Advanced Introduction to Machine Learning CMU-10715

Risk Minimization

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What have we seen so far?

Several classification & regression algorithms seem to work fine on training datasets:

- Linear regression
- Logistic regression
- Gaussian Processes
- Naïve Bayes classifier
- Support Vector Machines

- ❑How good are these algorithms on unknown test sets?
- ❑How many training samples do we need to achieve small error?
- ❑What is the smallest possible error we can achieve?

⇒ Learning Theory

Outline

- Risk and loss
  - Loss functions
  - Risk
  - Empirical risk vs True risk
  - Empirical Risk minimization
- Underfitting and Overfitting
- Classification
- Regression

Supervised Learning Setup

$\mathcal{D} = \{(X_1, Y_1), \ldots (X_n, Y_n)\}$ training data

$\{(X_{n+1}, Y_{n+1}), \ldots (X_m, Y_m)\}$ test data

Features: $X \in \mathcal{X} \subset \mathbb{R}^d$

Labels: $Y \in \mathcal{Y} \subset \mathbb{R}$

Generative model of the data: (train and test data)

$$X \sim \mu,\ \mu(A) = \Pr(X \in A)$$
$$Y \sim p(\cdot|X)$$

Regression: Labels: $\mathcal{Y} = [a, b] \subset \mathbb{R}$, or $\mathcal{Y} = \mathbb{R}$

Classification: Labels: $\mathcal{Y} = \{0, 1\}$

Loss

$\mathcal{D} = \{(X_1, Y_1), \ldots (X_n, Y_n)\}$ training data

$\{(X_{n+1}, Y_{n+1}), \ldots (X_m, Y_m)\}$ test data

Loss function: $L(x, y, f(x))$

where $L : \mathcal{X} \times \mathcal{Y} \times \mathbb{R} \to [0, \infty]$

It measures how good we are on a particular (x,y) pair.

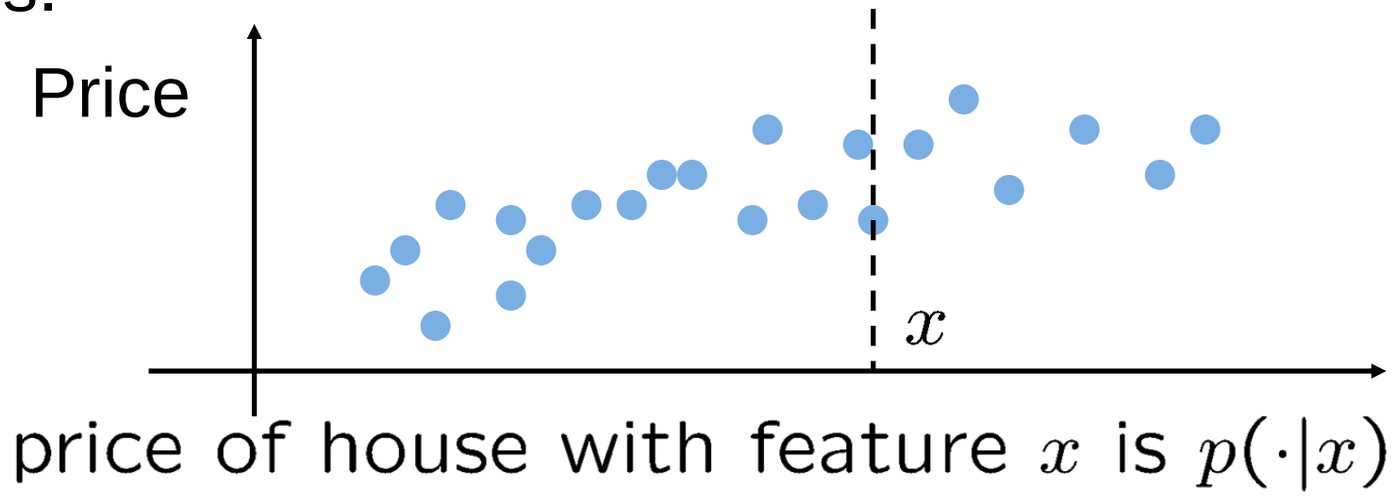
We want the loss $L(X_t, Y_t, f(X_t))$ to be small for many (X_t, Y_t) pairs in the test data.

Loss Examples

Classification loss:

$$L(x, y, f(x)) = \begin{cases} 1 & y \neq f(x) \\ 0 & y = f(x) \end{cases}$$

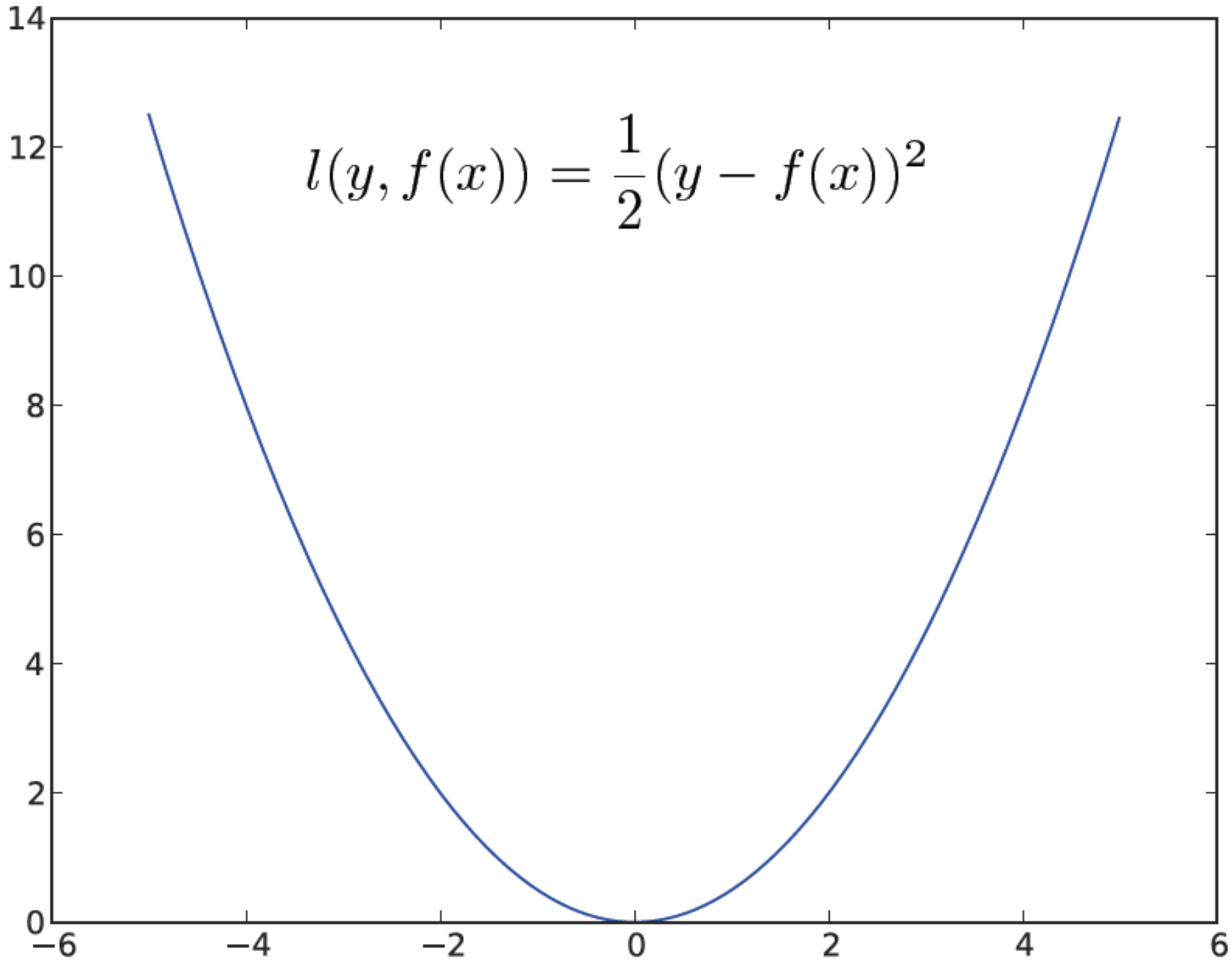
Regression: Predict house prices.



L_2 loss for regression: $L(x, y, f(x)) = (y - f(x))^2$

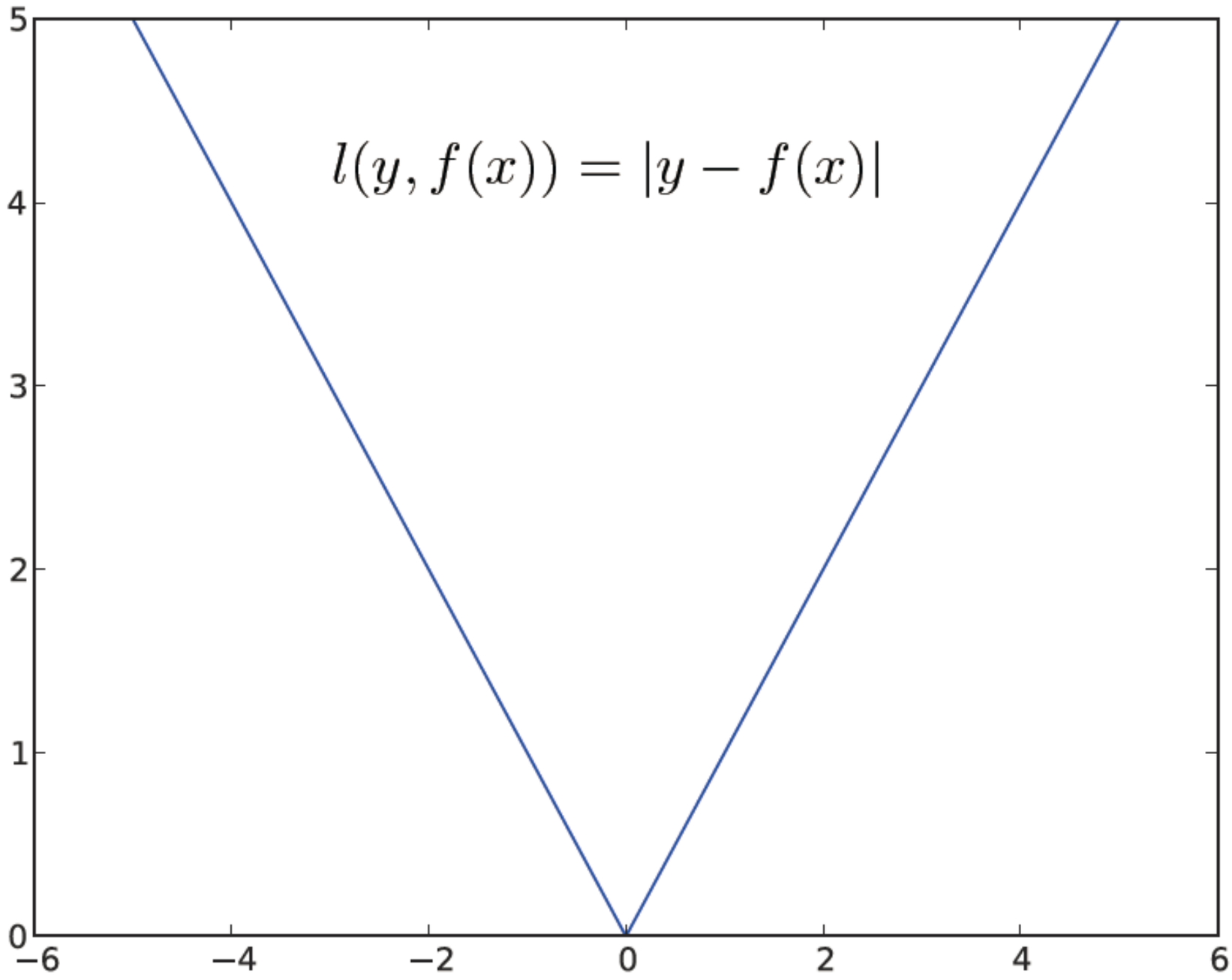
L_1 loss for regression: $L(x, y, f(x)) = |y - f(x)|$

Squared loss, L_2 loss



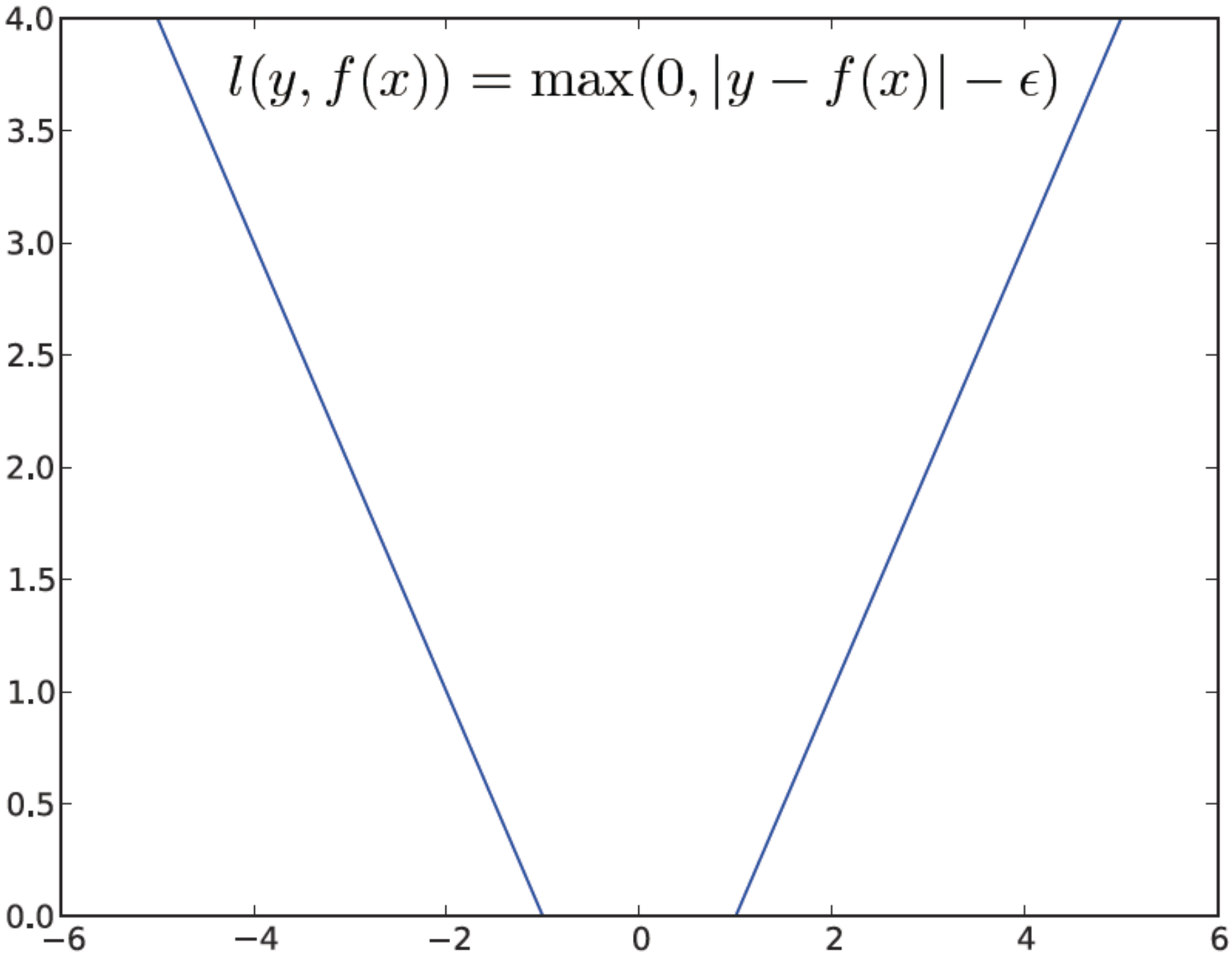
Picture form Alex

L_1 loss



Picture form Alex

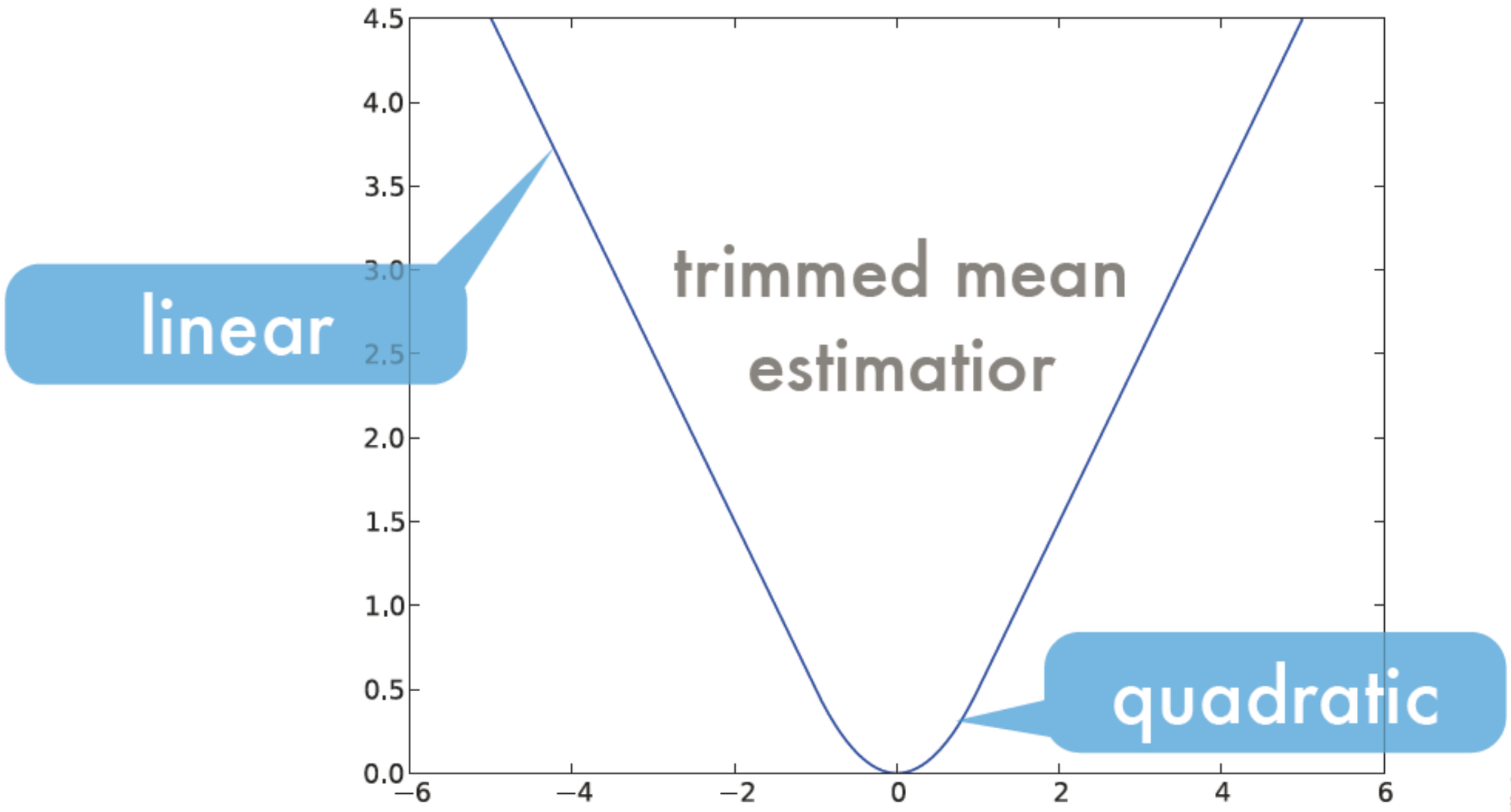
ε–insensitive loss



Picture form Alex

Huber's robust loss

$$l(y, f(x)) = \begin{cases} \frac{1}{2}(y - f(x))^2 & \text{if } |y - f(x)| < 1 \\ |y - f(x)| - \frac{1}{2} & \text{otherwise} \end{cases}$$



Picture form Alex

Risk

Risk of *f* classification/regression function:

$$R_{L,P}(f) = \int_{\mathcal{X}\times\mathcal{Y}} L(x, y, f(x))dP(x, y) = \mathbb{E}[L(X, Y, f(X))]$$

= The expected loss

$p(y, x)dydx$

$L(x, y, f(x))$: Loss function

$P(x, y)$: Distribution of the data.

Why do we care about this?

Why do we care about risk?

Risk of *f* classification/regression function:

$$R_{L,P}(f) = \int_{\mathcal{X}\times\mathcal{Y}} L(x, y, f(x))dP(x, y) \quad \text{=The expected loss}$$
$$= \mathbb{E}[L(X, Y, f(X))]$$

$p(y, x)dydx$

Our true goal is to minimize the loss of the test points!

$$f^* = \arg\min_f \frac{1}{m-n} \sum_{i=n+1}^{m} L(X_i, Y_i, f(X_i))$$

Usually we don't know the test points and their labels in advance…, but

$$\frac{1}{m-n} \sum_{i=n+1}^{m} L(X_i, Y_i, f(X_i)) \xrightarrow{m\to\infty} R_{L,P}(f) \quad \text{(LLN)}$$

That is why our goal is to minimize the risk.

Risk Examples

Risk: $R_{L,P}(f) = \int_{\mathcal{X}\times\mathcal{Y}} L(x, y, f(x)) dP(x, y)$ The expected loss

Classification loss: $L(x, y, f(x)) = \begin{cases} 1 & y \neq f(x) \\ 0 & y = f(x) \end{cases}$

Risk of classification loss:

$$R_{L,P}(f) = \int_{\mathcal{X}\times\mathcal{Y}} L(x, y, f(x)) dP(x, y) = \mathbb{E}[1_{\{f(X)\neq Y\}}] = \Pr(f(X) \neq Y)$$

L_2 loss for regression: $L(x, y, f(x)) = (y - f(x))^2$

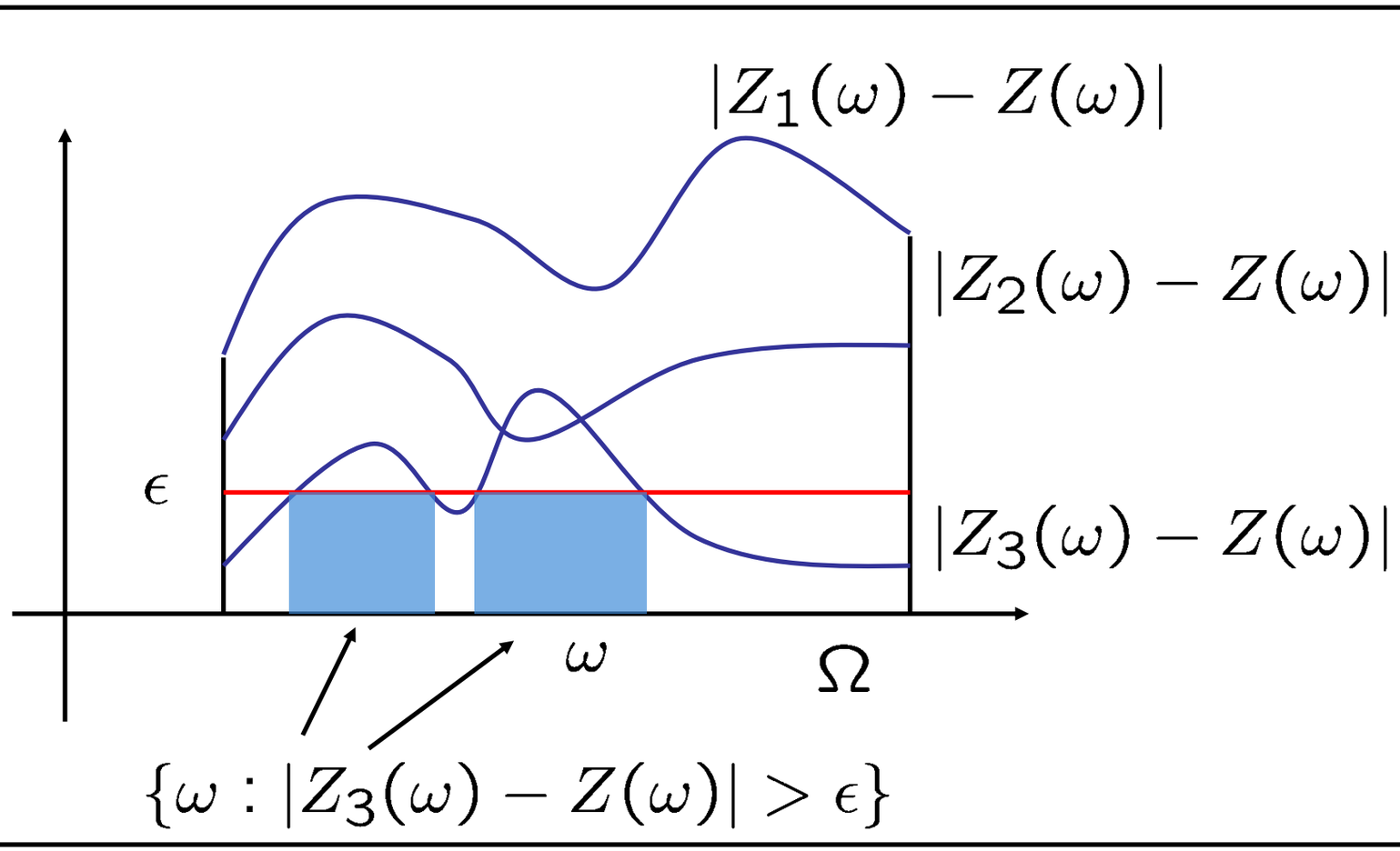
Risk of L_2 loss: $R_{L,P}(f) = \mathbb{E}[(Y - f(X))^2]$

Convergence in Probability

Notation: $Z_n \xrightarrow{p} Z$

Definition: $\forall \varepsilon > 0 \ \lim_{n\to\infty} \Pr\left(|Z_n - Z| \geq \varepsilon\right) = 0.$

$\forall \varepsilon > 0 \ \lim_{n\to\infty} \Pr\left(|Z_n - Z| < \varepsilon\right) = 1.$



This indeed measures how far the values of $Z_n(\omega)$ and $Z(\omega)$ are from each other.

Bayes Risk

$$R_{L,P}(f) = \int_{\mathcal{X}\times\mathcal{Y}} L(x, y, f(x))dP(x, y)$$ The expected loss

Definition: Bayes Risk

$$R^*_{L,P} = \inf_{f:\mathcal{X}\to\mathbb{R}} \int_{\mathcal{X}\times\mathcal{Y}} L(x, y, f(x))dP(x, y)$$

We consider all possible function f here

We don't know P, but we have i.i.d. training data sampled from P!

Goal of Learning:

Build a function f_D (using data D) whose risk $R_{L,P}(f_D)$ will be close to the Bayes risk $R^*_{L,P}$

The learning algorithm constructs this function f_D from the training data.

Consistency of learning methods

Risk is a random variable: $R_{L,P}(f_D) = \mathbb{E}[L(X, Y, f_D(X)|D]$

Definition:

A learning method is **univerally consistent** if **for all** $P(X, Y)$ distributions the risk converges to the Bayes risk when we increase the sample size

$$R_{L,P}(f_D) \xrightarrow{p} R^*_{L,P} \text{ as } n \to \infty.$$

Stone's theorem 1977: Many classification, regression algorithms are universally consistent for certain loss functions under certain conditions: kNN, Parzen kernel regression, SVM,…

Yayyy!!! ☺

Wait! This doesn't tell us anything about the rates…

No Free Lunch!

Devroy 1982: For every consistent learning method and for every fixed convergence rate a_n, $\exists$ P(X,Y) distribution such that the convergence rate of this learning method on P(X,Y) distributed data is slower than a_n

$$R_{L,P}(f_D) \xrightarrow{p} R^*_{L,P} \text{ as } n \to \infty \text{ with slower rate than } a_n$$

What can we do now?

What do we mean on rate?

$$R_{L,P}(f_D) \xrightarrow{p} R^*_{L,P} \text{ as } n \to \infty \text{ with slower rate than } a_n$$

Notation: (**stochastic rate, stochastic little o and big O**)

$$X_n = o_p(a_n) \Leftrightarrow X_n/a_n \xrightarrow{p} 0$$

$$X_n = O_p(a_n) \Leftrightarrow X_n/a_n = O_p(1) \qquad \textbf{(stochastically bounded)}$$

Definition: (**stochastically bounded**)

$X_n = O_p(1) \Leftrightarrow$ For all $\epsilon > 0$ there exisits $M = M(\epsilon) < \infty$ bound such that $\Pr(|X_n| > M) < \epsilon$ for all n

Example: (**CLT**) $\bar{X}_n - \mu = O_p(\frac{1}{n^{1/2}})$, but $\bar{X}_n \neq O_p(\frac{1}{n^{1/2}})$ (unless $\mu = 0$)

Empirical Risk and True Risk

Empirical Risk

For simplicity, let $L(x, y, f(x)) = L(y, f(x))$

Shorthand:

True risk of f (deterministic): $R(f) = R_{L,P}(f) = \mathbb{E}[L(Y, f(X)]$

Bayes risk: $R^* = R^*_{L,P} = \inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$

We dont know P, and hence we don't know $R(f)$ either.

Let us use the empirical counter part:

Empirical risk: $\widehat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i))$

Empirical Risk Minimization

$$R(f) = R_{L,P}(f) = \mathbb{E}[L(Y, f(X)] \qquad R^* = R^*_{L,P} = \inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$$

$$\widehat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i))$$

Law of Large Numbers:

For each fixed f, $\widehat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i)) \xrightarrow{n\to\infty} R(f)$

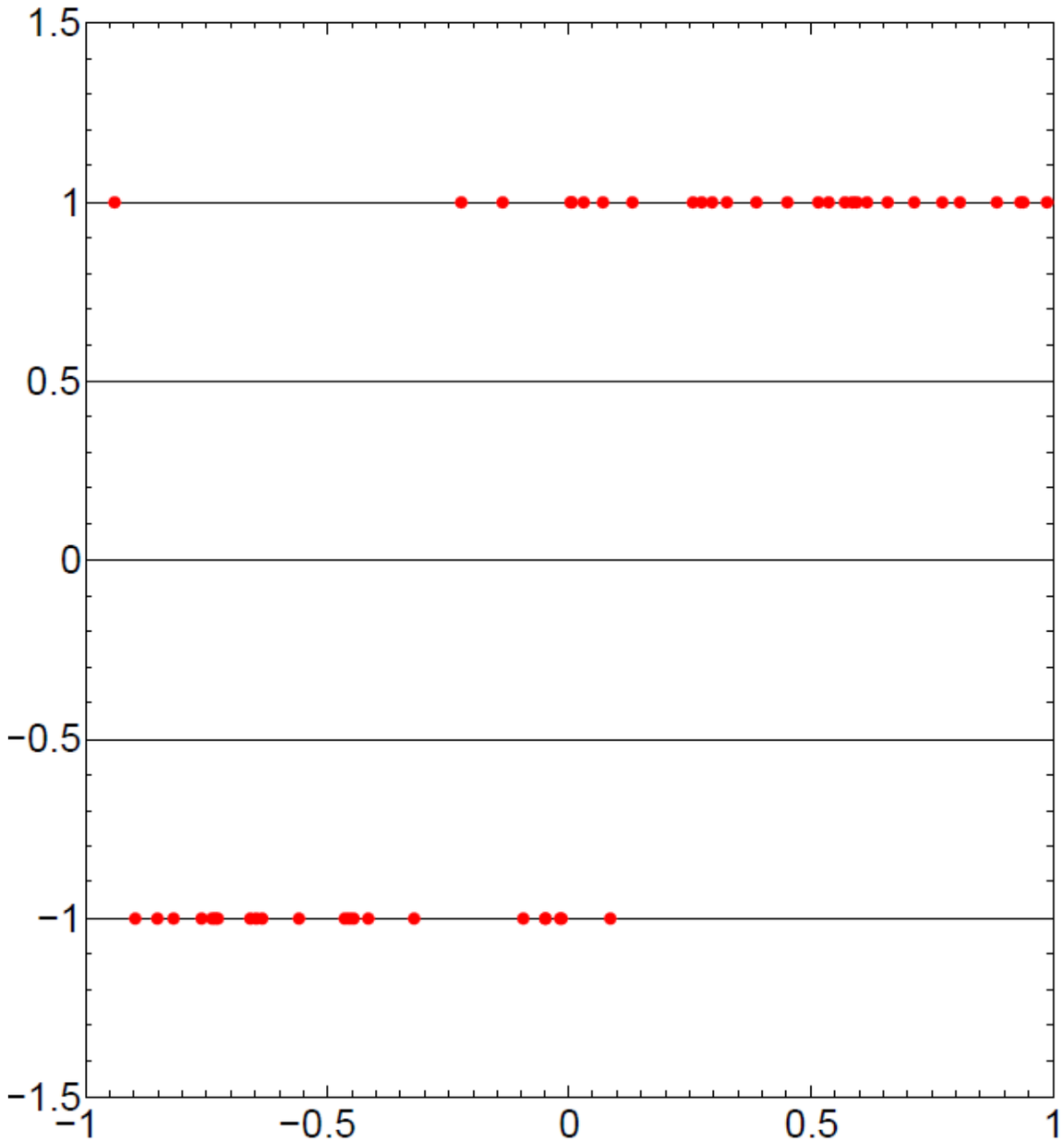
Empirical risk is converging to the Bayes risk

We need $\inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$, so let us calculate $\inf_{f:\mathcal{X}\to\mathbb{R}} \widehat{R}_n(f)$!

$$\inf_{f:\mathcal{X}\to\mathbb{R}} \widehat{R}_n(f) = \inf_{f:\mathcal{X}\to\mathbb{R}} \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i))$$

This is a **terrible idea** to optimize over all possible $f : \mathcal{X} \to \mathbb{R}$ functions! [Extreme overfitting]

Overfitting in Classification with ERM



Picture from David Pal

Generative model:

$$X \sim U[-1, 1]$$

$$\Pr(Y = 1|X > 0) = 0.9$$

$$\Pr(Y = -1|X > 0) = 0.1$$

$$\Pr(Y = 1|X < 0) = 0.1$$

$$\Pr(Y = -1|X < 0) = 0.9$$

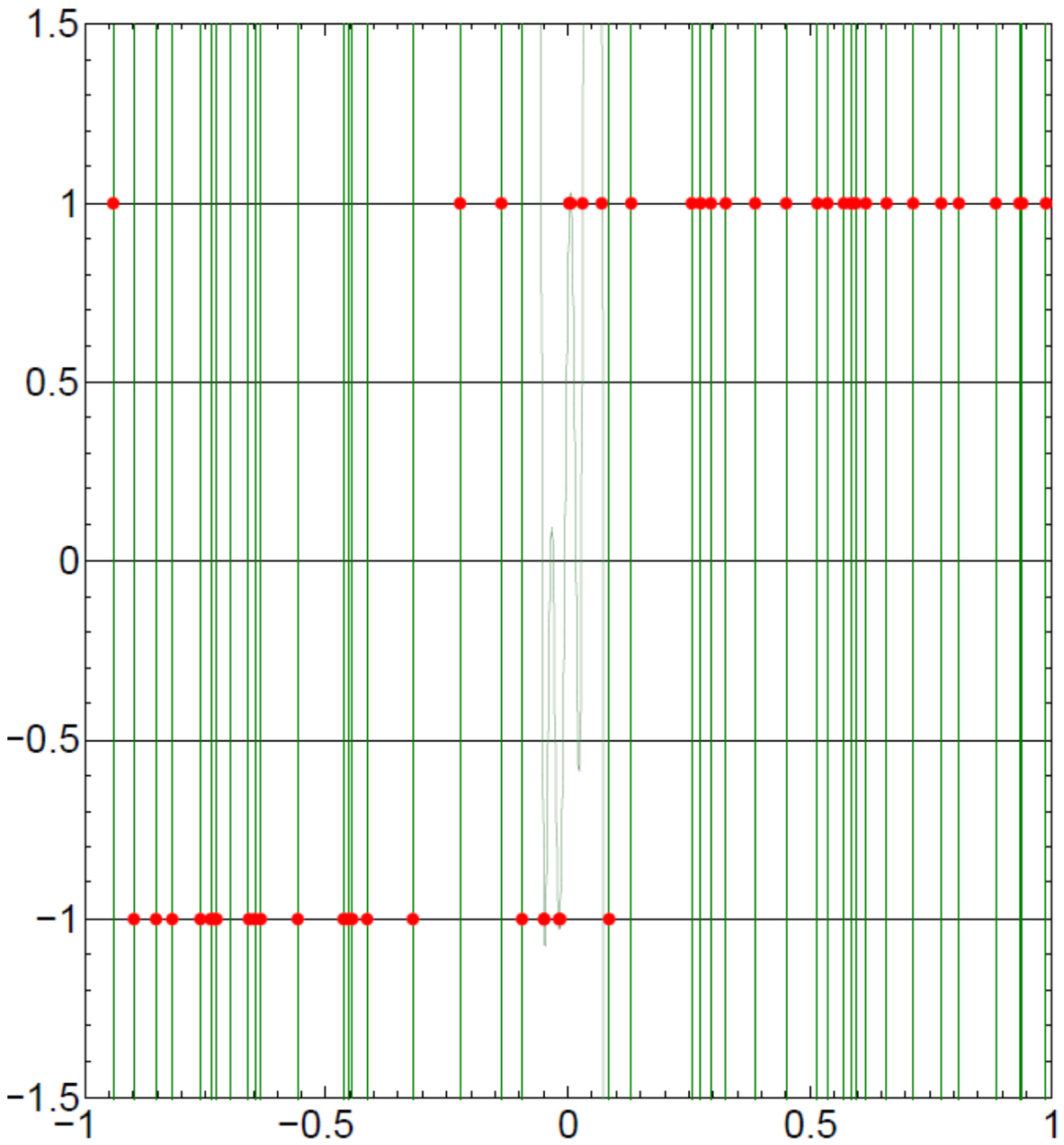
Bayes classifier:

$$f^* = \begin{cases} 1 & \text{if } x > 0 \\ -1 & \text{if } x \leq 0 \end{cases}$$

Bayes risk:

$$R^* = \Pr(Y \neq f^*(X)) = 0.1$$

Overfitting in Classification with ERM



Picture from David Pal

n-order thresholded polynomials

$$\mathcal{F} = \{f(x) = sign(\sum_{i=0}^{n} a_i x^i)\}$$

$$f_n^* = \arg\min_{f \in \mathcal{F}} \widehat{R}_n(f)$$

Empirical risk:

$$\widehat{R}_n(f_n^*) = 0$$

True risk of f_n^*=0.5

$$R(f_n^*) = \Pr(Y \neq f_n^*(X)) = 0.5$$

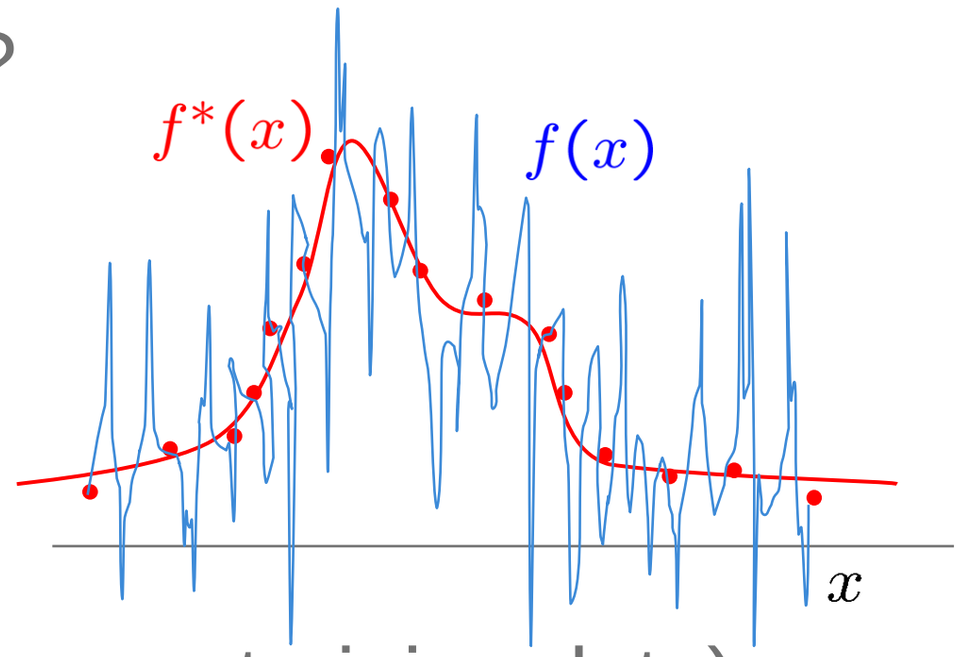
Bayes risk:

$$R^* = \Pr(Y \neq f^*(X)) = 0.1$$

Overfitting in Regression with ERM

Is the following predictor a good one?

$$f(x) = \begin{cases} Y_i, & x = X_i \text{ for } i = 1, \ldots, n \\ \text{any value}, & \text{otherwise} \end{cases}$$



What is its empirical risk? (performance on training data)

zero !

What about true risk?

> zero

Will predict very poorly on new random test point:

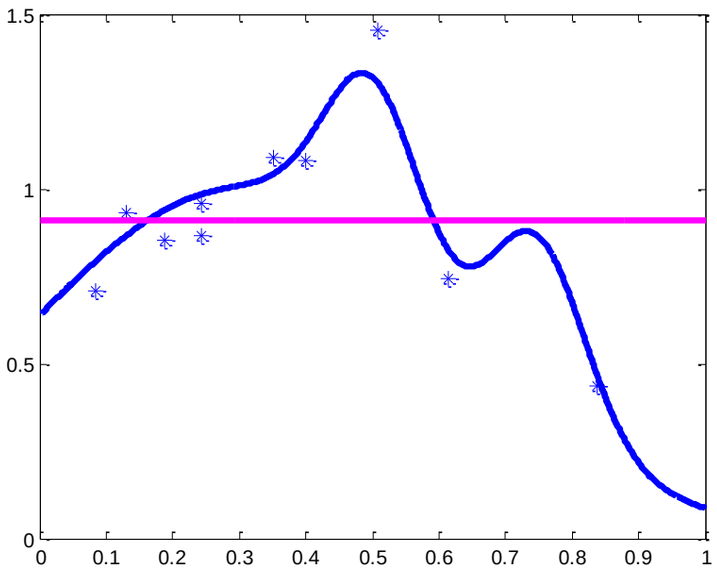
Large generalization error !

Overfitting in Regression

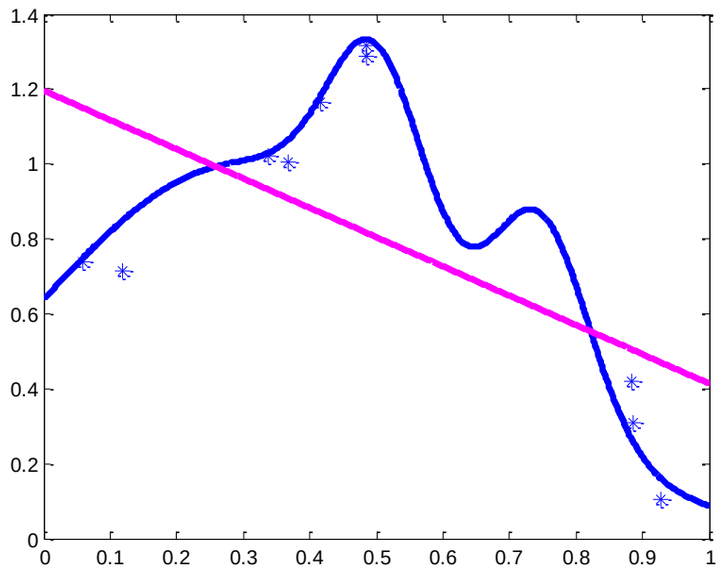
If we allow very complicated predictors, we could overfit the training data.

Examples: Regression (Polynomial of order k-1 – degree k)

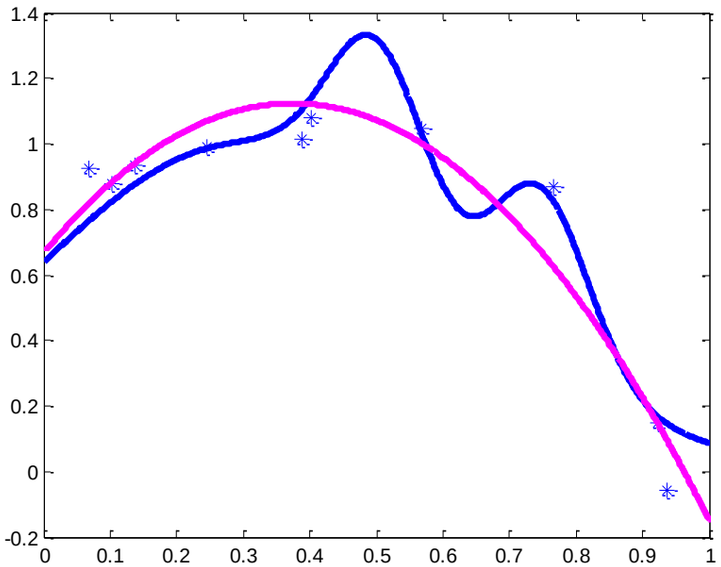
k=1
constant



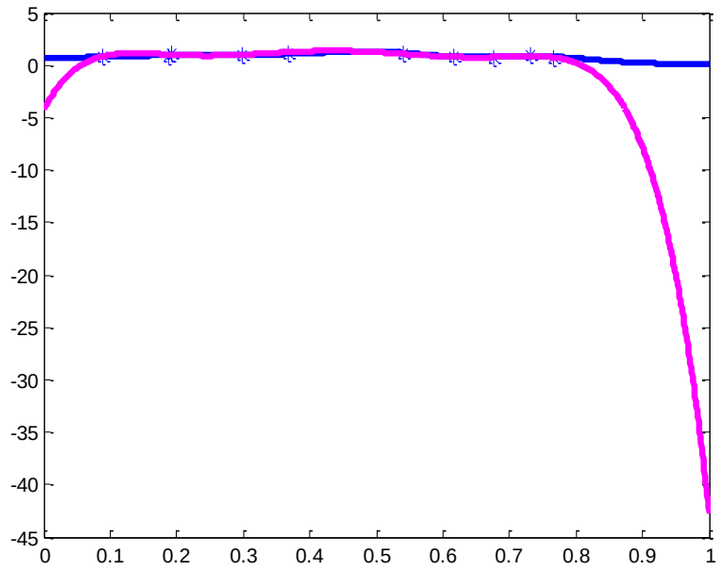
k=2
linear



k=3
quadratic



k=7
6th order



Solutions to Overfitting

Terrible idea to optimize over all possible $f : \mathcal{X} \to \mathbb{R}$ functions!
[Extreme overfitting]

$\Rightarrow$ minimize over a smaller function set $\mathcal{F}$.

Empirical risk minimization over the function set $\mathcal{F}$.

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

Solutions to Overfitting
Structural Risk Minimization

Empirical risk minimization over the function set $\mathcal{F}$.

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

Notation: $R_{\mathcal{F}}^* = \inf_{f \in \mathcal{F}} \mathbb{E}[L(Y, f(X))]$ Risk

$\widehat{R}_{n,\mathcal{F}}^* = \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i))$ Empirical risk

1st issue: $R_{\mathcal{F}}^* - R^* \geq 0$ needs to be small.

(Model error, Approximation error)

Risk in $\mathcal{F}$ - Bayes risk

Solution: **Structural Risk Minimzation (SRM)**

Let $\mathcal{F}_n$ increase with the smaple size n ($\mathcal{F}_{n+1} \supset \mathcal{F}_n$), and let $\mathcal{F}_{n+1}$ contain more complex functions than $\mathcal{F}_n$

Approximation error, Estimation error, PAC framework

Risk of the classifier *f*

Estimation error

Approximation error

$$R(f) - R(f^*) = R(f) - \inf_{f \in \mathcal{F}} R(f) + \inf_{f \in \mathcal{F}} R(f) - R(f^*)$$

R^*

$R^*_{\mathcal{F}}$

Best classifier in $\mathcal{F}$

R^*

Bayes risk

Probably Approximately Correct (PAC) learning framework

Learning algorithm produces $f_n^* = f_{n,\mathcal{F}}^*$ classifier. For each $\varepsilon, \delta >$ 0 we want to find n large enough such that $\Pr(\underbrace{R(f_n^*) - \inf_{f \in \mathcal{F}} R(f)}_{\text{Estimation error}} > \varepsilon) < \delta$

Solution to Overfitting

$$R^*_{\mathcal{F}} = \inf_{f \in \mathcal{F}} R(f) = \inf_{f \in \mathcal{F}} \mathbb{E}[L(Y, f(X))]$$

ERM on $\mathcal{F}$: $\widehat{R}^*_{n,\mathcal{F}} = \inf_{f \in \mathcal{F}} \widehat{R}_n(f) = \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i))$

2nd issue: $\widehat{R}^*_{n,\mathcal{F}} = \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i))$

$\inf_{f \in \mathcal{F}} \widehat{R}_n(f)$ might be a very difficult optimization problem in f

It might be not even convex in f

Solution:

Choose loss function L such that $\widehat{R}_n(f)$ will be convex in f

$$L(y, f(x)) = \begin{cases} 1 & y \neq f(x) \\ 0 & y = f(x) \end{cases} \Rightarrow \text{not convex } \widehat{R}_n(f)$$

Hinge loss $\Rightarrow$ convex $\widehat{R}_n(f)$

Quadratic loss $\Rightarrow$ convex $\widehat{R}_n(f)$

Big Picture

Ultimate goal: $R(f_n^*) - R^* = 0$

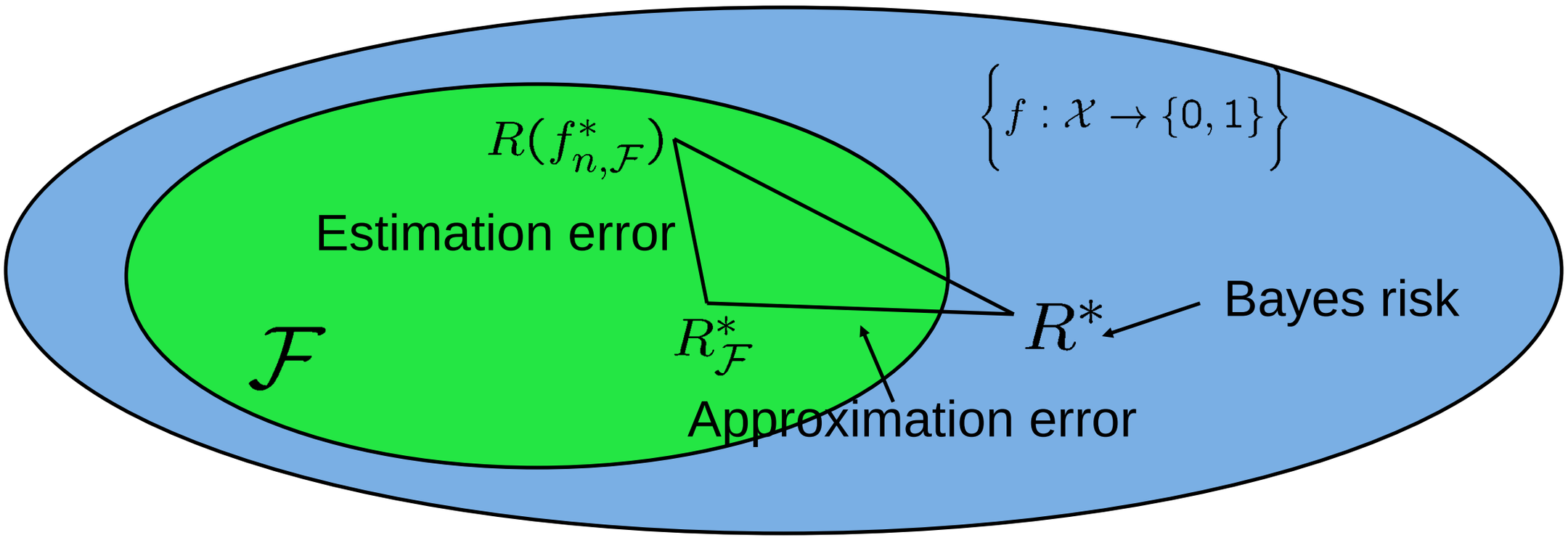
ERM: $f_n^* = f_{n,\mathcal{F}}^* = \arg\min_{f \in \mathcal{F}} \widehat{R}_n(f) = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n L(Y_i, f(X_i))$

Risk of the classifier $f_{n,\mathcal{F}}^*$ — Estimation error — Approximation error

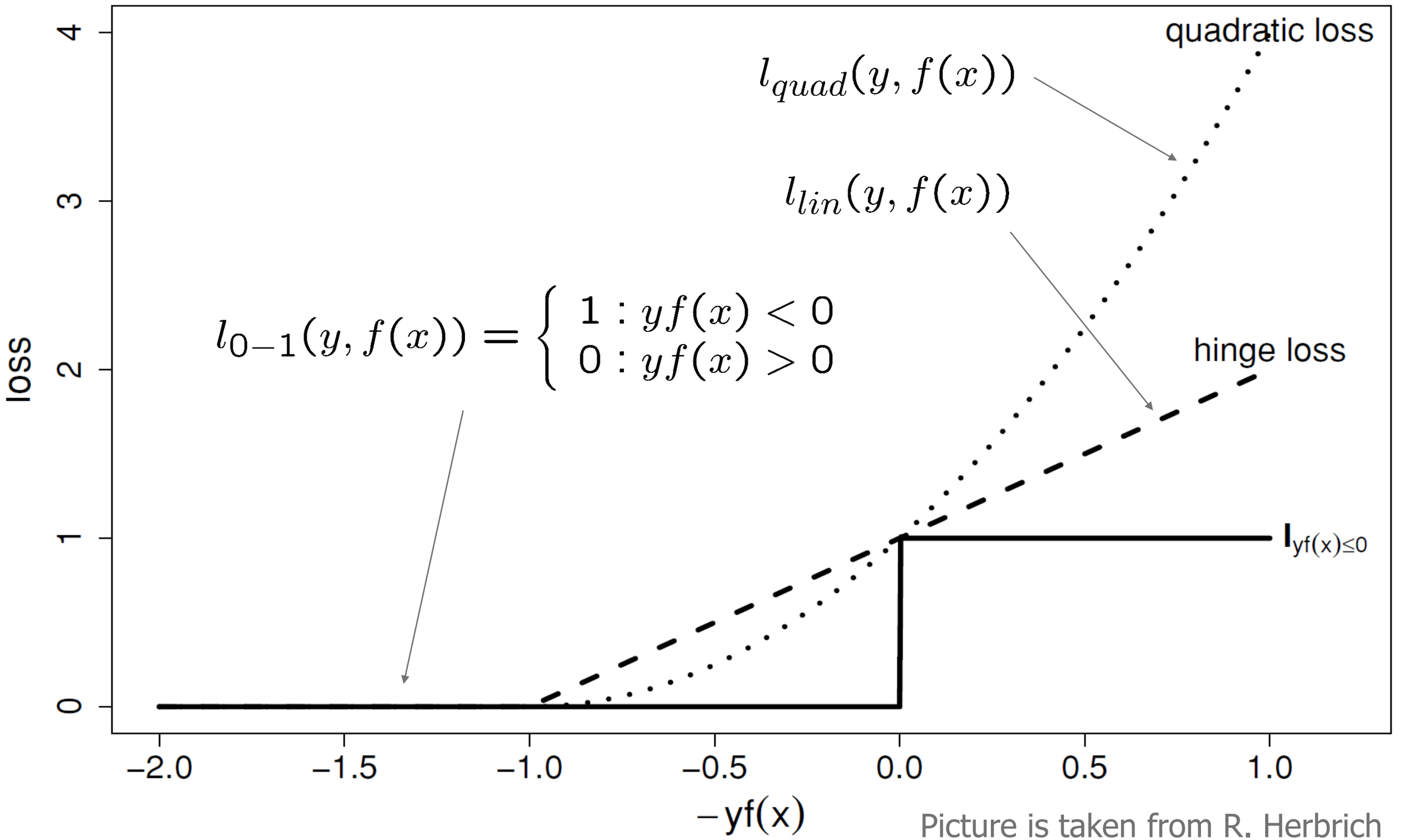
$$R(f_{n,\mathcal{F}}^*) - R^* = \overbrace{R(f_{n,\mathcal{F}}^*) - R_{\mathcal{F}}^*}^{\text{Estimation error}} + \overbrace{R_{\mathcal{F}}^* - R^*}^{\text{Approximation error}}$$

Bayes risk: $R^* = \inf_{g} R(g)$ (all measurable functions)

$R_{\mathcal{F}}^* = \inf_{g \in \mathcal{F}} R(g)$ — Best classifier in $\mathcal{F}$



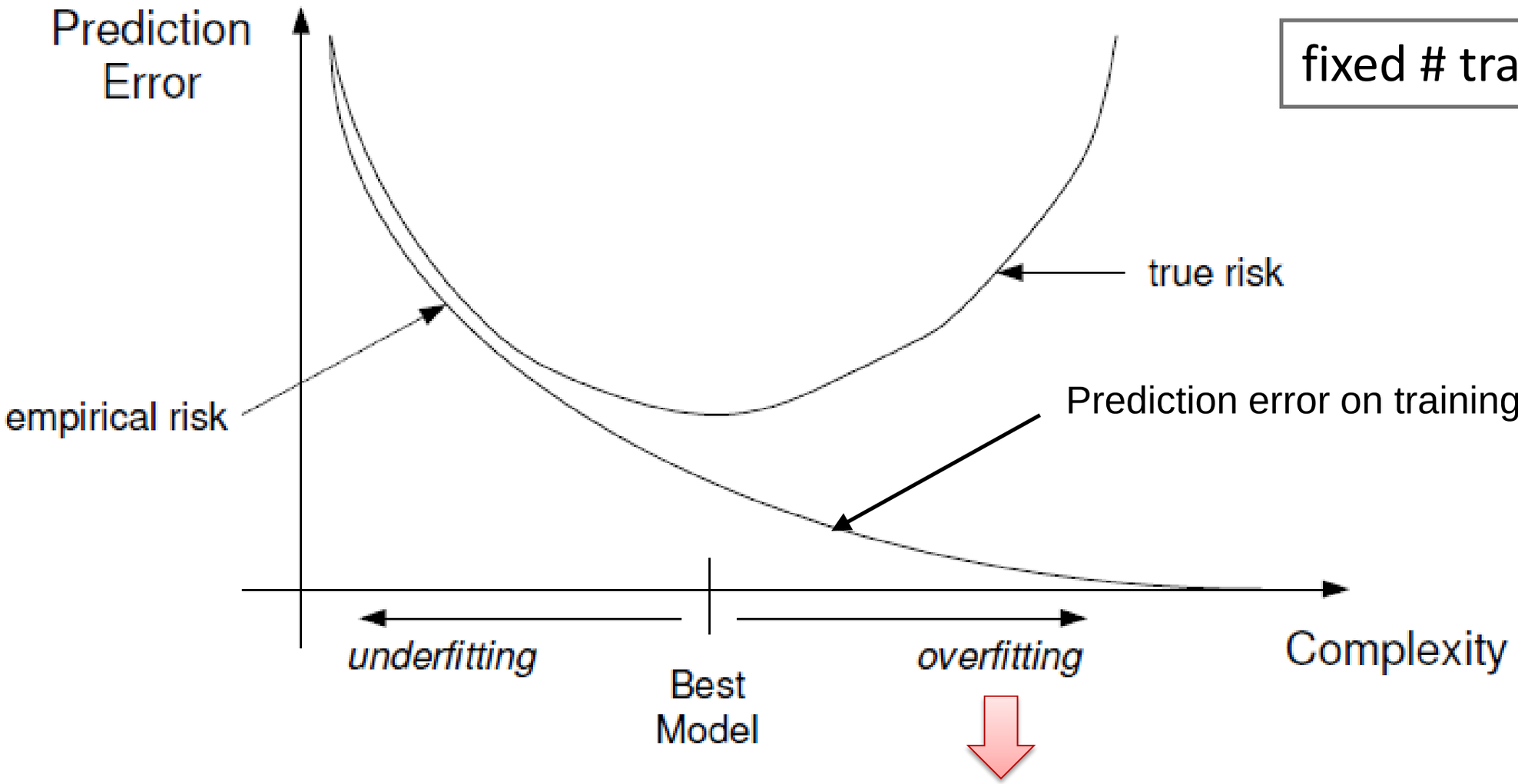
Approximation with the Hinge loss and quadratic loss



Picture is taken from R. Herbrich

Effect of Model Complexity

If we allow very complicated predictors, we could overfit the training data.

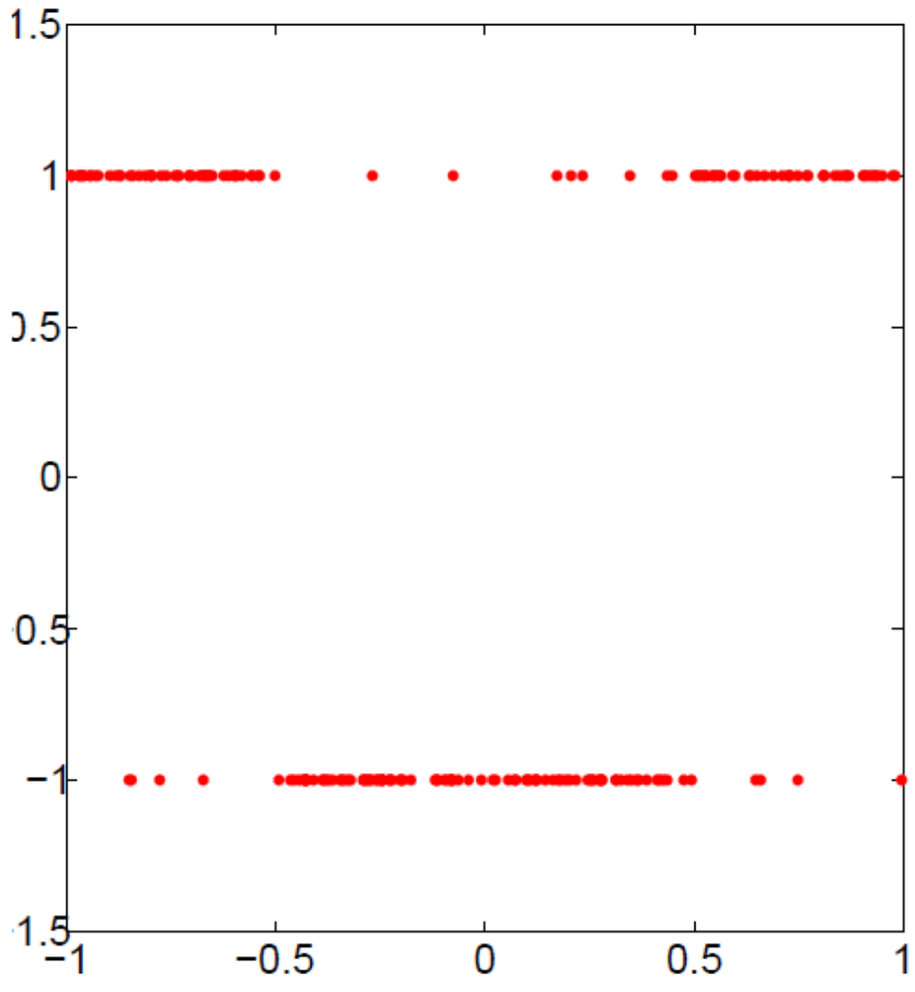


Empirical risk is no longer a good indicator of true risk

Underfitting

Let $\mathcal{F}$ be the class of thresholded polynomials of degree at most one.

$$\mathcal{F} = \{f : f(x) = \text{sign}(ax + b), a, b \in \mathbb{R}\}$$



$$X \sim U[-1, 1]$$

$$\Pr(Y = +1 | X \in (-0.5, 0.5)) = 0.9$$

$$\Pr(Y = -1 | X \in (-0.5, 0.5)) = 0.1$$

$$\Pr(Y = +1 | X \notin (-0.5, 0.5)) = 0.1$$

$$\Pr(Y = -1 | X \notin (-0.5, 0.5)) = 0.9$$

$$f^*(x) = \begin{cases} 1 & \text{if } x \notin (-0.5, 0.5) \\ -1 & \text{if } x \in (-0.5, 0.5) \end{cases}$$

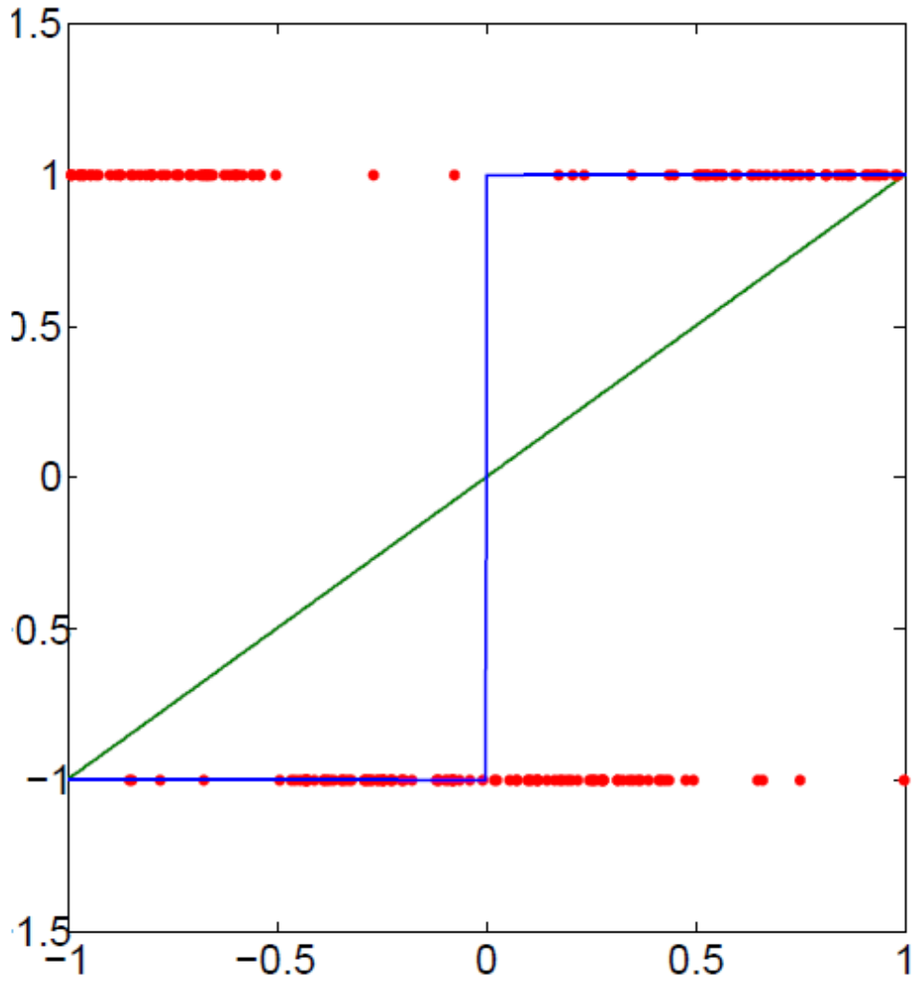
$$R^*_{\mathcal{F}} = \inf_{f \in \mathcal{F}} R(f) = \inf_{f \in \mathcal{F}} \mathbb{E}[L(Y, f(X))]$$

Bayes risk = 0.1

Underfitting

$$\mathcal{F} = \{f : f(x) = \text{sign}(ax + b), a, b \in \mathbb{R}\}$$

Best linear classifier:



$$R^*_{\mathcal{F}} = R(f^*_{\mathcal{F}}) = \inf_{f \in \mathcal{F}} \Pr[Y \neq f(X)]$$

$$= \frac{1}{4} \times 0.9 + \frac{1}{4} \times 0.1 + \frac{1}{4} \times 0.9 + \frac{1}{4} \times 0.1 = 0.5$$

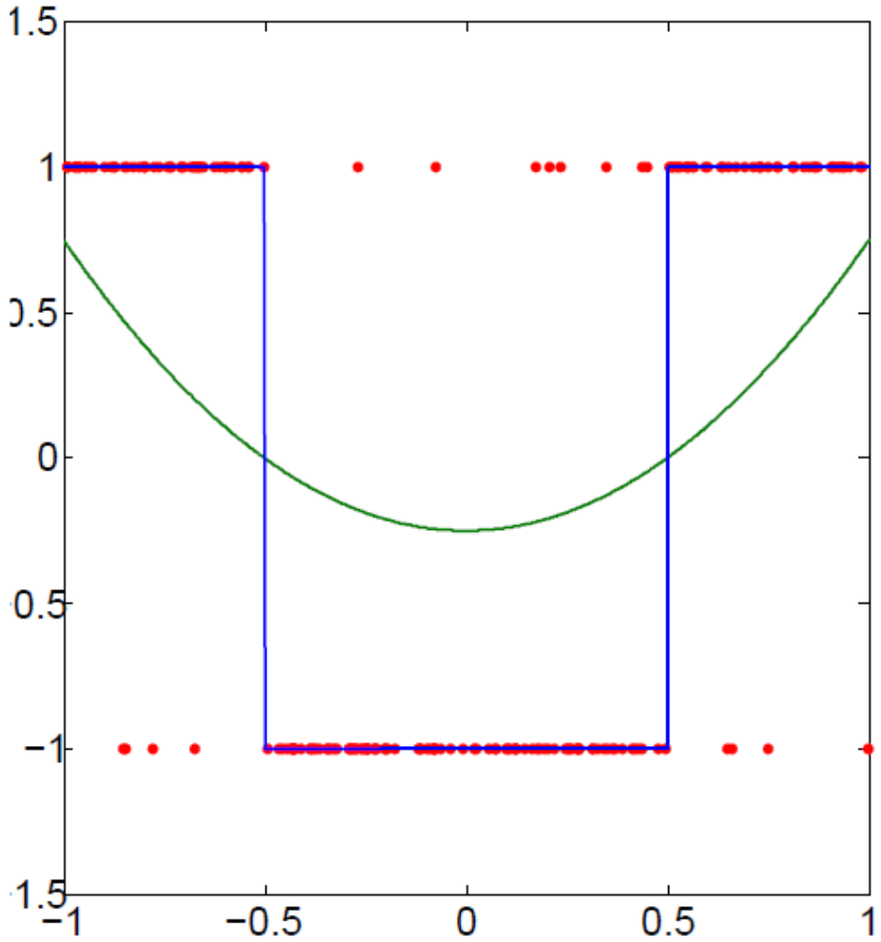
The empirical risk of the best linear classifier:

$$\widehat{R}_n(f^*_{\mathcal{F}}) \approx 0.5$$

Underfitting

$$\mathcal{F} = \{f : f(x) = \text{sign}(ax^2 + bx + c), a, b, c \in \mathbb{R}\}$$

Best quadratic classifier:



$$f^*_{\mathcal{F}} = \text{sign}((x - 0.5)(x + 0.5))$$

$$R^*_{\mathcal{F}} = R(f^*_{\mathcal{F}}) = \inf_{f \in \mathcal{F}} \Pr[Y \neq f(X)]$$
$$= \frac{1}{4} \times 0.1 + \frac{1}{4} \times 0.1 + \frac{1}{4} \times 0.1 + \frac{1}{4} \times 0.1 = 0.1$$

Same as the Bayes risk $\Rightarrow$ good fit!

Classification using the classification loss

The Bayes Classifier

$$L(y, f(x)) = \begin{cases} 1 & y \neq f(x) \\ 0 & y = f(x) \end{cases}$$

$$\begin{aligned} R^* &= \inf_{f:\mathcal{X}\to\mathbb{R}} R(f) \\ &= \inf_{f:\mathcal{X}\to\mathbb{R}} \mathbb{E}[L(Y, f(X))] \\ &= \inf_{f:\mathcal{X}\to\mathbb{R}} \Pr(Y \neq f(X)) \end{aligned} \qquad \begin{aligned} f^* &= \arg \inf_{f:\mathcal{X}\to\mathbb{R}} R(f) \\ &= \arg \inf_{f:\mathcal{X}\to\mathbb{R}} \mathbb{E}[L(Y, f(X))] \\ &= \arg \inf_{f:\mathcal{X}\to\mathbb{R}} \Pr(Y \neq f(X)) \end{aligned}$$

Lemma I: $\Pr(Y \neq f^*(X)) \leq \Pr(Y \neq f(X)) \quad \forall f$

Lemma II: $f^* = \begin{cases} 1 & \text{if } \eta(x) > 1/2 \\ 0 & \eta(x) \leq 1/2 \end{cases}$ $\qquad \eta(x) = \mathbb{E}[Y = 1|x]$

Proofs

Lemma I: Trivial from definition
Lemma II: Surprisingly long calculation

The Bayes Classifier

$R(f) = \Pr[Y \neq f(X)]$	$R^* = R(f^*) = \inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$	$f^* = \arg\inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$
	$R^*_{\mathcal{F}} = R(f^*_{\mathcal{F}}) = \inf_{f\in\mathcal{F}} R(f)$	$f^*_{\mathcal{F}} = \arg\inf_{f\in\mathcal{F}} R(f)$
$\widehat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} 1_{\{Y_i \neq f(X_i\}}$	$\widehat{R}^*_{n,\mathcal{F}} = \inf_{f\in\mathcal{F}} \widehat{R}_n(f)$	$f^*_{n,\mathcal{F}} = \arg\min_{f\in\mathcal{F}} \widehat{R}_n(f)$

This is what the learning algorithm produces

We will need these definitions, please copy it!

$R(f)$ = Risk

R^* = Bayes risk

$\widehat{R}_n(f)$ = Empricial risk

f^* = Bayes classifier

$f^*_n = f^*_{n,\mathcal{F}}$ = the classifier that the learning algorithm produces

The Bayes Classifier

$R(f) = \Pr[Y \neq f(X)]$	$R^* = R(f^*) = \inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$	$f^* = \arg\inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$
	$R^*_{\mathcal{F}} = R(f^*_{\mathcal{F}}) = \inf_{f\in\mathcal{F}} R(f)$	$f^*_{\mathcal{F}} = \arg\inf_{f\in\mathcal{F}} R(f)$
$\widehat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} 1_{\{Y_i \neq f(X_i)\}}$	$\widehat{R}^*_{n,\mathcal{F}} = \inf_{f\in\mathcal{F}} \widehat{R}_n(f)$	$f^*_{n,\mathcal{F}} = \arg\min_{f\in\mathcal{F}} \widehat{R}_n(f)$

This is what the learning algorithm produces

Theorem I: Bound on the Estimation error

The true risk of what the learning algorithm produces

$$|R(f^*_{n,\mathcal{F}}) - R^*_{\mathcal{F}}| \leq 2\sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)|$$

How far $f^*_{n,\mathcal{F}}$ is from the optimal in $\mathcal{F}$

$\sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)|$ can be used to get an upper bound for this

The Bayes Classifier

$R(f) = \Pr[Y \neq f(X)]$	$R^* = R(f^*) = \inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$	$f^* = \arg\inf_{f:\mathcal{X}\to\mathbb{R}} R(f)$
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$\widehat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n} 1_{\{Y_i \neq f(X_i)\}}$	$\widehat{R}^*_{n,\mathcal{F}} = \inf_{f\in\mathcal{F}} \widehat{R}_n(f)$	$f^*_{n,\mathcal{F}} = \arg\min_{f\in\mathcal{F}} \widehat{R}_n(f)$

This is what the learning algorithm produces

Theorem II:

$$|\widehat{R}_n(f^*_{n,\mathcal{F}}) - R(f^*_{n,\mathcal{F}})| \leq \sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)|$$

How far the empirical risk of $f^*_{n,\mathcal{F}}$ is from its true risk.

$\sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)|$ can be used to get an upper bound for this

Proofs

Theorem I: Not so long calculations.
Theorem II: Trivial

Corollary:

$$|\widehat{R}_n(f^*_{n,\mathcal{F}}) - R^*_{\mathcal{F}}| \leq 3 \sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)|$$

$\widehat{R}_n(f^*_{n,\mathcal{F}})$: Empirical risk of the learned classifier $f^*_{n,\mathcal{F}}$ (known)

$R^*_{\mathcal{F}}$: True risk of the best possible classifer in $\mathcal{F}$ (unknown)

Main message:

It's enough to derive upper bounds for

$$\sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)|$$

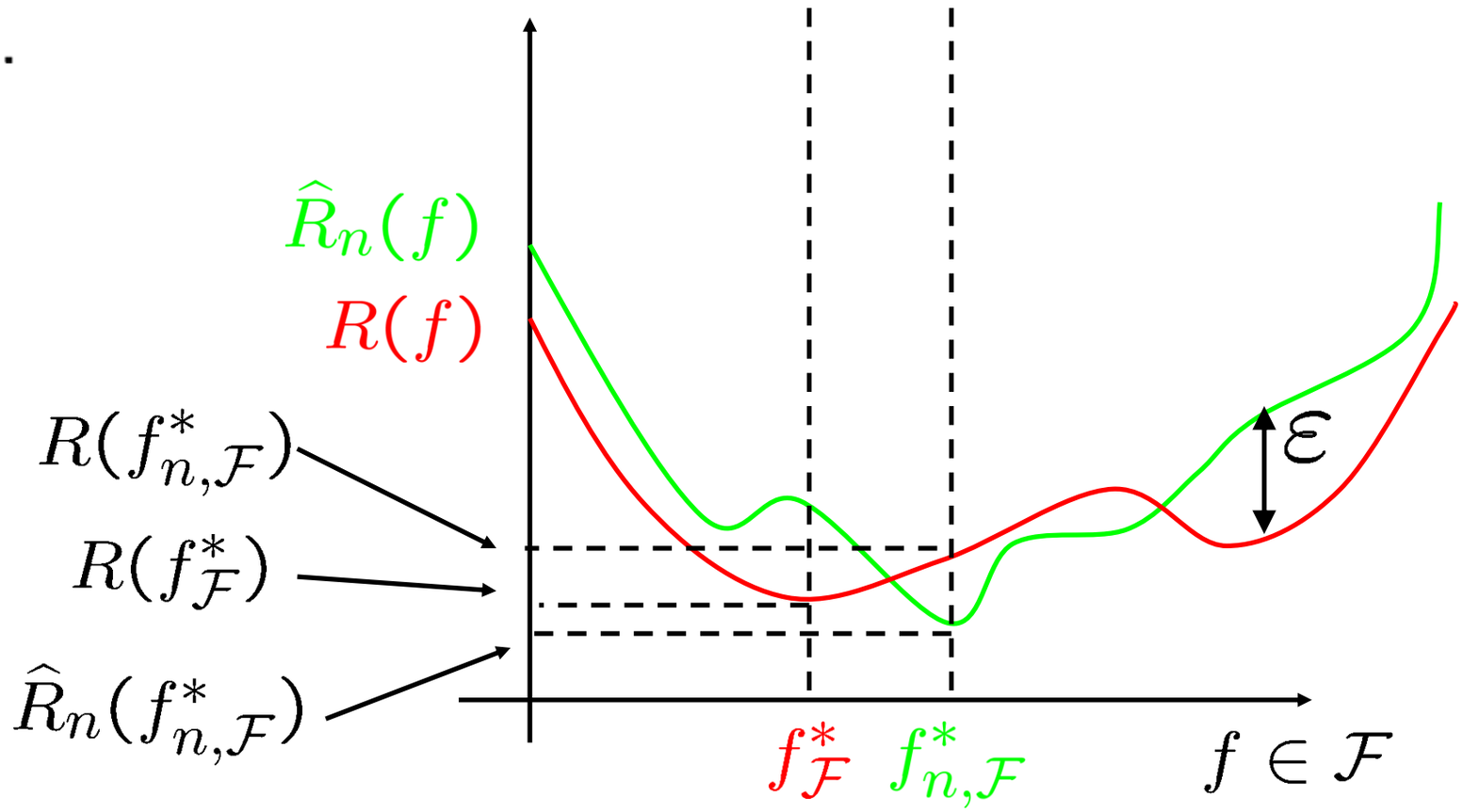
Illustration of the Risks

$$|\widehat{R}_n(f^*_{n,\mathcal{F}}) - R(f^*_{n,\mathcal{F}})| \leq \sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)| = \varepsilon$$

$$|R(f^*_{n,\mathcal{F}}) - R(f^*_{\mathcal{F}})| \leq 2 \sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)| = 2\varepsilon$$

$$|\widehat{R}_n(f^*_{n,\mathcal{F}}) - R(f^*_{\mathcal{F}})| \leq 3 \sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)| = 3\varepsilon$$

$\sup_{f\in\mathcal{F}} |R_n(f) - R(f)|$ can be used to get an upper bound for these.



It’s enough to derive upper bounds for

$$\sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)|$$

It is a random variable that we need to bound!
We will bound it with tail bounds!

Hoeffding's inequality (1963)

$$\left.\begin{array}{r} Z_1, ..., Z_n \text{ independent} \\ Z_i \in [a_i, b_i] \\ \varepsilon > 0 \end{array}\right\} \Rightarrow$$

$$\Rightarrow \Pr(|\frac{1}{n}\sum_{i=1}^{n}(Z_i - \mathbb{E}[Z_i])| > \varepsilon) \leq 2\exp\left(\frac{-2n\varepsilon^2}{\frac{1}{n}\sum_{i=1}^{n}(b_i - a_i)^2}\right)$$

Special case

$$Z_i \text{ is Bernoulli}(p) \Rightarrow \sum_{i=1}^{n} Z_i \text{ is Binomial}(n, p)$$

$$\Rightarrow \Pr(|\sum_{i=1}^{n}\frac{1}{n}(Z_i - \mathbb{E}[Z_i])| > \varepsilon) \leq 2\exp\left(\frac{-2n\varepsilon^2}{\frac{1}{n}\sum_{i=1}^{n}(1-0)^2}\right) = 2\exp\left(-2n\varepsilon^2\right)$$

Binomial distributions

Our goal is to bound $\sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)|$

$$\widehat{R}_n(f) = \frac{1}{n} \sum_{i=1}^{n} 1_{\{Y_i \neq f(X_i)\}} \Rightarrow n\widehat{R}_n(f) = \sum_{i=1}^{n} 1_{\{Y_i \neq f(X_i)\}} \sim Binom(n, p)$$

where $p = \mathbb{E}[1_{\{Y \neq f(X)\}}] = \Pr(Y \neq f(X)) = R(f)$

Bernoulli(p)

Let $Z_i = 1_{\{Y_i \neq f(X_i)\}} \sim \text{Bernoulli}(p)$

$$\Rightarrow |\widehat{R}_n(f) - R(f)| = |\frac{1}{n} \sum_{i=1}^{n} 1_{\{Y_i \neq f(X_i)\}} - p| = |\frac{1}{n} \sum_{i=1}^{n} Z_i - \mathbb{E}[Z_i]|$$

Therefore, from Hoeffding we have:

$$\Pr(|\widehat{R}_n(f) - R(f)| > \varepsilon) \leq 2 \exp\left(-2n\varepsilon^2\right)$$

Yuppie!!!

Inversion

From Hoeffding we have:

$$\Pr(|\widehat{R}_n(f) - R(f)| \geq \varepsilon) \leq 2\exp\left(-2n\varepsilon^2\right)$$

Let $2\exp\left(-2n\varepsilon^2\right) \leq \delta$

$$-2n\varepsilon^2 \leq \log(\delta/2)$$

$$\varepsilon^2 \geq \frac{\log(2/\delta)}{2n}$$

Therefore,

$$\Pr\left(|\widehat{R}_n(f) - R(f)| \geq \sqrt{\frac{\log(2/\delta)}{2n}}\right) \leq \delta$$

$$\Pr\left(|\widehat{R}_n(f) - R(f)| < \sqrt{\frac{\log(2/\delta)}{2n}}\right) \geq 1 - \delta$$

Usually $\delta = 0.05$ (5%), and $1 - \delta = 0.95$ (95%)

Union Bound

Our goal is to bound: $\sup_{f \in \mathcal{F}} |\hat{R}_n(f) - R(f)|$

We already know: $\Pr(|\hat{R}_n(f) - R(f)| > \varepsilon) \leq 2 \exp\left(-2n\varepsilon^2\right)$

Theorem: [tail bound on the 'deviation' in the worst case]

Let $\mathcal{F} = \{f : \mathcal{X} \to \{0, 1\}\}$, and $|\mathcal{F}| \leq N$

$$\Rightarrow \Pr\left(\sup_{f \in \mathcal{F}} |\hat{R}_n(f) - R(f)| > \varepsilon\right) \leq 2N \exp\left(-2n\varepsilon^2\right)$$

Worst case error

This is not the worst classifier in terms of classification accuracy!

Worst case means that the empirical risk of classifier *f* is the furthest from its true risk!

Proof: $\Pr(A \cup B) \leq \Pr(A) + \Pr(B)$

$$\Pr\left(\sup_{f \in \mathcal{F}} |\hat{R}_n(f) - R(f)| > \varepsilon\right) = \Pr\left(\bigcup_{f \in \mathcal{F}} \left\{|\hat{R}_n(f) - R(f)| > \varepsilon\right\}\right)$$

$$\Pr\left(\bigcup_{f \in \mathcal{F}} \left\{|\hat{R}_n(f) - R(f)| > \varepsilon\right\}\right) \leq \sum_{f \in \mathcal{F}} \Pr\left(|\hat{R}_n(f) - R(f)| > \varepsilon\right)$$

Inversion of Union Bound

We already know: Let $\mathcal{F} = \{f : \mathcal{X} \to \{0,1\}\}$, and $|\mathcal{F}| \leq N$

$$\Rightarrow \Pr\left(\sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)| > \varepsilon\right) \leq 2N \exp\left(-2n\varepsilon^2\right)$$

Let $2N \exp\left(-2n\varepsilon^2\right) \leq \delta \Rightarrow -2n\varepsilon^2 \leq \log(\delta/(2N)) \Rightarrow \varepsilon^2 \geq \frac{\log(2N/\delta)}{2n}$

Therefore,

$$\Pr\left(\sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)| \geq \sqrt{\frac{\log(N) + \log(2/\delta)}{2n}}\right) \leq \delta$$

$$\Pr\left(\sup_{f\in\mathcal{F}} |\widehat{R}_n(f) - R(f)| < \sqrt{\frac{\log(N) + \log(2/\delta)}{2n}}\right) \geq 1 - \delta$$

Inversion of Union Bound

$$\Pr\left(\sup_{f\in\mathcal{F}}|\widehat{R}_n(f)-R(f)|\geq\sqrt{\frac{\log(N)+\log(2/\delta)}{2n}}\right)\leq\delta$$

$$\Pr\left(\sup_{f\in\mathcal{F}}|\widehat{R}_n(f)-R(f)|<\sqrt{\frac{\log(N)+\log(2/\delta)}{2n}}\right)\geq 1-\delta$$

- The larger the *N*, the looser the bound
- This result is distribution free: True for all P(X,Y) distributions
- It is useless if N is big, or infinite… (e.g. all possible hyperplanes)

We will see later how to fix that. (Hint: McDiarmid, VC dimension…)

The Expected Error

Our goal is to bound: $\sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)|$

We already know: $\Pr\left(\sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)| > \varepsilon\right) \leq 2N \exp\left(-2n\varepsilon^2\right)$

(Tail bound, Concentration inequality)

Theorem: [Expected 'deviation' in the worst case]

Let $\mathcal{F} = \{f : \mathcal{X} \to \{0,1\}\}$, and $|\mathcal{F}| \leq N$

$$\Rightarrow \mathbb{E}\left[\sup_{f \in \mathcal{F}} |\widehat{R}_n(f) - R(f)|\right] \leq \sqrt{\frac{\log(2N)}{2n}}$$

Worst case deviation

This is not the worst classifier in terms of classification accuracy!
Worst case means that the empirical risk of classifier *f* is the furthest from its true risk!

Proof: we already know a tail bound. If $Y \geq 0$, then $\mathbb{E}[Y] = \int_0^\infty \Pr(Y \geq z) dz$

(From that actually we get a bit weaker inequality… oh well)

Thanks for your attention ☺