7. Statistical estimation

- maximum likelihood estimation
- optimal detector design
- experiment design

Parametric distribution estimation

- ullet 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

maximize (over x) $\log p_x(y)$

- y is observed value
- $l(x) = \log p_x(y)$ is called log-likelihood function
- ullet can add constraints $x\in C$ explicitly, or define $p_x(y)=0$ for $x\not\in C$
- ullet a convex optimization problem if $\log p_x(y)$ is concave in x for fixed y

Linear measurements with IID noise

linear measurement model

$$y_i = a_i^T x + v_i, \quad i = 1, \dots, m$$

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

maximum likelihood estimate: any solution x of

maximize
$$l(x) = \sum_{i=1}^{m} \log p(y_i - a_i^T x)$$

(y is observed value)

examples

ullet 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 ℓ_1 -norm solution

• uniform noise on [-a, a]:

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

ML estimate is any x with $|a_i^T x - y_i| \le a$

Logistic regression

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

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

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

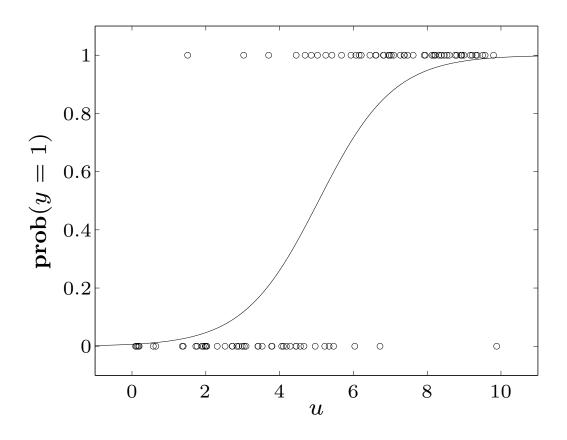
log-likelihood function (for $y_1 = \cdots = y_k = 1$, $y_{k+1} = \cdots = y_m = 0$):

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

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

concave in a, b

example (n = 1, m = 50 measurements)



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

(Binary) hypothesis testing

detection (hypothesis testing) problem

given observation of a random variable $X \in \{1, \dots, n\}$, 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

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

detection probability matrix:

$$D = \begin{bmatrix} Tp & Tq \end{bmatrix} = \begin{bmatrix} 1 - P_{\text{fp}} & P_{\text{fn}} \\ P_{\text{fp}} & 1 - P_{\text{fn}} \end{bmatrix}$$

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

multicriterion formulation of detector design

minimize (w.r.t.
$$\mathbf{R}_{+}^{2}$$
) $(P_{\mathrm{fp}}, P_{\mathrm{fn}}) = ((Tp)_{2}, (Tq)_{1})$ subject to $t_{1k} + t_{2k} = 1, \quad k = 1, \ldots, n$ $t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n$

variable $T \in \mathbf{R}^{2 \times n}$

scalarization (with weight $\lambda > 0$)

minimize
$$(Tp)_2 + \lambda (Tq)_1$$

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

an LP with a simple analytical solution

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

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

minimax detector

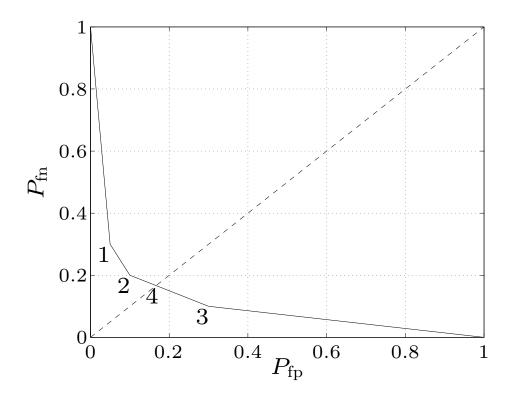
minimize
$$\max\{P_{\rm fp}, P_{\rm fn}\} = \max\{(Tp)_2, (Tq)_1\}$$

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

an LP; solution is usually not deterministic

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 $x \in \mathbf{R}^n$

- ullet 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

$$E = \mathbf{E} e e^T = \left(\sum_{i=1}^m a_i a_i^T\right)^{-1}$$

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

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

vector optimization formulation

minimize (w.r.t.
$$\mathbf{S}^n_+$$
) $E = \left(\sum_{k=1}^p m_k v_k v_k^T\right)^{-1}$ subject to $m_k \geq 0, \quad m_1 + \cdots + m_p = m$ $m_k \in \mathbf{Z}$

- 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

minimize (w.r.t.
$$\mathbf{S}_{+}^{n}$$
) $E = (1/m) \left(\sum_{k=1}^{p} \lambda_{k} v_{k} v_{k}^{T}\right)^{-1}$ subject to $\lambda \succeq 0, \quad \mathbf{1}^{T} \lambda = 1$

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

D-optimal design

minimize
$$\log \det \left(\sum_{k=1}^{p} \lambda_k v_k v_k^T\right)^{-1}$$
 subject to $\lambda \succeq 0$, $\mathbf{1}^T \lambda = 1$

interpretation: minimizes volume of confidence ellipsoids

dual problem

$$\begin{array}{ll} \text{maximize} & \log \det W + n \log n \\ \text{subject to} & v_k^T W v_k \leq 1, \quad k = 1, \dots, p \end{array}$$

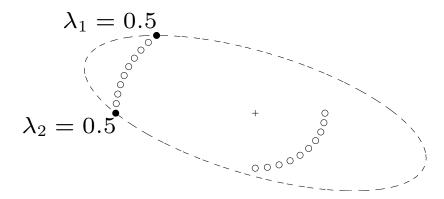
interpretation: $\{x \mid x^TWx \leq 1\}$ is minimum volume ellipsoid centered at origin, that includes all test vectors v_k

complementary slackness: for λ , W primal and dual optimal

$$\lambda_k(1 - v_k^T W v_k) = 0, \quad k = 1, \dots, p$$

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

example (p = 20)



design uses two vectors, on boundary of ellipse defined by optimal \boldsymbol{W}

derivation of dual of page 7–13

first reformulate primal problem with new variable X:

minimize
$$\log \det X^{-1}$$
 subject to $X = \sum_{k=1}^p \lambda_k v_k v_k^T, \quad \lambda \succeq 0, \quad \mathbf{1}^T \lambda = 1$

$$L(X, \lambda, Z, z, \nu) = \log \det X^{-1} + \mathbf{tr} \left(Z \left(X - \sum_{k=1}^{p} \lambda_k v_k v_k^T \right) \right) - z^T \lambda + \nu (\mathbf{1}^T \lambda - 1)$$

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

dual problem

$$\begin{array}{ll} \text{maximize} & n + \log \det Z - \nu \\ \text{subject to} & v_k^T Z v_k \leq \nu, \quad k = 1, \dots, p \end{array}$$

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

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