7. Statistical estimation

- maximum likelihood estimation
- optimal detector design
- experiment design

Parametric distribution estimation

- distribution estimation problem: estimate probability density $p(y)$ of a random variable from observed values
- parametric distribution estimation: choose from a family of densities $p_x(y)$, indexed by a parameter $x$

**maximum likelihood estimation**

$$\text{maximize (over } x) \quad \log p_x(y)$$

- $y$ is observed value
- $l(x) = \log p_x(y)$ is called log-likelihood function
- can add constraints $x \in C$ explicitly, or define $p_x(y) = 0$ for $x \notin C$
- a convex optimization problem if $\log p_x(y)$ is concave in $x$ for fixed $y$
Linear measurements with IID noise

linear measurement model

\[ y_i = a_i^T x + v_i, \quad i = 1, \ldots, m \]

- \( x \in \mathbb{R}^n \) is vector of unknown parameters
- \( v_i \) is IID measurement noise, with density \( p(z) \)
- \( y_i \) is measurement: \( y \in \mathbb{R}^m \) has density \( p_x(y) = \prod_{i=1}^{m} p(y_i - a_i^T x) \)

**maximum likelihood estimate:** any solution \( x \) of

\[
\text{maximize} \quad l(x) = \sum_{i=1}^{m} \log p(x_i - a_i^T x)
\]

(\( y \) is observed value)

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examples

- Gaussian noise \( \mathcal{N}(0, \sigma^2) \): \( p(z) = (2\pi\sigma^2)^{-1/2} e^{-z^2/(2\sigma^2)} \),

\[
l(x) = -\frac{m}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^{m} (a_i^T x - y_i)^2
\]

ML estimate is LS solution

- Laplacian noise: \( p(z) = (1/(2a)) e^{-|z|/a} \),

\[
l(x) = -m \log(2a) - \frac{1}{a} \sum_{i=1}^{m} |a_i^T x - y_i|
\]

ML estimate is \( \ell_1 \)-norm solution

- uniform noise on \( [-a, a] \):

\[
l(x) = \begin{cases} 
-m \log(2a) & |a_i^T x - y_i| \leq a, \quad i = 1, \ldots, m \\
-\infty & \text{otherwise}
\end{cases}
\]

ML estimate is any \( x \) with \( |a_i^T x - y_i| \leq a \)

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Logistic regression

random variable $y \in \{0, 1\}$ with distribution

$$p = \text{prob}(y = 1) = \frac{\exp(a^T u + b)}{1 + \exp(a^T u + b)}$$

- $a, b$ are parameters; $u \in \mathbb{R}^n$ are (observable) explanatory variables
- estimation problem: estimate $a, b$ from $m$ observations $(u_i, y_i)$

log-likelihood function (for $y_1 = \cdots = y_k = 1, y_{k+1} = \cdots = y_m = 0$):

$$l(a, b) = \log \left( \prod_{i=1}^{k} \frac{\exp(a^T u_i + b)}{1 + \exp(a^T u_i + b)} \frac{1}{\prod_{i=k+1}^{m} 1 + \exp(a^T u_i + b)} \right)$$

$$= \sum_{i=1}^{k} (a^T u_i + b) - \sum_{i=1}^{m} \log(1 + \exp(a^T u_i + b))$$

concave in $a, b$

example ($n = 1, m = 50$ measurements)

- circles show 50 points $(u_i, y_i)$
- solid curve is ML estimate of $p = \exp(a u + b)/(1 + \exp(a u + b))$
(Binary) hypothesis testing

detection (hypothesis testing) problem

given observation of a random variable \( X \in \{1, \ldots, n\} \), choose between:

- hypothesis 1: \( X \) was generated by distribution \( p = (p_1, \ldots, p_n) \)
- hypothesis 2: \( X \) was generated by distribution \( q = (q_1, \ldots, q_n) \)

randomized detector

- a nonnegative matrix \( T \in \mathbb{R}^{2 \times n} \), with \( 1^T T = 1 \)
- if we observe \( X = k \), we choose hypothesis 1 with probability \( t_{1k} \), hypothesis 2 with probability \( t_{2k} \)
- if all elements of \( T \) are 0 or 1, it is called a deterministic detector

Detection probability matrix:

\[
D = \begin{bmatrix} T_p & T_q \end{bmatrix} = \begin{bmatrix} 1 - P_{fp} & P_{fn} \\ P_{fp} & 1 - P_{fn} \end{bmatrix}
\]

- \( P_{fp} \) is probability of selecting hypothesis 2 if \( X \) is generated by distribution 1 (false positive)
- \( P_{fn} \) is probability of selecting hypothesis 1 if \( X \) is generated by distribution 2 (false negative)

Multicriterion formulation of detector design

\[
\begin{align*}
\text{minimize (w.r.t. } \mathbb{R}_+^2) & \quad (P_{fp}, P_{fn}) = ((T_p)_2, (T_q)_1) \\
\text{subject to} & \quad t_{1k} + t_{2k} = 1, \quad k = 1, \ldots, n \\
& \quad t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n
\end{align*}
\]

variable \( T \in \mathbb{R}^{2 \times n} \)
**scalarization** (with weight $\lambda > 0$)

minimize $\left(T_p\right)_2 + \lambda \left(T_q\right)_1$

subject to $t_{1k} + t_{2k} = 1, \quad t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n$

an LP with a simple analytical solution

$$(t_{1k}, t_{2k}) = \begin{cases} (1, 0) & p_k \geq \lambda q_k \\ (0, 1) & p_k < \lambda q_k \end{cases}$$

- a deterministic detector, given by a likelihood ratio test
- if $p_k = \lambda q_k$ for some $k$, any value $0 \leq t_{1k} \leq 1$, $t_{1k} = 1 - t_{2k}$ is optimal ($i.e.$, Pareto-optimal detectors include non-deterministic detectors)

**minimax detector**

minimize $\max\{P_{fp}, P_{fn}\} = \max\{(T_p)_2, (T_q)_1\}$

subject to $t_{1k} + t_{2k} = 1, \quad t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n$

an LP; solution is usually not deterministic

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**example**

$$P = \begin{bmatrix} 0.70 & 0.10 \\ 0.20 & 0.10 \\ 0.05 & 0.70 \\ 0.05 & 0.10 \end{bmatrix}$$

solutions 1, 2, 3 (and endpoints) are deterministic; 4 is minimax detector
Experiment design

$m$ linear measurements $y_i = a_i^T x + w_i$, $i = 1, \ldots, m$ of unknown $x \in \mathbb{R}^n$

- measurement errors $w_i$ are IID $\mathcal{N}(0, 1)$
- ML (least-squares) estimate is
  \[
  \hat{x} = \left( \sum_{i=1}^m a_i a_i^T \right)^{-1} \sum_{i=1}^m y_i a_i
  \]

- error $e = \hat{x} - x$ has zero mean and covariance
  \[
  E = \mathbb{E} e e^T = \left( \sum_{i=1}^m a_i a_i^T \right)^{-1}
  \]

  confidence ellipsoids are given by $\{x \mid (x - \hat{x})^T E^{-1} (x - \hat{x}) \leq \beta\}$

experiment design: choose $a_i \in \{v_1, \ldots, v_p\}$ (a set of possible test vectors) to make $E$ ‘small’

vector optimization formulation

\[
\begin{align*}
\text{minimize (w.r.t. } S^n_+) & \quad E = \left( \sum_{k=1}^p m_k v_k v_k^T \right)^{-1} \\
\text{subject to} & \quad m_k \geq 0, \quad m_1 + \cdots + m_p = m \\
& \quad m_k \in \mathbb{Z}
\end{align*}
\]

- variables are $m_k$ (# vectors $a_i$ equal to $v_k$)
- difficult in general, due to integer constraint

relaxed experiment design

assume $m \gg p$, use $\lambda_k = m_k / m$ as (continuous) real variable

\[
\begin{align*}
\text{minimize (w.r.t. } S^p_+) & \quad E = \left( \frac{1}{m} \right) \left( \sum_{k=1}^p \lambda_k v_k v_k^T \right)^{-1} \\
\text{subject to} & \quad \lambda \succeq 0, \quad 1^T \lambda = 1
\end{align*}
\]

- common scalarizations: minimize $\log \det E$, $\text{tr} E$, $\lambda_{\max}(E)$, \ldots
- can add other convex constraints, e.g., bound experiment cost $c^T \lambda \leq B$
**D-optimal design**

\[
\begin{align*}
\text{minimize} \quad & \log \det \left( \sum_{k=1}^{p} \lambda_k v_k v_k^T \right)^{-1} \\
\text{subject to} \quad & \lambda_k \geq 0, \quad \mathbf{1}^T \lambda = 1
\end{align*}
\]

interpretation: minimizes volume of confidence ellipsoids

**dual problem**

\[
\begin{align*}
\text{maximize} \quad & \log \det W + n \log n \\
\text{subject to} \quad & v_k^T W v_k \leq 1, \quad k = 1, \ldots, p
\end{align*}
\]

interpretation: \( \{ x \mid x^T W x \leq 1 \} \) is minimum volume ellipsoid centered at origin, that includes all test vectors \( v_k \)

**complementary slackness:** for \( \lambda, W \) primal and dual optimal

\[
\lambda_k (1 - v_k^T W v_k) = 0, \quad k = 1, \ldots, p
\]

optimal experiment uses vectors \( v_k \) on boundary of ellipsoid defined by \( W \)

**example** \( (p = 20) \)

\[
\begin{align*}
\lambda_1 &= 0.5 \\
\lambda_2 &= 0.5
\end{align*}
\]

design uses two vectors, on boundary of ellipse defined by optimal \( W \)
derivation of dual of page 7–13

first reformulate primal problem with new variable $X$:

\[
\begin{align*}
\text{minimize} & \quad \log \det X^{-1} \\
\text{subject to} & \quad X = \sum_{k=1}^{P} \lambda_k v_k v_k^T, \quad \lambda \succeq 0, \quad 1^T \lambda = 1 \\
\end{align*}
\]

\[
L(X, \lambda, Z, z, \nu) = \log \det X^{-1} + \text{tr} \left( Z \left( X - \sum_{k=1}^{P} \lambda_k v_k v_k^T \right) \right) - z^T \lambda + \nu(1^T \lambda - 1)
\]

- minimize over $X$ by setting gradient to zero: $-X^{-1} + Z = 0$
- minimum over $\lambda_k$ is $-\infty$ unless $-v_k^T Z v_k - z_k + \nu = 0$

**dual problem**

\[
\begin{align*}
\text{maximize} & \quad n + \log \det Z - \nu \\
\text{subject to} & \quad v_k^T Z v_k \leq \nu, \quad k = 1, \ldots, p \\
\end{align*}
\]

change variable $W = Z/\nu$, and optimize over $\nu$ to get dual of page 7–13