# Speeding up Monte Carlo Integration: Control Neighbors for Optimal Convergence

**Rémi LELUC**

*Ecole Polytechnique, Institut Polytechnique de Paris, France*

Joint work with François Portier, Johan Segers and Aigerim Zhuman

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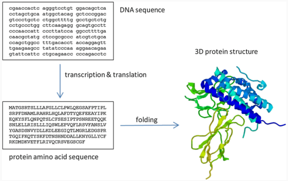
# Motivation: Machine Learning recent advances

AlphaGo (2016)



AlphaFold (2018)

GPT-3/4(2020/2023)

**"Intelligence"**

=

Data + Models + **Algorithms** + Computing Power

# Motivation: need for integral estimators

**Central Question:** *Integration*

Computation of an *integral* through probabilistic objective $\mathcal{F}$

$$\mathcal{F}(\theta) = \mathbb{E}_{\pi_\theta(x)}[f(x)] = \int_{\mathcal{X}} f(x)\pi_\theta(x)\mathrm{d}x. \quad (1)$$

**Main issue:** intractability and computational cost

- **(RL)** Trajectory $\tau = (s_0, a_0, \dots, s_{T-1}, a_{T-1})$ with policy $\pi_\theta$ and cumulative return $\mathcal{R}(\tau) = \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t)$.

$$\mathcal{F}(\theta) = \mathbb{E}_{\pi_\theta(\tau)}[\mathcal{R}(\tau)]$$

*(2016) AlphaGo A.I. beats champion Lee Sedol in Go.*

- **(VI)** $\mathcal{F}$ optimises the log-likelihood $\log p(x|z)$ under a regularization constraint which promotes closeness between the density $q$ and the prior distribution $p(z)$

$$\text{ELBO} = \mathcal{F}(\theta) = \mathbb{E}_{q_\theta(z|x)}[\log p(x|z)] - \text{KL}(q_\theta(z|x)||p(z)).$$

# Advantages of Random estimates

***Easy and Practical***

→ Requires only three steps: sampling, evaluating, averaging

***Randomness as a Strength***

→ Naturally escape local optima

→ Complete exploration of the search space

***Large-Scale learning***

→ simple, scalable, parallelizable

→ in supervised learning, deterministic gradient scales as $O(nd)$, stochastic version reduces to $O(d)$ operations

***Theoretical justifications***[1]

→ deterministic methods $O(n^{-s/d})$

→ optimal random procedure $O(n^{-1/2}n^{-s/d})$

[1](Novak, 2016): Some results on the complexity of numerical integration

# Integration $\mathcal{F}$

## Monte Carlo Integration & Variance Reduction

# Monte Carlo integration

### Underlying integration problem

Let $(\mathcal{X}, \mathcal{A}, \pi)$ be a probability space, $f : \mathcal{X} \to \mathbb{R}$ with $f \in L_2(\pi)$.

- **Goal:**

$$\pi(f) := \int_{\mathcal{X}} f(x)\pi(\mathrm{d}x) = \mathbb{E}_\pi[f(X)].$$

- **Constraints:** $f$ is unknown (black-box) or no approximation is sufficiently accurate, sampling from $\pi$ may be hard.

Let $X_1, ..., X_n \overset{\text{i.i.d.}}{\sim} \pi$, naive Monte Carlo estimator $\hat{\alpha}_n^{\mathrm{mc}}(f)$ of $\pi(f)$ is

$$\hat{\alpha}_n^{\mathrm{mc}}(f) := \frac{1}{n}\sum_{i=1}^{n} f(X_i) \tag{2}$$

### Research Questions

- How to reduce the variance of Monte Carlo estimates?
- How to sample from $\pi$?
- How to achieve optimal convergence rates?

Ref: Metropolis and Ulam (1949); Robert and Casella (1999); Evans and Swartz (2000); Glasserman (2004); Owen (2013); Novak (2016); Chopin and Gerber (2024)

# Complexity rates for integration error

**Definition: Root Mean Squared Error (RMSE)**

The error $\delta_n$ of a procedure $\hat{\alpha}_n(f)$ that approximates $\pi(f)$ is

$$\delta_n = \mathbb{E}\left[|\hat{\alpha}_n(f) - \pi(f)|^2\right]^{1/2}$$

$\rightarrow$ Lipschitz integrands[2], **optimal rate** in $O(n^{-1/2}n^{-1/d})$ (Novak, 2016)

| | |
|---|---|
| **OLS control variates** (Portier and Segers, 2019) | $O(n^{-1/2}m^{-1/d})$ |
| **Determinantal sampling** (Bardenet and Hardy, 2020) | $O(n^{-1/2}n^{-1/2d})$ |
| **Control Functionals** (Oates et al., 2017) | $O(n^{-7/12})$ |
| **Cubic Stratification** (Haber, 1966; Chopin and Gerber, 2024) | $O(n^{-1/2}n^{-1/d})$ |

[2] for integrand with $s$ bounded derivatives, rate in $O(n^{-1/2}n^{-s/d})$

# General view of Control Variates

## Control Functionals

- Build surrogate function $\hat{f}$ with known integral $\pi(\hat{f})$
- Use centered variables $\hat{f}(X_i) - \pi(\hat{f})$ to derive the following enhanced Monte Carlo estimate with control variates

$$\hat{\alpha}_n^{(CV)}(f) = \frac{1}{n}\sum_{i=1}^{n}\left\{f(X_i) - \left(\hat{f}(X_i) - \pi(\hat{f})\right)\right\}$$

## Approximation in $L_2(\pi)$

Let $(X_1, \dots X_n) \sim \pi$. Suppose that $\hat{f}$ depends only on a surrogate sample $\tilde{X}_1, \dots, \tilde{X}_N$ which is independent from $(X_1, \dots X_n)$, then

$$\mathbb{E}\left[|\hat{\alpha}_n^{(CV)}(f) - \pi(f)|^2\right] \leq \frac{1}{n}\mathbb{E}\left[\int (f - \hat{f})^2 \mathrm{d}\pi\right].$$

# Control Functionals examples

- **RKHS approximation:** (Oates, Girolami, and Chopin, 2017)

Ridge regression in Hilbert space $\mathcal{H}$

$$\hat{f} \in \arg\min_{\varphi \in \mathcal{H}} \frac{1}{N} \sum_{i=1}^{N} (f(\tilde{X}_i) - \varphi(\tilde{X}_i))^2 + \lambda \|\varphi\|_{\mathcal{H}}^2$$

- **Basis functions:** (Portier and Segers, 2019; Leluc et al., 2021)

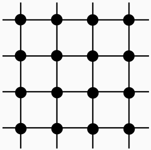
Use $m$ basis functions $h_1, \ldots, h_m$ to fit OLS:

$$\hat{f} = \hat{\beta}_n^\top h, \qquad \left(\hat{\alpha}_n, \hat{\beta}_n\right) = \arg\min_{(\alpha,\beta) \in \mathbb{R} \times \mathbb{R}^m} \|f^{(n)} - \alpha \mathbb{1}_n - H\beta\|_2^2$$

- **Partitioning and Stratification:** (Chopin and Gerber, 2024)

$(\tilde{X}_1, \ldots, \tilde{X}_N)$ is the $(1/\ell)$-equidistant grid of $[0,1]^d$ with $N = \ell^d$, $\ell \geq 1$ and $(R_i)_{i=1,\ldots,N}$ is the partition of $[0,1]^d$ made of the rectangles.

$$\hat{f}(x) = \sum_{i=1}^{N} f(\tilde{X}_i) \mathbb{1}_{R_i}(x)$$



# Nearest Neighbors

## Control Neighbors

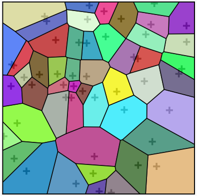
$$\hat{\alpha}_n^{(CVNN)}(f) = \frac{1}{n}\sum_{i=1}^{n}\left\{f(X_i) - \left(\hat{f}_n^{(i)}(X_i) - \pi(\hat{f}_n)\right)\right\}$$

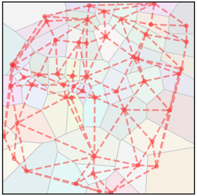
**Leave-one-out Nearest Neighbors:**

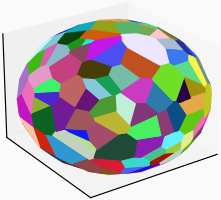
Take same sample $(X_1, \ldots, X_n)$ and define

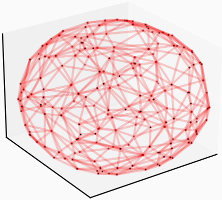
$$\hat{f}_n(x) = \sum_{j=1}^{n} f(X_j)\mathbb{1}_{S_{n,j}}(x), \qquad \hat{f}_n^{(i)}(x) = \sum_{j\neq i} f(X_j)\mathbb{1}_{S_{n,j}^{(i)}}(x)$$

where $S_{n,j}$ are **Voronoï cells**









# Control Neighbors properties

## Control Neighbors

$$\hat{\alpha}_n^{(CVNN)}(f) = \frac{1}{n}\sum_{i=1}^{n}\left\{f(X_i) - \left(\hat{f}_n^{(i)}(X_i) - \pi(\hat{f}_n)\right)\right\}$$

- (a) (Same framework as naive MC) does not require the existence of control variates with known integrals
- (b) (Quadrature Rule) $\hat{\alpha}_n = \sum_{i=1}^{n} w_{n,i} f(X_i)$, for **quadrature weights** $w_{n,i}$ **that do not depend on the function** $f$.
- (c) (Practical tool box) The weights $w_{n,i}$ are built using efficient nearest neighbors estimates (Bentley, 1975; Pedregosa et al., 2011)

## Complexity rate for integration error of Control Neighbors

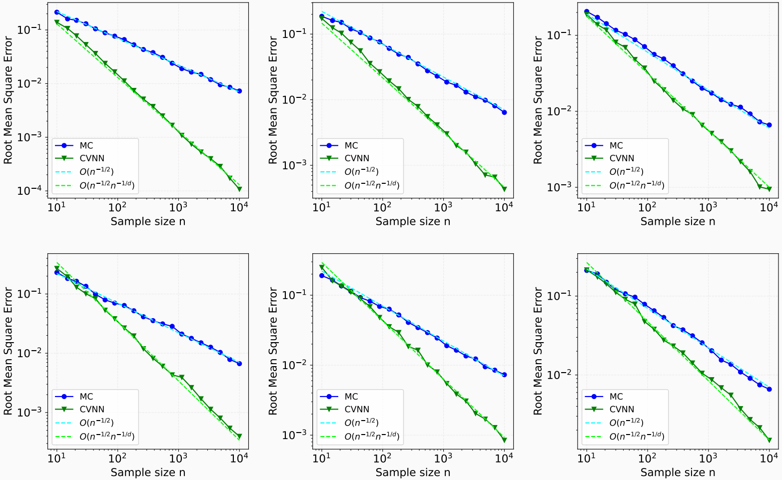
$$\mathbb{E}\left[|\hat{\alpha}_n^{(CVNN)}(f) - \pi(f)|^2\right]^{1/2} \lesssim n^{-1/2} n^{-s/d}$$

$$|\hat{\alpha}_n^{(CVNN)}(f) - \pi(f)| \lesssim \sqrt{\log(1/\varepsilon)}(\log n)^{1+s/d} n^{-1/2} n^{-s/d}$$

(with proba greater than $1-\varepsilon$)

# Control Neighbors on synthetic integrands

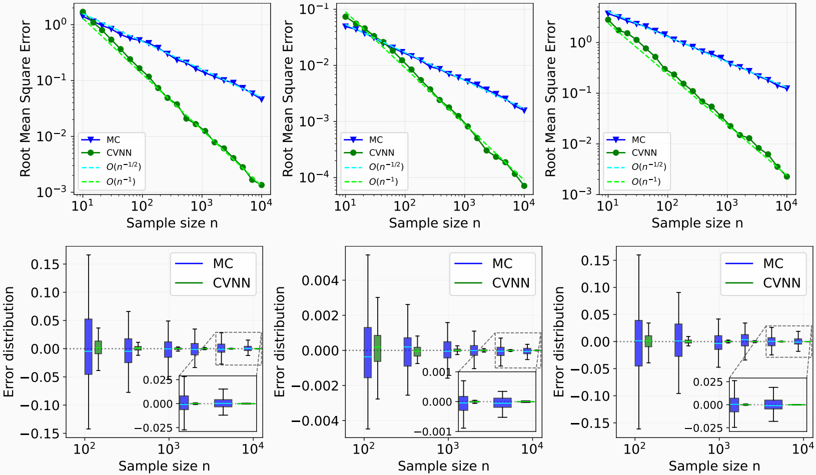
- $f_1(x_1, \ldots, x_d) = \sin(\pi(\frac{2}{d}\sum_{i=1}^{d} x_i - 1))$ with $\pi = \mathbb{1}_{[0,1]^d}$
- $f_2(x_1, \ldots, x_d) = \sin(\frac{\pi}{d}\sum_{i=1}^{d} x_i)$ with $\pi = \mathcal{N}_d(0, I_d)$




Error curves for $f_1$(top) and $f_2$(bottom) with $d \in \{2; 3; 4\}$

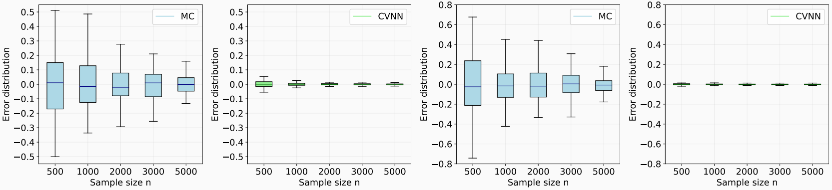
# Control Neighbors on Sphere $\mathbb{S}^2$

$$f_3(x,y,z) = \cos(x+y+z),\ f_4(x,y,z) = \cos(x)\cos(y)\cos(z),\ f_5(x,y,z) = \exp(x-y)$$

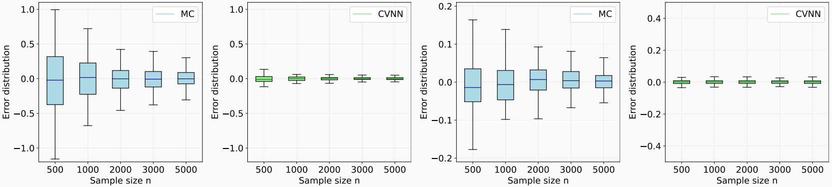



RMSE and boxplots for $f_3$(left), $f_4$(center) and $f_5$(right)

# Control Neighbors for Option Pricing




Black-Scholes model with spot price $S_0 = 100$, strike $K = S_0$, maturity $T = 2$ months, risk-free rate $r = 0.1$, constant volatility $\sigma = 0.3$, barrier price $H = 130$.(left: "Up-In"/right: "Up-Out")

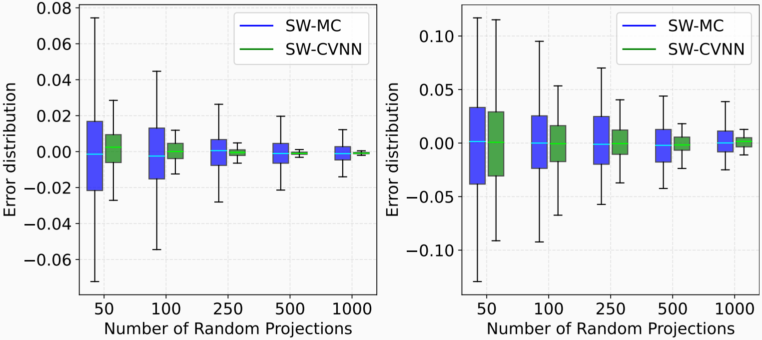



Heston Model with spot ptice $S_0 = 100$, strike $K = S_0$, barrier price $H = 130$, maturity $T = 2$ months, risk-free rate $r = 0.1$, initial volatility $v_0 = 0.1$, long-run average variance $\theta = 0.02$, rate of mean reversion $\kappa = 4$, instanteneous correlation $\rho = 0.8$ and volatility of volatility $\xi = 0.9$.(left: "Up-In"/right: "Up-Out")

# Control Neighbors for Sliced-Wasserstein

• Compare standard Monte Carlo estimate (SW-MC) with the proposed control neighbors estimate (SW-CVNN) when computing the Sliced-Wasserstein distance between two Gaussian distributions $SW_2(P, Q)$.

•$P = \mathcal{N}_q(m_X, \sigma_X^2 \mathrm{I}_q)$ and $Q = \mathcal{N}_q(m_Y, \sigma_Y^2 \mathrm{I}_q)$, $m_X, m_Y \sim \mathcal{N}(0, \mathrm{I}_q)$ and $\sigma_X = 2$ and $\sigma_Y = 5$, empirical distributions $P_m$ and $Q_m$ based on $m = 2\,000$ samples, $n \in \{50; 100; 250; 500; 1000\}$.




Boxplots of Sliced-Wasserstein estimates SW-MC and SW-CVNN for Gaussian distributions on $\mathbb{R}^q$ with $q \in \{3; 6\}$. The boxplots are obtained over $100$ replications.

# Conclusion

- We have explored the use of **nearest neighbors** in the construction of control variates for variance reduction in Monte Carlo integration.

- We have shown that for Hölder integrands of regularity $s \in (0, 1]$ on bounded metric spaces of dimension $d$ as measured by a sufficiently regular probability distribution, a **faster rate of convergence**, in $\mathcal{O}(n^{-1/2} n^{-s/d})$ as $n \to \infty$, is possible through the construction of a control variate via leave-one-out neighbors.

- (**Theory**) Theoretical guarantees are given both in terms of bounds on the root mean squared error and as concentration inequalities (requiring an additional logarithmic factor).

- (**Practice**) In numerical experiments, the method enjoyed a notable error reduction with respect to Monte Carlo integration.

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