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Estimation and Inference for smooth DNNs.

Blessing of dimension

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2 “Modern” theory of statistical estimation. An overview

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- Training procedure
- Nonlinear least squares
- Calming
- Noise reduction

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Which **dimension**?

Which **dimension**?

Number of **features** d ?

Which **dimension**?

Number of **features** d ?

or

Which **dimension**?

Number of **features** d ?

or

number of **parameters** p of the model?

Coincide for **linear** models.

- Full parameter dimension p does not enter the accuracy guarantees;
- what matters?
 - effective dimension p ;
 - geometric properties (like strong convexity) of the objective function;
- A proper extension of the parameter space can be useful and helpful to improve geometric properties of the objective function without increasing the effective dimension.

Given data $(Y_i, \mathbf{X}_i)$ with response Y_i and regressors $\mathbf{X}_i \in \mathbb{R}^d$.

Aim: to build a network with a small prediction error $Y_i - m(\mathbf{X}_i)$.

Shallow network: $\mathbb{X} = \sigma(W\mathbf{X})$,

Deep NN: $\mathbb{X} = \mathbb{X}^{(K)} = \text{DNN}(\mathbf{X}) \in \mathbb{R}^M$,

$$\text{DNN}(\mathbf{X}) = \sigma(W^{(K)}\sigma(W^{(K-1)}\dots\sigma(W^{(1)}\mathbf{X}))),$$

where $M = M^{(K)}$ is the number of nodes in the last hidden layer,
 $W^{(k)} = (w_{mj})$ is a weighting $M_k \times M_{k-1}$ -matrix with rows $W_m^{(k)}$, and σ
is an entry-wise activating function.

Prediction by linear regression on $\mathbb{X}$:

$$m(\mathbf{X}_i) = \mathbb{X}_i^\top \beta = \underbrace{\sigma(W\mathbf{X}_i)^\top}_{\text{shallow}} \beta.$$

Model (shallow): $\text{DNN}(\mathbf{X}_i \mid W) = \sigma(W \mathbf{X}_i)$.

Model (deep): $W = (W^{(1)}, \dots, W^{(K)})$,

$$\text{DNN}(\mathbf{X} \mid W) = \sigma(W^{(K)} \sigma(W^{(K-1)} \dots \sigma(W^{(1)} \mathbf{X}))) .$$

Method (MLE):

$$m(\mathbf{X}_i \mid W, \beta) = \text{DNN}(X_i \mid W)^\top \beta ,$$

$$L(W, \beta) = \sum_{i=1}^n |Y_i - m(\mathbf{X}_i \mid W, \beta)|^2 ,$$

$$(\widehat{W}, \widehat{\beta}) = \underset{W, \beta}{\operatorname{argmin}} L(W, \beta) .$$

Issues: Non-convexity, lack of identifiability, overparametrization.

- [Schmidt-Hieber, 2020]. Nonparametric regression using deep neural networks with ReLU activation function, Kolmogorov-Arnold representation,
- [Zuowei Shen et al., 2020], Deep Network Approximation Characterized by Number of Neurons,
- [Fan et al., 2024], How do noise tails impact on deep ReLU networks? polynomial noise, tails, Huber, DNN approximation,
- [Kohler and Krzyzak, 2022], Analysis of the rate of convergence of an over-parametrized deep neural network estimate learned by gradient descent,
- [Shen et al., 2022], Approximation with CNNs in Sobolev Space: with Applications to Classification,
- [Liu et al., 2022], Benefits of Overparameterized Convolutional Residual Networks: Function Approximation under Smoothness Constraint,
- [Simionescu-Badea, 2022], Analysis of the rate of convergence of fully connected deep neural network regression estimates with smooth activation,

- [Chen et al., 2019], Efficient Approximation of Deep ReLU Networks for Functions on Low Dimensional Manifolds,
- [Kohler et al., 2019], Estimation of a Function of Low Local Dimensionality by DNN,
- [Jiao et al., 2021], Deep Nonparametric Regression on Approximately Low-dim Manifolds,
- [Liu et al., 2021], Besov Function Approximation ... on Low-Dim Manifolds ... ,
- [Cloninger and Klock, 2021], A deep network construction that adapts to intrinsic dimensionality beyond the domain,
- [Zhang et al., 2023], Effective Minkowski Dimension of Deep Nonparametric Regression: Function Approximation and Statistical Theories,
- [Shen et al., 2023], RePU DNN, manifolds, Differentiable Neural Networks with RePU Activation: with Applications ...
- [Jiao et al., 2023], Deep nonparametric regression on approximate manifolds

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Let $L(\mathbf{v})$ be a random function (loss, empirical risk, negative log-likelihood). Consider

$$\tilde{\mathbf{v}} = \operatorname{argmin}_{\mathbf{v}} L(\mathbf{v}); \quad \mathbf{v}^* = \operatorname{argmin}_{\mathbf{v}} \mathbb{E} L(\mathbf{v});$$

Includes MLE, LSE, LAD, Minimum Contrast, and many others procedures.

Aim: describe $\tilde{\mathbf{v}} - \mathbf{v}^*$ (estimation loss) and $L(\tilde{\mathbf{v}}) - L(\mathbf{v}^*)$ (excess).

Perturbed optimization: $L(\mathbf{v})$ is a perturbation of $f(\mathbf{v}) = \mathbb{E} L(\mathbf{v})$ by a stochastic component

$$\zeta(\mathbf{v}) = L(\mathbf{v}) - \mathbb{E} L(\mathbf{v}).$$

- **Truth** $\boldsymbol{v}^* \stackrel{\text{def}}{=} \operatorname{argmin}_{\boldsymbol{v}} \mathbb{E} L(\boldsymbol{v})$;
- **MLE** $\tilde{\boldsymbol{v}} \stackrel{\text{def}}{=} \operatorname{argmin}_{\boldsymbol{v}} L(\boldsymbol{v})$;
- **Fisher information** $\mathbb{F}(\boldsymbol{v}) = \nabla^2 \mathbb{E} L(\boldsymbol{v})$, $\mathbb{F} = \mathbb{F}(\boldsymbol{v}^*)$;
- **Effective sample size** $\mathbb{N} \stackrel{\text{def}}{=} \lambda_{\min}(\mathbb{F})$;
- **Score** $\zeta(\boldsymbol{v}) \stackrel{\text{def}}{=} L(\boldsymbol{v}) - \mathbb{E} L(\boldsymbol{v})$, $\nabla \zeta = \nabla \zeta(\boldsymbol{v}^*)$;
- **Effective dimension** $\mathbb{p} \stackrel{\text{def}}{=} \operatorname{tr}(\mathbb{F}^{-1} \operatorname{Var}(\nabla \zeta))$;

■ **Concentration** (requires $p \ll N$)

$$\|\mathbb{F}^{1/2}(\tilde{\mathbf{v}} - \mathbf{v}^*)\| \lesssim \sqrt{p}.$$

■ **Fisher expansion** (requires $p \ll N$)

$$\|\mathbb{F}^{1/2}(\tilde{\mathbf{v}} - \mathbf{v}^* + \mathbb{F}^{-1} \nabla \zeta)\| \lesssim \frac{\|\mathbb{F}^{-1} \nabla \zeta\|^2}{\sqrt{N}}.$$

■ **Wilks expansion** [Wilks, 1938] (requires $p \ll N$)

$$\left| L(\tilde{\mathbf{v}}) - L(\mathbf{v}^*) + \frac{1}{2} \|\mathbb{F}^{-1/2} \nabla \zeta\|^2 \right| \lesssim \frac{\|\mathbb{F}^{-1} \nabla \zeta\|^{3/2}}{\sqrt{N}}.$$

[Spokoiny, 2024].

Consider a penalized MLE for a penalty function $\text{pen}_G(\mathbf{v})$

$$\tilde{\mathbf{v}}_G = \underset{\mathbf{v}}{\operatorname{argmin}} L_G(\mathbf{v}) = \underset{\mathbf{v}}{\operatorname{argmin}} \{L(\mathbf{v}) + \text{pen}_G(\mathbf{v})\}.$$

Typical examples: $\text{pen}_G(\mathbf{v}) = \|G\mathbf{v}\|^2/2$ and $\text{pen}_\lambda(\mathbf{v}) = \lambda\|\mathbf{v}\|_1$.

Consider three optimization problems

$$\tilde{\mathbf{v}}_G = \underset{\mathbf{v}}{\operatorname{argmin}} L_G(\mathbf{v}),$$

$$\mathbf{v}_G^* = \underset{\mathbf{v}}{\operatorname{argmin}} \mathbb{E} L_G(\mathbf{v}),$$

$$\mathbf{v}^* = \underset{\mathbf{v}}{\operatorname{argmin}} \mathbb{E} L(\mathbf{v}).$$

The penalized MLE $\tilde{\mathbf{v}}_G$ estimates rather $\mathbf{v}_G^*$ than $\mathbf{v}^*$.

$$\mathbf{v}_G^* = \operatorname{argmin}_{\mathbf{v}} \mathbb{E} L_G(\mathbf{v}) = \operatorname{argmin}_{\mathbf{v}} \{ \mathbb{E} L(\mathbf{v}) + \operatorname{pen}_G(\mathbf{v}) \},$$

$$\mathbf{v}^* = \operatorname{argmin}_{\mathbf{v}} \mathbb{E} L(\mathbf{v}).$$

Proposition

Define

$$\mathbb{F}_G \stackrel{\text{def}}{=} \nabla^2 \mathbb{E} L_G(\mathbf{v}_G^*) = \mathbb{F} + \nabla^2 \operatorname{pen}_G(\mathbf{v}_G^*),$$

$$\mathbf{M}_G \stackrel{\text{def}}{=} \nabla \operatorname{pen}_G(\mathbf{v}^*).$$

Then

$$\| \mathbb{F}_G^{1/2} (\mathbf{v}_G^* - \mathbf{v}^* + \mathbb{F}_G^{-1} \mathbf{M}_G) \| \lesssim \frac{\| \mathbb{F}_G^{-1/2} \mathbf{M}_G \|^2}{\sqrt{N}}.$$

Fix $Q: \mathbb{R}^p \rightarrow \mathbb{R}^q$

$$\mathbf{p}_Q \stackrel{\text{def}}{=} \text{tr} \text{Var}(Q \mathbf{F}_G^{-1} \nabla \zeta), \quad \text{variance}$$

$$\mathbf{b}_Q = \|Q \mathbf{F}_G^{-1} \mathbf{M}_G\| = \|Q \mathbf{F}_G^{-1} \nabla \text{pen}_G(\mathbf{v}^*)\| \quad \text{bias}$$

$$\begin{aligned} \mathcal{R}_Q &\stackrel{\text{def}}{=} \mathbb{E}\{\|Q \mathbf{F}_G^{-1}(\nabla \zeta + \mathbf{M}_G)\|^2 \mathbb{I}_{\Omega(\mathbf{x})}\} \quad \text{squared risk} \\ &\leq \mathbf{p}_Q + \mathbf{b}_Q^2. \end{aligned}$$

Then $\tilde{\mathbf{v}}_G - \mathbf{v}^* \approx \mathbf{F}_G^{-1}(\nabla \zeta + \mathbf{M}_G)$ and

$$(1 - \alpha_Q)^2 \mathcal{R}_Q \leq \mathbb{E}\{\|Q(\tilde{\mathbf{v}}_G - \mathbf{v}^*)\|^2 \mathbb{I}_{\Omega(\mathbf{x})}\} \leq (1 + \alpha_Q)^2 \mathcal{R}_Q.$$

[Spokoyny, 2024].

- **Stochastic linearity**: the stochastic component $\zeta(\mathbf{v}) = L(\mathbf{v}) - \mathbb{E}L(\mathbf{v})$ is linear in $\mathbf{v}$ or $\nabla\zeta(\mathbf{v}) \equiv \nabla\zeta$;
- **Sub-gaussian** tails for $\nabla\zeta$;
- **Convexity**: $\mathbb{E}L_G(\mathbf{v})$ is strongly convex in $\mathbf{v}$;
- **Smoothness**: $\mathbb{E}L_G(\mathbf{v})$ is third order smooth in uniform gateaux sense (**self-concordance**);

- The results are **dimension- and coordinate-free**. The **ambient dimension** $p \leq \infty$ is unimportant; only the **effective dimension** p matters. Can be controlled by a choice of penalization, replacing model reduction. The results require $p \ll N$.
- All the remainder are **explicit** and can be handled. Helpful for further analysis of iterative procedures like stochastic optimization, EM-procedures, etc.
- Conditions are restrictive. **Convexity** is the most critical, but can be ensured by extending the parameter set (**blessing of dimension**) and **localization**.
- The main tool is **perturbed optimization**, [Spokoiny, 2025b, Spokoiny, 2025a].

Let $f(\mathbf{v})$ be a smooth convex function,

$$\mathbf{v}^* = \operatorname{argmin}_{\mathbf{v}} f(\mathbf{v}), \quad \mathbb{F} = \nabla^2 f(\mathbf{v}^*).$$

Let another function $g(\mathbf{v})$ satisfy for some vector $\mathbf{A}$

$$g(\mathbf{v}) - g(\mathbf{v}^*) = \langle \mathbf{v} - \mathbf{v}^*, \mathbf{A} \rangle + f(\mathbf{v}) - f(\mathbf{v}^*).$$

Define

$$\mathbf{v}^\circ \stackrel{\text{def}}{=} \operatorname{argmin}_{\mathbf{v}} g(\mathbf{v}), \quad g(\mathbf{v}^\circ) = \min_{\mathbf{v}} g(\mathbf{v}).$$

Aim: evaluate the quantities $\mathbf{v}^\circ - \mathbf{v}^*$ and $g(\mathbf{v}^\circ) - g(\mathbf{v}^*)$.

Consider $\mathbf{v}^* \stackrel{\text{def}}{=} \operatorname{argmin} f(\mathbf{v})$, $\mathbf{v}^\circ \stackrel{\text{def}}{=} \operatorname{argmin}\{f(\mathbf{v}) + \langle \mathbf{v}, \mathbf{A} \rangle\}$.

$(\mathcal{T}_3^*)$ $f(\mathbf{v})$ is strongly convex, $D^2 \leq \mathbb{F} \stackrel{\text{def}}{=}} \nabla^2 f(\mathbf{v}^*)$, and

$$\sup_{\mathbf{u}: \|D\mathbf{u}\| \leq r} \sup_{\mathbf{z} \in \mathbb{R}^p} \frac{|\langle \nabla^3 f(\mathbf{v}^* + \mathbf{u}), \mathbf{z}^{\otimes k} \rangle|}{\|D\mathbf{z}\|^3} \leq \tau_3.$$

Proposition ([Spokoiny, 2025b, Spokoiny, 2025a])

Assume $(\mathcal{T}_3^*)$ at $\mathbf{v}^*$ with D^2 , r , and τ_3 s.t.

$$r \geq \frac{3}{2} \|D \mathbb{F}^{-1} \mathbf{A}\|, \quad \tau_3 \|D \mathbb{F}^{-1} \mathbf{A}\| < \frac{4}{9}.$$

Then $\|D(\mathbf{v}^\circ - \mathbf{v}^*)\| \leq (3/2) \|D \mathbb{F}^{-1} \mathbf{A}\|$ and moreover,

$$\|D^{-1} \mathbb{F}(\mathbf{v}^\circ - \mathbf{v}^* - \mathbb{F}^{-1} \mathbf{A})\| \leq \frac{3}{4} \tau_3 \|D \mathbb{F}^{-1} \mathbf{A}\|^2.$$

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Model:

$$L(W, \beta) = \frac{1}{2} \sum_{i=1}^n |Y_i - \sigma(W \mathbf{X}_i)^\top \beta|^2$$

MLE:

$$(\widehat{W}, \widehat{\beta}) = \underset{W, \beta}{\operatorname{argmin}} L(W, \beta).$$

Issue: The major assumptions of stochastic linearity and convexity are not fulfilled.

$\mathbf{Y} = (Y_1, \dots, Y_n)^\top \in \mathbb{R}^n$, $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n)^\top$ – observations,
 $m(\mathbf{v}) = (m(\mathbf{X}_1, \mathbf{v}), \dots, m(\mathbf{X}_n, \mathbf{v}))^\top$, regression function.

Nonlinear least squares (Gauss, Legendre):

$$\hat{\mathbf{v}} = \underset{\mathbf{v}}{\operatorname{argmin}} L(\mathbf{v}) = \underset{\mathbf{v}}{\operatorname{argmin}} \|\mathbf{Y} - m(\mathbf{v})\|^2.$$

Hessian

$$\nabla^2 L(\mathbf{v}) = \nabla m(\mathbf{v}) \nabla m(\mathbf{v})^\top - \{\mathbf{Y} - m(\mathbf{v})\}^\top \nabla^2 m(\mathbf{v}).$$

Noiseless case: $\mathbf{Y} = m(\mathbf{v}^*)$, $\mathbf{v} \approx \mathbf{v}^*$

$$\nabla^2 L(\mathbf{v}) \approx \nabla m(\mathbf{v}) \nabla m(\mathbf{v})^\top.$$

Gauss–Newton iterations; [Gratton et al., 2007]. Requires “small noise”.

Original problem

$$L(W, \beta) = \frac{1}{2} \|\mathbf{Y} - \sigma(W\mathbf{X})^\top \beta\|^2.$$

- Introduce $\mathbb{X} = \sigma(W\mathbf{X})$ and $m = \mathbb{X}^\top \beta$;
- Replace the structural relations by **structural penalty**
 $\lambda^* \|\mathbb{X} - \sigma(W\mathbf{X})\|^2/2$ and $\lambda^* \|m - \mathbb{X}^\top \beta\|^2/2$ (later $\lambda^* = 1$)

For $\mathbf{v} = (W, \mathbb{X}, \beta, m)$, results in

$$\mathcal{L}(\mathbf{v}) = \frac{1}{2} \|\mathbf{Y} - m\|^2 + \frac{1}{2} \|\mathbb{X} - \sigma(W\mathbf{X})\|^2 + \frac{1}{2} \|m - \mathbb{X}^\top \beta\|^2.$$

Dimension **before** calming:

$$p = \dim(W) + \dim(\beta) =$$

Dimension **before** calming:

$$p = \dim(W) + \dim(\beta) = dM + M.$$

Dimension **after** calming:

$$\begin{aligned} p &= \dim(W) + \dim(\mathbb{X}) + \dim(m) + \dim(\beta) \\ &= \end{aligned}$$

Dimension **before** calming:

$$p = \dim(W) + \dim(\beta) = dM + M.$$

Dimension **after** calming:

$$\begin{aligned} p &= \dim(W) + \dim(\mathbb{X}) + \dim(m) + \dim(\beta) \\ &= dM + nM + n + M \gg nd + n. \end{aligned}$$

DNN require very good (purified) data satisfying the **small noise** condition.

Noise reduction by presmoothing by $\mathcal{S} : \mathbf{Y} \rightarrow \mathbf{Z} \stackrel{\text{def}}{=} \mathcal{S}\mathbf{Y}$:

$$\mathcal{L}(\mathbf{v}) = \frac{\mu^2}{2} \|\mathbf{Z} - \mathbf{z}\|^2 + \frac{1}{2} \|\mathbf{X} - \sigma(W\mathbf{X})\|^2 + \frac{1}{2} \|\mathbf{z} - \mathcal{S}\mathbf{X}^\top \boldsymbol{\beta}\|^2.$$

Example: **convolutional networks**.

Identifiability issue: partially resolved by ridge penalties:

$$\begin{aligned} \mathcal{L}(\mathbf{v}) = & \frac{\mu^2}{2} \|\mathbf{Z} - \mathbf{z}\|^2 + \frac{1}{2} \|\mathbf{z} - \mathcal{S} \mathbf{X}^\top \boldsymbol{\beta}\|^2 + \frac{1}{2} \|\mathbf{X} - \sigma(W \mathbf{X})\|^2 \\ & + \frac{\lambda_W}{2} \|W - W_0\|^2 + \frac{\lambda_X}{2} \|\mathbf{X} - \mathbf{X}_0\|^2 + \frac{\lambda_\beta}{2} \|\boldsymbol{\beta} - \boldsymbol{\beta}_0\|^2 + \frac{\lambda_z}{2} \|\mathbf{z} - \mathbf{z}_0\|^2. \end{aligned}$$

The **estimator** $\tilde{\mathbf{v}} = (\tilde{W}, \tilde{\mathbf{X}}, \tilde{\boldsymbol{\beta}}, \tilde{\mathbf{z}})$ and the **background truth** $\mathbf{v}^* = (W^*, \mathbf{X}^*, \boldsymbol{\beta}^*, \mathbf{z}^*)$:

$$\tilde{\mathbf{v}} = \underset{\mathbf{v}}{\operatorname{argmin}} \mathcal{L}(\mathbf{v}), \quad \mathbf{v}^* = \underset{\mathbf{v}}{\operatorname{argmin}} \mathbb{E} \mathcal{L}(\mathbf{v}).$$

The main results describe the error of estimation $\tilde{\mathbf{v}} - \mathbf{v}^*$.

Construction can be extended to a K -layer network using recurrence

$$\mathbb{X}^{(k)} = \sigma(W^{(k)} \mathbb{X}^{(k-1)})$$

for $k = 1, \dots, K$ and $\mathbb{X}^{(0)} = \mathbf{X}$. With $\mathbb{X} = (\mathbb{X}^{(1)}, \dots, \mathbb{X}^{(K)})$ and $W = (W^{(1)}, \dots, W^{(K)})$, this leads to the log-likelihood

$$\begin{aligned} \mathcal{L}(\mathbf{v}) = \mathcal{L}(W, \mathbb{X}, \beta, \mathbf{z}) = & \frac{\mu^2}{2} \|\mathbf{Z} - \mathbf{z}\|^2 \\ & + \frac{1}{2} \|\mathbf{z} - \mathcal{S} \mathbb{X}^{(K)\top} \beta\|^2 + \frac{1}{2} \sum_{k=1}^K \|\mathbb{X}^{(k)} - \sigma(W^{(k)} \mathbb{X}^{(k-1)})\|^2 \\ & + \frac{\lambda_{\mathbf{W}}}{2} \|W - W_0\|^2 + \frac{\lambda_{\mathbb{X}}}{2} \|\mathbb{X} - \mathbb{X}_0\|^2 + \frac{\lambda_{\beta}}{2} \|\beta - \beta_0\|^2 + \frac{\lambda_{\mathbf{z}}}{2} \|\mathbf{z} - \mathbf{z}_0\|^2. \end{aligned}$$

Parameter dimension **before** calming: with $M^{(0)} = d$

$$p = \sum_{k=1}^K \dim(W^{(k)}) + \dim(\beta) =$$

Parameter dimension **before** calming: with $M^{(0)} = d$

$$p = \sum_{k=1}^K \dim(W^{(k)}) + \dim(\beta) = \sum_{k=1}^K M^{(k-1)} M^k + M^{(K)}.$$

Dimension **after** calming: $\boldsymbol{v} = (W, \mathbb{X}, \beta, \boldsymbol{z})$

$$p = \sum_{k=1}^K \{ \dim(W^{(k)}) + \dim(\mathbb{X}^{(k)}) \} + \dim(\beta) + \dim(\boldsymbol{z})$$

=

Parameter dimension **before** calming: with $M^{(0)} = d$

$$p = \sum_{k=1}^K \dim(W^{(k)}) + \dim(\beta) = \sum_{k=1}^K M^{(k-1)} M^{(k)} + M^{(K)}.$$

Dimension **after** calming: $\mathbf{v} = (W, \mathbb{X}, \beta, \mathbf{z})$

$$\begin{aligned} p &= \sum_{k=1}^K \{ \dim(W^{(k)}) + \dim(\mathbb{X}^{(k)}) \} + \dim(\beta) + \dim(\mathbf{z}) \\ &= \sum_{k=1}^K \{ M^{(k-1)} M^{(k)} + n M^{(k)} \} + M^{(K)} + q. \end{aligned}$$

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For $\mathbf{v} = (W, \mathbf{X}, \boldsymbol{\beta}, \mathbf{z})$, and a starting point $\mathbf{v} = (W_0, \mathbf{X}_0, \boldsymbol{\beta}_0, \mathbf{z}_0)$ consider

$$\begin{aligned} \mathcal{L}(\mathbf{v}) = & \frac{\mu^2}{2} \|\mathbf{Z} - \mathbf{z}\|^2 + \frac{1}{2} \|\mathbf{z} - \mathcal{S} \mathbf{X}^\top \boldsymbol{\beta}\|^2 + \frac{1}{2} \|\mathbf{X} - \sigma(W \mathbf{X})\|^2 \\ & + \frac{\lambda_W}{2} \|W - W_0\|^2 + \frac{\lambda_X}{2} \|\mathbf{X} - \mathbf{X}_0\|^2 + \frac{\lambda_\beta}{2} \|\boldsymbol{\beta} - \boldsymbol{\beta}_0\|^2 + \frac{\lambda_z}{2} \|\mathbf{z} - \mathbf{z}_0\|^2. \end{aligned}$$

Sufficient condition for local convexity: for $\mathbf{v} \in U(\mathbf{v}^*)$:

$$\mathcal{F}(\mathbf{v}) = \nabla^2 \mathcal{L}(\mathbf{v}) > 0.$$

$$\begin{aligned}\mathcal{L}(\mathbf{v}) = & \frac{\mu^2}{2} \|\mathbf{Z} - \mathbf{z}\|^2 + \frac{1}{2} \|\mathbf{z} - \mathcal{S} \mathbf{X}^\top \boldsymbol{\beta}\|^2 + \frac{1}{2} \|\mathbf{X} - \sigma(W \mathbf{X})\|^2 \\ & + \frac{\lambda_{\mathbf{w}}}{2} \|W - W_0\|^2 + \frac{\lambda_{\mathbf{x}}}{2} \|\mathbf{X} - \mathbf{X}_0\|^2 + \frac{\lambda_{\boldsymbol{\beta}}}{2} \|\boldsymbol{\beta} - \boldsymbol{\beta}_0\|^2 + \frac{\lambda_{\mathbf{z}}}{2} \|\mathbf{z} - \mathbf{z}_0\|^2.\end{aligned}$$

Later $\lambda_{\mathbf{w}} = \lambda_{\boldsymbol{\beta}} = \lambda_{\mathbf{z}} = 0$ provided $\mu^2 > 3$.

Lemma

Fix $\mathbf{v} = (W, \mathbf{X}, \boldsymbol{\beta}, \mathbf{z})$ with $\mathbf{X} = \sigma(W \mathbf{X})$ and $\mathbf{z} = \mathcal{S} \mathbf{X}^\top \boldsymbol{\beta}$. Then for any $\mathbf{u} = (\mathbf{w}, \mathbf{x}, \mathbf{b}, \mathbf{h})$

$$\begin{aligned}\frac{d^2}{dt^2} \mathcal{L}(\mathbf{v} + t\mathbf{u}) \Big|_{t=0} = & (\mu^2 + \lambda_{\mathbf{z}}) \|\mathbf{h}\|^2 + \lambda_{\mathbf{x}} \|\mathbf{x}\|^2 + \lambda_{\boldsymbol{\beta}} \|\mathbf{b}\|^2 + \lambda_{\mathbf{w}} \|\mathbf{w}\|^2 \\ & + \sum_{i=1}^n \sum_{m=1}^M \left\{ \sigma'(W_m \mathbf{X}_i) \mathbf{w}_m \mathbf{X}_i - \mathbf{x}_{mi} \right\}^2 + \|\mathbf{h} - \mathcal{S}(\mathbf{X}^\top \mathbf{b} + \mathbf{x}^\top \boldsymbol{\beta})\|^2.\end{aligned}$$

For $\mathbf{v} = (W, \mathbf{X}, \boldsymbol{\beta}, \mathbf{z})$, define

$$\mathbb{F}_m(\mathbf{v}) = \mathbb{F}_m(W_m) \stackrel{\text{def}}{=} \sum_{i=1}^n \sigma'(W_m \mathbf{X}_i)^2 \mathbf{X}_i \mathbf{X}_i^\top + \frac{4}{3} \lambda_{\mathbf{w}} \mathbb{I}_d,$$

$$\mathcal{F}_{\mathbf{w}\mathbf{w}}(\mathbf{v}) = \mathcal{F}_{\mathbf{w}\mathbf{w}}(W) = \text{block}\{\mathbb{F}_1(W_1), \dots, \mathbb{F}_M(W_M)\}.$$

Lemma

Let $\mathbf{A} = \mathcal{S}^\top \mathcal{S}$, $\mu^2 \geq 3$, $\lambda_{\mathbf{x}} \geq \frac{1}{3} + \frac{3b_0^2 \|\mathbf{A}\|_{\text{op}}}{2}$. Let also $\mathbf{X} = \sigma(W\mathbf{X})$, $\mathbf{z} = \mathcal{S}\mathbf{X}^\top \boldsymbol{\beta}$, and $\|\boldsymbol{\beta}\| \leq b_0$

$$\mathcal{F}(\mathbf{v}) \geq \text{block}\left\{ \frac{3}{4} \mathcal{F}_{\mathbf{w}\mathbf{w}}, \left(\lambda_{\mathbf{x}} - \frac{1}{3} - \frac{3b_0^2 \|\mathbf{A}\|_{\text{op}}}{2} \right) \mathbb{I}_{\mathbf{x}}, \right. \\ \left. \frac{1}{2} \mathbf{X} \mathbf{A} \mathbf{X}^\top + \lambda_{\boldsymbol{\beta}} \mathbb{I}_{\boldsymbol{\beta}}, (\mu^2 - 3) \mathbb{I}_{\mathbf{z}} \right\}.$$

Introduce a full dimensional metric tensor $\mathcal{D}$ by

$$\mathcal{D}^2 \stackrel{\text{def}}{=} \text{block}\{D_{\mathbb{W}}^2, \mathbb{I}_{\mathbb{X}}, D_{\beta}^2, \mu^2 \mathbb{I}_z\},$$

$$D_{\mathbb{W}}^2 \stackrel{\text{def}}{=} \frac{1}{4} \text{block}\{\mathbb{F}_1, \dots, \mathbb{F}_M\}, \quad D_{\beta}^2 \stackrel{\text{def}}{=} \frac{1}{2} \mathbb{X}^* \mathbb{A} \mathbb{X}^{*\top} + \lambda_{\beta} \mathbb{I}_{\beta},$$

$$\mathbb{F}_m(W_m) = \sum_{i=1}^n \sigma'(W_m \mathbf{X}_i)^2 \mathbf{X}_i \mathbf{X}_i^{\top} + 4\lambda_{\mathbb{W}} \mathbb{I}_d.$$

With $\sigma(t) = \alpha^{-1} \log(1 + e^{\alpha t})$, define

$$N^{-1/2} = \max_{m \leq M, i \leq n} \left\{ \frac{\sigma''(W_m^* \mathbf{X}_i)}{\sigma'(W_m^* \mathbf{X}_i)} \|\mathbb{F}_m^{-1/2} \mathbf{X}_i\| \right\}, \quad N_1^{-1/2} = \|D_{\beta}^{-1}\|.$$

Under $\|\beta\| \leq b_0$, $\mathbb{X} \mathbb{A} \mathbb{X}^{\top} \leq 2 \mathbb{X}^* \mathbb{A} \mathbb{X}^{*\top}$, smoothness cond. holds with

$$\tau_3 \stackrel{\text{def}}{=} 6\sqrt{e} N^{-1/2} + 6(b_0 + 1) N_1^{-1/2}.$$

For the score vector $\nabla\zeta$, it holds $\nabla\zeta = (0, 0, 0, \nabla_z\zeta)$ with

$$\nabla_z\zeta = \mu^2(\mathbf{Z} - \mathbb{E}\mathbf{Z}), \quad \text{Var}(\nabla_z\zeta) = \text{Var}(\mathcal{S}\mathbf{Y}) = \mu^2 \text{Var}(\mu\mathcal{S}\boldsymbol{\varepsilon}).$$

With $\mathcal{F} = \mathcal{F}(\mathbf{v}^*) = \nabla^2 \mathcal{L}(\mathbf{v}^*)$, the **effective dimension**

$$\mathfrak{p} \stackrel{\text{def}}{=} \text{tr}\{\mathcal{F}^{-1} \text{Var}(\nabla\zeta)\}.$$

Then $\mathcal{F}^{-1} \leq \mathcal{D}^{-2}$ and

$$\|\mathcal{D}\mathcal{F}^{-1}\nabla\zeta\| \leq \|\mathcal{D}^{-1}\nabla\zeta\| = \|\mu\mathcal{S}\boldsymbol{\varepsilon}\|,$$

$$\mathfrak{p} \leq \text{tr}\{\mathcal{D}^{-2} \text{Var}(\nabla\zeta)\} \leq \mathbb{E}\|\mu\mathcal{S}\boldsymbol{\varepsilon}\|^2.$$

The **effective radius** $r_{\mathcal{D}}$ fulfills with $\mathbb{W}^2 \stackrel{\text{def}}{=} \text{Var}(\mu\mathcal{S}\boldsymbol{\varepsilon})$

$$r_{\mathcal{D}} \leq z(\mathbb{W}^2, \mathbf{x}) \leq \sqrt{\text{tr } \mathbb{W}^2} + \sqrt{2\mathbf{x} \|\mathbb{W}^2\|} \approx \sqrt{\mathfrak{p}}.$$

Identifiability of the product $\mathbf{X}^\top \boldsymbol{\beta}$ after restricting to a bounded set

$$\mathcal{R}^\circ \stackrel{\text{def}}{=} \{ \mathbf{v} = (W, \mathbf{X}, \boldsymbol{\beta}, z) : \|\boldsymbol{\beta}\| \leq b_0, \mathbf{X} \mathbf{A} \mathbf{X}^\top \leq 2 \mathbf{X}^* \mathbf{A} \mathbf{X}^{*\top} \}.$$

Here $\mathbf{A} = \boldsymbol{\mathcal{S}}^\top \boldsymbol{\mathcal{S}}$ and b_0 is a fixed constant, e.g. $b_0 = 2$.

Theorem

Let $\mu^2 \geq 3$, $\lambda_{\mathbf{X}} \geq 1/3 + 3b_0^2 \|\mathbf{A}\|_{\text{op}}/2$, and $r_{\mathcal{D}} \tau_3 \leq 4/9$. For any $\mathcal{Q} : \mathbb{R}^{\bar{p}} \rightarrow \mathbb{R}^q$, on a random set $\Omega(\mathbf{x})$ with $\mathbb{P}(\Omega(\mathbf{x})) \geq 1 - e^{-x}$

$$\|\mathcal{Q}(\tilde{\mathbf{v}} - \mathbf{v}^* + \mathcal{F}^{-1} \nabla \zeta)\| \leq \|\mathcal{Q} \mathcal{D}^{-1}\| \frac{3\tau_3}{4} \|\mu \boldsymbol{\mathcal{S}} \boldsymbol{\varepsilon}\|^2.$$

where $\mathcal{D}^2 = \text{block}\{D_{\mathbf{w}}^2, \mathbb{I}_{\mathbf{X}}, D_{\boldsymbol{\beta}}^2, \mathbb{I}_z\}$,

$$D_{\mathbf{w}}^2 \stackrel{\text{def}}{=} \frac{3}{4} \text{block}\{\mathbb{F}_1, \dots, \mathbb{F}_M\}, \quad D_{\boldsymbol{\beta}}^2 \stackrel{\text{def}}{=} \frac{1}{2} \mathbf{X}^* \mathbf{A} \mathbf{X}^{*\top} + \lambda_{\boldsymbol{\beta}} \mathbb{I}_{\boldsymbol{\beta}}.$$

Theorem

Introduce

$$\mathbb{p}_Q \stackrel{\text{def}}{=} \mathbb{E} \{ \| Q \mathcal{F}^{-1} \nabla \zeta \|^2 \mathbb{1}_{\Omega(\mathbf{x})} \} ,$$

assume $\mathbb{E} \{ \| S \varepsilon \|^4 \mathbb{1}_{\Omega(\mathbf{x})} \} \leq C_4^2 \mathbb{p}^2$, and define

$$\alpha_Q \stackrel{\text{def}}{=} \frac{\| Q \mathcal{D}^{-1} \| (3/4) \tau_3 C_4 \mathbb{p}}{\sqrt{\mathbb{p}_Q}} .$$

If $\alpha_Q < 1$ then

$$(1 - \alpha_Q)^2 \mathbb{p}_Q \leq \mathbb{E} \{ \| Q (\tilde{\mathbf{v}} - \mathbf{v}^*) \|^2 \mathbb{1}_{\Omega(\mathbf{x})} \} \leq (1 + \alpha_Q)^2 \mathbb{p}_Q .$$

Denote $\mathcal{I} = \mu \mathcal{F}^{-1}$ and $\boldsymbol{\xi} = \mu \mathcal{S} \boldsymbol{\varepsilon}$. Then

$$\mathcal{F}^{-1} \nabla \zeta = (\mathcal{I}_{\mathbf{w}z} \boldsymbol{\xi}, \mathcal{I}_{\mathbf{x}z} \boldsymbol{\xi}, \mathcal{I}_{\beta z} \boldsymbol{\xi}, \mathcal{I}_{zz} \boldsymbol{\xi}),$$

$$D_{\mathbf{w}}^2 \stackrel{\text{def}}{=} \frac{1}{4} \text{block}\{\mathbf{F}_1, \dots, \mathbf{F}_M\}, \quad D_{\beta}^2 \stackrel{\text{def}}{=} \frac{1}{2} \mathbf{X}^* \mathbf{A} \mathbf{X}^{*\top} + \lambda_{\beta} \mathbb{I}_{\beta}.$$

Corollary

On $\Omega(\mathbf{x})$, with $\mathcal{I} = \mathcal{F}^{-1}$,

$$\|D_{\mathbf{w}}(\widetilde{W} - W^* + \mathcal{I}_{\mathbf{w}z} \boldsymbol{\xi})\| \leq (3/4) \tau_3 \|\boldsymbol{\xi}\|^2,$$

$$\|\widetilde{\mathbf{X}} - \mathbf{X}^* + \mathcal{I}_{\mathbf{x}z} \boldsymbol{\xi}\| \leq (3/4) \tau_3 \|\boldsymbol{\xi}\|^2,$$

$$\|D_{\beta}(\widetilde{\beta} - \beta^* + \mathcal{I}_{\beta z} \boldsymbol{\xi})\| \leq (3/4) \tau_3 \|\boldsymbol{\xi}\|^2,$$

$$\|\widetilde{z} - z^* + \mathcal{I}_{zz} \boldsymbol{\xi}\| \leq (3/4) \tau_3 \|\boldsymbol{\xi}\|^2$$

Construction can be extended to a K -layer network using recurrence

$$\mathbb{X}^{(k)} = \sigma(W^{(k)} \mathbb{X}^{(k-1)})$$

for $k = 1, \dots, K$ and $\mathbb{X}^{(0)} = \mathbf{X}$. With $\mathbb{X} = (\mathbb{X}^{(1)}, \dots, \mathbb{X}^{(K)})$ and $W = (W^{(1)}, \dots, W^{(K)})$, this leads to the log-likelihood

$$\begin{aligned} \mathcal{L}(\mathbf{v}) = \mathcal{L}(W, \mathbb{X}, \beta, z) = & \frac{\mu^2}{2} \|\mathbf{Z} - \mathbf{z}\|^2 \\ & + \frac{1}{2} \|\mathbf{z} - \mathcal{S} \mathbb{X}^{(K)\top} \beta\|^2 + \frac{1}{2} \sum_{k=1}^K \|\mathbb{X}^{(k)} - \sigma(W^{(k)} \mathbb{X}^{(k-1)})\|^2 \\ & + \frac{\lambda_{\mathbb{X}, K}}{2} \sum_{k=1}^K \|\mathbb{X}^{(k)} - \mathbb{X}_0^{(k)}\|^2 + \frac{\lambda_{\mathbb{W}}}{2} \sum_{k=1}^K \|W^{(k)} - W_0^{(k)}\|^2 \\ & + \frac{\lambda_{\beta}}{2} \|\beta - \beta_0\|^2 + \frac{\lambda_z}{2} \|\mathbf{z} - \mathbf{z}_0\|^2. \end{aligned}$$

Lemma

Fix $\mathbf{v} = (W, \mathbb{X}, \beta, \mathbf{z})$ with $\mathbb{X}^{(k)} = \sigma(W^{(k)} \mathbf{X}^{(k-1)})$, $\mathbf{z} = \mathcal{S} \mathbb{X}^{(K)\top} \beta$.

For any $\mathbf{u} = (\mathbf{w}, \mathbb{x}, \mathbf{b}, \mathbf{h})$ with $\mathbf{w} = (\mathbf{w}^{(k)}) \in \mathbb{R}^{n_{\mathbf{w}}}$,

$\mathbb{x} = (\mathbf{x}^{(k)}) \in \mathbb{R}^{n \times d}$, $\mathbf{b} \in \mathbb{R}^{M_K}$, and $\mathbf{h} \in \mathbb{R}^q$, it holds

$$\begin{aligned} \left. \frac{d^2}{dt^2} \mathcal{L}(\mathbf{v} + t\mathbf{u}) \right|_{t=0} &= \lambda_{\mathbb{x}} \|\mathbb{x}\|^2 + \lambda_{\mathbf{w}} \|\mathbf{w}\|^2 + (1 + \lambda_{\mathbf{h}}) \|\mathbf{h}\|^2 + \lambda_{\beta} \|\mathbf{b}\|^2 \\ &+ \sum_{k=1}^K \sum_{m=1}^{M_k} \sum_{i=1}^n \left\{ \sigma'(W_m^{(k)} \mathbb{X}_i^{(k-1)}) \left(\mathbf{w}_m^{(k)} \mathbb{X}_i^{(k-1)} + W_m^{(k)} \mathbf{x}_i^{(k-1)} \right) - \mathbf{x}_{mi}^{(k)} \right\}^2 \\ &+ \left\| \mathbf{h} - \mathcal{S}(\mathbb{X}^{(K)\top} \mathbf{b} + \mathbb{x}^{(K)\top} \beta) \right\|^2 + \lambda_{\mathbb{x}, K} \|\mathbb{x}^{(K)}\|^2. \end{aligned}$$

With $\mathbf{v}^{(k)} = (W^{(k)}, \mathbb{X}^{(k-1)})$, define for $k \leq K$ and $m \leq M_k$

$$\mathbb{F}_m^{(k)}(\mathbf{v}^{(k)}) \stackrel{\text{def}}{=} \sum_{i=1}^n \sigma'(W_m^{(k)} \mathbb{X}_i^{(k-1)})^2 \mathbb{X}_i^{(k-1)} \mathbb{X}_i^{(k-1)\top} + \lambda_k \mathbb{I}_{M_k},$$

$$\mathbb{F}^{(k)}(\mathbf{v}^{(k)}) \stackrel{\text{def}}{=} \text{block}\{\mathbb{F}_1^{(k)}(\mathbf{v}^{(k)}), \dots, \mathbb{F}_{M_k}^{(k)}(\mathbf{v}^{(k)})\}.$$

Similarly define for $k = 2, \dots, K$ and $i = 1, \dots, n$

$$\mathbb{G}_i^{(k)}(\mathbf{v}^{(k)}) \stackrel{\text{def}}{=} \sum_{m=1}^{M_k} \sigma'(W_m^{(k)} \mathbb{X}_i^{(k-1)})^2 W_m^{(k)\top} W_m^{(k)},$$

$$\mathbb{G}^{(k)}(\mathbf{v}^{(k)}) \stackrel{\text{def}}{=} \text{block}\{\mathbb{G}_1^{(k)}(\mathbf{v}^{(k)}), \dots, \mathbb{G}_n^{(k)}(\mathbf{v}^{(k)})\}.$$

Also set $\mathbb{G}^{(1)}(\mathbf{v}^{(1)}) \equiv 0$.

Lemma

Let $\mathbf{X}^{(k)} \equiv \sigma(W^{(k)} \mathbf{X}^{(k-1)})$, $k = 1, \dots, K$. Also, assume $\|\beta\| \leq b_0$ and

$$\max_{i=1,\dots,n} \max_{k=1,\dots,K} \frac{3}{2} \|\mathbf{G}_i^{(k)}(\mathbf{v}^{(k)})\|_{\text{op}} \leq G_0 \leq \lambda_{\mathbf{X}} - 1/3.$$

Then it holds with and $\mathbf{A} = \mathcal{S}\mathcal{S}^\top$

$$\mathcal{F}(\mathbf{v}) \geq \text{block} \left\{ \frac{1}{2} \mathbf{F}^{(1)}(\mathbf{v}^{(1)}), \mathbb{I}_{\mathbf{X}^{(1)}}, \dots, \frac{1}{2} \mathbf{F}^{(K)}(\mathbf{v}^{(K)}), \mathbb{I}_{\mathbf{X}^{(K)}}, \right. \\ \left. \frac{1}{2} \mathbf{X}^{(K)} \mathbf{A} \mathbf{X}^{(K)\top} + \lambda_{\beta} \mathbb{I}_{\beta}, (\mu^2 - 3) \mathbb{I}_z \right\}.$$

1 Introduction

2 “Modern” theory of statistical estimation. An overview

3 Regression using DNN

- Training procedure
- Nonlinear least squares
- Calming
- Noise reduction

4 DNN regression. Theoretical study

5 Conclusion

- Only **effective dimension** p matters, **full dimension** p irrelevant;
- **Blessing of dimension**: extension of parameter space (**calming**) may improve geometric properties of the objective function without changing the effective dimension;
- **Small noise** condition: DNN training requires “small noise” condition (purified data), may be improved by presmoothing;
- (Local) **strong convexity** helps to study theoretical guarantees of the trained DNN and convergence of alternating optimization;
- Each **layer** $\mathbb{X}^{(k)}$ and each **weighting matrix** $W^{(k)}$ can be studied separately;
- No need of **backward propagation**;
- ...

- (Parametric) lower bounds. Please, ask about
- LASSO-type procedures. Issue $\|v\|_1$ is non-smooth.
 Idea: replace by a smooth penalty ensuring $p \asymp \#(\text{active set})$.
- Other models including
 - dimension reduction, manifold learning
 - density estimation
 - error-in-operator models
 - matrix completion
 - inference for stochastic processes
 - statistical nonlinear inverse problems, PDEs
 - ...
- adaptation, parameter/penalty choice
- higher-order expansions, estimation of smooth functionals.

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