## PATTERN RECOGNITION and MACHINE LEARNING

CHAPTER 2: PROBABILITY DISTRIBUTIONS

## Parametric Distributions

Basic building blocks: $p(\mathbf{x} \mid \boldsymbol{\theta})$
Need to determine $\boldsymbol{\theta}$ given $\left\{\mathbf{x}_{1}, \ldots, \mathrm{x}_{N}\right\}$ Representation: $\boldsymbol{\theta}^{\star}$ or $p(\boldsymbol{\theta})$ ?

Recall Curve Fitting

$$
p(t \mid x, \mathbf{x}, \mathbf{t})=\int p(t \mid x, \mathbf{w}) p(\mathbf{w} \mid \mathbf{x}, \mathbf{t}) \mathrm{d} \mathbf{w}
$$



## Binary Variables (1)

Coin flipping: heads=1, tails=0

$$
p(x=1 \mid \mu)=\mu
$$

Bernoulli Distribution

$$
\begin{aligned}
\operatorname{Bern}(x \mid \mu) & =\mu^{x}(1-\mu)^{1-x} \\
\mathbb{E}[x] & =\mu \\
\operatorname{var}[x] & =\mu(1-\mu)
\end{aligned}
$$

## Binary Variables (2)

## $N$ coin flips:

$$
p(m \text { heads } \mid N, \mu)
$$

## Binomial Distribution

$$
\begin{gathered}
\operatorname{Bin}(m \mid N, \mu)=\binom{N}{m} \mu^{m}(1-\mu)^{N-m} \\
\mathbb{E}[m] \equiv \sum_{m=0}^{N} m \operatorname{Bin}(m \mid N, \mu)=N \mu \\
\operatorname{var}[m] \equiv \sum_{m=0}^{N}(m-\mathbb{E}[m])^{2} \operatorname{Bin}(m \mid N, \mu)=N \mu(1-\mu)
\end{gathered}
$$

## Binomial Distribution



## Parameter Estimation (1)

## ML for Bernoulli

Given: $\mathcal{D}=\left\{x_{1}, \ldots, x_{N}\right\}, m$ heads (1), N-m tails (0)

$$
\begin{gathered}
p(\mathcal{D} \mid \mu)=\prod_{n=1}^{N} p\left(x_{n} \mid \mu\right)=\prod_{n=1}^{N} \mu^{x_{n}}(1-\mu)^{1-x_{n}} \\
\ln p(\mathcal{D} \mid \mu)=\sum_{n=1}^{N} \ln p\left(x_{n} \mid \mu\right)=\sum_{n=1}^{N}\left\{x_{n} \ln \mu+\left(1-x_{n}\right) \ln (1-\mu)\right\} \\
\mu_{\mathrm{ML}}=\frac{1}{N} \sum_{n=1}^{N} x_{n}=\frac{m}{N}
\end{gathered}
$$

## Parameter Estimation (2)

Example: $\quad \mathcal{D}=\{1,1,1\} \rightarrow \mu_{\mathrm{ML}}=\frac{3}{3}=1$
Prediction: all future tosses will land heads up

Overfitting to $\mathcal{D}$

## Beta Distribution

Distribution over $\mu \in[0,1]$.

$$
\begin{aligned}
\operatorname{Beta}(\mu \mid a, b) & =\frac{\Gamma(a+b)}{\Gamma(a) \Gamma(b)} \mu^{a-1}(1-\mu)^{b-1} \\
\mathbb{E}[\mu] & =\frac{a}{a+b} \\
\operatorname{var}[\mu] & =\frac{a b}{(a+b)^{2}(a+b+1)}
\end{aligned}
$$

## Bayesian Bernoulli

$$
\begin{aligned}
p\left(\mu \mid a_{0}, b_{0}, \mathcal{D}\right) & \propto p(\mathcal{D} \mid \mu) p\left(\mu \mid a_{0}, b_{0}\right) \\
& =\left(\prod_{n=1}^{N} \mu^{x_{n}}(1-\mu)^{1-x_{n}}\right) \operatorname{Beta}\left(\mu \mid a_{0}, b_{0}\right) \\
& \propto \mu^{m+a_{0}-1}(1-\mu)^{(N-m)+b_{0}-1} \\
& \propto \operatorname{Beta}\left(\mu \mid a_{N}, b_{N}\right) \\
a_{N}= & a_{0}+m \quad b_{N}=b_{0}+(N-m)
\end{aligned}
$$

The Beta distribution provides the conjugate prior for the Bernoulli distribution.

## Beta Distribution



## Prior • Likelihood = Posterior





## Properties of the Posterior

As the size of the data set, $N$, increase

$$
\begin{aligned}
a_{N} & \rightarrow m \\
b_{N} & \rightarrow N-m \\
\mathbb{E}[\mu] & =\frac{a_{N}}{a_{N}+b_{N}} \rightarrow \frac{m}{N}=\mu_{\mathrm{ML}} \\
\operatorname{var}[\mu] & =\frac{a_{N} b_{N}}{\left(a_{N}+b_{N}\right)^{2}\left(a_{N}+b_{N}+1\right)} \rightarrow 0
\end{aligned}
$$

## Prediction under the Posterior

What is the probability that the next coin toss will land heads up?

$$
\begin{aligned}
p\left(x=1 \mid a_{0}, b_{0}, \mathcal{D}\right) & =\int_{0}^{1} p(x=1 \mid \mu) p\left(\mu \mid a_{0}, b_{0}, \mathcal{D}\right) \mathrm{d} \mu \\
& =\int_{0}^{1} \mu p\left(\mu \mid a_{0}, b_{0}, \mathcal{D}\right) \mathrm{d} \mu \\
& =\mathbb{E}\left[\mu \mid a_{0}, b_{0}, \mathcal{D}\right]=\frac{a_{N}}{b_{N}}
\end{aligned}
$$

## Multinomial Variables

$$
\begin{gathered}
\text { 1-of- } K \text { coding scheme: } \mathbf{x}=(0,0,1,0,0,0)^{\mathrm{T}} \\
p(\mathbf{x} \mid \boldsymbol{\mu})=\prod_{k=1}^{K} \mu_{k}^{x_{k}} \\
\forall k: \mu_{k} \geqslant 0 \quad \text { and } \sum_{k=1}^{K} \mu_{k}=1 \\
\mathbb{E}[\mathbf{x} \mid \boldsymbol{\mu}]=\sum_{\mathbf{x}} p(\mathbf{x} \mid \boldsymbol{\mu}) \mathbf{x}=\left(\mu_{1}, \ldots, \mu_{K}\right)^{\mathrm{T}}=\boldsymbol{\mu} \\
\sum_{\mathbf{x}} p(\mathbf{x} \mid \boldsymbol{\mu})=\sum_{k=1}^{K} \mu_{k}=1
\end{gathered}
$$

## ML Parameter estimation

Given: $\mathcal{D}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{N}\right\}$

$$
p(\mathcal{D} \mid \boldsymbol{\mu})=\prod_{n=1}^{N} \prod_{k=1}^{K} \mu_{k}^{x_{n k}}=\prod_{k=1}^{K} \mu_{k}^{\left(\sum_{n} x_{n k}\right)}=\prod_{k=1}^{K} \mu_{k}^{m_{k}}
$$

Ensure $\sum_{k} \mu_{k}=1$, use a Lagrange multiplier, $\lambda$.

$$
\begin{gathered}
\sum_{k=1}^{K} m_{k} \ln \mu_{k}+\lambda\left(\sum_{k=1}^{K} \mu_{k}-1\right) \\
\mu_{k}=-m_{k} / \lambda \quad \mu_{k}^{\mathrm{ML}}=\frac{m_{k}}{N}
\end{gathered}
$$

## The Multinomial Distribution

$$
\begin{aligned}
\operatorname{Mult}\left(m_{1}, m_{2}, \ldots, m_{K} \mid \boldsymbol{\mu}, N\right) & =\binom{N}{m_{1} m_{2} \ldots m_{K}} \prod_{k=1}^{K} \mu_{k}^{m_{k}} \\
\mathbb{E}\left[m_{k}\right] & =N \mu_{k} \\
\operatorname{var}\left[m_{k}\right] & =N \mu_{k}\left(1-\mu_{k}\right) \\
\operatorname{cov}\left[m_{j} m_{k}\right] & =-N \mu_{j} \mu_{k}
\end{aligned}
$$

## The Dirichlet Distribution

$$
\begin{aligned}
& \operatorname{Dir}(\boldsymbol{\mu} \mid \boldsymbol{\alpha})=\frac{\Gamma\left(\alpha_{0}\right)}{\Gamma\left(\alpha_{1}\right) \cdots \Gamma\left(\alpha_{K}\right)} \prod_{k=1}^{K} \mu_{k}^{\alpha_{k}-1} \\
& \alpha_{0}=\sum_{k=1}^{K} \alpha_{k} \\
& \text { Conjugate prior for the } \\
& \text { multinomial distribution. }
\end{aligned}
$$

## Bayesian Multinomial (1)

$$
\begin{gathered}
p(\boldsymbol{\mu} \mid \mathcal{D}, \boldsymbol{\alpha}) \propto p(\mathcal{D} \mid \boldsymbol{\mu}) p(\boldsymbol{\mu} \mid \boldsymbol{\alpha}) \propto \prod_{k=1}^{K} \mu_{k}^{\alpha_{k}+m_{k}-1} \\
p(\boldsymbol{\mu} \mid \mathcal{D}, \boldsymbol{\alpha})=\operatorname{Dir}(\boldsymbol{\mu} \mid \boldsymbol{\alpha}+\mathbf{m}) \\
=\frac{\Gamma\left(\alpha_{0}+N\right)}{\Gamma\left(\alpha_{1}+m_{1}\right) \cdots \Gamma\left(\alpha_{K}+m_{K}\right)} \prod_{k=1}^{K} \mu_{k}^{\alpha_{k}+m_{k}-1}
\end{gathered}
$$

## Bayesian Multinomial (2)


$\alpha_{k}=10^{-1}$

$\alpha_{k}=10^{0}$

$\alpha_{k}=10^{1}$

## The Gaussian Distribution



## Central Limit Theorem

The distribution of the sum of $N$ i.i.d. random variables becomes increasingly Gaussian as $N$ grows.
Example: $N$ uniform $[0,1]$ random variables.




## Geometry of the Multivariate Gaussian

$$
\begin{aligned}
& \Delta^{2}=(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) \\
& \boldsymbol{\Sigma}^{-1}=\sum_{i=1}^{D} \frac{1}{\lambda_{i}} \mathbf{u}_{i} \mathbf{u}_{i}^{\mathrm{T}} \\
& \Delta^{2}=\sum_{i=1}^{D} \frac{y_{i}^{2}}{\lambda_{i}} \\
& y_{i}=\mathbf{u}_{i}^{\mathrm{T}}(\mathbf{x}-\boldsymbol{\mu})
\end{aligned}
$$



## Moments of the Multivariate Gaussian (1)

$$
\begin{aligned}
\mathbb{E}[\mathbf{x}] & =\frac{1}{(2 \pi)^{D / 2}} \frac{1}{|\boldsymbol{\Sigma}|^{1 / 2}} \int \exp \left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\} \mathbf{x} \mathrm{d} \mathbf{x} \\
& =\frac{1}{(2 \pi)^{D / 2}} \frac{1}{|\boldsymbol{\Sigma}|^{1 / 2}} \int \exp \left\{-\frac{1}{2} \mathbf{z}^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} \mathbf{z}\right\}(\mathbf{z}+\boldsymbol{\mu}) \mathrm{d} \mathbf{z}
\end{aligned}
$$

thanks to anti-symmetry of $z$

$$
\mathbb{E}[\mathbf{x}]=\mu
$$

## Moments of the Multivariate Gaussian (2)

$$
\begin{gathered}
\mathbb{E}\left[\mathbf{x x ^ { \mathrm { T } }}\right]=\boldsymbol{\mu} \boldsymbol{\mu}^{\mathrm{T}}+\boldsymbol{\Sigma} \\
\operatorname{cov}[\mathbf{x}]=\mathbb{E}\left[(\mathbf{x}-\mathbb{E}[\mathbf{x}])(\mathbf{x}-\mathbb{E}[\mathbf{x}])^{\mathrm{T}}\right]=\boldsymbol{\Sigma}
\end{gathered}
$$


$(a)$



## Partitioned Gaussian Distributions

$$
\begin{gathered}
p(\mathbf{x})=\mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
\mathbf{x}=\binom{\mathbf{x}_{a}}{\mathbf{x}_{b}} \quad \boldsymbol{\mu}=\binom{\boldsymbol{\mu}_{a}}{\boldsymbol{\mu}_{b}} \quad \boldsymbol{\Sigma}=\left(\begin{array}{ll}
\boldsymbol{\Sigma}_{a a} & \boldsymbol{\Sigma}_{a b} \\
\boldsymbol{\Sigma}_{b a} & \boldsymbol{\Sigma}_{b b}
\end{array}\right) \\
\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1}
\end{gathered} \quad \boldsymbol{\Lambda}=\left(\begin{array}{ll}
\boldsymbol{\Lambda}_{a a} & \boldsymbol{\Lambda}_{a b} \\
\boldsymbol{\Lambda}_{b a} & \boldsymbol{\Lambda}_{b b}
\end{array}\right) .
$$

## Partitioned Conditionals and Marginals

$$
\begin{gathered}
p\left(\mathbf{x}_{a} \mid \mathbf{x}_{b}\right)=\mathcal{N}\left(\mathbf{x}_{a} \mid \boldsymbol{\mu}_{a \mid b}, \boldsymbol{\Sigma}_{a \mid b}\right) \\
\boldsymbol{\Sigma}_{a \mid b}=\boldsymbol{\Lambda}_{a a}^{-1}=\boldsymbol{\Sigma}_{a a}-\boldsymbol{\Sigma}_{a b} \boldsymbol{\Sigma}_{b b}^{-1} \boldsymbol{\Sigma}_{b a} \\
\boldsymbol{\mu}_{a \mid b}=\boldsymbol{\Sigma}_{a \mid b}\left\{\boldsymbol{\Lambda}_{a a} \boldsymbol{\mu}_{a}-\boldsymbol{\Lambda}_{a b}\left(\mathbf{x}_{b}-\boldsymbol{\mu}_{b}\right)\right\} \\
=\boldsymbol{\mu}_{a}-\boldsymbol{\Lambda}_{a a}^{-1} \boldsymbol{\Lambda}_{a b}\left(\mathbf{x}_{b}-\boldsymbol{\mu}_{b}\right) \\
=\boldsymbol{\mu}_{a}+\boldsymbol{\Sigma}_{a b} \boldsymbol{\Sigma}_{b b}^{-1}\left(\mathbf{x}_{b}-\boldsymbol{\mu}_{b}\right) \\
\\
p\left(\mathbf{x}_{a}\right)=\int p\left(\mathbf{x}_{a}, \mathbf{x}_{b}\right) \mathrm{d} \mathbf{x}_{b} \\
\end{gathered}
$$

## Partitioned Conditionals and Marginals




## Bayes' Theorem for Gaussian Variables

Given

$$
\begin{aligned}
p(\mathbf{x}) & =\mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}, \mathbf{\Lambda}^{-1}\right) \\
p(\mathbf{y} \mid \mathbf{x}) & =\mathcal{N}\left(\mathbf{y} \mid \mathbf{A} \mathbf{x}+\mathbf{b}, \mathbf{L}^{-1}\right)
\end{aligned}
$$

we have

$$
\begin{aligned}
p(\mathbf{y}) & =\mathcal{N}\left(\mathbf{y} \mid \mathbf{A} \boldsymbol{\mu}+\mathbf{b}, \mathbf{L}^{-1}+\mathbf{A} \mathbf{\Lambda}^{-1} \mathbf{A}^{\mathrm{T}}\right) \\
p(\mathbf{x} \mid \mathbf{y}) & =\mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\Sigma}\left\{\mathbf{A}^{\mathrm{T}} \mathbf{L}(\mathbf{y}-\mathbf{b})+\boldsymbol{\Lambda} \boldsymbol{\mu}\right\}, \boldsymbol{\Sigma}\right)
\end{aligned}
$$

where

$$
\boldsymbol{\Sigma}=\left(\boldsymbol{\Lambda}+\mathbf{A}^{\mathrm{T}} \mathbf{L} \mathbf{A}\right)^{-1}
$$

## Maximum Likelihood for the Gaussian (1)

Given i.i.d. data $\mathbf{X}=\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{N}\right)^{\mathrm{T}}$, the log likelihood function is given by

$$
\ln p(\mathbf{X} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})=-\frac{N D}{2} \ln (2 \pi)-\frac{N}{2} \ln |\boldsymbol{\Sigma}|-\frac{1}{2} \sum_{n=1}^{N}\left(\mathbf{x}_{n}-\boldsymbol{\mu}\right)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_{n}-\boldsymbol{\mu}\right)
$$

Sufficient statistics

$$
\sum_{n=1}^{N} \mathbf{x}_{n} \quad \sum_{n=1}^{N} \mathbf{x}_{n} \mathbf{x}_{n}^{\mathrm{T}}
$$

## Maximum Likelihood for the Gaussian (2)

Set the derivative of the log likelihood function to zero,

$$
\frac{\partial}{\partial \boldsymbol{\mu}} \ln p(\mathbf{X} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})=\sum_{n=1}^{N} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_{n}-\boldsymbol{\mu}\right)=0
$$

and solve to obtain

Similarly

$$
\boldsymbol{\mu}_{\mathrm{ML}}=\frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{n}
$$

$$
\boldsymbol{\Sigma}_{\mathrm{ML}}=\frac{1}{N} \sum_{n=1}^{N}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}\right)\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}\right)^{\mathrm{T}}
$$

## Maximum Likelihood for the Gaussian (3)

Under the true distribution

$$
\begin{aligned}
\mathbb{E}\left[\boldsymbol{\mu}_{\mathrm{ML}}\right] & =\boldsymbol{\mu} \\
\mathbb{E}\left[\boldsymbol{\Sigma}_{\mathrm{ML}}\right] & =\frac{N-1}{N} \boldsymbol{\Sigma}
\end{aligned}
$$

Hence define

$$
\widetilde{\boldsymbol{\Sigma}}=\frac{1}{N-1} \sum_{n=1}^{N}\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}\right)\left(\mathbf{x}_{n}-\boldsymbol{\mu}_{\mathrm{ML}}\right)^{\mathrm{T}}
$$

## Sequential Estimation

Contribution of the $N^{\text {th }}$ data point, $\mathbf{x}_{N}$

$$
\begin{aligned}
\boldsymbol{\mu}_{\mathrm{ML}}^{(N)} & =\frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{n} \\
& =\frac{1}{N} \mathbf{x}_{N}+\frac{1}{N} \sum_{n=1}^{N-1} \mathbf{x}_{n} \\
& =\frac{1}{N} \mathbf{x}_{N}+\frac{N-1}{N} \boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)} \\
& =\boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)}+\frac{1}{N}\left(\mathbf{x}_{N}-\boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)}\right) \\
\longrightarrow & \\
& \\
& \text { correction given } \mathbf{x}_{N}
\end{aligned}
$$

## The Robbins-Monro Algorithm (1)

Consider $\theta$ and $z$ governed by $p(z, \theta)$ and define the regression function

$$
f(\theta) \equiv \mathbb{E}[z \mid \theta]=\int z p(z \mid \theta) \mathrm{d} z
$$

Seek $\theta^{\star}$ such that $f\left(\theta^{\star}\right)=0$.

## The Robbins-Monro Algorithm (2)



Assume we are given samples from $p(z, \theta)$, one at the time.

## The Robbins-Monro Algorithm (3)

Successive estimates of $\theta^{\star}$ are then given by

$$
\theta^{(N)}=\theta^{(N-1)}-a_{N-1} z\left(\theta^{(N-1)}\right)
$$

Conditions on $a_{N}$ for convergence :

$$
\lim _{N \rightarrow \infty} a_{N}=0 \quad \sum_{N=1}^{\infty} a_{N}=\infty \quad \sum_{N=1}^{\infty} a_{N}^{2}<\infty
$$

## Robbins-Monro for Maximum Likelihood (1)

Regarding

$$
-\lim _{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^{N} \frac{\partial}{\partial \theta} \ln p\left(x_{n} \mid \theta\right)=\mathbb{E}_{x}\left[-\frac{\partial}{\partial \theta} \ln p(x \mid \theta)\right]
$$

as a regression function, finding its root is equivalent to finding the maximum likelihood solution $\theta_{\mathrm{ML}}$. Thus

$$
\theta^{(N)}=\theta^{(N-1)}-a_{N-1} \frac{\partial}{\partial \theta^{(N-1)}}\left[-\ln p\left(x_{N} \mid \theta^{(N-1)}\right)\right] .
$$

## Robbins-Monro for Maximum Likelihood (2)

Example: estimate the mean of a Gaussian.

$$
\begin{aligned}
z & =\frac{\partial}{\partial \mu_{\mathrm{ML}}}\left[-\ln p\left(x \mid \mu_{\mathrm{ML}}, \sigma^{2}\right)\right] \\
& =-\frac{1}{\sigma^{2}}\left(x-\mu_{\mathrm{ML}}\right)
\end{aligned}
$$

The distribution of $z$ is Gaussian with mean $\mu-\mu_{\mathrm{ML}}$.

For the Robbins-Monro update equation, $a_{N}=\sigma^{2} / N$.


## Bayesian Inference for the Gaussian (1)

Assume $\sigma^{2}$ is known. Given i.i.d. data $\mathbf{x}=\left\{x_{1}, \ldots, x_{N}\right\}$, the likelihood function for $\mu$ is given by

$$
p(\mathbf{x} \mid \mu)=\prod_{n=1}^{N} p\left(x_{n} \mid \mu\right)=\frac{1}{\left(2 \pi \sigma^{2}\right)^{N / 2}} \exp \left\{-\frac{1}{2 \sigma^{2}} \sum_{n=1}^{N}\left(x_{n}-\mu\right)^{2}\right\} .
$$

This has a Gaussian shape as a function of $\mu$ (but it is not a distribution over $\mu$ ).

## Bayesian Inference for the Gaussian (2)

Combined with a Gaussian prior over $\mu$,

$$
p(\mu)=\mathcal{N}\left(\mu \mid \mu_{0}, \sigma_{0}^{2}\right)
$$

this gives the posterior

$$
p(\mu \mid \mathbf{x}) \propto p(\mathbf{x} \mid \mu) p(\mu)
$$

Completing the square over $\mu$, we see that

$$
p(\mu \mid \mathbf{x})=\mathcal{N}\left(\mu \mid \mu_{N}, \sigma_{N}^{2}\right)
$$

## Bayesian Inference for the Gaussian (3)

... where

$$
\begin{aligned}
\mu_{N} & =\frac{\sigma^{2}}{N \sigma_{0}^{2}+\sigma^{2}} \mu_{0}+\frac{N \sigma_{0}^{2}}{N \sigma_{0}^{2}+\sigma^{2}} \mu_{\mathrm{ML}}, \quad \mu_{\mathrm{ML}}=\frac{1}{N} \sum_{n=1}^{N} x_{n} \\
\frac{1}{\sigma_{N}^{2}} & =\frac{1}{\sigma_{0}^{2}}+\frac{N}{\sigma^{2}}
\end{aligned}
$$

Note:

|  | $N=0$ | $N \rightarrow \infty$ |
| :---: | :---: | :---: |
| $\mu_{N}$ | $\mu_{0}$ | $\mu_{\mathrm{ML}}$ |
| $\sigma_{N}^{2}$ | $\sigma_{0}^{2}$ | 0 |

## Bayesian Inference for the Gaussian (4)

Example: $p(\mu \mid \mathbf{x})=\mathcal{N}\left(\mu \mid \mu_{N}, \sigma_{N}^{2}\right)$ for $N=0,1,2$ and 10 .


## Bayesian Inference for the Gaussian (5)

Sequential Estimation

$$
\begin{aligned}
p(\mu \mid \mathbf{x}) & \propto p(\mu) p(\mathbf{x} \mid \mu) \\
& =\left[p(\mu) \prod_{n=1}^{N-1} p\left(x_{n} \mid \mu\right)\right] p\left(x_{N} \mid \mu\right) \\
& \propto \mathcal{N}\left(\mu \mid \mu_{N-1}, \sigma_{N-1}^{2}\right) p\left(x_{N} \mid \mu\right)
\end{aligned}
$$

The posterior obtained after observing $N-1$ data points becomes the prior when we observe the $N^{\text {th }}$ data point.

## Bayesian Inference for the Gaussian (6)

Now assume $\mu$ is known. The likelihood function for $\lambda=1 / \sigma^{2}$ is given by

$$
p(\mathbf{x} \mid \lambda)=\prod_{n=1}^{N} \mathcal{N}\left(x_{n} \mid \mu, \lambda^{-1}\right) \propto \lambda^{N / 2} \exp \left\{-\frac{\lambda}{2} \sum_{n=1}^{N}\left(x_{n}-\mu\right)^{2}\right\} .
$$

This has a Gamma shape as a function of $\lambda$.

## Bayesian Inference for the Gaussian (7)

The Gamma distribution

$$
\begin{gathered}
\operatorname{Gam}(\lambda \mid a, b)=\frac{1}{\Gamma(a)} b^{a} \lambda^{a-1} \exp (-b \lambda) \\
\mathbb{E}[\lambda]=\frac{a}{b}
\end{gathered} \quad \operatorname{var}[\lambda]=\frac{a}{b^{2}} \quad .
$$





## Bayesian Inference for the Gaussian (8)

Now we combine a Gamma prior, $\operatorname{Gam}\left(\lambda \mid a_{0}, b_{0}\right)$, with the likelihood function for $\lambda$ to obtain

$$
p(\lambda \mid \mathbf{x}) \propto \lambda^{a_{0}-1} \lambda^{N / 2} \exp \left\{-b_{0} \lambda-\frac{\lambda}{2} \sum_{n=1}^{N}\left(x_{n}-\mu\right)^{2}\right\}
$$

which we recognize as $\operatorname{Gam}\left(\lambda \mid a_{N}, b_{N}\right)$ with

$$
\begin{aligned}
& a_{N}=a_{0}+\frac{N}{2} \\
& b_{N}=b_{0}+\frac{1}{2} \sum_{n=1}^{N}\left(x_{n}-\mu\right)^{2}=b_{0}+\frac{N}{2} \sigma_{\mathrm{ML}}^{2} .
\end{aligned}
$$

## Bayesian Inference for the Gaussian (9)

If both $\mu$ and $\lambda$ are unknown, the joint likelihood function is given by

$$
\begin{aligned}
& p(\mathbf{x} \mid \mu, \lambda)=\prod_{n=1}^{N}\left(\frac{\lambda}{2 \pi}\right)^{1 / 2} \exp \left\{-\frac{\lambda}{2}\left(x_{n}-\mu\right)^{2}\right\} \\
& \\
& \propto\left[\lambda^{1 / 2} \exp \left(-\frac{\lambda \mu^{2}}{2}\right)\right]^{N} \exp \left\{\lambda \mu \sum_{n=1}^{N} x_{n}-\frac{\lambda}{2} \sum_{n=1}^{N} x_{n}^{2}\right\} .
\end{aligned}
$$

We need a prior with the same functional dependence on $\mu$ and $\lambda$.

## Bayesian Inference for the Gaussian (10)

## The Gaussian-gamma distribution

$$
\begin{aligned}
& p(\mu, \lambda)=\mathcal{N}\left(\mu \mid \mu_{0},(\beta \lambda)^{-1}\right) \operatorname{Gam}(\lambda \mid a, b) \\
& \propto \quad \exp \{\underbrace{-\frac{\beta \lambda}{2}\left(\mu-\mu_{0}\right)^{2}}\} \underbrace{\lambda^{a-1} \exp \{-b \lambda\}}
\end{aligned}
$$

- Quadratic in $\mu$. - Gamma distribution over $\lambda$.
- Linear in $\lambda . \quad$ - Independent of $\mu$.


## Bayesian Inference for the Gaussian (11)

The Gaussian-gamma distribution


## Bayesian Inference for the Gaussian (12)

Multivariate conjugate priors

- $\boldsymbol{\mu}$ unknown, $\boldsymbol{\Lambda}$ known: $p(\boldsymbol{\mu})$ Gaussian.
- $\boldsymbol{\Lambda}$ unknown, $\boldsymbol{\mu}$ known: $p(\boldsymbol{\Lambda})$ Wishart,

$$
\mathcal{W}(\boldsymbol{\Lambda} \mid \mathbf{W}, \nu)=B|\boldsymbol{\Lambda}|^{(\nu-D-1) / 2} \exp \left(-\frac{1}{2} \operatorname{Tr}\left(\mathbf{W}^{-1} \boldsymbol{\Lambda}\right)\right)
$$

- $\boldsymbol{\Lambda}$ and $\boldsymbol{\mu}$ unknown: $p(\boldsymbol{\mu}, \boldsymbol{\Lambda})$ GaussianWishart, $p\left(\boldsymbol{\mu}, \boldsymbol{\Lambda} \mid \boldsymbol{\mu}_{0}, \beta, \mathbf{W}, \nu\right)=$

$$
\mathcal{N}\left(\boldsymbol{\mu} \mid \boldsymbol{\mu}_{0},(\beta \boldsymbol{\Lambda})^{-1}\right) \mathcal{W}(\boldsymbol{\Lambda} \mid \mathbf{W}, \nu)
$$

## Student's t-Distribution

$$
\begin{aligned}
p(x \mid \mu, a, b) & =\int_{0}^{\infty} \mathcal{N}\left(x \mid \mu, \tau^{-1}\right) \operatorname{Gam}(\tau \mid a, b) \mathrm{d} \tau \\
& =\int_{0}^{\infty} \mathcal{N}\left(x \mid \mu,(\eta \lambda)^{-1}\right) \operatorname{Gam}(\eta \mid \nu / 2, \nu / 2) \mathrm{d} \eta \\
& =\frac{\Gamma(\nu / 2+1 / 2)}{\Gamma(\nu / 2)}\left(\frac{\lambda}{\pi \nu}\right)^{1 / 2}\left[1+\frac{\lambda(x-\mu)^{2}}{\nu}\right]^{-\nu / 2-1 / 2} \\
& =\operatorname{St}(x \mid \mu, \lambda, \nu)
\end{aligned}
$$

where

$$
\lambda=a / b \quad \eta=\tau b / a \quad \nu=2 a .
$$

Infinite mixture of Gaussians.

## Student's t-Distribution



|  | $\nu=1$ | $\nu \rightarrow \infty$ |
| :---: | :---: | :---: |
| $\operatorname{St}(x \mid \mu, \lambda, \nu)$ | Cauchy | $\mathcal{N}\left(x \mid \mu, \lambda^{-1}\right)$ |

## Student's t-Distribution

Robustness to outliers: Gaussian vs t-distribution.



## Student's t-Distribution

The $D$-variate case:

$$
\begin{aligned}
\operatorname{St}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Lambda}, \nu) & =\int_{0}^{\infty} \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu},(\eta \boldsymbol{\Lambda})^{-1}\right) \operatorname{Gam}(\eta \mid \nu / 2, \nu / 2) \mathrm{d} \eta \\
& =\frac{\Gamma(D / 2+\nu / 2)}{\Gamma(\nu / 2)} \frac{|\boldsymbol{\Lambda}|^{1 / 2}}{(\pi \nu)^{D / 2}}\left[1+\frac{\Delta^{2}}{\nu}\right]^{-D / 2-\nu / 2}
\end{aligned}
$$

Where $\Delta^{2}=(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu})$.
Properties:

$$
\begin{aligned}
\mathbb{E}[\mathbf{x}] & =\boldsymbol{\mu}, & & \text { if } \nu>1 \\
\operatorname{cov}[\mathbf{x}] & =\frac{\nu}{(\nu-2)} \boldsymbol{\Lambda}^{-1}, & & \text { if } \nu>2 \\
\operatorname{mode}[\mathbf{x}] & =\boldsymbol{\mu} & &
\end{aligned}
$$

## Periodic variables

- Examples: calendar time, direction, ...
- We require

$$
\begin{aligned}
p(\theta) & \geqslant 0 \\
\int_{0}^{2 \pi} p(\theta) \mathrm{d} \theta & =1 \\
p(\theta+2 \pi) & =p(\theta) .
\end{aligned}
$$

## von Mises Distribution (1)

This requirement is satisfied by

$$
p\left(\theta \mid \theta_{0}, m\right)=\frac{1}{2 \pi I_{0}(m)} \exp \left\{m \cos \left(\theta-\theta_{0}\right)\right\}
$$

where

$$
I_{0}(m)=\frac{1}{2 \pi} \int_{0}^{2 \pi} \exp \{m \cos \theta\} \mathrm{d} \theta
$$

is the $0^{\text {th }}$ order modified Bessel function of the $1^{\text {st }}$ kind.

## von Mises Distribution (4)


$3 \pi / 4$
$m=5, \theta_{0}=\pi / 4$
$m=1, \theta_{0}=3 \pi / 4$

## Maximum Likelihood for von Mises

Given a data set, $\mathcal{D}=\left\{\theta_{1}, \ldots, \theta_{N}\right\}$, the log likelihood function is given by

$$
\ln p\left(\mathcal{D} \mid \theta_{0}, m\right)=-N \ln (2 \pi)-N \ln I_{0}(m)+m \sum_{n=1}^{N} \cos \left(\theta_{n}-\theta_{0}\right)
$$

Maximizing with respect to $\theta_{0}$ we directly obtain

$$
\theta_{0}^{\mathrm{ML}}=\tan ^{-1}\left\{\frac{\sum_{n} \sin \theta_{n}}{\sum_{n} \cos \theta_{n}}\right\} .
$$

Similarly, maximizing with respect to $m$ we get

$$
\frac{I_{1}\left(m_{\mathrm{ML}}\right)}{I_{0}\left(m_{\mathrm{ML}}\right)}=\frac{1}{N} \sum_{n=1}^{N} \cos \left(\theta_{n}-\theta_{0}^{\mathrm{ML}}\right)
$$

which can be solved numerically for $m_{\mathrm{ML}}$.

## Mixtures of Gaussians (1)

## Old Faithful data set




## Mixtures of Gaussians (2)

Combine simple models into a complex model:

$$
p(\mathbf{x})=\sum_{k=1}^{K} \pi_{k} \underbrace{\mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)}_{\text {Mixing coefficient }}
$$



$$
\forall k: \pi_{k} \geqslant 0 \quad \sum_{k=1}^{K} \pi_{k}=1
$$

## Mixtures of Gaussians (3)



## Mixtures of Gaussians (4)

Determining parameters $\boldsymbol{\mu}, \boldsymbol{\Sigma}$, and $\boldsymbol{\pi}$ using maximum log likelihood

$$
\ln p(\mathbf{X} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})=\sum_{n=1}^{N} \underbrace{\ln \left\{\sum_{k=1}^{K} \pi_{k} \mathcal{N}\left(\mathbf{x}_{n} \mid \boldsymbol{\mu}_{k}, \boldsymbol{\Sigma}_{k}\right)\right\}}_{\text {Log of a sum; no closed form maximum. }}
$$

Solution: use standard, iterative, numeric optimization methods or the expectation maximization algorithm (Chapter 9).

## The Exponential Family (1)

$$
p(\mathbf{x} \mid \boldsymbol{\eta})=h(\mathbf{x}) g(\boldsymbol{\eta}) \exp \left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right\}
$$

where $\boldsymbol{\eta}$ is the natural parameter and

$$
g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right\} \mathrm{d} \mathbf{x}=1
$$

so $g(\boldsymbol{\eta})$ can be interpreted as a normalization coefficient.

## The Exponential Family (2.1)

## The Bernoulli Distribution

$$
\begin{aligned}
p(x \mid \mu) & =\operatorname{Bern}(x \mid \mu)=\mu^{x}(1-\mu)^{1-x} \\
& =\exp \{x \ln \mu+(1-x) \ln (1-\mu)\} \\
& =(1-\mu) \exp \left\{\ln \left(\frac{\mu}{1-\mu}\right) x\right\}
\end{aligned}
$$

Comparing with the general form we see that

$$
\eta=\ln \left(\frac{\mu}{1-\mu}\right) \quad \text { and SO } \quad \mu=\underbrace{\sigma(\eta)=\frac{1}{1+\exp (-\eta)}}_{\text {Logistic sigmoid }}
$$

## The Exponential Family (2.2)

The Bernoulli distribution can hence be written as

$$
p(x \mid \eta)=\sigma(-\eta) \exp (\eta x)
$$

where

$$
\begin{aligned}
u(x) & =x \\
h(x) & =1 \\
g(\eta) & =1-\sigma(\eta)=\sigma(-\eta)
\end{aligned}
$$

## The Exponential Family (3.1)

## The Multinomial Distribution

$$
p(\mathbf{x} \mid \boldsymbol{\mu})=\prod_{k=1}^{M} \mu_{k}^{x_{k}}=\exp \left\{\sum_{k=1}^{M} x_{k} \ln \mu_{k}\right\}=h(\mathbf{x}) g(\boldsymbol{\eta}) \exp \left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)
$$

where, $\mathbf{x}=\left(x_{1}, \ldots, x_{M}\right)^{\mathrm{T}}, \boldsymbol{\eta}=\left(\eta_{1}, \ldots, \eta_{M}\right)^{\mathrm{T}}$ and

$$
\begin{aligned}
\eta_{k} & =\ln \mu_{k} \\
\mathbf{u}(\mathbf{x}) & =\mathbf{x} \\
h(\mathbf{x}) & =1 \\
g(\boldsymbol{\eta}) & =1
\end{aligned}
$$

NOTE: The ' ${ }_{k}$ parameters are not independent since the corresponding $\mu_{k}$ must satisfy

$$
\sum_{k=1}^{M} \mu_{k}=1
$$

## The Exponential Family (3.2)

Let $\mu_{M}=1-\sum_{k=1}^{M-1} \mu_{k}$. This leads to

$$
\eta_{k}=\ln \left(\frac{\mu_{k}}{1-\sum_{j=1}^{M-1} \mu_{j}}\right) \text { and } \mu_{k}=\underbrace{\frac{\exp \left(\eta_{k}\right)}{1+\sum_{j=1}^{M-1} \exp \left(\eta_{j}\right)}}_{\operatorname{sottmax}} .
$$

Here the $\eta_{k}$ parameters are independent. Note that

$$
0 \leqslant \mu_{k} \leqslant 1 \text { and } \sum_{k=1}^{M-1} \mu_{k} \leqslant 1 .
$$

## The Exponential Family (3.3)

The Multinomial distribution can then be written as

$$
p(\mathbf{x} \mid \boldsymbol{\mu})=h(\mathbf{x}) g(\boldsymbol{\eta}) \exp \left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)
$$

where

$$
\begin{aligned}
\boldsymbol{\eta} & =\left(\eta_{1}, \ldots, \eta_{M-1}, 0\right)^{\mathrm{T}} \\
\mathbf{u}(\mathbf{x}) & =\mathbf{x} \\
h(\mathbf{x}) & =1 \\
g(\boldsymbol{\eta}) & =\left(1+\sum_{k=1}^{M-1} \exp \left(\eta_{k}\right)\right)^{-1} .
\end{aligned}
$$

## The Exponential Family (4)

## The Gaussian Distribution

$$
\begin{aligned}
p\left(x \mid \mu, \sigma^{2}\right) & =\frac{1}{\left(2 \pi \sigma^{2}\right)^{1 / 2}} \exp \left\{-\frac{1}{2 \sigma^{2}}(x-\mu)^{2}\right\} \\
& =\frac{1}{\left(2 \pi \sigma^{2}\right)^{1 / 2}} \exp \left\{-\frac{1}{2 \sigma^{2}} x^{2}+\frac{\mu}{\sigma^{2}} x-\frac{1}{2 \sigma^{2}} \mu^{2}\right\} \\
& =h(x) g(\boldsymbol{\eta}) \exp \left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(x)\right\}
\end{aligned}
$$

where

$$
\begin{array}{rlrl}
\boldsymbol{\eta} & =\binom{\mu / \sigma^{2}}{-1 / 2 \sigma^{2}} & & h(\mathbf{x})=(2 \pi)^{-1 / 2} \\
\mathbf{u}(x) & =\binom{x}{x^{2}} & g(\boldsymbol{\eta})=\left(-2 \eta_{2}\right)^{1 / 2} \exp \left(\frac{\eta_{1}^{2}}{4 \eta_{2}}\right) .
\end{array}
$$

## ML for the Exponential Family (1)

From the definition of $g(\boldsymbol{\eta})$ we get

$$
\nabla g(\boldsymbol{\eta}) \underbrace{\int h(\mathbf{x}) \exp \left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right\} \mathrm{d} \mathbf{x}}_{1 / g(\boldsymbol{\eta})}+\underbrace{g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right\} \mathbf{u}(\mathbf{x}) \mathrm{d} \mathbf{x}}_{\mathbb{E}[\mathbf{u}(\mathbf{x})]}=0
$$

Thus

$$
-\nabla \ln g(\boldsymbol{\eta})=\mathbb{E}[\mathbf{u}(\mathbf{x})]
$$

## ML for the Exponential Family (2)

Give a data set, $\mathrm{X}=\left\{\mathrm{x}_{1}, \ldots, \mathrm{x}_{N}\right\}$, the likelihood function is given by

$$
p(\mathbf{X} \mid \boldsymbol{\eta})=\left(\prod_{n=1}^{N} h\left(\mathbf{x}_{n}\right)\right) g(\boldsymbol{\eta})^{N} \exp \left\{\boldsymbol{\eta}^{\mathrm{T}} \sum_{n=1}^{N} \mathbf{u}\left(\mathbf{x}_{n}\right)\right\} .
$$

Thus we have

$$
-\nabla \ln g\left(\boldsymbol{\eta}_{\mathrm{ML}}\right)=\frac{1}{N} \underbrace{\sum_{n=1}^{N} \mathbf{u}\left(\mathbf{x}_{n}\right)}_{\text {Sufficient statistic }}
$$

## Conjugate priors

For any member of the exponential family, there exists a prior

$$
p(\boldsymbol{\eta} \mid \boldsymbol{\chi}, \nu)=f(\boldsymbol{\chi}, \nu) g(\boldsymbol{\eta})^{\nu} \exp \left\{\nu \boldsymbol{\eta}^{\mathrm{T}} \boldsymbol{\chi}\right\} .
$$

Combining with the likelihood function, we get
$p(\boldsymbol{\eta} \mid \mathbf{X}, \boldsymbol{\chi}, \nu) \propto g(\boldsymbol{\eta})^{\nu+N} \exp \left\{\boldsymbol{\eta}^{\mathrm{T}}\left(\sum_{n=1}^{N} \mathbf{u}\left(\mathbf{x}_{n}\right)+\nu \boldsymbol{\chi}\right)\right\}$.
Prior corresponds to $\nu$ pseudo-observations with value $\boldsymbol{\chi}$.

## Noninformative Priors (1)

With little or no information available a-priori, we might choose a non-informative prior.

- $\lambda$ discrete, $K$-nomial : $p(\lambda)=1 / K$.
- $\lambda \in[a, b]$ real and bounded: $p(\lambda)=1 / b-a$.
- $\lambda$ real and unbounded: improper!

A constant prior may no longer be constant after a change of variable; consider $p(\lambda)$ constant and $\lambda=\eta^{2}$ :

$$
p_{\eta}(\eta)=p_{\lambda}(\lambda)\left|\frac{\mathrm{d} \lambda}{\mathrm{~d} \eta}\right|=p_{\lambda}\left(\eta^{2}\right) 2 \eta \propto \eta
$$

## Noninformative Priors (2)

Translation invariant priors. Consider

$$
p(x \mid \mu)=f(x-\mu)=f((x+c)-(\mu+c))=f(\widehat{x}-\widehat{\mu})=p(\widehat{x} \mid \widehat{\mu}) .
$$

For a corresponding prior over $\mu$, we have

$$
\int_{A}^{B} p(\mu) \mathrm{d} \mu=\int_{A-c}^{B-c} p(\mu) \mathrm{d} \mu=\int_{A}^{B} p(\mu-c) \mathrm{d} \mu
$$

for any $A$ and $B$. Thus $p(\mu)=p(\mu-c)$ and $p(\mu)$ must be constant.

## Noninformative Priors (3)

Example: The mean of a Gaussian, $\mu$; the conjugate prior is also a Gaussian,

$$
p\left(\mu \mid \mu_{0}, \sigma_{0}^{2}\right)=\mathcal{N}\left(\mu \mid \mu_{0}, \sigma_{0}^{2}\right)
$$

As $\sigma_{0}^{2} \rightarrow \infty$, this will become constant over $\mu$.

## Noninformative Priors (4)

Scale invariant priors. Consider $p(x \mid \sigma)=(1 / \sigma) f(x / \sigma)$ and make the change of variable $\widehat{x}=c x$

$$
p_{\widehat{x}}(\widehat{x})=p_{x}(x)\left|\frac{\mathrm{d} x}{\mathrm{~d} \widehat{x}}\right|=p_{x}\left(\frac{\widehat{x}}{c}\right) \frac{1}{c}=\frac{1}{c \sigma} f\left(\frac{\widehat{x}}{c \sigma}\right)=p_{x}(\widehat{x} \mid \widehat{\sigma}) .
$$

For a corresponding prior over $\sigma$, we have

$$
\int_{A}^{B} p(\sigma) \mathrm{d} \sigma=\int_{A / c}^{B / c} p(\sigma) \mathrm{d} \sigma=\int_{A}^{B} p\left(\frac{1}{c} \sigma\right) \frac{1}{c} \mathrm{~d} \sigma
$$

for any $A$ and $B$. Thus $p(\sigma) \propto 1 / \sigma$ and so this prior is improper too. Note that this corresponds to $p(\ln \sigma)$ being constant.

## Noninformative Priors (5)

Example: For the variance of a Gaussian, $\sigma^{2}$, we have

$$
\mathcal{N}\left(x \mid \mu, \sigma^{2}\right) \propto \sigma^{-1} \exp \left\{-((x-\mu) / \sigma)^{2}\right\} .
$$

If $\lambda=1 / \sigma^{2}$ and $p(\sigma) \propto 1 / \sigma$, then $p(\lambda) \propto 1 / \lambda$.
We know that the conjugate distribution for $\lambda$ is the Gamma distribution,

$$
\operatorname{Gam}\left(\lambda \mid a_{0}, b_{0}\right) \propto \lambda^{a_{0}-1} \exp \left(-b_{0} \lambda\right)
$$

A noninformative prior is obtained when $a_{0}=0$ and $b_{0}=0$.

## Nonparametric Methods (1)

Parametric distribution models are restricted to specific forms, which may not always be suitable; for example, consider modelling a multimodal distribution with a single, unimodal model.

Nonparametric approaches make few assumptions about the overall shape of the distribution being modelled.

## Nonparametric Methods (2)

Histogram methods partition the data space into distinct bins with widths $\Delta_{i}$ and count the number of observations, $n_{i}$, in each bin.

$$
p_{i}=\frac{n_{i}}{N \Delta_{i}}
$$

- Often, the same width is used for all bins, $\Delta_{i}=\Delta$.
$-\Delta$ acts as a smoothing parameter.


## Nonparametric Methods (3)

Assume observations drawn from a density $p(\mathbf{x})$ and consider a small region $\mathcal{R}$ containing x such that

$$
P=\int_{\mathcal{R}} p(\mathbf{x}) \mathrm{d} \mathbf{x}
$$

The probability that $K$ out of $N$ observations lie inside $\mathcal{R}$ is $\operatorname{Bin}(K \mid N, P)$ and if $N$ is large

If the volume of $\mathcal{R}, V$, is sufficiently small, $p(\mathbf{x})$ is approximately constant over $\mathcal{R}$ and

$$
P \simeq p(\mathbf{x}) V
$$

Thus

$$
p(\mathbf{x})=\frac{K}{N V}
$$

$V$ small, yet $K>0$, therefore $N$ large?

$$
K \simeq N P
$$

## Nonparametric Methods (4)

Kernel Density Estimation: fix $V$, estimate $K$ from the data. Let $\mathcal{R}$ be a hypercube centred on $\mathbf{x}$ and define the kernel function (Parzen window)

$$
k\left(\left(\mathbf{x}-\mathbf{x}_{n}\right) / h\right)= \begin{cases}1, & \left|\left(x_{i}-x_{n i}\right) / h\right| \leqslant 1 / 2, \quad i=1, \ldots, D \\ 0, & \text { otherwise. }\end{cases}
$$

It follows that
$K=\sum_{n=1}^{N} k\left(\frac{\mathbf{x}-\mathbf{x}_{n}}{h}\right)$ and hence $p(\mathbf{x})=\frac{1}{N} \sum_{n=1}^{N} \frac{1}{h^{D}} k\left(\frac{\mathbf{x}-\mathbf{x}_{n}}{h}\right)$.

## Nonparametric Methods (5)

To avoid discontinuities in $p(x)$, use a smooth kernel, e.g. a Gaussian

$$
p(\mathbf{x})=\frac{1}{N} \sum_{n=1}^{N} \frac{1}{\left(2 \pi h^{2}\right)^{D / 2}}
$$

$$
\exp \left\{-\frac{\left\|\mathbf{x}-\mathbf{x}_{n}\right\|^{2}}{2 h^{2}}\right\}
$$

Any kernel such that

$$
\begin{aligned}
k(\mathbf{u}) & \geqslant 0 \\
\int k(\mathbf{u}) \mathrm{d} \mathbf{u} & =1
\end{aligned}
$$


will work.

## Nonparametric Methods (6)

## Nearest Neighbour

Density Estimation: fix $K$, estimate $V$ from the data.
Consider a hypersphere centred on $\mathbf{x}$ and let it grow to a volume, $V^{\star}$, that includes $K$ of the given $N$ data points. Then

$$
p(\mathrm{x}) \simeq \frac{K}{N V^{\star}} .
$$



## Nonparametric Methods (7)

Nonparametric models (not histograms) requires storing and computing with the entire data set.

Parametric models, once fitted, are much more efficient in terms of storage and computation.

## K-Nearest-Neighbours for Classification (1)

Given a data set with $N_{k}$ data points from class $\mathcal{C}_{k}$ and $\sum_{k} N_{k}=N$, we have

$$
p(\mathbf{x})=\frac{K}{N V}
$$

and correspondingly

$$
p\left(\mathbf{x} \mid \mathcal{C}_{k}\right)=\frac{K_{k}}{N_{k} V} .
$$

Since $p\left(\mathcal{C}_{k}\right)=N_{k} / N$, Bayes' theorem gives

$$
p\left(\mathcal{C}_{k} \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{p(\mathbf{x})}=\frac{K_{k}}{K} .
$$

## K-Nearest-Neighbours for Classification (2)




## K-Nearest-Neighbours for Classification (3)





- K acts as a smother
- For $N \rightarrow \infty$, the error rate of the 1-nearest-neighbour classifier is never more than twice the optimal error (obtained from the true conditional class distributions).

