Inference

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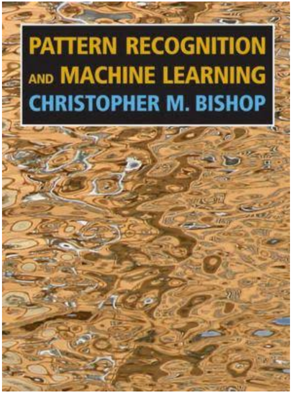
July 16, 2023

Contents

Main reference

I will mainly follow chapters two *Probability distributions* and three *Linear models for regression* from Bishop (2016).



Contents

The Gaussian distribution

- One-dimensional

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi)^{\frac{1}{2}}(\sigma^2)^{\frac{1}{2}}} \exp\left\{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right\}$$

- D-dimensional

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\Sigma) = \frac{1}{(2\pi)^{D/2}\Sigma^{\frac{1}{2}}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\intercal}\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

The Gaussian is the maximum entropy distribution (Cover and Thomas, 1991)

Definition 1 (Differential entropy)

The differential entropy $h(X)$ of a continuous random variable X with a density $f(x)$ is defined as

$$h(X) = -\int_S f(X) \log f(x)\ dx$$

where S is the support set of the random variable.

Theorem 1 (The Gaussian is the maximum entropy distribution)

Let the random vector $X \in \mathbb{R}^n$ have zero mean and covariance K. Then $h(X) \leq \frac{1}{2} \log(2\pi e)^n |K|$, with equality if $X \sim \mathcal{N}(0, K)$.

The central limit theorem (Papoulis and Pillai, 2002)

Theorem 2 (The central limit theorem)

Given n independent and identically distributed random vectors $\mathbf{X}_i$, with mean vector $\boldsymbol{\mu} = E\{\mathbf{X}_i\}$ and covariance matrix $\boldsymbol{\Sigma}$. Then

$$\sqrt{n}(\bar{\mathbf{X}}_n - \boldsymbol{\mu}) \rightarrow \mathcal{N}(0, \Sigma)$$

with convergence in distribution.

Very useful properties of the Gaussian distribution (Bishop, 2016)

Theorem 3 (Marginals and conditionals of Gaussians are Gaussians)

Given $\mathbf{x} = \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix}$ *such that*

$$
\begin{aligned}
p(\mathbf{x}) &= \mathcal{N}\left(\mathbf{x} \,\middle|\, \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}\right) \\
&= \mathcal{N}\left(\mathbf{x} \,\middle|\, \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix}, \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}^{-1}\right)
\end{aligned}
$$

Then

$$
\begin{aligned}
p(\mathbf{x}_a|\mathbf{x}_b) &= \mathcal{N}\left(\mathbf{x}_a \,\middle|\, \boldsymbol{\mu}_a - \Lambda_{aa}^{-1}\Lambda_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b), \Lambda_{aa}^{-1}\right) && (1) \\
&= \mathcal{N}\left(\mathbf{x}_a \,\middle|\, \boldsymbol{\mu}_a + \Sigma_{ab}\Sigma_{bb}^{-1}(\mathbf{x}_b - \boldsymbol{\mu}_b), \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}\right) && (2) \\
p(\mathbf{x}_b) &= \mathcal{N}\left(\mathbf{x}_b \,\middle|\, \boldsymbol{\mu}_b, \Sigma_{bb}\right) && (3)
\end{aligned}
$$

Very useful properties of the Gaussian distribution (Bishop, 2016)

Theorem 4 (Marginals and conditionals of the linear Gaussian model)

Given the linear Gaussian model

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

Then

$$
\begin{aligned}
p(\mathbf{t}) &= \mathcal{N}(\mathbf{t}|A\boldsymbol{\mu} + \mathbf{b}, L^{-1} + A\Lambda^{-1}A^{\intercal}) \\
p(\mathbf{x}|\mathbf{t}) &= \mathcal{N}(\mathbf{x}|\Sigma\{A^{\intercal}L(\mathbf{t} - \mathbf{b}) + \Sigma\boldsymbol{\mu}\}, \Sigma)
\end{aligned}
$$

where

$$
\Sigma = (\Lambda + A^{\intercal}LA)^{-1}
$$

Very useful properties of the Gaussian distribution (Bishop, 2016)

The conditional, $p(\mathbf{x}|\mathbf{t})$, of the linear Gaussian model is the fundamental result used in the derivation of

1. Bayesian linear regression (Bishop, 2016),
2. Gaussian process regression (Williams and Rasmussen, 2006),
3. Gaussian process factor analysis (Yu et al., 2009),
4. linear dynamical systems (Durbin and Koopman, 2012).

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 1)

Claim 1 (Quadratic form of Gaussian log pdf)

$p(\mathbf{x})$ is a Gaussian pdf with mean $\boldsymbol{\mu}$ and precision matrix Λ if and only if $\int p(\mathbf{x})d\mathbf{x} = 1$ and

$$\log p(\mathbf{x}) = -\frac{1}{2}(\mathbf{x}^\mathsf{T}\Lambda\mathbf{x} - 2\mathbf{x}^\mathsf{T}\Lambda\boldsymbol{\mu}) + K \tag{4}$$

where K is a constant that does not depend on $\mathbf{x}$.

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 1)

Proof of Claim 1.

$\rightarrow$)

$$
\begin{aligned}
p(\mathbf{x}) &= \frac{1}{(2\pi)^{D/2}\Lambda^{-\frac{1}{2}}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \Lambda (\mathbf{x}-\boldsymbol{\mu})\right\} \\
\log p(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \Lambda (\mathbf{x}-\boldsymbol{\mu}) - \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
&= -\frac{1}{2}(\mathbf{x}^\intercal \Lambda \mathbf{x} - 2\mathbf{x}^\intercal \Lambda \boldsymbol{\mu}) - \frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} - \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
&= -\frac{1}{2}(\mathbf{x}^\intercal \Lambda \mathbf{x} - 2\mathbf{x}^\intercal \Lambda \boldsymbol{\mu}) + K
\end{aligned}
$$

with $K = -\frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} - \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}})$.

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 1)

Proof of Claim 1.

$\leftarrow$)

$$
\begin{aligned}
\log p(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x}^\intercal \Lambda \mathbf{x} - 2\mathbf{x}^\intercal \Lambda \boldsymbol{\mu}) + K \\
\log p(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x}^\intercal \Lambda \mathbf{x} - 2\mathbf{x}^\intercal \Lambda \boldsymbol{\mu}) - \frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} - \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
&\quad + K + \frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
&= -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\intercal \Lambda (\mathbf{x} - \boldsymbol{\mu}) - \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
&\quad + K + \frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
&= \log N(\mathbf{x}|\boldsymbol{\mu}, \Lambda) + K + \frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}}) \\
p(\mathbf{x}) &= N(\mathbf{x}|\boldsymbol{\mu}, \Lambda) \exp\left(K + \frac{1}{2}\boldsymbol{\mu}^\intercal \Lambda \boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}})\right)
\end{aligned}
\tag{5}
$$

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 1)

Proof of Claim 1.

$\leftarrow$) cont

$$
\begin{aligned}
1 &= \int p(\mathbf{x}) d\mathbf{x} \\
&= \int N(\mathbf{x}|\boldsymbol{\mu}, \Lambda) \exp\left(K + \frac{1}{2}\boldsymbol{\mu}^{\intercal}\Lambda\boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}})\right) d\mathbf{x} \\
&= \exp\left(K + \frac{1}{2}\boldsymbol{\mu}^{\intercal}\Lambda\boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}})\right) \int N(\mathbf{x}|\boldsymbol{\mu}, \Lambda) d\mathbf{x} \\
&= \exp\left(K + \frac{1}{2}\boldsymbol{\mu}^{\intercal}\Lambda\boldsymbol{\mu} + \log((2\pi)^{D/2}\Lambda^{-\frac{1}{2}})\right)
\end{aligned}
$$

From Eq. 5 then $p(\mathbf{x}) = N(\mathbf{x}|\boldsymbol{\mu}, \Lambda)$.

$\square$

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 1)

Proof of Theorem 3, Eq. 1.

$$p(\mathbf{x}_a|\mathbf{x}_b) = \frac{p(\mathbf{x}_a, \mathbf{x}_b)}{p(\mathbf{x}_b)} = \frac{p(\mathbf{x})}{p(\mathbf{x}_b)}$$

$$\log p(\mathbf{x}_a|\mathbf{x}_b) = \log p(\mathbf{x}) - \log p(\mathbf{x}_b) = \log p(\mathbf{x}) + K$$

Therefore, the terms of $\log p(\mathbf{x}_a|\mathbf{x}_b)$ that depend on $\mathbf{x}_a$ are those of $\log p(\mathbf{x})$.
Steps for the proof:

1. isolate the terms of $\log p(\mathbf{x})$ that depend on $\mathbf{x}_a$,
2. notice that these term has the quadratic form of Claim 1, therefore $p(\mathbf{x}_a|\mathbf{x}_b)$ is Gaussian,
3. identify $\boldsymbol{\mu}$ and Λ in this quadratic form.

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 1)

Proof of Theorem 3, Eq. 1.

$$
\begin{aligned}
p(\mathbf{x}) &= \frac{1}{(2\pi)^{D/2}|\Lambda|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \Lambda (\mathbf{x}-\boldsymbol{\mu})\right) \\
\log p(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\intercal \Lambda (\mathbf{x}-\boldsymbol{\mu}) + K_1 \\
&= -\frac{1}{2}[(\mathbf{x}_a-\boldsymbol{\mu}_a)^\intercal, (\mathbf{x}_b-\boldsymbol{\mu}_b)^\intercal] \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix} \begin{bmatrix} \mathbf{x}_a-\boldsymbol{\mu}_a \\ \mathbf{x}_b-\boldsymbol{\mu}_b \end{bmatrix} + K_1 \\
&= -\frac{1}{2}\left\{(\mathbf{x}_a-\boldsymbol{\mu}_a)^\intercal \Lambda_{aa}(\mathbf{x}_a-\boldsymbol{\mu}_a) + 2(\mathbf{x}_a-\boldsymbol{\mu}_a)^\intercal \Lambda_{ab}(\mathbf{x}_b-\boldsymbol{\mu}_b)\right. \\
&\quad \left. +(\mathbf{x}_b-\boldsymbol{\mu}_b)^\intercal \Lambda_{bb}(\mathbf{x}_b-\boldsymbol{\mu}_b)\right\} + K_1 \\
&= -\frac{1}{2}\left\{\mathbf{x}_a^\intercal \Lambda_{aa}\mathbf{x}_a - 2\mathbf{x}_a^\intercal(\Lambda_{aa}\boldsymbol{\mu}_a - \Lambda_{ab}(\mathbf{x}_b-\boldsymbol{\mu}_b))\right\} + K_2 \\
&= -\frac{1}{2}\left\{\mathbf{x}_a^\intercal \Lambda_{aa}\mathbf{x}_a - 2\mathbf{x}_a^\intercal\Lambda_{aa}(\boldsymbol{\mu}_a - \Lambda_{aa}^{-1}\Lambda_{ab}(\mathbf{x}_b-\boldsymbol{\mu}_b))\right\} + K_2
\end{aligned}
$$

Comparing the last equation with Eq. 4 we see that $\Lambda = \Lambda_{aa}$, $\boldsymbol{\mu} = \boldsymbol{\mu}_a - \Lambda_{aa}^{-1}\Lambda_{ab}(\mathbf{x}_b-\boldsymbol{\mu}_b)$ and conclude that $p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_a - \Lambda_{aa}^{-1}\Lambda_{ab}(\mathbf{x}_b-\boldsymbol{\mu}_b), \Lambda_{aa})$ □

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 2)

Claim 2 (Inverse of a partitioned matrix)

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} M & -MBD^{-1} \\ -D^{-1}CM & D^{-1} + D^{-1}CMBD^{-1} \end{pmatrix} \tag{6}$$

where

$$M = (A - BD^{-1}C)^{-1}$$

Proof.

Exercise. Hint: verify that the multiplication of the inverse of the matrix in the right hand side of Eq. 6 with the matrix in the left hand side of the same equation is the identiy matrix.

Proof: the conditional of a Gaussian is a Gaussian (Theorem 3, Eq. 2)

Proof of Theorem 3, Eq. 2.

Using the definition

$$\begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}^{-1} = \begin{pmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{pmatrix}$$

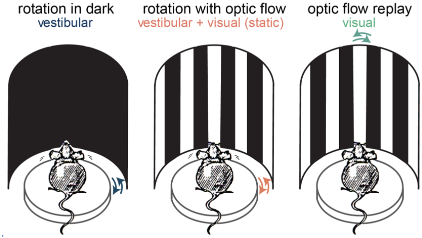
and using Eq. 6, we obtain

$$\begin{aligned} \Lambda_{aa} &= (\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba})^{-1} \\ \Lambda_{ab} &= -(\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba})^{-1}\Sigma_{ab}\Sigma_{bb}^{-1} \end{aligned}$$

Replacing the above equations in Eq. 1 we obtain Eq. 2. □

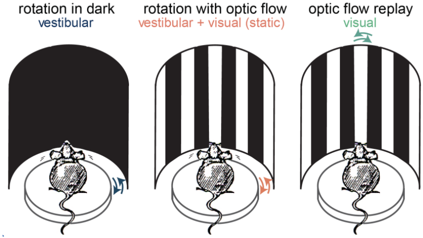
Contents

Linear regression example

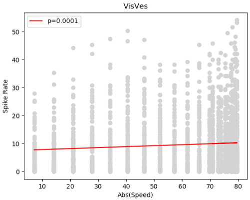


Keshavarzi et al., 2021

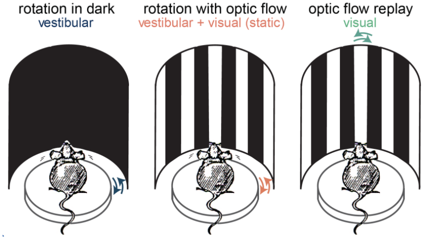
Linear regression example



Keshavarzi et al., 2021



Linear regression example



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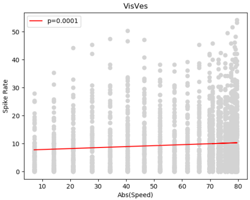


Is there a linear relation between the speed of rotation and the firing rate of visual cells?

Linear regression model

simple linear regression model

$$y(x_i, \mathbf{w}) = w_0 + w_1 x_i = [1, x_i] \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = [\phi_0(x_i), \phi_1(x_i)] \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$
$$= \phi(x_i)^\intercal \mathbf{w}$$

polynomial regression model

$$y(x_i, \mathbf{w}) = w_0 + w_1 x_i + w_2 x_i^2 + w_3 x_i^3 = [1, x_i, x_i^2, x_i^3] \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix}$$
$$= [\phi_0(x_i), \phi_1(x_i), \phi_2(x_i), \phi_3(x_i)] \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix} = \phi(x_i)^\intercal \mathbf{w}$$

basis functions linear regression model

$$y(x_i, \mathbf{w}) = \phi(x_i)^\intercal \mathbf{w} = \sum_{j=1}^{M} w_j \phi_j(x_i)$$

Linear regression model

$$
\begin{aligned}
\mathbf{y}(\mathbf{x}, \mathbf{w}) &= \begin{bmatrix} y(x_1, \mathbf{w}) \\ y(x_2, \mathbf{w}) \\ \dots \\ y(x_N, \mathbf{w}) \end{bmatrix} = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \dots & \phi_M(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \dots & \phi_M(x_2) \\ \vdots & \vdots & \dots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) & \dots & \phi_M(x_N) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_M \end{bmatrix} \\
&= \mathbf{\Phi} \mathbf{w}
\end{aligned}
$$

where $\mathbf{y}(\mathbf{x}, \mathbf{w}) \in \mathbb{R}^N, \mathbf{\Phi} \in \mathbb{R}^{N \times M}, \mathbf{w} \in \mathbb{R}^M$.

Basis functions for regression

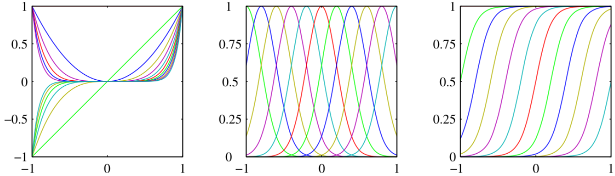


Figure 3.1 Examples of basis functions, showing polynomials on the left, Gaussians of the form (3.4) in the centre, and sigmoidal of the form (3.5) on the right.

Bishop (2016))

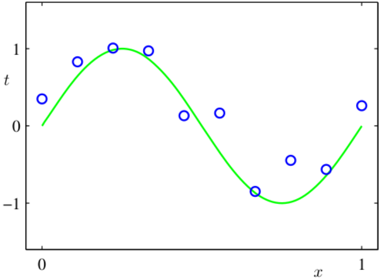
polynomial $\phi_i(x) = x^i$

Gaussian $\phi_i(x) = \exp(-\frac{(x-\mu_i)^2}{2\sigma^2})$

sigmoidal $\phi_i(x) = \frac{1}{1+\exp(-\frac{x-\mu_i}{\sigma^2})}$

Example dataset

Figure 1.2 Plot of a training data set of $N = 10$ points, shown as blue circles, each comprising an observation of the input variable x along with the corresponding target variable t. The green curve shows the function $\sin(2\pi x)$ used to generate the data. Our goal is to predict the value of t for some new value of x, without knowledge of the green curve.



Bishop (2016)

Least-squares estimation of model parameters (Trefethen and Bau III, 1997)

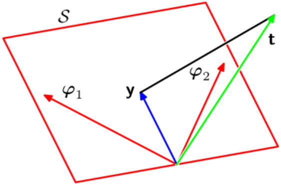
Definition 2 (Least-squares problem)

Given $\mathbf{\Phi} \in \mathbb{R}^{N \times M}$, $N \geq M$, $\mathbf{t} \in \mathbb{R}^N$, find $\mathbf{w} \in \mathbb{R}^M$ such that $||\mathbf{t} - \mathbf{\Phi w}||_2$ is minimized.

Theorem 5 (Least-squares solution)

Let $\mathbf{\Phi} \in \mathbb{R}^{N \times M} (N \geq M)$ and $\mathbf{t} \in \mathbb{R}^N$ be given. A vector $\mathbf{w} \in \mathbb{R}^M$ minimizes $||\mathbf{r}||_2 = ||\mathbf{t} - \mathbf{\Phi w}||_2$, thereby solving the least-squares problem, if and only if $\mathbf{r} \perp range(\mathbf{\Phi})$, that is, $\mathbf{\Phi}^\mathsf{T}\mathbf{r} = 0$, or equivalently, $\mathbf{\Phi}^\mathsf{T}\mathbf{\Phi w} = \mathbf{\Phi}^\mathsf{T}\mathbf{t}$, or again equivalently, $P\mathbf{t} = \mathbf{\Phi w}$.

Figure 3.2 Geometrical interpretation of the least-squares solution, in an N-dimensional space whose axes are the values of $t_1, \ldots, t_N$. The least-squares regression function is obtained by finding the orthogonal projection of the data vector $\mathbf{t}$ onto the subspace spanned by the basis functions $\phi_j(\mathbf{x})$ in which each basis function is viewed as a vector φ_j of length N with elements $\phi_j(\mathbf{x}_n)$.



Bishop (2016)

Code for least-squares estimation of model parameters

- overfitting
- cross validation
- larger datasets allow more complex models

Maximum-likelihood estimation of model parameters

Definition 3 (Likelihood function)

For a statistical model characterized by a probability density function $f(\mathbf{x}|\theta)$ (or probability mass function $P_\theta(X = \mathbf{x})$) the likelihood function is a function of the parameters θ, $\mathcal{L}(\theta) = f(\mathbf{x}|\theta)$ (or $\mathcal{L}(\theta) = P_\theta(\mathbf{x})$).

Definition 4 (Maximum likelihood parameters estimates)

The maximum likelihood parameters estimates are the parameters that maximimize the likelihood function.

$$\theta_{ML} = \arg\max_{\theta} \mathcal{L}(\theta)$$

Maximum-likelihood estimation for the basis function linear regression model

If model observations as

$$\mathbf{t} \sim \mathcal{N}(\mathbf{t}|\mathbf{\Phi}\mathbf{w}, \beta^{-1}I_N)$$

then the likelihood function is

$$\mathcal{L}(\mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\phi^{\intercal}(x_n)\mathbf{w}, \beta^{-1})$$

and the maximum likelihood parameters estimates are

$$\mathbf{w}_{ML} = (\mathbf{\Phi}^{\intercal}\mathbf{\Phi})^{-1}\mathbf{\Phi}^{\intercal}\mathbf{t} \tag{7}$$

$$\frac{1}{\beta_{ML}} = \frac{1}{N}\sum_{n=1}^{N}(t_n - \phi(\mathbf{x}_n)^{\intercal}\mathbf{w}_{ML})^2 \tag{8}$$

Note: if errors are assumed to be Normal, the maximum-likelihood and least-squares coefficients estimates are equal.

Exercise

Exercise 1

Derive the formulas for the maximum likelihood estimates of the coefficients, $\mathbf{w}$, *and noise precision,* β, *of the basis functions linear regression model given in Eqs. 7 and 8.*

References

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