Deep Neural Networks for PDEs

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Short Reading List

1. Ian Goodfellow and Yoshua Bengio and Aaron Courville: Deep Learning; MIT Press, 2016
2. Aurelien Geron: Hands-On Machine Learning with Scikit-Learn and TensorFlow; O'Reilley, 2017
3. Brian Steele and John Chandler and Swarna Reddy: Algorithms for Data Science; Springer, 2017
4. Alan Jeffrey: Applied Partial Differential Equations – An Introduction; Academic Press, 2002

Syllabus

1. PDEs and the Curse of Dimensionality
2. A Crash Course in Statistical Learning Theory (including a Detour to Variational Autoencoders)
3. PDEs as Learning Problem
4. Solving linear Kolmogorov Equations by means of Neural Network Based Learning

PDEs and the Curse of Dimensionality

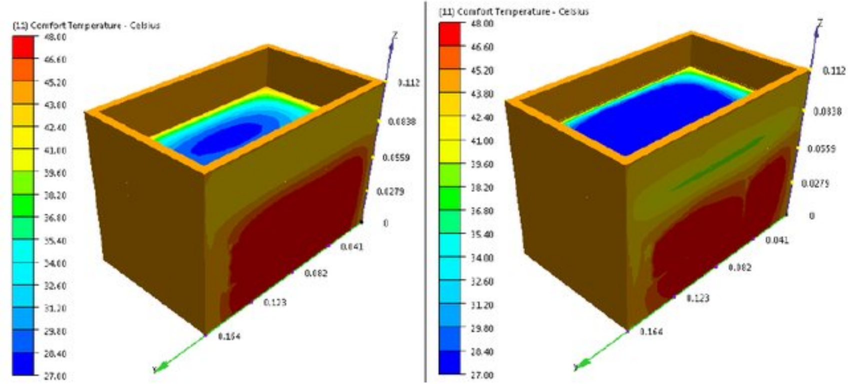
PDEs

A PDE for the function $u(x_1, \dots, x_d)$ is an equation of the form

$$\mathcal{F}\left(x_1, \dots, x_d, u, \frac{\partial u}{\partial x_1}, \dots \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1 \partial x_1}, \dots, \frac{\partial^2 u}{\partial x_1 \partial x_d}, \dots\right) = 0.$$

together with suitable boundary conditions.

Heat Equation



$$\frac{\partial u}{\partial t}(t,x) = \frac{\partial^2 u}{\partial x_1 \partial x_1} + \frac{\partial^2 u}{\partial x_2 \partial x_2} + \frac{\partial^2 u}{\partial x_3 \partial x_3} + g(t,x), \quad u(0,x) = \varphi(x)$$

$t \in (0,\infty), x \in \mathbb{R}^3;\ d = 4.$

Explicit Solution of Heat Equation if $g = 0$

Let $u(t, x)$ satisfy

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$t \in (0,\infty), x \in \mathbb{R}^3$; $d = 4$.
Then

$$u(t,x) = \frac{1}{(4\pi t)^{3/2}} \int_{\mathbb{R}^3} \varphi(y) \exp(-|x-y|^2/4t) dy.$$

Fluid Dynamics

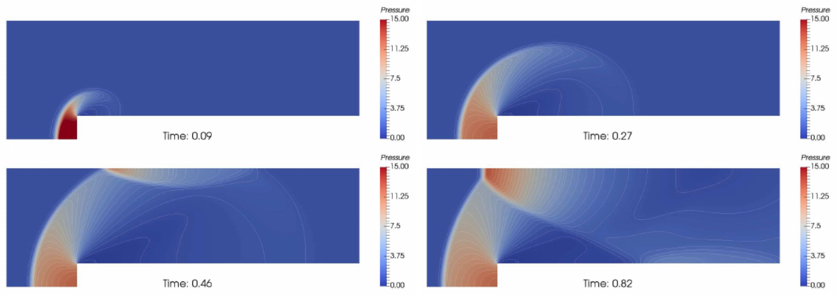


Figure 8: Mach 3 wind tunnel: Polynomial degree $K = 40$, $35k$ Vertices, Maxwellian molecules, $28.9M$ total DoFs. Coloring: pressure, contour lines: density. Computations were carried out on the Euler cluster of ETH Zurich (Xeon E5-2697 v2) with 360 cores.

$$\frac{\partial u}{\partial t}(t,x,v) + v \cdot \nabla u(t,x,v) = Qu(t,x,v)$$

$t \in (0,\infty), x, v \in \mathbb{R}^3$; $d = 7$.

Schrödinger Equation

Wave function of non-relativistic quantum mechanical system of N electons in a field of K nuclei of charge Z_ν and fixed position $R_\mu \in \mathbb{R}^3$

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N;t) = -\frac{1}{2}\sum_{\xi=1}^{N}\Delta_i\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N;t) -$$

$$\sum_{\xi=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|\mathbf{r}_\xi - R_\nu|}\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N;t) + \frac{1}{2}\sum_{\xi=1}^{N}\sum_{\eta=1}^{N}\frac{1-\delta_{\xi,\eta}}{|\mathbf{r}_\xi - \mathbf{r}_\eta|},$$

$t \in (0,\infty)$, $\mathbf{r}_1,\ldots,\mathbf{r}_N \in \mathbb{R}^3$; $d = 3N+1$.

Black-Scholes Equation

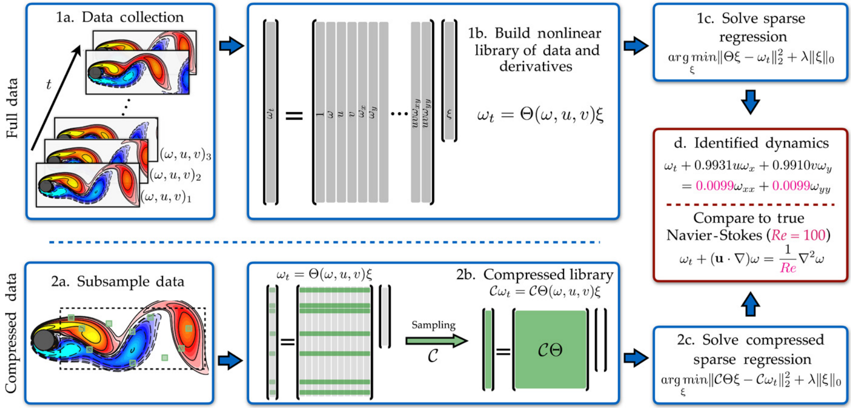
Pricing a portfolio of N financial derivatives

$$\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\sum_{i,j=1}^{N} x_i x_j \beta_i \beta_j \langle \varsigma_i, \varsigma_j \rangle_{\mathbb{R}^N} \left(\frac{\partial^2 u}{\partial x_i \partial x_j}\right)(t,x) + \sum_{i=1}^{N} \mu_i x_i \left(\frac{\partial u}{\partial x_i}\right)(t,x)$$

$$u(0,x) = \max\{K - \sum_{i=1}^{N} c_i x_i, 0\}$$

$t \in (0,\infty)$, $x \in \mathbb{R}^N$; $d = N+1$.

Learning the PDE [Rudy et.al. (2017)]



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Want to approximate $u(x)$ for $x \in [0,1]^d$.

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$$\frac{u_{i_1,\dots,i_l+1,\dots,i_d} - u_{i_1,\dots,i_l,\dots,i_d}}{\epsilon} \sim \frac{\partial}{\partial x_l} u(i_1\epsilon,\dots,i_d\epsilon),$$
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and so on,

- and solve the discrete system

$$\mathcal{F}\left(i_1\epsilon, \ldots, i_d\epsilon, u_{i_1,\ldots,i_d}, \frac{u_{i_1+1,\ldots,i_d} - u_{i_1,\ldots,i_d}}{\epsilon}, \ldots\right) = 0$$
$$(i_1, \ldots, i_d) \in \{0, \ldots, \lfloor \epsilon^{-1} \rfloor\}^d.$$

Curse of Dimensionality

The system

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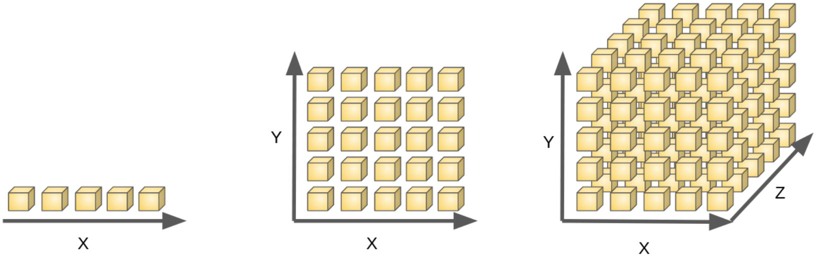
Curse of Dimensionality



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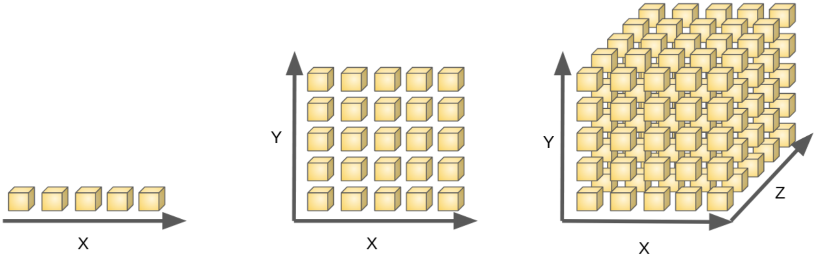
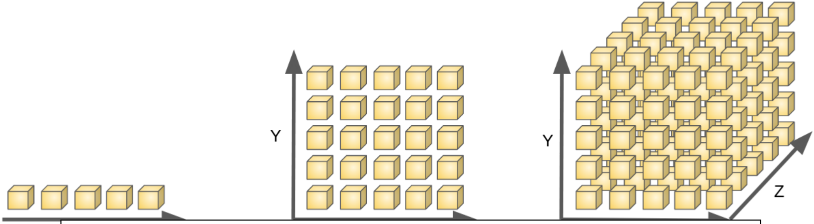


The complexity of approximating a general d-dimensional function scales exponentially in d.

Curse of Dimensionality



The ... ction

Suppose we have a problem where we aim to approximate a d-dimensional function. An algorithm to solve the problem suffers from the curse of dimensionality if its computational complexity depends exponentially on the dimension d.

Black-Scholes Equation

- Pricing a portfolio of N financial derivatives

$$\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\sum_{i,j=1}^{N} x_i x_j \beta_i \beta_j \langle \varsigma_i, \varsigma_j \rangle_{\mathbb{R}^N} (\frac{\partial^2 u}{\partial x_i \partial x_j})(t,x) + \sum_{i=1}^{N} \mu_i x_i (\frac{\partial u}{\partial x_i})(t,x)$$

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- Complexity of finite difference method: $2^{100} - 2^{1000}$.
- Number of atoms in the universe: 2^{250}.

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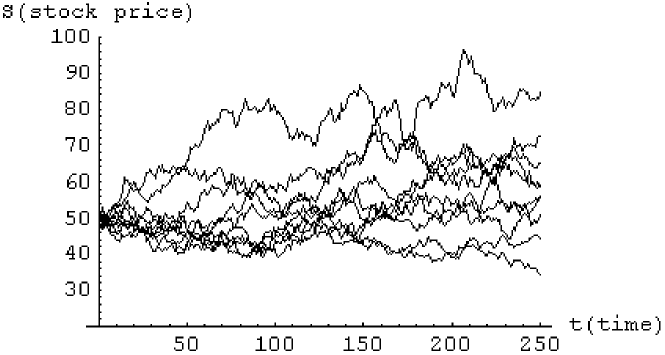

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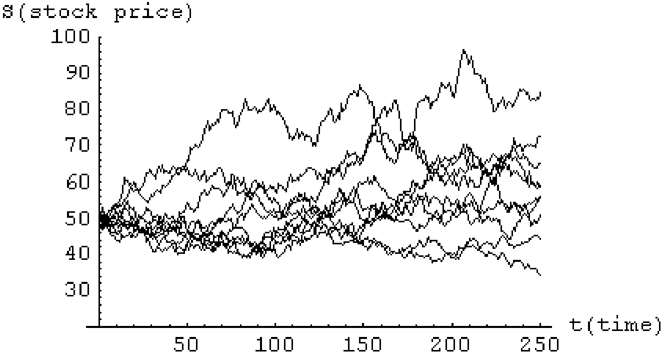

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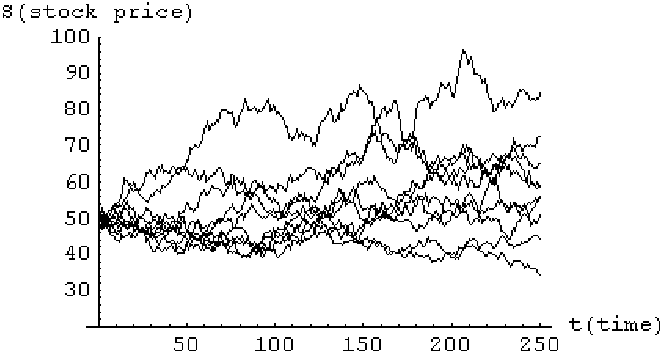

- Option pricing is extremely relevant and has to be done every day in the financial industry
- All algorithms for the solution of the Black-Scholes equation suffer from the curse of dimensionality!

MNIST

MNIST Database for handwritten digit recognition http://yann.lecun.com/exdb/mnist/

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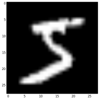

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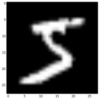

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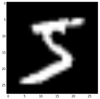

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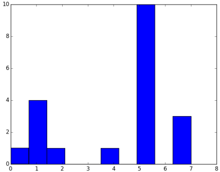

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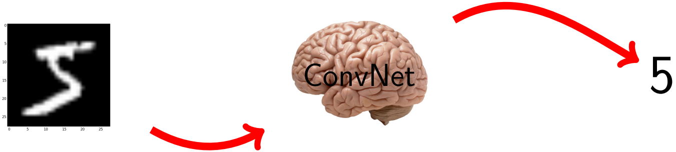

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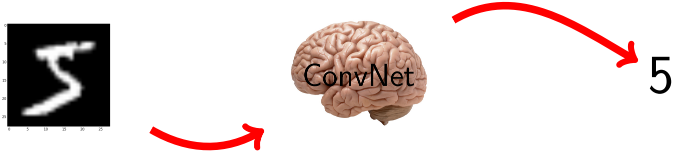

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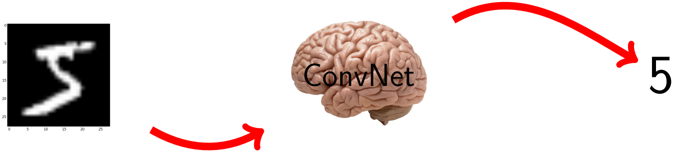

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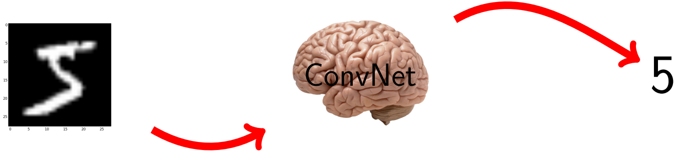

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Can this also be used for the solution of PDEs?

A Crash Course in Statistical Learning Theory

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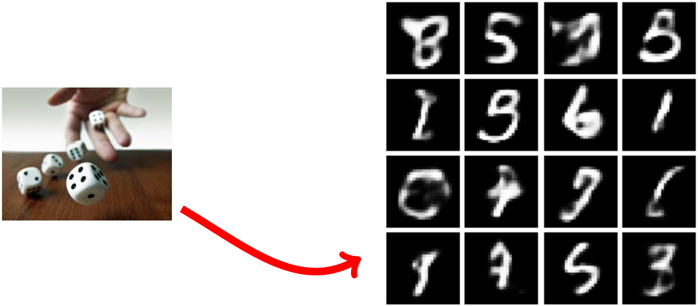

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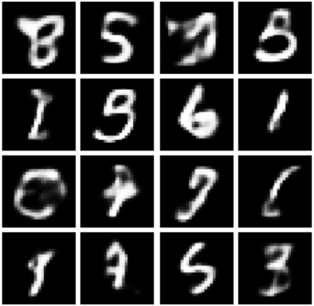

$\boxed{\rightsquigarrow \textbf{Variational Autoencoder Demo}}$

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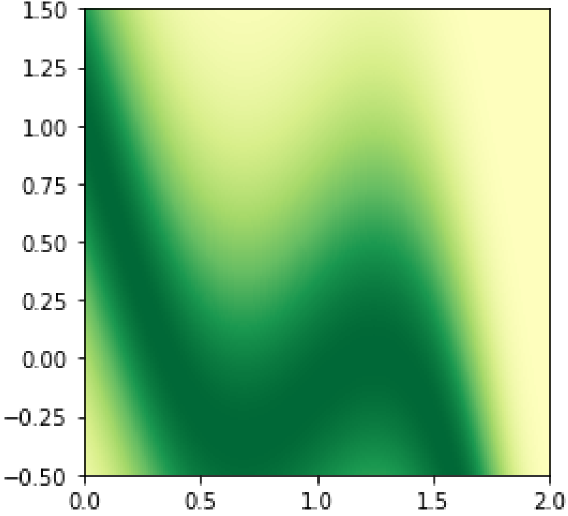

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If we knew the data distribution (X, Y), the best functional relation between X and Y would simply be $\mathbb{E}[Y|X = x]$!

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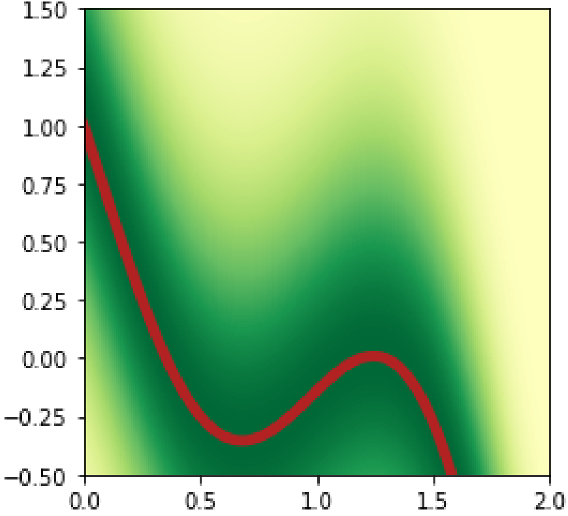

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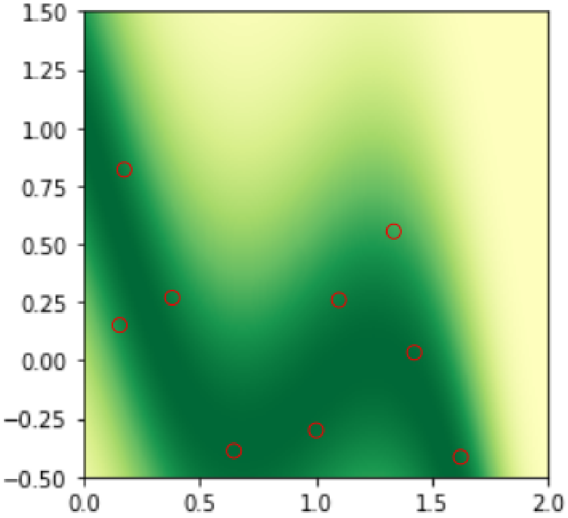

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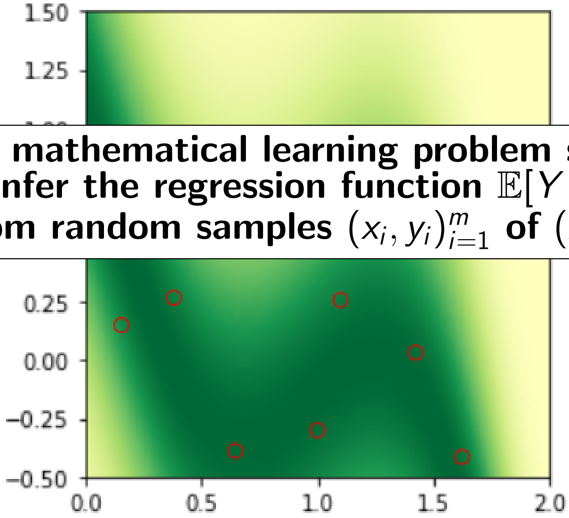

A mathematical learning problem seeks to infer the regression function $\mathbb{E}[Y|X = x]$ from random samples $(x_i, y_i)_{i=1}^m$ of (X, Y).

Mathematical Formulation

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- Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and let $X : \Omega \to \mathbb{R}^d$ and $Y : \Omega \to \mathbb{R}^n$ be random vectors. Find the best functional relationship $\hat{U} : \mathbb{R}^d \to \mathbb{R}^n$ between these vectors in the sense that

$$\begin{aligned}
\hat{U} &= \underset{U:\mathbb{R}^d \to \mathbb{R}^n}{\operatorname{argmin}} \int_\Omega |U(X(\omega)) - Y(\omega)|^2 d\mathbb{P}(\omega) \\
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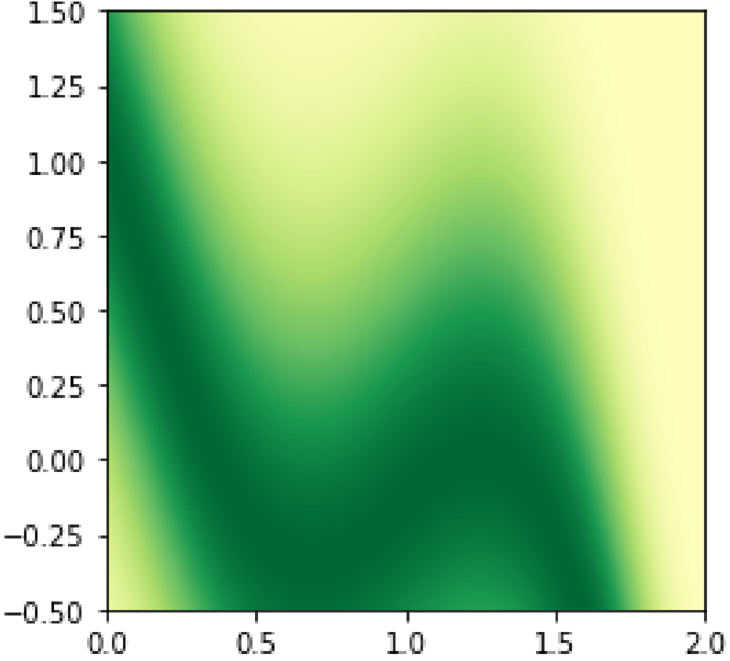
$\hat{U}$ is called the *regression function*.


1.50
1.25
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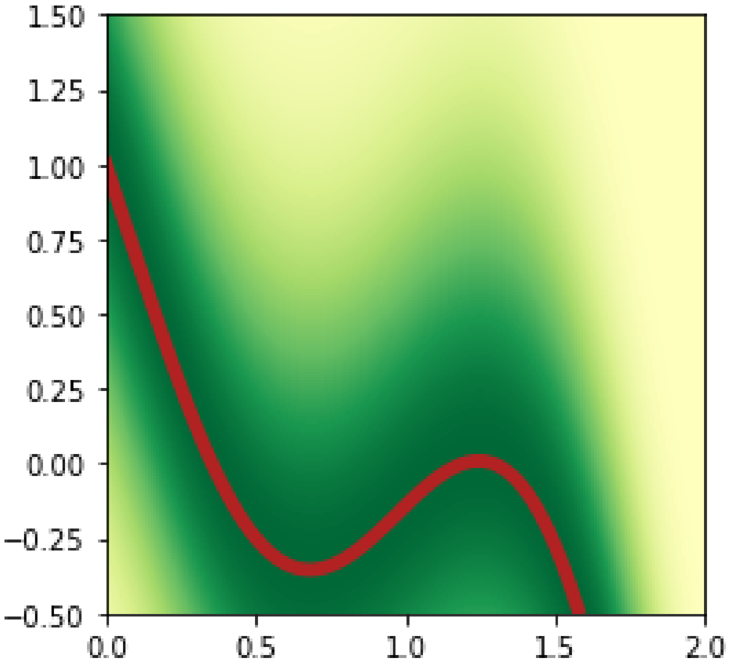
1.5
2.0



1.50
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−0.25
−0.50
0.0
0.5
1.0
1.5
2.0

Statistical Learning Theory

- Let $z = \big((x_1, y_1), \ldots, (x_m, y_m)\big)$ be m realizations of samples independently drawn according to (X, Y). For a function $U\colon \mathbb{R}^d \to \mathbb{R}^k$ define the *empirical risk* of U by

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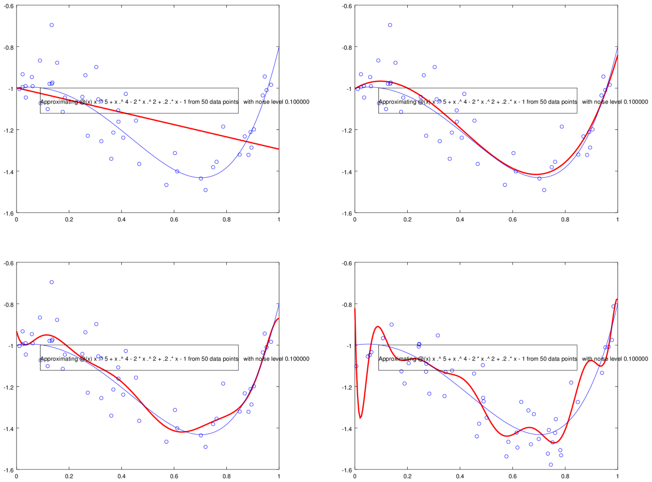
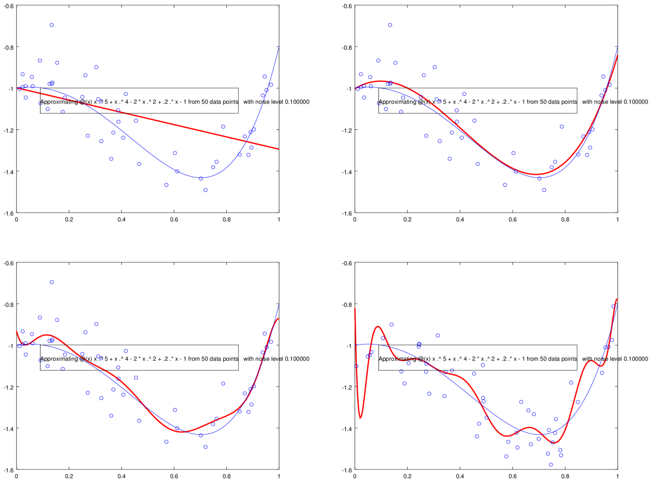
- Example $\mathcal{H} = \{\text{Polynomials of degree} \leq p\}$.



Approximating @(x) x .^ 5 + x .^ 4 - 2 * x .^ 2 + .2 .* x - 1 from 50 data points with noise level 0.100000
-0.6
-0.8
-1
-1.2
-1.4
-1.6
0
0.2
0.4
0.6
0.8
1



Degree too low: underfitting. Degree to high: overfitting!

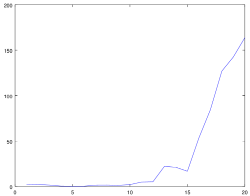


Figure: Error with Polynomial Degree

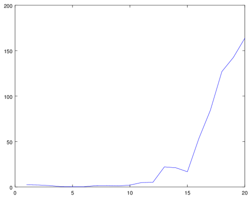


Figure: Error with Polynomial Degree

Bias-Variance-Problem

"Capacity" of the hypothesis space has to be adapted to the complexity of the target function and the sample size!

Bias-Variance Decomposition

Let (X, Y) data generating r.v.'s and $\hat{U}$ the regression function. Let $\mathbf{z} = (x_i, y_i)_{i=1}^m$ i.i.d. samples, $\mathcal{H}$ a hypothesis class and $\hat{U}_{\mathcal{H},\mathbf{z}}$ the empirical regression function. We seek to understand the error

$$\epsilon := \mathcal{E}(\hat{U}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\hat{U}) = \mathbb{E}|\hat{U}_{\mathcal{H},\mathbf{z}}(X) - \hat{U}(X)|^2$$

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Let $U_{\mathcal{H}} := \operatorname{argmin}_{U\in\mathcal{H}} \mathbb{E}|U(X) - \hat{U}(X)|^2$,
$\epsilon_{approx} := \mathbb{E}|U_{\mathcal{H}}(X) - \hat{U}(X)|^2$ the *approximation error* and
$\epsilon_{generalize} := \mathcal{E}(U_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(U_{\mathcal{H}})$ the *generalization error*. Then
$\epsilon = \epsilon_{approx} + \epsilon_{generalize}$.

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Main Theorem [e.g., Cucker-Zhou (2007)]

If $m \gtrsim \frac{\ln(\mathcal{N}(\mathcal{H}, c\cdot\eta))}{\eta^2}$ (and very strong conditions hold), then $\epsilon_{generalize} \leq \eta$ w.h.p. where $\mathcal{N}(\mathcal{H}, s)$ is the s-covering number of $\mathcal{H}$ w.r.t. L^∞ .

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Problems for Data Science Applications:

- **Assumption that data is iid is debatable**
- **Different asymptotic regime in deep learning (where often $\#$DOFs $>>$ $\#$training samples)**
- **Without knowing $\mathbb{P}_{(X,Y)}$ it is impossible to control the approximation error.**

w.r.t. L^∞ .

PDEs as Learning Problems

Explicit Solution of Heat Equation if $g = 0$

Let $u(t, x)$ satisfy

$$\frac{\partial u}{\partial t}(t, x) = \frac{\partial^2 u}{\partial x_1 \partial x_1} + \frac{\partial^2 u}{\partial x_2 \partial x_2} + \frac{\partial^2 u}{\partial x_3 \partial x_3}, \quad u(0, x) = \varphi(x)$$

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The solution $u(t,x)$ of the PDE can be interpreted as solution to the learning problem with data distribution (X,Y), where $X \sim \mathcal{U}[u,v]^3$ and $Y = \varphi(Z_t^X)$ and $Z_t^X \sim \mathcal{N}(x, t^{1/2} I)$!

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We will see in a minute that similar properties hold for a much more general class of PDEs!

Linear Kolmogorov Equations

Given $\Sigma : \mathbb{R}^d \to \mathbb{R}^{d \times d}$, $\mu : \mathbb{R}^d \to \mathbb{R}^d$ and initial value $\varphi : \mathbb{R}^d \to \mathbb{R}$, find $u : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}$ with

$$\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\mathrm{Trace}\left(\Sigma(x)\Sigma^T(x)\mathrm{Hess}_x u(t,x)\right) + \mu(x) \cdot \nabla_x u(t,x),$$
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- Examples include convection-diffusion equations and Black-Scholes Equation.
- Standard methods such as sparse grid methods, sparse tensor product methods, spectral methods, finite element methods or finite difference methods are incapable of solving such equations in high dimensions ($d = 100$)!

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- **Pricing Problem:** $u(0,x) = ??$.

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Then (Feynman-Kac)

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Lemma (Beck-Becker-G-Jafaari-Jentzen (2018))

Let $X \sim \mathcal{U}_{[a,b]^d}$ and let $Y = \varphi(Z_X^T)$. The solution $\hat{U}$ of the mathematical learning problem with data distribution (X, Y) is given by

$$\hat{U}(x) = u(T, x), \quad x \in [a, b]^d,$$

where u solves the corresponding Kolmogorov equation.

Solving linear Kolmogorov Equations by means of Neural Network Based Learning

The Vanilla DL Paradigm

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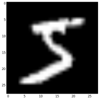
- Every image is given as a 28×28 matrix $x \in \mathbb{R}^{28\times 28} \sim \mathbb{R}^{784}$:



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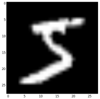
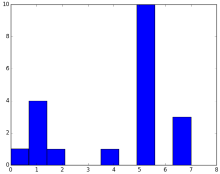


- Every label is given as a 10-dim vector $y \in \mathbb{R}^{10}$ describing the 'probability' of each digit



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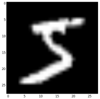

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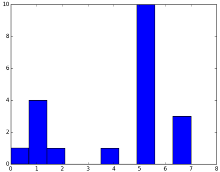

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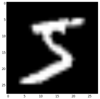

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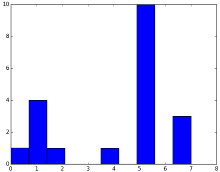

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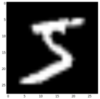

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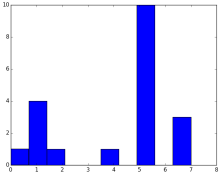

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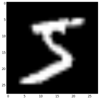

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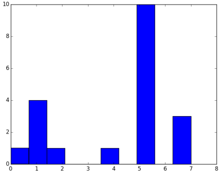

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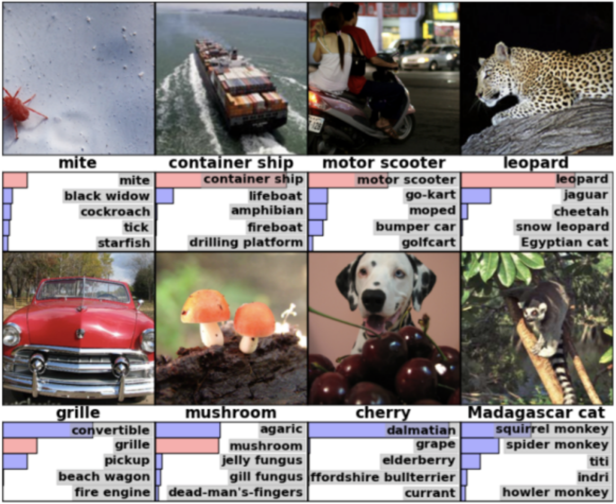
- Typically solved by stochastic first order optimization methods.

Description of Image Content

ImageNet Challenge



Deep Learning Algorithm

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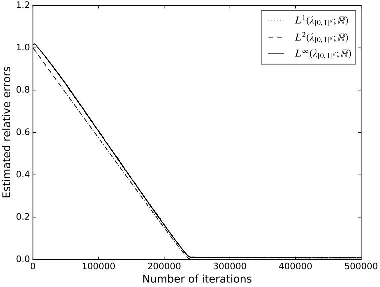
2. Apply the Deep Learning Paradigm to this training data ...meaning that
   (i) we pick a network architecture $(N_0 = d, N_1, \ldots, N_L = 1)$, and let $\mathcal{H} = \mathcal{H}^\sigma_{(N_0,\ldots,N_L)}$ and
   (ii) attempt to approximately compute

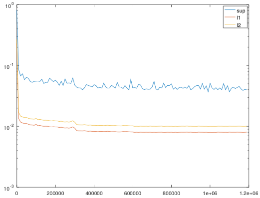
$$\hat{U}_{\mathcal{H},\mathbf{z}} = \operatorname*{argmin}_{U \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^m (U(x_i) - y_i)^2$$

   in Tensorflow.



Number of steps	Relative $L^1(\lambda_{[0,1]^d};\mathcal{R})$-error	Relative $L^2(\lambda_{[0,1]^d};\mathcal{R})$-error	Relative $L^\infty(\lambda_{[0,1]^d};\mathcal{R})$-error	Runtime in seconds
0	0.998253	0.998254	1.003524	0.5
10000	0.957464	0.957536	0.993083	44.6
50000	0.786743	0.786806	0.828184	220.8
100000	0.574013	0.574060	0.605283	440.8
150000	0.361564	0.361594	0.384105	661.0
200000	0.001419	0.001784	0.010423	880.8
500000	0.001419	0.001784	0.010423	2200.7
750000	0.001419	0.001784	0.010423	3300.6

Figure: Estimated errors associated to the solution $u(1,\cdot)$ of the 100-dimensional parabolic PDE $\frac{\partial u}{\partial t}(t,x) = \Delta_x u(t,x)$, $u(0,x) = |x|^2$, $x \in [0,1]^{100}$.



Number of steps	Relative $L^1(\lambda_{[90,110]^d};\mathcal{R})$-error	Relative $L^2(\lambda_{[90,110]^d};\mathcal{R})$-error	Relative $L^\infty(\lambda_{[90,110]^d};\mathcal{R})$-error	Runtime in seconds
0	1.004285	1.004286	1.009524	1
25000	0.842938	0.843021	0.87884	110.2
50000	0.684955	0.685021	0.719826	219.5
100000	0.371515	0.371551	0.387978	437.9
150000	0.064605	0.064628	0.072259	656.2
250000	0.001220	0.001538	0.010039	1092.6
500000	0.000949	0.001187	0.005105	2183.8
750000	0.000902	0.001129	0.006028	3275.1

Figure: Estimated errors associated to the solution $u(T,\cdot)$ of the 100-dimensional uncorrelated Black Scholes PDE $\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\sum_{i=1}^{d} |\sigma_i x_i|^2 (\frac{\partial^2 u}{\partial x_i^2})(t,x) + \sum_{i=1}^{d} \mu_i x_i (\frac{\partial u}{\partial x_i})(t,x)$, $u(0,x) = \exp(-rT)\max\{\max_{i\in\{1,2,\ldots,d\}} x_i - 100, 0\}$, $x \in [90,110]^{100}$.

Number of steps	Relative $L^1(\lambda_{[90,110]^d};\mathcal{R})$-error	Relative $L^2(\lambda_{[90,110]^d};\mathcal{R})$-error	Relative $L^\infty(\lambda_{[90,110]^d};\mathcal{R})$-error	Runtime in seconds
0	1.003383	1.003385	1.011662	0.8
25000	0.631420	0.631429	0.640633	112.1
50000	0.269053	0.269058	0.275114	223.3
100000	0.000752	0.000948	0.00553	445.8
150000	0.000694	0.00087	0.004662	668.2
250000	0.000604	0.000758	0.006483	1119.3
500000	0.000493	0.000615	0.002774	2292.8
750000	0.000471	0.00059	0.002862	3466.8

Figure: Estimated errors associated to the solution $u(T,\cdot)$ of the 100-dimensional correlated Black Scholes PDE $\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\sum_{i,j=1}^{d} x_i x_j \beta_i \beta_j \langle \varsigma_i, \varsigma_j \rangle_{\mathbb{R}^d} \big(\frac{\partial^2 u}{\partial x_i \partial x_j}\big)(t,x) + \sum_{i=1}^{d} \mu_i x_i \big(\frac{\partial u}{\partial x_i}\big)(t,x)$, $u(0,x) = \exp(-\mu T) \max\big\{110 - \min_{i\in\{1,2,\dots,d\}}\{x_i\}, 0\big\}$, $x \in [90,110]^{100}$.

Number of steps	Relative $L^1(\lambda_{[90,110]^d};\mathcal{R})$-error	Relative $L^2(\lambda_{[90,110]^d};\mathcal{R})$-error	Relative $L^\infty(\lambda_{[90,110]^d};\mathcal{R})$-error	Runtime in seconds
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All computations were performed in single precision (float32) on a NVIDIA GeForce GTX 1080 GPU with 1974 MHz core clock and 8 GB GDDR5X memory with 1809.5 MHz clock rate. The underlying system consisted of an Intel Core i7-6800K CPU with 64 GB DDR4-2133 memory running Tensorflow 1.5 on Ubuntu 16.04.

Some Theoretical Results

Linear Affine Kolmogorov Equations

Given $\Sigma : \mathbb{R}^d \to \mathbb{R}^{d\times d}$, $\mu : \mathbb{R}^d \to \mathbb{R}^d$ affine and initial value $\varphi : \mathbb{R}^d \to \mathbb{R}$, find $u : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}$ with

$$\frac{\partial u}{\partial t}(t,x) = \frac{1}{2}\mathrm{Trace}\left(\Sigma(x)\Sigma^T(x)\mathrm{Hess}_x u(t,x)\right) + \mu(x)\cdot\nabla_x u(t,x),$$
$$(t,x) \in [0,T]\times\mathbb{R}^d, \quad u(0,x) = \varphi(x).$$

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Theorem [G-Hornung-Jentzen-Von Wurstenberger (2018)], simplified version

Suppose that $\varphi \in \mathcal{H}^\sigma_{(N_0,\dots,N_L)}$ (or can be well approximated by NNs). Then for all $\epsilon > 0$ there is Φ_ϵ with $\mathrm{size}(\Phi_\epsilon) \lesssim \mathrm{size}(\varphi)\cdot\epsilon^{-2}$ and

$$\sup_{x\in[a,b]^d} |u(T,x) - R_\sigma(\Phi_\epsilon)(x)| \le \epsilon.$$

The implicit constant depends at most polynomially on the dimension $d = N_0$.

Option Pricing without Curse of Dimensionality

Theorem [Berner-G-Jentzen (2018)], very special case

Let $\varphi(x) = \min\{\max\{\max(x_i - K_i), 0\}, R\}$ or $\varphi(x) = \min\{\max\{\sum_{i=1}^{d} x_i - K, 0\}, R\}$ (or any typical option). Then for all $\epsilon > 0$ there is $\Phi_\epsilon \in \mathcal{H}^{ReLU}_{(N_0,\ldots,N_L)}$ with $\mathrm{size}(\Phi_\epsilon) = \mathcal{O}(\epsilon^{-2})$ and

$$\frac{1}{(b-a)^{d/2}} \left(\int_{[a,b]^d} |u(T,x) - R_\sigma(\Phi_\epsilon)(x)|^2 dx \right)^{1/2} \leq \epsilon.$$

Such networks can be found by solving the ERM problem with $m \sim \epsilon^{-4}$ samples. The implicit constants depend at most polynomially on the dimension $d = N_0$!

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Due to compositional structure of NNs, all results hold also for options operating on options...

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Wrap Up

- Several PDEs can be reformulated as learning problem
- Neural network based numerical solution of high-dimensional PDEs is extremely promising both empirically and mathematically – and it is possible to prove real theorems!
- Specifically, we can prove that these methods are capable of overcoming the curse of dimensionality for an important class of PDEs arising in computational finance.
- We can observe these properties in simulations.

Thank You!

Questions?

Literature

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