Overcoming the curse of dimensionality: from nonlinear Monte Carlo to deep learning

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Friday, April 22nd, 2022

Computational problems from

- **Financial Engineering** (Evaluations of risks and financial products),
- **Operations Research** (Optimal control, optimal use of resources),
- **Environmental Sciences** (Landscape Ecology, modelling of Biodiversity),
- **Filtering** (Chemical engineering, Kushner and Zakai equations)

often require approximations for high-dimensional functions such as $u\colon [0,1]^d \to \mathbb{R}$ for $d \in \mathbb{N}$ large.

Approximations methods such as finite element methods, finite differences, sparse grids suffer under *the curse of dimensionality* (Bellman 1957).

Monte Carlo method based on Feynman-Kac formula:
high-dimensional linear partial differential equations (PDEs)

Deep learning based methods for high-dimensional PDEs:
E, Han, J 2017 *CIMS*, Han, J, E 2018 *PNAS*,
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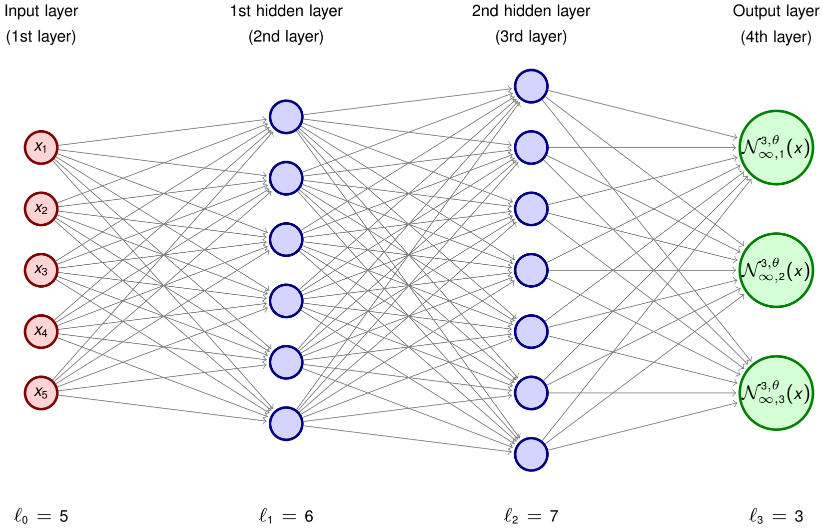

Input layer
(1st layer)
1st hidden layer
(2nd layer)
2nd hidden layer
(3rd layer)
Output layer
(4th layer)
x_1
x_2
x_3
x_4
x_5
$\mathcal{N}^{3,\theta}_{\infty,1}(x)$
$\mathcal{N}^{3,\theta}_{\infty,2}(x)$
$\mathcal{N}^{3,\theta}_{\infty,3}(x)$
$\ell_0 = 5$
$\ell_1 = 6$
$\ell_2 = 7$
$\ell_3 = 3$

Hamiltonian–Jacobi–Bellman equations

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
10000	11.87860	0.00022705	11.89099	0.00104	0.00001909	1687.680

Approximations for $u(1,0)$; Layer: $\ell_0 = d$, $\ell_1 = \ell_2 = d + 10$, $\ell_3 = 1$; Time steps: 24; 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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assume $|g_d(x)| + \|(\nabla g_d)(x)\| \leq \kappa d^\kappa (1 + \|x\|^\kappa)$, *let* $\mathfrak{M}_l\colon \mathbb{R}^l \to \mathbb{R}^l$, $l \in \mathbb{N}$, *satisfy* $\mathfrak{M}_l(x_1, \ldots, x_l) = (\max\{x_1, 0\}, \ldots, \max\{x_l, 0\})$, *let*

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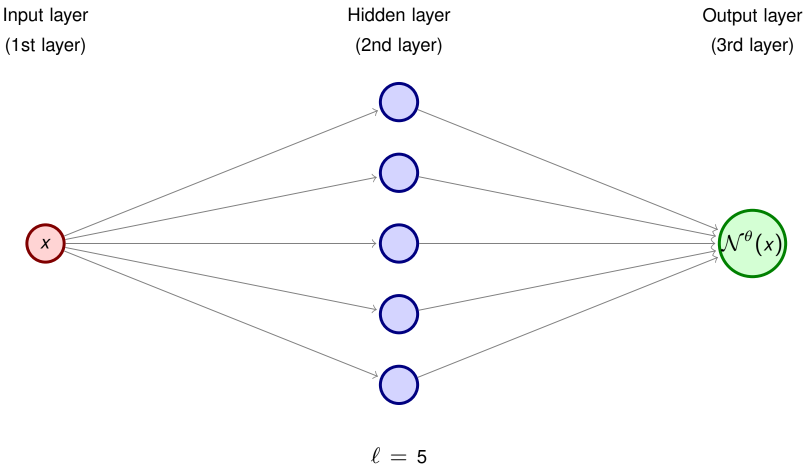

Input layer
(1st layer)
Hidden layer
(2nd layer)
Output layer
(3rd layer)
x
$\mathcal{N}^\theta(x)$
$\ell = 5$

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let $\mathcal{R}\colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}$ *satisfy* $\mathcal{R}(\theta) = \int_{[a,b]^{\ell_0}} \|\mathcal{N}^{L,\theta}(x) - f(x)\|^2\, \mathfrak{p}(x)\, \mathrm{d}x$, *let* $\mathcal{G}\colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}^{\mathcal{P}}$ *be generalized gradient of* $\mathcal{R}$, *and let* $\Theta \in C([0,\infty), \mathbb{R}^{\mathcal{P}})$ *satisfy* $\liminf_{t\to\infty}\|\Theta_t\| < \infty$ *and* $\forall\, t \in [0,\infty)\colon \Theta_t = \Theta_0 - \int_0^t \mathcal{G}(\Theta_s)\,\mathrm{d}s$. *Then there exist* $\vartheta \in \mathbb{R}^{\mathcal{P}}$, $\mathfrak{C}, \beta \in (0,\infty)$ *with* $0 \in \partial\mathcal{R}(\vartheta)$ *such that* $\forall\, t \in [0,\infty)$:

$$\|\Theta_t - \vartheta\| \le \mathfrak{C}(1+t)^{-\beta} \qquad \text{and} \qquad |\mathcal{R}(\Theta_t) - \mathcal{R}(\vartheta)| \le \mathfrak{C}(1+t)^{-1}.$$

Theorem (J, Riekert 2021 *JML* (revision requested) (Eberle, J, Riekert, Weiss 2021))

Let $L \in \mathbb{N}$, $\ell_0, \ell_1, \dots, \ell_L \in \mathbb{N}$, $a \in \mathbb{R}$, $b \in [a, \infty)$, $\mathcal{P} = \sum_{k=1}^{L} \ell_k(\ell_{k-1} + 1)$, *let* $f\colon [a,b]^{\ell_0} \to \mathbb{R}^{\ell_L}$ *and* $\mathfrak{p}\colon [a,b]^{\ell_0} \to [0,\infty)$ *be piecewise polynomial, for every* $k \in \{1, \dots, L\}$, $\theta \in \mathbb{R}^{\mathcal{P}}$ *let* $\mathfrak{w}^{k,\theta} \in \mathbb{R}^{\ell_k \times \ell_{k-1}}$ *and* $\mathfrak{b}^{k,\theta} \in \mathbb{R}^{\ell_k}$ *satisfy*

$$\mathfrak{w}^{k,\theta}_{i,j} = \theta_{(i-1)\ell_{k-1}+j+\sum_{h=1}^{k-1}\ell_h(\ell_{h-1}+1)} \qquad \text{and} \qquad \mathfrak{b}^{k,\theta}_i = \theta_{\ell_k\ell_{k-1}+i+\sum_{h=1}^{k-1}\ell_h(\ell_{h-1}+1)},$$

let $\mathfrak{M}\colon (\cup_{n\in\mathbb{N}}\mathbb{R}^n) \to (\cup_{n\in\mathbb{N}}\mathbb{R}^n)$ *satisfy* $\mathfrak{M}(x) = (\max\{x_1, 0\}, \dots, \max\{x_n, 0\})$, *for every* $\theta \in \mathbb{R}^{\mathcal{P}}$ *let* $\mathcal{N}^{k,\theta}\colon \mathbb{R}^{\ell_0} \to \mathbb{R}^{\ell_k}$, $k \in \{1, \dots, L\}$, *satisfy*

$$\mathcal{N}^{1,\theta}(x) = \mathfrak{b}^{1,\theta} + \mathfrak{w}^{1,\theta}x \quad \text{and} \quad \mathcal{N}^{k+1,\theta}(x) = \mathfrak{b}^{k+1,\theta} + \mathfrak{w}^{k+1,\theta}(\mathfrak{M}(\mathcal{N}^{k,\theta}(x))),$$

let $\mathcal{R}\colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}$ *satisfy* $\mathcal{R}(\theta) = \int_{[a,b]^{\ell_0}} \|\mathcal{N}^{L,\theta}(x) - f(x)\|^2\, \mathfrak{p}(x)\, dx$, *let* $\mathcal{G}\colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}^{\mathcal{P}}$ *be generalized gradient of* $\mathcal{R}$, *and let* $\Theta \in C([0,\infty), \mathbb{R}^{\mathcal{P}})$ *satisfy* $\liminf_{t\to\infty}\|\Theta_t\| < \infty$ *and* $\forall\, t \in [0,\infty)\colon \Theta_t = \Theta_0 - \int_0^t \mathcal{G}(\Theta_s)\, ds$. *Then there exist* $\vartheta \in \mathbb{R}^{\mathcal{P}}$, $\mathfrak{C}, \beta \in (0,\infty)$ *with* $0 \in \partial\mathcal{R}(\vartheta)$ *such that* $\forall\, t \in [0,\infty)$:

$$\|\Theta_t - \vartheta\| \le \mathfrak{C}(1+t)^{-\beta} \qquad \text{and} \qquad |\mathcal{R}(\Theta_t) - \mathcal{R}(\vartheta)| \le \mathfrak{C}(1+t)^{-1}.$$

Theorem (J, Riekert 2021 *JML* (revision requested) (Eberle, J, Riekert, Weiss 2021))

Let $L \in \mathbb{N}$, $\ell_0, \ell_1, \ldots, \ell_L \in \mathbb{N}$, $a \in \mathbb{R}$, $b \in [a, \infty)$, $\mathcal{P} = \sum_{k=1}^{L} \ell_k(\ell_{k-1} + 1)$, *let* $f\colon [a,b]^{\ell_0} \to \mathbb{R}^{\ell_L}$ *and* $\mathfrak{p}\colon [a,b]^{\ell_0} \to [0,\infty)$ *be piecewise polynomial, for every* $k \in \{1, \ldots, L\}$, $\theta \in \mathbb{R}^{\mathcal{P}}$ *let* $\mathfrak{w}^{k,\theta} \in \mathbb{R}^{\ell_k \times \ell_{k-1}}$ *and* $\mathfrak{b}^{k,\theta} \in \mathbb{R}^{\ell_k}$ *satisfy*

$$\mathfrak{w}^{k,\theta}_{i,j} = \theta_{(i-1)\ell_{k-1}+j+\sum_{h=1}^{k-1}\ell_h(\ell_{h-1}+1)} \qquad \text{and} \qquad \mathfrak{b}^{k,\theta}_{i} = \theta_{\ell_k\ell_{k-1}+i+\sum_{h=1}^{k-1}\ell_h(\ell_{h-1}+1)},$$

let $\mathfrak{M}\colon (\cup_{n\in\mathbb{N}}\mathbb{R}^n) \to (\cup_{n\in\mathbb{N}}\mathbb{R}^n)$ *satisfy* $\mathfrak{M}(x) = (\max\{x_1, 0\}, \ldots, \max\{x_n, 0\})$, *for every* $\theta \in \mathbb{R}^{\mathcal{P}}$ *let* $\mathcal{N}^{k,\theta}\colon \mathbb{R}^{\ell_0} \to \mathbb{R}^{\ell_k}$, $k \in \{1, \ldots, L\}$, *satisfy*

$$\mathcal{N}^{1,\theta}(x) = \mathfrak{b}^{1,\theta} + \mathfrak{w}^{1,\theta}x \quad \text{and} \quad \mathcal{N}^{k+1,\theta}(x) = \mathfrak{b}^{k+1,\theta} + \mathfrak{w}^{k+1,\theta}(\mathfrak{M}(\mathcal{N}^{k,\theta}(x))),$$

let $\mathcal{R}\colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}$ *satisfy* $\mathcal{R}(\theta) = \int_{[a,b]^{\ell_0}} \|\mathcal{N}^{L,\theta}(x) - f(x)\|^2 \, \mathfrak{p}(x)\, dx$, *let* $\mathcal{G}\colon \mathbb{R}^{\mathcal{P}} \to \mathbb{R}^{\mathcal{P}}$ *be generalized gradient of* $\mathcal{R}$, *and let* $\Theta \in C([0,\infty), \mathbb{R}^{\mathcal{P}})$ *satisfy* $\liminf_{t\to\infty}\|\Theta_t\| < \infty$ *and* $\forall\, t \in [0,\infty)\colon \Theta_t = \Theta_0 - \int_0^t \mathcal{G}(\Theta_s)\, ds$. *Then there exist* $\vartheta \in \mathbb{R}^{\mathcal{P}}$, $\mathfrak{C}, \beta \in (0,\infty)$ *with* $0 \in \partial\mathcal{R}(\vartheta)$ *such that* $\forall\, t \in [0,\infty)\colon$

$$\|\Theta_t - \vartheta\| \le \mathfrak{C}(1+t)^{-\beta} \qquad \text{and} \qquad |\mathcal{R}(\Theta_t) - \mathcal{R}(\vartheta)| \le \mathfrak{C}(1+t)^{-1}.$$

Many thanks for your attention!