## 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

$$
y_{i}=a_{i}^{T} x+v_{i}, \quad i=1, \ldots, m
$$

- $x \in \mathbf{R}^{n}$ 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 $p_{x}(y)=\prod_{i=1}^{m} p\left(y_{i}-a_{i}^{T} x\right)$
maximum likelihood estimate: any solution $x$ of

$$
\operatorname{maximize} \quad l(x)=\sum_{i=1}^{m} \log p\left(y_{i}-a_{i}^{T} x\right)
$$

( $y$ is observed value)

## examples

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

$$
l(x)=-\frac{m}{2} \log \left(2 \pi \sigma^{2}\right)-\frac{1}{2 \sigma^{2}} \sum_{i=1}^{m}\left(a_{i}^{T} x-y_{i}\right)^{2}
$$

ML estimate is LS solution

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

$$
l(x)=-m \log (2 a)-\frac{1}{a} \sum_{i=1}^{m}\left|a_{i}^{T} x-y_{i}\right|
$$

ML estimate is $\ell_{1}$-norm solution

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

$$
l(x)= \begin{cases}-m \log (2 a) & \left|a_{i}^{T} x-y_{i}\right| \leq a, \quad i=1, \ldots, m \\ -\infty & \text { otherwise }\end{cases}
$$

ML estimate is any $x$ with $\left|a_{i}^{T} x-y_{i}\right| \leq a$

## Logistic regression

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

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

- $a, b$ 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 $y_{1}=\cdots=y_{k}=1, y_{k+1}=\cdots=y_{m}=0$ ):

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

concave in $a, b$
example ( $n=1, m=50$ measurements)


- circles show 50 points $\left(u_{i}, y_{i}\right)$
- 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 $p=\left(p_{1}, \ldots, p_{n}\right)$
- hypothesis 2: $X$ was generated by distribution $q=\left(q_{1}, \ldots, q_{n}\right)$


## 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 $t_{1 k}$, hypothesis 2 with probability $t_{2 k}$
- if all elements of $T$ are 0 or 1 , it is called a deterministic detector
detection probability matrix:

$$
D=\left[\begin{array}{cc}
T p & T q
\end{array}\right]=\left[\begin{array}{cc}
1-P_{\mathrm{fp}} & P_{\mathrm{fn}} \\
P_{\mathrm{fp}} & 1-P_{\mathrm{fn}}
\end{array}\right]
$$

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

$$
\begin{array}{ll}
\operatorname{minimize}\left(\text { w.r.t. } \mathbf{R}_{+}^{2}\right) & \left(P_{\mathrm{fp}}, P_{\mathrm{fn}}\right)=\left((T p)_{2},(T q)_{1}\right) \\
\text { subject to } & t_{1 k}+t_{2 k}=1, \quad k=1, \ldots, n \\
& t_{i k} \geq 0, \quad i=1,2, \quad k=1, \ldots, n
\end{array}
$$

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

$$
\begin{array}{ll}
\operatorname{minimize} & (T p)_{2}+\lambda(T q)_{1} \\
\text { subject to } & t_{1 k}+t_{2 k}=1, \quad t_{i k} \geq 0, \quad i=1,2, \quad k=1, \ldots, n
\end{array}
$$

an LP with a simple analytical solution

$$
\left(t_{1 k}, t_{2 k}\right)= \begin{cases}(1,0) & p_{k} \geq \lambda q_{k} \\ (0,1) & p_{k}<\lambda q_{k}\end{cases}
$$

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

$$
\begin{array}{ll}
\operatorname{minimize} & \max \left\{P_{\mathrm{fp}}, P_{\mathrm{fn}}\right\}=\max \left\{(T p)_{2},(T q)_{1}\right\} \\
\text { subject to } & t_{1 k}+t_{2 k}=1, \quad t_{i k} \geq 0, \quad i=1,2, \quad k=1, \ldots, n
\end{array}
$$

an LP; solution is usually not deterministic
example

$$
P=\left[\begin{array}{ll}
0.70 & 0.10 \\
0.20 & 0.10 \\
0.05 & 0.70 \\
0.05 & 0.10
\end{array}\right]
$$


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

- 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 $\left\{x \mid(x-\hat{x})^{T} E^{-1}(x-\hat{x}) \leq \beta\right\}$
experiment design: choose $a_{i} \in\left\{v_{1}, \ldots, v_{p}\right\}$ (a set of possible test vectors) to make $E$ 'small'
vector optimization formulation

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

- 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

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

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


## $D$-optimal design

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

interpretation: minimizes volume of confidence ellipsoids

## dual problem

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

interpretation: $\left\{x \mid x^{T} W x \leq 1\right\}$ is minimum volume ellipsoid centered at origin, that includes all test vectors $v_{k}$
complementary slackness: for $\lambda, W$ primal and dual optimal

$$
\lambda_{k}\left(1-v_{k}^{T} W v_{k}\right)=0, \quad k=1, \ldots, p
$$

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 $X$ :

$$
\begin{array}{cl}
\begin{array}{l}
\text { minimize } \\
\text { subject to } \quad \\
\log \operatorname{det} X^{-1} \\
\end{array}=\sum_{k=1}^{p} \lambda_{k} v_{k} v_{k}^{T}, \quad \lambda \succeq 0, \quad \mathbf{1}^{T} \lambda=1 \\
L(X, \lambda, Z, z, \nu)=\log \operatorname{det} X^{-1}+\operatorname{tr}\left(Z\left(X-\sum_{k=1}^{p} \lambda_{k} v_{k} v_{k}^{T}\right)\right)-z^{T} \lambda+\nu\left(\mathbf{1}^{T} \lambda-1\right)
\end{array}
$$

- 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

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

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

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