Foundations of machine learning

Statistical decision theory

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Outline

- Basic definitions
- Optimality criteria
- Relationships between optimality criteria
- Analogies to microeconomics
- Two justifications of the Bayesian approach

Takeaways for this part of class

1. A general framework to think about what makes a “good” estimator, test, etc.
2. How the foundations of statistics relate to those of microeconomic theory.
3. In what sense the set of Bayesian estimators contains most “reasonable” estimators.

Examples of decision problems

- Decide whether or not the hypothesis of no racial discrimination in job interviews is true
- Provide a forecast of the unemployment rate next month
- Provide an estimate of the returns to schooling
- Pick a portfolio of assets to invest in
- Decide whether to reduce class sizes for poor students
- Recommend a level for the top income tax rate

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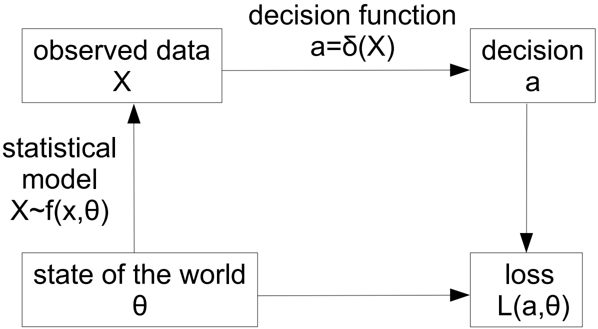
Components of a general statistical decision problem

- Observed data X
- A statistical decision a
- A state of the world θ
- A loss function $L(a, \theta)$ (the negative of utility)
- A statistical model $f(X|\theta)$
- A decision function $a = \delta(X)$

How they relate

- underlying state of the world θ
  $\Rightarrow$ distribution of the observation X.
- decision maker: observes $X \Rightarrow$ picks a decision a
- her goal: pick a decision that minimizes loss $L(a, \theta)$
  (θ unknown state of the world)
- X is useful $\Leftrightarrow$ reveals some information about θ
  $\Leftrightarrow f(X|\theta)$ does depend on θ.
- problem of statistical decision theory:
  find decision functions δ which "make loss small."

Graphical illustration



Examples

- investing in a portfolio of assets:
  - X: past asset prices
  - a: amount of each asset to hold
  - θ: joint distribution of past and future asset prices
  - L: minus expected utility of future income
- decide whether or not to reduce class size:
  - X: data from project STAR experiment
  - a: class size
  - θ: distribution of student outcomes for different class sizes
  - L: average of suitably scaled student outcomes, net of cost

Practice problem

For each of the examples on slide 2, what are

- the data X,
- the possible actions a,
- the relevant states of the world θ, and
- reasonable choices of loss function L?

Loss functions in estimation

- goal: find an a
- which is close to some function μ of θ.
- for instance: $\mu(\theta) = E[X]$
- loss is larger if the difference between our estimate and the true value is larger

Some possible loss functions:

1. **squared error** loss,
$$L(a, \theta) = (a - \mu(\theta))^2$$
2. **absolute error** loss,
$$L(a, \theta) = |a - \mu(\theta)|$$

Loss functions in testing

- goal: decide whether $H_0 : \theta \in \Theta_0$ is true
- decision $a \in \{0,1\}$ (accept / reject)

Possible loss function:

$$L(a,\theta) = \begin{cases} 1 & \text{if } a = 1,\ \theta \in \Theta_0 \\ c & \text{if } a = 0,\ \theta \notin \Theta_0 \\ 0 & \text{else.} \end{cases}$$

	truth	
decision a	$\theta \in \Theta_0$	$\theta \notin \Theta_0$
0	0	c
1	1	0

Risk function

$$R(\delta,\theta) = E_\theta[L(\delta(X),\theta)].$$

- expected loss of a decision function δ
- R is a function of the true state of the world θ.
- crucial intermediate object in evaluating a decision function
- small $R \Leftrightarrow$ good δ
- δ might be good for some θ, bad for other θ.
- Decision theory deals with this trade-off.

Example: estimation of mean

- observe $X \sim N(\mu, 1)$
- want to estimate μ
- $L(a, \theta) = (a - \mu(\theta))^2$
- $\delta(X) = \alpha + \beta \cdot X$

Practice problem (Estimation of means)

Find the risk function for this decision problem.

Variance / Bias trade-off

Solution:

$$\begin{aligned} R(\delta,\mu) &= E[(\delta(X)-\mu)^2] \\ &= \mathrm{Var}(\delta(X)) + \mathrm{Bias}(\delta(X))^2 \\ &= \beta^2\,\mathrm{Var}(X) + (\alpha+\beta E[X]-E[X])^2 \\ &= \beta^2 + (\alpha+(\beta-1)\mu)^2. \end{aligned}$$

- equality 1 and 2: always true for squared error loss
- Choosing β (and α) involves a trade-off of bias and variance,
- this trade-off depends on μ.

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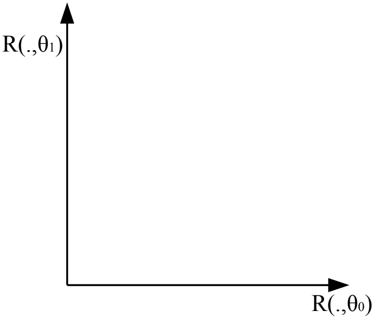
- Ranking provided by the risk function is multidimensional:
- a ranking of performance between decision functions for every θ
- To get a global comparison of their performance, have to aggregate this ranking into a global ranking.
- preference relationship on space of risk functions
  $\Rightarrow$ preference relationship on space of decision functions

Illustrations for intuition

- Suppose θ can only take two values,
- $\Rightarrow$ risk functions are points in a 2D-graph,
- each axis corresponds to $R(\delta, \theta)$ for $\theta = \theta_0, \theta_1$.



Three approaches to get a global ranking

1. **partial ordering**:
   a decision function is better relative to another
   if it is better for *every* θ

2. complete ordering, **weighted average**:
   a decision function is better relative to another
   if a weighted average of risk across θ is lower
   weights $\sim$ prior distribution

3. complete ordering, **worst case**:
   a decision function is better relative to another
   if it is better under its worst-case scenario.

Approach 1: Admissibility

Dominance:
δ is said to dominate another function δ' if

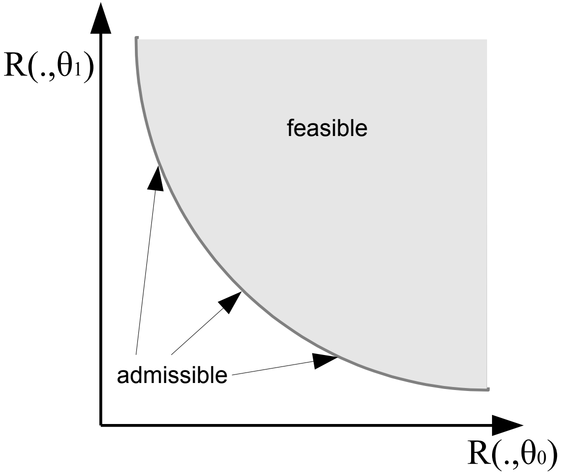
$$R(\delta, \theta) \leq R(\delta', \theta)$$

for all θ, and

$$R(\delta, \theta) < R(\delta', \theta)$$

for at least one θ.

Admissibility:
decisions functions which are not dominated are called admissible,
all other decision functions are inadmissible.


R(.,θ1)
feasible
admissible
R(.,θ0)

- admissibility $\sim$ "Pareto frontier"
- Dominance only generates a partial ordering of decision functions.
- in general: many different admissible decision functions.

Practice problem

- you observe $X_i \sim^{iid} N(\mu, 1)$, $i = 1, \ldots, n$ for $n > 1$
- your goal is to estimate μ, with squared error loss
- consider the estimators
  1. $\delta(X) = X_1$
  2. $\delta(X) = \frac{1}{n} \sum_i X_i$
- can you show that one of them is inadmissible?

Approach 2: Bayes optimality

- natural approach for economists:
- trade off risk across different θ
- by assigning weights $\pi(\theta)$ to each θ

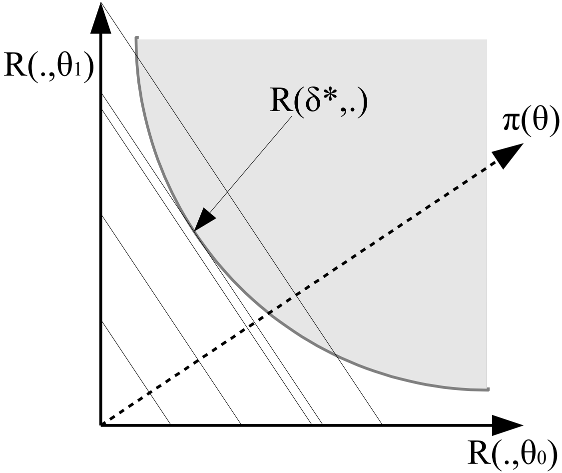
Integrated risk:

$$R(\delta, \pi) = \int R(\delta, \theta)\pi(\theta)d\theta.$$

Bayes decision function:
minimizes integrated risk,

$$\delta^* = \underset{\delta}{\operatorname{argmin}}\ R(\delta, \pi).$$

- Integrated risk $\sim$ linear indifference planes in space of risk functions
- prior $\sim$ normal vector for indifference planes


R(.,θ1)
R(δ*,.)
π(θ)
R(.,θ0)

Decision weights as prior probabilities

- suppose $0 < \int \pi(\theta) d\theta < \infty$
- then wlog $\int \pi(\theta) d\theta = 1$ (normalize)
- if additionally $\pi \geq 0$
- then π is called a prior distribution

Posterior

- suppose π is a prior distribution
- **posterior distribution:**

$$\pi(\theta|X) = \frac{f(X|\theta)\pi(\theta)}{m(X)}$$

- normalizing constant $=$ prior likelihood of X

$$m(X) = \int f(X|\theta)\pi(\theta)d\theta$$

Practice problem

- you observe $X \sim N(\theta, 1)$
- consider the prior
$$\theta \sim N(0, \tau^2)$$
- calculate
  1. $m(X)$
  2. $\pi(\theta|X)$

Posterior expected loss

$$R(\delta, \pi|X) := \int L(\delta(X), \theta)\pi(\theta|X)d\theta$$

Proposition

Any Bayes decision function δ^*
can be obtained by minimizing $R(\delta, \pi|X)$
through choice of $\delta(X)$ for every X.

Practice problem

Show that this is true.

Hint: show first that

$$R(\delta, \pi) = \int R(\delta(X), \pi|X)m(X)dX.$$

Bayes estimator with quadratic loss

- assume quadratic loss, $L(a, \theta) = (a - \mu(\theta))^2$
- posterior expected loss:

$$\begin{aligned} R(\delta, \pi | X) &= E_{\theta|X}\left[L(\delta(X), \theta)|X\right] \\ &= E_{\theta|X}\left[(\delta(X) - \mu(\theta))^2 | X\right] \\ &= \text{Var}(\mu(\theta)|X) + (\delta(X) - E[\mu(\theta)|X])^2 \end{aligned}$$

- Bayes estimator minimizes posterior expected loss $\Rightarrow$

$$\delta^*(X) = E[\mu(\theta)|X].$$

Practice problem

- you observe $X \sim N(\theta, 1)$
- your goal is to estimate θ, with squared error loss
- consider the prior

$$\theta \sim N(0, \tau^2)$$

- for any δ, calculate
  1. $R(\delta(X), \pi | X)$
  2. $R(\delta, \pi)$
  3. the Bayes optimal estimator δ^*

Practice problem

- you observe X_i iid., $X_i \in \{1,2,\dots,k\}$, $P(X_i = j) = \theta_j$
- consider the so called Dirichlet prior, for $\alpha_j > 0$:

$$\pi(\theta) = const. \cdot \prod_{j=1}^{k} \theta_j^{\alpha_j - 1}$$

- calculate $\pi(\theta|X)$
- look up the Dirichlet distribution on Wikipedia
- calculate $E[\theta|X]$

Approach 3: Minimaxity

- Don't want to pick a prior?
- Can instead always assume the worst.
- worst $=\theta$ which maximizes risk

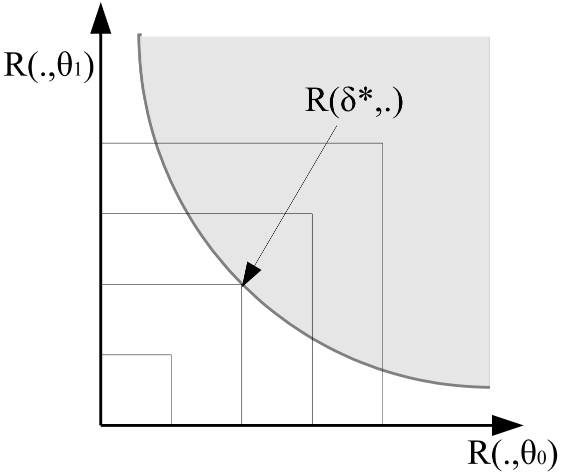
worst-case risk:

$$\overline{R}(\delta)=\sup_{\theta} R(\delta,\theta).$$

minimax decision function:

$$\delta^{*}=\underset{\delta}{\operatorname{argmin}}\ \overline{R}(\delta)=\underset{\delta}{\operatorname{argmin}}\ \sup_{\theta} R(\delta,\theta).$$

(does not always exist!)


R(.,θ1)
R(δ*,.)
R(.,θ0)

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Proposition (Minimax decision functions)

If δ^* is admissible with constant risk,
then it is a minimax decision function.

Proof:

- picture!
- Suppose that δ' had smaller worst-case risk than δ^*
- Then

$$R(\delta', \theta') \leq \sup_{\theta} R(\delta', \theta) < \sup_{\theta} R(\delta^*, \theta) = R(\delta^*, \theta'),$$

- used constant risk in the last equality
- This contradicts admissibility.

- despite this result,
  minimax decision functions are very hard to find
- Example:
  - if $X \sim N(\mu, I)$, $\dim(X) \geq 3$, then
  - X has constant risk (mean squared error) as estimator for μ
  - but: X is not an admissible estimator for μ
    therefore not minimax
  - We will discuss dominating estimator in the next part of class.

Proposition (Bayes decisions are admissible)

Suppose:

- δ^* is the Bayes decision function
- $\pi(\theta) > 0$ for all θ, $R(\delta^*, \pi) < \infty$
- $R(\delta^*, \theta)$ is continuous in θ

Then δ^* is admissible.

(We will prove the reverse of this statement in the next section.)

Sketch of proof:

- picture!
- Suppose δ^* is not admissible
- $\Rightarrow$ dominated by some δ'
  i.e. $R(\delta', \theta) \leq R(\delta^*, \theta)$ for all θ with strict inequality for some θ
- Therefore

$$R(\delta', \pi) = \int R(\delta', \theta)\pi(\theta)d\theta < \int R(\delta^*, \theta)\pi(\theta)d\theta = R(\delta^*, \pi)$$

- This contradicts δ^* being a Bayes decision function.

Proposition (Bayes risk and minimax risk)

The Bayes risk
$R(\pi) := \inf_\delta R(\delta, \pi)$
is never larger than the minimax risk
$\overline{R} := \inf_\delta \sup_\theta R(\delta, \theta)$.

Proof:

$$
\begin{aligned}
R(\pi) &= \inf_\delta R(\delta, \pi) \\
&\leq \sup_\pi \inf_\delta R(\delta, \pi) \\
&\leq \inf_\delta \sup_\pi R(\delta, \pi) \\
&\leq \inf_\delta \sup_\theta R(\delta, \theta) = \overline{R}.
\end{aligned}
$$

If there exists a prior π^* such that $R(\pi) = \overline{R}$, it is called the least favorable distribution.

Analogies to microeconomics

1) Welfare economics

statistical decision theory	social welfare analysis
different parameter values θ	different people i
risk $R(.,\theta)$	individuals' utility $u_i(.)$
dominance	Pareto dominance
admissibility	Pareto efficiency
Bayes risk	social welfare function
prior	welfare weights (distributional preferences)
minimaxity	Rawlsian inequality aversion

2) choice under uncertainty / choice in strategic interactions

statistical decision theory	**strategic interactions**
dominance of decision functions	dominance of strategies
Bayes risk	expected utility
Bayes optimality	expected utility maximization
minimaxity	(extreme) ambiguity aversion

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Two justifications of the Bayesian approach
justification 1 – the complete class theorem

- last section: every Bayes decision function is admissible
  (under some conditions)
- the reverse also holds true (under some conditions):
  every admissible decision function is Bayes,
  or the limit of Bayes decision functions
- can interpret this as:
  all reasonable estimators are Bayes estimators
- will state a simple version of this result

Preliminaries

- set of risk functions that correspond to some δ is the **risk set**,

$$\mathscr{R} := \{r(.) = R(., \delta) \text{ for some } \delta\}$$

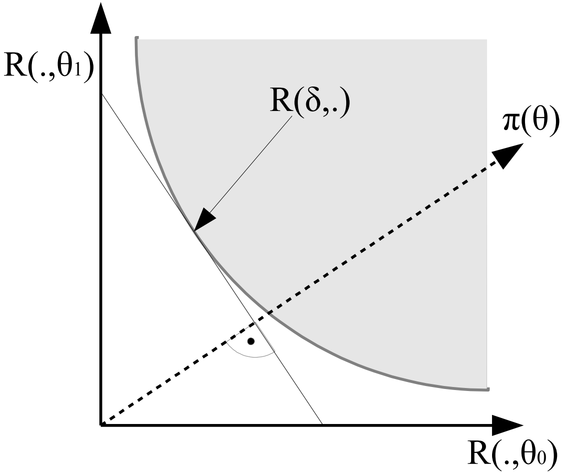
- will assume **convexity** of $\mathscr{R}$
  – no big restriction, since we can always randomly "mix" decision functions
- a class of decision functions δ is a **complete class** if it contains every admissible decision function δ^*

Theorem (Complete class theorem)

Suppose

- the set Θ of possible values for θ is compact
- the risk set $\mathscr{R}$ is convex
- all decision functions have continuous risk

Then the Bayes decision functions constitute a complete class:
For every admissible decision function δ^*, there exists a prior distribution π such that δ^* is a Bayes decision function for π.


R(.,θ1)
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Intuition for the complete class theorem

- any choice of decision procedure has to trade off risk across θ
- slope of feasible risk set
  = relative "marginal cost" of decreasing risk at different θ
- pick a risk function on the admissible frontier
- can rationalize it with a prior
  = "marginal benefit" of decreasing risk at different θ
- for example, minimax decision rule:
  rationalizable by least favorable prior
  slope of feasible set at constant risk admissible point
- analogy to social welfare: any policy choice or allocation corresponds to distributional preferences / welfare weights

Proof of complete class theorem:

- application of the separating hyperplane theorem, to the space of functions of θ, with the inner product

$$\langle f,g\rangle = \int f(\theta)g(\theta)d\theta.$$

- for intuition: focus on binary θ, $\theta \in \{0,1\}$, and $\langle f,g\rangle = \sum_\theta f(\theta)g(\theta)$
- Let δ^* be admissible. Then $R(.,\delta^*)$ belongs to the lower boundary of $\mathscr{R}$.
- convexity of $\mathscr{R}$, separating hyperplane theorem separating $\mathscr{R}$ from (infeasible) risk functions dominating δ^*

- $\Rightarrow$ there exists a function $\tilde{\pi}$ (with finite integral) such that for all δ

$$\langle R(.,\delta^*),\tilde{\pi}\rangle \leq \langle R(.,\delta),\tilde{\pi}\rangle.$$

- by construction $\tilde{\pi} \geq 0$
- thus $\pi := \tilde{\pi}/\int\tilde{\pi}$ defines a prior distribution.
- δ^* minimizes

$$\langle R(.,\delta^*),\pi\rangle = R(\delta^*,\pi)$$

  among the set of feasible decision functions
- and is therefore the optimal Bayesian decision function for the prior π.

justification 2 – subjective probability theory

- going back to Savage (1954) and Anscombe and Aumann (1963).
- discussed in chapter 6 of
  Mas-Colell, A., Whinston, M., and Green, J. (1995), *Microeconomic theory*, Oxford University Press
- and maybe in Econ 2010 / Econ 2059.

- Suppose a decision maker ranks risk functions $R(., \delta)$ by a **preference relationship** $\succeq$
- properties $\succeq$ might have:
  1. **completeness**: any pair of risk functions can be ranked
  2. **monotonicity**: if the risk function R is (weakly) lower than R' for all θ, than R is (weakly) preferred
  3. **independence**:

$$R^1 \succeq R^2 \Leftrightarrow \alpha R^1 + (1-\alpha)R^3 \succeq \alpha R^2 + (1-\alpha)R^3$$

     for all R^1, R^2, R^3 and $\alpha \in [0,1]$

- Important: this independence has nothing to do with statistical independence

Theorem

If $\succeq$ is complete, monotonic, and satisfies independence, then there exists a prior π such that

$$R(.,\delta^1) \succeq R(.,\delta^2) \Leftrightarrow R(\pi,\delta^1) \leq R(\pi,\delta^2).$$

Intuition of proof:

- Independence and completeness imply linear, parallel indifference sets
- monotonicity makes sure prior is non-negative

Sketch of proof:
Using independence repeatedly, we can show that for all $R^1, R^2, R^3 \in \mathbb{R}^{\mathscr{X}}$, and all $\alpha > 0$,

1. $R^1 \succeq R^2$ iff $\alpha R^1 \succeq \alpha R^2$,
2. $R^1 \succeq R^2$ iff $R^1 + R^3 \succeq R^2 + R^3$,
3. $\{R : R \succeq R^1\} = \{R : R \succeq 0\} + R^1$,
4. $\{R : R \succeq 0\}$ is a convex cone.
5. $\{R : R \succeq 0\}$ is a half space.

The last claim requires completeness. It immediately implies the existence of π. Monotonicity implies that π is not negative.

Remark

- personally, I’m more convinced by the complete class theorem than by normative subjective utility theory
- admissibility seems a very sensible requirement
- whereas “independence” of the preference relationship seems more up for debate

References

Robert, C. (2007). The Bayesian choice: from decision-theoretic foundations to computational implementation. *Springer Verlag, chapter 2.*

Casella, G. and Berger, R. L. (2001). Statistical inference. *Duxbury Press, chapter 7.3.4.*