

Estimation ability of deep learning with connection to sparse estimation in function space

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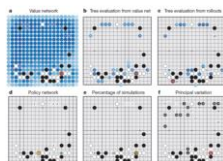
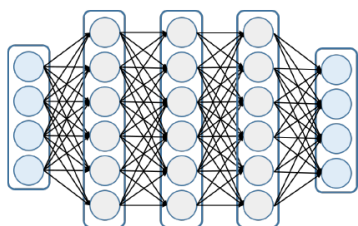
4TU.AMI Meeting on Mathematics of Deep Learning

@TU Delft, Science Centre

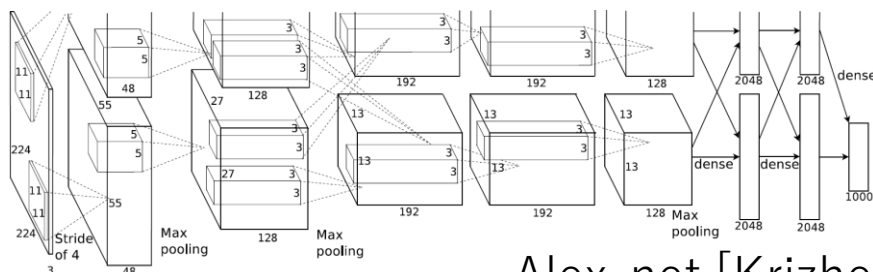
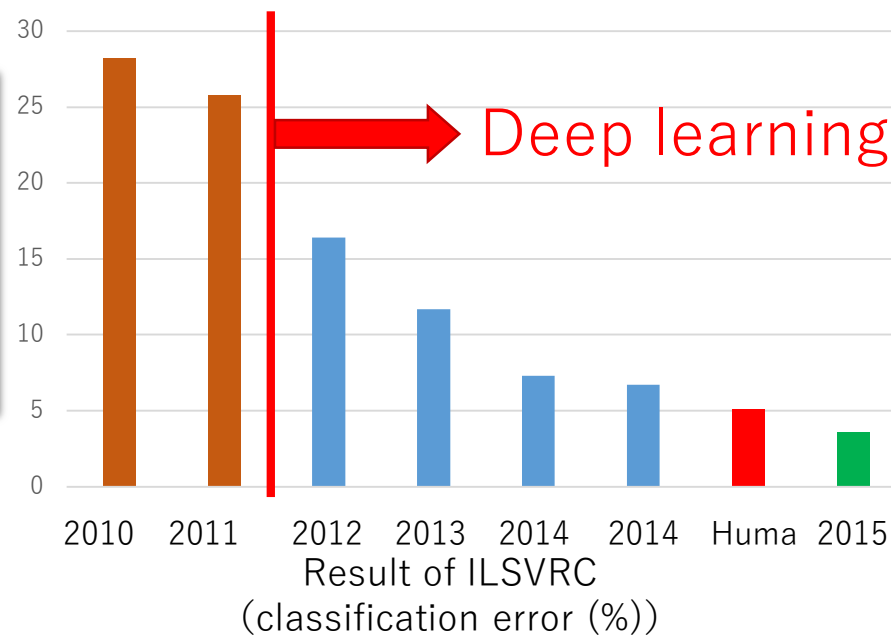
Theory of Deep Learning

Deep learning

- High performance
- Applied to services in several industries:
Google Deepmind, Facebook AI Lab., Baidu, ...

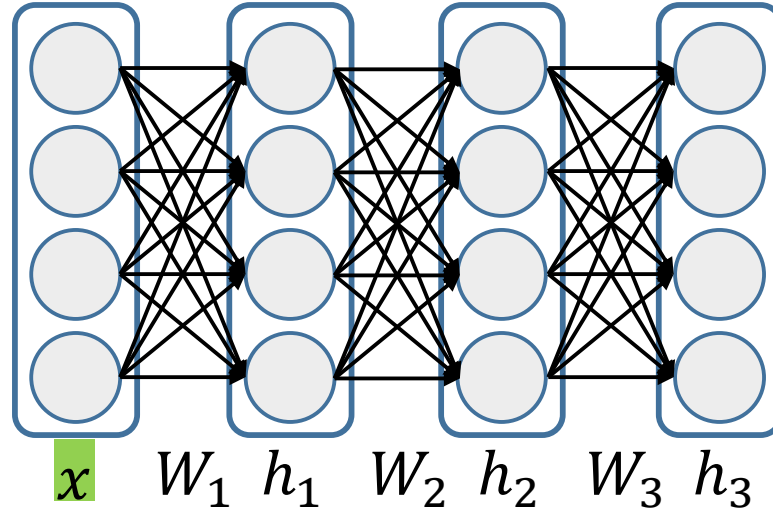


• High performance in several applications
• But, theoretical understanding is not satisfactory (Big issue all over the world)

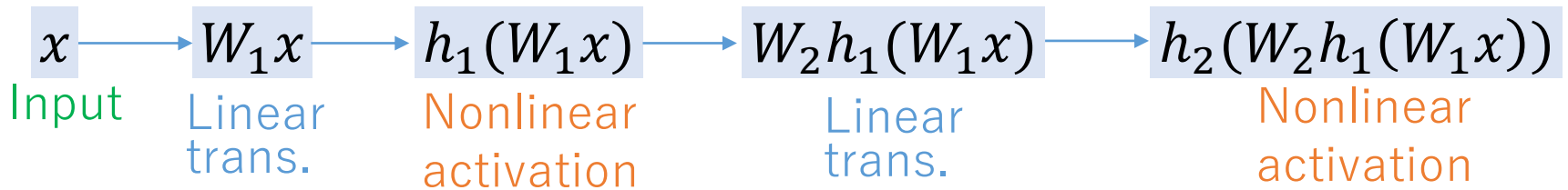


Alex-net [Krizhevsky, Sutskever + Hinton, 2012]

Structure of deep NN



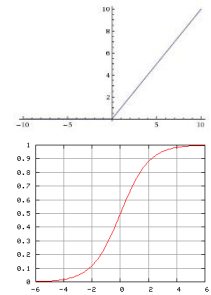
Repeat “linear transform” and “nonlinear activation.”



$$h_1(u) = [h_{11}(u_1), h_{12}(u_2), \dots, h_{1d}(u_d)]^T$$

- \star ReLU (Rectified Linear Unit) : $h(u) = \max\{u, 0\}$

- Sigmoid function : $h(u) = \frac{1}{1 + e^{-u}}$

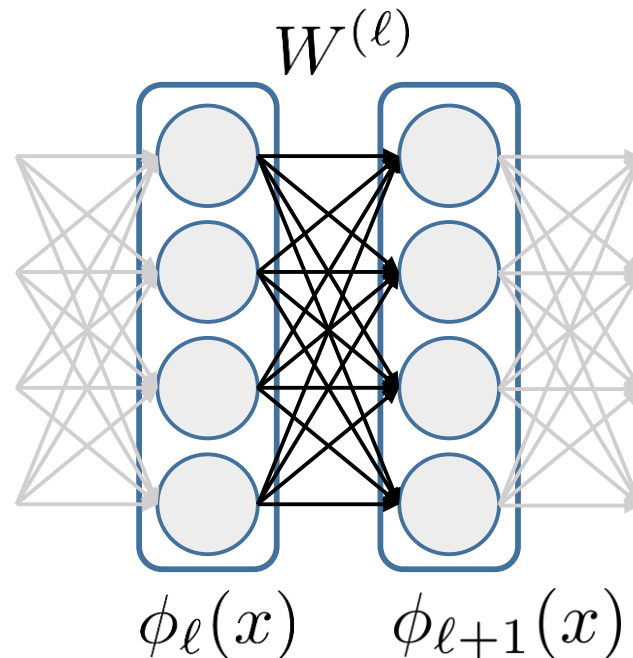


Fully connected layer

- ℓ -th layer

$$\phi_{\ell+1}(x) = \eta(W^{(\ell)}\phi_{\ell}(x) + b^{(\ell)})$$

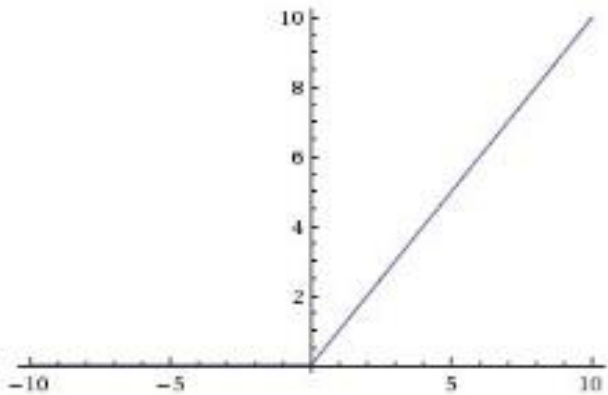
$$W^{(\ell)} \in \mathbb{R}^{m_{\ell+1} \times m_{\ell}} \quad b^{(\ell)} \in \mathbb{R}^{m_{\ell+1}}$$



Examples of activation functions

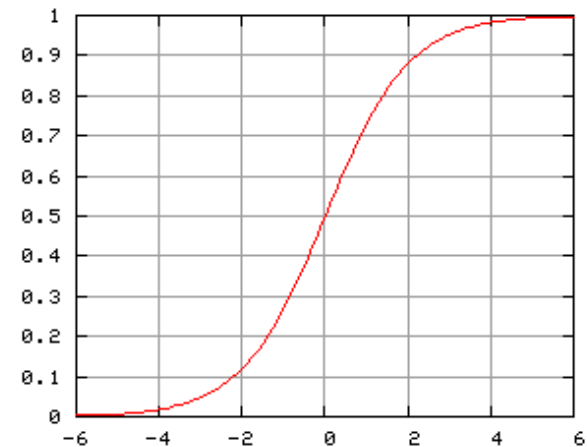
★ReLU (Rectified Linear Unit)

$$\eta(u) = \max\{u, 0\}$$



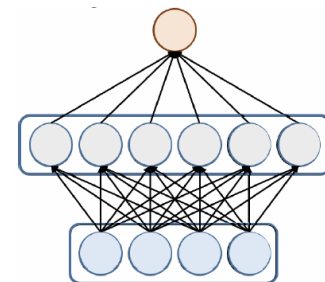
Sigmoid function

$$\eta(u) = \frac{1}{1 + e^{-u}}$$



Universal Approximator

$$f(x) = \sum_{j=1}^m v_j \eta(w_j^\top x + b_j)$$



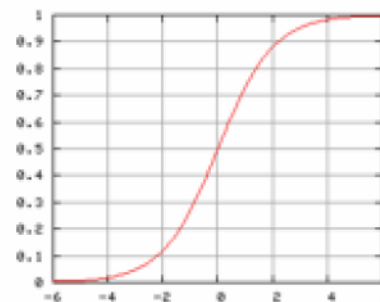
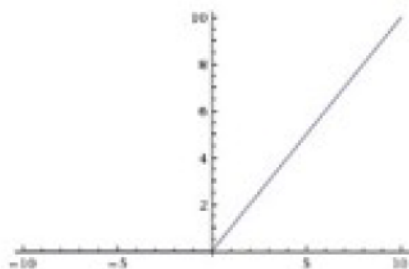
Taking $m \rightarrow \infty$, we can approximate “any function” with “any precision.”

η can be sigmoid or ReLU.

Activation functions:

ReLU: $\eta(u) = \max\{u, 0\}$

Sigmoid: $\eta(u) = \frac{1}{1 + \exp(-u)}$



2015

Shinji Ueda, Masahito

Unbounded, admissible

$L_1(\mathbb{R}^n), L_2(\mathbb{R}^n)$

K is any compact set.

Ref: 園田, “ニューラルネットの積分表現理論”, 2015.

Adaptivity of deep learning

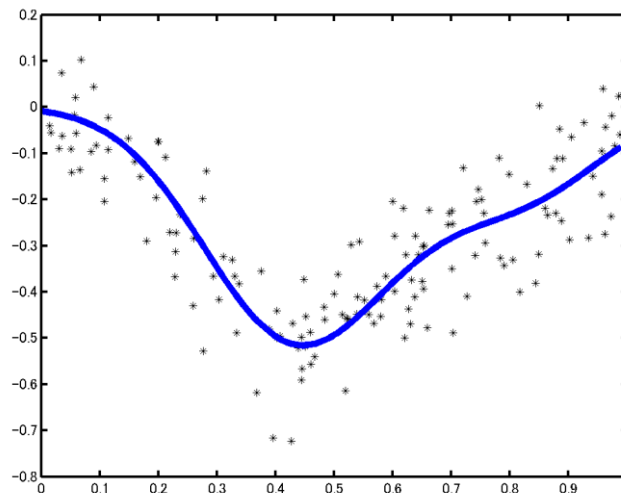
- Deep learning shows good performances in various tasks.
 - “Adaptivity” of deep learning
 - Besov space and its variants.
 - Deep learning can outperform non-adaptive method and linear estimators.
 - Extension of the theory to more general space.
- Suzuki: Adaptivity of deep ReLU network for learning in Besov and mixed smooth Besov spaces: optimal rate and curse of dimensionality. ICLR2019.
- Oono&Suzuki: Approximation and Non-parametric Estimation of ResNet-type Convolutional Neural Networks. ICML2019.
- Hayakawa&Suzuki: On the minimax optimality and superiority of deep neural network learning over sparse parameter spaces. arXiv:1905.09195.
- Suzuki&Nitanda: Deep learning is adaptive to intrinsic dimensionality of model smoothness in anisotropic Besov space. arXiv:1910.12799, 2019.

Non-parametric regression

$$y_i = f^\circ(x_i) + \xi_i \quad (i = 1, \dots, n)$$

where $\xi_i \sim N(0, \sigma^2)$ and $x_i \in [0, 1]^d \sim P_X(X)$ (i.i.d.).

We estimate f° from $(x_i, y_i)_{i=1}^n$.



Estimation error:

$$\mathbb{E}[\|\hat{f} - f^\circ\|_{L_2(P)}^2] < ?$$

A similar argument can be applied to classification.

Relation to existing work

Hölder

Normal data

[Schmidt-Hieber, 2018]
[Yarotsky, 2017]
Deep learning with ReLU
activation achieves minimax
rate in Hölder space:

$$n^{-\frac{2s}{2s+d}}$$

Besov

[Suzuki, 2019]
Minimax rate in Besov space:

$$n^{-\frac{2s}{2s+d}}$$

Kernel method (linear est.):

$$n^{-\frac{2s - 2d(1/p - 1/2)_+}{2s+d - 2d(1/p - 1/2)_+}}$$

Anisotropic Besov

[Suzuki&Nitanda, 2019]
Minimax rate:

$$n^{-\frac{2\bar{s}}{2\bar{s}+1}} \quad \bar{s} := \left(\frac{1}{s_1} + \dots + \frac{1}{s_d} \right)^{-1}$$

Kernel method (linear est.):

$$n^{-\frac{2(s_{\min} - D/p + d/2)}{2(s_{\min} - D/p + d/2) + d}}$$

High dimensional
structured data

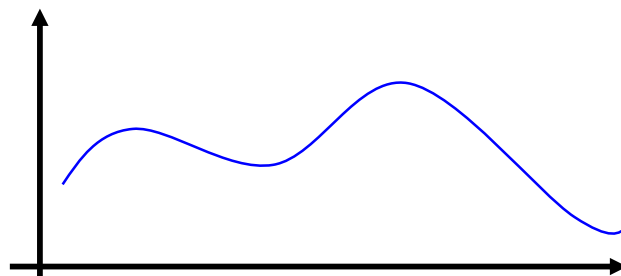
- [Schmidt-Hieber, 2018]:
composition of Holder.
- [Schmidt-Hieber, 2019]
[Nakada&Imaizumi, 2019]:
Low dim structure.

$$n^{-\frac{2s}{2s+D}}$$

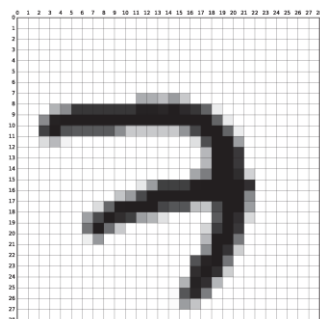
(D : intrinsic dim.)

Two quantities

- Smoothness



- Dimensionality



(a) MNIST sample belonging to the digit '7'.

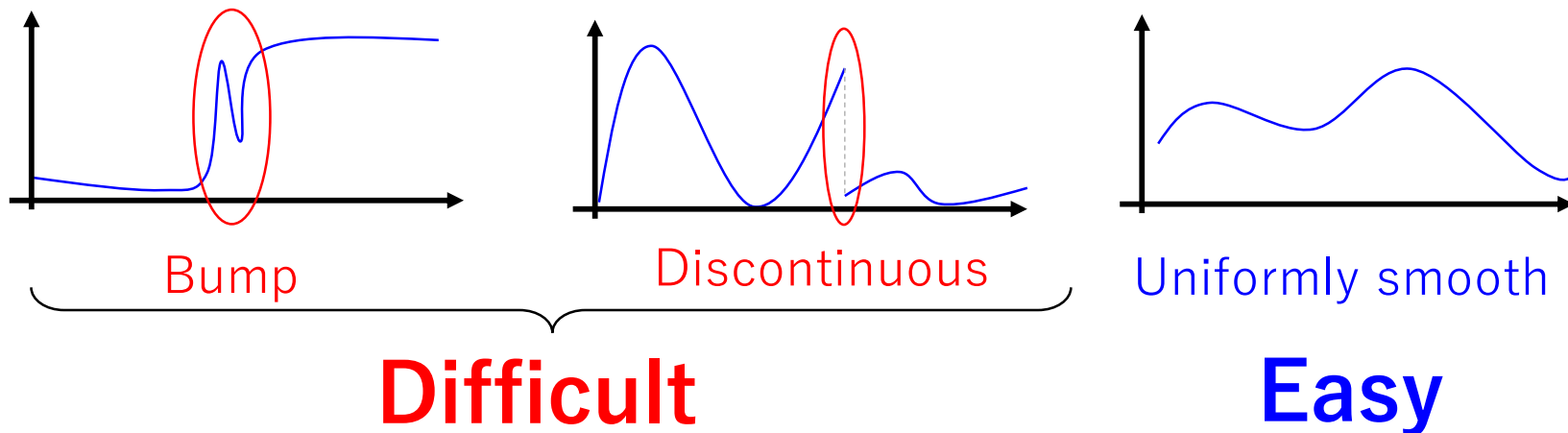


(b) 100 samples from the MNIST training set.

Smoothness

[Suzuki: Adaptivity of deep ReLU network for learning in Besov and mixed smooth Besov spaces: optimal rate and curse of dimensionality. ICLR2019]

In machine learning, there appears various types of functions:



If we overly adapt to bump, the model becomes unnecessarily large. → overfitting.
 If we adapt to smooth part, bump can not be estimated. → underfitting.

“Adaptivity” is important

Theorem

Deep learning can achieve the minimax optimal rate to estimate functions in the Besov space ($B_{p,q}^s$).
 (DL can adaptively estimate various types of functions.)

Convergence rate comparison (smoothness)

Linear estimator (shallow method)

Deep learning

e.g., kernel ridge regression:

$$\hat{f}(x) = K_{x,X}(K_{X,X} + \lambda I)^{-1}Y$$

$$n^{-\frac{2s - 2(1/p - 1/2)_+}{2s + 1 - 2(1/p - 1/2)_+}} \gg n^{-\frac{2s}{2s + 1}}$$

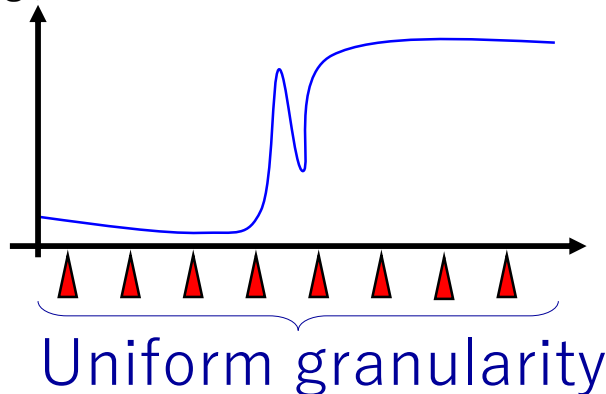
Sub-optimal

Optimal

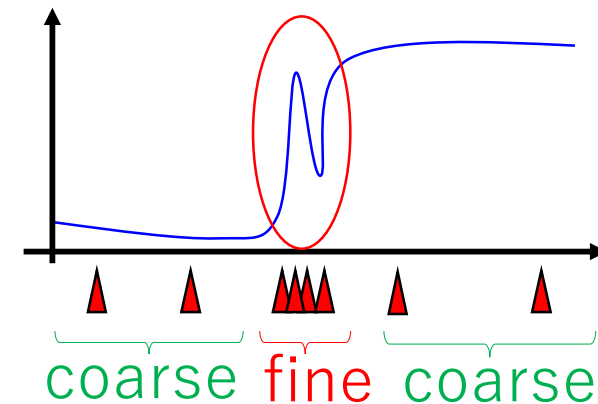
(n : sample size, p : uniformity of smoothness, s : smoothness)

Linear method

(e.g., kernel method)



Deep learning

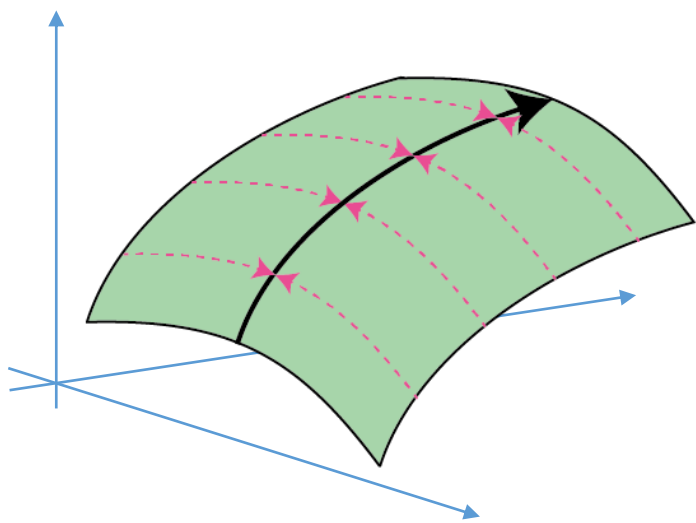


Dimensionality

- High dimensional data
→ Curse of dimensionality

Low dimensionality of the true function:

- The true function can be very smooth (constant) in several directions.
- Data is usually distributed on a low-dimensional sub-manifold.



The estimator should find in which direction the true function is smooth.

Theorem

Deep learning is minimax-optimal also in the anisotropic Besov space.

Convergence rate comparison (dimensionality)

Linear estimator (shallow method)

Deep learning

$$n^{-\frac{2(s_{\min} - D/p + d/2)}{2(s_{\min} - D/p + d/2) + d}} \gg n^{-\frac{2\tilde{s}}{2\tilde{s} + 1}}$$

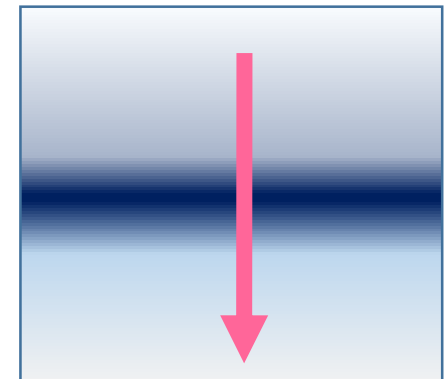
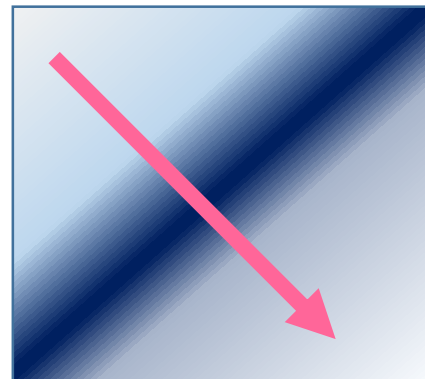
Sub-optimal

(n : sample size, s : smoothness)

Optimal

$$\tilde{s} := \left(\frac{1}{s_1} + \dots + \frac{1}{s_d} \right)^{-1}$$

Linear estimator can not find
smooth directions.
(lack of feature extraction ability)



Hölder, Sobolev, Besov space

$$\Omega = [0, 1]^d \subset \mathbb{R}^d$$

- Hölder space ($\mathcal{C}^\beta(\Omega)$)

$$\|f\|_{\mathcal{C}^\beta} = \max_{|\alpha| \leq m} \|\partial^\alpha f\|_\infty + \max_{|\alpha|=m} \sup_{x \in \Omega} \frac{|\partial^\alpha f(x) - \partial^\alpha f(y)|}{|x - y|^{\beta-m}}$$

- Sobolev space ($W_p^k(\Omega)$)

$$\|f\|_{W_p^k} = \left(\sum_{|\alpha| \leq k} \|D^\alpha f\|_{L^p(\Omega)}^p \right)^{\frac{1}{p}}$$

- Besov space ($B_{p,q}^s(\Omega)$) ($0 < p, q \leq \infty, 0 < s \leq m$)

$$\omega_m(f, t)_p := \sup_{\|h\| \leq t} \left\| \sum_{j=0}^m (-1)^{m-j} \binom{m}{j} f(\cdot + jh) \right\|_{L^p(\Omega)},$$

$$\|f\|_{B_{p,q}^s(\Omega)} = \|f\|_{L^p(\Omega)} + \left(\int_0^\infty [t^{-s} \omega_m(f, t)_p]^q \frac{dt}{t} \right)^{1/q}.$$

Spatial homogeneity
of smoothness

Smoothness

Relation between the spaces

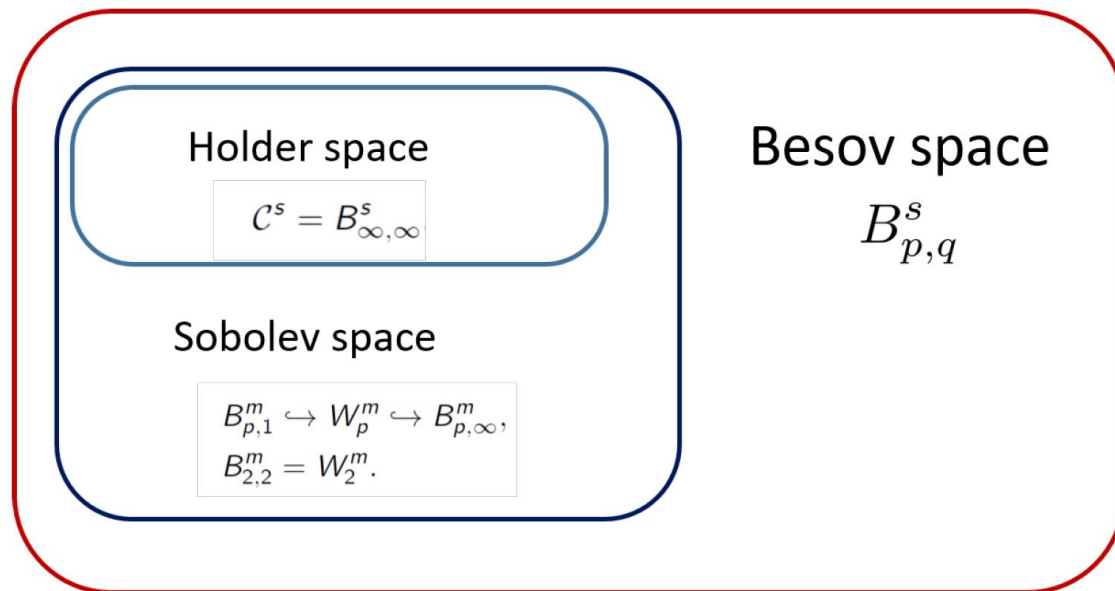
- For $m \in \mathbb{N}$,

$$B_{p,1}^m \hookrightarrow W_p^m \hookrightarrow B_{p,\infty}^m,$$

$$B_{2,2}^m = W_2^m.$$

- For $0 < s < \infty$ and $s \notin \mathbb{N}$,

$$C^s = B_{\infty,\infty}^s.$$

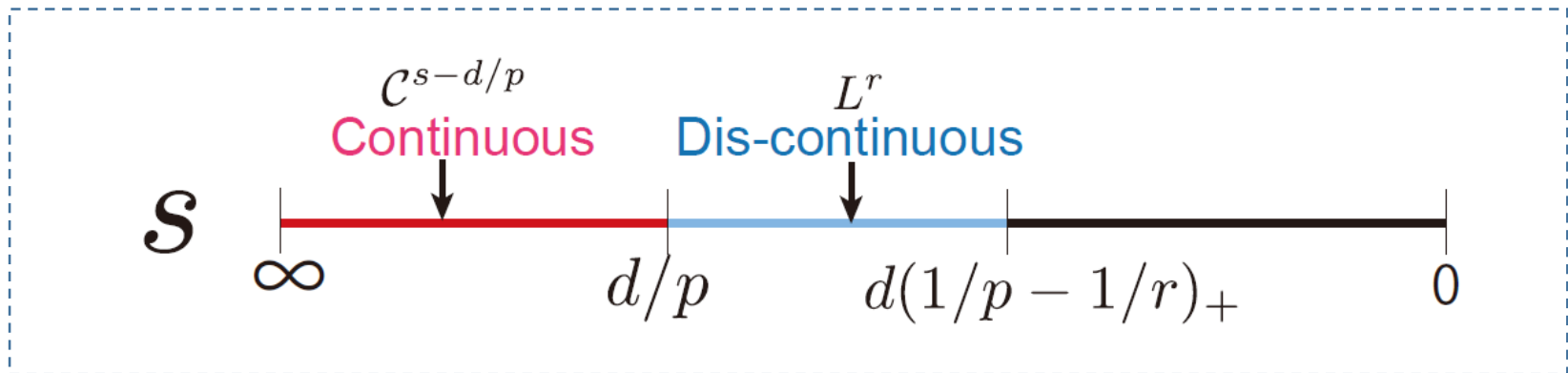


- Continuous regime: $s > d/p$

$$B_{p,q}^s \hookrightarrow C^0$$

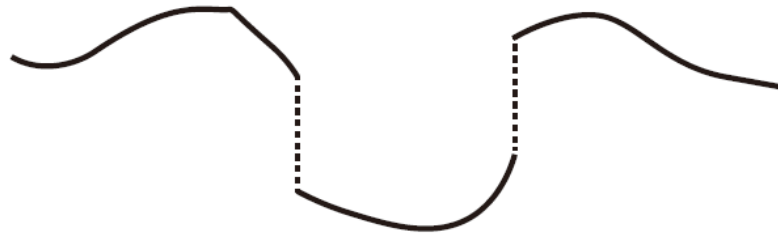
- L^r -integrability : $s \geq d(1/p - 1/r)_+$

$$B_{p,q}^s \hookrightarrow L^r$$

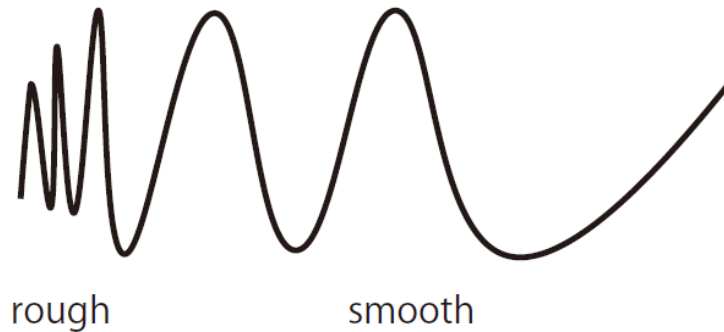


- $B_{1,1}^1([0, 1]) \subset \{\text{bounded total variation}\} \subset B_{1,\infty}^1([0, 1])$

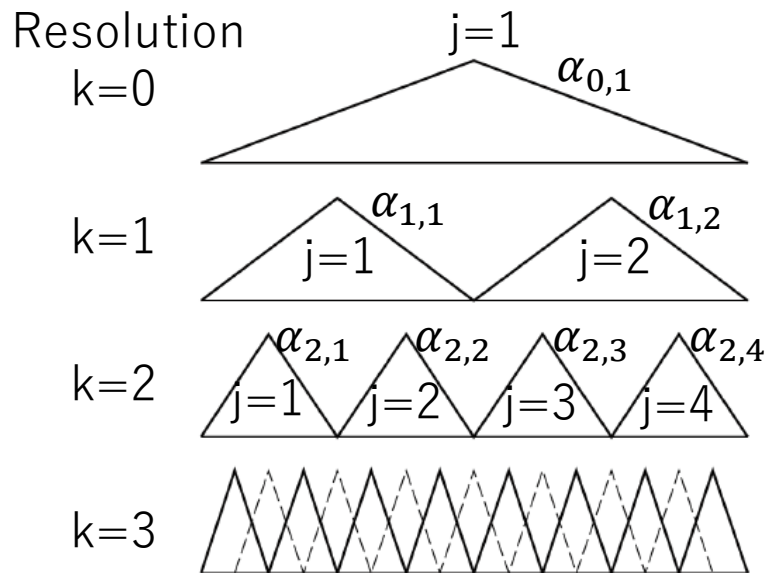
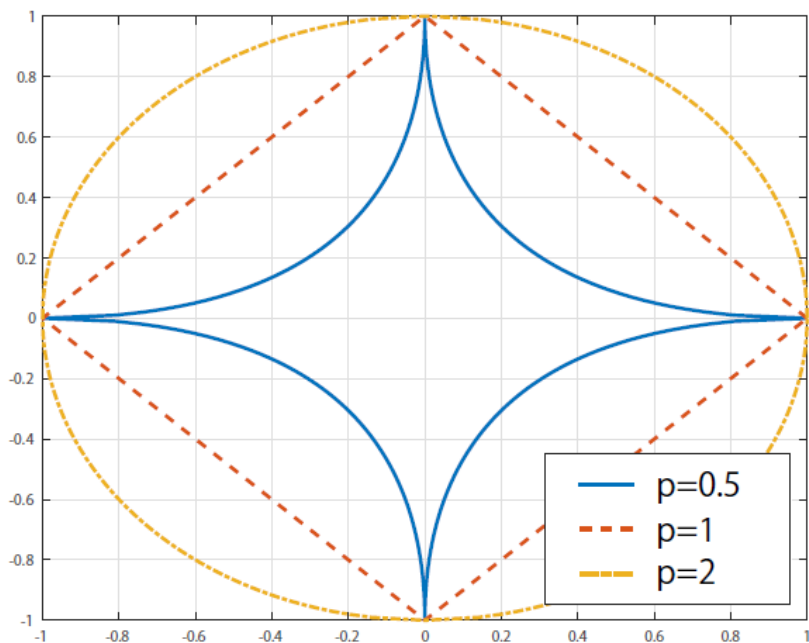
- **Discontinuity:** $d/p > s$



- **Spatial inhomogeneity of smoothness:** small p



Connection to wavelet



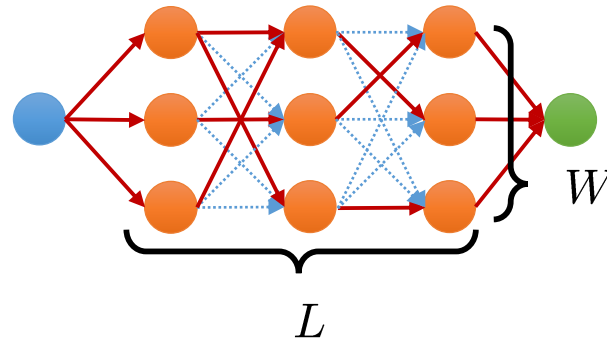
Multiresolution expansion

$$f = \sum_{k \in \mathbb{N}^+} \sum_{j \in J(k)} \alpha_{k,j} \mathcal{N}_{k,j}^{(d)}$$

$$\|f\|_{B_{p,q}^s} \simeq \left[\sum_{k=0}^{\infty} \left\{ 2^{sk} \left(2^{-kd} \sum_{j \in J(k)} |\alpha_{k,j}|^p \right)^{1/p} \right\}^q \right]^{1/q}$$

Sparse coefficients \rightarrow spatial inhomogeneity of smoothness
(non-convexity)

Deep learning model

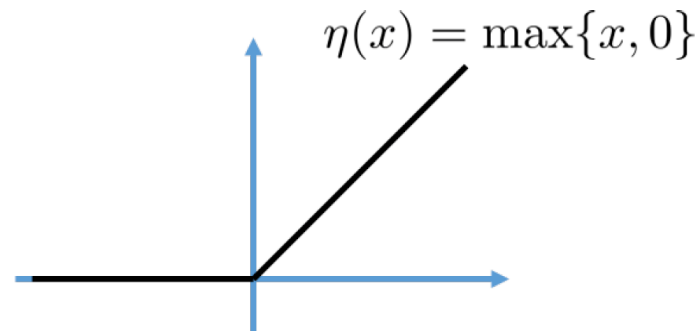


$$f(x) = (W^{(L)}\eta(\cdot) + b^{(L)}) \circ (W^{(L-1)}\eta(\cdot) + b^{(L-1)}) \circ \dots \circ (W^{(1)}x + b^{(1)})$$

$$\mathcal{F}(L, W, S, B) \left\{ \begin{array}{l} \bullet \text{ Depth : } L \\ \bullet \text{ Width : } W \\ \bullet \text{ Sparsity : } S \\ \bullet \text{ Norm bound : } B \end{array} \right.$$

Set of deep NN models

- Activation function is ReLU



Approximation in Besov space

- Assume $0 < p, q, r \leq \infty$, $0 < s < \infty$, and following condition:

$$s > d(1/p - 1/r)_+ \quad (L^r\text{-integrable})$$

- m is an integer s.t. $s < \min\{m, m - 1 + 1/p\}$.

Approximation ability of deep neural network

For an integer N , let depth L , width W , sparsity S , norm bound B be

$$\begin{aligned} L &= O(\log(N)), & W &= O(N), \\ S &= O(N \log(N)), & B &= O(N^{(d/p-s)_+}), \end{aligned}$$

Then, deep NN can approximate elements in Besov space as

$$\sup_{f^o \in U(B_{p,q}^s([0,1]^d))} \inf_{\check{f} \in \mathcal{F}(L,W,S,B)} \|f^o - \check{f}\|_{L^r([0,1]^d)} \lesssim N^{-s/d}.$$

Pinkus (1999), Mhaskar (1996): $p = r$ and $1 \leq p$, ReLU activation is excluded.
 Petrushev (1998): $p = r = 2$, ReLU is excluded ($s \leq k + 1 + (d - 1)/2$).

Comparison

Under the condition $s > d(1/p - 1/r)_+$, we have

$$\sup_{f^\circ \in U(B_{p,q}^s([0,1]^d))} \inf_{\check{f} \in \mathcal{F}(L,W,S,B)} \|f^\circ - \check{f}\|_{L^r([0,1]^d)} \lesssim N^{-s/d}.$$

- For $p = q = \infty$, it is reduced to Yarotsky (2016) (Hölder space)
- **Adaptive nonlinear** approx. must be used (Dung, 2011)

Linear approx. (Linear width) :

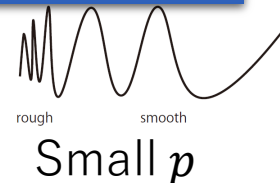
$$\begin{cases} N^{-s/d + (1/p - 1/r)_+} \\ N^{-s/d + 1/p - 1/2} \end{cases} \begin{cases} \text{either } (0 < p \leq r \leq 2), \\ \text{or } (2 \leq p \leq r \leq \infty), \\ \text{or } (0 < r \leq p \leq \infty), \end{cases}$$

$p \neq r$
is important

Non-adaptive approx. (N-term)

$$\begin{cases} N^{-s/d + (1/p - 1/r)_+} & (1 < p < 2 < r \leq \infty, s > d/p), \\ N^{-s/d + 1/p - 1/2} & (1 < p < 2 < r \leq \infty, s > d/p), \\ N^{-s/d} & (2 \leq p < r \leq \infty, s > d/2), \end{cases}$$

- Adaptivity of deep NN
- Good feature extractor



This difference does not appear for Hölder space

- Chui et al. (1994) and Bölcskei et al. (2017) dealt with a “smooth” activation with $\lim_{x \rightarrow \infty} \eta(x)/x^k \rightarrow 1$, $\lim_{x \rightarrow -\infty} \eta(x)/x^k = 0$ with $k \geq 2$ under $1 \leq p$. Mhaskar and Micchelli (1992) studied $s = k + 1$. Mhaskar (1993) studied $k \geq 2$ and $s = k + 1$, Mhaskar (1996) considered the Sobolev space W_p^m with a “bump” activation function (excluding ReLU).

Estimation error analysis

- Least squares estimator

$$\hat{f} = \arg \min_{\bar{f}: f \in \mathcal{F}(L, W, S, B)} \sum_{i=1}^n (y_i - \bar{f}(x_i))^2$$

where $\bar{f} = \min\{\max\{f, -F\}, F\}$ (clipping).

Theorem (estimation error)

Suppose $\|f^\circ\|_{B_{p,q}^s} \leq 1$, $\|f^\circ\|_\infty \leq 1$ and $0 < p, q \leq \infty$, $s > d(1/p - 1/2)_+$.

Then, by setting $N \asymp n^{\frac{d}{2s+d}}$, we have

$$\mathbb{E}[\|f^\circ - \hat{f}\|_{L^2(P_X)}^2] \leq n^{-\frac{2s}{2s+d}} \log(n)^3.$$

For $p = q = \infty$, it is reduced to Schmidt-Hieber (2017).

Linear estimator

Linear estimator: an estimator which is linear to $(y_i)_{i=1}^n$.

“Shallow” method

$$X_n = (x_1, \dots, x_n)$$

$$\hat{f}(x) = \sum_{i=1}^n \varphi(x; X_n) \underline{y_i}$$

Linear

Examples

- Kernel ridge estimator
- Sieve estimator
- Nadaraya-Watson estimator
- k-NN estimator

Kernel ridge regression:

$$\hat{f}(x) = K_{x,X} (K_{X,X} + \lambda I)^{-1} \underline{Y}$$

Comparison to other methods

- Linear estimators (Donoho & Johnstone, 1994)
(Kernel ridge estimator, Sieve estimator, Nadaraya-Watson, ...)

$$n^{-\frac{2s - 2d(1/p - 1/2)_+}{2s + d - 2d(1/p - 1/2)_+}}$$

- Deep learning \checkmark

$$n^{-\frac{2s}{2s + d}}$$

There appears
difference when
 $p < 2$

When p is small ($p < 2$), deep learning dominates
→ Spatial inhomogeneity of smoothness
(adaptivity to produce appropriate bases)

c.f., piece-wise smooth function: Imaizumi&Fukumizu, 2018.

Intuition

$$\check{f}(x) = \sum_{j=1}^N \beta_j \varphi_j(x)$$

Coefficient

Basis

$$n^{-\frac{2s-2d(1/p-1/2)_+}{2s+d-2d(1/p-1/2)_+}}$$

Pre-specified: Non-adaptive method

➤ Kernel ridge regression, ...

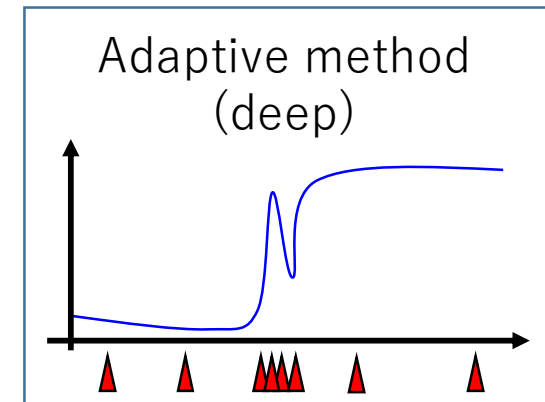
Estimated: Adaptive method

➤ Deep learning, sparse estimator, ...

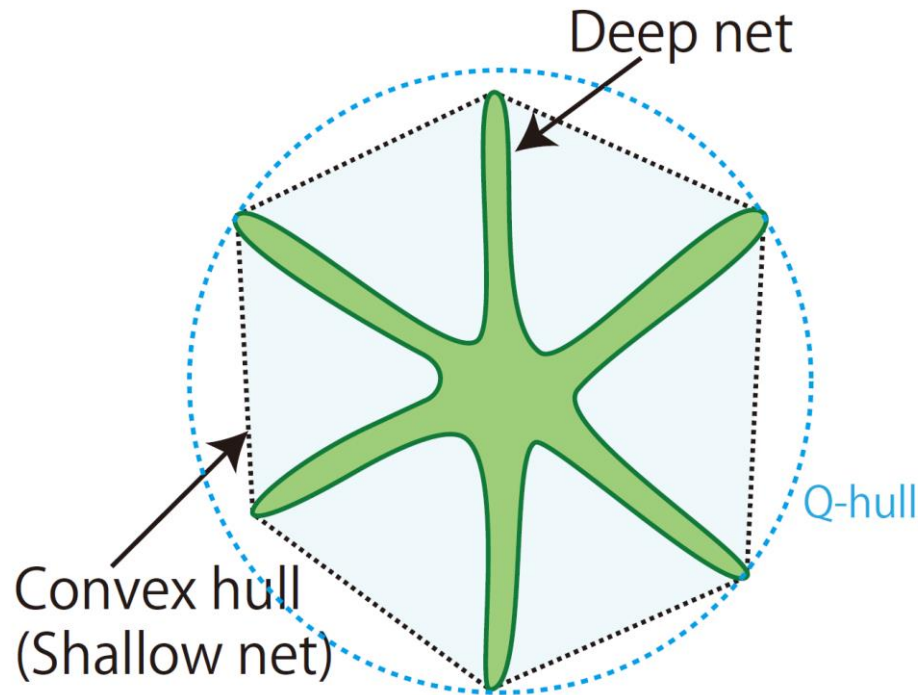
$$n^{-\frac{2s}{2s+d}}$$

Difference between deep and sparse learning:

- Sparse:
 - Choose important bases from a pre-specified set of bases.
- Deep:
 - Construct bases directly.



Why does this difference happen?



$$\inf_{\hat{f}: \text{Linear}} \sup_{f^o \in \mathcal{F}} \mathbb{E}[\|\hat{f} - f^o\|_{L_2(P)}^2] = \inf_{\hat{f}: \text{Linear}} \sup_{f^o \in \text{conv}(\mathcal{F})} \mathbb{E}[\|\hat{f} - f^o\|_{L_2(P)}^2]$$

A blue bracket connects the $\sup_{f^o \in \mathcal{F}}$ term in the left-hand side to the $\sup_{f^o \in \text{conv}(\mathcal{F})}$ term in the right-hand side.

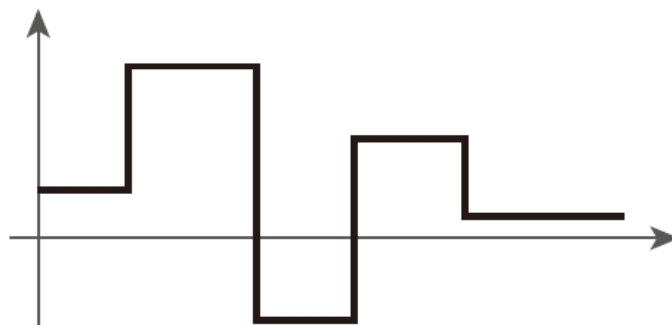
With additional conditions, it can be extended to “Q-hull.”

Simple example

[Hayakawa&Suzuki: 2019]

$$J_K = \left\{ a_0 + \sum_{i=1}^K a_i \mathbf{1}_{[t_i, 1]} \mid t_i \in (0, 1], |a_0|, \sum_{i=1}^K |a_i| \leq 1 \right\}$$

→ Its convex hull includes the **functions of bounded variation**.



Theorem

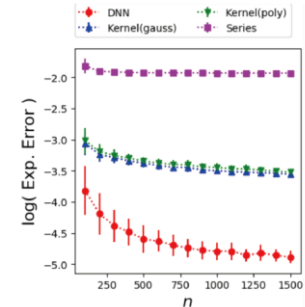
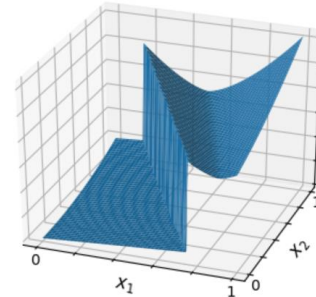
$$\inf_{\hat{f}: \text{Linear}} \sup_{f^o \in J_K} \mathbb{E} \left[\|\hat{f} - f^o\|_{L_2(P)}^2 \right] \geq \Omega \left(\frac{1}{\sqrt{n}} \right).$$

Deep learning : $o\left(\frac{1}{n}\right)$

Examples (1)

- **Piece-wise smooth function** (Imaizumi & Fukumizu, 2018)

$$f^\circ(x) = \sum_{k=1}^K \mathbf{1}_{R_k}(x) h_k(x)$$



where R_k is a region with smooth boundary and h_k is a smooth function.

- Deep is better than a kernel method (linear estimator).

- **Low dimensional feature extractor** (Schmidt-Hieber, 2018)

$$f^\circ(x) = g(w^\top x)$$

Dim. reduction

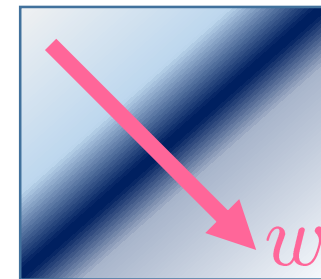
g is a univariate smooth function.

$$n^{-\frac{2s}{2s+1}} \lll n^{-\frac{2s}{2s+d}}$$

Deep

Wavelet series estimator

: suffers from curse of dim.



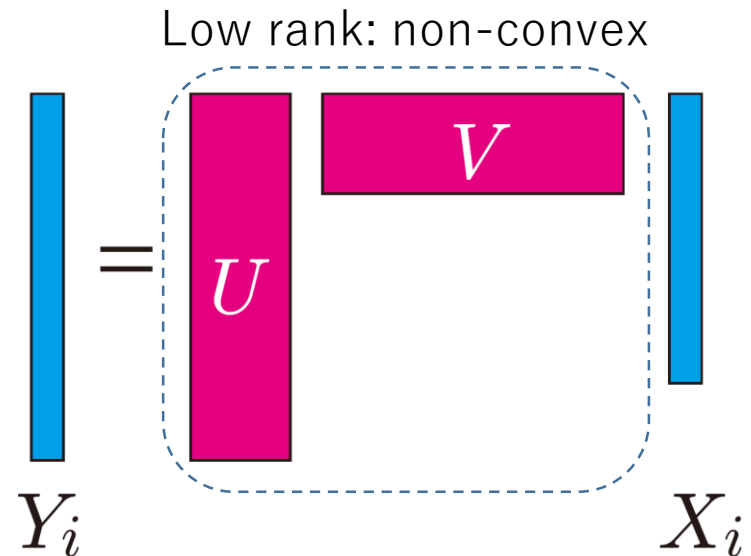
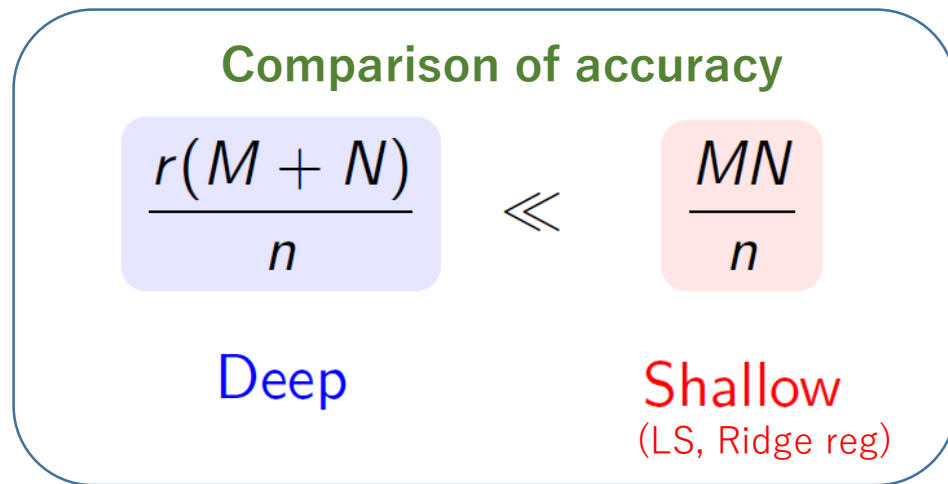
Example (2)

- Reduced rank regression

$$Y_i = UVX_i + \xi_i \quad (i = 1, \dots, n)$$

where $Y_i \in \mathbb{R}^M$, $X_i \in \mathbb{R}^N$ and $U \in \mathbb{R}^{M \times r}$, $V \in \mathbb{R}^{r \times N}$ ($r \ll M, N$).

- Linear estimator $\hat{f}(x) = \sum_{i=1}^n Y_i \varphi(X_1, \dots, X_n, x)$,
- Deep learning $\hat{f}(x) = \hat{U} \hat{V} x$.



Convex hull of the low rank model is full-rank.

Curse of dimensionality

Curse of dimensionality

Estimation error bound :

$$n^{-\frac{2s}{2s+d}}$$

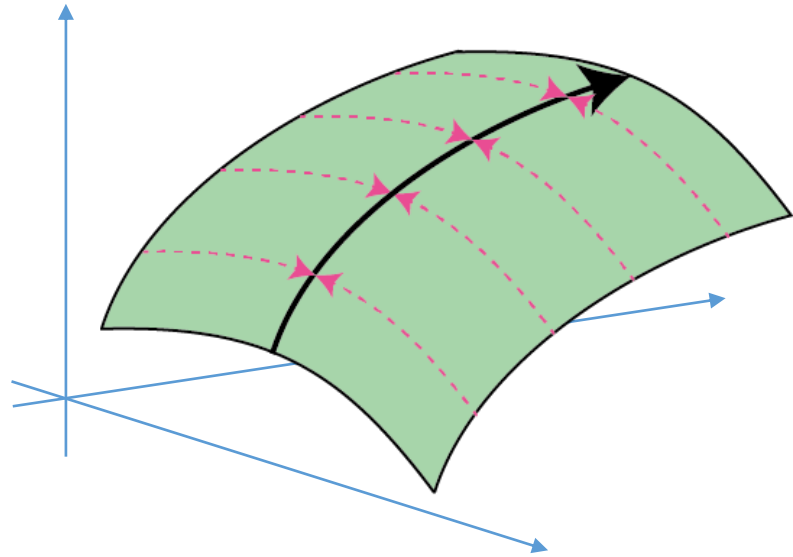
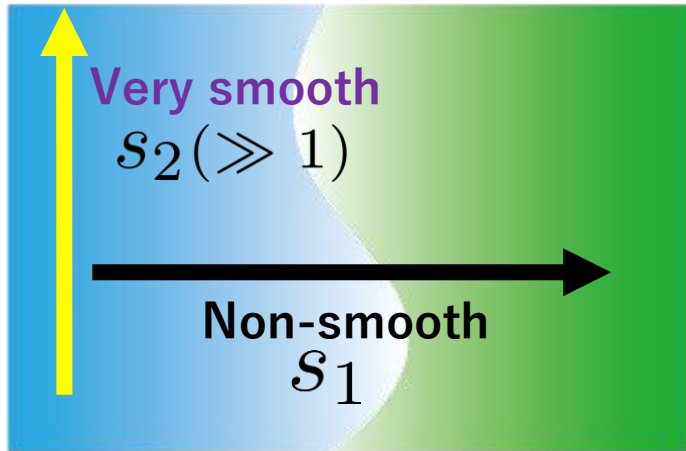
Approximation error bound :

$$N^{-\frac{s}{d}}$$

→ Curse of dimensionality

Anisotropic Besov space

[Suzuki&Nitanda: Deep learning is adaptive to intrinsic dimensionality of model smoothness in anisotropic Besov space. arXiv:1910.12799, 2019.]



$$f^\circ \in B_{p,q}^{(s_1, \dots, s_d)} \quad \bar{s} := \left(\frac{1}{s_1} + \dots + \frac{1}{s_d} \right)^{-1}$$

$$n^{-\frac{2\bar{s}}{2\bar{s}+1}}$$

Deep

- Curse of dimensionality is avoided.
- Minimax optimal.

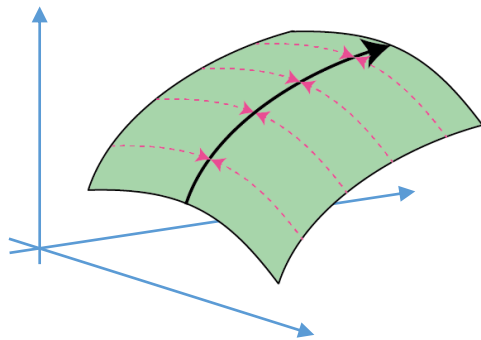
[Ibragimov & Khas'minskii (1984),
Nyssbaum (1983, 1987), Kerkyacharian et
al. (2001)]

Deep composition model

$$f^\circ(x) = h_H \circ \dots \circ h_1(x)$$

$h_\ell : \mathbb{R}^{m_\ell} \rightarrow \mathbb{R}^{m_{\ell+1}}$: included in an anisotropic Besov space $(B_{p,q}^{\beta^{(\ell)}})$.

Example:



$$f^\circ(x) = h \circ \underline{\varphi(x)}$$

Coordinate in the manifold
(feature extractor)

Theorem

$$\mathbb{E}[\|\hat{f} - f^\circ\|_{L^2(P_X)}^2] \lesssim \max_{\ell \in [H]} n^{-\frac{2\tilde{\beta}^{*(\ell)}}{2\tilde{\beta}^{*(\ell)}+1}} \log(n)^3$$

Deep learning

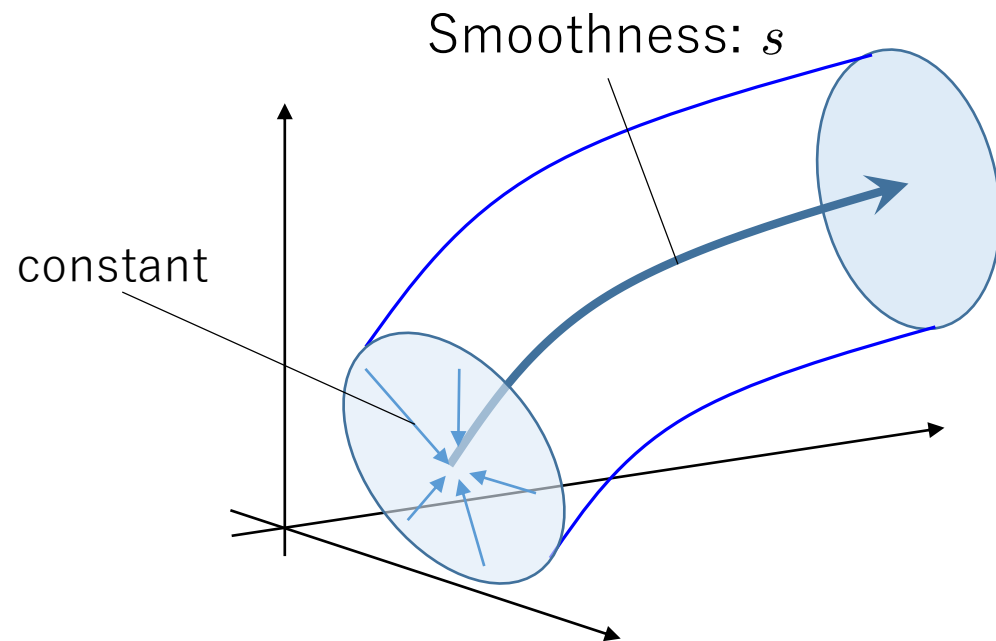
This is minimax optimal.

$$\tilde{\beta}^{(\ell)} := \left(\frac{1}{\beta_1^{(\ell)}} + \dots + \frac{1}{\beta_{m_\ell}^{(\ell)}} \right)^{-1}$$

$$\tilde{\beta}^{*(\ell)} := \tilde{\beta}^{(\ell)} \prod_{k=\ell+1}^H [(\min_j \beta_j^{(k)} - 1/p) \wedge 1]$$

Example

Data on smooth manifold



- The true function varies only one direction in the manifold.
- Invariant against noise injection to other directions.

Deep

$$n^{-\frac{2s}{2s+1}}$$

Intrinsic dimensionality: $d = 1$

Naïve evaluation: $n^{-\frac{2s}{2s+d}}$

c.f., Manifold regression:

- Classic method: Yang & Dunson (2016), Bickel & Li (2007), Yang & Tokdar (2015)
- Deep learning: Nakada & Imaizumi (2019), Schmidt-Hieber (2019)

Comparison to linear estimator

$$f^\circ(x) = g(Wx) \quad (W \in \mathbb{R}^{D \times d}, g \in B_{p,q}^s([0,1]^D))$$

f° depends only D -dimensional subspace.

Deep

$$n^{-\frac{2s}{2s+D}}$$

$$\left(n^{-\frac{2s}{2s+d/2}} \text{ when } D = \frac{d}{2} \right)$$

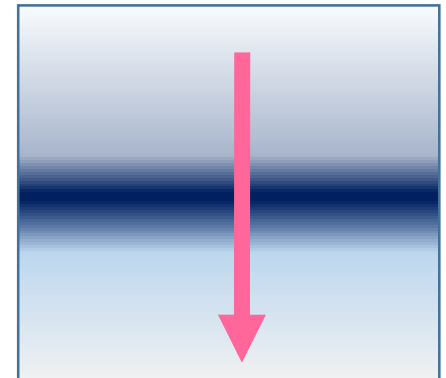
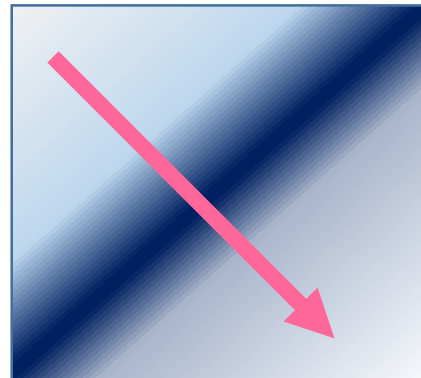
\ll

Linear estimator

$$n^{-\frac{2(s-D/p+d/2)}{2(s-D/p+d/2)+d}} \vee n^{-\frac{2s}{2s+D}}$$

$$\left(n^{-\frac{2s}{2s+d}} \text{ when } D = \frac{d}{2} \text{ and } p = 1 \right)$$

Deep can ease curse of dim.,
but linear estimators directly
suffers from curse of dim.



Adaptivity of deep learning

- The ReLU-DNN has high adaptivity to shape of the target functions (spatial inhomogeneity of smoothness).

$$\|\hat{f} - f^\circ\|_{L^2(P)}^2 = O(n^{-2s/(2s+d)} \log(n)^3)$$

- DNN outperforms non-adaptive methods.

[Besov]

$$\text{(DNN)} \quad n^{-\frac{2s}{2s+d}} \ll n^{-\frac{2(s-d(1/p-1/2))}{2s+d-2d(1/p-1/2)}} \quad (\text{linear method})$$

[Anisotropic Besov]

$$\text{(DNN)} \quad n^{-\frac{2\bar{s}}{2\bar{s}+1}} \ll n^{-\frac{2s_{\min}}{2s_{\min}+d}} \quad (\text{linear method})$$

Deep learning \approx Sparse estimation in infinite dim. space