Foundations of Deep Learning overview

16 August 2019

In this talk

Will be covered

- nonparametric supervised offline regression

Will NOT be covered

- unsupervised
- online
- density estimation
- reinforcement learning
- beyond i.i.d
- generative models
- adversarial learning
- computational complexity
- approximation power

Plan

Generalization [1]–[4]

$$Z = (X, Y) \text{ — r.v.} \quad X \in \mathcal{X}, Y \in \mathcal{Y}$$

loss $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$

population risk $L : \mathfrak{M}(\mathcal{Y}^{\mathcal{X}}) \to \mathbb{R}$

$$L(f) = \mathbb{E}_Z[\ell(f(X), Y)]$$

Aim:

$$f^\star = \arg\min_{f \in \mathfrak{M}(\mathcal{Y}^{\mathcal{X}})} L(f)$$

Simplification: level 1.a

Issue

$\mathfrak{M}(\mathcal{Y}^{\mathcal{X}})$ is too large, not parametrizable

Solution

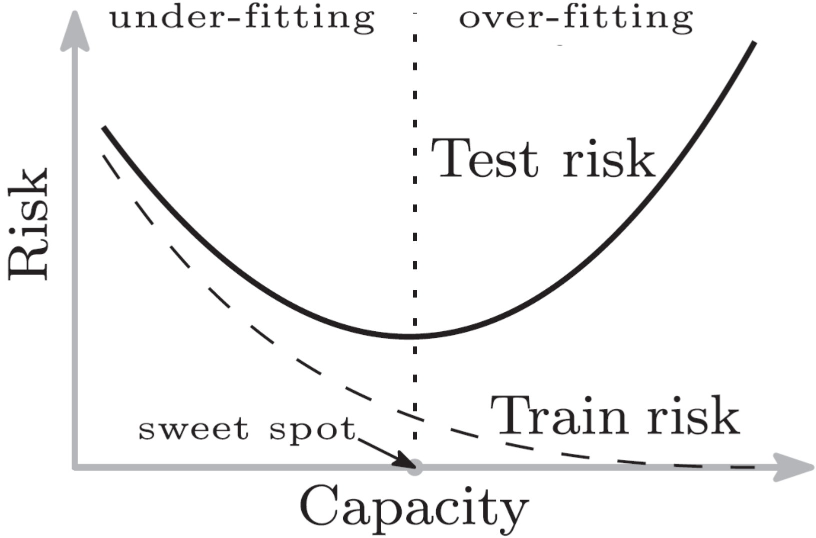
Introduce $\mathcal{F} \subset \mathfrak{M}(\mathcal{Y}^{\mathcal{X}})$ — parametric function class, incapsulates inductive bias

bias-variance trade-off

for $f_{\mathcal{F}} = \arg\min_{f \in \mathcal{F}} L(f)$, any $f \in \mathcal{F}$:

$$\underbrace{L(f) - L(f^{\star})}_{\text{total risk}} = \underbrace{L(f) - L(f_{\mathcal{F}})}_{\text{estimation risk}} + \underbrace{L(f_{\mathcal{F}}) - L(f^{\star})}_{\text{approximation risk}}$$

Classic risk curve



Simplification: level 1.b

Issue

L is defined with unknown $\mathbb{P}_Z$

Solution

Sample i.i.d $(X_i', Y_i')_{i=1}^m$ from $\mathbb{P}_Z$ and define empirical risk

$$\tilde{L}(f) = \frac{1}{m} \sum_{i=1}^{m} \ell(f(X_i'), Y_i')$$

Law of Large Numbers

If $f \perp\!\!\!\perp (X_i', Y_i')^m$ then $\tilde{L}(f) - L(f) \to 0$

Inconsistency

Aim:

$$\tilde{f} = \arg\min_{f \in \mathcal{F}} \tilde{L}(f)$$

$\tilde{f}$ defined by stochastic objective $\tilde{L}(f)$ that depends on $(X_i', Y_i')^m$, but $\tilde{f}$ must not depend on $(X_i', Y_i')^m$ to use LLN

Simplification: level 2

Issue

$\tilde{f}$ depends on $(X_i', Y_i')^m$

Solution

Generate a copy: i.i.d $(X_i, Y_i)_{i=1}^n$ from $\mathbb{P}_Z$ and build

$$\hat{L}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(X_i), Y_i) \qquad \hat{f} = \arg\min_{f \in \mathcal{F}} \hat{L}(f)$$

Simplification: level 3

Issue

$\hat{L}(f)$ can still be non-convex, NP hard to optimize

Solution

fix a learning algorithm $\mathcal{A}$ and take

$$\hat{f} = \mathcal{A}(\{Z_i\}^n, \Gamma)$$

Use intrinsic properties of the algorithm to build generalization guarantees

Power system example

Power system state estimation problem via non-convex recovery:

$$\text{given } X_i = M_i \text{ and } Y_i = m_i$$

$$\text{minimize} \sum_i (x^* M_i x - m_i)^2$$

Power engineering aim: get $\|xx^* - vv^*\|$ small
Machine Learning aim: get $\mathbb{E}_{M,m}[x^* M x - m]^2$ small

Statistical Learning Theory

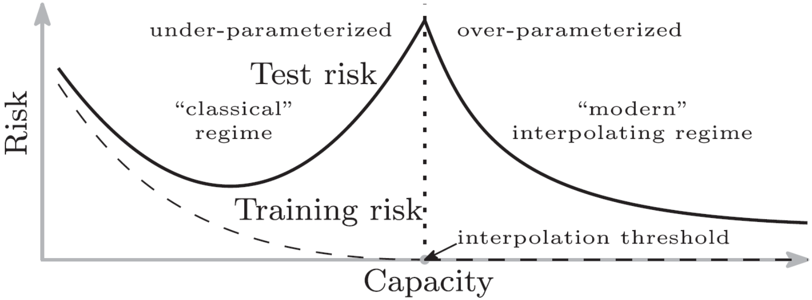
Bounds on Excess Risk

$$L(f) - L(f_{\mathcal{F}}) = [L(f) - \hat{L}(f)] + [\hat{L}(f) - \hat{L}(f_{\mathcal{F}})] + [\hat{L}(f_{\mathcal{F}}) - L(f_{\mathcal{F}})]$$

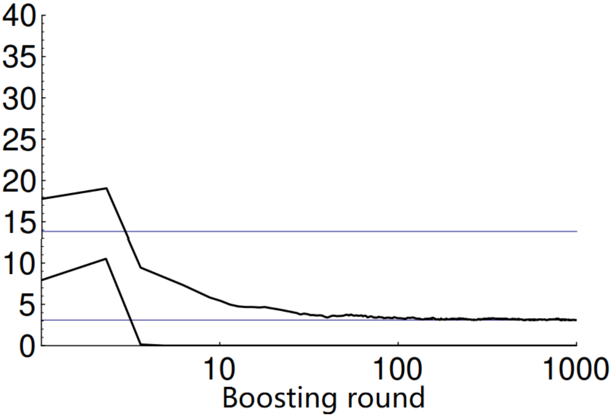
$$\mathbb{E}_n L(\hat{f}) - L(f_{\mathcal{F}}) \leq \mathbb{E}_n[L(\hat{f}) - \hat{L}(\hat{f})] \leq \mathbb{E}_n \sup_{f \in \mathcal{F}} |L(f) - \hat{L}(f)|$$

Note: exist bounds with compression argument and stability argument, which do not rely on properties of $\mathcal{F}$, but on $\hat{f}$ instead

Modern risk curve [5]

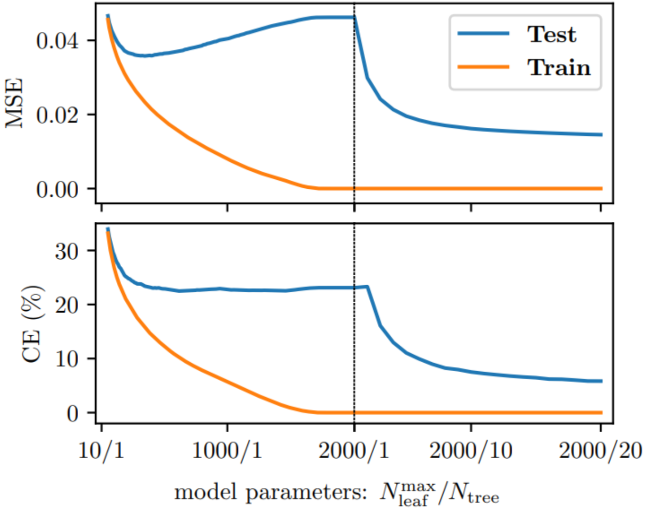


"Modern" risk curve

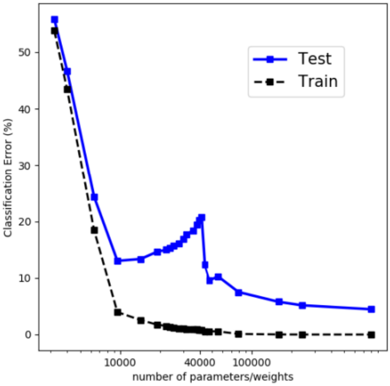


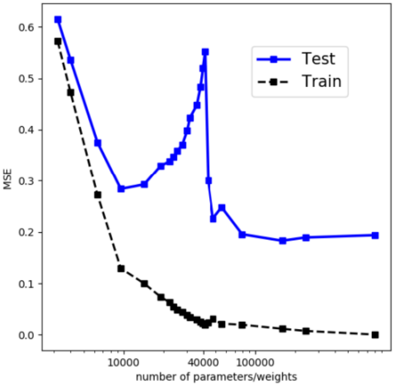
NIPS tutorial by P.Bartlett, 1998

More examples: random forest [5]



More examples: neural net [5]





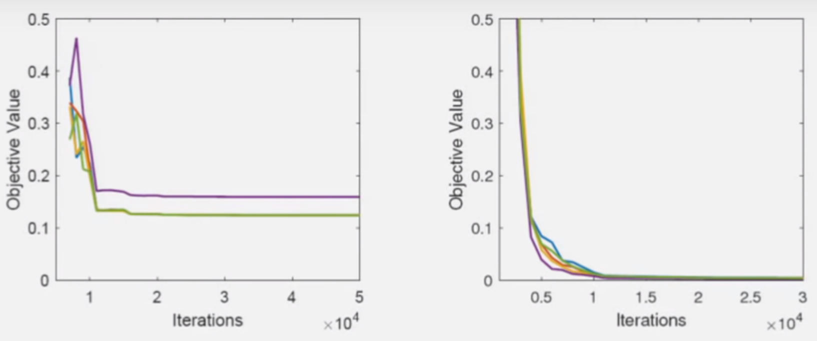
Questions

Phenomenon: good test risk with zero *regression* train loss on *noisy* data

1. When is zero train loss achievable? (optimization)
2. In which of these cases does test risk go down? (generalization)
3. What is the gain compared to the amount of computation?

State of the art: optimization [7], [8]

Observation: larger architectures are easier to train [6]



There is a phase transition

State of the art: optimization [7], [8]

Taxometry of results on overparametrization

- Static: All solutions (SOSP) are global
  - Shallow, quadratic activation: $\textit{width} \gtrsim \min\{\textit{dim}, \sqrt{n}\}$ [9], [10]
  - Deep, leaky ReLU: $\textit{width} \gtrsim n$ [11], [12]
- Dynamic: SGD finds global solution near a random initialization (SGD learns something competitive to the best in RKHS) [13]–[16]
  - $\textit{width} \gtrsim n^2$ at least and depth-dependent

Note: under regularity conditions, SGD converges to a second-order stationary point [17], [18]

Reproducing Kernel Hilbert Space (RKHS)

$\mathcal{H}$ — Hilbert (complete inner product vector) space of real-valued functions on $\mathcal{X}$. It is a RKHS iff there is $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that

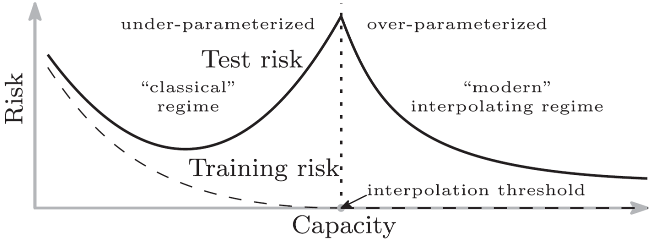
$$\sum_{i,j} c_i c_j K(x_i, x_j) \geq 0$$

$$\mathcal{H} \longleftrightarrow K$$

Usually, $K(x, y) = \langle \phi(x), \phi(y) \rangle$ where $\phi : \mathcal{X} \to \mathcal{V}$

Examples: Gaussian $e^{-\frac{\|x-y\|^2}{\sigma}}$; Neural Tangent Kernel (NTK) [19], [20]

State of the art: generalization



What happens after interpolation threshold: implicit regularization

- by $\|W_1\| \dots \|W_L\|$ for linear neural nets [21]
- by $\|f\|_{\mathcal{H}}$ for Random Fourier Features [5], [22]

Note: [23] characterizes the effect of overparametrization on generalization in linear regression

Neural Network learning routine [24]–[27]

Steps:

- Model Selection
- Initialization
- Learning algorithm
- Regularization

Routine:

1. reach interpolation
2. regularize

Model selection: Neural architecture search [40]

- Adjustable parameters: layer structure (dense, convolutional, recurrent, attention), activation function, learning properties
- Hierarchical search space [28], [29]
- Search strategy: Evolution [30], [31], Bayessian optimization [32], [33], Reinforcement Learning [34], continuous relaxation [35], incremental learning [36]

- First benchmark dated by May 2019 [37]
- Modern NN models seem to tolerate adaptation to common data sets [38], [39]

Initialization: random

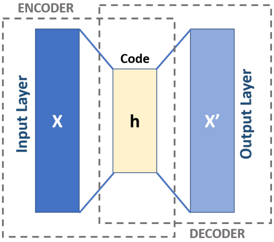
$$\text{Xavier: } W^{(l)} \sim \mathcal{N}(0, \frac{2}{p^{l-1}}); \quad b^{(l)} = 0 \quad [41]$$

$$\text{He: } W^{(l)} \sim \mathcal{N}(0, \frac{2}{p^{l-1} + p^{l}}); \quad b^{(l)} = 0 \quad [42]$$

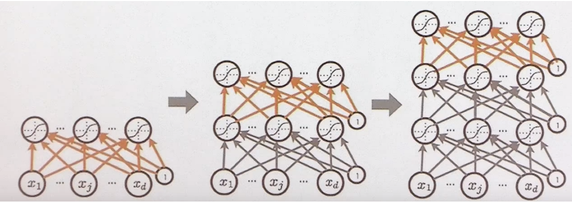
Initialization: Unsupervised pre-training [43]

Autoencoder

$$\phi : \mathcal{X} \to \mathcal{Y}$$
$$\psi : \mathcal{Y} \to \mathcal{X}$$
$$\phi^*, \psi^* = \arg\min_{\phi,\psi} \mathbb{E}\ell[(\psi \circ \phi)(X), X]$$



Greedy layer-wise pre-training: stack encoders

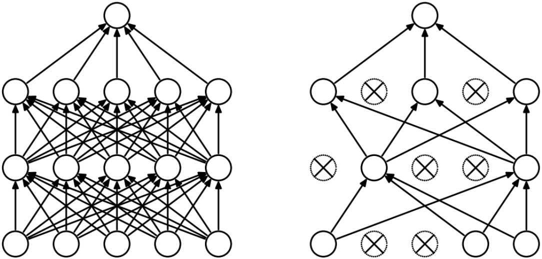


Learning algorithm: SGD

Objective: $\min_\theta \frac{1}{n}\sum_{i=1}^{n} \ell(\Phi(X_i, \theta), Y_i)$
mini-batch SGD: $\theta^{t+1} = \theta^t - \frac{\alpha}{|\mathcal{B}|}\sum_{i\in\mathcal{B}} \nabla_\theta \ell(\Phi(X_i, \theta^t), Y_i)$
Modern version: faster convergence/saddles fighting

- Momentum[44]:
  $\theta^{t+1} = \theta^t - v^{t+1}; v^{t+1} = \gamma v^t + \frac{\alpha}{|\mathcal{B}|}\sum_{i\in\mathcal{B}} \nabla_\theta \ell(\Phi(X_i, \theta^t), Y_i)$
- Nesterov[45]: in the above $\Phi(X_i, \theta^t) \to \Phi(X_i, \theta^t - \gamma v^t)$
- Adagrad/Adadelta/RMSprop — adaptive learning rate (keep exponentially decaying average of past gradients)
- Batch normalization: $\hat{x}^i = \alpha \frac{x^i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \varepsilon}} + \beta$; $\sigma_\mathcal{B}$ and $\mu_\mathcal{B}$ — std div and mean of the batch, α and β to be learned

Regularization: Dropout [48]



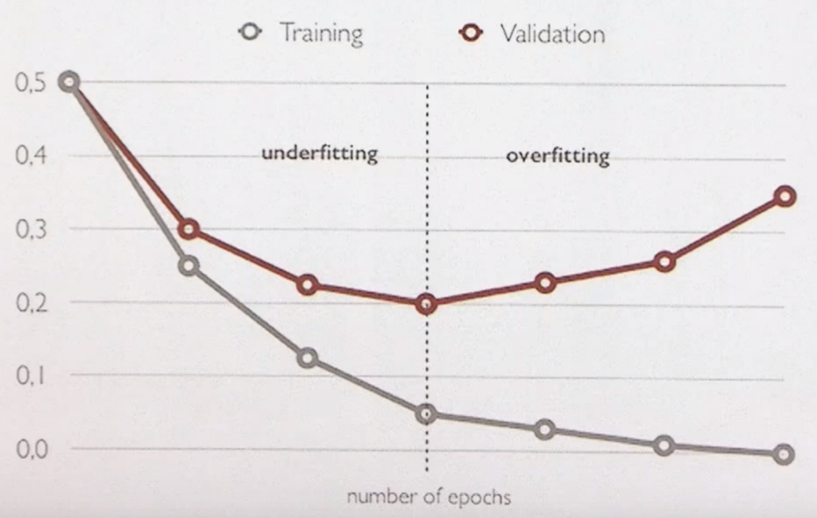
(a) Standard Neural Net (b) After applying dropout.

$z^t \in \{0,1\}^p$ — random, p — number of parameters

SGD+dropout: $\theta^{t+1} = \theta^t - \frac{\alpha}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla_\theta \ell(\underbrace{\Phi(X_i, \theta^t, z^t)}_{\text{output of dropout neurons is 0}}, Y_i) \underbrace{\otimes z^t}_{\text{gradient of dropout is 0}}$

Note: "Dropout-stable" solutions posses the property of Landscape Connectivity [46]; dropout acts as explicit regularization in Stochastic Matrix Factorization [47]

Regularization: Early stopping



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