Robust and efficient identification of neural networks

Sampling recovery and related problems
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May 2021

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Outline

- Approximation of multivariate functions
- Structural assumptions: active variables, SPAM's, ...
- Ridge functions - single neurons:
  - Recovery algorithms
  - Lower bounds
- Sums of ridge functions - one layer neural networks:
  - Non-linear optimization
  - Whitening
  - ...

Classical task of approximation/sampling:
Given a function f with some properties (i.e. from some set) and few its function values $y_1 = f(x_1), \dots, y_n = f(x_n)$ generate a function g, which is close to f in some sense.

Typically, the error (i.e. the distance of f and g) decays with n. Well known for many classical function spaces, like Sobolev spaces, Besov spaces, Triebel-Lizorkin spaces, etc.

Typical decay: $n^{-s/d}$

Birman, Solomyak, Temlyakov, Kudryavtsev, Kashin, DeVore, Maiorov, Cohen, Kruglyak, Heinrich, Novak, Triebel, Sickel, Ullrich and many many others ...

Curse of dimension

Many classical problems suffer from exponential dependence of the results on d!

Example: Approximation of smooth functions
Let $\mathcal{F}_d := \{f : [0,1]^d \to \mathbb{R}, \|D^\alpha f\|_\infty \le 1, \alpha \in \mathbb{N}_0^d\}$
Smoothness does not help!. . . ?!
Infinitely differentiable functions on $\Omega = [0,1]^d$:

Novak, Woźniakowski (2009): Initial error is the same as error of uniform approximation for $n \le 2^{\lfloor d/2 \rfloor} - 1$
. . . curse of dimension!
. . . the number of sampling points must grow exponentially in d

Structural assumptions

- **Active variables:**

R. DeVore, G. Petrova, and P. Wojtaszczyk: Approximation of functions of few variables in high dimensions, Constr. Appr. 2011:

$$f(x_1,\dots,x_d) := g(x_{i_1},\dots,x_{i_\ell}),\quad \ell \ll N.$$

1-Lipschitz function f can be recovered uniformly with accuracy ε from $C(\ell)\varepsilon^{-\ell}\log_2 d$ sampling points.

Use of low-rank matrix recovery:
H. Tyagi, V. Cevher, Learning non-parametric basis independent models from point queries via low-rank methods, ACHA 2014

Revisited also in
K. Schnass, J.V., Compressed learning of high-dimensional sparse functions, Proceedings of ICASSP '11
S. Foucart, Sampling schemes and recovery algorithms for functions of few coordinate variables, J. Compl. 2020

Structural assumptions

• **Sparse additive models:** H. Tyagi and J. Vybiral: Learning non-smooth sparse additive models from point queries in high dimensions, Constr. Appr. 2019:

$r_0 = 1,\ f : [-1,1]^d \to \mathbb{R}$

$$f(x) = \sum_{j \in \mathcal{S}_1} \phi_j(x_j),$$

where $x = (x_1, \ldots, x_d)$ and $\mathcal{S}_1 \subset \{1, \ldots, d\}$ with $|\mathcal{S}_1| \ll d$

$r_0 = 2,\ f : [-1,1]^d \to \mathbb{R}$

$$f(x) = \sum_{j \in \mathcal{S}_1} \phi_j(x_j) + \sum_{(j_1,j_2) \in \mathcal{S}_2} \phi_{(j_1,j_2)}(x_{j_1}, x_{j_2}),$$

with $\mathcal{S}_2 \subset \binom{\{1,\ldots,d\}}{2}$ and $|\mathcal{S}_2| \ll \binom{d}{2}$

Ridge functions

Ridge functions

Let $g : \mathbb{R} \to \mathbb{R}$ and $a \in \mathbb{R}^d \setminus \{0\}$.
Ridge function with *ridge profile* g and *ridge vector* a is the function

$$f(x) := g(\langle a, x \rangle).$$

Constant along the hyperplane $a^\perp = \{y \in \mathbb{R}^d : \langle y, a \rangle = 0\}$ and its translates.

More general, if $g : \mathbb{R}^k \to \mathbb{R}$ and $A \in \mathbb{R}^{k \times d}$ with $k \ll d$ then

$$f(x) := g(Ax)$$

is a $k-$*ridge function*.

Ridge functions in approximation theory

Approximation of a function by functions from the dictionary

$$D_{\mathrm{ridge}} = \{\varrho(\langle k, x\rangle - b) : k \in \mathbb{R}^d, b \in \mathbb{R}\}$$

- Fundamentality
- Greedy algorithms

Lin & Pinkus, Fundamentality of ridge functions, J. Approx. Theory 75 (1993), no. 3, 295–311

Cybenko, Approximation by superpositions of a sigmoidal function, Math. Control Signals Systems 2 (1989), 303–314

Leshno, Lin, Pinkus & Schocken, Multilayer feedforward networks with a nonpolynomial activation function can approximate any function, Neural Networks 6 (1993), 861–867

Ridge functions: Approximation algorithms

$k=1$: $f(x)=g(\langle a,x\rangle)$, $\quad \|a\|_2=1$, $\quad g$ smooth

Approximation has two parts: approximation of g and of a

Recovery of a - from $\nabla f(x)$:

$$\nabla f(x)=g'(\langle a,x\rangle)a, \nabla f(0)=g'(0)a.$$

After recovering a, the problem becomes essentially one-dimensional and one can use arbitrary sampling method to approximate g.

$g'(0)\neq 0\ldots g'(0)=1$

A.Cohen, I.Daubechies, R.DeVore, G.Kerkyacharian, D.Picard, '12
Capturing ridge functions in high dimensions from point queries

- $\boldsymbol{k = 1 : f(x) = g(\langle a, x\rangle)}$
- $f : [0,1]^d \to \mathbb{R}$
- $g \in C^s([0,1])$, $1 < s$
- $\|g\|_{C^s} \leq M_0$
- $\boldsymbol{\|a\|_{\ell_q^d} \leq M_1, 0 < q \leq 1}$
- $\boldsymbol{a \geq 0}$

Then

$$\|f - \hat{f}\|_\infty \leq CM_0 \left\{ L^{-s} + M_1 \left(\frac{1 + \log(d/L)}{L} \right)^{1/q-1} \right\}$$

using $3L + 2$ sampling points

- First sampling along the diagonal $\frac{i}{L}\mathbf{1} = \frac{i}{L}(1, \ldots, 1), i = 0, \ldots, L$:

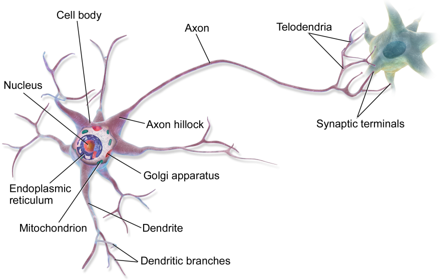
$$f\left(\frac{i}{L}\mathbf{1}\right) = g\left(\left\langle \frac{i}{L}\mathbf{1}, a\right\rangle\right) = g(i\|a\|_1/L)$$

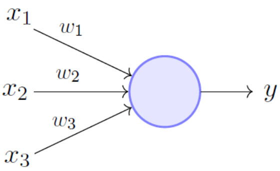
- Recovery of g on a grid of $[0, \|a\|_1]$
- Finding i_0 with largest $g((i_0 + 1)\|a\|_1/L) - g(i_0\|a\|_1/L)$
- Approximating $D_{\varphi_j} f(i_0/L \cdot \mathbf{1}) = g'(i_0\|a\|_1/L)\langle a, \varphi_j\rangle$ by first order differences
- Then recovery of a from $\langle a, \varphi_1\rangle, \ldots, \langle a, \varphi_m\rangle$ by methods of compressed sensing (CS)

Further results:

- M. Fornasier, K. Schnass, and J.V., Learning functions of few arbitrary linear parameters in high dimensions, Found. Comput. Math. (2012)
  $\rightsquigarrow$ Recovery algorithm for ridge functions on a ball
- A. Kolleck and J.V., On some aspects of approximation of ridge functions, J. Appr. Theory (2015)
  $\rightsquigarrow$ Ridge functions on cubes and other topics
- S. Mayer, T. Ullrich, and J.V., Entropy and sampling numbers of classes of ridge functions, Constr. Appr. (2015)
  $\rightsquigarrow$ Lower bounds, entropy numbers
- B.Doerr and S. Mayer, The recovery of ridge functions on the hypercube suffers from the curse of dimensionality, J. Compl. (2021)
  $\rightsquigarrow$ Ridge functions on cubes, lower bounds

Motivated by biological research on human brain and neurons
W. McCulloch, W. Pitts (1943); M. Minsky, S. Papert (1969)





Perceptron Model (Minsky-Papert in 1969)

Artificial Neuron

...gets activated if a linear combination of its inputs grows over a certain threshold...

- Inputs $x = (x_1, \dots, x_n) \in \mathbb{R}^n$
- Weights $w = (w_1, \dots, w_n) \in \mathbb{R}^n$
- Comparing $\langle w, x \rangle$ with a threshold $b \in \mathbb{R}$
- Plugging the result into the "activation function" - jump (or smoothed jump) function σ

Artificial neuron is a function

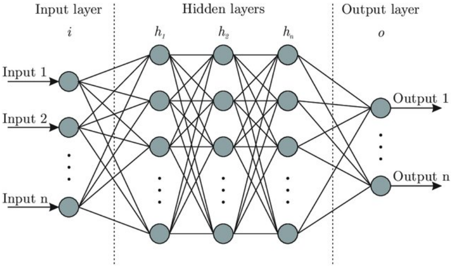
$$x \to \sigma(\langle x, w \rangle - b),$$

where $\sigma : \mathbb{R} \to \mathbb{R}$ might be $\sigma(x) = \text{sign}(x)$ or $\sigma(x) = e^x/(1 + e^x)$, etc.

Artificial neural networks

Artificial neural network is a directed, acyclic graph of artificial neurons

- Input: $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$
- First layer of neurons:
  $y_1 = \sigma(\langle x, w_1^1 \rangle - b_1^1), \ldots, y_{n_1} = \sigma(\langle x, w_{n_1}^1 \rangle - b_{n_1}^1)$
- The outputs $y = (y_1, \ldots, y_{n_1})$ become inputs for the next layer . . . ; last layer outputs $y \in \mathbb{R}$



M. Fornasier, J.V., I. Daubechies,
Robust and resource efficient identification of shallow neural networks by fewest samples
to appear in IMA: Information and Inference

Recovery of

$$f(x) = \sum_{j=1}^{m} g_j(\langle a_j, x\rangle)$$

- one layer of a neural network

- Special case of $f(x) = g(Ax)$, but we would like to have m onedimensional problems, and not one m-dimensional
- We would like to identify $a_1, \dots, a_m$, then $g_1, \dots, g_m$

- **Step 1.:** Sampling of

$$\nabla f(x) = \sum_{j=1}^{m} g_j'(\langle a_j, x\rangle) a_j$$

at different points gives elements of

$$A = \operatorname{span}\{a_1, \dots, a_m\} \subset \mathbb{R}^d$$

- We sample (only) differences and obtain an approximation $\tilde{A} \sim A$, upper bound on $\|P_A - P_{\tilde{A}}\|_F$
- $\bar{A}$ - matrix, columns are a basis of $\tilde{A}$
- We consider

$$\tilde{f}(y) = \sum_{i=1}^{m} g_i(\langle \bar{A}^T a_i, y\rangle) = \sum_{i=1}^{m} g_i(\langle a_i, \bar{A}y\rangle)$$

Recovery of individual a_i's for $d = m$?

- **Step 2.:** Second order derivatives:

$$\nabla^2 f(x) = \sum_{j=1}^{m} g_j''(\langle a_j, x\rangle) a_j \otimes a_j$$

- Put

$$\mathcal{A} = \operatorname{span}\{a_i \otimes a_i : i = 1, \dots, m\} \subset \mathbb{R}^{m \times m}$$

- We can recover $\tilde{\mathcal{A}} \sim \mathcal{A}$ - an approximation of $\mathcal{A}$

- **Step 3.:** We try to find matrices in $\tilde{\mathcal{A}}$, which are close to $a_i \otimes a_i \in \mathcal{A}$

- We look for matrices in $\tilde{\mathcal{A}}$ with the "smallest" rank

- We analyze the non-convex problem

$$(\star) \qquad \arg\max \ \|M\|, \quad \text{s.t.} \quad M \in \tilde{\mathcal{A}}, \|M\|_F \leq 1$$

- Every algorithm, which is able to find an approximation of $a_1 \otimes a_1$ can also land close to $a_j \otimes a_j$, $j = 2, \ldots, m$, hence **it must be non-convex**

Analysis of $(\star)$:
- Let M be a local maximizer of $(\star)$
- Eigenvalues $\lambda_1, \ldots, \lambda_m$, eigenvectors $u_1, \ldots, u_m$
- Then

$$u_j^T X u_j = \lambda_j \langle X, M \rangle \quad \text{for every } X \in \tilde{\mathcal{A}}$$

and every j with $|\lambda_j| = \|M\|$
- If $a_1, \ldots, a_m$ are nearly orthonormal, then $|\lambda_1| = \|M\|$ is unique and

$$2 \sum_{k=2}^{m} \frac{(u_1^T X u_k)^2}{|\lambda_1 - \lambda_k|} \leq \|M\| \cdot \|X - \langle X, M \rangle_F M\|_F^2 \quad \text{for all } X \in \tilde{\mathcal{A}}$$

second Hadamard variation formula

The Algorithm leads to $\hat{a}$ with $\|\hat{a} - a_{j_0}\|_2$ small.

Whitening: If a_i's are not orthonormal, we consider (any) positive definite

$$G = \sum_{i=1}^{m} \xi_i a_i \otimes a_i \in \mathcal{A}$$

and its singular value decomposition

$$G = UDU^T,$$

then $W := D^{-1/2} U^T$ is the so-called *whitening matrix* and $\{\sqrt{\xi_i} W a_i : i = 1, \ldots, m\}$ is an orthonormal basis.

Passive sampling: sampling points preselected at random from a distribution with known density

Identification of g_i's:
- $(\hat{a}_j)_{j=1}^m$ an approximation of $(a_j)_{j=1}^m$
- $(\hat{b}_j)_{j=1}^m$ the dual basis to $(\hat{a}_j)_{j=1}^m$
- $\hat{g}_j(t) := f(t\hat{b}_j)$.

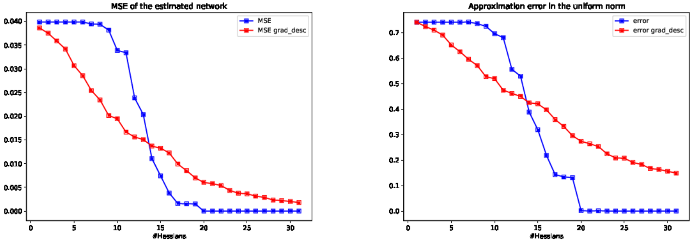


Figure: Average approximation error of 10 random networks with $m = 20, \varepsilon = 1$ in terms of MSE (left), uniform norm (right). The errors were measured over 10^5 datapoints generated uniform at random on the ball B_1^d.

Thank you for your attention!