Control Variates Selection for Monte-Carlo Integration

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Joint work with François Portier and Johan Segers

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Machine Learning Summer School (MLSS) 2020

Outline

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Introduction

- Solve deterministic problems by a stochastic approach

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- Simple, Flexible, Scalable

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- Solve deterministic problems by a stochastic approach
- Simple, Flexible, Scalable
- Many fields of applications that include: physical science, engineering, climate change, biology, applied statistics, artificial intelligence for games, finance and business.

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- Evaluate the function at nodes $f(X_1), \ldots, f(X_n)$.
- Compute an approximation of $P(f)$ based on $((X_1, f(X_1)), \ldots, (X_n, f(X_n)))$.

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- Let $X_1, ..., X_n \overset{\text{i.i.d}}{\sim} P$ be an independent random sample from P on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The naive Monte-Carlo estimator of $P(f)$ is given by the empirical mean

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- The Monte-Carlo estimator $P_n(f)$ of $P(f)$ is unbiased and has variance $\sigma^2(f)/n$, where $\sigma^2(f) = P[(f - P(f))^2]$. By the central limit theorem, we have the convergence in distribution

$$\boxed{\sqrt{n}(P_n(f) - P(f)) \xrightarrow[n \to +\infty]{d} \mathcal{N}(0, \sigma^2(f))}$$

Popular Methods

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- Control variates

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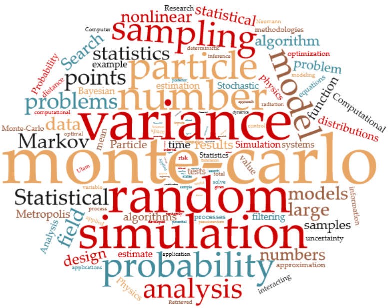
- Antithetic variates
- Control variates
- Importance sampling
- Sequential Monte-Carlo/MCMC



Books: **Evans** (Approximating integrals via Monte Carlo and deterministic methods,2000), **Robert** (Monte Carlo Statistical Methods,2005), **Glasserman** (Monte Carlo Methods in Financial Engineering,2003)

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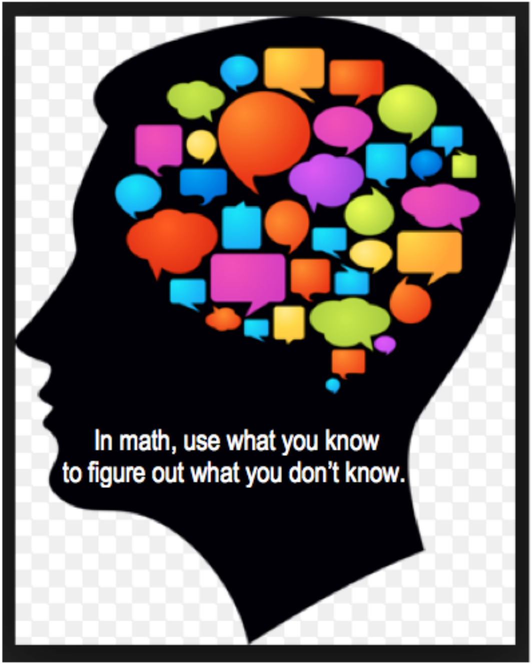
In math, use what you know
to figure out what you don't know.

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- The control variates are functions $h_1, ...h_m \in L^2(P)$ with known expectations. Assume that $P(h_k) = 0$ for all $k = 1, ..., m$. Let $h = (h_1, \ldots, h_m)^T$ denote the $\mathbb{R}^m$-valued function with the m control variates as elements.

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- For $\beta = (\beta_1, \dots, \beta_m)^T \in \mathbb{R}^m$, $P(f - \beta^T h) = P(f)$, so $P_n(f - \beta^T h)$ is an unbiased estimator of $P(f)$.

Control Variates estimator

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- Class of Monte-Carlo estimators

$$\boxed{\hat{I}_n^{(\mathrm{cv})}(f,\beta) = \frac{1}{n}\sum_{i=1}^{n}\left\{f(X_i) - \beta^T h(X_i)\right\}}, (\beta \in \mathbb{R}^m)$$

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- Minimize the variance to find optimal β

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- If $\beta^*(f)$ would be known, the use of control variates would always reduce the variance of the basic Monte Carlo estimator.

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- The integral $P(f)$ thus appears as the intercept of a linear regression model with response f and explanatory variables $h_1, \ldots, h_m$,

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- (Hilbert projection) Normal equation: $P(hh^T)\beta^\star(f) = P(hf)$
- Need to estimate the Gram matrix $P(hh^T)$ and $P(hf)$

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- $f^{(n)} = (f(X_1), \ldots, f(X_n))^T \in \mathbb{R}^n$ is the vector of evaluations of f.
- $\mathbb{1}_n = (1, \ldots, 1)^T \in \mathbb{R}^n$, $\|\cdot\|_2$ denotes the Euclidean norm and H is the random $n \times m$ matrix defined by $H = \left(h_j(X_i)\right)_{\substack{i=1,\ldots,n \\ j=1,\ldots,m}}$.

$$\boxed{\hat{\alpha}_n^{\mathrm{ols}}(f) = P_n[f - \hat{\beta}_n^{\mathrm{ols}}(f)^T h] = \sum_{i=1}^n w_{n,i} f(X_i)}$$

Control Variates in the literature

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- Variance reduction via regularization $\hookrightarrow$ **Regularised Zero-Variance Control Variates for High-Dimensional Variance Reduction**, South, L. F., C. J. Oates, A. Mira, and C. Drovandi (2018)

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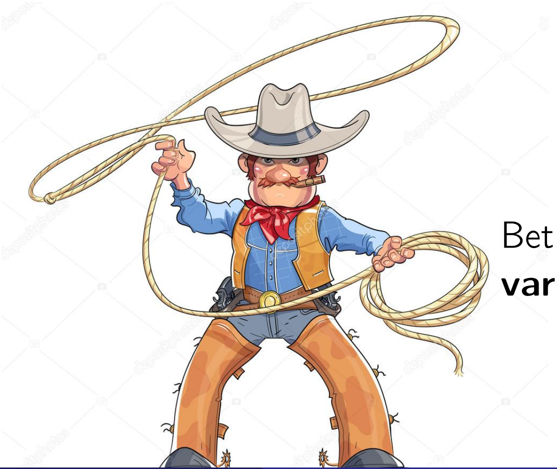

Bet on sparsity

variable selection !

Lasso Monte-Carlo (LASSOMC)

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- Adding ℓ_1-penalization leads to

$$\boxed{\left(\hat{\alpha}_n^{\mathrm{lasso}}(f), \hat{\beta}_n^{\mathrm{lasso}}(f)\right) = \operatorname*{arg\,min}_{(\alpha,\beta)\in\mathbb{R}\times\mathbb{R}^m} \frac{1}{2n}\|f^{(n)} - \alpha\mathbb{1}_n - H\beta\|_2^2 + \lambda\|\beta\|_1}$$

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- Lasso takes advantage of *sparse* regression models.The *active set* associated to the coefficient vector $\beta \in \mathbb{R}^m$ is

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- The number of elements in $S^\star = S(\beta^\star(f))$, denoted by $\ell^\star := |S^\star|$, quantifies the level of sparsity associated to the regression model.

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- Lasso to select the active variables among a large number of control variates, then compute OLSMC using only the variables selected at the previous stage.
- Let $\hat{S} = \{k \in \{1, \ldots, m\} : \hat{\beta}^{\text{lasso}}_{N,k}(f) > 0\}$ denote the estimated active set of control variates based on the subsample of size N. The LSLASSOMC estimate $\hat{\alpha}^{\text{lslasso}}_n(f)$ of $P(f)$ is defined by

$$\boxed{\left(\hat{\alpha}^{\text{lslasso}}_n(f), \hat{\beta}^{\text{lslasso}}_n(f)\right) \in \operatorname*{arg\,min}_{(\alpha,\beta)\in\mathbb{R}\times\mathbb{R}^{\hat{\ell}}} \|f^{(n)} - \alpha \mathbb{1}_n - H_{\hat{S}}\beta\|_2^2}$$

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Non-asymptotic Error Analysis

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Assumptions: **sub-gaussian** residuals with factor τ, **linearly independent** and **bounded** control variates, appropriate λ
$(U_h = \max_{j=1,\dots,m} \sup_{x \in \mathcal{X}} |h_j(x)|, \gamma = \lambda_{\min}(G), \zeta_h = U_h^2/\gamma)$

Concentration inequalities (Leluc,Portier,Segers, 2019)

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- Methods in competition: OLSMC, LassoMC, LSLassoMC(X)

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d	k	Degree threshold				
		1	3	5	10	12
3	12	3	19	55	285	454
5	10	5	55	251	3 001	6 157
8	3	8	164	1 214	20 993	36 813

Table: Number of control variates by degrees

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- initialize $\lambda = \lambda_{max}$ and decrease it to have more and more control variates until their number lies in the range $[c_1\sqrt{n}, c_2\sqrt{n}]$.

Numerical experiments

- λ is selected by imposing a lower bound and an upper bound on the number of activated random variables $\rightarrow$ dichotomic search.
- initialize $\lambda = \lambda_{max}$ and decrease it to have more and more control variates until their number lies in the range $[c_1\sqrt{n}, c_2\sqrt{n}]$.

n	N	$\lfloor 3\sqrt{n} \rfloor$	$\lfloor 12\sqrt{n} \rfloor$
2 000	700	134	536
5 000	1 000	212	848
10 000	2 000	300	1 200

Table: Parameters setting with range $(c_1\sqrt{n}, c_2\sqrt{n})$ of selected control variates.

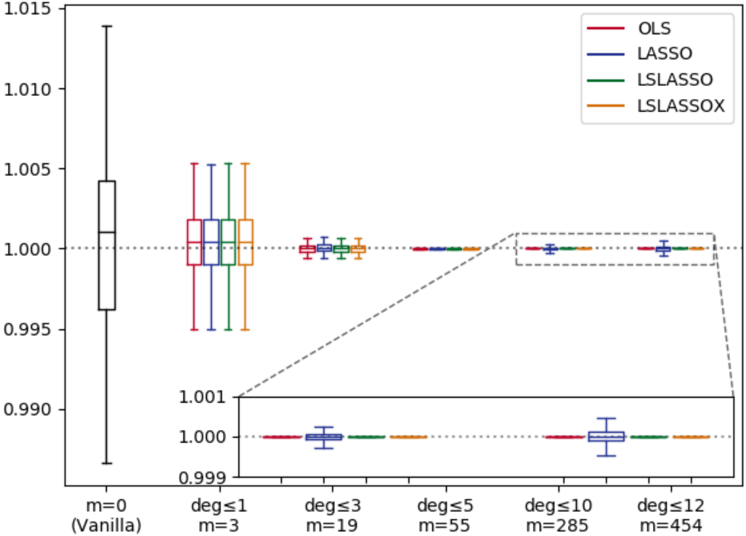

Figure: $\varphi, d = 3, n = 10\,000, N = 2\,000$.

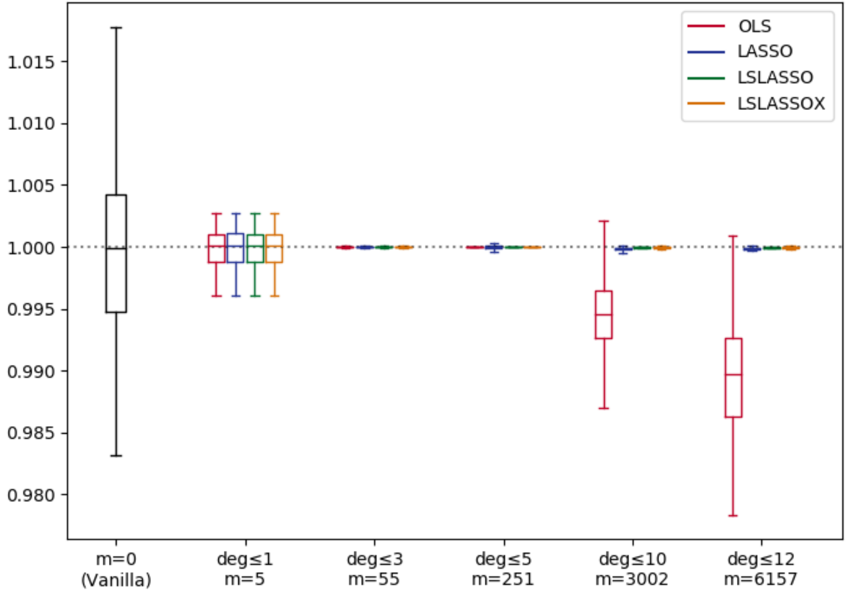

Figure: $g_3, d = 5, n = 2\,000, N = 700.$

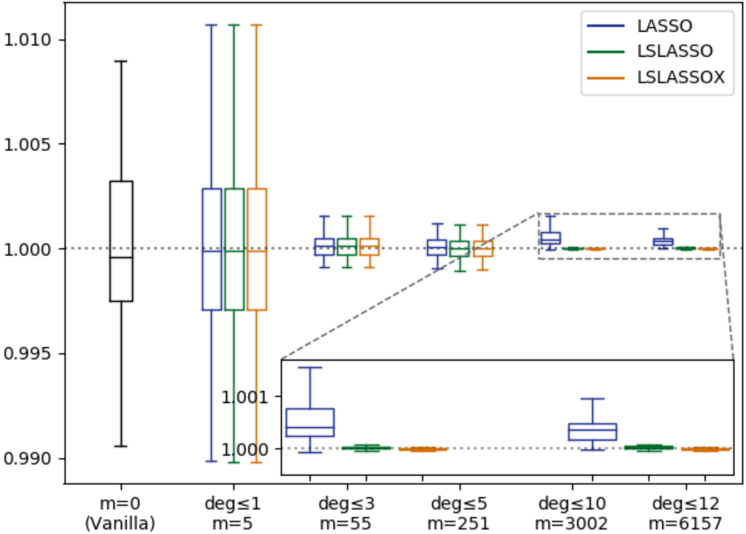

Figure: $f_1, d = 5, n = 5\,000, N = 1\,000.$

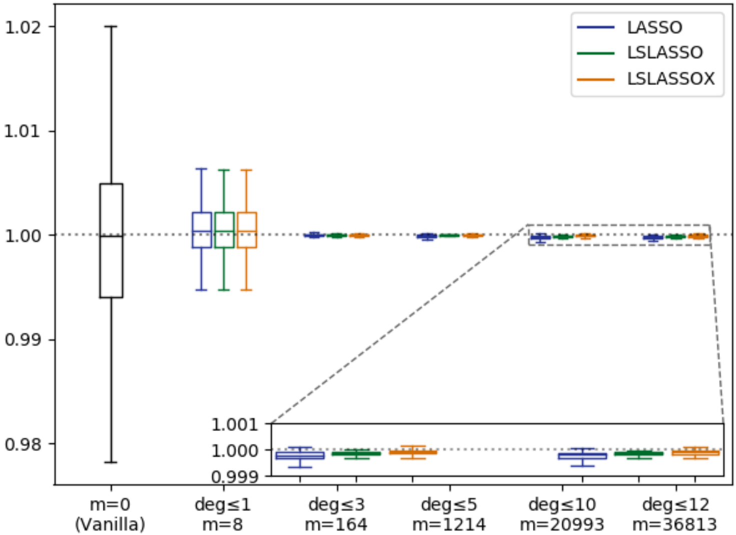

Figure: $g_4, d = 8, n = 2\,000, N = 700.$

Outline

Conclusion

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- The particular variance reduction technique of control variates offers many advantages as it relies on a simple and intuitive paradigm.
- Regularizing the ordinary least squares estimator by preselecting appropriate control variates via the Lasso turns out to increase the accuracy without additional computational cost.
- The proposed numerical method performs better than any other state of the art method.

Questions and Answers

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Assumptions

- The control variates $h_1, \dots, h_m \in L^2(P)$ are **linearly independent**. As a consequence, the **Gram matrix** $G := P(hh^T) \in \mathbb{R}^m$ is **positive definite** and its smallest eigenvalue $\gamma := \lambda_{\min}(G)$ is positive.
- The residual function $\epsilon = f - P(f) - \beta^\star(f)^T h$ satisfies $\epsilon \in \mathcal{G}(\tau^2)$ for some $\tau > 0$, that is, $\int_{\mathcal{X}} \exp(\lambda x)\, \epsilon(x)\, P(dx) \leq \exp(\lambda^2 \tau^2 / 2), \forall \lambda \in \mathbb{R}$.
- The control variates $h_1, \dots, h_m \in L^2(P)$ are **uniformly bounded**. Put $U_h := \max_{j=1,\dots,m} \sup_{x \in \mathcal{X}} |h_j(x)|$
- We have **orthogonality between active and inactive control variates** $P(h_j h_k) = 0$ for all $j \in \{1, \dots, m\} \setminus S^\star$ and all $k \in S^\star$.

Support recovery

Assumptions: **sub-gaussian** residuals, **linearly independent** and **bounded** control variates, appropriate λ
$(U_h = \max_{j=1,\dots,m} \sup_{x\in\mathcal{X}} |h_j(x)|, \gamma = \lambda_{\min}(G))$

Support recovery LASSOMC (Leluc,Portier,Segers, 2019)

For all $\delta \in (0,1)$, all integer n such that $n \geq 70(\ell^\star U_h^2/\gamma^\star)^2 \log(10\ell^\star m/\delta)$, and all λ such that

$$17 U_h \sqrt{\log(10m/\delta)}\tau/\sqrt{n} \leq \lambda \leq (\gamma^\star/(3\sqrt{\ell^\star})) \min_{k\in S^\star} |\beta_k^\star(f)|,$$

it holds that, with probability at least $1-\delta$, the LASSO solution $\hat{\beta}_n^{\text{lasso}}(f)$ is unique and the true active set is recovered, $\text{supp}(\hat{\beta}_n^{\text{lasso}}(f)) = S^\star$.