Convergence analysis for the gradient descent optimization method in the training of artificial neural networks with ReLU activation for piecewise linear target functions

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Let $d, H, \mathcal{P} \in \mathbb{N}$, $\mathscr{a} \in \mathbb{R}$, $\mathscr{b} > \mathscr{a}$, $u \in C([\mathscr{a}, \mathscr{b}]^d, \mathbb{R})$ satisfy $\mathcal{P} = dH + 2H + 1$, let $\mu \colon \mathcal{B}([\mathscr{a}, \mathscr{b}]^d) \to [0, \infty)$ be finite measure, let $\mathcal{L}_H \colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}$ satisfy $\forall\, \theta \in \mathbb{R}^{\mathcal{P}}$:

$$\mathcal{L}_H(\theta) = \int_{[\mathscr{a},\mathscr{b}]^d} \left[u(x) - \theta_{\mathcal{P}} - \sum_{i=1}^H \theta_{H(d+1)+i} \max\{\theta_{Hd+i} + \sum_{j=1}^d \theta_{(i-1)d+j} x_j, 0\} \right]^2 \mu(\mathrm{d}x),$$

let $\mathcal{G}_H \colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}^{\mathcal{P}}$ be an appropriately generalized gradient of $\mathcal{L}_H$, and let $\Theta \in C([0, \infty), \mathbb{R}^{\mathcal{P}})$ satisfy for all $t \in [0, \infty)$ that $\Theta_t = \Theta_0 - \int_0^t \mathcal{G}_H(\Theta_s)\, \mathrm{d}s$.

Theorem (Cheridito, J, Riekert, Rossmannek 2021; J, Riekert 2021)

Assume for all $x, y \in [\mathscr{a}, \mathscr{b}]^d$ that $u(x) = u(y)$. Then there exist no non-global local minima and no saddle points of $\mathcal{L}$ and $\lim_{t\to\infty} \mathcal{L}_H(\Theta_t) = 0$.

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Assume $\mu \ll \lambda_{[\mathscr{a},\mathscr{b}]^d}$ and $\sup_{t\in[0,\infty)} \|\Theta_t\| < \infty$. Then there exists $\vartheta \in (\mathcal{G}_H)^{-1}(\{0\})$ such that $\lim_{t\to\infty} \mathcal{L}_H(\Theta_t) = \mathcal{L}_H(\vartheta)$.

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Assume $\mu \sim \lambda_{[a,b]}$ with a Lipschitz continuous density, assume that u is piecewise affine linear, let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space, for every $H, k \in \mathbb{N}$, $\gamma \in \mathbb{R}$ let $\Theta_n^{H,k,\gamma} \colon \Omega \to \mathbb{R}^{3H+1}$, $n \in \mathbb{N}_0$, and $\mathbf{k}_n^{H,k,\gamma} \colon \Omega \to \mathbb{N}$, $n \in \mathbb{N}_0$, be random variables satisfying for all $n \in \mathbb{N}_0$ that

$$\Theta_{n+1}^{H,k,\gamma} = \Theta_n^{H,k,\gamma} - \gamma \mathcal{G}_H(\Theta_n^{H,k,\gamma}) \quad \text{and} \quad \mathbf{k}_n^{H,k,\gamma} \in \arg\min_{\ell \in \{1,\dots,k\}} \mathcal{L}_H(\Theta_n^{H,\ell,\gamma}),$$

and assume for all $H \in \mathbb{N}$, $\gamma \in \mathbb{R}$ that $\Theta_0^{H,k,\gamma}$, $k \in \mathbb{N}$, are i.i.d. standard normal. Then $\exists\, \mathfrak{g} > 0 \colon \forall\, \gamma \in (0, \mathfrak{g}] \colon$

$$\liminf_{H\to\infty} \liminf_{K\to\infty} \mathbb{P}\Big(\limsup_{n\to\infty} \mathcal{L}_H\big(\Theta_n^{H,\mathbf{k}_n^{H,K,\gamma},\gamma}\big) = 0\Big) = 1.$$

Proof based on Fehrman, Gess, J 2020 *JMLR*.

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Proof based on Fehrman, Gess, J 2020 *JMLR*.

Appendix

Let $d, H, \mathcal{P} \in \mathbb{N}$, $a \in \mathbb{R}$, $b \in (a, \infty)$, $f \in C([a, b]^d, \mathbb{R})$ satisfy $\mathcal{P} = dH + 2H + 1$, let $\mathfrak{R}_r \in C(\mathbb{R}, \mathbb{R})$, $r \in \mathbb{N} \cup \{\infty\}$, satisfy for all $x \in \mathbb{R}$ that $(\bigcup_{r \in \mathbb{N}} \{\mathfrak{R}_r\}) \subseteq C^1(\mathbb{R}, \mathbb{R})$, $\mathfrak{R}_\infty(x) = \max\{x, 0\}$, $\sup_{r \in \mathbb{N}} \sup_{y \in [-|x|, |x|]} |(\mathfrak{R}_r)'(y)| < \infty$, and

$$\limsup_{r \to \infty} \big(|\mathfrak{R}_r(x) - \mathfrak{R}_\infty(x)| + |(\mathfrak{R}_r)'(x) - \mathbb{1}_{(0,\infty)}(x)|\big) = 0,$$

let $\mu \colon \mathcal{B}([a, b]^d) \to [0, \infty]$ be a finite measure, let $\mathcal{L}_r \colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}$, $r \in \mathbb{N} \cup \{\infty\}$, satisfy for all $r \in \mathbb{N} \cup \{\infty\}$, $\theta = (\theta_1, \ldots, \theta_{\mathcal{P}}) \in \mathbb{R}^{\mathcal{P}}$ that

$$\mathcal{L}_r(\theta) = \int_{[a,b]^d} \big(f(x_1, \ldots, x_d) \\ - \theta_{\mathcal{P}} - \textstyle\sum_{i=1}^{H} \theta_{H(d+1)+i} \big[\mathfrak{R}_r(\theta_{Hd+i} + \sum_{j=1}^{d} \theta_{(i-1)d+j} x_j)\big]\big)^2 \, \mu(\mathrm{d}(x_1, \ldots, x_d)),$$

let $\mathcal{G} \colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}^{\mathcal{P}}$ satisfy for all $\theta \in \{\vartheta \in \mathbb{R}^{\mathcal{P}} \colon ((\nabla \mathcal{L}_r)(\vartheta))_{r \in \mathbb{N}} \text{ is convergent}\}$ that $\mathcal{G}(\theta) = \lim_{r \to \infty} (\nabla \mathcal{L}_r)(\theta)$, and let $\Theta \in C([0, \infty), \mathbb{R}^{\mathcal{P}})$ satisfy

$$\forall\, t \in [0, \infty) \colon \Theta_t = \Theta_0 - \int_0^t \mathcal{G}(\Theta_s)\, \mathrm{d}s.$$

Lemma

There exists an open $U \subseteq \mathbb{R}^{\mathcal{P}}$ such that $\int_{\mathbb{R}^{\mathcal{P}} \setminus U} 1 \, \mathrm{d}x = 0$, $(\mathcal{L}_\infty)|_U \in C^1(U, \mathbb{R})$, and $\nabla((\mathcal{L}_\infty)|_U) = \mathcal{G}|_U$.

Let $d, H, \mathcal{P} \in \mathbb{N}$, $\mathscr{a} \in \mathbb{R}$, $\mathscr{b} \in (\mathscr{a}, \infty)$, $f \in C([\mathscr{a}, \mathscr{b}]^d, \mathbb{R})$ satisfy $\mathcal{P} = dH + 2H + 1$, let $\mathfrak{R}_r \in C(\mathbb{R}, \mathbb{R})$, $r \in \mathbb{N} \cup \{\infty\}$, satisfy for all $x \in \mathbb{R}$ that $(\bigcup_{r\in\mathbb{N}}\{\mathfrak{R}_r\}) \subseteq C^1(\mathbb{R}, \mathbb{R})$, $\mathfrak{R}_\infty(x) = \max\{x, 0\}$, $\sup_{r\in\mathbb{N}} \sup_{y\in[-|x|,|x|]} |(\mathfrak{R}_r)'(y)| < \infty$, and

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Assume $\mu = \lambda_{[\mathscr{a}, \mathscr{b}]}$, *let* $\alpha, \beta \in \mathbb{R}$, *satisfy for all* $x \in [\mathscr{a}, \mathscr{b}]$ *that* $f(x) = \alpha x + \beta$, *and assume* $\sup_{t \in [0, \infty)} (H - 1) \|\Theta_t\| < \infty$, *and* $\mathcal{L}_\infty(\Theta_0) < \frac{\alpha^2 (\mathscr{b} - \mathscr{a})^3}{12(2\lfloor H/2 \rfloor + 1)^4}$. *Then*

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Consider

$$\frac{\partial u}{\partial t} = \Delta_x u - \|\nabla_x u\|^2$$

with $u(0,x) = \sqrt{\|x\|}$ for $t \in [0,1]$, $x \in \mathbb{R}^d$.

d	Mean	Std. dev.	Ref. value	rel. L^1-error	Std. dev. rel. error	avg. runtime
10	2.07017	0.00634850	2.04629	0.01167	0.00310245	58.200
50	3.15098	0.00275839	3.13788	0.00417	0.00087906	58.359
100	3.75329	0.00136920	3.74471	0.00229	0.00036564	58.329
200	4.46734	0.00079688	4.46172	0.00126	0.00017860	58.159
300	4.94586	0.00087736	4.94105	0.00097	0.00017756	58.819
500	5.62126	0.00045092	5.61735	0.00070	0.00008027	57.670
1000	6.68594	0.00040334	6.68335	0.00039	0.00006035	66.546
5000	9.97266	0.00047098	9.99835	0.00257	0.00004711	393.894
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$$\frac{\partial u}{\partial t} = \Delta_x u - \|\nabla_x u\|^2$$

with $u(0, x) = \sqrt{\|x\|}$ for $t \in [0, 1]$, $x \in \mathbb{R}^d$.

d	Mean	Std. dev.	Ref. value	rel. L^1-error	Std. dev. rel. error	avg. runtime
10	2.07017	0.00634850	2.04629	0.01167	0.00310245	58.200
50	3.15098	0.00275839	3.13788	0.00417	0.00087906	58.359
100	3.75329	0.00136920	3.74471	0.00229	0.00036564	58.329
200	4.46734	0.00079688	4.46172	0.00126	0.00017860	58.159
300	4.94586	0.00087736	4.94105	0.00097	0.00017756	58.819
500	5.62126	0.00045092	5.61735	0.00070	0.00008027	57.670
1000	6.68594	0.00040334	6.68335	0.00039	0.00006035	66.546
5000	9.97266	0.00047098	9.99835	0.00257	0.00004711	393.894
10000	11.87860	0.00022705	11.89099	0.00104	0.00001909	1687.680

Approximations for $u(1, 0)$; Time steps: 24;

SGD steps: 500 ($d < 10^4$), 600 ($d = 10^4$); Learning rates: $\frac{1}{10}$, $\frac{1}{100}$, $\frac{1}{1000}$

Beck, Becker, Cheridito, J, Neufeld 2019 *SISC* (to appear)

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Full history recursive Multilevel-Picard method: Let $T > 0, L, p \geq 0, \Theta = \cup_{n=1}^{\infty} \mathbb{Z}^n$, $\forall\, d \in \mathbb{N}$ let $g_d \in C(\mathbb{R}^d, \mathbb{R})$ satisfy $\forall\, x \in \mathbb{R}^d \colon |g_d(x)| \leq L(1 + \|x\|^p)$, let $f \colon \mathbb{R} \to \mathbb{R}$ be Lipschitz, let $(\Omega, \mathcal{F}, \mathbb{P})$ probab. sp., let $W^{d,\theta} \colon [0, T] \times \Omega \to \mathbb{R}^d$, $d \in \mathbb{N}$, $\theta \in \Theta$, be i.i.d. Brownian motions, let $S^\theta \colon [0, T] \times \Omega \to \mathbb{R}$, $\theta \in \Theta$, i.i.d. continuous satisfying $\forall\, t \in [0, T]$, $\theta \in \Theta$ that S^θ_t is $\mathcal{U}_{[t,T]}$-distributed, assume that $(S^\theta)_{\theta \in \Theta}$ and $(W^{d,\theta})_{\theta \in \Theta, d \in \mathbb{N}}$ are independent, let $U^{d,\theta}_{n,M} \colon [0, T] \times \mathbb{R}^d \times \Omega \to \mathbb{R}$, $d, n, M \in \mathbb{Z}$, $\theta \in \Theta$, satisfy $\forall\, d, M \in \mathbb{N}$, $n \in \mathbb{N}_0$, $\theta \in \Theta$, $t \in [0, T]$, $x \in \mathbb{R}^d$:

$$U^{d,\theta}_{n,M}(t, x) = \sum_{m=1}^{M^n} \frac{g_d(x + W^{d,(\theta,0,-m)}_{T-t}) \mathbb{1}_{\mathbb{N}}(n)}{M^n} + \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U^{d,(\theta,l,m)}_{l,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) - \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U^{d,(\theta,l,m)}_{l-1,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \Bigg]$$

and $\forall\, d, n \in \mathbb{N}$ let $\mathrm{Cost}_{d,n} \in \mathbb{N}$ be the comp. cost of $U^{d,0}_{n,n}(0, 0)$.

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$$\begin{aligned} U^{d,\theta}_{n,M}(t,x) &= \sum_{m=1}^{M^n} \frac{g_d(x + W^{d,(\theta,0,-m)}_{T-t}) \mathbb{1}_{\mathbb{N}}(n)}{M^n} \\ &\quad + \Bigg[\sum_{l=0}^{n-1} \tfrac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U^{d,(\theta,l,m)}_{l,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \\ &\qquad - \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U^{d,(\theta,-l,m)}_{l-1,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \Bigg] \end{aligned}$$

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$$
\begin{aligned}
U^{d,\theta}_{n,M}(t,x) &= \sum_{m=1}^{M^n} \frac{g_d(x + W^{d,(\theta,0,-m)}_{T-t})\mathbb{1}_{\mathbb{N}}(n)}{M^n} \\
&\quad + \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U^{d,(\theta,l,m)}_{l,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \\
&\qquad - \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U^{d,(\theta,-l,m)}_{l-1,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \Bigg]
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- \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U_{l-1,M}^{d,(\theta,-l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \Bigg]
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$$+ \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U^{d,(\theta,l,m)}_{l,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big)$$
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- \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U^{d,(\theta,-l,m)}_{l-1,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \Bigg]
\end{aligned}
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and $\forall\, d, n \in \mathbb{N}$ let $\text{Cost}_{d,n} \in \mathbb{N}$ be the comp. cost of $U^{d,0}_{n,n}(0, 0)$.

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$$
\begin{aligned}
U^{d,\theta}_{n,M}(t,x) &= \sum_{m=1}^{M^n} \frac{g_d(x + W^{d,(\theta,0,-m)}_{T-t}) \mathbb{1}_{\mathbb{N}}(n)}{M^n} \\
&\quad + \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U^{d,(\theta,l,m)}_{l,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \\
&\qquad - \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U^{d,(\theta,l,m)}_{l-1,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \Bigg]
\end{aligned}
$$

and $\forall\, d, n \in \mathbb{N}$ let $\mathrm{Cost}_{d,n} \in \mathbb{N}$ be the comp. cost of $U^{d,0}_{n,n}(0,0)$.

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$$
\begin{aligned}
U_{n,M}^{d,\theta}(t, x) &= \sum_{m=1}^{M^n} \frac{g_d(x + W_{T-t}^{d,(\theta,0,-m)}) \mathbb{1}_{\mathbb{N}}(n)}{M^n} \\
&\quad + \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U_{l,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \\
&\qquad - \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U_{l-1,M}^{d,(\theta,-l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \Bigg]
\end{aligned}
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and $\forall\, d, n \in \mathbb{N}$ let $\mathrm{Cost}_{d,n} \in \mathbb{N}$ be the comp. cost of $U_{n,n}^{d,0}(0, 0)$.

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$$U_{n,M}^{d,\theta}(t, x) = \sum_{m=1}^{M^n} \frac{g_d(x + W_{T-t}^{d,(\theta,0,-m)}) \mathbb{1}_{\mathbb{N}}(n)}{M^n} + \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U_{l,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) - \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U_{l-1,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \Bigg]$$

and $\forall\, d, n \in \mathbb{N}$ let $\mathrm{Cost}_{d,n} \in \mathbb{N}$ be the comp. cost of $U_{n,n}^{d,0}(0, 0)$.

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$$+ \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U_{l,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big)$$
$$- \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U_{l-1,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \Bigg]$$

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$$- \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U_{l-1,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \Bigg]$$

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$$
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- \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U^{d,(\theta,l,m)}_{l-1,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \Bigg]
\end{aligned}
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$$+ \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U_{l,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big)$$

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$$
\begin{aligned}
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+ \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U_{l,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \\
- \mathbb{1}_{\mathbb{N}}(l)\, f\Big(U_{l-1,M}^{d,(\theta,l,m)}\big(S_t^{(\theta,l,m)}, x + W_{S_t^{(\theta,l,m)}-t}^{d,(\theta,l,m)}\big)\Big) \Bigg]
\end{aligned}
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$$
\begin{aligned}
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&\quad + \Bigg[\sum_{l=0}^{n-1} \frac{(T-t)}{M^{n-l}} \sum_{m=1}^{M^{n-l}} f\Big(U^{d,(\theta,l,m)}_{l,M}\big(S^{(\theta,l,m)}_t, x + W^{d,(\theta,l,m)}_{S^{(\theta,l,m)}_t - t}\big)\Big) \\
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\end{aligned}
$$

and $\forall\, d, n \in \mathbb{N}$ let $\mathrm{Cost}_{d,n} \in \mathbb{N}$ be the comp. cost of $U^{d,0}_{n,n}(0, 0)$.

Then

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and

(ii) $\forall\, \delta > 0\colon$ there exist $n\colon \mathbb{N}\times(0,\infty)\to\mathbb{N}$ and $C>0\colon$ $\forall\, d\in\mathbb{N}, \varepsilon>0\colon$

$$\left(\mathbb{E}\left[\left|u_d(0,0) - U^{d,0}_{n_{d,\varepsilon},n_{d,\varepsilon}}(0,0)\right|^2\right]\right)^{1/2} \leq \varepsilon$$

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