

Convergence analysis for gradient descent optimization methods in the training of ReLU neural networks

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Let $T, p, \kappa > 0$, let $f: \mathbb{R} \rightarrow \mathbb{R}$ be Lipschitz, $\forall d \in \mathbb{N}$ let $g_d \in C^1(\mathbb{R}^d, \mathbb{R})$ and $u_d: [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}$ be an at most poly. grow. solution of

$$\frac{\partial u_d}{\partial t} = \Delta_x u_d + f(u_d) \quad \text{with} \quad u_d(0, \cdot) = g_d,$$

assume $|g_d(x)| + \|(\nabla g_d)(x)\| \leq \kappa d^\kappa (1 + \|x\|^\kappa)$, let $\mathcal{A}_l: \mathbb{R}^l \rightarrow \mathbb{R}^l$, $l \in \mathbb{N}$, satisfy $\mathcal{A}_l(x_1, \dots, x_l) = (\max\{x_1, 0\}, \dots, \max\{x_l, 0\})$, let

$$\mathbf{N} = \cup_{L \in \mathbb{N}} \cup_{l_0, \dots, l_L \in \mathbb{N}} \left(\times_{n=1}^L (\mathbb{R}^{l_n \times l_{n-1}} \times \mathbb{R}^{l_n}) \right),$$

let $\mathcal{R}: \mathbf{N} \rightarrow \cup_{a,b=1}^{\infty} C(\mathbb{R}^a, \mathbb{R}^b)$ satisfy for all $L \in \mathbb{N}$, $l_0, \dots, l_L \in \mathbb{N}$,

$\Phi = ((W_1, B_1), \dots, (W_L, B_L)) \in \times_{n=1}^L (\mathbb{R}^{l_n \times l_{n-1}} \times \mathbb{R}^{l_n})$, $x_0 \in \mathbb{R}^{l_0}, \dots, x_L \in \mathbb{R}^{l_L}$ with $\forall n \in \{1, \dots, L\}: x_n = \mathcal{A}_{l_n}(W_n x_{n-1} + B_n)$ that

$$(\mathcal{R}\Phi)(x_0) = W_L x_{L-1} + B_L,$$

let $\mathcal{P}: \mathbf{N} \rightarrow \mathbb{N}$ be the number of parameters, and let $(G_{d,\varepsilon})_{d \in \mathbb{N}, \varepsilon \in (0,1]} \subseteq \mathbf{N}$ satisfy

$\mathcal{P}(G_{d,\varepsilon}) \leq \kappa d^\kappa \varepsilon^{-\kappa}$ and $|g_d(x) - (\mathcal{R}G_{d,\varepsilon})(x)| \leq \varepsilon \kappa d^\kappa (1 + \|x\|^\kappa)$. Then

$\exists (U_{d,\varepsilon})_{d \in \mathbb{N}, \varepsilon \in (0,1]} \subseteq \mathbf{N}$, $c > 0: \forall d \in \mathbb{N}, \varepsilon \in (0, 1]:$

$$\left[\int_{[0,T] \times [0,1]^d} |u_d(y) - (\mathcal{R}U_{d,\varepsilon})(y)|^p dy \right]^{1/p} \leq \varepsilon \quad \text{and} \quad \mathcal{P}(U_{d,\varepsilon}) \leq c d^c \varepsilon^{-c}.$$

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Let $T, p, \kappa > 0$, let $f: \mathbb{R} \rightarrow \mathbb{R}$ be Lipschitz, $\forall d \in \mathbb{N}$ let $g_d \in C^1(\mathbb{R}^d, \mathbb{R})$ and $u_d: [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}$ be an at most poly. grow. solution of

$$\frac{\partial u_d}{\partial t} = \Delta_x u_d + f(u_d) \quad \text{with} \quad u_d(0, \cdot) = g_d,$$

assume $|g_d(x)| + \|(\nabla g_d)(x)\| \leq \kappa d^\kappa (1 + \|x\|^\kappa)$, let $\mathcal{A}_l: \mathbb{R}^l \rightarrow \mathbb{R}^l$, $l \in \mathbb{N}$, satisfy $\mathcal{A}_l(x_1, \dots, x_l) = (\max\{x_1, 0\}, \dots, \max\{x_l, 0\})$, let

$$\mathbf{N} = \cup_{L \in \mathbb{N}} \cup_{l_0, \dots, l_L \in \mathbb{N}} \left(\times_{n=1}^L (\mathbb{R}^{l_n \times l_{n-1}} \times \mathbb{R}^{l_n}) \right),$$

let $\mathcal{R}: \mathbf{N} \rightarrow \cup_{a,b=1}^\infty C(\mathbb{R}^a, \mathbb{R}^b)$ satisfy for all $L \in \mathbb{N}$, $l_0, \dots, l_L \in \mathbb{N}$,

$\Phi = ((W_1, B_1), \dots, (W_L, B_L)) \in \times_{n=1}^L (\mathbb{R}^{l_n \times l_{n-1}} \times \mathbb{R}^{l_n})$, $x_0 \in \mathbb{R}^{l_0}, \dots, x_L \in \mathbb{R}^{l_L}$ with $\forall n \in \{1, \dots, L\}: x_n = \mathcal{A}_{l_n}(W_n x_{n-1} + B_n)$ that

$$(\mathcal{R}\Phi)(x_0) = W_L x_{L-1} + B_L,$$

let $\mathcal{P}: \mathbf{N} \rightarrow \mathbb{N}$ be the number of parameters, and let $(G_{d,\varepsilon})_{d \in \mathbb{N}, \varepsilon \in (0,1]} \subseteq \mathbf{N}$ satisfy

$\mathcal{P}(G_{d,\varepsilon}) \leq \kappa d^\kappa \varepsilon^{-\kappa}$ and $|g_d(x) - (\mathcal{R}G_{d,\varepsilon})(x)| \leq \varepsilon \kappa d^\kappa (1 + \|x\|^\kappa)$. Then

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

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

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

Appendix

Let $d, H, P \in \mathbb{N}$, $a \in \mathbb{R}$, $\theta \in (a, \infty)$, $f \in C([a, \theta]^d, \mathbb{R})$ 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

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

let $\mu: \mathcal{B}([a, \theta]^d) \rightarrow [0, \infty]$ be a measure, let $\mathcal{L}_r: \mathbb{R}^P \rightarrow \mathbb{R}$, $r \in \mathbb{N} \cup \{\infty\}$, satisfy for all $r \in \mathbb{N} \cup \{\infty\}$, $\theta = (\theta_1, \dots, \theta_P) \in \mathbb{R}^P$ that

$$\begin{aligned} \mathcal{L}_r(\theta) &= \int_{[a, \theta]^d} (f(x_1, \dots, x_d) \\ &\quad - \theta_P - \sum_{i=1}^H \theta_{H(d+1)+i} [\mathfrak{R}_r(\theta_{Hd+i} + \sum_{j=1}^d \theta_{(i-1)d+j} x_j)])^2 \mu(d(x_1, \dots, x_d)), \end{aligned}$$

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

$$\forall t \in [0, \infty): \Theta_t = \Theta_0 - \int_0^t \mathcal{G}(\Theta_s) ds.$$

Lemma

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

Let $d, H, \mathcal{P} \in \mathbb{N}$, $a \in \mathbb{R}$, $\vartheta \in (a, \infty)$, $f \in C([a, \vartheta]^d, \mathbb{R})$ satisfy

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

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- 3 it holds for all $\theta \in \mathcal{G}^{-1}(\{0\})$ that θ is a global minima of \mathcal{L}_∞ , and
- 4 it holds that $\limsup_{t \rightarrow \infty} \mathcal{L}_\infty(\Theta_t) = 0$.

Theorem (Cheridito J Rossmannek 2021, J Rieker 2021)

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

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

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

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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;

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

Hamiltonian-Jacobi-Bellman equations

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

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Then

- (i) $\forall d \in \mathbb{N}$: there exists $u_d: [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}$ at most polyn. grow. solution of

$$\frac{\partial u_d}{\partial t} + \frac{1}{2} \Delta_x u_d + f(u_d) = 0 \quad \text{with} \quad u_d(T, \cdot) = g_d$$

and

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

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

and

$$\text{Cost}_{d, n_d, \varepsilon} \leq C d^{1+p(1+\delta)} \varepsilon^{-(2+\delta)}.$$

Extensions: Algorithms/Simulations/Proofs: Fully nonlinear PDEs (Beck, E, J 2018 *JNS*), Optimal stopping (Becker, Cheridito, J 2018 *JMLR*), Uniform errors (Beck, Becker, Grohs, Jaafari, J 2018), Semilinear PDEs/CVA (Hutzenthaler, J, von Wurstemberger 2019 *EJP*, Hutzenthaler, J, Kruse, Nguyen 2020), Nonlipschitz nonlinearities (Beck, Hornung, Hutzenthaler, Jentzen, Kruse 2019 *J. Numer. Math.*), Gradient dependent nonlinearities (Hutzenthaler, J, Kruse 2019), Elliptic PDEs (Beck, Gonon, J 2020), Discrete problems (Beck, J, Kruse 2020), . . .

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