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

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

- 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

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

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

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

(y is observed value)

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 ℓ_1-norm solution

- uniform noise on $[-a, a]$:

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

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

Logistic regression

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

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

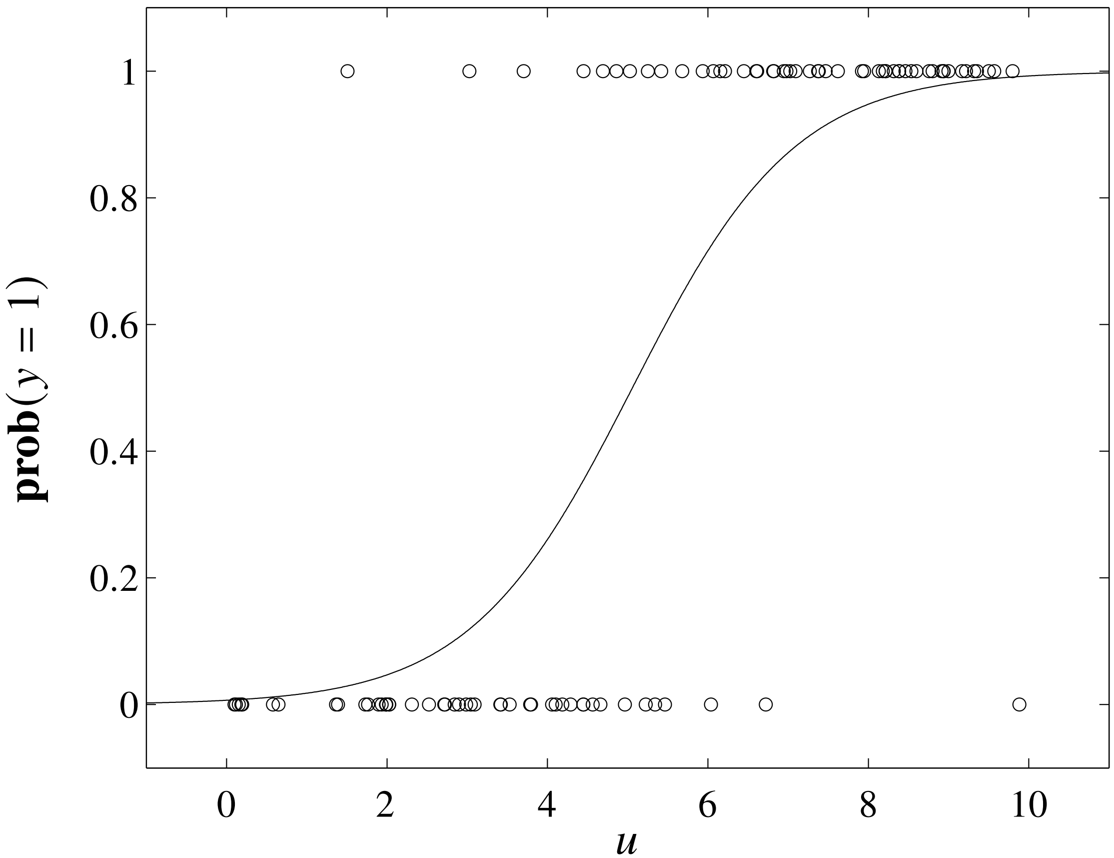
- a, b are parameters; $u \in \mathbf{R}^n$ are (observable) explanatory variables
- estimation problem: estimate a, b from m observations (u_i, y_i)

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

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

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 $X \in \{1, \ldots, n\}$, 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 $T \in \mathbf{R}^{2\times n}$, 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}
- if all elements of T are 0 or 1, it is called a deterministic detector

Detection probability matrix

$$D = \left[\begin{array}{cc} Tp & Tq \end{array} \right] = \left[\begin{array}{cc} 1 - P_{\rm fp} & P_{\rm fn} \\ P_{\rm fp} & 1 - P_{\rm fn} \end{array} \right]$$

- $P_{\rm fp}$ 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

$$\begin{array}{ll} \text{minimize (w.r.t. } \mathbf{R}^2_+) & (P_{\rm fp}, P_{\rm fn}) = ((Tp)_2, (Tq)_1) \\ \text{subject to} & t_{1k} + t_{2k} = 1, \quad k = 1, \ldots, n \\ & t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n \end{array}$$

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

Scalarization (with weight $\lambda > 0$)

$$\begin{array}{ll} \text{minimize} & (Tp)_2 + \lambda(Tq)_1 \\ \text{subject to} & t_{1k} + t_{2k} = 1, \quad t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n \end{array}$$

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)

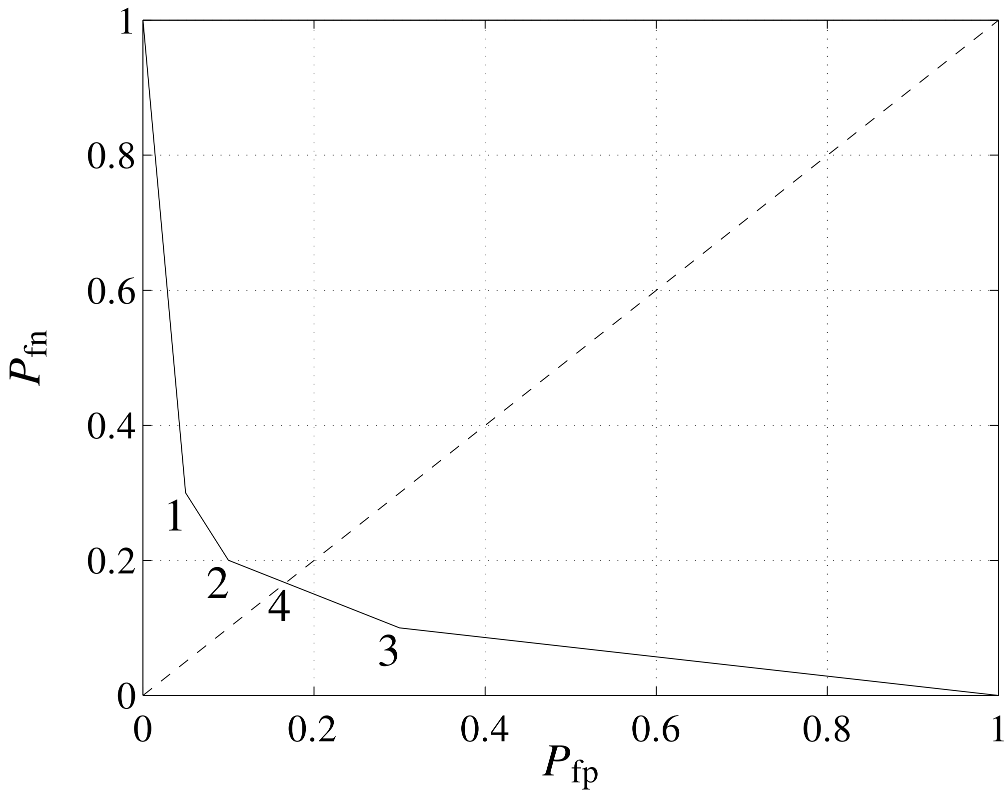
Minimax detector

$$\begin{array}{ll} \text{minimize} & \max\{P_{\text{fp}}, P_{\text{fn}}\} = \max\{(Tp)_2, (Tq)_1\} \\ \text{subject to} & t_{1k} + t_{2k} = 1, \quad t_{ik} \geq 0, \quad i = 1, 2, \quad k = 1, \ldots, n \end{array}$$

an LP; solution is usually not deterministic

Example

$$\begin{bmatrix} p_1 & q_1 \\ p_2 & q_2 \\ p_3 & q_3 \\ p_4 & q_4 \end{bmatrix} = \begin{bmatrix} 0.70 & 0.10 \\ 0.20 & 0.10 \\ 0.05 & 0.70 \\ 0.05 & 0.10 \end{bmatrix}$$



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

Experiment design

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

- 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

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

  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

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

- 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

$$
\begin{array}{ll}
\text{minimize (w.r.t. } \mathbf{S}_+^n) & E = (1/m)\left(\sum_{k=1}^p \lambda_k v_k v_k^T\right)^{-1} \\
\text{subject to} & \lambda \succeq 0, \quad \mathbf{1}^T\lambda = 1
\end{array}
$$

- 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

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

interpretation: minimizes volume of confidence ellipsoids

Dual problem

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

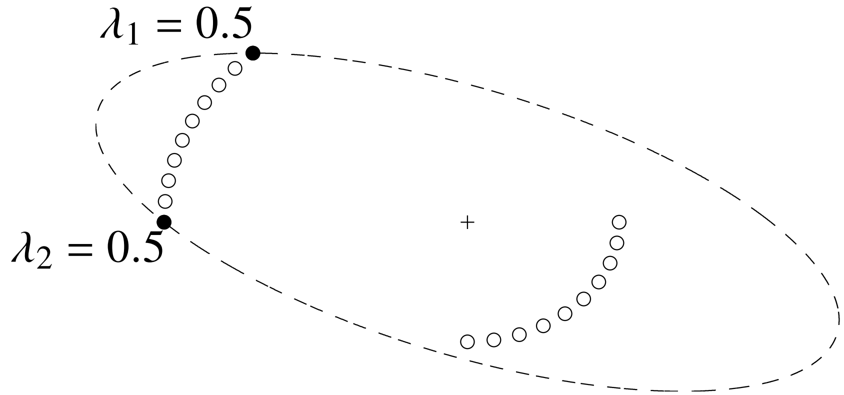
interpretation: $\{x \mid x^T W x \leq 1\}$ is minimum volume ellipsoid centered at origin, that includes all test vectors v_k

Complementary slackness: for λ, 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 ($p = 20$)



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:

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

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

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

dual problem

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

change variable $W = Z/\nu$, and optimize over ν to get dual of page 7.13