

Lecture 3: Bayesian Decision Theory

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Outline

- 1 Bibliography
- 2 Bayesian decision theory
- 3 Bayes classifier
- 4 Cost-sensitive
- 5 Margin-based
- 6 Multi-class
- 7 Regression
- 8 Summary

Main references

- Duda, Hart & Stork (DHS) - Chapter 2
- Bishop - Chapter 1.5










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Bayesian decision theory

Bayesian decision theory addresses the problem of making *optimal decisions under uncertainty*.

- **A decision rule** prescribes what decision to make based on observed input (e.g., grant the credit).
- **Uncertainty**: Usually Y is not a deterministic function of X but instead we assume a probability distribution $P(y|x)$ that determines the probability of observing class y for the given features x .

		x (features)			y (label)
		Income	Credit card	Previous loans	Repaid?
Applicant 1		1.5k		✓	
Applicant 2		2.7k		✗	
Applicant 3		2.2k		✓	

Notation

Let's assume $\mathcal{Y} = \{-1, 1\}$ and $p(x, y)$ denotes the **joint density** of the probability measure P on $\mathcal{X} \times \mathcal{Y}$, which satisfies that:

$$p(y|x) = \frac{p(x|y) \times p(y)}{p(x)},$$

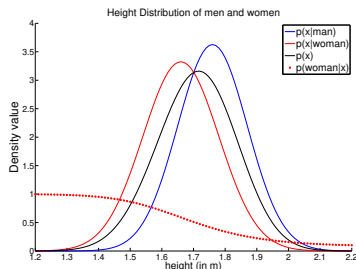
where

- $P(y|x)$ denotes the **posterior probability** and corresponds to the probability that we observe y after observing x .
- $p(x|y)$ denotes the **class-conditional density (or likelihood)** and models the occurrence of the features x of class y .
- $P(y)$ denotes the **prior probability** of a class y and reflects our knowledge of how likely we expect a certain class before we can actually observe any data.
- $P(x)$ denotes the **marginal distribution (or evidence)** of the features x and models the cumulated occurrence of features over all classes $y \in \mathcal{Y}$.

Example I

Goal: Predict sex of a person (i.e., $Y = \{\text{male}, \text{female}\}$) using height as feature (i.e., $\mathcal{X} = \mathbb{R}$). How do we find the optimal **classification rule**?

- Based on prior knowledge, i.e., classify x as female if $P(\text{female}) \geq P(\text{male})$.
- Based on class conditional density, i.e., classify x as female if $p(x|\text{female}) \geq p(x|\text{male})$.
- Based on posterior probability, i.e., classify x as female if $P(\text{female}|x) \geq P(\text{male}|x)$.



Example II

Goal: Predict sex of a person (i.e., $Y = \{\text{male}, \text{female}\}$) using height as feature (i.e., $\mathcal{X} = \mathbb{R}$). How do we find the optimal **classification rule**?

- Based on prior knowledge, i.e., classify x as female if $P(\text{female}) \geq P(\text{male})$.
 - Always decides same class for all x . $P(\text{error}|x) = P(\text{error}) = \min[Pr(\text{male}), P(\text{female})]$.
- Based on class conditional density, i.e., classify x as female if $P(x|\text{female}) \geq P(x|\text{male})$.
 - For an observed feature vector x , $P(\text{error}|x) = \min[Pr(x|\text{male}), P(x|\text{female})]$.
- Based on posterior probability, i.e., classify x as female if $P(\text{female}|x) \geq P(\text{male}|x)$.
 - For an observed feature vector x , $P(\text{error}|x) = \min[Pr(\text{male}|x), P(\text{female}|x)]$.

Goal: Predict type of fish (i.e., $Y = \{\omega_1, \omega_2\}$) using a set of features (i.e., $\mathcal{X} = \mathbb{R}^d$) such as length, width, lightness, etc.

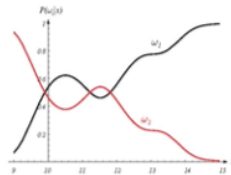

$$P(\omega_i/x)$$


FIGURE 2.2. Posterior probabilities for the particular priors $P(a_1) = 2/3$ and $P(a_2) = 1/3$ for the class-conditional probability densities shown in Fig. 2.1. Thus in this case, given that a pattern is measured to have feature value $x = 14$, the probability it is in category a_2 is roughly 0.08, and that it is in a_1 is 0.92. At every x , the posteriors sum to 1.0. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

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Bayes Decision Rule

The **Bayes (optimal) decision rule** given by:

$$y^* = \arg \max_i P(\omega_i|x),$$

is optimal, i.e., it minimizes $P(error|x)$ for all x and thus $P(error)$, which are given (in binary cases) by:

$$P(error|x) = \min[Pr(\omega_1|x), P(\omega_2|x).]$$

and

$$P(error) = \int P(error|x)p(x)dx$$

It minimizes $P(error|x)$ for all x and thus also $P(error)$. Why?

Loss function and risk

Quantitative measure of error:

Definition (Loss function)

A **loss function** L is a mapping $L : \mathcal{Y} \times \mathcal{Y} \rightarrow [0, \infty)$.

Examples:

Classification: 0-1-loss, $L(\hat{y}(x), y) = \mathbb{1}_{\hat{y}(x) \neq y}$

Regression: squared loss, $L(\hat{y}(x), y) = (y - \hat{y}(x))^2$

Loss function and risk

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Definition (Risk)

The **risk** or **expected loss** of a learning rule $f : \mathcal{X} \rightarrow \mathcal{Y}$ is defined as

$$R_L(\hat{y}) = \mathbb{E}[L(\hat{y}(X), Y)] = \mathbb{E}[\mathbb{E}[L(\hat{y}(X), Y)|X]].$$

Note: $\mathbb{E}[\mathbb{E}[L(\hat{y}(X), Y)|X]] = \int_{\mathbb{R}^d} \left[\int_{\mathbb{R}} L(\hat{y}(x), y) p(y|x) dy \right] p(x) dx.$

Bayes optimal risk

Definition

The **Bayes optimal risk** is given by

$$R_L^* = \inf_{\hat{y}} \{R(\hat{y}) \mid \hat{y} \text{ measurable}\}.$$

A function \hat{y}_L^* which minimizes the above functional is called **Bayes optimal learning rule** (with respect to the loss L).

Note: since we minimize over all measurable \hat{y} , the minimizer of $\mathbb{E}[L(\hat{y}(X), Y)]$ can be found by **pointwise minimization** of

$$\mathbb{E}[L(\hat{y}(X), Y) | X = x]$$

Classification: $\mathbb{E}[L(\hat{y}(X), Y) | X = x] = \sum_{y \in \mathcal{Y}} L(\hat{y}(x), y) P(Y = y | X = x).$

Regression: $\mathbb{E}[L(\hat{y}(X), Y) | X = x] = \int_{\mathcal{Y}} L(\hat{y}(x), y) p(y | X = x) dy.$

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Bayes classifier

Binary Classification: $\mathcal{Y} = \{-1, 1\}$.

0-1-loss: $L(\hat{y}(x), y) = \mathbb{1}_{\hat{y}(x)y \leq 0}$ is the canonical loss for classification.

Risk is the **probability of error**:

$$R(\hat{y}) = \mathbb{E}[\mathbb{1}_{\hat{y}(X)Y \leq 0}] = P(\hat{y}(X)Y \leq 0) = P(\hat{y}(X) \neq Y) = P(\text{error}).$$

Bayes classifier

Binary Classification: $\mathcal{Y} = \{-1, 1\}$.

0-1-loss: $L(\hat{y}(x), y) = \mathbb{1}_{\hat{y}(x)y \leq 0}$ is the canonical loss for classification.

Risk is the **probability of error**:

$$R(\hat{y}) = \mathbb{E}[\mathbb{1}_{\hat{y}(X)Y \leq 0}] = P(\hat{y}(X)Y \leq 0) = P(\hat{y}(X) \neq Y) = P(\text{error}).$$

Minimizaton of the risk: The risk (and thus probability of error) is minimized by the Bayesian decision rule since the risk decomposes as:

$$\begin{aligned} R(f) &= \mathbb{E}[\mathbb{1}_{\hat{y}(X)Y \leq 0}] = \mathbb{E}_X[\mathbb{E}_{Y|X}[\mathbb{1}_{\hat{y}(X)Y \leq 0}|X]] \\ &= \mathbb{E}_X[\mathbb{1}_{\hat{y}(X)=-1}P(Y = 1|X) + \mathbb{1}_{\hat{y}(X)=1}P(Y = -1|X)]. \end{aligned}$$

The minimizing function $\hat{y}^* : \mathcal{X} \rightarrow \{-1, 1\}$ is called the **Bayes classifier**

$$\hat{y}^*(x) = \begin{cases} +1 & \text{if } P(Y = 1|X = x) > P(Y = -1|X = x) \\ -1 & \text{else} \end{cases}$$

Regression function

Definition

The **regression function** $\eta(x)$ is defined as

$$\eta(x) = \mathbb{E}[Y|X = x].$$

Binary classification $\mathcal{Y} = \{-1, 1\}$,

$$\begin{aligned}\eta(x) &= \mathbb{E}[Y|X = x] = P(Y = 1|X = x) - P(Y = -1|X = x) \\ &= 2P(Y = 1|X = x) - 1.\end{aligned}$$

Bayes classifier as a margin-based classifier:

$$\hat{y}^*(x) = \text{sign } \eta(x).$$

Bayes error

The **Bayes error** (risk of the Bayes classifier):

$$\begin{aligned} R^* &= \mathbb{E}_X [\min\{P(Y = 1|X), P(Y = -1|X)\}] \\ &= \int_{\mathbb{R}^d} \min\{p(x|Y = 1)P(Y = 1), p(x|Y = -1)P(Y = -1)\} dx. \\ &\implies 0 \leq R^* \leq \frac{1}{2} \end{aligned}$$

Bayes error

The **Bayes error** (risk of the Bayes classifier):

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Proposition

The Bayes risk R^ satisfies,*

$$R^* \leq \min\{P(Y = 1), P(Y = -1)\}.$$

To do: Proof.

Additional results: Error bounds for Normal features (Chapter 2.8 [DHS]).

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Cost-sensitive classification

Problem: Cost of errors is not always equal.

Example: Cancer detection from x-ray images
(cancer $Y = 1$, no cancer $Y = -1$)
cost of not detecting cancer (false negatives) is much higher
than wrongly assigning a healthy person to be ill
(false positives).

	positive Prediction	negative Prediction
positive cases	true positives	false negatives
negative cases	false positives	true negatives

Cost matrix and Risk

Cost matrix:

$$C_{ij} = C(Y = i, \hat{y}_c(X) = j).$$

	positive Prediction	negative Prediction
positive cases	0	$C(Y = 1, \hat{y}_c(X) = -1)$
negative cases	$C(Y = -1, \hat{y}_c(X) = 1)$	0

Cost sensitive 0-1-loss:

$$\begin{aligned}
 R^C(f) &= \mathbb{E}[C(Y, \hat{y}_c(X)) \mathbb{1}_{\hat{y}_c(X) \neq Y}] \\
 &= \mathbb{E}_X[C_{1,-1} \mathbb{1}_{\hat{y}_c(X)=-1} P(Y = 1|X) + C_{-1,1} \mathbb{1}_{\hat{y}_c(X)=1} P(Y = -1|X)].
 \end{aligned}$$

Classification rule

Cost sensitive Bayes classifier:

$$\hat{y}_c^*(x) = \begin{cases} +1 & \text{if } C_{1,-1} P(Y = 1|X = x) > C_{-1,1} P(Y = -1|X = x) \\ -1 & \text{else} \end{cases}$$

A new threshold for the regression function:

$$\hat{y}_c(x) = \text{sign} \left[\eta(x) - \frac{C_{-1,1} - C_{1,-1}}{C_{-1,1} + C_{1,-1}} \right],$$

where $\eta(x) = \mathbb{E}[Y|X = x] = 2P(Y = 1|X = x) - 1$.

Observation : If $C_{-1,1} = C_{1,-1}$ (same costs for both classes), then we recover the standard Bayes classifier.

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Margin-based classification

In practice we only have access to *training data* $(X_i, Y_i)_{i=1}^n$ sampled from the (unknown) probability measure P on $\mathcal{X} \times \mathcal{Y}$ (Lecture 4).

Classification Problem: We aim to learn a mapping function (classifier) of the form $\hat{y} : \mathcal{X} \rightarrow \{-1, 1\}$ that minimizes the 0-1-loss (and thus the probability of error). Unfortunately, finding a function that minimizes the 0-1-loss leads often to a hard optimization problem. Instead, we can minimize an alternative loss function which is easier to optimize.

Margin-based classification: Provides an “easier” approach to solve a classification problem as a regression problem by finding the function $f : \mathcal{X} \rightarrow \mathbb{R}$ that minimizes a surrogate convex loss, i.e., by :

- Using a **surrogate convex** loss function which upper bounds the 0-1-loss.
- Defining the classifier $\hat{y} : \mathcal{X} \rightarrow \{-1, 1\}$ as

$$\hat{y}(x) = \text{sign } f(x).$$

Loss function I

Definition (Convex margin-based loss function)

A function $L : \mathbb{R} \rightarrow \mathbb{R}_+$ is a **convex margin-based loss function** if

- $L(y, f(x)) = L(y f(x))$, where function (of the product) $y f(x) \in \mathbb{R}$ is called the **functional margin**,
- L is convex,
- L upper bounds the 0-1-loss.

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- L is convex,
- L upper bounds the 0-1-loss.

Examples:

hinge loss (soft margin loss)

$$L(y f(x)) = \max(0, 1 - y f(x))$$

truncated squared loss

$$L(y f(x)) = \max(0, 1 - y f(x))^2$$

exponential loss

$$L(y f(x)) = \exp(-y f(x))$$

logistic loss

$$L(y f(x)) = \log(1 + \exp(-y f(x)))$$

Loss function II

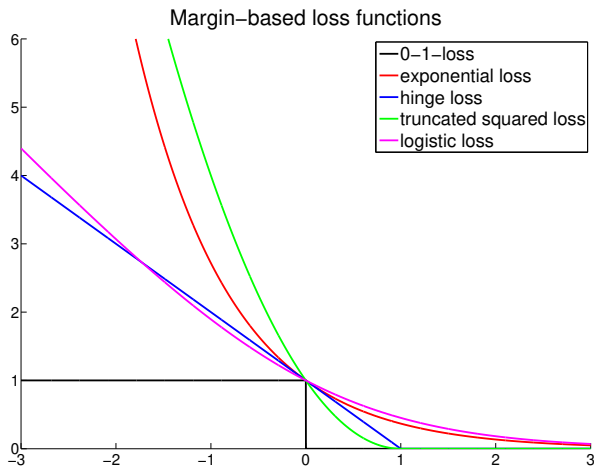


Figure: Image from Prof. Hein

Optimality I

Problem: Different loss measure \implies Different optimal function

Question: Let, $f_L^* : \mathcal{X} \rightarrow \mathbb{R}$, be the function which minimizes the risk R_L ,

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

where L is a convex margin-based loss function (surrogate of the 0-1-loss). Does the sign of f_L^* agree with the Bayes classifier $\hat{y}^*(x)$? I.e.,

$$\hat{y}^*(x) \stackrel{?}{=} \text{sign } f_L^*(x).$$

Optimality I

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$$\hat{y}^*(x) \stackrel{?}{=} \text{sign } f_L^*(x).$$

Definition

A margin-based loss function $L : \mathbb{R} \rightarrow [0, \infty)$ is **classification calibrated** if for all $\eta(x) \neq 0$, then

$$\text{sign } f_L^*(x) = \hat{y}^*(x) = \text{sign } \eta(x),$$

i.e., f_L^* has the same sign as the Bayes classifier \hat{y}^* .

Note: $\eta(x) = \mathbb{E}[Y|X = x] = P(Y = 1|X = x) - P(Y = -1|X = x)$

Optimality II

Cost sensitive risk functional based on convex margin-based loss:

$$R_L^C(f) = \mathbb{E}_X[C_{1,-1} L(f(X)) P(Y = 1|X) + C_{-1,1} L(-f(X)) P(Y = -1|X)]$$

$$f_{C,L}^* = \arg \min \{R_L^C(f) \mid f \text{ measurable}\}.$$

Definition

A margin-based loss function $L : \mathbb{R} \rightarrow [0, \infty)$ is **cost-sensitive classification calibrated** if for all $\eta(x) \neq \frac{C_{-1,1} - C_{1,-1}}{C_{1,-1} + C_{-1,1}}$ we have

$$\text{sign } f_{C,L}^*(x) = \hat{y}_C^*(x) = \text{sign} \left[\eta(x) - \frac{C_{-1,1} - C_{1,-1}}{C_{1,-1} + C_{-1,1}} \right],$$

that is $f_{C,L}^*$ has the same sign as the Bayes classifier \hat{y}_C^* .

Optimality III

Examples of surrogate convex losses for classification with their optimal solution:

Loss	Loss function $L(y f(x))$	Optimal function
hinge (soft-margin)	$\max(0, 1 - y f(x))$	$f_L^*(x) = \begin{cases} 1 & \text{if } \eta(x) > 0 \\ -1 & \text{if } \eta(x) < 0 \end{cases}$
truncated squared	$\max(0, 1 - y f(x))^2$	$f_L^*(x) = \eta(x),$
exponential	$\exp(-y f(x))$	$f_L^*(x) = \frac{1}{2} \log \frac{1+\eta(x)}{1-\eta(x)},$
logistic	$\log(1 + \exp(-y f(x)))$	$f_L^*(x) = \log \frac{1+\eta(x)}{1-\eta(x)}.$

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Multi-class Classification

$$\mathcal{Y} = \{1, \dots, K\} \text{ (no order!)}$$

Multi-class risk of the 0-1-loss:

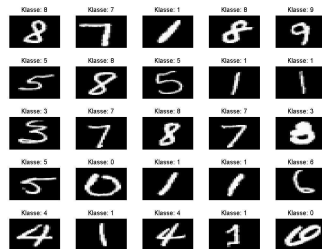
$$R(\hat{y}) = \mathbb{E}[\mathbb{1}_{\hat{y}(X) \neq Y}] = \mathbb{E}[\mathbb{E}[\mathbb{1}_{\hat{y}(X) \neq Y} | X]] = \mathbb{E}\left[\sum_{k=1}^K \mathbb{1}_{\hat{y}(X) \neq k} P(Y = k | X)\right].$$

Multi-class Bayes classifier:

$$\hat{y}^*(x) = \arg \max_{k \in \{1, \dots, K\}} P(Y = k | X = x),$$

Multi-class Bayes risk:

$$R^* = \mathbb{E}\left[1 - \max_{k \in \{1, \dots, K\}} P(Y = k | X)\right].$$



Multi-class Classification II

Idea: Decompose multi-class problem into binary classification problems,

- **one-vs-all:** The multi-class problem is decomposed into K binary problems. Each class versus all other classes $\Rightarrow K$ classifiers $\{f_i\}_{i=1}^K$.

$$f_{OVA}(x) = \arg \max_{i=1,\dots,K} f_i(x),$$

where ideally $f_i(x) = P(Y = i|x)$.

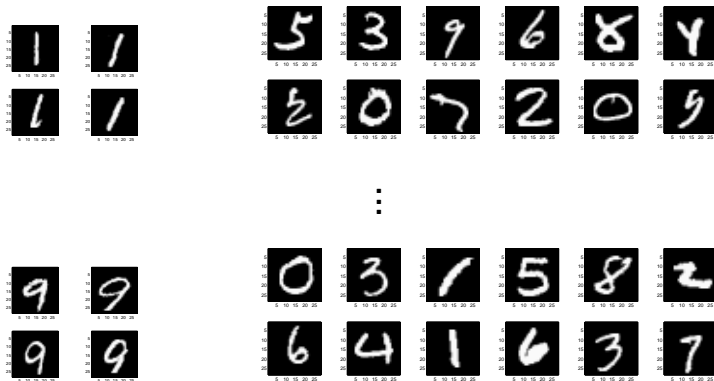
- **one-vs-one:** The multi-class problem is decomposed into $\binom{K}{2}$ binary problems. Each class versus each other class. Each binary classifier f_{ij} votes for one class. Final classification by majority vote,

$$f_{OVO}(x) = \arg \max_{i=1,\dots,K} \sum_{\substack{j=1 \\ j \neq i}}^K \mathbb{1}_{f_{ij}(x) > 0},$$

where ideally $f_{ij}(x) = P(Y = i|x) - P(Y = j|x)$.

One-vs-all

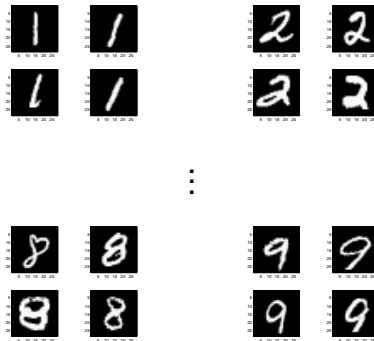
Decompose multi-class problem into K binary classification problems,



Handwritten digits: $K = 10 \implies 10$ binary classification problems.

One-vs-one

Decompose multi-class problem into $\binom{K}{2}$ binary classification problems,



Handwritten digits: $K = 10 \implies 45$ binary classification problems.

Optimality

Theorem

The one-vs-all and one-vs-one multi-class schemes lead to the Bayes optimal solution for the multi-class problem if the binary classifiers f_i and f_{ij} for all $i, j \in \mathcal{Y}$ are strictly monotonically increasing functions of the conditional distribution.

Proof.

One-vs-all: Given that f_i are strictly monotonically increasing functions of the conditional distribution, i.e., $f_{ij}(x) = g(P(Y = i|X = x))$ with $g()$ being a strictly monotonically increasing function, we have that

$$\arg \max_{i=1,\dots,K} f_i(x) = \arg \max_{i=1,\dots,K} g(P(Y = i|X = x)) = \arg \max_{i=1,\dots,K} Pr(Y = i|X = x) = \hat{y}^*.$$

Optimality

Theorem

The one-vs-all and one-vs-one multi-class schemes lead to the Bayes optimal solution for the multi-class problem if the binary classifiers f_i and f_{ij} for all $i, j \in \mathcal{Y}$ are strictly monotonically increasing functions of the conditional distribution.

Proof.

One-vs-one: Given that f_{ij} are strictly monotonically increasing functions of the conditional distribution, i.e., $f_{ij}(x) = g(P_{ij}(Y = i|x))$ with

$P_{ij}(Y = i|x) = \frac{P(Y=i|X=x)}{P(Y=i|X=x)+P(Y=j|X=x)}$, and that the binary optimal classifier fulfills that $f_{ij}^* = -f_{ji}^*$, then

$$\begin{aligned} \arg \max_{i=1,\dots,K} \sum_{\substack{j=1 \\ j \neq i}}^K \mathbb{1}_{f_{ij}^*(x) > 0} &= \arg \max_{i=1,\dots,K} \sum_{\substack{j=1 \\ j \neq i}}^K \mathbb{1}_{f_{ij}^*(x) > f_{ji}^*(x)} = \arg \max_{i=1,\dots,K} \sum_{\substack{j=1 \\ j \neq i}}^K \mathbb{1}_{g(P_{ij}(Y=i|x)) > g(P_{ij}(Y=j|x))} \\ &= \arg \max_{i=1,\dots,K} \sum_{\substack{j=1 \\ j \neq i}}^K \mathbb{1}_{P_{ij}(Y=i|x) > P_{ij}(Y=j|x)} = \arg \max_{i=1,\dots,K} \sum_{\substack{j=1 \\ j \neq i}}^K \mathbb{1}_{P(Y=i|x) > P(Y=j|x)} = \arg \max_{i=1,\dots,K} P(Y = i|x) \end{aligned}$$

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Regression

Regression: output space $\mathcal{Y} = \mathbb{R}$,

Risk: $R(f) = \mathbb{E}[L(Y, f(X))] = \mathbb{E}_X[\mathbb{E}_{Y|X}[L(Y, f(X)) | X]]$

Loss function: $L(y, f(x))$ (often plotted with $|y - f(x)|$ as argument).

Loss function	Optimal regressor
Squared loss: $L(y, f(x)) = (y - f(x))^2$	$f_L^*(x) = \mathbb{E}_Y[Y X = x]$
L_1 - loss: $L(y, f(x)) = y - f(x) $	$f_L^*(x) = \text{Median}(Y X = x)$
ε-insensitive : $L(y, f(x)) = (y - f(x) - \varepsilon) \mathbb{1}_{ y - f(x) > \varepsilon}$	not unique
Huber's robust loss: $L(y, f(x)) = \begin{cases} \frac{1}{2\varepsilon}(y - f(x))^2 & \text{if } y - f(x) \leq \varepsilon \\ y - f(x) - \frac{\varepsilon}{2} & \text{if } y - f(x) > \varepsilon \end{cases}$	unknown

Observation: In regression problems, the optimal regression function depends on the considered loss.

Loss functions for regression III

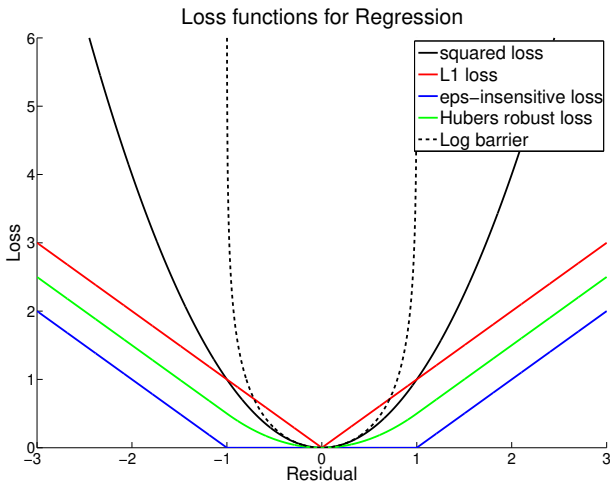


Figure: Image from Prof. Hein

Median is more stable than the mean

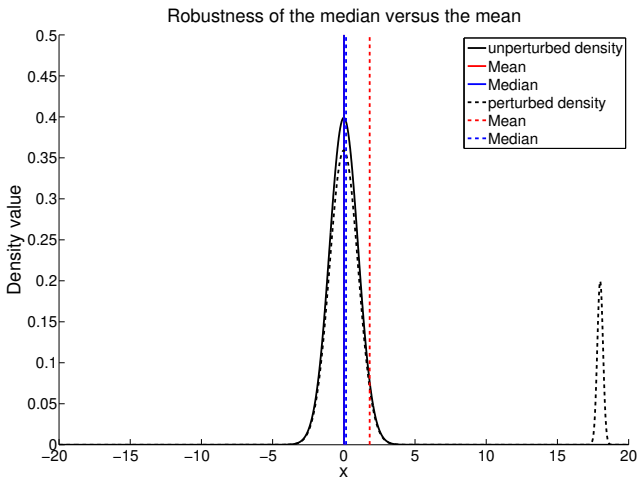


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Summary

- Bayesian decision theory allows us to make optimal decisions under uncertainty.
- The optimal binary classifier is the Bayes classifier and selects the class that maximizes the posterior $P(Y|x)$ for each feature vector x .
- Bayes classifier can be extended to *cost-sensitive learning* and the *multi-class* setting. For multi-class problems we have seen two approaches: one-versus-all and one-versus-one.
- Margin-based classifiers allows us to solve classification problems by minimizing a surrogate loss function that is easier to optimize than the 0-1-loss.
- In contrast, in regression problems, the optimal regression function is loss-dependent.
- Next lecture we will see how to solve regression and classification problems using data!