# Benign Overfitting

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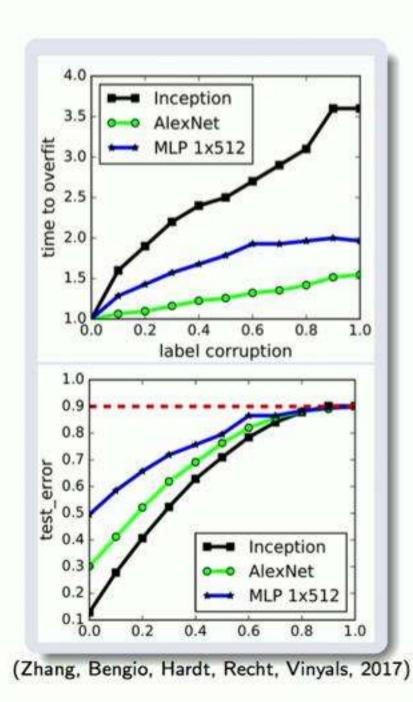
Gábor Lugosi



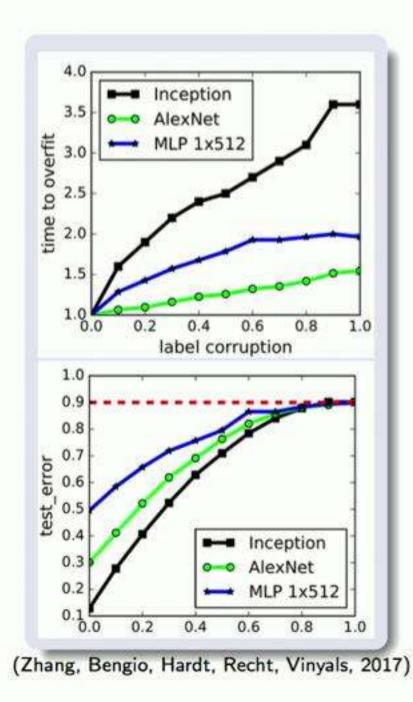
Alexander Tsigler

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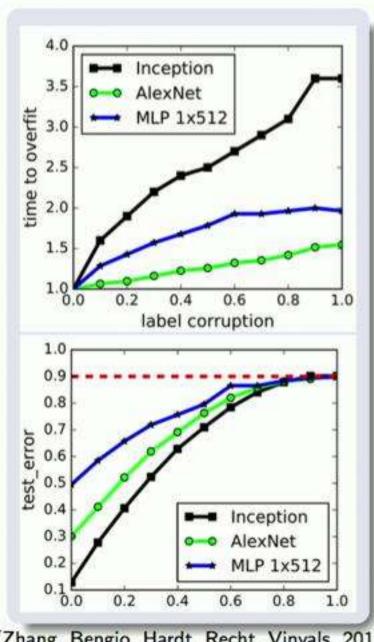


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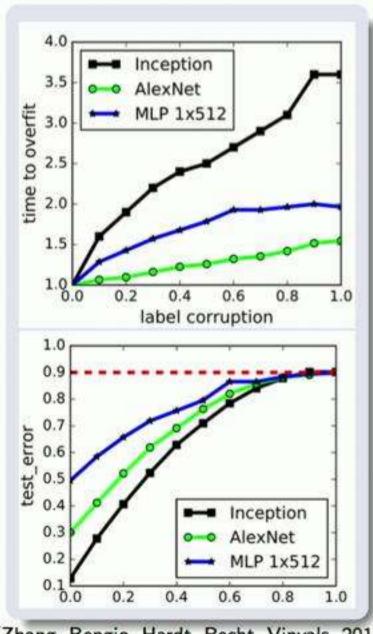
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This is especially important for nonparametric methods, that is, those for which the number of parameters grows with the sample size.

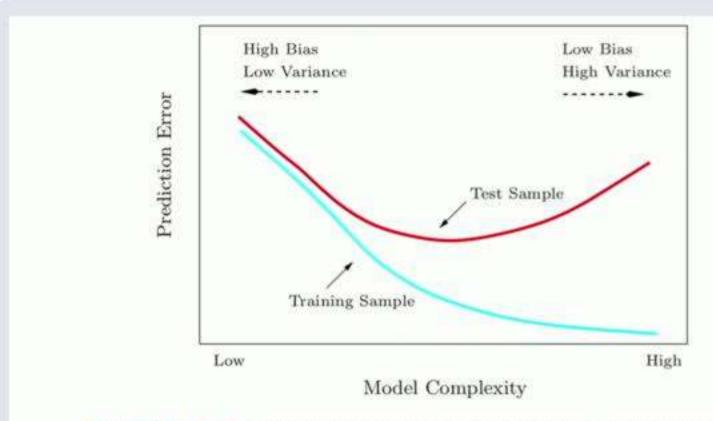
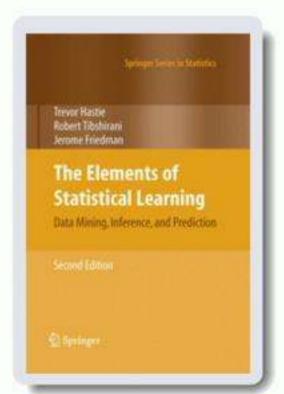


FIGURE 2.11. Test and training error as a function of model complexity.

Figure 2.11 shows the typical behavior of the test and training error, as model complexity is varied. The training error tends to decrease whenever we increase the model complexity, that is, whenever we fit the data harder. However with too much fitting, the model adapts itself too closely to the training data, and will not generalize well (i.e., have large test error). In

"... interpolating fits... [are] unlikely to predict future data well at all."



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2. How to Construct Nonparametric Regression Estimates?

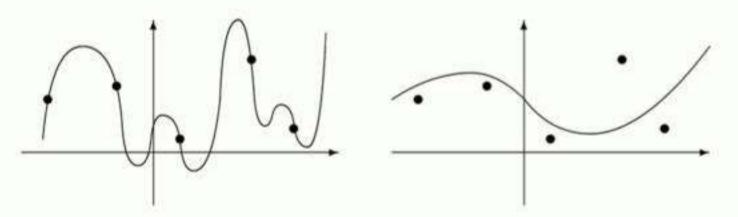
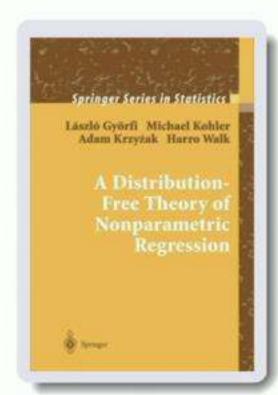


Figure 2.3. The estimate on the right seems to be more reasonable than the estimate on the left, which interpolates the data.

over  $\mathcal{F}_n$ . Least squares estimates are defined by minimizing the empirical  $L_2$  risk over a general set of functions  $\mathcal{F}_n$  (instead of (2.7)). Observe that it doesn't make sense to minimize (2.9) over all (measurable) functions f, because this may lead to a function which interpolates the data and hence is not a reasonable estimate. Thus one has to restrict the set of functions over



# Benign Overfitting

# A new statistical phenomenon: good prediction with zero training error for regression loss

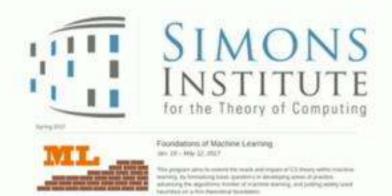
- Statistical wisdom says a prediction rule should not fit too well.
- But deep networks are trained to fit noisy data perfectly, and they predict well.

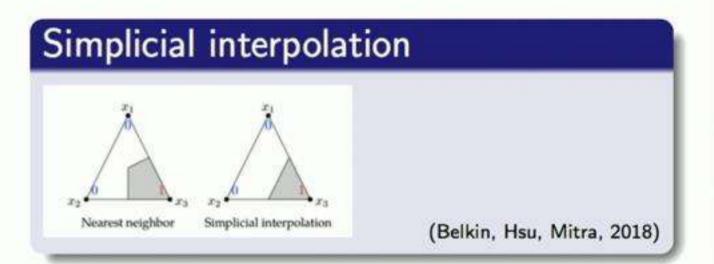


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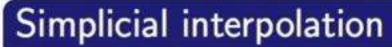
Foundations of Machine Learning

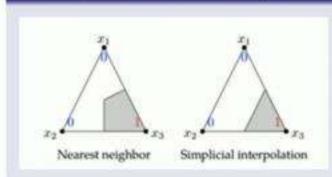
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(Belkin, Hsu, Mitra, 2018)

### Kernel smoothing with singular kernels

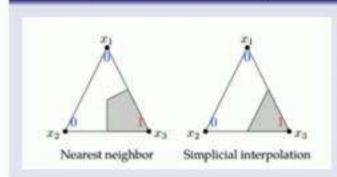
$$\hat{f}(x) = \sum_{i=1}^{n} \frac{y_i K_h(x - x_i)}{\sum_{i=1}^{n} K_h(x - x_i)} \quad \text{with } K_h(x) = \frac{1}{h||x||^{\alpha}}.$$

Minimax rates possible (with suitable h).

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## Simplicial interpolation



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## Linear regression with $d \approx n$

Kernels defined in terms of the Euclidean inner product

(Liang and Rakhlin, 2018)

ullet Linear regression with  $d,n o\infty$ ,  $d/n o\gamma$  (Hastie, Montanari, Rosset, Tibshirani, 2019)

# Outline

- Linear regression
- Characterizing benign overfitting
- Deep learning
- Adversarial examples

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$$\Sigma := \mathbb{E} x x^{\top} = \sum_{i} \lambda_{i} v_{i} v_{i}^{\top}, \quad \text{(assume } \lambda_{1} \geq \lambda_{2} \geq \cdots \text{)}$$

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- Data:  $X \in \mathbb{H}^n$ ,  $y \in \mathbb{R}^n$ .
- Estimator  $\hat{\theta} = (X^{T}X)^{\dagger} X^{T} y$ , which solves

$$\min_{\theta \in \mathbb{H}} \quad \|\theta\|^2$$
  
s.t. 
$$\|X\theta - y\|^2 = \min_{\beta} \|X\beta - y\|^2.$$

## Excess prediction error

$$R(\hat{\theta}) := \mathbb{E}_{(x,y)} \left( y - x^{\top} \hat{\theta} \right)^{2} - \underbrace{\min_{\theta} \mathbb{E} \left( y - x^{\top} \theta \right)^{2}}_{\text{optimal prediction error}}$$

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$$= \mathbb{E}_{(x,y)} \left[ \left( y - x^{\top} \hat{\theta} \right)^{2} - \left( y - x^{\top} \theta^{*} \right)^{2} \right]$$

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So  $\Sigma$  determines the importance of parameter directions.

(Recall that 
$$\Sigma = \sum_{i} \lambda_{i} v_{i} v_{i}^{\top}$$
 for orthonormal  $v_{i}$ ,  $\lambda_{1} \geq \lambda_{2} \geq \cdots$ .)

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- When can the label noise be hidden in  $\hat{\theta}$  without hurting predictive accuracy?

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Also, 
$$\frac{r_0(\Sigma)}{\ln(1+r_0(\Sigma))} \ge \kappa n$$
 implies for some  $\theta^*$ ,  $\Pr(R(\hat{\theta}) \ge 1/c) \ge 1/4$ .

### Definition (Effective Ranks)

Recall that  $\lambda_1 \geq \lambda_2 \geq \cdots$  are the eigenvalues of  $\Sigma$ .

For  $k \ge 0$ , if  $\lambda_{k+1} > 0$ , define the effective ranks

$$r_k(\Sigma) = \frac{\sum_{i>k} \lambda_i}{\lambda_{k+1}}, \qquad \qquad R_k(\Sigma) = \frac{\left(\sum_{i>k} \lambda_i\right)^2}{\sum_{i>k} \lambda_i^2}.$$

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#### Lemma

$$1 \leq r_k(\Sigma) \leq R_k(\Sigma) \leq r_k^2(\Sigma)$$
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- ② If  $rank(\Sigma) = p$ , we can write

$$r_0(\Sigma) = \mathrm{rank}(\Sigma) s(\Sigma), \qquad R_0(\Sigma) = \mathrm{rank}(\Sigma) S(\Sigma),$$
 with  $s(\Sigma) = \frac{1/p \sum_{i=1}^p \lambda_i}{\lambda_1}, \qquad S(\Sigma) = \frac{\left(1/p \sum_{i=1}^p \lambda_i\right)^2}{1/p \sum_{i=1}^p \lambda_i^2}.$ 

Both s and S lie between 1/p ( $\lambda_2 \approx 0$ ) and 1 ( $\lambda_i$  all equal).

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  - Small eigenvalues: roughly equal (but they can be more assymmetric if there are many more than n of them).

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$$R(\hat{\theta}) = (\hat{\theta} - \theta^*)^{\top} \Sigma (\hat{\theta} - \theta^*)$$
$$\approx \theta^{*\top} (I - \hat{\Sigma}\hat{\Sigma}^{\dagger}) (\Sigma - \hat{\Sigma}) (I - \hat{\Sigma}^{\dagger}\hat{\Sigma}) \theta^*$$

$$+\,\sigma^2\mathrm{tr}\,\bigg(\Big(X^\top X\Big)^\dagger\,\Sigma\bigg).$$

$$R(\hat{\theta}) = \left(\hat{\theta} - \theta^*\right)^{\top} \mathbf{\Sigma} \left(\hat{\theta} - \theta^*\right).$$

### The excess risk

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- So  $XX^{\top} \succeq \rho I$ .  $\hat{\theta} = (X^{\top}X)^{\dagger} X^{\top} y$ c.f. ridge regression:  $\hat{\theta} = (X^{\top}X + \rho I)^{-1} X^{\top} y$ .

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Total prediction error bound: 
$$\frac{k}{n} + n \sum_{i > k} \lambda_i^2 \rho^{-2} = \frac{k}{n} + \frac{n}{R_k(\Sigma)}$$
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- And otherwise, the excess expected loss is at least a constant.

# Benign Overfitting: A Characterization

#### Theorem

For universal constants b, c, and any linear regression problem  $(\theta^*, \sigma^2, \Sigma)$  with  $\lambda_n > 0$ , if  $k^* = \min\{k \ge 0 : r_k(\Sigma) \ge bn\}$ ,

With high probability,

$$R(\hat{\theta}) \leq c \left( \|\theta^*\|^2 \|\Sigma\| \sqrt{\frac{r_0(\Sigma)}{n}} + \sigma^2 \left( \frac{k^*}{n} + \frac{n}{R_{k^*}(\Sigma)} \right) \right),$$

$$\mathbb{E}R(\hat{\theta}) \geq \frac{\sigma^2}{c} \min \left\{ \frac{k^*}{n} + \frac{n}{R_{k^*}(\Sigma)}, 1 \right\}.$$

Also, 
$$\frac{r_0(\Sigma)}{\ln(1+r_0(\Sigma))} \ge \kappa n$$
 implies for some  $\theta^*$ ,  $\Pr(R(\hat{\theta}) \ge 1/c) \ge 1/4$ .

We say  $\Sigma$  is asymptotically benign if

$$\lim_{n\to\infty}\left(\|\Sigma\|\sqrt{\frac{r_0(\Sigma)}{n}}+\frac{k_n^*}{n}+\frac{n}{R_{k_n^*}(\Sigma)}\right)=0,$$

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If  $\lambda_i = i^{-\alpha} \ln^{-\beta} (i+1)$ , then  $\Sigma$  is benign iff  $\alpha = 1$  and  $\beta > 1$ .

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The  $\lambda_i$  must be almost diverging!!?!?

### Example: Finite dimension, plus isotropic noise

If

$$\lambda_{k,n} = \begin{cases} e^{-k} + \epsilon_n & \text{if } k \leq p_n, \\ 0 & \text{otherwise,} \end{cases}$$

then  $\Sigma_n$  is benign iff

- $p_n = \omega(n)$ ,
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$$(n \ge 40 \Longrightarrow ne^{-n} < 2^{-52})$$

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Universal phenomenon: fast converging  $\lambda_i$ ,  $p_n \gg n$ , noise in all directions.

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**3** Components of  $\Sigma^{-1/2}x$  are independent subgaussian:

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e.g., see (Rakhlin and Zhai, 2018)

# Outline

- Linear regression
- Characterizing benign overfitting
- Deep learning
- Adversarial examples

# Implications for deep learning

### Neural networks versus linear prediction

For wide enough randomly initialized neural networks, gradient descent dynamics quickly converge to (approximately) a min-norm interpolating solution with respect to a certain kernel.

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For wide enough randomly initialized neural networks, gradient descent dynamics quickly converge to (approximately) a min-norm interpolating solution with respect to a certain kernel.

For example, for

$$f(x) = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} a_i \sigma\left(\langle w_i, x \rangle\right),\,$$

the corresponding (random) kernel is

$$K^{m}(x,x_{j}):=\frac{1}{m}\sum_{i=1}^{m}a_{i}^{2}\sigma'\left(\langle w_{i},x\rangle\right)\sigma'\left(\langle w_{i},x_{j}\rangle\right)\langle x,x_{j}\rangle.$$

(Xie, Liang, Song, '16), (Jacot, Gabriel, Hongler '18), (Li and Liang, 2018), (Du, Poczós, Zhai, Singh, 2018), (Du, Lee, Li, Wang, Zhai, 2018), (Arora, Du, Hu, Li, Wang, 2019).

(No generalization results for prediction rules that interpolate noisy data.)

# Implications for deep learning

### Neural networks versus linear prediction

- What can we say about realistic deep networks?
- The characterization of benign overfitting in linear regression requires  $x = \sum^{1/2} z$  for a vector z with *independent* components.

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Label noise appears in  $\hat{\theta}$ 

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We can find a unit norm  $\Delta$   $\Delta \propto x^{\top} (xx^{\top})^{-1} \epsilon$  such that perturbing an input x by  $\Delta$  changes the output enormously: even if  $\Delta^{\top} \theta^* = 0$ ,

$$\left\| (x + \Delta)^{\top} \hat{\theta} - x^{\top} \hat{\theta} \right\|^{2} \geq \frac{\sigma}{\sqrt{\lambda_{k^{*}+1}}} \geq \sqrt{\frac{n}{\operatorname{tr}(\Sigma)}} \sigma.$$

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- But it leads to huge sensitivity to (adversarial) perturbations.