Report

Shagadatov Nurlan

January 21, 2019

1 Variance reduced estimator

$$f(X_p) = \mathbb{E}\left[f(X_p)|\zeta_j\right] + \sum_{k\in\mathbb{N}_0^d\setminus\{0\}}\sum_{l=j+1}^{p} a_{p,l,k}(X_{l-1})\mathbf{H}_{\mathbf{k}}(Z_l),$$

$$a_{p,l,k}(x) = \mathbb{E}\left[f(X_p)\mathbf{H}_{\mathbf{k}}(Z_l)|X_{l-1}=x\right]$$

$$M_{K,n}^N(f) = \sum_{\mathbf{k}:\ 0<\|\mathbf{k}\|\le K}\sum_{p=N+1}^{N+n}\omega_{p,n}^N\sum_{l=N+1}^{p} a_{p,l,\mathbf{k}}(X_{l-1})\mathbf{H}_{\mathbf{k}}(Z_l) \tag{1}$$

$$= \sum_{\mathbf{k}:\ 0<\|\mathbf{k}\|\le K}\sum_{l=N+1}^{N+n}\bar{a}_{l,\mathbf{k}}(X_{l-1})\mathbf{H}_{\mathbf{k}}(Z_l)$$

with $\|\mathbf{k}\| = \max_i k_i$ and

$$\pi_{K,n}^N(f) = \pi_n^N(f) - M_{K,n}^N(f)$$

2 Algorithm 1

The coefficients $a_{p,l,k}$ can be alternatively represented as

$$a_{p,l,k}(x) = \mathbb{E}\left[\mathbf{H}_{\mathbf{k}}(\xi)Q_{p,l}(x-\gamma_l\mu(x)+\sqrt{\gamma_l}\xi)\right]$$

with $Q_{p,l}(x) = \mathbb{E}\left[f(X_p)|\,X_l=x\right]$. On the other hand, due to (almost) time-homogenous markov chain generated by ULA, functions $Q_{p,l}$ can be approximated via regression depending only on number of lags $p-l$:

$$Q_{p,l}(x) = \mathbb{E}\left[f(X_p)|X_l=x\right] = G_{p-l}(x) = \mathbb{E}\left[f(\Phi^{p-l}(x,\xi))\right]$$

Thus we have:

$$\forall l: \quad G_r(x) = \mathbb{E}\left[f(X_{l+r})|X_l=x\right]$$

Consequently, functions G_r could be estimated using regression:

$$\hat{G}_r = \arg\min_{\psi\in\Psi}\sum_{s=1}^{N_{train}}\sum_{l=N+1}^{N+n-r}\left|f(X_{l+r}^{(s)}) - \psi(X_l^{(s)})\right|^2$$

where $1\le r\le n-1$ and $\hat{G}_0(x) = f(x)$

Lemma (decay of coefficients). Suppose that $f,\mu\in C^1(\mathbb{R})$, $0<b_\mu\le\mu'(x)\le B_\mu$ and $B_\mu\gamma_l\le 1$, then

$$\|a_{p,l,\mathbf{k}}\|_\infty \le \sqrt{\gamma_l}\,\|f'\|_\infty\exp\left(-b_\mu\sum_{r=l+1}^{p}\gamma_r\right), \quad \mathbf{k}\in\mathbb{N}^d\setminus\{\mathbf{0}\}$$

Therefore, we can reduce number of estimations by approximation $Q_{p,l}$ for $p-l<\tilde{n}(U,d)$. It allows us to construct small amount of training trajectories (and even use only target trajectory) to approximate conditional expectations $Q_{p,l}$.

Eventually, we have truncated version of algorithm to compute variance reduced estimator:

$$\pi^N_{K,n}(f)=\pi^N_n(f)-M^N_{K,n,\tilde{n}}(f)$$

where

$$\widehat{M}^N_{K,n,\tilde{n}}=\sum_{0<\|k\|\le K}\sum_{p=N+1}^{N+n}\omega^N_{p,n}\sum_{l=N+1}^{p}\widehat{a}_{p,l,k}(X_{l-1})\mathbf{H}_{\mathbf{K}}(Z_l)\mathbb{I}\{p-l<\tilde{n}\}$$

2.1 Polynomial approximation

In order to compute coefficients $a_{p,l,k}$ we need to compute expectations according to distribution of Z_l. This could be done by fast integration methods, such as FFT. On the other hand, in case of ULA we can derive explicit formula using polynomial approximation for $Q_{p,l}$. Suppose we constructed a polynomial approximation for $Q_{p,l}(x)$ of the form:

$$\widehat{Q}_{p,l}(x)=\sum_{\|\mathbf{s}\|\le m}\beta_{\mathbf{s}}x^{\mathbf{s}},\quad s=(s_1,\dots,s_d)$$

for some $\beta_{\mathbf{s}}\in\mathbb{R}$. Then using the identity

$$\xi^j=j!\sum_{r=0}^{j/2}\frac{1}{2^r r!\sqrt{(j-2r)!}}H_{j-2r}(\xi),\quad \xi\in\mathbb{R},$$

we derive

$$\begin{aligned}\widehat{a}_{p,l,\mathbf{k}}(x) &= \mathsf{E}\left[\mathbf{H}_{\mathbf{k}}(x)Q_{p,l}(x-\gamma\mu(x)+\sqrt{\gamma}\xi)\right]= \\ &= \sum_{\|\mathbf{s}\|\le m}\beta_{\mathbf{s}}\,\mathsf{E}\left[\prod_{i=1}^{d}H_{k_i}(\xi_i)(x_i-\gamma\mu_i(x)+\sqrt{\gamma}\xi_i)^{s_i}\right] \\ &= \sum_{\|\mathbf{s}\|\le m}\beta_{\mathbf{s}}\prod_{i=1}^{d}E_i\end{aligned}$$

with

$$\begin{aligned}E_i &= \mathsf{E}\left[H_{k_i}(\xi_i)(x_i-\gamma\mu_i(x)+\sqrt{\gamma}\xi_i)^{s_i}\right] \\ &= \sum_{j=0}^{s_i}\sum_{r=0}^{j/2}j!\frac{1}{2^r}\frac{1}{r!\sqrt{(t-2r)!}}\binom{s_i}{j}\left[x_i-\gamma\mu_i(x)\right]^{s_i-j}\gamma^{j/2}\int_{\mathbb{R}}H_{k_i}(y)H_{j-2r}(y)\varphi(y)\,dy\end{aligned}$$

and

$$\int_{\mathbb{R}}H_{k_i}(y)H_{j-2r}(y)\varphi(y)\,dy=\delta_{k_i,j-2r}.$$

3 Algorithm 2

$$\begin{aligned}\bar{a}_{l,\mathbf{k}}(x) &= \sum_{p=l}^{N+n}\omega^N_{p,n}a_{p,l,\mathbf{k}}(x) \\ &= \mathsf{E}\left[\left(\sum_{p=l}^{N+n}\omega^N_{p,n}f(X_p)\right)\mathbf{H}_{\mathbf{k}}(Z_l)\,\middle|\,X_{l-1}=x\right].\end{aligned}$$

$$\bar{Q}_l(x) = \sum_{p=N+1}^{N+n} Q_{p,l}(x) = \mathsf{E}\left[\sum_{p=l}^{N+n} \omega_{p,n}^N f(X_p) \middle| X_l = x\right], \quad l = N+1, \ldots, N+n.$$

$$\widehat{Q}_l = \arg\min_{\psi\in\Psi} \sum_{s=1}^{N_{tr}} \left| \sum_{p=l}^{N+n} \omega_{p,n}^N f(X_p^{(s)}) - \psi(X_l^{(s)}) \right|^2 \tag{2}$$

$$\widehat{a}_{l,k}(x) = \mathsf{E}\left[\phi_k(\xi)\,\widehat{Q}_l(\Phi_l(x,\xi)) \middle| \mathcal{D}_{tr}\right]$$

3.1 Truncation

Due to definition of $\bar{a}_{l,\mathbf{k}}$ and small γ_i we have that

$$\mathbb{E}\left[\omega_{p,n}^N f(X_p)\mathbf{H}_{\mathbf{k}}(Z_l) \,|X_{l-1} = x\right] \to 0$$

as $p - l \to \infty$
Therefore, we have truncated version of algorithm

$$\widehat{Q}_{l,\tilde{n}} = \arg\min_{\psi\in\Psi} \sum_{s=1}^{N_{tr}} \left| \sum_{p=l}^{min\{l+\tilde{n},N+n\}} \omega_{p,n}^N f(X_p^{(s)}) - \psi(X_l^{(s)}) \right|^2 \tag{3}$$

$$\widehat{a}_{l,k,\tilde{n}}(x) = \mathsf{E}\left[\phi_k(\xi)\,\widehat{Q}_{l,\tilde{n}}(\Phi_l(x,\xi)) \middle| \mathcal{D}_{tr}\right]$$

$$\widehat{M}_{K,n,\tilde{n}}^N = \sum_{0<\|k\|\le K} \sum_{l=N+1}^{N+n} \widehat{a}_{l,k,\tilde{n}}(X_{l-1})\mathbf{H}_{\mathbf{K}}(Z_l)$$

3.2 Polynomial approximation

The same as $a_{p,l,k}$

4 Experiment 1. Gaussian mixture (2d, 8d)

$$\pi(x) = \frac{1}{2(2\pi)^{p/2}}\left(e^{-\frac{\|x-a\|_2^2}{2}} + e^{-\frac{\|x+a\|_2^2}{2}}\right), \quad x \in \mathbb{R}^p$$

$$U(x) = \frac{1}{2}\|x-a\|_2^2 - \log(1 + e^{-2x^T a})$$

$$\bigtriangledown U(x) = x - a + 2a(1 + e^{2x^T a})^{-1}$$

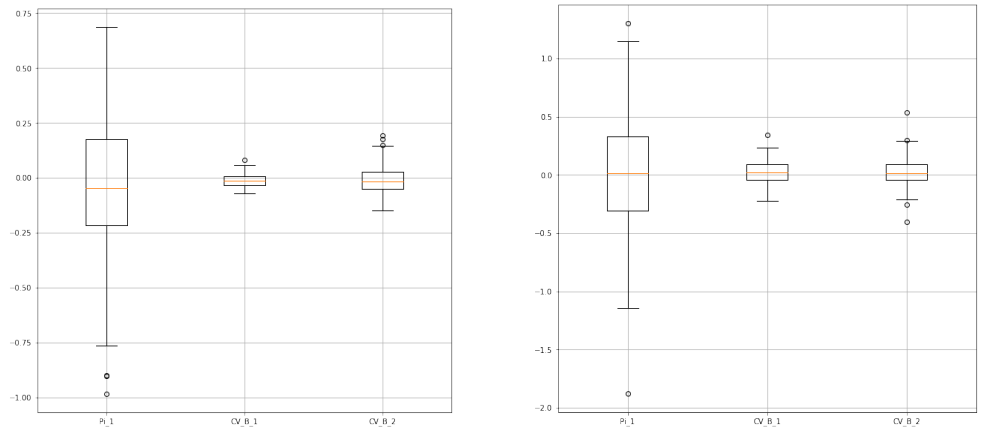
$$m = 1 - \|a\|_2^2, \quad M = 1, \quad L_U = \frac{1}{2}\|a\|_2^3$$

$$a = (\frac{1}{\sqrt{2d}}, \ldots, \frac{1}{\sqrt{2d}})$$

Results:

1. $d = 2, f(x) = x_1 + x_2$

   (a) Algorithm 1: $n = 1000, N_{train} = 100, \Psi = \{\text{polinomials } \max_{\deg} = 3\}, K = 2, \tilde{n} = 100$
   K = 1: 109.1 (0.0929643537005 -> 0.000837575184641)
   K = 2: 107.1 (0.0929643537005 -> 0.000852084051565)



(a) d = 2 (b) d = 8

Figure 1: Gaussian mixture boxplot

(b) Algorithm 2 :$n = 1000, N_{train} = 1000, \Psi = \{\text{polinomials } \max_{\deg} = 2\}, K = 2, \tilde{n} = 60$
K = 1 : 23.34 (0.0929643537005 -> 0.003982653841986601)
K = 2 : 24.76 (0.0929643537005 -> 0.003753718582081946)

2. $d = 8, f(x) = \sum_{i=1}^{d} x_i$

(a) Algorithm 1 $n = 1000, N_{train} = 50, \Psi = \{\text{polinomials } \max_{\deg} = 1\}, K = 1, \tilde{n} = 100$
K = 1 : 33.2 (0.3247338706361704 -> 0.00978211277392896)

(b) Algorithm 2 $n = 1000, N_{train} = 1000, \Psi = \{\text{polinomials } \max_{\deg} = 1\}, K = 1, \tilde{n} = 60$
K = 1 : 20.1 (0.3247338706361704 -> 0.016168075573709376)

5 Experiment 2. Binary Logistic regression

Training set: $\{(X_i, Y_i)\}_{i=1,..,n}$, $X_i \in \mathbb{R}^p$ and $Y_i \in \{0, 1\}$

$$r(\theta, x) = \mathbb{P}(Y_i = 1, X_i = x) = \frac{e^{\theta^T x}}{(1 + e^{\theta^T x})}$$

Let π_0 is prior probability density on θ, which is Gaussian with zero mean and covariance matrix proportional to the inverse of the Gram matrix $\mathbf{\Sigma}_X = \frac{1}{n}\sum_{i=1}^{n} X_i X_i^T$, then posterior:

$$\pi(\theta) \propto \exp\left\{-Y^T X\theta - \sum_{i=1}^{n} \log(1 + e^{-\theta^T X_i}) - \frac{\lambda}{2}\|\mathbf{\Sigma}_X^{1/2}\theta\|_2^2\right\}$$

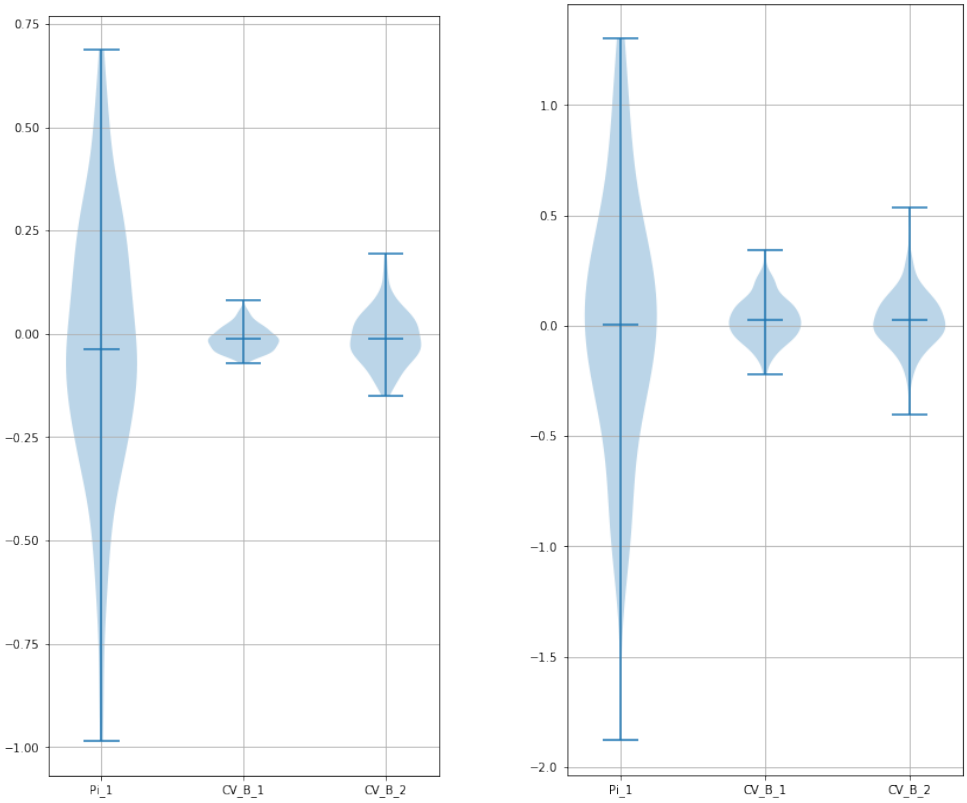
$$f(\theta) = Y^T X\theta + \sum \log(1 + e^{-\theta^T X_i}) + \lambda/2\|\mathbf{\Sigma}_X^{1/2}\theta\|_2^2$$

$$\bigtriangledown f(\theta) = X^T Y - \sum \frac{X_i}{1 + e^{\theta^T X_i}} + \lambda \mathbf{\Sigma}_X \theta$$

Lipschitz constant: $L_g = 0.1\|\sum \|AX_i\|_2 AX_i X_i^T A\|_2$
X has been generated from a Rademacher distribution and then normalized to have Euclidean norm equal to one. Y_i was drawn from Bernoulli distribution with parameter $r((1, 1, .., 1)^T, x)$.
Results:

1. $d = 2, f(x) = x_1 + x_2$

(a) Algorithm 1: $n = 1000, N_{train} = 50, \Psi = \{\text{polinomials } \max_{\deg} = 3\}, K = 1, \tilde{n} = 10$
K = 1: 117.44 ($2.18 * 10^{-4} -> 1.858 * 10^{-6}$)



(a) d = 2 (b) d = 8

Figure 2: Gaussian mixture violinplot

(b) Algorithm 2 :$n = 1000, N_{train} = 50, \Psi = \{\text{polinomials max}_{\text{deg}} = 2\}, K = 1, \tilde{n} = 3$
K = 1 : 9.4 (2.18 * $10^{-4} -> 2.32 * 10^{-5}$)

2. $d = 8, f(x) = \sum_{i=1}^{d} x_i$

   (a) Algorithm 1 $n = 1000, N_{train} = 50, \Psi = \{\text{polinomials max}_{\text{deg}} = 1\}, K = 1, \tilde{n} = 100$
   K = 1 : 38.67 (1.44 * $10^{-3} -> 3.71 * 10^{-5}$)

(b) Algorithm 2 $n = 1000, N_{train} = 500, \Psi = \{\text{polinomials max}_{\text{deg}} = 1\}, K = 1, \tilde{n} = 3$
K = 1 : 19.5 (1.44 * $10^{-3} -> 7.37 * 10^{-5}$)

6 CV and ZV

6.1 Papamarkou, Mira, Girolami Zero Variance estimator (ZV)

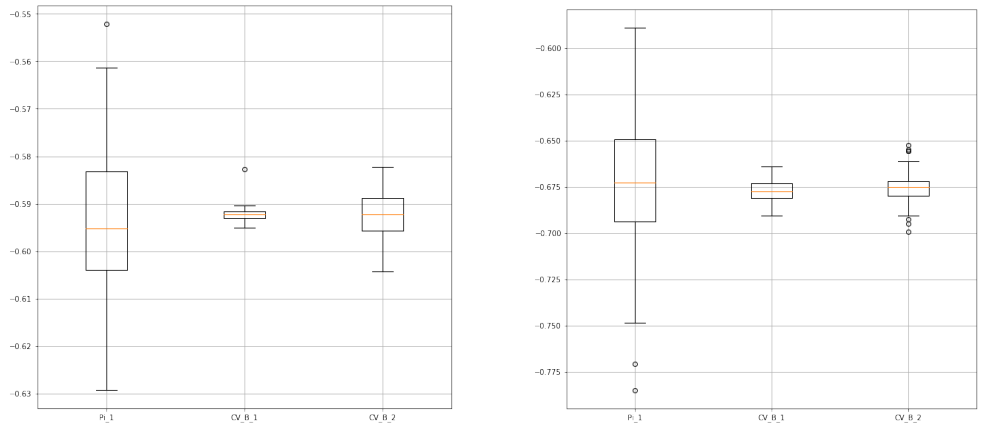
$$\tilde{f}(x) = f(x) + \frac{H\left[\psi(x)\right]}{\sqrt{\pi(x)}}$$

$$H\left[\psi(x)\right] = -\frac{1}{2}\Delta_x\left[\psi(x)\right] + \frac{\psi(x)}{2\sqrt{\pi(x)}}\Delta_x\left[\sqrt{\pi(x)}\right]$$

where $\Delta_x := \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$

$$\psi(x) = P(x)\sqrt{\pi(x)}$$

$$\tilde{f}(x) = f(x) - \frac{1}{2}\Delta_x\left[P(x)\right] + \nabla_x\left[P(x)\right] z(x)$$



(a) d = 2 (b) d = 8

Figure 3: Logistic regression boxplot

$$z(x) = -\frac{1}{2}\nabla_x \left[ln(\pi(x))\right] = \frac{1}{2}\nabla_x \left[U(x)\right]$$

First degree polynomials:

$$P(x) = a^T x$$

$$\nabla_x \left[P(x)\right] = a^T, \quad \Delta_x \left[P(x)\right] = 0$$

$$\tilde{f}(x) = f(x) + a^T z(x)$$

Optimal a:

$$a = -Var^{-1}\left[z(x)\right] * Cov\left[f(x), z(x)\right]$$

$$\hat{a} = -\hat{Var}_{(n)}^{-1}\left[z(x)\right] * \hat{Cov}_{(n)}\left[f(x), z(x)\right]$$

where

$$\hat{Var}_{(n)}\left[z(x)\right] = \frac{1}{n-1}\sum_{i=1}^{n}\left(z(X_i) - \mu\left[z(X_i)\right]\right)\left(z(X_i) - \mu\left[z(X_i)\right]\right)^T$$

$$\hat{Cov}_{(n)}\left[f(x), z(x)\right] = \frac{1}{n-1}\sum_{i=1}^{n}\left(f(X_i) - \mu\left[f(X_i)\right]\right)\left(z(X_i) - \mu\left[z(X_i)\right]\right)$$

$$\pi_n^{ZV_1}(f) = \frac{1}{n}\sum_{k=1}^{n}\left\{f(X_k) + \hat{a}^T \nabla U(X_k)\right\}$$

Second degree polynomials:

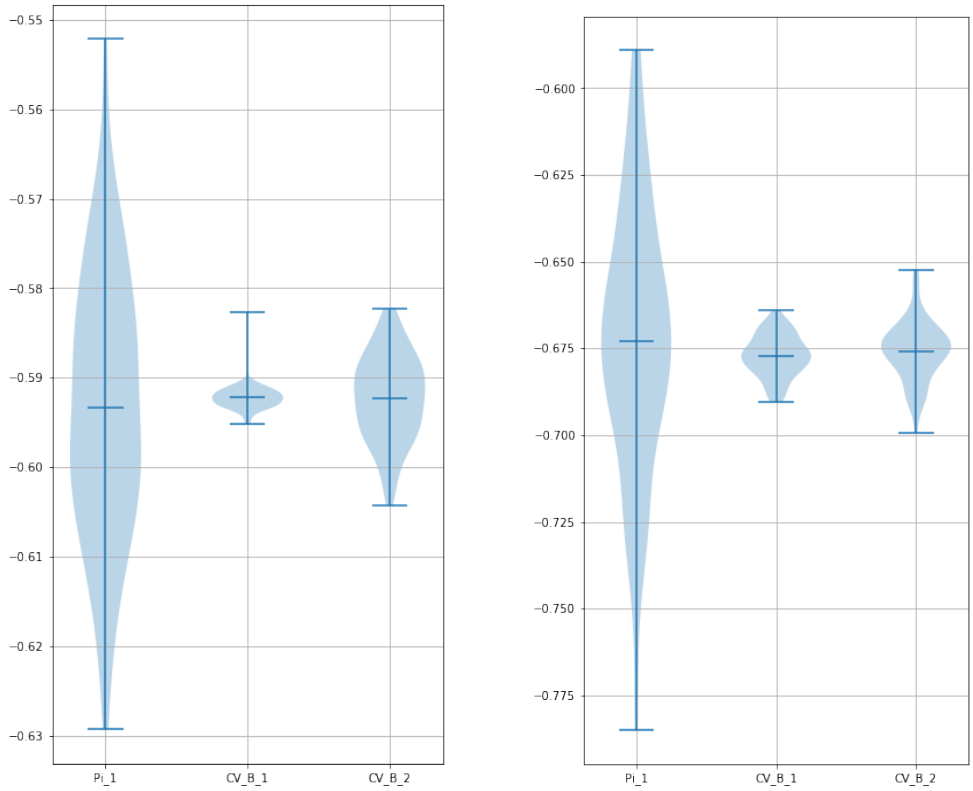
$$P(x) = c^T x + \frac{1}{2}x^T B x$$

where B is symmetric

$$\nabla_x \left[P(x)\right] = (c + Bx)^T, \quad \Delta_x \left[P(x)\right] = tr(B)$$

$$\tilde{f}(x) = f(x) - \frac{1}{2}tr(B) + (c + Bx)^T z(x)$$

It can be represented as:



(a) d = 2 (b) d = 8

Figure 4: Logistic regression violinplot

$$\tilde{(f)}(x) = f(x) + a^T w(x)$$

where

$$a = [c_1, \ldots, c_d, b_{11}, \ldots, b_{dd}, b_{12}, \ldots, b_{ij}, \ldots]^T$$

$$w(x) = \left[z_1, \ldots, z_d, x_1 z_1 - \frac{1}{2}, \ldots, x_d z_d - \frac{1}{2}, x_2 z_1 + x_1 z_2, \ldots, x_j z_i + x_i z_j, \ldots\right]^T$$

and optimal $a(c, B)$:

$$a^* = -Var\left[w(x)\right]^{-1} Cov\left[f(x), w(x)\right]$$

$$\hat{a}^* = -\hat{Var}_{(n)}\left[w(x)\right]^{-1} \hat{Cov}_{(n)}\left[f(x), w(x)\right]$$

6.2 N. Brosse Zero-variance estimator (CV)

define generator: $\mathfrak{L}\varphi = - < \nabla U, \nabla\varphi > + \Delta\varphi$

Note: $\mathfrak{L}\varphi = \frac{2H\left[\varphi\sqrt{\pi(x)}\right]}{\sqrt{\pi(x)}}$

$$\pi_n^{CV} = \frac{1}{n}\sum_{k=1}^{n}\left\{f(X_k) + \mathfrak{L}\left(\hat{\theta}_n^*(f)^T\psi(X_k)\right)\right\}$$

optimal θ:

$$\hat{\theta}_n^* = H_n^+\left[\frac{1}{n}\sum_{k=1}^{n}\psi(X_k)\left\{f(X_k) - \hat{\pi}_n(f)\right\}\right]$$

where

$$(H_n)_{ij} = \frac{1}{n}\sum_{k=1}^{n} \langle \nabla\psi_i(X_k), \nabla\psi_j(X_k)\rangle$$

First degree polynomials:

$$\psi = (\psi_1, \dots, \psi_d)$$

$$\psi_i(x) = x_i$$

$$(H_n)_{ij} = \frac{1}{n}\sum_{k=1}^{n} \langle \nabla\psi_i(X_k), \nabla\psi_j(X_k)\rangle = \delta_{ij} \quad \Rightarrow H_n = I$$

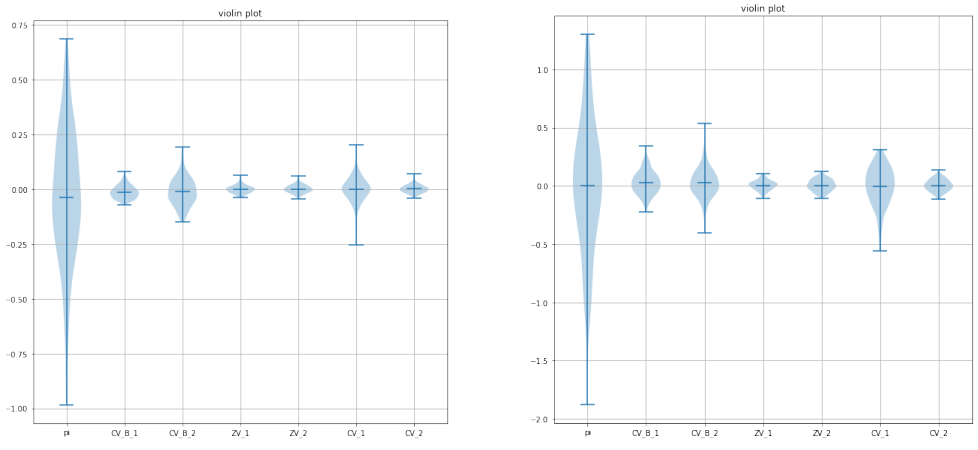
$$\hat{\theta}_n^*(f) = \frac{1}{n}\sum_{k=1}^{n} X_k \left\{f(X_k) - \hat{\pi}_n(f)\right\}$$

$$\pi_n^{CV_1}(f) = \frac{1}{n}\sum_{k=1}^{n} \left\{f(X_k) - \left\langle \nabla U(X_k), \hat{\theta}_n^*(f)\right\rangle\right\}$$

$$\hat{\theta}_n^*(f) = \left[\hat{Cov}_n(x_1, f(x)), \dots, \hat{Cov}_n(x_d, f(x))\right]^T$$

Second degree polynomials:

$$\psi = \left(x_1, \dots, x_d, x_1^2, \dots, x_2^2, x_1x_2, \dots\right)$$

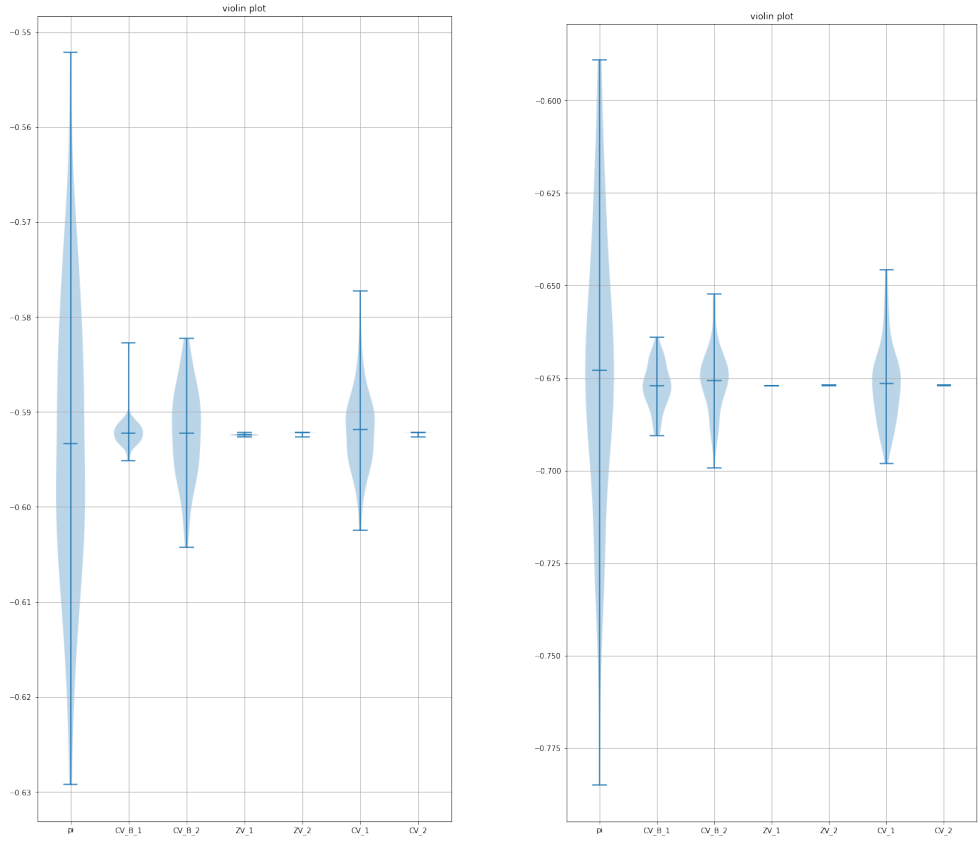


(a) d = 2 (b) d = 8

Figure 5: Gaussian mixture violins ($\mathrm{cv}_B 1 - algorithm1, cv_B 2 - algorithm2, ZV, CV$)

7 Conclusion

Eventually, we have that algorithm 1 is more effective than algorithm 2, however time consumption is considerably bigger. In addition, parameter $\tilde{n}$ in algorithm 1 is less significant and influences on final result slightly ($\tilde{n} = \infty$ doesn't work properly because expectation should convergence to zero with the distance from X_l, but we accumulate error and estimation is wrong), while $\tilde{n}$ in algorithm 2 strongly influences on result (requires the right selection to reduce variance, $\tilde{n} = \infty$ doesn't work). Unfortunately, ZV and CV are more effective (variance reduction and time consumption) than new control variates, however optimisation of algorithm 1 to run trough trajectory by "window" could reduce required number of train trajectory (train by window in repository). Additionaly algorithm from old version of article (algo 1, direct estimation of the coefficient $\bar{a}_{l,k}$) also works with right truncation $\tilde{n}$, but best variance reduction is lower in comparison with algorithm 2 (regression for $\bar{Q}_l$).



(a) d = 2 (b) d = 8

Figure 6: Logistic regression violins ($\mathrm{cv}_B 1 - algorithm1, cv_B 2 - algorithm2, ZV, CV$)