## Chapter 31

## Probability and random variables

ap, prob

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### 31.1 Introduction (s.prob,intro)

This appendix summarizes some facts from probability and statistics that are used in developing and analyzing image reconstruction algorithms. This is not intended to be a tutorial introduction; for review see [1].

### 31.2 Conditional probability (s.prob,cond)

For two events $A$ and $B$, the definition of conditional probability is:

$$
\begin{equation*}
\mathrm{P}\{A \mid B\}=\frac{\mathrm{P}\{A, B\}}{\mathrm{P}\{B\}} \tag{31.2.1}
\end{equation*}
$$

Bayes rule is:

$$
\begin{equation*}
\mathrm{P}\{A \mid B\}=\frac{\mathrm{P}\{B \mid A\} \mathrm{P}\{A\}}{\mathrm{P}\{B\}} \tag{31.2.2}
\end{equation*}
$$

If $\left\{A_{i}\right\}$ are disjoint (mutually exclusive) events and $\mathrm{P}\left\{\bigcup_{i} A_{i}\right\}=1$, then the total probability relation is:

$$
\begin{equation*}
\mathrm{P}\{B\}=\sum_{i} \mathrm{P}\left\{B \mid A_{i}\right\} \mathrm{P}\left\{A_{i}\right\} \tag{31.2.3}
\end{equation*}
$$

### 31.3 Discrete distributions

### 31.3.1 Binomial and Multinomial (s,prob,nomial)

Random variable $X$ has a binomial distribution with parameter p if

$$
\mathrm{P}\{X=x\}= \begin{cases}\mathrm{p}, & x=1 \\ 1-\mathrm{p}, & x=0\end{cases}
$$

Random variables $X_{1}, \ldots, X_{M}$ have a multinomial distribution with parameters $\mathrm{p}_{1}, \ldots, \mathrm{p}_{M}$ and $N$ if

$$
\begin{equation*}
\mathrm{P}\left\{X_{1}=x_{1}, \ldots, X_{M}=x_{M}\right\}=\binom{N}{x_{1} x_{2} \ldots x_{M}} \prod_{m=1}^{M} \mathrm{p}_{m} \mathbb{I}_{\left\{\sum_{m=1}^{M} x_{m}=N\right\}} \tag{31.3.1}
\end{equation*}
$$

where $\binom{N}{x_{1} x_{2} \ldots} x_{M} . ~=\frac{N!}{\prod_{m=1}^{M} x_{m}!}$.

### 31.3.2 Poisson (s,prob,poisson)

A Poisson [2, p. 206] random variable $N$ with mean $\mu_{0}$ has the following probability mass function (PMF):

$$
\mathrm{P}\{N=k\}=\frac{1}{k!} \mathrm{e}^{-\mu_{0}} \mu_{0}^{k}, \quad k=0,1, \ldots
$$

We write $N \sim$ Poisson $\left\{\mu_{0}\right\}$. The above PMF is the usual form, but to be more precise, one should consider the case where $\mu_{0}=0$, and write the PMF as follows:

$$
\mathrm{P}\{N=k\}= \begin{cases}1, & \mu_{0}=0, k=0  \tag{31.3.2}\\ \frac{1}{k!} \mathrm{e}^{-\mu_{0}} \mu_{0}^{k}, & \mu_{0}>0, k=0,1, \ldots \\ 0, & \text { otherwise }\end{cases}
$$

The fellowing sections review properties of Poisson random variables are useful for statistical image reconstruction algorithms.

### 31.3.2.1 Moments

The most important moments of $N \sim \operatorname{Poisson}\left\{\mu_{0}\right\}$ are $\mathrm{E}[N]=\mu_{0}, \operatorname{Var}\{N\}=\mu_{0}, \mathrm{E}\left[N^{4}\right]=\mu_{0}+7 \mu_{0}^{2}+6 \mu_{0}^{3}+\mu_{0}^{4}$, $\operatorname{Var}\left\{N^{2}\right\}=\mu_{0}+6 \mu_{0}^{2}+4 \mu_{0}^{3}$. [wiki]

### 31.3.2.2 Bernoulli thinning

Suppose a source transmits $N$ photons of a certain energy along a ray passing through an object towards a specified pixel on the detector. We assume $N$ is a Poisson random variable with mean $\mu_{0}$ as in (31.3.2). Each of the $N$ transmitted photons may either pass unaffected ("survive" passage) or may interact with the object. These are Bernoulli trials since the photons interact independently. From Beer's law [3] we know that the probability of surviving passage is given by

$$
\mathrm{p}=\mathrm{e}^{-\int \mu(z) \mathrm{d} z}
$$

The number of photons $M$ that pass unaffected through the object is a random variable, and this process is called Bernoulli thinning or Bernoulli selection. From Beer's law [3]:

$$
\begin{equation*}
\mathrm{P}\{M=m \mid N=n\}=\binom{n}{m} \mathrm{p}^{m}(1-\mathrm{p})^{n-m}, \quad m=0, \ldots, n . \tag{31.3.3}
\end{equation*}
$$

Using total probability:

$$
\begin{aligned}
\mathrm{P}\{M=m\} & =\sum_{n=0}^{\infty} \mathrm{P}\{M=m \mid N=n\} \mathrm{P}\{N=n\} \\
& =\sum_{n=m}^{\infty}\binom{n}{m} \mathrm{p}^{m}(1-\mathrm{p})^{n-m} \frac{1}{n!} \mathrm{e}^{-\mu_{0}} \mu_{0}^{n}=\frac{1}{m!} \mathrm{e}^{-\mu_{0} \mathrm{p}}\left(\mu_{0} \mathrm{p}\right)^{m}, \quad m=0,1, \ldots
\end{aligned}
$$

Therefore the distribution of photons that survive passage is also Poisson, with mean $\mathrm{E}[M]=\mu_{0} \mathrm{p}$.

### 31.3.2.3 Poisson conditionals

It also is useful to examine the reverse of (31.3.3). By applying Bayes' rule, for $0 \leq m \leq n$ :

$$
\begin{aligned}
\mathrm{P}\{N=n \mid M=m\} & =\frac{\mathrm{P}\{M=m \mid N=n\} \mathrm{P}\{N=n\}}{\mathrm{P}\{M=m\}} \\
& =\frac{\binom{n}{m} p^{m}(1-p)^{n-m} \frac{1}{n!} \mathrm{e}^{-\mu_{0}} \mu_{0}^{n}}{\frac{1}{m!} \mathrm{e}^{-\mu_{0} p}\left(\mu_{0} p\right)^{m}} \\
& =\frac{1}{(n-m)!}\left(\mu_{0}-\mu_{0} p\right)^{n-m} \mathrm{e}^{-\left(\mu_{0}-\mu_{0} p\right)} \\
& =\frac{1}{(n-m)!}(\mathrm{E}[N]-\mathrm{E}[M])^{n-m} \mathrm{e}^{-(\mathrm{E}[N]-\mathrm{E}[M])}
\end{aligned}
$$

Thus, conditioned on $M$, the random variable $N-M$ has a Poisson distribution with mean $\mathrm{E}[N]-\mathrm{E}[M]$. In particular,

$$
\mathrm{E}[N-M \mid M]=\mathrm{E}[N]-\mathrm{E}[M]
$$

which is useful in deriving the transmission EM algorithm [4, 5].

### 31.3.2 4 Sums of Poisson random variables

Suppose $Y=\sum_{k=1}^{K} X_{k}$ where $X_{k} \sim \operatorname{Poisson}\left\{\mu_{k}\right\}$. Then $Y \sim \operatorname{Poisson}\left\{\sum_{k=1}^{K} \mu_{k}\right\}$. Interestingly, there is a converse for this result called Raikov's theorem [6]. If two independent nonnegative random variables have a sum that has a Poisson distribution, then the two random variables also have a Poisson distribution.

### 31.3.2.5 Poisson conditioning and multinomials

Suppose $Y=\sum_{k=1}^{K} X_{k}$ where $X_{k} \sim$ Poisson $\left\{\mu_{k}\right\}$ with each $\mu_{k} \geq 0$. Then, conditioned on the event $[Y=y]$, the collection of random variables $\left(X_{1}, \ldots, X_{K}\right)$ has a multinomial distribution with

$$
\mathrm{E}\left[X_{j} \mid Y=y\right]= \begin{cases}\frac{\mu_{j}}{\sum_{k} \mu_{k}} y, & \sum_{k} \mu_{k}>0, y \geq 0  \tag{31.3.4}\\ 0, & \sum_{k} \mu_{k}=0, y=0 \\ \text { undefined, } & \sum_{k} \mu_{k}=0, y>0\end{cases}
$$

Proof:
Using Bayes rule and the Poisson distributions of the independent $X_{k}$ values:

$$
\begin{aligned}
& \mathrm{P}\left\{X_{1}=x_{1}, \ldots, X_{K}=x_{K} \mid Y=y\right\} \\
& \quad=\frac{\mathrm{P}\left\{Y=y \mid X_{1}=x_{1}, \ldots, X_{K}=x_{K}\right\} \mathrm{P}\left\{X_{1}=x_{1}, \ldots, X_{K}=x_{K}\right\}}{\mathrm{P}\{Y=y\}} \\
& \quad=\mathbb{I}_{\left\{y=x_{1}+\cdots+x_{K}\right\}} \frac{\prod_{k=1}^{K} \mu_{k}^{x_{k}} \mathrm{e}^{-\mu_{k}} / x_{k}!}{\left[\sum_{k} \mu_{k}\right]^{y} \mathrm{e}^{-\sum_{k} \mu_{k} / y!}} \\
& \quad=\mathbb{I}_{\left\{y=x_{1}+\cdots+x_{K}\right\}}\binom{y}{x_{1} \cdots x_{K}} \prod_{j=1}^{K}\left(\frac{\mu_{j}}{\sum_{k} \mu_{k}}\right)^{x_{k}},
\end{aligned}
$$

which is a multinomial distribution with means given by (31.3.4).
One can also show that

$$
\begin{equation*}
\mathrm{E}\left[\prod_{j} t_{j}^{X_{j}} \mid Y=y\right]=\left(\frac{\sum_{k} t_{k} \mu_{k}}{\sum_{k} \mu_{k}}\right)^{y} \tag{31.3.5}
\end{equation*}
$$

a fact that is somewhat useful in deriving an $\alpha$-EM algorithm for Poisson data; see Problem 18.6 and Problem 31.1.

### 31.3.2.6 Poisson sums of multinomials

Let $X_{l}$ be independently and identically distributed multinomial random variables with parameters $\left(p_{1}, \ldots, p_{J} ; 1\right)$, i.e., $\mathrm{P}\left\{X_{l}=j\right\}=\mathrm{p}_{j}, j=1, \ldots, J$. Let $N \sim \operatorname{Poisson}\left\{\mu_{0}\right\}$ and define $Y_{j}=\sum_{l=1}^{N} \mathbb{I}_{\left\{X_{l}=j\right\}}$. Then the $\left\{Y_{j}\right\}$ values have independent Poisson distributions with means $\mathrm{E}\left[Y_{j}\right]=\mu_{0} \mathrm{p}_{j}$.
Proof:
By construction, conditioned in $[N=n]$ the $Y_{j}$ values have a multinomial distribution with parameters $\left(p_{1}, \ldots, p_{J} ; n\right)$. Thus by total probability:

$$
\mathrm{P}\left\{Y_{1}=y_{1}, \ldots, Y_{J}=y_{J}\right\}=\sum_{n=0}^{\infty} \mathrm{P}\left\{Y_{1}=y_{1}, \ldots, Y_{J}=y_{J} \mid N=n\right\} \mathrm{P}\{N=n\}
$$

The only nonzero term in this sum is when $n=\sum_{j=1}^{J} y_{j}$. Thus

$$
\begin{equation*}
\mathrm{P}\left\{Y_{1}=y_{1}, \ldots, Y_{J}=y_{J}\right\}=\frac{n!}{\prod_{j=1}^{J} y_{j}!} \prod_{j=1}^{J} \mathrm{p}_{j}^{y_{j}} \frac{1}{n!} \mathrm{e}^{-\mu_{0}} \mu_{0}^{n}=\prod_{j=1}^{J} \frac{\left(\mu_{0} \mathrm{p}_{j}\right)^{y_{j}}}{y_{j}!} \mathrm{e}^{-\mu_{0} \mathrm{p}_{j}} \tag{31.3.6}
\end{equation*}
$$

### 31.3.2.7 Moments of random sums of IID random variables

Let $X_{1}, X_{2}, \ldots$ denote IID random variables with mean $\mu_{X}$ and variance $\sigma_{X}^{2}$. Often in imaging problems we need the moments of a sum of a random number $N$ of these:

$$
Y=\sum_{n=1}^{N} X_{n}
$$

Often $N$ has a Poisson distribution, but the moments of $Y$ can be found more generally. Using iterated expectation, the mean of $Y$ is:

$$
\begin{equation*}
\mathrm{E}[Y]=\mathrm{E}[\mathrm{E}[Y \mid N]]=\mathrm{E}\left[N \mu_{X}\right]=\mathrm{E}[N] \mu_{X} \tag{31.3.7}
\end{equation*}
$$

Similarly, the second moment of $Y$ is

$$
\begin{aligned}
\mathrm{E}\left[Y^{2}\right] & =\mathrm{E}\left[\mathrm{E}\left[Y^{2} \mid N\right]\right]=\mathrm{E}\left[\sum_{n=1}^{N} \sum_{m=1}^{N} \mathrm{E}\left[X_{n} X_{m}\right]\right]=\mathrm{E}\left[N \mathrm{E}\left[X_{n}^{2}\right]+\left(N^{2}-N\right) \mu_{X}^{2}\right] \\
& =\mathrm{E}\left[N\left(\sigma_{X}^{2}+\mu_{X}^{2}\right)+\left(N^{2}-N\right) \mu_{X}^{2}\right]=\mathrm{E}\left[N \sigma_{X}^{2}+N^{2} \mu_{X}^{2}\right]=\mathrm{E}[N] \sigma_{X}^{2}+\left(\sigma_{N}^{2}+\mathrm{E}^{2}[N]\right) \mu_{X}^{2}
\end{aligned}
$$

Thus the variance of a random sum is

$$
\begin{equation*}
\operatorname{Var}\{Y\}=\mathrm{E}\left[Y^{2}\right]-\mathrm{E}^{2}[Y]=\mathrm{E}[N] \sigma_{X}^{2}+\left(\sigma_{N}^{2}+\mathrm{E}^{2}[N]\right) \mu_{X}^{2}-\mathrm{E}^{2}[N] \mu_{X}^{2}=\mathrm{E}[N] \sigma_{X}^{2}+\sigma_{N}^{2} \mu_{X}^{2} \tag{31.3.8}
\end{equation*}
$$

### 31.4 Continuous distributions

### 31.4.1 Normal or gaussian (s,prob,gauss)

For a gaussian random vector $\boldsymbol{X}$, we write $\boldsymbol{X} \sim \mathrm{N}(\boldsymbol{\mu}, \boldsymbol{K})$ as a short hand for the joint normal pdf

$$
\begin{equation*}
\mathrm{p}(\boldsymbol{x})=\frac{1}{\sqrt{\operatorname{det}\{2 \pi \boldsymbol{K}\}}} \mathrm{e}^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\prime} \boldsymbol{K}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})} \tag{31.4.1}
\end{equation*}
$$

The covariance matrix $\boldsymbol{K}$ is always symmetric positive-semidefinite and is usually positive definite.
We say $\boldsymbol{X} \sim \mathrm{N}\left(\boldsymbol{\mu}_{\boldsymbol{X}}, \boldsymbol{K}_{\boldsymbol{X}}\right)$ and $\boldsymbol{Y} \sim \mathrm{N}\left(\boldsymbol{\mu}_{\boldsymbol{Y}}, \boldsymbol{K}_{\boldsymbol{Y}}\right)$ are jointly distributed gaussian random vectors with covariance $\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}$ if $\left[\begin{array}{l}\boldsymbol{X} \\ \boldsymbol{Y}\end{array}\right] \sim \mathrm{N}(\boldsymbol{\mu}, \boldsymbol{K})$ where $\boldsymbol{\mu}=\left[\begin{array}{l}\boldsymbol{\mu}_{\boldsymbol{X}} \\ \boldsymbol{\mu}_{\boldsymbol{Y}}\end{array}\right]$ and $\boldsymbol{K}=\left[\begin{array}{ll}\boldsymbol{K}_{\boldsymbol{X}} & \operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\} \\ \operatorname{Cov}\{\boldsymbol{Y}, \boldsymbol{X}\} & \boldsymbol{K}_{\boldsymbol{Y}}\end{array}\right]$.

If $\boldsymbol{X}$ and $\boldsymbol{Y}$ are jointly distributed gaussian random vectors, then

$$
\mathrm{E}[\boldsymbol{X} \mid \boldsymbol{Y}=\boldsymbol{y}]=\mathrm{E}[\boldsymbol{X}]+\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}[\operatorname{Cov}\{\boldsymbol{Y}\}]^{-1}(\boldsymbol{y}-\mathrm{E}[\boldsymbol{Y}])
$$

and

$$
\operatorname{Cov}\{\boldsymbol{X} \mid \boldsymbol{Y}=\boldsymbol{y}\}=\operatorname{Cov}\{\boldsymbol{X}\}-\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}[\operatorname{Cov}\{\boldsymbol{Y}\}]^{-1} \operatorname{Cov}\{\boldsymbol{Y}, \boldsymbol{X}\}
$$

If two jointly distributed gaussian random variables are uncorrelated, then they are independent.
Two random variables can each have gaussian distributions yet still not be jointly gaussian distributed; see Problem 3.37.

The following property of gaussian random vectors is useful for deriving Stein's unbiased risk estimate (SURE). If $\boldsymbol{Z} \sim \mathrm{N}\left(\boldsymbol{x}, \sigma^{2} \boldsymbol{I}\right)$ and if $\boldsymbol{h}(\boldsymbol{z})$ is a $n_{\mathrm{p}}$-dimensional vector function for which $\mathrm{E}\left[\left|\frac{\partial}{\partial z_{j}} h_{j}(\boldsymbol{z})\right|\right]<\infty$ for $j=1, \ldots, n_{\mathrm{p}}$, then [7]:

$$
\begin{equation*}
\mathrm{E}\left[\sum_{j=1}^{n_{\mathrm{p}}} h_{j}(\boldsymbol{z}) x_{j}\right]=\mathrm{E}\left[\sum_{j=1}^{n_{\mathrm{p}}} h_{j}(\boldsymbol{z}) z_{j}\right]-\sigma^{2} \mathrm{E}[\operatorname{div}\{\boldsymbol{h}(\boldsymbol{z})\}], \tag{31.4.2}
\end{equation*}
$$

where the divergence is defined as $\operatorname{div}\{\boldsymbol{h}(\boldsymbol{z})\} \triangleq \sum_{j=1}^{n_{\mathrm{p}}} \frac{\partial}{\partial z_{j}} h_{j}(\boldsymbol{z})$.

### 31.4.2 Transformations (s,prob,xform)

The following theorem generalizes the usual such formulas found in engineering probability texts for transformations of random vectors.

Theorem 31.4.1 (See [8, 9] for proofs.)
Let $g: \mathbb{R}^{n} \rightarrow \mathbb{R}^{n}$ be one-to-one and assume that $h=g^{-1}$ is continuous. Assume that, on an open set $\mathcal{S} \subseteq \mathbb{R}^{n}, h$ is continuously differentiable with Jacobian determinant ${ }^{1}|\operatorname{det}\{\nabla h(\boldsymbol{x})\}| \triangleq\left|\operatorname{det}\left\{\frac{\partial}{\partial x_{j}} h_{i}(\boldsymbol{x})\right\}\right|$. Suppose random vector $\boldsymbol{X}$ has pdf $\mathrm{p}(\boldsymbol{x})$ and

$$
\begin{equation*}
\mathrm{P}\left\{\boldsymbol{X} \in h\left(\mathcal{S}^{c}\right)\right\}=\int_{\mathcal{S}^{c}} \mathrm{p}(\boldsymbol{x}) \mathrm{d} \boldsymbol{x}=0 \tag{31.4.3}
\end{equation*}
$$

where $\mathcal{S}^{c}$ denotes the set complement (in $\mathbb{R}^{n}$ ) of $\mathcal{S}$, and $h(\mathcal{A})=\{h(\boldsymbol{x}): \boldsymbol{x} \in \mathcal{A}\}$. Then the pdf of the random vector $\boldsymbol{Y}=g(\boldsymbol{X})$ is given by

$$
\begin{equation*}
\mathrm{p}(\boldsymbol{y})=|\operatorname{det}\{\nabla h(\boldsymbol{y})\}| \mathrm{p}(h(\boldsymbol{y})), \quad \boldsymbol{y} \in \mathcal{S}, \tag{31.4.4}
\end{equation*}
$$

and is zero otherwise.

### 31.5 Covariances (s.prob,cov)

The covariance of a random vector $\boldsymbol{X}$ is defined by:

$$
\operatorname{Cov}\{\boldsymbol{X}\} \triangleq \mathrm{E}\left[(\boldsymbol{X}-\mathrm{E}[\boldsymbol{X}])(\boldsymbol{X}-\mathrm{E}[\boldsymbol{X}])^{\prime}\right]
$$

The cross covariance of a random vector $\boldsymbol{X}$ and a random vector $\boldsymbol{Y}$ is defined by:

$$
\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\} \triangleq \mathrm{E}\left[(\boldsymbol{X}-\mathrm{E}[\boldsymbol{X}])(\boldsymbol{Y}-\mathrm{E}[\boldsymbol{Y}])^{\prime}\right]
$$

## Properties of covariance

[^0]- Covariances are positive-semidefinite matrices: $\operatorname{Cov}\{\boldsymbol{X}\} \succeq \mathbf{0}$
- $\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}=\mathrm{E}\left[\boldsymbol{X} \boldsymbol{Y}^{\prime}\right]-\mathrm{E}[\boldsymbol{X}] \mathrm{E}\left[\boldsymbol{Y}^{\prime}\right]$
- $\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}=\operatorname{Cov}\{\boldsymbol{Y}, \boldsymbol{X}\}^{\prime}$
- $\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{X}\}=\operatorname{Cov}\{\boldsymbol{X}\}$
- $\operatorname{Cov}\{a \boldsymbol{X}+b, c \boldsymbol{Y}+d\}=a c^{*} \operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}$
- $\operatorname{Cov}\{\boldsymbol{A} \boldsymbol{X}, \boldsymbol{B} \boldsymbol{Y}+d\}=\boldsymbol{A} \operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\} \boldsymbol{B}^{\prime}$
- In particular, $\operatorname{Var}\left\{X_{i}\right\}=\boldsymbol{e}_{i}^{\prime} \operatorname{Cov}\{\boldsymbol{X}\} \boldsymbol{e}_{i}$, where $\boldsymbol{e}_{i}$ denotes the $i$ th unit vector
- If non-random vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ have the same size as $\boldsymbol{X}$ and $\boldsymbol{Y}$ respectively, then a version of the Schwarz Inequality is:

$$
\left|\boldsymbol{u}^{\prime} \operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\} \boldsymbol{v}\right| \leq \sqrt{\operatorname{Var}\left\{\boldsymbol{u}^{\prime} \boldsymbol{X}\right\} \operatorname{Var}\left\{\boldsymbol{v}^{\prime} \boldsymbol{Y}\right\}}=\sqrt{\boldsymbol{u}^{\prime} \operatorname{Cov}\{\boldsymbol{X}\} \boldsymbol{u}} \sqrt{\boldsymbol{v}^{\prime} \operatorname{Cov}\{\boldsymbol{Y}\} \boldsymbol{v}}
$$

- In particular, if $X$ and $Y$ are scalar random variables, then the correlation coefficient $\rho_{X, Y} \triangleq \frac{\operatorname{Cov}\{X, Y\}}{\sqrt{\operatorname{Var}\{X\} \operatorname{Var}\{Y\}}}$ is bounded by unity: $\left|\rho_{\boldsymbol{X}, \boldsymbol{Y}}\right| \leq 1$.
- If $\boldsymbol{X}$ and $\boldsymbol{Y}$ are independent r.v.s, then $E[\boldsymbol{X} \boldsymbol{Y}]=\mathrm{E}[\boldsymbol{X}] \mathrm{E}[\boldsymbol{Y}]]$ so $\operatorname{Cov}\{\boldsymbol{X}, \boldsymbol{Y}\}=\mathbf{0}$.
- The reverse is not true in general (uncorrelated does not ensure independence); an exception is gaussian.
- $\operatorname{Cov}\left\{\sum_{i} \boldsymbol{X}_{i}, \sum_{j} \boldsymbol{Y}_{j}\right\}=\sum_{i} \sum_{j} \operatorname{Cov}\left\{\boldsymbol{X}_{i}, \boldsymbol{Y}_{j}\right\}$
- If $\mathrm{E}[\boldsymbol{X}]=\boldsymbol{\mu}$, then using (28.1.7):

$$
\begin{align*}
\mathrm{E}\left[\boldsymbol{X}^{\prime} \boldsymbol{B} \boldsymbol{X}\right] & =\mathrm{E}\left[\operatorname{trace}\left\{\boldsymbol{X}^{\prime} \boldsymbol{B} \boldsymbol{X}\right\}\right]=\mathrm{E}\left[\operatorname{trace}\left\{\boldsymbol{B} \boldsymbol{X} \boldsymbol{X}^{\prime}\right\}\right]=\operatorname{trace}\left\{\boldsymbol{B} \mathrm{E}\left[\boldsymbol{X} \boldsymbol{X}^{\prime}\right]\right\} \\
& =\boldsymbol{\mu}^{\prime} \boldsymbol{B} \boldsymbol{\mu}+\operatorname{trace}\{\boldsymbol{B} \operatorname{Cov}\{\boldsymbol{X}\}\} \tag{31.5.1}
\end{align*}
$$

### 31.6 Standard errors (s.,prob,stderr)

We often estimate the mean, variance, or standard deviation from a sample of $n$ elements and present the estimates with standard errors or error bars (in plots) as well. A standard error of a statistic (or estimator) is the (estimated) standard deviation of the statistic. An error bar is, in a plot, a line which is centered at the estimate with length that is double the standard error. Standard errors mean the statistical fluctuation of estimators, and they are important particularly when one compares two estimates (for example, whether one quantity is higher than the other in a statistically meaningful way). Here we review the standard errors of frequently used estimators of the mean, variance, and standard deviation [10].

### 31.6.1 Normal one sample problem

Let $X_{1}, \ldots, X_{n}$ denote a random sample from $\mathrm{N}\left(\mu, \sigma^{2}\right)$ where both $\mu$ and $\sigma$ are unknown parameters. Define the following two statistics (sample mean and sample variance):

$$
\bar{X}=\frac{1}{n} \sum_{i=1}^{n} X_{i} \text { and } S^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}
$$

### 31.6.2 Mean estimator

The uniformly minimum variance unbiased (UMVU) estimator of $\mu$ is $\bar{X}[11, \mathrm{p} .92]$. Because $\bar{X} \sim \mathcal{N}\left(\mu, \sigma^{2} / n\right)$, the standard error of $\bar{X}$ is

$$
\sigma_{\bar{X}}=\sqrt{\operatorname{Var}\{\bar{X}\}}=\frac{\sigma}{\sqrt{n}}
$$

Hence the natural estimate of $\sigma_{\bar{X}}$ is $\hat{\sigma}_{\bar{X}}=\hat{\sigma} / \sqrt{n}$ For $\hat{\sigma}$, see §31.6.4.

### 31.6.3 Variance estimator

From [11, p. 92], $S^{2}$ is UMVU for $\sigma^{2}$ and

$$
\begin{equation*}
\frac{(n-1) S^{2}}{\sigma^{2}} \sim \chi_{n-1}^{2} \tag{31.6.1}
\end{equation*}
$$

Because the chi-squared distribution with $n-1$ degrees of freedom $\left(\chi_{n-1}^{2}\right)$ has variance $2(n-1)$ [11, p. 31], the standard error of $S^{2}$ is

$$
\sigma_{S^{2}}=\sqrt{\operatorname{Var}\left\{S^{2}\right\}}=\sigma^{2} \sqrt{\frac{2}{n-1}}
$$

Hence the natural estimate is $\hat{\sigma}_{S^{2}}=S^{2} \sqrt{2 /(n-1)}$. It is useful to note

$$
\sigma_{S^{2}} / \sigma^{2}=\hat{\sigma}_{S^{2}} / S^{2}=\sqrt{\frac{2}{n-1}}
$$

Because $\sigma^{2}$ and $S^{2}$ have the square of the units of $X_{i}$, often it is preferable to report estimates of $\sigma$, as described next.

### 31.6.4 Standard deviation estimator

The UMVU estimator of $\sigma$ is $K_{n} S[11$, p. 92] where

$$
K_{n}=\sqrt{\frac{n-1}{2}} \frac{\Gamma\left(\frac{n-1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)}=\sqrt{\frac{n-1}{2}} e^{\ln \Gamma\left(\frac{n-1}{2}\right)-\ln \Gamma\left(\frac{n}{2}\right)},
$$

where the second form is more numerically stable for large values of $n$ when using the "ln gamma function." By setting $K_{n}=1, S$ is a common choice in practice but it is slightly biased. Because

$$
\frac{\sqrt{n-1}}{\sigma} S \sim \chi_{n-1}
$$

[see (31.6.1)] and the chi distribution with $n-1$ degrees of freedom $\left(\chi_{n-1}\right)$ has variance [12, p. 49: typo corrected]

$$
V_{n}=2\left(\frac{n-1}{2}-\frac{\Gamma^{2}\left(\frac{n}{2}\right)}{\Gamma^{2}\left(\frac{n-1}{2}\right)}\right)
$$

the standard error of $K_{n} S$ is

$$
\sigma_{K_{n} S}=\sqrt{\operatorname{Var}\left\{K_{n} S\right\}}=\sigma K_{n} \sqrt{\frac{V_{n}}{n-1}}
$$

To investigate the asymptotic behavior of $\sigma_{K_{n} S}$, we need the following approximation [13, P. 602]:

$$
\begin{equation*}
\frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n-1}{2}\right)}=\sqrt{\frac{n-1}{2}}\left(1-\frac{1}{4(n-1)}+O\left(\frac{1}{n^{2}}\right)\right) \tag{31.6.2}
\end{equation*}
$$

Using (31.6.2), it can be shown that

$$
K_{n}=1+O\left(\frac{1}{n}\right)
$$

and

$$
\begin{aligned}
\sigma_{K_{n} S} & =\frac{\sigma}{\sqrt{2(n-1)}}\left(1+O\left(\frac{1}{n}\right)\right) \\
& =\frac{\sigma}{\sqrt{2(n-1)}}+O\left(\frac{1}{n \sqrt{n}}\right)
\end{aligned}
$$

To summarize,

$$
\begin{align*}
\sigma_{K_{n} S} / \sigma & =\hat{\sigma}_{K_{n} S} /\left(K_{n} S\right)=\frac{K_{n} \sqrt{V_{n}}}{\sqrt{n-1}} \\
& \approx \frac{1}{\sqrt{2(n-1)}} \text { for large } n \tag{31.6.3}
\end{align*}
$$

Fig. 31.6.1 shows a plot of $K_{n}, \sqrt{V_{n}}$, and $K_{n} \sqrt{V_{n}}$ versus $n$. For $n>10$, it seems reasonable to use $K_{n}=1$ and the approximation (31.6.3) for the standard error.


Figure 31.6.1: This plot shows that $K_{n}$ and $\sqrt{V_{n}}$ approach 1 and $1 / \sqrt{2}$, respectively, as $n$ increases.

### 31.7 Fisher information and Cramér-Rao bound (s.prob,fish)

For a statistical model with measurements $\boldsymbol{y}$ distributed according to a distribution $\mathrm{p}(\boldsymbol{y} ; \boldsymbol{x})$ that depends on a parameter vector $\boldsymbol{x}$, an important quantity is the Fisher information matrix defined by

$$
\begin{equation*}
\mathbf{F}(\boldsymbol{x}) \triangleq \mathrm{E}[\nabla \mathrm{~L}(\boldsymbol{x}) \nabla \mathrm{L}(\boldsymbol{x})] \tag{31.7.1}
\end{equation*}
$$

where $\mathrm{L}(\boldsymbol{x}) \triangleq \log \mathrm{p}(\boldsymbol{y} ; \boldsymbol{x})$ denotes the $\log$ likelihood associated with the measurement statistics. Under suitable regularity conditions, an equivalent expression is

$$
\begin{equation*}
\mathbf{F}(\boldsymbol{x})=-\mathrm{E}\left[\nabla^{2} \mathrm{~L}(\boldsymbol{x})\right] \tag{31.7.2}
\end{equation*}
$$

Example 31.7.1 For the linear gaussian model $\boldsymbol{y}=\boldsymbol{A} \boldsymbol{x}+\boldsymbol{\varepsilon}$ where $\boldsymbol{\varepsilon} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Pi})$, the log-likelihood is $\mathrm{L}(\boldsymbol{x}) \equiv$ $-\frac{1}{2}(\boldsymbol{y}-\boldsymbol{A} \boldsymbol{x})^{\prime} \boldsymbol{\Pi}^{-1}(\boldsymbol{y}-\boldsymbol{A} \boldsymbol{x})$ and $\nabla \mathrm{L}(\boldsymbol{x})=\boldsymbol{A}^{\prime} \boldsymbol{\Pi}^{-1}(\boldsymbol{y}-\boldsymbol{A x})=\boldsymbol{A}^{\prime} \boldsymbol{\Pi}^{-1} \varepsilon$ so the Fisher information is

$$
\mathbf{F}=\mathrm{E}\left[A^{\prime} \Pi^{-1} \varepsilon \varepsilon^{\prime} \Pi^{-1} A\right]=\boldsymbol{A}^{\prime} \Pi^{-1} \mathrm{E}\left[\varepsilon \varepsilon^{\prime}\right] \boldsymbol{\Pi}^{-1} \boldsymbol{A}=\boldsymbol{A}^{\prime} \Pi^{-1} \boldsymbol{A}
$$

More generally, for the nonlinear gaussian model $\boldsymbol{y}=\boldsymbol{\mu}(\boldsymbol{x})+\varepsilon$ where $\varepsilon \sim \mathbf{N}(\mathbf{0}, \boldsymbol{\Pi})$, the log-likelihood is $\mathrm{L}(\boldsymbol{x}) \equiv-\frac{1}{2}(\boldsymbol{y}-\boldsymbol{\mu}(\boldsymbol{x}))^{\prime} \boldsymbol{\Pi}^{-1}(\boldsymbol{y}-\boldsymbol{\mu}(\boldsymbol{x}))$ and $\nabla \mathrm{L}(\boldsymbol{x})=(\nabla \boldsymbol{\mu}(\boldsymbol{x})) \boldsymbol{\Pi}^{-1}(\boldsymbol{y}-\boldsymbol{\mu}(\boldsymbol{x}))=(\nabla \boldsymbol{\mu}(\boldsymbol{x})) \boldsymbol{\Pi}^{-1} \varepsilon$, where $\nabla \boldsymbol{\mu}(\boldsymbol{x})$ denotes the $n_{\mathrm{p}} \times n_{\mathrm{d}}$ gradient of $\boldsymbol{\mu}: \mathbb{R}^{n_{\mathrm{p}}} \rightarrow \mathbb{R}^{n_{\mathrm{d}}}$. So the Fisher information is

$$
\begin{equation*}
\mathbf{F}=\mathrm{E}\left[\nabla \boldsymbol{\mu}(\boldsymbol{x}) \boldsymbol{\Pi}^{-1} \varepsilon \varepsilon^{\prime} \boldsymbol{\Pi}^{-1} \nabla \boldsymbol{\mu}(\boldsymbol{x})\right]=\nabla \boldsymbol{\mu}(\boldsymbol{x}) \boldsymbol{\Pi}^{-1} \mathrm{E}\left[\varepsilon \varepsilon^{\prime}\right] \boldsymbol{\Pi}^{-1} \nabla \boldsymbol{\mu}(\boldsymbol{x})=\nabla \boldsymbol{\mu}(\boldsymbol{x}) \boldsymbol{\Pi}^{-1} \nabla \boldsymbol{\mu}(\boldsymbol{x}) . \tag{31.7.3}
\end{equation*}
$$

One reason the Fisher information matrix is important is that under certain regularity conditions, maximum likelihood estimators (MLE) $\hat{\boldsymbol{x}}$ asymptotically have gaussian distributions with covariance $\mathbf{F}^{-1}$. Furthermore, the Cramér-Rao lower bound (CRB) [wiki] states that if $\hat{\boldsymbol{x}}$ is an unbiased estimator for $\boldsymbol{x}$, then the covariance of $\hat{\boldsymbol{x}}$ satisfies

$$
\begin{equation*}
\operatorname{Cov}\{\hat{\boldsymbol{x}}\} \succ \mathbf{F}^{-1} \tag{31.7.4}
\end{equation*}
$$

See $\S 25.18$ for a concise derivation. The only estimator that can achieve the lower bound is the MLE. Even for finite sample sizes, the CRB is often a good approximation to the covariance of a ML estimate:

$$
\operatorname{Cov}\{\hat{\boldsymbol{x}}\} \approx \mathbf{F}^{-1}
$$

### 31.8 Gauss-Markov theorem (s.,prob,gauss-markov)

The Gauss-Markov theorem is a particularly important result from statistical estimation theory that serves as a guide for designing estimators including image reconstruction methods.

Consider the linear model $\boldsymbol{y}=\boldsymbol{A} \boldsymbol{x}+\boldsymbol{\varepsilon}$ where we assume that the noise is zero mean: $\mathrm{E}[\varepsilon]=\mathbf{0}$ and has known covariance: $\operatorname{Cov}\{\varepsilon\}=\boldsymbol{K}$. Note that no other assumptions about the distribution of $\varepsilon$ are made. Now suppose that our goal is to find an unbiased linear estimator of $\boldsymbol{x}$ that has the "smallest possible" variability. This is known as the best linear unbiased estimator (BLUE). Specifically, for a linear estimator of the form

$$
\hat{\boldsymbol{x}}=\boldsymbol{B} \boldsymbol{y}
$$

for some matrix $\boldsymbol{B}$, we want to minimize trace $\{\operatorname{Cov}\{\hat{\boldsymbol{x}}\}\}$ subject to the constraint that $\mathrm{E}[\hat{\boldsymbol{x}}]=\boldsymbol{x}$ for any $\boldsymbol{x}$, i.e., that $\boldsymbol{B} \boldsymbol{A}=\boldsymbol{I}$. The solution is $[14,15]$

$$
\boldsymbol{B}=\left[\boldsymbol{A}^{\prime} \boldsymbol{K}^{-1} \boldsymbol{A}\right]^{-1} \boldsymbol{A}^{\prime} \boldsymbol{K}^{-1}
$$

In other words, the best $\hat{\boldsymbol{x}}$ solves the following weighted least-squares (WLS) problem:

$$
\hat{\boldsymbol{x}}=\underset{\boldsymbol{x}}{\arg \min }\|\boldsymbol{y}-\boldsymbol{A} \boldsymbol{x}\|_{\boldsymbol{W}^{1 / 2}}^{2}=\left[\boldsymbol{A}^{\prime} \boldsymbol{W} \boldsymbol{A}\right]^{-1} \boldsymbol{A}^{\prime} \boldsymbol{W} \boldsymbol{y}
$$

where the weighting is the inverse of the noise covariance:

$$
\boldsymbol{W}=\boldsymbol{K}^{-1}
$$

Therefore, when feasible, we should include weighting based on the inverse of the data covariance for least-squares data consistency terms. Generalizations of this argument to biased estimators are also available [16].

The covariance of this BLUE is

$$
\operatorname{Cov}\{\hat{\boldsymbol{x}}\}=\boldsymbol{B} \operatorname{Cov}\{\boldsymbol{y}\} \boldsymbol{B}^{\prime}=\left[\boldsymbol{A}^{\prime} \boldsymbol{K}^{-1} \boldsymbol{A}\right]^{-1} .
$$

### 31.9 Variable-projection methods for nonlinear least-squares (s.prob,varpro)

For problems with gaussian noise, the ML estimate $\hat{\boldsymbol{\theta}}$ of a parameter vector $\boldsymbol{\theta}$ minimizes a WLS cost function:

$$
\hat{\boldsymbol{\theta}}=\underset{\boldsymbol{\theta}}{\arg \min } \frac{1}{2}\|\boldsymbol{y}-\overline{\boldsymbol{y}}(\boldsymbol{\theta})\|_{\boldsymbol{W}^{1 / 2}}^{2}
$$

where $\overline{\boldsymbol{y}}(\boldsymbol{\theta})$ denotes the model for the measurements. A typical optimization method used for this minimization problem is the Levenberg-Marquardt method [17, 18]. There are a variety of nonlinear least-squares estimation problems where the model is linear in some of the unknown parameters and nonlinear in the other parameters. Mathematically, the overall parameter vector has the form $\boldsymbol{\theta}=(\boldsymbol{x}, \boldsymbol{\alpha})$ where

$$
\overline{\boldsymbol{y}}(\boldsymbol{\theta})=\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{x}
$$

In these cases, the WLS problem becomes

$$
\underset{\boldsymbol{x}, \boldsymbol{\alpha}}{\arg \min } \frac{1}{2}\|\boldsymbol{y}-\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{x}\|_{\boldsymbol{W}^{1 / 2}}^{2} .
$$

This joint estimation problem can be simplified by exploiting the partially linear structure of the model. The resulting approach is called the variable projection method [19].

For any given $\boldsymbol{\alpha}$, the minimizer over $\boldsymbol{x}$ is a linear WLS problem with solution

$$
\hat{\boldsymbol{x}}(\boldsymbol{\alpha})=\underset{\boldsymbol{x}}{\arg \min } \frac{1}{2}\|\boldsymbol{y}-\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{x}\|_{\boldsymbol{W}^{1 / 2}}^{2}=\boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2} \boldsymbol{y}
$$

where $\boldsymbol{B}(\boldsymbol{\alpha}) \triangleq \boldsymbol{W}^{1 / 2} \boldsymbol{A}(\boldsymbol{\alpha})$ and $\boldsymbol{B}^{\dagger}$ denotes the pseudo-inverse of $\boldsymbol{B}$. Usually such problems are over determined, i.e., $\boldsymbol{B}$ is a "tall" matrix with full column rank, in which case

$$
\boldsymbol{B}^{\dagger}=\left[\boldsymbol{B}^{\prime} \boldsymbol{B}\right]^{-1} \boldsymbol{B}^{\prime}
$$

Substituting $\hat{\boldsymbol{x}}(\boldsymbol{\alpha})$ back into the original cost function, the minimization over $\boldsymbol{\alpha}$ becomes

$$
\hat{\boldsymbol{\alpha}}=\underset{\boldsymbol{\alpha}}{\arg \min } \frac{1}{2}\|\boldsymbol{y}-\boldsymbol{A}(\boldsymbol{\alpha}) \hat{\boldsymbol{x}}(\boldsymbol{\alpha})\|_{\boldsymbol{W}^{1 / 2}}^{2}=\underset{\boldsymbol{\alpha}}{\arg \min } \frac{1}{2}\left\|\boldsymbol{y}-\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2} \boldsymbol{y}\right\|_{\boldsymbol{W}^{1 / 2}}^{2}
$$

Now note that (after some simplification):

$$
\begin{gathered}
\left\|\boldsymbol{y}-\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2} \boldsymbol{y}\right\|_{\boldsymbol{W}^{1 / 2}}^{2}=\boldsymbol{y}^{\prime}\left(\boldsymbol{I}-\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2}\right)^{\prime} \boldsymbol{W}\left(\boldsymbol{I}-\boldsymbol{A}(\boldsymbol{\alpha}) \boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2}\right) \boldsymbol{W}^{1 / 2} \boldsymbol{y} \\
=\boldsymbol{y}^{\prime} \boldsymbol{W} \boldsymbol{y}-\boldsymbol{y}^{\prime} \boldsymbol{W}^{1 / 2} \boldsymbol{B}(\boldsymbol{\alpha}) \boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2} \boldsymbol{y}
\end{gathered}
$$

The first term is independent of $\boldsymbol{\alpha}$, so the nonlinear optimization problem simplifies to

$$
\begin{aligned}
\hat{\boldsymbol{\alpha}} & =\underset{\boldsymbol{\alpha}}{\arg \max } \boldsymbol{y}^{\prime} \boldsymbol{W}^{1 / 2} \boldsymbol{B}(\boldsymbol{\alpha}) \boldsymbol{B}^{\dagger}(\boldsymbol{\alpha}) \boldsymbol{W}^{1 / 2} \boldsymbol{y} \\
& =\underset{\alpha}{\arg \max } \boldsymbol{y}^{\prime} \boldsymbol{W} \boldsymbol{A}(\boldsymbol{\alpha})\left[\boldsymbol{A}^{\prime}(\boldsymbol{\alpha}) \boldsymbol{W} \boldsymbol{A}(\boldsymbol{\alpha})\right]^{-1} \boldsymbol{A}^{\prime}(\boldsymbol{\alpha}) \boldsymbol{W} \boldsymbol{y} .
\end{aligned}
$$

Because $\operatorname{dim}(\boldsymbol{\alpha})<\operatorname{dim}(\boldsymbol{\theta})$, less computation is needed to find $\hat{\boldsymbol{\alpha}}$ using this approach. After one finds $\hat{\boldsymbol{\alpha}}$, the final estimate for $\boldsymbol{x}$ is $\hat{\boldsymbol{x}}(\hat{\boldsymbol{\alpha}})$. In the special case where the matrix $\boldsymbol{B}(\boldsymbol{\alpha})$ has orthonormal columns for every possible parameter $\boldsymbol{\alpha}$, then $\boldsymbol{B}^{\dagger}=\boldsymbol{B}^{\prime}$ and the computation further simplifies to

$$
\begin{equation*}
\underset{\boldsymbol{\alpha}}{\arg \max }\left\|\boldsymbol{A}^{\prime}(\boldsymbol{\alpha}) \boldsymbol{W} \boldsymbol{y}\right\|^{2} \tag{31.9.1}
\end{equation*}
$$

The variable projection method has been generalized beyond least squares problems [20]. To avoid expensive exhaustive search over $\boldsymbol{\alpha}$, one can use cover trees methods [21].

Example 31.9.1 Consider the problem of finding the phase of a sinusoid from equally spaced samples: $\bar{y}_{m}(\boldsymbol{\theta})=$ $\sqrt{\frac{1}{M}} x_{1}+\sqrt{\frac{2}{M}} x_{2} \cos (2 \pi m / M+\alpha), \quad m=0, \ldots, M-1$, where $\boldsymbol{\theta}=\left(x_{1}, x_{2}, \alpha\right)$. In this case, if $\boldsymbol{W}=\boldsymbol{I}$, then $\boldsymbol{B}=[\boldsymbol{u} \boldsymbol{c}(\alpha)]$ where $\boldsymbol{u}=\sqrt{\frac{1}{M}} \mathbf{1}$ and $c_{m}(\alpha)=\sqrt{\frac{2}{M}} \cos (2 \pi m / M+\alpha)$. One can verify that this matrix $\boldsymbol{B}(\alpha)$ is orthonormal for any value of $\alpha$. Thus, from (31.9.1) the LS estimate of $\alpha$ is given by by the maximizer of $\left\|\boldsymbol{B}^{\prime}(\alpha) \boldsymbol{y}\right\|^{2}=$ $\left|\boldsymbol{u}^{\prime} \boldsymbol{y}\right|^{2}+\left|\boldsymbol{c}^{\prime}(\alpha) \boldsymbol{y}\right|^{2}$. The first term is independent of $\alpha$, so $\hat{\alpha}$ is the maximizer of $\left|\boldsymbol{c}^{\prime}(\alpha) \boldsymbol{y}\right|=\left|\sum_{m=0}^{M-1} c_{m}^{*}(\alpha) y_{m}\right|=$ $\left|\sum_{m=0}^{M-1} \cos (2 \pi m / M+\alpha) y_{m}\right|=\left|\operatorname{real}\left\{\sum_{m=0}^{M-1} \mathrm{e}^{-\imath 2 \pi m / M} \mathrm{e}^{-\imath \alpha} y_{m}\right\}\right|=\left|\operatorname{real}\left\{\mathrm{e}^{-\imath \alpha} Y_{1}\right\}\right|=\left|\left|Y_{1}\right| \cos \left(\angle Y_{1}-\alpha\right)\right|$. where the first DFT coefficient is $Y_{1}=\sum_{m=0}^{M-1} \mathrm{e}^{-\imath 2 \pi m / M} y_{m}$ and we have assumed that $\boldsymbol{y}$ is real. Thus the LS estimate is $\hat{\alpha}=\angle Y_{1}+k \pi$ where $k$ is any integer.

### 31.10 Entropy (s.,prob,entropy)

The entropy of a random variable, as defined by Shannon [22, 23], is often used (and abused) in imaging problems. In particular, it is useful for multi-modality image registration problems. It has also been studied extensively as a regularization method for image recovery problems.

### 31.10.1 Shannon entropy

For a discrete random variable $X$ having probability mass function (PMF) $\left\{\mathrm{p}_{k}, k=1, \ldots, K\right\}$, the entropy of $X$ is defined by ${ }^{2}$

$$
\begin{equation*}
\mathrm{H}\{X\}=-\sum_{k=1}^{K} \mathrm{p}_{k} \log \mathrm{p}_{k} \tag{31.10.1}
\end{equation*}
$$

Note that like expectation $\mathrm{E}[X]$ and variance $\operatorname{Var}\{X\}$, entropy is defined in terms of the distribution of $X$ and is thus a constant, not a random variable. This definition of entropy has several desirable properties. For example, one can show that

$$
\begin{equation*}
0 \leq \mathrm{H} \leq \log K \tag{31.10.2}
\end{equation*}
$$

The upper bound is achieved by the (discrete) uniform distribution where $\mathrm{p}_{k}=1 / K$. This is the "most random" distribution for a discrete random variable taking $K$ distinct values. The lower bound is achieved when $X$ takes only one value (with probability one), e.g., when $\mathrm{p}_{1}=1, \mathrm{p}_{2}=\cdots=\mathrm{p}_{K}=0$. Such a random variable is not random at all.

In some image recovery problems, notably those based on maximum entropy methods, the 2 D array of image values $f[m, n]$ is treated as if it represents a 2D probability mass function (after suitable normalization), and the "entropy" of such an image is defined as

$$
\begin{equation*}
\mathrm{H}=-\sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \frac{|f[m, n]|}{s} \log \left(\frac{|f[m, n]|}{s}\right) \tag{31.10.3}
\end{equation*}
$$

where $s \triangleq \sum_{m=0}^{M-1} \sum_{n=0}^{N-1}|f[m, n]|$. Often the normalization factor $s$ is ignored. Given an imaging model $g=\boldsymbol{A} f$, typically under-determined, one can try to find $f[m, n]$ to maximize H subject to $\|g=\boldsymbol{A} f\| \leq \varepsilon$. Because the upper bound in (31.10.2) is achieved for uniform, rather than impulsive, distributions, one can expect that the maximum entropy image will be among the smoother images that are sufficiently consistent with the data.

Consider a $N \times M$ digital image $f[m, n]$ with a finite number gray levels $\left\{f_{k}\right\}$, e.g., $\{0,1, \ldots, 255\}$. Whether this image should be viewed as a deterministic function or as a random process is a question of modeling and philosophy. However, one can always define a random variable $X$ by selecting one pixel at random and letting $X$ be the value of the selected pixel. This will be a discrete-valued random variable having probability mass function

$$
\begin{equation*}
\mathrm{p}_{k}=\mathrm{P}\left\{X=f_{k}\right\}=\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \mathbb{I}_{\left\{f[m, n]=f_{k}\right\}} \tag{31.10.4}
\end{equation*}
$$

MIRT
See hist_bin_int.m.
This PMF is simply the histogram of the values of the image $f[m, n]$, normalized by $M N$. Another definition of the entropy of the image $f[m, n]$ uses this PMF:

$$
\begin{align*}
\mathrm{H}_{f} & =\mathrm{H}\{X\}=-\sum_{k=1}^{K} \mathrm{p}_{k} \log \mathrm{p}_{k}  \tag{31.10.5}\\
& =-\sum_{k=1}^{K}\left(\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \mathbb{I}_{\left\{f[m, n]=f_{k}\right\}}\right) \log \left(\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \mathbb{I}_{\left\{f[m, n]=f_{k}\right\}}\right) . \tag{31.10.6}
\end{align*}
$$

Note that this definition differs considerably from (31.10.3), as illustrated in the following example.
Example 31.10.1 Consider an $N \times M$ image $f[m, n]$ that is completely uniform: $f[m, n]=c$. In this case, (31.10.3) evaluates to its maximum $\mathrm{H}=\log (M N)$, whereas (31.10.6) evaluates to its minimum $\mathrm{H}=0$.

[^1]Now suppose that the image $f[m, n]$ is continuous valued, e.g., arbitrary real or complex numbers. (This situation arises in many image registration problems because even if the initial images are discrete valued, interpolation operations can lead to arbitrary gray scale values.) In this situation, the standard "histogram" definition of entropy given in (31.10.6) may not be useful. For example, if every image pixel has a different value, then $K=M N$ and (31.10.6) reduces to $\mathrm{H}=\log (M N)$.

For continuous-valued images, one might be inclined to seek a continuous analogue of (31.10.1). For a continuous random variable with probability density function $\mathrm{p}(x)$, its differential entropy is defined by

$$
\begin{equation*}
\mathrm{h}=-\int \mathrm{p}(x) \log \mathrm{p}(x) \mathrm{d} x \tag{31.10.7}
\end{equation*}
$$

Example 31.10.2 If $X \sim \mathrm{~N}\left(\mu, \sigma^{2}\right)$ then, using (31.4.1), its differential entropy is $\mathrm{h}=\frac{1}{2}\left(1+\log \left(2 \pi \sigma^{2}\right)\right)$, which increases monotonically with $\sigma^{2}$. More generally, if $\boldsymbol{X} \sim \mathbf{N}(\boldsymbol{\mu}, \boldsymbol{K}) \in \mathbb{R}^{d}$ then $\mathrm{h}=\frac{1}{2}(d+\log (\operatorname{det}\{2 \pi \boldsymbol{K}\}))$.

The definition (31.10.7) lacks some of the desirable properties of (31.10.1). For example it can take negative values, as illustrated in Example 31.10 .2 when $\sigma^{2}<1 /(2 \pi e)$. Furthermore, the distribution $\mathrm{p}(x)$ is rarely known in practice for images so this expression seems to be of limited use for inverse problems. One could estimate $\mathrm{p}(x)$ from an image $f[m, n]$ using a kernel density estimate, also known as the Parzen window method:

$$
\hat{\mathrm{p}}(x)=\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} q(f[m, n]-x)
$$

for some nonnegative function $q(\cdot)$ (called the kernel or window) that integrates to unity. Choosing the width of the kernel requires care [24-26]. However, one would still need to sample $x$ to perform numerical calculations, so it seems more direct to work with discrete $x$ values directly as described next.

A simple way to apply (31.10.1) to continuous-valued images would be to quantize those values into $K$ bins. For example, if the image values lie in the range $[0,100)$ then one could use $K$ bins of the form $\mathcal{B}_{k}=[k \Delta,(k+1) \Delta)$ where in this case $\Delta=100 / K$, covering that interval. By analogy with (31.10.4), define the PMF of the quantized values as

$$
\begin{equation*}
\mathrm{p}_{k}=\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \mathbb{I}_{\left\{f[m, n] \in \mathcal{B}_{k}\right\}} \tag{31.10.8}
\end{equation*}
$$

and then use (31.10.1) to define entropy. (Even for discrete-valued images one can use (31.10.8) by neglecting the least-significant bits [27].
MIRT See jf_histn.m.
A limitation of this definition is that $\mathrm{H} \rightarrow \log (M N)$ as $\Delta \rightarrow 0$, if the image values are distinct. Therefore, choosing the bin size $\Delta$ is delicate. Note that if $\Delta$ is small, then $\mathrm{p}_{k} \approx \Delta \mathrm{p}\left(x_{k}\right)$ where $x_{k}=k \Delta$, so

$$
\mathrm{H}=-\sum_{k} \mathrm{p}_{k} \log \mathrm{p}_{k} \approx-\sum_{k} \Delta \mathrm{p}\left(x_{k}\right) \log \left(\Delta \mathrm{p}\left(x_{k}\right)\right) \approx \mathrm{h}-\log \Delta .
$$

Unfortunately, the simple quantization method (31.10.8) is not a continuous function of the image, which prevents the use of gradient-based methods for optimization.

Inspired by the interpolation method of [28], an alternative approach is to use a differentiable kernel $\psi(t)$ to "interpolate" the histogram as follows:

$$
\begin{equation*}
\mathrm{p}_{k}=\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \psi(f[m, n] / \Delta-k), \quad k=k_{\min }, \ldots, k_{\max } \tag{31.10.9}
\end{equation*}
$$

where we assume $\psi(\cdot)$ is nonnegative and satisfies the interpolation property

$$
\sum_{k=-\infty}^{\infty} \psi(t-k)=1, \forall t \in \mathbb{R}
$$

so that $\sum_{k=k_{\min }}^{k_{\max }} \mathrm{p}_{k}=1$ (provided we choose $k_{\min }$ and $k_{\max }$ properly as discussed below). Choosing $\Delta$ and $\psi$ is still important because typically $\mathrm{H} \rightarrow 0$ as $\Delta \rightarrow \infty$ and $\mathrm{H} \rightarrow \log (M N)$ as $\Delta \rightarrow 0$. It might appear that (31.10.9) requires $O(M N K)$ computation. But if we use a kernel $\psi$ with finite support $(-W / 2, W / 2)$, then for each $k$ we need only
evaluate $\psi(t-k)$ for values of $t$ for which $t-k$ lies in the support interval, i.e., $k-W / 2<t<k+W / 2$. For a given data value, the only pertinent values of $k$ are those integers for which $t-W / 2<k<t+W / 2$, i.e.,

$$
\begin{equation*}
\lfloor t-W / 2\rfloor+1 \leq k \leq\lceil t+W / 2\rceil-1 \tag{31.10.10}
\end{equation*}
$$

The number of such $k$ values is $\lceil t+W / 2\rceil-\lfloor t-W / 2\rfloor-1 \leq\lceil W\rceil$ using (29.12.2). So this method requires $O(M N\lceil W\rceil)$ computation if implemented efficiently.

Based on (31.10.10), the smallest and largest relevant values of $k$ are respectively $k_{\min }=\left\lfloor f_{\min } / \Delta-W / 2\right\rfloor+1$ and $k_{\text {max }}=\left\lfloor f_{\text {min }} / \Delta+W / 2\right\rfloor-1$.

If $\psi(\cdot)$ is differentiable, then $\mathrm{p}_{k}$ is a differentiable function of the image, facilitating gradient-based optimization. Substituting (31.10.9) into (31.10.1) and differentiating the resulting entropy definition yields

$$
\begin{aligned}
\frac{\partial}{\partial f[m, n]} \mathrm{H} & =-\sum_{k}\left[\left(\frac{\partial}{\partial f} \mathrm{p}_{k}\right) \log \mathrm{p}_{k}+\frac{\mathrm{p}_{k}}{\mathrm{p}_{k}}\left(\frac{\partial}{\partial f} \mathrm{p}_{k}\right)\right]=-\sum_{k}\left(\frac{\partial}{\partial f} \mathrm{p}_{k}\right) \log \mathrm{p}_{k}-\frac{\partial}{\partial f} \sum_{k} \mathrm{p}_{k} \\
& =-\sum_{k}\left(\frac{\partial}{\partial f} \mathrm{p}_{k}\right) \log \mathrm{p}_{k}=\frac{1}{M N \Delta}\left(\sum_{k} \dot{\psi}(f[m, n] / \Delta-k) \log \mathrm{p}_{k}\right)
\end{aligned}
$$

Again, by using an interpolator $\psi$ with finite support, gradient computation is also $O(M N\lceil W\rceil)$. In particular, by using a quadratic B -spline for $\psi$, the derivative operation is akin to linear interpolation.
See kde_pmf1.m and kde_pmf2.m
The literature describes many methods for choosing the parameter $\Delta$. One simple rule of thumb that has been advocated for a gaussian window $q(\cdot)$ is to choose

$$
\Delta=0.9 \min (\sigma, \mathrm{IQR} / 1.34) /(M N)^{1 / 5}
$$

where $\sigma$ is the sample standard deviation of the image values and IQR is the inter-quartile range [29, p. 48]. For another kernel $\psi$, such as a quadratic B-spline, one can scale $\Delta$ according to the relative FWHM of $\psi$ and a gaussian kernel.
MIRT See kde_pmf_width.

### 31.10.2 Joint entropy

For a pair of discrete random variables $X, Y$ having joint probability mass function $\mathrm{p}_{k l}=\mathrm{P}\left\{X=x_{k}, Y=y_{l}\right\}$, for $k=1, \ldots, K, l=1, \ldots, L$, the joint entropy of $X$ and $Y$ is defined by

$$
\begin{equation*}
\mathrm{H}\{X, Y\}=-\sum_{k=1}^{K} \sum_{l=1}^{L} \mathrm{p}_{k l} \log \mathrm{p}_{k l} . \tag{31.10.11}
\end{equation*}
$$

An important property of this definition is

$$
\begin{equation*}
\max (\mathrm{H}\{X\}, \mathrm{H}\{Y\}) \leq \mathrm{H}\{X, Y\} \leq \mathrm{H}\{X\}+\mathrm{H}\{Y\} \tag{31.10.12}
\end{equation*}
$$

The latter inequality is called subadditivity. The upper bound is reached when $X$ and $Y$ are stastistically independent. Joint entropy has been studied for multi-modality image registration problems [27, 30-32] and for certain multimodality regularization methods [33-35].

Given a pair of images $f[m, n]$ and $g[m, n]$ (possibly continuous valued), the joint histogram analog of (31.10.9) is

$$
\mathrm{p}_{k l}=\frac{1}{M N} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \psi\left(f[m, n] / \Delta_{f}-k\right) \psi\left(g[m, n] / \Delta_{g}-l\right), \quad k=1, \ldots, K, \quad l=1, \ldots, L
$$

where now it may be appropriate to allow $\Delta_{f}$ and $\Delta_{g}$ to differ.

### 31.10.3 Mutual information

A related quantity for a pair of jointly distributed random variables is their mutual information:

$$
\begin{equation*}
\mathrm{MI}(X, Y)=\mathrm{H}\{X\}+\mathrm{H}\{Y\}-\mathrm{H}\{X, Y\} \tag{31.10.13}
\end{equation*}
$$

This quantity has been used for multi-modality image registration problems [28, 36, 37]. It also has been explored for multi-modality regularization methods [33, 38, 39]. Numerous variations have been proposed, e.g., [40, 41], including normalized mutual information

$$
\begin{equation*}
\mathrm{NMI}(X, Y)=\frac{\mathrm{H}\{X\}+\mathrm{H}\{Y\}}{\mathrm{H}\{X, Y\}} \tag{31.10.14}
\end{equation*}
$$

and entropy correlation coefficient

$$
\begin{equation*}
\mathrm{ECC}(X, Y)=\sqrt{2-2 \frac{\mathrm{H}\{X, Y\}}{\mathrm{H}\{X\}+\mathrm{H}\{Y\}}} . \tag{31.10.15}
\end{equation*}
$$

An important practical consideration in all such similarity measures for image registration is whether they exhibit overlap invariance [42, 43].

### 31.10.4 Cross entropy

Yet another related quantity that has been used in imaging problems is the cross entropy of two random variables [44, 45], defined by (cf. §18.4.3):

$$
\mathrm{H}\{X\}+\mathrm{D}(\boldsymbol{p} \| \boldsymbol{q})=\left(-\sum_{k} \mathrm{p}_{k} \log \mathrm{p}_{k}\right)+\left(\sum_{k} \mathrm{p}_{k} \log \frac{\mathrm{p}_{k}}{\mathrm{q}_{k}}-\mathrm{p}_{k}+\mathrm{q}_{k}\right)=-\sum_{k} \mathrm{p}_{k} \log \mathrm{q}_{k}
$$

where $\mathrm{p}_{k}$ denotes the PMF of $X$ and $\mathrm{q}_{k}$ denotes the PMF of $Y$. This quantity has been used for multi-modality regularization methods [46-48] and for image reconstruction [46, 47, 49-53].

### 31.11 Problems (s,prob,prob)

Problem 31.1 Prove (31.3.5).
(Solve?)
Problem 31.2 Random variable $\boldsymbol{x}$ has a mixture distribution: $\mathrm{p}(\boldsymbol{x})=\sum_{k} \pi_{k} \mathrm{p}_{k}(\boldsymbol{x})$ where $\pi_{k} \geq 0$ and $\sum_{k} \pi_{k}=1$ and $\mathrm{p}_{k}(\boldsymbol{x})$ is the distribution of $\boldsymbol{x}$ for the kth class. Assume that the conditional distribution $\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{x})$ of the measurements $\boldsymbol{y}$ is independent of the class of $\boldsymbol{x}$. Show that the MMSE estimate of $\boldsymbol{x}$ from $\boldsymbol{y}$ is

$$
\hat{\boldsymbol{x}}=\sum_{k} \pi_{k} \frac{\mathrm{p}\left(\boldsymbol{y} \mid \mathcal{A}_{k}\right)}{\mathrm{p}(y)} \mathrm{E}\left[\boldsymbol{x} \mid \boldsymbol{y}, \mathcal{A}_{k}\right],
$$

where $\mathcal{A}_{k}$ denotes the event that $\boldsymbol{x}$ is drawn from the kth class, i.e., $\mathrm{p}_{k}(\boldsymbol{x})=\mathrm{p}\left(\boldsymbol{x} \mid \mathcal{A}_{k}\right)$. This estimator expression simplifies further when $\boldsymbol{x}$ is a mixture of gaussians and $\boldsymbol{y} \mid \boldsymbol{x} \sim \mathrm{N}(\boldsymbol{A} \boldsymbol{x}, \boldsymbol{\Pi})$.

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[^0]:    ${ }^{1}$ We use $|\operatorname{det}\{\boldsymbol{A}\}|$ to denote the absolute value of the determinant of a matrix $\boldsymbol{A}$.

[^1]:    ${ }^{2}$ In digital communications, often the logarithm base 2 is used, but this is just a scale factor that is unimportant for imaging problems.

