Analysis of the Generalization Error: Empirical Risk Minimization Over Deep Neural Networks Overcomes the Curse of Dimensionality in the Numerical Approximation of Black-Scholes PDEs

Julius Berner¹, Philipp Grohs^{1,2}, Arnulf Jentzen³

¹Faculty of Mathematics, University of Vienna
²Research Platform DataScience@UniVienna, University of Vienna
³Department of Mathematics, ETH Zürich



GAMM, 2019



Suitable Learning Problems for $d \in \mathbb{N}$

- input data: $X_d \sim U([u,v]^d)$
- label: random variable Y_d with $\|Y_d\|_{L^\infty} \leq D$

Definition (learning problem \Rightarrow regression function)

$$\widehat{f}_d = \operatorname*{argmin}_{f \,:\, \mathbb{R}^d o \mathbb{R}} \mathbb{E} \Big[\big(f(X_d) - Y_d \big)^2 \Big]$$

Suitable Learning Problems for $d \in \mathbb{N}$

- input data: $X_d \sim U([u,v]^d)$
- label: random variable Y_d with $\|Y_d\|_{L^\infty} \leq D$

Definition (learning problem \Rightarrow regression function)

$$\widehat{f}_d = \operatorname*{argmin}_{f : \ \mathbb{R}^d \to \mathbb{R}} \mathbb{E}\Big[\big(f(X_d) - Y_d \big)^2 \Big]$$

- training data: $((X_d^{(i)},Y_d^{(i)}))_{i\in\mathbb{N}}$ i.i.d. with $(X_d^{(1)},Y_d^{(1)})\sim (X_d,Y_d)$
- hypothesis class: $\mathcal{H}_d \subseteq C([u, v]^d)$ compact

Definition (ERM \Rightarrow empirical target function)

$$\widehat{f}_{m,\mathcal{H}_d} \in \operatorname*{argmin}_{f \in \mathcal{H}_d} \frac{1}{m} \sum_{i=1}^m \left(f(X_d^{(i)}) - Y_d^{(i)} \right)^2$$

Berner, Grohs, Jentzen

Analysis of the Generalization Error

Neural Networks as Hypothesis Class

- affine linear mapping: $\mathcal{A}_{W,B}(x) := Wx + B$
- ReLU activation: ρ(x) := max{x, 0}
- clipping function: $C_D(x) := \min\{|x|, D\} \operatorname{sgn}(x)$
- network architecture: $\mathbf{a} \in \mathbb{N}^{l+2}$

Definition (hypothesis class of clipped ReLU networks)

$$\mathcal{N}_{\mathbf{a},R} := \left\{ f \middle| \begin{array}{c} f = \mathcal{C}_D \circ \mathcal{A}_{W_l,B_l} \circ \varrho \circ \mathcal{A}_{W_{l-1},B_{l-1}} \circ \varrho \circ \cdots \circ \mathcal{A}_{W_0,B_0}, \\ W_i \in [-R,R]^{\mathbf{a}_{i+1} \times \mathbf{a}_i}, B_i \in [-R,R]^{\mathbf{a}_{i+1}}, i = 0, \dots, I \end{array} \right\}$$

Neural Networks as Hypothesis Class

- affine linear mapping: $\mathcal{A}_{W,B}(x) := Wx + B$
- ReLU activation: ρ(x) := max{x, 0}
- clipping function: $C_D(x) := \min\{|x|, D\} \operatorname{sgn}(x)$
- network architecture: $\mathbf{a} \in \mathbb{N}^{l+2}$

Definition (hypothesis class of clipped ReLU networks)

$$\mathcal{N}_{\mathbf{a},R} := \left\{ f \mid \begin{array}{c} f = \mathcal{C}_D \circ \mathcal{A}_{W_l,B_l} \circ \varrho \circ \mathcal{A}_{W_{l-1},B_{l-1}} \circ \varrho \circ \cdots \circ \mathcal{A}_{W_0,B_0}, \\ W_i \in [-R,R]^{\mathbf{a}_{i+1} \times \mathbf{a}_i}, B_i \in [-R,R]^{\mathbf{a}_{i+1}}, i = 0, \dots, I \end{array} \right\}$$

Definition (size of the hypothesis class)

$$size(\mathcal{N}_{\mathbf{a},R}) := max \left\{ R, \sum_{i=0}^{l} a_{i+1}a_i + a_{i+1} \right\}$$

Berner, Grohs, Jentzen

Analysis of the Generalization Error

Generalization without Curse

Assumption (approximation without Curse)

Assume there are $\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}$ with size $(\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}) \in \mathcal{O}(\operatorname{\textit{poly}}(d,\varepsilon^{-1}))$ and

$$\min_{f\in\mathcal{N}_{\mathbf{a}_{d,\varepsilon}},R_{d,\varepsilon}}\frac{1}{(v-u)^d}\left\|f-\widehat{f}_d\right\|_{L^2[u,v]^d}^2\leq\varepsilon.$$

Generalization without Curse

Assumption (approximation without Curse)

Assume there are $\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}$ with size $(\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}) \in \mathcal{O}(\operatorname{\textit{poly}}(d,\varepsilon^{-1}))$ and

$$\min_{f\in\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}}\frac{1}{(v-u)^{d}}\left\|f-\widehat{f}_{d}\right\|_{L^{2}[u,v]^{d}}^{2}\leq\varepsilon.$$

Theorem (generalization without curse)

Then there exists $m \in \mathcal{O}(\operatorname{\textit{poly}}(d, \varepsilon^{-1}) \ln(\varrho^{-1}))$ with

$$\mathbb{P}\left[\frac{1}{(v-u)^d}\left\|\widehat{f}_{m,\mathcal{N}_{\mathbf{a}_{d,\varepsilon}},R_{d,\varepsilon}}-\widehat{f}_d\right\|_{L^2[u,v]^d}^2\leq\varepsilon\right]\geq 1-\varrho.$$

Generalization without Curse

Assumption (approximation without Curse)

Assume there are $\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}$ with size $(\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}) \in \mathcal{O}(\operatorname{\textit{poly}}(d,\varepsilon^{-1}))$ and

$$\min_{f\in\mathcal{N}_{\mathbf{a}_{d,\varepsilon},R_{d,\varepsilon}}}\frac{1}{(v-u)^{d}}\left\|f-\widehat{f}_{d}\right\|_{L^{2}[u,v]^{d}}^{2}\leq\varepsilon.$$

Theorem (generalization without curse)

Then there exists $m \in \mathcal{O}(\operatorname{\textit{poly}}(d, \varepsilon^{-1}) \ln(\varrho^{-1}))$ with

$$\mathbb{P}\left[\frac{1}{(v-u)^d}\left\|\widehat{f}_{m,\mathcal{N}_{\mathbf{a}_{d,\varepsilon}},R_{d,\varepsilon}}-\widehat{f}_d\right\|_{L^2[u,v]^d}^2\leq\varepsilon\right]\geq 1-\varrho.$$

Proof: covering number of $\mathcal{N}_{\mathbf{a},R}$ and Hoeffding's inequality

Berner, Grohs, Jentzen

Partial Summary

Assume

- X_d uniformly distributed
- Y_d uniformly bounded
- i.i.d. training data
- \hat{f}_d can be approximated by ReLU networks without curse

Main Result

Partial Summary

Assume

- X_d uniformly distributed
- Y_d uniformly bounded
- i.i.d. training data
- \widehat{f}_d can be approximated by ReLU networks without curse

Then $f_{m,\mathcal{N}_{a,B}}$ (solution of to the ERM problem)

- approximates \hat{f}_d within accuracy ε with high probability
- with size($\mathcal{N}_{\mathsf{a},R}$) and m scaling polynomially in d and ε^{-1}

Main Result

Partial Summary

Assume

- X_d uniformly distributed
- Y_d uniformly bounded
- i.i.d. training data
- \hat{f}_d can be approximated by ReLU networks without curse

Then $f_{m,\mathcal{N}_{a,B}}$ (solution of to the ERM problem)

- approximates \hat{f}_d within accuracy ε with high probability
- with size($\mathcal{N}_{a,R}$) and *m* scaling polynomially in *d* and ε^{-1}

Can the assumptions be satisfied?

Kolmogorov PDE

- initial condition: $\varphi_d \in C(\mathbb{R}^d, [-D, D])$
- coefficient functions: $\sigma_d \colon \mathbb{R}^d \to R^{d \times d}$, $\mu_d \colon \mathbb{R}^d \to \mathbb{R}^d$ affine linear

Definition (Kolmogorov equation)

$$\begin{cases} \frac{\partial F_d}{\partial t}(t,x) = \frac{1}{2} \operatorname{Trace} \left(\sigma_d(x) \sigma_d^{\mathsf{T}}(x) \operatorname{Hess}_x F_d(t,x) \right) + \left\langle \mu_d(x), \nabla_x F_d(t,x) \right\rangle \\ F_d(0,x) = \varphi_d(x) \end{cases}$$

for every $t \in [0, T]$, $x \in \mathbb{R}^d$

Kolmogorov PDE

- initial condition: $\varphi_d \in C(\mathbb{R}^d, [-D, D])$
- coefficient functions: $\sigma_d \colon \mathbb{R}^d \to R^{d \times d}$, $\mu_d \colon \mathbb{R}^d \to \mathbb{R}^d$ affine linear

Definition (Kolmogorov equation)

$$\begin{cases} \frac{\partial F_d}{\partial t}(t,x) = \frac{1}{2} \operatorname{Trace} \left(\sigma_d(x) \sigma_d^{\mathsf{T}}(x) \operatorname{Hess}_x F_d(t,x) \right) + \left\langle \mu_d(x), \nabla_x F_d(t,x) \right\rangle \\ F_d(0,x) = \varphi_d(x) \end{cases}$$

for every $t \in [0, T]$, $x \in \mathbb{R}^d$

 \Rightarrow goal: approximately compute the function (end value)

$$[u,v]^d \ni x \mapsto F_d(T,x)$$

Learning Problem

let Y_d := φ_d(S_T^{X_d}) where S^{X_d} is the solution processes to the stochastic differential equation (SDE)

$$\begin{cases} dS_t^{X_d} = \sigma_d(S_t^{X_d}) dB_t^d + \mu_d(S_t^{X_d}) dt \\ S_0^{X_d} = X_d \end{cases}$$

Learning Problem

let Y_d := φ_d(S_T^{X_d}) where S^{X_d} is the solution processes to the stochastic differential equation (SDE)

$$\begin{cases} dS_t^{X_d} = \sigma_d(S_t^{X_d}) dB_t^d + \mu_d(S_t^{X_d}) dt \\ S_0^{X_d} = X_d \end{cases}$$

Theorem (regression function is solution to PDE - Beck et al. '18) For a.e. $x \in [u, v]^d$ it holds that

$$F_d(T,x)=\widehat{f}_d(x).$$

Learning Problem

let Y_d := φ_d(S_T^{X_d}) where S^{X_d} is the solution processes to the stochastic differential equation (SDE)

$$\begin{cases} dS_t^{X_d} = \sigma_d(S_t^{X_d}) dB_t^d + \mu_d(S_t^{X_d}) dt \\ S_0^{X_d} = X_d \end{cases}$$

Theorem (regression function is solution to PDE - Beck et al. '18) For a.e. $x \in [u, v]^d$ it holds that

$$F_d(T,x)=\widehat{f}_d(x).$$

Proof: Feynman-Kac formula $F_d(T, x) = \mathbb{E}[\varphi_d(S_T^x)]$ and representation of regression function $\hat{f}_d(x) = \mathbb{E}[Y_d|X_d = x]$

Approximation without Curse

- assume φ_d can be approximated by ReLU networks without curse of dimensionality
- \Rightarrow satisfied for applications in financial engineering

Approximation without Curse

- assume φ_d can be approximated by ReLU networks without curse of dimensionality
- \Rightarrow satisfied for applications in financial engineering

Theorem (approximation without curse - Grohs et al. '18)

Then there are $\mathcal{N}_{\mathbf{a},R}$ with size $(\mathcal{N}_{\mathbf{a},R}) \in \mathcal{O}(\textit{poly}(d, \varepsilon^{-1}))$ and

$$\min_{f\in\mathcal{N}_{\mathbf{a},R}}\frac{1}{(v-u)^d}\|f-F_d(T,\cdot)\|_{L^2[u,v]^d}^2\leq\varepsilon.$$

Approximation without Curse

- assume φ_d can be approximated by ReLU networks without curse of dimensionality
- \Rightarrow satisfied for applications in financial engineering

Theorem (approximation without curse - Grohs et al. '18)

Then there are $\mathcal{N}_{\mathbf{a},R}$ with size $(\mathcal{N}_{\mathbf{a},R}) \in \mathcal{O}(\mathit{poly}(d, \varepsilon^{-1}))$ and

$$\min_{f\in\mathcal{N}_{\mathbf{a},R}}\frac{1}{(v-u)^d}\|f-F_d(T,\cdot)\|_{L^2[u,v]^d}^2\leq\varepsilon.$$

Proof: Monte-Carlo mean squared error and representation of SDE solution

ERM without Curse

Our assumptions are satisfied!

Generalization Result

ERM without Curse

Our assumptions are satisfied!

Corollary (ERM solves the Kolmogorov PDE without curse) There exists $N_{a,R}$ and m with

• size($\mathcal{N}_{\mathbf{a},R}$) $\in \mathcal{O}(\operatorname{\textit{poly}}(d,\varepsilon^{-1}))$

•
$$m \in \mathcal{O}(\operatorname{\textit{poly}}(d, \varepsilon^{-1}) \ln(\varrho^{-1}))$$

•
$$\mathbb{P}\left[\frac{1}{(v-u)^d}\left\|\widehat{f}_{m,\mathcal{N}_{\mathbf{a},R}}-\widehat{F}_d(T,\cdot)\right\|_{L^2[u,v]^d}^2\leq\varepsilon\right]\geq 1-\varrho.$$

Proof: approximation without curse implies generalization without curse

Pricing of European Options without Curse

- capped European put option: $\varphi_d(x) = \min \left\{ \max \left\{ D - \sum_{i=1}^d c_{d,i} x_i, 0 \right\}, D \right\}$
- \Rightarrow exactly representable by a neural network with size scaling linearly in d

Pricing of European Options without Curse

• capped European put option:

$$\varphi_d(x) = \min \left\{ \max \left\{ D - \sum_{i=1}^d c_{d,i} x_i, 0 \right\}, D \right\}$$

⇒ exactly representable by a neural network with size scaling linearly in d⇒ quantitative version: there exist $\mathbf{a} = (d, a_1, a_2, 1)$, R and m with

• size
$$(\mathcal{N}_{\mathbf{a},R}) \in \mathcal{O}(d^2 \varepsilon^{-2})$$

• $m \in \mathcal{O}(d^2 \varepsilon^{-4} \ln(d \varepsilon^{-1} \varrho^{-1}))$
• $\mathbb{P}\left[\frac{1}{(v-u)^d} \left\| \widehat{f}_{m,\mathcal{N}_{\mathbf{a},R}} - F_d(T, \cdot) \right\|_{L^2[u,v]^d}^2 \le \varepsilon\right] \ge 1 - \varrho.$

Numerical Experiments (Beck et al. '18)

Number of	Relative	Relative	Relative	Runtime
descent steps	L ¹ -error	L ² -error	L^{∞} -error	in seconds
0	1.004285	1.004286	1.009524	1
100000	0.371515	0.371551	0.387978	437.9
250000	0.001220	0.001538	0.010039	1092.6
500000	0.000949	0.001187	0.005105	2183.8

Table: ERM with a = (100, 200, 200, 1) for a Black-Scholes PDE on $[90, 110]^{100}$

Thank you for your Attention!

Preprint available on arXiv:



Berner, J., Grohs, P., and Jentzen, A.

Analysis of the generalization error: Empirical risk minimization over deep artificial neural networks overcomes the curse of dimensionality in the numerical approximation of Black-Scholes partial differential equations. arXiv:1809.03062 (9 2018).