambda_n)$$

Approximate Bayesian Computation



When $p(y_n|x_n)$ is untractable or impossible to compute in reasonable time

$$\begin{cases} X_n = F_n(X_{n-1}, W_n) & \xrightarrow{\mathcal{X}_n = (X_n, Y_n)} \\ Y_n = H_n(X_n, V_n) & \xrightarrow{\mathcal{X}_n = (X_n, Y_n)} \\ & Y_n^{\epsilon} = Y_n + \epsilon V_n^{\epsilon} \end{cases} \\ \downarrow \\ \mathsf{Law} \left(X \mid Y^{\epsilon} = y \right) \simeq_{\epsilon \downarrow 0} \mathsf{Law} \left(X \mid Y = y \right) \\ & \downarrow \end{cases}$$

Feynman-Kac model with the Markov chain and the potentials :

$$\mathcal{X}_n = (X_n, Y_n)$$
 and $G_n(\mathcal{X}_n) = p(Y_n^{\epsilon}|Y_n)$

Interacting Kalman-Filters

$$X_n = (X_n^1, X_n^2) \text{ with } X_n^1 \text{ Markov and } (X_n^2, Y_n) | X^1 \text{ linear-gaussian model}$$
$$\begin{cases} X_n^2 &= A_n(X_n^1) X_{n-1}^2 + B_n(X_n^1) W_n \\ Y_n &= C_n(X_n^1) X_n^2 + D_n(X_n^1) V_n \\ & \downarrow \end{cases}$$

 $\mathsf{Law}\left(X_n^2 \ \left| \ X^1, \ Y_p = y_p, \ p < n\right.\right) = \eta_{X^1,n} = \mathrm{Kalman} \ \mathrm{gaussian} \ \mathrm{predictor}$

Interacting Kalman-Filters

$$X_n = (X_n^1, X_n^2) \text{ with } X_n^1 \text{ Markov and } (X_n^2, Y_n) | X^1 \text{ linear-gaussian model}$$

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 $\mathsf{Law}\left(X_n^2 \mid X^1, \ Y_p = y_p, \ p < n\right) = \eta_{X^1,n} = \mathrm{Kalman \ gaussian \ predictor}$

Integration over $X^1 \Rightarrow Law((X^1, X^2) \mid Y) =$ Feynman-Kac model

with the reference Markov chain and the gaussian potential

$$\mathcal{X}_{n} = (X_{n}^{1}, \eta_{X^{1}, n}) \& G_{n}(\mathcal{X}_{n}) = \int p(Y_{n} \mid (x_{n}^{1}, x_{n}^{2})) \eta_{X^{1}, n}(dx_{n}^{2})$$

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Uncertainty propagations in numerical codes



Law (Inputs $\mathcal{I} \mid$ Outputs $\mathcal{O} = C(\mathcal{I}) \in$ Reference or Critical event)

$$\mu = \operatorname{Law}(\mathcal{I}) A = \{\mathcal{I} : C(\mathcal{I}) \in B\} \} \longrightarrow \mathbb{P}(\mathcal{I} \in A) = \mu(A) \& \operatorname{Law}(\mathcal{I} \mid \mathcal{I} \in A) = \mu_A$$

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Uncertainty propagations in numerical codes



Law (Inputs $\mathcal{I} \mid$ Outputs $\mathcal{O} = C(\mathcal{I}) \in$ Reference or Critical event)

$$\begin{array}{l} \mu = \operatorname{Law}(\mathcal{I}) \\ A = \{\mathcal{I} : C(\mathcal{I}) \in B\} \end{array} \right\} \longrightarrow \mathbb{P}\left(\mathcal{I} \in A\right) = \mu(A) \& \operatorname{Law}\left(\mathcal{I} \mid \mathcal{I} \in A\right) = \mu_A \end{array}$$

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Multi-level decomposition

$$h_n = 1_{A_n} \text{ with } A_n \downarrow \implies \mu_{A_n}(dx) \propto \left\{ \prod_{0 \leq p \leq n} h_p(x) \right\} \ \mu(dx)$$

Feynman-Kac representation

 $(X_{n-1} \rightsquigarrow X_n) = \text{an MCMC move with target } \mu_{A_n} \quad \& \quad G_n = \mathbf{1}_{A_{n+1}}$

Stochastic particle sampling methods

Bayesian statistical learning

Concentration inequalities

Current population models Particle free energy Genealogical tree models Backward particle models

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Current population models

Constants (c_1, c_2) related to (bias,variance), c universal constant Test funct. $\|f_n\| \leq 1$

▶ \forall ($x \ge 0, n \ge 0, N \ge 1$), the probability of the event

$$\left[\eta_n^N - \eta_n\right](f) \le \frac{c_1}{N} \left(1 + x + \sqrt{x}\right) + \frac{c_2}{\sqrt{N}} \sqrt{x}$$

is greater than $1 - e^{-x}$.

►
$$x = (x_i)_{1 \le i \le d} \rightsquigarrow (-\infty, x] = \prod_{i=1}^d (-\infty, x_i]$$
 cells in $E_n = \mathbb{R}^d$.
 $F_n(x) = \eta_n (1_{(-\infty, x]}) \text{ and } F_n^N(x) = \eta_n^N (1_{(-\infty, x]})$

 $\forall \ (y \ge 0, n \ge 0, N \ge 1)$, the probability of the following event

$$\sqrt{N} \|F_n^N - F_n\| \le c \sqrt{d (y+1)}$$

is greater than $1 - e^{-x}$.

Particle free energy models

Constants (c_1, c_2) related to (bias, variance), c universal constant.

▶ \forall ($y \ge 0, n \ge 0, N \ge 1, \epsilon \in \{+1, -1\}$), the probability of the event

$$\frac{\epsilon}{n}\log\frac{\mathcal{Z}_n^N}{\mathcal{Z}_n} \le \frac{c_1}{N} \ \left(1 + x + \sqrt{x}\right) + \frac{c_2}{\sqrt{N}} \ \sqrt{x}$$

is greater than $1 - e^{-x}$.

Note : $(0 \le \epsilon \le 1 \Rightarrow (1 - e^{-\epsilon}) \lor (e^{\epsilon} - 1) \le 2\epsilon)$

$$e^{-\epsilon} \le \frac{z^N}{z} \le e^{\epsilon} \Rightarrow \left|\frac{z^N}{z} - 1\right| \le 2\epsilon$$

Genealogical tree models := η_n^N (in path space)

Constants (c_1, c_2) related to (bias,variance), c universal constant $\mathbf{f_n}$ test function $\|\mathbf{f_n}\| \leq 1$.

▶ \forall ($y \ge 0, n \ge 0, N \ge 1$), the probability of the event

$$\left[\eta_n^{\mathcal{N}}-\mathbb{Q}_n
ight](f)\leq c_1\;rac{n+1}{\mathcal{N}}\;\left(1+x+\sqrt{x}
ight)+c_2\;\sqrt{rac{(n+1)}{\mathcal{N}}}\;\sqrt{x}$$

is greater than $1 - e^{-x}$.

▶ \mathcal{F}_n = indicator fct. \mathbf{f}_n of cells in $\mathbf{E}_n = (\mathbb{R}^{d_0} \times ..., \times \mathbb{R}^{d_n})$ $\forall (y \ge 0, n \ge 0, N \ge 1)$, the probability of the following event

$$\sup_{\mathbf{f}_{\mathbf{n}}\in\mathcal{F}_n}\left|\eta_n^N(\mathbf{f}_{\mathbf{n}})-\mathbb{Q}_n(\mathbf{f}_{\mathbf{n}})\right|\leq c~(n+1)~\sqrt{\frac{\sum_{0\leq p\leq n}d_p}{N}}~(x+1)$$

is greater than $1 - e^{-x}$.

Backward particle models

Constants (c_1, c_2) related to (bias,variance), c universal constant. **f**_n normalized additive functional with $||f_p|| \le 1$.

▶ \forall ($x \ge 0, n \ge 0, N \ge 1$), the probability of the event

$$\left[\mathbb{Q}_n^N-\mathbb{Q}_n
ight](ar{\mathbf{f}}_n)\leq c_1\;rac{1}{N}\;(1+(x+\sqrt{x}))+c_2\;\sqrt{rac{x}{N(n+1)}}$$

is greater than $1 - e^{-x}$.

f_{a,n} normalized additive functional w.r.t. f_p = 1_{(-∞,a]}, a ∈ ℝ^d = E_n
 .
 ∀ (x ≥ 0, n ≥ 0, N ≥ 1), the probability of the following event

$$\sup_{\mathbf{a}\in\mathbb{R}^d} \left|\mathbb{Q}_n^N(\mathbf{f}_{\mathbf{a},\mathbf{n}}) - \mathbb{Q}_n(\mathbf{f}_{\mathbf{a},\mathbf{n}})\right| \leq c \ \sqrt{\frac{d}{N}}(x+1)$$

is greater than $1 - e^{-x}$.