PML Script for Lectures by Oswin

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Contents

On this Document

This document is intended as a short script to provide a) the necessary background for the course and b) to provide lecture notes for the lectures given by Oswin. The background sections are 1 and 2 followed by the sections for individual lecture content.

The background part is written in a concise and compressed way to quickly look up basic relations and properties. It assumes that the reader has some familiarity with Machine Learning in general. For a less concise description,

we refer to Bishop, Pattern Recognition and Machine-Learning, Chapters 1-4. Each section in this document contains references to the chapters in the book, even though our content has a different order than Bishop and is somewhat more formal.

Background material As probability theory stands on the shoulder of giants, we need a rich knowledge of different areas of math. This includes, among others, results from Linear Algebra: properties of matrix determinants, matrix inverses and matrix decompositions. We recommend the matrix cookbook as a quick reference as well as a look nto your old material on Linear Algebra.

Structure We write proofs of statements in blocks

> **Proof:** The proof.

These blocks can be skipped on a first read through, even though we encourage the reader to work through them later on. Another important block are Notation blocks:

> **Notation:** We write ...

These should not be skipped as they will often change how we write equations in the following.

Errors This document is version 1.0. Even though we checked derivations and text several times, there can be errors in the document. We are happy to correct any error you find.

Contents Sections 1 and 2 are necessary background of probability distribution with focus on the multivariate normal distribution. We will come back to these properties often throughout the course. Chapter 3 and 4 are content of the first lecture and give an introduction to Bayesian and Frequentist probability as well as Generalized Linear Models.

1 Random Variables

Every algorithm interacting with the real world must be able to handle uncertainty. Uncertainty arises from a number of sources, be it incomplete or missing information, inaccuracies of a measurement or true randomness introduced by physical systems. Probability theory is the branch of mathematics that aims to formally describe uncertainty. A proper introduction to probability theory requires deep knowledge in analysis, topology and measure theory, which we can not provide in this script. Instead, we will introduce the key concepts in a depth that is sufficient for this course. This means that sometimes we do not treat a topic with the necessary technical rigor required. We therefore assume that all operations (integral etc) are well-defined in the context we use them in. This script still assumes that the reader is somewhat familiar with the topic and serves mostly as a reminder and to introduce a common notation. An a little bit more basic introduction is given in (Bishop, chapters 1.2, pages 12-20).

The key concept of probability theory is that of a *random variable*. A random variable X models the process of how random observations are generated. Random variables take values on a state space Ω and an *observation* or *realization* of a random variable is a value $x \in \Omega$ that is observed as an outcome of a random experiment. If the set of values of X taken in Ω is countable, we call X a discrete random variable, otherwise, if X takes values that are continuous in Ω, we call X a continuous random variable.

Independent of the type of random variable, the probability that X takes a value in a given set $S \subseteq \Omega$ is $P(X \in S) \in [0, 1]$ and $P(X \in \Omega) = 1$. If X is discrete, the probability of observing value x is given by the *probability mass function* (pmf) $P(X = x) \geq 0$. The probability $P(X \in S)$ can be written in terms of the pmf by summing over all elements in S

$$P(X \in S) = \sum_{x \in S} P(X = x) \ . \tag{1}$$

If X is continuous, the probability of observing a specific event $P(X = x)$ is zero and thus the pmf can not be used to describe continuous random variables. Instead, we use the *probability density function* (pdf) $p(X = x) \geq 0$ and its relation to $P(X \in S)$ is given by integration

$$P(X \in S) = \int_S p(X = x)\, dx \ . \tag{2}$$

For both pmf and pdf, we have $P(\emptyset) = 0$, $P(S) = 1$

Notation: The process of defining a random variable is often written in a shortcut form. Given a pdf $p(x)$ we can write $X \sim p(x)$ to define a random variable X with samples distributed according to $p(x)$. Here, the state space Ω is defined implicitly via the input space of p. This notation is most commonly used in conjunction with known distributions. This gives rise to notations like $X \sim \mathcal{N}(\mu, \sigma^2)$ or $X \sim \mathcal{N}(x; \mu, \sigma^2)$ to define a random variable that follows a normal distribution with specified mean and variance. The latter notation also serves as a shortcut to defining the pdf $p(x) = \mathcal{N}(x; \mu, \sigma^2)$.

In the following we will assume that random variables are continuous, if not stated otherwise. However, all definitions hold for discrete variables analogously.

The concept of a probability of a single random variable can be extended to a set of random variables. For two random variables X, Y with state spaces Ω_X, Ω_Y, the *joint probability* of observing a specific tuple of outcomes in a set $S \subseteq \Omega_X \times \Omega_Y$ is given by

$$P((X, Y) \in S) = \int_S p(X = x, Y = y)\, dx\, dy \ . \tag{3}$$

If only a subset of random variables is of interest, the joint distribution can be *marginalized* to obtain the probability of only the variables of interest. The resulting distribution is called the *marginal*. Sampling from the marginal distribution is the same as sampling from the joint, while ignoring the values of the variables which are not of interest. In the pdf, marginalization is done via integration of all variables which are not of interest. For example, to obtain the marginal of X from the pair X, Y we compute the marginal pdf

$$p(X = x) = \int_{\Omega_Y} p(X = x, Y = y)\, dy \ . \tag{4}$$

We say that a set of random variables is independent, if their joint pdf can be written as the product of marginals

$$p(X = x, Y = y) = p(X = x)p(Y = y) \ . \tag{5}$$

Finally, we can compute the probability of X taking a specific value conditioned on a specific value that we have already observed, $Y = y$. The *conditional distribution* is given by

$$p(X = x|Y = y) = \frac{p(X = x, Y = y)}{\int_{\Omega_X} p(X = x', Y = y)\, dx'} = \frac{p(X = x, Y = y)}{p(Y = y)} \tag{6}$$

The joint distribution can be written in terms of conditional and marginal distribution

$$p(X = x, Y = y) = p(X = x|Y = y)p(Y = y) = p(Y = y|X = x)p(X = x) \ , \tag{7}$$

and if two variables are independent, then the conditional distribution is the same as the marginal

$$p(X = x|Y = y) = P(X = x) \ . \tag{8}$$

Notation: There are a number of different notations in the literature for the pdf. Common notations include $p_X(x)$, $f_X(x)$ or simply $p(X)$ or $p(x)$. The latter is most commonly used in the machine-learning literature and often the differentiation between the random variable X and an outcome x is not made.
Similarly, there are several shortcuts to describe the relations between multiple random variables. For example the conditional $X|Y$ is itself taken as a random variable (the random variable of X after observing Y).
In the following, we will write $p(x)$ instead of $p(X = x)$ if it is clear from the context, which random variable we mean.

1.1 Transformations and Expectations of random variables

If we observe a random variable X taking values on state-space $\Omega_X = \mathbb{R}^d$ several times, we obtain realizations $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$. Their sample average is given by

$$\hat{x} = \frac{1}{N} \sum_{i=1}^{N} x_i \ . \tag{9}$$

The mean of X, $E[X]$ is the integral

$$E[X] = \int_{\Omega_X} p(x) x dx \ . \tag{10}$$

The relation between the sample average and the mean is given by the *weak law of large numbers*: If X has finite variance, then in the limit of infinite samples the sample average converges to the mean

$$E[X] = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} x_i \ . \tag{11}$$

We can transform a random variable given a function $f : \Omega_X \to \Omega_Z$. Applying f to an observation x of X gives a new random variable Z with realizations, $z = f(x)$. As shortcut, we write

$$Z = f(X) \ . \tag{12}$$

In the case that $\Omega_X = \Omega_Z = \mathbb{R}^d$ and f is a bijective function, we can write the probability density of Z in terms of the inverse function $f^{-1} : \Omega_Z \to \Omega_X$ and the determinant of its Jacobian $J_{f^{-1}}(z)$

$$p(z) = p(X = f^{-1}(z))|\det J_{f^{-1}}(z)| \ . \tag{13}$$

The Jacobian of a function g is the matrix of partial derivatives:

$$J_g(x) = \begin{pmatrix} \frac{\partial g_1(x)}{\partial x_1} & \dots & \frac{\partial g_1(x)}{\partial x_d} \\ \vdots & \dots & \vdots \\ \frac{\partial g_d(x)}{\partial x_1} & \dots & \frac{\partial g_d(x)}{\partial x_d} \end{pmatrix} \tag{14}$$

Proof: This can be derived directly using integration by substitution, which in the multi-dimensional case reads:

$$\int_{g(S)} h(x)\, dx = \int_S h(g(z))|\det J_g(z)|\, dz \ ,$$

assuming that g is bijective and has a continuous derivative. The reader might not be familiar with the multi-variate version and can consider the case of one-dimensional substitution instead.

Let $S \subseteq \Omega_Z$. The probability of $P(Z \in S)$ is given by:

$$\begin{aligned} P(Z \in S) &= \int_S p(Z = z)\, dz \\ &= \int_{f^{-1}(S)} p(X = x)\, dx \\ &= \int_S p(X = f^{-1}(z))|\det J_{f^{-1}}(z)|\, dz \end{aligned}$$

In the first step we used, that due to bijectivity, observing a value z of random variable Z entails observation of a unique value x of random variable X. Thus $P(Z \in S) = P(X \in f^{-1}(S))$. The next step is direct application of integration by substitution for multiple variables.
We obtain the final result by comparing the first and last integral pointwise.

With a similar derivation, we can show that the expectation of Z can be written directly in terms of f and X,

$$E[Z] = \int_{\Omega_Z} p(Z = z) z\, dz = \int_{\Omega_X} p(X = x) f(x)\, dx \ . \tag{15}$$

This relation is useful, because often it is much easier to compute the integral of the right hand side, than to start with the left hand side. It is worth noting that this relation holds under much weaker assumptions than required by the change of variable formula and invertibility of f is not required. Indeed, the assumptions are so weak that most statisticians use it without checking the requirements (or even knowing of their existence), which led to its name of *the law of the unconscious statistician* (LOTUS). It is fair to say, that LOTUS will hold for all functions considered in machine-learning.

Notation: We will introduce another helpful shortcut and directly write $E[f(X)]$ instead of $E[Z]$. Further, if more than one random variable appears in an expression and we don't intend to take the expectation over all, we specify the random variable to integrate over. For example, given two random variables X, Y and the transformed variable $Z = f(X, Y)$, then $E_Y[f(X, Y)]$ only computes the expectation over Y, keeping X constant. The result is still a random variable as a transformation of X.

We will state a few important properties of the expectation. Let X, Y be two independent d-dimensional random variables. Then for the sum $X + Y$ it holds:

$$E[X + Y] = E[X] + E[Y] \tag{16}$$

For their product, it holds:

$$E[X \cdot Y] = E[X] \cdot E[Y] \tag{17}$$

For transformed variables, it is difficult to find an expression in the general case. However, if f is an affine linear function, then

$$E[f(X)] = f(E[X]) \ . \tag{18}$$

When f is a convex function, then we have *Jensen's Inequality*:

$$E[f(X)] \geq f(E[X]) \ . \tag{19}$$

While the expectation gives a description for the average location of a sample, the variance is used to obtain an estimate of the spread. For a random variable X with state-space $\mathbb{R}$ the variance can be defined as the expected squared distance from the mean:

$$\mathrm{Var}(X) = E[(X - E[X])^2] \ . \tag{20}$$

A way to measure dependency of X on another real-valued variable Y is the covariance

$$\mathrm{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])] \ . \tag{21}$$

The covariance measures a linear relationship between X and Y: if X becomes larger, then Y tends to change as well and its expected rate of change is given by $\mathrm{Cov}(X, Y)$. Computing the covariance of a variable with itself gives the variance, $\mathrm{Var}(X) = \mathrm{Cov}(X, X)$. Further, if X and Y are independent their covariance is 0, due to property (17) of the mean. The converse does not hold as dependent variables can have covariance 0.

For a random rector $X \in \mathbb{R}^d$, the set of variances and covariances between all pairs of variables in X can be computed using the covariance matrix:

$$\mathrm{Cov}(X) = \begin{pmatrix} \mathrm{Cov}(X_1, X_1) & \dots & \mathrm{Cov}(X_1, X_d) \\ \vdots & \dots & \vdots \\ \mathrm{Cov}(X_d, X_1) & \dots & \mathrm{Cov}(X_d, X_d) \end{pmatrix} = E[(X - E[X])(X - E[X])^T] \ .$$

The diagonal elements of the covariance matrix give the variances of the variables and the off-diagonal elements each give the covariance between pairs of elements.

2 The Normal distribution

Due to it importance to machine-learning, we will quickly reintroduce the key concepts of the normal distribution. We will then extend it to the multivariate case and show some of its most important properties. Many of these properties will be usable throughout the course, even for very advanced non-linear models. As additional reading, we refer to (Bishop, chapter 2.3-2.3.2, pages 78-90). As always, the reader is encouraged to skip the proofs at a first read through.

We call a random variable X with state space $\mathbb{R}$ normal distributed with mean μ and variance σ^2, or in short $X \sim \mathcal{N}(\mu, \sigma^2)$, if it has pdf

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{\sigma^2}} \tag{22}$$

Notation: The normal distribution is an example of a parameterized distribution. If it is clear in the context which parameters and value swe mean, we will just write $p(x)$. If we want to clarify the existence or choice of parameters, we will write them in form of a conditional pdf, for example $p(x|\mu, \sigma^2)$.

The normal distribution has a few important properties:

Affine transformations Let $\epsilon \sim \mathcal{N}(0, 1)$, $a, b \in \mathbb{R}$, then

$$Z = a + b\epsilon \tag{23}$$

is a normal distributed random variable $Z \sim \mathcal{N}(a, b^2)$.

Summation Let $X \sim \mathcal{N}(\mu_X, \sigma_X^2)$, $Y \sim \mathcal{N}(\mu_Y, \sigma_Y^2)$, then

$$Z = X + Y \tag{24}$$

is a normal distributed random variable $Z \sim \mathcal{N}(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2)$.

Notation: For the second result it is important that both variables, X and Y are independent. Following common ML notation, we treat independently defined random variables as independent if not mentioned otherwise. If we assume dependence, we denote this by making the parameters of one variable a function of the other, e.g., $Y \sim \mathcal{N}(\mu_Y(X), \sigma_Y^2(X))$.

A result of these two properties is that any linear combination of normal distributed random variables is normally distributed. We extend the definition to the multivariate distribution by focusing on this property:

Definition: Let $\epsilon \in \mathbb{R}^N$ be a random variable with elements distributed as $\epsilon_i \sim \mathcal{N}(0,1)$, $i = 1, \ldots, N$. Further, let $A \in \mathbb{R}^{d \times N}$, $\mu \in \mathbb{R}^d$. A random variable of the form

$$X = \mu + A\epsilon \tag{25}$$

is called Multivariate Normal Distributed with mean $E[X] = \mu$ and variance $\Sigma = AA^T$, or in short

$$X \sim \mathcal{N}(\mu, \Sigma) \ .$$

This definition is indirect as it gives us neither a density nor a distribution function, but it provides a direct way to create normal distributed random variables. A more commonly used definition is the following:

PDF of the Multivariate Normal Distribution: Let $X \sim \mathcal{N}(\mu, \Sigma)$, where $\mu \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$ is a symmetric positive definite matrix. Then X has pdf

$$p(x) = \frac{1}{\sqrt{2\pi}^d \sqrt{\det \Sigma}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right) \ . \tag{26}$$

These two definitions are not equivalent, because the second definition only encompasses a subset of normal distributed variables: the first definition allows a choice of A such, that $\Sigma = AA^T$ is only positive semi-definite, which means that $\det \Sigma = 0$. In this case, equation (26) includes a division by zero. This is why typically in a machine-learning course only the second version is presented: handling of normal distributions with semi-definite covariance matrix is more difficult. We give the full definition here because a proper handling of Gaussian Processes later in this course requires the full definition, but unless explicitly stated, we will assume that X has a pdf. For completeness, we need to show that the pdf described by (26) belongs to a random variable that can be created via (25). The statement we want to show is:

Let X be a multivariate normal distributed random variable following (25). If A is invertible, then X has pdf (26). Conversely, if X has pdf (26), then it can be written in form (25) with A invertible.

Proof: We will begin with the first part of the statement. First of all, we note that invertibility of A requires that $N = d$ and thus A is a $d \times d$ matrix. Since the elements of ϵ are independent normally distributed

variables, its pdf is

$$p(\epsilon) = \prod_{i=1}^{d} p(\epsilon_i) = \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}\epsilon_i^2} = \frac{1}{\sqrt{2\pi}^d} \exp\left(-\frac{1}{2}\epsilon^T\epsilon\right)$$

By (25), X can be written as transformation of a random variable using the affine function $f(x) = \mu + Ax$ and $X = f(\epsilon)$. Since A is invertible, f is an invertible function with inversion $f^{-1}(x) = A^{-1}(x-\mu)$ and Jacobian $J_{f^{-1}}(x) = A^{-1}$. This allows us to use the change of variables formula (13)

$$\begin{aligned} p(X = x) &= p(\epsilon = f^{-1}(x))|\det J_{f^{-1}}(x)| \\ &= p(\epsilon = A^{-1}(x-\mu))|\det(A^{-1})| \\ &= \frac{\det A^{-1}}{\sqrt{2\pi}^d} \exp\left(-\frac{1}{2}(x-\mu)^T(A^{-1})^T A^{-1}(x-\mu)\right) \end{aligned}$$

To write this in terms of Σ, we first note that $\Sigma^{-1} = (A^{-1})^T A^{-1}$. To write $|\det J_{f^{-1}}(x)|$ in terms of Σ, we use properties of the determinant and obtain $\det\Sigma = \det(AA^T) = (\det A)^2$ and $|\det J_{f^{-1}}(x)| = 1/|\det A| = 1/\sqrt{\det\Sigma}$. Inserting this in the previous result gives (26).

To show the opposite direction, we need to show that for every Σ a matching A exists. This can be done using the eigenvalue decomposition. Since Σ is symmetric positive definite, it has a symmetric eigenvalue composition

$$\Sigma = \sum_{i=1}^{d} \lambda_i v_i v_i^T \quad ,$$

where λ_1 are the eigenvalues and v_i the corresponding eigenvectors with property $v_i^T v_i = 1$ and $v_i^T v_j = 0$, $i \neq j$. Since Σ is positive definite, $\lambda_i > 0$. We now construct A as

$$A = \sum_{i=1}^{d} \sqrt{\lambda_i} v_i v_i^T \quad .$$

It can be verified easily, that $AA^T = \Sigma$ and A is invertible as $\sqrt{\lambda_i} > 0$

The relation between (25) and the pdf (26) is important, because in practice it it often easier to show that a random variable has a multivariate normal distribution via (25), than to manipulate the pdf and its integrals. We will use this approach in the following to derive a few of the most important properties of multivariate normal random variables: Their mean and variance and rules for calculating the marginals, conditionals, projections and summation.

Standard Multivariate normal Let $\epsilon \in \mathbb{R}^d$ be a random vector with elements $\epsilon_i \sim \mathcal{N}(0,1)$. Then, ϵ follows a multivariate normal distribution, $\epsilon \sim \mathcal{N}(0, I_d)$, where 0 is the d-dimensional zero vector and I_d the d-dimensional identity matrix. This distribution is called he standard multivariate normal distribution.

Proof: This follows directly from property (25) with $\mu_X = 0$ and $A = I_d$.

Mean and Covariance Let $X \sim \mathcal{N}(\mu_x, \Sigma_X)$. Its mean is

$$E[X] = \mu \tag{27}$$

and its covariance matrix is

$$\text{Cov}(X) = \Sigma_X \tag{28}$$

Proof: We start by the observation of (25), that there exists an A, such, that $X = \mu_X + A\epsilon$, where $\epsilon \sim \mathcal{N}(0, I_d)$.
Then using property (18) of the mean we obtain:

$$E[X] = E[\mu_X + A\epsilon] = \mu_X + AE[\epsilon] = \mu_X$$

The last step holds, since the mean of a univariate standard normal variable is 0 and thus the vector is the zero-vector.

$$\begin{aligned}
\text{Cov}[X] &= E[(X - E[X])(X - E[X])^T] \\
&= E[(\mu_X + A\epsilon - \mu_X)(\mu_X + A\epsilon - \mu_X)^T] \\
&= E[A\epsilon\epsilon^T A^T] \\
&= A \underbrace{E[\epsilon\epsilon^T]}_{I_d} A^T = \Sigma_X
\end{aligned}$$

In the first step, we used equation (25) and the value for the mean of X we computed earlier. Then we simplified and applied property (18) of the mean. Finally, we used that the variance of standard normally distributed random variables is 1 and covariance between independent variables is 0 and thus $E[\epsilon\epsilon^T]$ is the identity matrix.

Marginal and Conditional distribution Let $X \sim \mathcal{N}(\mu_x, \Sigma_X)$ be a d-dimensional multivariate random variable. We consider marginalizing a subset of these variables, or computing the conditional distribution of a subset of variables. For simplicity we split X in two blocks: $X_1 \in \mathbb{R}^k$ and $X_2 \in \mathbb{R}^{d-k}$. With

this block split, we can write both Σ_X and μ_X in block notation

$$X = \left[\begin{array}{c} X_1 \\ \hline X_2 \end{array}\right], \ \mu_X = \left[\begin{array}{c} \mu_1 \\ \hline \mu_2 \end{array}\right], \ \Sigma_X = \left[\begin{array}{c|c} \Sigma_{11} & \Sigma_{12} \\ \hline \Sigma_{21} & \Sigma_{22} \end{array}\right]$$

Then, the marginal distribution of X_1 is $\mathcal{N}(\mu_1, \Sigma_{11})$ and the conditional distribution $X_2|X_1$ with pdf $p(x_2|x_1)$ is $\mathcal{N}(\mu_{2|1}, \Sigma_{2|1})$, where

$$\mu_{2|1} = \mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(X_1 - \mu_1), \qquad \Sigma_{2|1} = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{21}^T \tag{29}$$

The results for the marginal of X_2 and the conditional $X_1|X_2$ can be obtained by permuting the order of X_1 and X_2 in the random vector and exchanging the blocks of μ_X and Σ_X accordingly.

Proof: We start by the observation of (25), that there exists an A, such, that $X = \mu_X + A\epsilon$ where $\epsilon \sim \mathcal{N}(0, I_d)$. Moreover, it can be shown that there exist an A that fulfills the form

$$A = \left[\begin{array}{c|c} A_{11} & 0 \\ \hline A_{21} & A_{22} \end{array}\right], \text{ with } A_{22} \text{ invertible.}$$

(This can be shown constructively using the Cholesky decomposition algorithm. We skip this part for brevity of presentation.)

To obtain a more concrete description of A we relate the values using $\Sigma_X = AA^T$ and using blockwise matrix multiplication, we have

$$\begin{aligned} \left[\begin{array}{c|c} \Sigma_{11} & \Sigma_{12} \\ \hline \Sigma_{21} & \Sigma_{22} \end{array}\right] &= \left[\begin{array}{c|c} A_{11}A_{11}^T + 0 \cdot 0 & A_{11}A_{21}^T + 0 \cdot A_{22}^T \\ \hline A_{21}A_{11}^T + A_{22} \cdot 0 & A_{22}A_{22}^T + A_{21}A_{21}^T \end{array}\right] \\ &= \left[\begin{array}{c|c} A_{11}A_{11}^T & A_{11}A_{21}^T \\ \hline A_{21}A_{11}^T & A_{22}A_{22}^T + A_{21}A_{21}^T \end{array}\right] \end{aligned}$$

By comparing both sides block by block, we obtain the relations

$$\begin{aligned} A_{11}A_{11}^T &= \Sigma_{11} \\ A_{21} &= \Sigma_{21}(A_{11}^T)^{-1} \\ A_{22}A_{22}^T &= \Sigma_{22} - A_{21}A_{21}^T = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{21}^T \end{aligned}$$

With that, $X = \mu_X + A\epsilon$ can be written in block notation using the same split of ϵ in ϵ_1 and ϵ_2:

$$\left[\begin{array}{c} X_1 \\ \hline X_2 \end{array}\right] = \left[\begin{array}{c} \mu_1 \\ \hline \mu_2 \end{array}\right] + \left[\begin{array}{c|c} A_{11} & 0 \\ \hline A_{21} & A_{22} \end{array}\right] \left[\begin{array}{c} \epsilon_1 \\ \hline \epsilon_2 \end{array}\right] \tag{30}$$

Comparing the left and right side reveals $X_1 = \mu_1 + A_{11}\epsilon_1$ and thus $X_1 \sim \mathcal{N}(\mu_1, \Sigma_{11})$ by equation (25). This shows the marginalization part.

For the conditional distribution $X_2|X_1$, we assume that X_1 is observed and therefore fixed. Thus $X_2|X_1$ are all samples from the joint that lead to this value of X_1. When considering this in the generating transformation (30), this means as X_1 appears on the left side, we have to compute its effect on the right hand side. We have shown already, that $X_1 = \mu_1 + A_{11}\epsilon_1$, thus with X_1 fixed, ϵ_1 is fixed as well and

$$\epsilon_1 = A_{11}^{-1}(X_1 - \mu_1) \ .$$

The same equation for X_2 is given by the second row of (30) and

$$X_2 = \mu_2 + A_{21}\epsilon_1 + A_{22}\epsilon_2 = \mu_2 + A_{21}A_{11}^{-1}(X_1 - \mu_1) + A_{22}\epsilon_2 \ .$$

Thus, X_2 follows a multivariate distribution by (25) with mean $\mu_{2|1} = \mu_2 + A_{21}A_{11}^{-1}(X_1 - \mu_1)$ and covariance $\Sigma_{2|1} = A_{22}A_{22}^T$. Using the three value relations between A and Σ_X above, we obtain the result.

Joint of dependent normals with shifted means Let $X \sim \mathcal{N}(\mu_X, \Sigma_X)$ be a d-dimensional multivariate random variable and $Y|X \sim \mathcal{N}(\mu_Y + AX, \Sigma_Y)$. Then the joint distribution of both variables is

$$\left[\begin{array}{c} X \\ \hline Y \end{array}\right] \sim \mathcal{N}\left(\left[\begin{array}{c} \mu_X \\ \hline \mu_Y + A\mu_X \end{array}\right], \left[\begin{array}{c|c} \Sigma_X & \Sigma_X A^T \\ \hline A\Sigma_X & \Sigma_Y + A\Sigma_X A^T \end{array}\right]\right) \ . \tag{31}$$

This statement is the inverse of the previous statement: In (29) we obtained that $X_2|X_1$ is normally distributed with its only dependence on the value of X_1 being the shifted mean. Now we show, that two multivariate normal distributed random variables that depend on each other by a mean shift are jointly multivariate normal.

Proof: The proof follows by stating (25) for the joint distribution.

Closed under linear Transformations Let $X \sim \mathcal{N}(\mu_x, \Sigma_X)$ be a d-dimensional multivariate random variable. Further, let $Q \in \mathbb{R}^{k \times d}$, then

$$Z = QX$$

is a multivariate normal random variable with $Z \sim \mathcal{N}(Q\mu_X, Q\Sigma_X Q^T)$

Proof: Let $\epsilon \sim \mathcal{N}(0, I_d)$. Further, let A_X be a matrix such, that $\Sigma_X = A_X A_X^T$. Then $X = \mu_X + A_X\epsilon$ and

$$Z = QX = Q(\mu_X + A_X\epsilon) = \underbrace{Q\mu_X}_{\mu_Z} + \underbrace{QA_X}_{A_Z}\epsilon = \mu_Z + A_Z\epsilon.$$

This meets the definition of a multivariate normal distribution by (25) and Z has covariance

$$\Sigma_Z = A_Z A_Z^T = Q A_X A_X^T Q^T = Q \Sigma_X Q^T \ .$$

Sum of Multivariate Random Variables Let $X \sim \mathcal{N}(\mu_x, \Sigma_X)$, $Y \sim \mathcal{N}(\mu_y, \Sigma_Y)$ be d-dimensional multivarate random variables. Then,

$$Z = X + Y \tag{32}$$

is a multivariate normal random variable with $Z \sim \mathcal{N}(\mu_X + \mu_Y, \Sigma_X + \Sigma_Y)$.

Proof: We can construct the result directly from the previous result on linear transformations. We treat X, Y as two blocks of a $2d$ dimensional random variable T and it is straight forward to show that T is a multivariate normal distributed random variable (e.g., as special case of the joint of dependent normals property) with

$$T = \left[\frac{X}{Y}\right] \sim \mathcal{N}\left(\left[\frac{\mu_X}{\mu_Y}\right], \left[\begin{array}{c|c} \Sigma_X & 0 \\ \hline 0 & \Sigma_Y \end{array}\right]\right) \ .$$

We define as linear transformation the block-matrix constructed by concatenating two d-dimensional identity matrices I_d, $Q = [I_d | I_d] \in \mathbb{R}^{d \times 2d}$ and $Z = Q \cdot T = X + Y$. Then, using the projection property, we obtain the end result.

3 Interpretations of Probability

While probability theory introduces the formal foundations for handling uncertainty and randomness, mathematics is not directly concerned with the real world. The formal definition of probability does not tell us how to interpret the values we compute. Two fundamentally different interpretations of probabilities are actively used in Machine Learning: the Frequentist and the Bayesian perspective. The choice of perspective can lead to quite different methods for modeling data.

Let us start with two simple examples to illustrate the problem. Consider first that we want to throw a fair coin 100 times. Before throwing the coin, we can ask "What is the probability that a fair coin will come up heads at least 60 times?". We then throw the coin 100 times and observe that it comes up heads 63 times. This is an unlikely event, so an immediate question arising is: "After observing the outcome, what is the probability that the coin is fair?".

In the two cases we use the word probability with a different meaning. In the first question, probability refers to the *frequency* of an outcome. If we repeated this experiment 1000 times, we would expect that the coin comes up heads more than 60 times in around 2.8% of repetitions and the weak law of large numbers tells us that as the number of repetitions increase, we expect less of a deviation from this number. In this sense, this interpretation of probability is in principle a verifiable fact (at least in our experiment, where we have the luxury that we can repeat it numerous times).

In the second question, we interpret probability as an *uncertainty over a held belief*. The coin might be fair but we have observed an unlikely event providing evidence that the coin gives heads more often than tails and this observation changes our belief over the coins fairness. Most importantly, this interpretation of probability does not refer to verifiable facts - the coin is either fair or biased, independent of our beliefs.

In the real world, these two interpretations of probability exist side by side in our decision processes. A recent scientific example was the possible observation of neutrinos travelling faster than light by the OPERA collaboration in 2011. Neutrinos were produced at CERN in Geneva and sent towards a detector at Gran Sasso in Italy. The time-difference between time of production and time of observation provides an estimate of the speed at which the particles travel. This observation is noisy, since at both ends the instruments only have limited precision. Therefore the experiment was repeated a large number of times. The result was that neutrinos moved too quickly: they arrived on average around 60.7ns faster than they would if they travelled with speed of light and the time difference was several time larger than what was expected due to random measurement imprecision.

The first reaction of the scientific community was, that this was most likely a data fluke or an error in the experiment. So the collaboration tested everything, repeated the experiment and gathered enough data so that the probability of observing a random fluctuation this large was less than 1 in 10 Million - the common threshold for an effect to be considered a scientific discovery in particle

physics. This only lead many scientists to *belief stronger* that there is an error in the experiment. And they were right. Half a year later, a loose cable was found that slowed down the time signal of the high-precision clock. A repetition of the experiment then verified that the new expected travel time was within the error margin of the experiment assuming that neutrinos are not travelling faster than the speed of light.

This example sheds light on the two interpretations of probability. In the first, we only consider uncertainty over verifiable facts: is the difference in travel time larger than we would expect? It does neither provide evidence towards the reason why these differences are observed, nor does it provide direct guidance towards which decision to take: it could be either a real effect or the experiment is faulty and there is no information that can discern between the two.

In the second interpretation, our beliefs of a truth are affected by the prior belief: evidence towards faster than light neutrinos lead scientists to belief that the experiment is faulty, because their *prior* belief of the world is that the probability of an error in the experiment is much larger than a particle travelling faster than light. This is also why gathering more experimental data using the same experimental equipment did not sway their opinion: gathering more data only rules out the chance of observing a random fluctuation, but does not rule out persistent errors in the measurement equipment.

3.1 Bayesianism and Frequentism

The two aforementioned interpretations each have a name in the scientific community. Approaches that interpret probabilities as the frequency of an event are called *Frequentist* and statisticians who favour this interpretation are called *Frequentists*. Approaches using the second interpretation are called *Bayesian* and statisticians using these approaches are called *Bayesians*. This name refers to the importance of Bayes' Theorem to incorporating the prior belief into the evidence. Still, the use of Bayes' theorem does not make a theory Bayesian, as it is a fact derived from probability theory and used by Frequentists as well - it is the interpretation of the resulting probabilities as a belief, which is the important distinction.

There are very strong opinions in the statistics community about which approach is the "better" one. This is because both approaches can be used to make decisions: While Frequentism does not model decisions directly, a Frequentist can still decide to adapt the option that is supported most by the data. For example, we can decide that a coin should be discarded and replaced by a new if it lands heads more than 60 times out of a 100. This decision would at worst discard 1.7% of fair coins on average, while discarding most of strongly biased coins (e.g. a coin with probability of heads $\geq 65\%$ has at least a 82.7% chance of being discarded) . This decision process does not entail a belief over whether a discarded coin is biased or not: depending on the actual frequency of biased coins, almost none or all discarded coins might be fair.

A Bayesian would incorporate their prior belief about the relative proportions of fair and unfair coins into the model to obtain a final belief that the

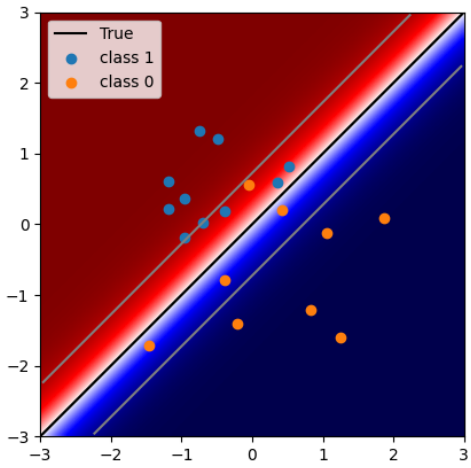


Figure 1: Visualization of our logistic regression toy experiment. The samples drawn (points) are assigned labels (colors) based on the class-probability $p(y = 1|x, \theta)$ (background coloring) for a chosen value of θ. The decision boundary of the classifier is shown as the black line labeled "True". Blue background means $p(y = 0|x, \theta) > p(y = 1|x, \theta)$, red means the opposite.

decision is based on. The decision would then be to only keep coins which are believed to be fair (e.g. $P(\text{Coin is fair}|\text{Data}) > 0.8$). The Frequentist would argue that by incorporating the prior belief, the decision becomes subjective: it is not only the evidence that partakes in the decision, but also the prior. The Bayesian would in turn argue that not using prior knowledge sometimes leads to nonsensical decisions, like adapting that Neutrinos might travel faster than light (to which the Frequentist would argue that of course they would not favour that and instead would propose to gather data via an independent replication to rule out an error in this experiment. By this point, the reader might guess, that these discussions between Bayesians and Frequentists are rarely fruitful).

In the following, we will try to keep a neutral view on the two approaches. While this topic is also covered in (Bishop, chapters 1.2.3, 1.5, 3.4), it is important to keep in mind that Bishop declares himself a Bayesian and he is arguing for the adaptation of the Bayesian approach. Similarly, while this text tries to stay neutral, it is written by someone who was educated in the Frequentist view.

We will introduce the two approaches in a formal way and shed light on their predictions. As a running example, we will use the case of logistic regression in a binary classification problem. We assume, we are given a Dataset $\mathcal{D} = \{(x^{(1)}, y^{(1)}), \dots, (x^{(\ell)}, y^{(\ell)})\}$, where the $x^{(i)} \in \mathbb{R}^2$ are the inputs and $y^{(i)} \in \{0, 1\}$ are the labels assigned to point $x^{(i)}$. Our goal is to find the parameters θ of a linear model $f_\theta(x) = \theta_1 x_1 + \theta_2 x_2 + \theta_3$ that separates between points of both classes. The probability of a label y given a point x in this model is

$$p(y = 1|x, \theta) = \text{sigmoid}(\theta_1 x_1 + \theta_2 x_2 + \theta_3) \tag{33}$$

A visualisation of this data and task is given in Figure 1.

3.2 The Bayesian view

In the Bayesian view we assume that the unknown parameter vector θ is a random variable symbolizing the distribution of our beliefs. Our initial beliefs about the parameter before seeing any data are encoded via the *prior distribution* $p(\theta)$. The dataset $\mathcal{D}$ is considered fixed: this is the evidence that we use to update our prior belief $p(\theta)$ to the *posterior* belief $p(\theta|\mathcal{D})$.

We assume that $\mathcal{D}$ is produced by a data generative process. For example, in logistic regression, we assume that a learning problem and its dataset are generated by first sampling the unknown model parameters θ from $p(\theta)$, then sample datapoints $x^{(i)}$ from a distribution $p(x)$ and then acquire labels using a distribution $p(y|x, \theta)$, or

$$p(\mathcal{D}, \theta) = p(\theta)p(\mathcal{D}|\theta) = p(\theta) \prod_{i=1}^{\ell} p(x^{(i)})p(y^{(i)}|x, \theta) \ . \tag{34}$$

Since we do not observe θ in this generative process and are only left with the dataset, we can only compute our belief over the distribution of the parameters

after observing the data. Assuming that our model (34) is correct, we compute $p(\theta|\mathcal{D})$ using Bayes' Theorem :

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D},\theta)}{\int_{\Omega_\theta} p(\mathcal{D},\theta')d\theta'} = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})} \quad . \tag{35}$$

The quantity $p(\mathcal{D})$ is constant in the model. It is the normalisation constant that ensures that $\int p(\theta|\mathcal{D})d\theta = 1$. This quantity is often very difficult to compute.

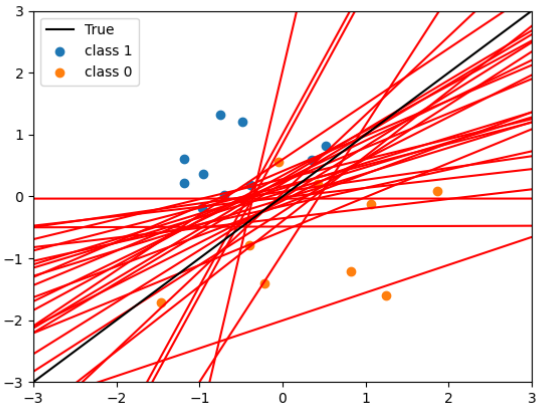
To visualize the distribution using logistic regression, we can obtain samples from $p(\theta|\mathcal{D})$ (with algorithms covered later in the course) and plot the resulting models. As prior $p(\theta)$ we use a standard normal distribution for each parameter. In Figure 2a we show the decision boundaries obtained for different sampled values of θ given a dataset with $\ell = 20$ elements. The red lines mark the points where $p(y = 1|x, \theta) = 1/2$. There is quite some variation in the obtained samples, even though a majority is pointing in the correct direction and pass in-between the data points. This variation is reduced as we increase the size of the dataset to $\ell = 100$ (Figure 2b) at which point most of the obtained boundaries separate the two classes well. This is an important property of Bayesian approaches. As the number of points is low, the prior dominates the samples and thus, if the prior has a large variation, the posterior distribution will retain some of it and will still be affected by it.

This is true independently of the chosen prior. If we change the choice of prior to a less fitting strong prior belief, the quality of the obtained models decreases. In Figure 2c we have changed the prior distribution of the offset θ_3 to a normal distribution with mean 5 and variance 0.1. In this case, even with $\ell = 100$ samples in the dataset, the decision boundaries still don't separate the two classes at a good location and the obtained decision boundaries are shifted upwards. Moreover, the posterior distribution shows low variation, similar to the case in Figure 2b. Thus, the variance of the posterior does not give information about the quality of the model. If the prior distribution is confidently wrong, the posterior is likely confidently wrong as well, unless a large amount of data is provided. Of course, if the provided prior is confident and right, then the posterior will be much better and samples will approximate the true parameters with high precision, even if only little data is available.

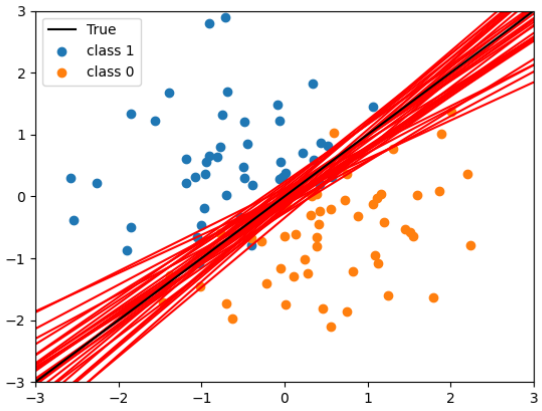
So far we have only computed a distribution of parameters via the posterior distribution, but in practice we often have to decide on a concrete model to use. There are a few common options. The most well-known is the maximum-a-posteriori estimate (MAP), which picks the θ that maximizes $p(\theta|\mathcal{D})$:

$$\theta^{MAP} = \arg\max_\theta p(\theta|\mathcal{D}) = \arg\max_\theta p(\mathcal{D}|\theta)p(\theta) \quad . \tag{36}$$

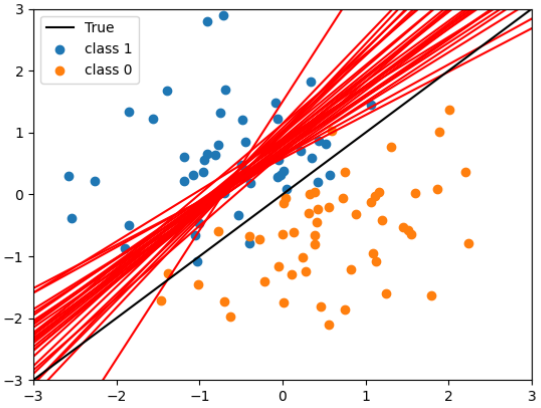
This approach does not require computing $p(\mathcal{D})$ as it is a constant over all queried values of θ. However, picking the point with the largest value of the posterior pdf is not equivalent to picking a point that is representative of the distribution. This point might be far away from the majority of sampled points.



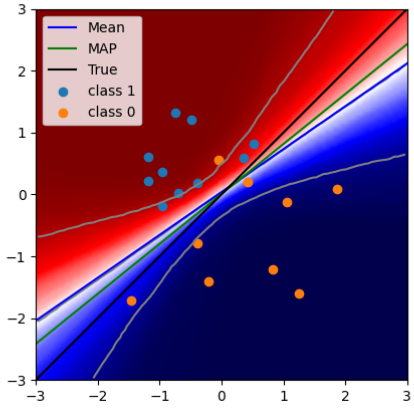
(a) $\ell = 20$



(b) $\ell = 100$



(c) Bad prior, $\ell = 100$



(d) Model selection

Figure 2: a+b) samples from the posterior distribution using datasets with different number of points ℓ. The training data is plotted as points, colors indicate the label of the dots. c) Same as b) but with a different prior distribution. d) Plot of the Mean (blue, eq (37)), MAP (green, eq. (36)) and a-posteriori distribution (background, grey lines, eq. (38))

Another estimate is the mean

$$\hat{\theta} = E[\theta|\mathcal{D}] = \int p(\theta|\mathcal{D})\theta \; d\theta \;\; . \tag{37}$$

In practice this value can not be computed and is instead replaced by taking the sample mean over a set of sampled parameter vectors. Of course it is debatable, whether taking the mean of sampled parameter values is a sensible operation in our model. The solution that many Bayesians favour is defining a new distribution, called the *posterior predictive*

$$p(y|x, \mathcal{D}) = \int p(\theta|\mathcal{D})p(y|x, \theta)d\theta \;\; . \tag{38}$$

This approach samples a number of parameter values $\theta^{(i)}$ from $p(\theta|\mathcal{D})$ and then for each of them computes the distribution of labels $p(y|x, \theta^{(i)})$ for a given query input x. The prediction is the average of the label distributions. A decision is then taken, for example by picking the label y with the highest probability. For our logistic regression example, we visualize the three different solutions in Figure 2d. Both the MAP and mean solution differ from each other, but they are each a linear model. If we compare the posterior predictive (color background and grey lines in Figure 2d) and compare it to the original model Figure 1, it becomes clear that the distribution of label uncertainty is different. The shape formed by the grey lines in the posterior distribution is closer to an hourglass, than a straight line. This takes into account the spread of the samples in Figure 2a. The uncertainty of the direction of the decision boundary transforms to an uncertainty of its position in sample space. This uncertainty increases as we get further away from the midpoint of the data distribution, giving rise to the hourglass shape.

The biggest criticism of the Bayesian approach is the explicit choice of a prior that affects the final selection of models. This is because in a pure Bayesian approach, it is impossible to verify the quality of a prior. This sounds counter-dtive, because when comparing the results in Figures 2b&2c, it seems obvious which prior leads to a better data fit. To see the difficulty in evaluating priors, we have to look back at our data generative process (34). As long as $p(y|x, \theta)$ never assigns probability 0 to a label, we can obtain a dataset that includes an unlucky pick of labels. Thus, the posterior reflects a balance between picking a model we believe can be true and still somewhat aligns with a dataset that includes a few "unlucky" labels.

Given the difficulty of assessing a prior, how can we pick priors in the real world? After all, in many applications the fitted parameters are abstract and have no obvious meaning. There are several common techniques:

- Complexity arguments. A natural choice of prior in machine learning is one that penalizes model complexity. In the presence of little data, we prefer a simple model and as more data becomes available, we allow the chosen parameters to represent one that is more complex. In our logistic regression example, the complexity of the model can be measured in the

norm $\|\theta\|$, as with increasing norm the model becomes more confident in its predictions and the probabilities are closer to 0 and 1. The normal distribution prior with zero mean used in our example does this.

- Weak priors: Sometimes no usable prior knowledge is available. In this case, a weak prior can be used that assigns prior probability to a wide range of parameters. This can be done by picking a normal distribution with a very large variance.

- Sometimes, we have a strong intuition about the general form of a prior, but don't know its parameters. In this case, we can parameterize the prior with its own set of parameters η and then add another prior distribution $p(\eta)$. The resulting prior on θ is then

$$p(\theta) = \int_{\Omega_\eta} p(\theta|\eta)p(\eta)d\eta \tag{39}$$

  This is called a hierarchical prior because as the number of data points increases, we begin to favour specific choices of η which then pick a prior for the parameters θ.

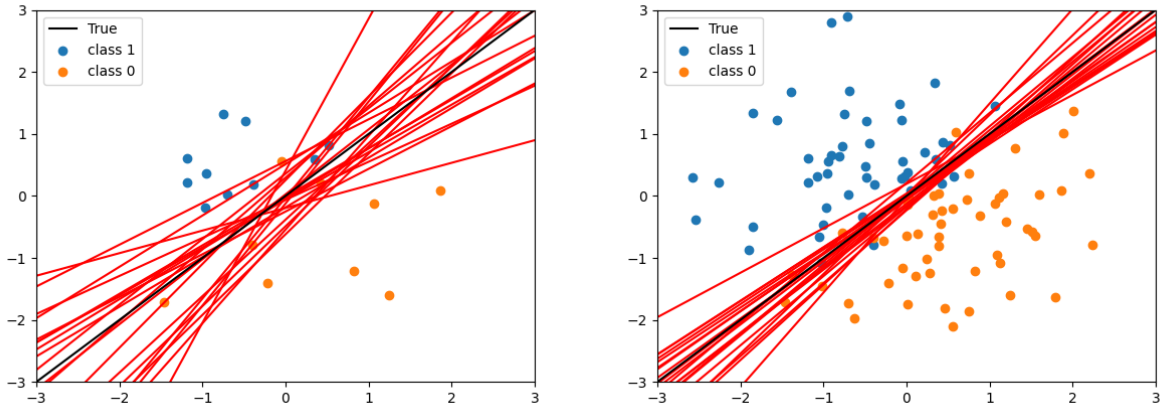
Bayesian model selection The hierarchical prior approach can be used to perform Bayesian model selection: the task of picking the model, or prior, that models the data best. In this, we pick η as an index for the chosen prior and then each $p(\theta|\eta)$ represents a choice of prior. For example, we can pick $p(\theta|\eta = 1)$ as a standard normal distribution to penalize model complexity, while $p(\theta|\eta = 2)$ encodes a different prior which we could have obtained by analysis of the learning problem in question (this analysis might be faulty and thus give rise to the bad prior case we discussed previously). Then, we pick a prior over η, for example a uniform distribution over choices. With this model, computing $p(\theta|\mathcal{D})$ automatically averages over the posterior distribution of η. this happens, since

$$p(\theta|\mathcal{D}) = \int_{\Omega_\eta} p(\theta|\eta, \mathcal{D})p(\eta|\mathcal{D})\ d\eta\ , \tag{40}$$

where $p(\theta|\eta, \mathcal{D})$ is the posterior distribution of the model parameters under the choice of prior indexed by η. This way, as more data is used, $p(\eta|\mathcal{D})$ becomes more and more concentrated over a single η: The degree of our belief over which prior is correct increases.

3.3 The Frequentist view

The Frequentist approach takes almost the opposite point of view when it comes to the basic assumptions. Here, we assume that the parameter values θ^* we search in a learning task are unknown, but fixed. Instead, we consider the dataset as a random variable and an estimator (or learning algorithm) is used



(a) $\ell = 20$ (b) $\ell = 100$

Figure 3: a+b) samples from the distribution $p(\theta|\theta^*, \mathcal{A})$ using datasets with different number of points ℓ. The training data is plotted as points, colors indicate the label of the dots.

to estimate the parameter values given the data. The point of view taken here is that for a given task, there exist optimal model parameters and the quality of a) our Dataset $\mathcal{D}$ and b) our estimator $\mathcal{A}$ are deciding factors in how close our estimates can get to the true parameters. Since we rarely have control over a), the focus of Frequentist approaches lies on selection of good estimators b).

Even if the estimator is deterministic, every time we obtain a new dataset for a given task the estimated parameter values will vary slightly and θ is distributed as

$$p(\theta|\theta^*, \mathcal{A}) = \int p(\mathcal{D}|\theta^*) p(\theta|\mathcal{A}, \mathcal{D}) \, d\mathcal{D} \ . \tag{41}$$

Here, $p(\mathcal{D}|\theta^*)$ uses a generative process similar to (34), except that we assume that θ^* is already drawn and therefore constant. The distribution $p(\theta|\mathcal{A}, \mathcal{D})$ is the distribution of parameter vectors returned by $\mathcal{A}$ given a sampled dataset. If the algorithm is deterministic, the distribution is a delta-peak, putting all probability mass on a single point.

Again, we can visualize this using the logistic-regression toy experiment. We sample a set of datasets $\mathcal{D}^{(i)}$ from our generative process for fixed θ^* and for each dataset, we obtain an estimate $\theta^{(i)}$ by applying the estimator to the dataset. As estimator, we use maximum likelihood:

$$\theta^{(i)} = \arg\max_{\theta} p(\mathcal{D}^{(i)}|\theta) \tag{42}$$

The results for datasets of sizes $\ell = 20$ and $\ell = 100$ are given in Figures 3a&3b. We can again see that with a small dataset, there is a lot of variation in the

obtained models, which decreases as the number of data points increases.

This is a property of the chosen maximum likelihood estimator, but is not true for all estimators. For example consider the estimator that always returns the zero-vector, or the MAP estimate using the "bad" prior used in Figure 2c. Both estimators always show a small (or zero) variance, but model the data poorly. Thus, similar to the Bayesian case, the spread of the distribution $p(\theta|\theta^*, \mathcal{A})$ does not carry information about the quality of the estimator that produced it. If we want to select estimators based on their ability to model the data well, we need a different measure.

Risk measures are used to compare different estimators. They use a loss-function $L(\theta, \theta^*)$ that assign a loss based on the difference between true and estimated value. With this, we define the risk as the expected loss over $p(\theta|\theta^*, \mathcal{A})$, the distribution of estimated parameters using $\mathcal{A}$ as estimator integrated over all possible datasets

$$\mathcal{R}(\mathcal{A}, \theta^*) = \int p(\theta|\theta^*, \mathcal{A}) L(\theta, \theta^*) d\theta \tag{43}$$

A popular choice for the loss is the squared error $L(\theta, \theta^*) = \|\theta - \theta^*\|^2$. Intuitively, with this loss, the risk is the average squared distance between estimated and true parameter value. If the estimator is also unbiased, i.e., $E[\theta] = \theta^*$ the measure directly computes the variance of θ.

Example: We throw a coin N times and record the results as a dataset with outcomes $x_1, \ldots, x\ell$, $x_i \in \{0, 1\}$, where 1 stands for heads. The samples x_i follow a Bernoulli distribution $x_i \sim \text{Bernoulli}(\theta^*)$, where $\theta^* \in [0, 1]$ is the probability of the coin to land heads. As estimator $\mathcal{A}$ of θ^*, we pick the sample mean

$$\theta = \frac{1}{\ell} \sum_{i=1}^{\ell} x_i \ .$$

In this case, the data distribution of the generating process is known and the random variable $Z = \ell\theta$ follows a Binomial distribution. From this we can compute the risk using the squared loss (try deriving this yourself) and obtain:

$$R(\mathcal{A}, \theta^*) = \frac{1}{\ell} \theta^* (1 - \theta^*)$$

The risk as defined above depends on the value θ^*. Since this value is unknown, it seems difficult to compare estimators in practice as different estimators might perform better for different values of θ^*. What we would like to have is a single number. One option is to consider the *minimax risk*, that is the

maximum risk over all θ^*,

$$\mathcal{R}_{\max}(\mathcal{A}) = \max_{\theta^*} \mathcal{R}(\mathcal{A}, \theta^*) \ .$$

Example: In the previous coin experiment, the minimax risk over all $\theta^* \in [0, 1]$ is obtained for $\theta^* = 1/2$ and

$$\mathcal{R}_{\max}(\mathcal{A}) = \max_{\theta^*} \frac{1}{\ell}\theta^*(1-\theta^*) = \frac{1}{4\ell} \ .$$

The minimax risk is dominated by the worst-case performance and is thus very pessimistic or even infinite. An average risk would be preferable, but the average risk requires to define a prior distribution on θ^*, $p(\theta^*)$. The resulting risk is called the Bayes-Risk:

$$\mathcal{R}_{\text{Bayes}}(\mathcal{A}) = \int p(\theta^*)\mathcal{R}(\mathcal{A}, \theta^*)d\theta^* \ .$$

The Bayes-Risk is accepted in the Frequentist community if there is a natural choice of $p(\theta^*)$.

Example: Linear Classifiers are estimators. A linear classifier assigns a label to a point based on which side of the decision boundary it lies:

$$h(x) = \text{sign}(\phi^T x)$$

Here, ϕ is the parameter vector selected by the learning procedure. Thus, the model $h(x)$ is itself an estimator of the unknown label y^* of the query point x. We can therefore compute a risk-measure for this estimator. For classification, we can use the classification loss as risk measure that returns 1 if the wrong label is assigned

$$L(y, y^*) = \begin{cases} 0, \text{ if } y = y^* \\ 1, \text{ if } y \neq y^* \end{cases} \ .$$

The risk is then the expected miss-classification rate averaged over the samples of a specific class

$$\mathcal{R}(f, y^*) = \int p(x|y^*)L(h(x), y^*)\ dx \ .$$

The minimax risk is then just the miss-classification rate of the the class with highest risk. If we use the true label probability as prior, the Bayes risk is the proportion of miss-classified points

$$\mathcal{R}_{\text{Bayes}}(f) = \int p(x, y^*)L(h(x), y^*)\ dx\ dy^*$$

In applications, even if there is a natural choice of prior, the Bayes risk can typically not be computed, since we lack an analytical expression for it. Instead, if pairs $(\theta^*, \mathcal{D})$ sampled from the prior are available, we can compute the *empirical* Bayes risk by using known test sets, i.e., samples of problems with datasets $\mathcal{D}^{(i)}$, $i = 1, \ldots, N$ and parameters $(\theta^*)^{(i)}$. An estimator can generate estimates $\theta^{(i)}$ for each dataset and we can evaluate them using the expected loss

$$R_{\text{emp}}(\mathcal{A}) = \frac{1}{N} \sum_{i=1}^{N} L(\theta^{(i)}, (\theta^*)^{(i)}) \ . \tag{44}$$

Example: When evaluating the risk(=miss-classification rate) of a classifier, the data distribution is typically unknown. Instead, we can obtain a test set of labeled data $x^{(i)}, (y^*)^{(i)}$. The empirical Bayes risk is

$$R_{\text{emp}}(\mathcal{A}) \frac{1}{N} \sum_{i=1}^{N} L(h(x^{(i)}), (y^*)^{(i)}) \ .$$

Statistical Testing a Nutshell. If we have to choose an estimator, we can base this decision on the empirical risk, for example by picking the estimator with the smallest risk. However, even if the estimator is fixed, the empirical risk is a random variable due to its dependence on the test dataset, which in the Frequentist view is random. Thus, it is unclear whether for two estimators $\mathcal{A}_1$, $\mathcal{A}_2$ the observation that $R_{\text{emp}}(\mathcal{A}_1) < R_{\text{emp}}(\mathcal{A}_2)$ also implies $R_{\text{Bayes}}(\mathcal{A}_1) < R_{\text{Bayes}}(\mathcal{A}_2)$. Therefore, the correct approach is to test, whether the observed differences are so large compared to the variance of the empirical risk, that it is unlikely to be a random deviation. In case that the result is unlikely, the better of two models can be adapted, similarly to how we described it in the problem of the fair coin throw in the beginning of the chapter. This strategy is called statistical testing and one of the hallmarks of Frequentist methodology.

Importance to Bayesianism The importance of statistical testing also extends deep into Bayesian methodology, for two reasons. First, at all steps of statistical modeling we have to make assumptions about the model and distributions, for example in the generative model (34). Second, we are often not interested in the likelihood of the data under our model, but instead have fixed performance metrics, for example the miss-classification risk.

Therefore, model evaluation is key to ensure that our model also performs well in reality. Aside of model comparison, there are also more cross-overs between both approaches. For example, instead of a hierarchical prior, we can use the maximum likelihood estimate of the parameters of the prior. This gives rise to *empirical Bayes* methodology.

4 Generalized Linear Models

This chapter covers parts of the following chapters in the Bishop book: 3.1, 3.3, 4.3.

Independent of which statistical view is adapted, most machine learning approaches rely on the assumption of a generative model for the dataset $\mathcal{D}$. The most common is the the generative model in supervised learning for the dataset $\mathcal{D} = \{(x^{(1)}, y^{(1)}), \dots, (x^{(\ell)}, y^{(\ell)})\}$, as we have stated in (34) and repeat here:

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{\ell} p(x^{(i)}) p(y^{(i)}|x^{(i)}, \theta) \tag{45}$$

Notation: In supervised learning, we are interested in learning the relation $p(y^{(i)}|x, \theta)$ while we assume that $p(x)$ is given by an implicit distribution of samples: we want to predict the label for an input but do not want to model the distribution of inputs. Therefore, $p(x)$ is independent of our learned model and in all learning methods $p(x)$ will cancel out at some point. For example, when computing the posterior from (45) using a prior $p(\theta)$, we have

$$\begin{aligned} p(\theta|\mathcal{D}) &= \frac{p(\theta) \prod_{i=1}^{\ell} p(x^{(i)}) p(y^{(i)}|x^{(i)}, \theta)}{\int_{\Omega_\theta} p(\theta') \prod_{i=1}^{\ell} p(x^{(i)}) p(y^{(i)}|x^{(i)}, \theta') d\theta'} \\ &= \frac{p(\theta) \prod_{i=1}^{\ell} p(y^{(i)}|x^{(i)}, \theta)}{\int_{\Omega_\theta} p(\theta) \prod_{i=1}^{\ell} p(y^{(i)}|x^{(i)}, \theta') d\theta'} \end{aligned}$$

therefore, we will drop $p(x)$ in the following. This is equivalent to conditioning on $x^{(1)}, \dots, x^{(\ell)}$ as first step.

With logistic regression, we have already considered an example for binary labels $y^{(i)} \in \{0, 1\}$

$$p(y = 1|x, \theta) = \text{sigmoid}(f_\theta(x)) \ , \tag{46}$$

where $f_\theta(x) = \theta^T x$ is a linear model. Here, we used the sigmoid function

$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$

to map between the model prediction and the probability of a label. But we could have used any function that maps from a real input to the interval $(0, 1)$. The question is therefore: What is the significance of the choice and how does it affect our model?

Linear Regression To answer this question, we look first at a different case, linear regression. Here, our labels are real valued, $y \in \mathbb{R}$ and our task is to find the parameters of a linear function f_θ such, that the predictions $f_\theta(x^{(i)})$ are as

close as possible to $y^{(i)}$. We assume that the $y^{(i)}$ are noisy observations. This means that the labels assigned to a random point X are the response of the true underlying model $g(X)$, corrupted by random noise, which is typically assumed to be additive:

$$Y = g(X) + \epsilon \tag{47}$$

Here, ϵ is some random variable, modeling the measurement noise. Consequently, our labels are samples from this generative model

$$y^{(i)} = g(x^{(i)}) + \epsilon^{(i)} \quad . \tag{48}$$

A frequent assumption is that $\epsilon \sim \mathcal{N}(0, \sigma_Y^2)$ and therefore

$$p(y|x) = \mathcal{N}(y; g(x), \sigma_Y^2) \quad . \tag{49}$$

Of course we don't know $g(x)$, but assuming it is a linear function, our generative model takes the form

$$p(y|x, \theta) = \mathcal{N}(y; \theta^T x, \sigma_Y^2) \quad . \tag{50}$$

Binary Classification For the binary classification case, we can try to adapt the model of linear regression and investigate possible alternatives to generalize (47) to binary labels. A possible generalization is as follows: We take $g(x)$ and view it as a function of class-membership: if $g(X) > 0$, then the label is 1, otherwise 0. Of course, since our predictions are affected by incomplete information and measurement noise, labels are not assigned based on $g(X)$ but $g(X) + \epsilon$, where ϵ now models our uncertainty about the class membership. Thus, labels are Bernoulli distributed random variables generated by

$$Y = \begin{cases} 1, & \text{if } g(X) + \epsilon > 0 \\ 0, & \text{otherwise} \end{cases} \quad . \tag{51}$$

The probability that $Y = 1$ can be computed easily, since $Y = 1$ entails $g(X) + \epsilon > 0$ and thus

$$P(y = 1|x) = P(\epsilon > -g(X)) = 1 - P(\epsilon \leq -g(X)) = 1 - \int_{-\infty}^{-g(X)} p(\epsilon)\, d\epsilon \quad .$$

The function $P(\epsilon \leq t)$ for a univariate random variable is the cumulative distribution function (cdf).

Logistic Regression To derive logistic regression, we need to pick ϵ as distributed according to the standard logistic distribution with state space $\mathbb{R}$ and pdf

$$p(\epsilon) = \frac{\exp(-\epsilon)}{(1 + \exp(-\epsilon))^2} \quad .$$

The cdf is given by

$$P(\epsilon \leq t) = \frac{1}{1 + \exp(-x))} = \text{sigmoid}(t)$$

And using properties of the sigmoid, we obtain:

$$P(y = 1|x) = 1 - P(\epsilon \leq -g(x)) = 1 - \text{sigmoid}(-g(x)) = \text{sigmoid}(g(x))$$

Replacing $g(X)$ by our model, we obtain the original result in equation (46).

Probit regression The choice of the logistic distribution for ϵ was arbitrary. After all, why shouldn't we use $\epsilon \sim \mathcal{N}(0, 1)$? If we do this, we can not write down the solution in such a nice closed form anymore, since

$$P(\epsilon < t) = \Phi(x) = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}x^2)\ dx$$

does not have a closed form solution. The resulting model is called probit regression, based on the name for $\Phi(t)$, probit function. Even though, we can not compute the integral analytically, there are still efficient algorithms to compute $\Phi(t)$.

If that works, why do most people prefer logistic regression? Next to the fact that the sigmoid function can be written down easily using known primitives, there is an important statistical difference between the two models. The logistic distribution has much heavier tails than the normal distribution. That means that even at the same variance, the samples spread out over a larger area. Thus, the logistic regression is much more resilient to outliers, as it expects labels from the opposite class even further away from the boundary.

Generalized Linear Models We want to generalize the models we have discussed so far. We will call a model a generalized linear model, if it has the form

$$f_\theta(x) = \theta^T \phi(x) \ ,$$

where $\phi : \mathbb{R}^d \to \mathbb{R}^N$ is a feature mapping from the d dimensional input points x to a set of N features. Further, the linear model must be based on a likelihood function

$$p(y|x, \theta) = p(y|f_\theta(x)) \ .$$

The simplest example for ϕ is

$$\phi(x) = \begin{pmatrix} x \\ 1 \end{pmatrix} \ ,$$

which simply adds a constant value to the input. this allows incorporating a bias term in the linear model. But any set of non-linear features are allowed, as long as they are independent of θ.

Finally, lets take a look at a Frequentist and Bayesian example.

4.1 Logistic Regression Revisited

We have already taken a look at Frequentist Maximum Likelihood estimation in the logistic regression example where we maximized

$$\arg\max_\theta p(\mathcal{D}|\theta) = \arg\max \prod_{i=1}^{\ell} p(y^{(i)}|x^{(i)},\theta) = \arg\min_\theta \underbrace{-\sum_{i=1}^{\ell} \log p(y^{(i)}|x^{(i)},\theta)}_{E(\theta)} \ .$$

This searches the model that describes the data best, independent of any prior considerations about good values of θ. To find the maximum algorithmically, we perform gradient descent on the gradient of $E(\theta)$

$$\nabla E(\theta) = -\sum_{i=1}^{\ell} \nabla_\theta \log p(y^{(i)}|x^{(i)},\theta) \ .$$

or use any other algorithm that finds minima of the error function.

4.2 Example: Bayesian Linear Regression

Returning to Linear regression, we can take a full Bayesian approach. We assume that our model has the form $f_\theta(x) = \theta^T x$ and its parameters have a prior distribution of $\theta \sim \mathcal{N}(0, \Sigma_\theta)$. This amounts to a choice of $\phi(x) = x$ in the previous chapter and we make this explicit choice just for the sake of simplicity of presentation: all derivations are the same when replacing x by $\phi(x)$. As before, we assume that the noise is normal distributed and $\epsilon \sim \mathcal{N}(0, \sigma_y^2)$. This leads to the likelihood function

$$p(y|x,\theta) = \mathcal{N}(y; \theta^T x, \sigma_y^2) \ .$$

For simplicity, we will store the datapoints in a design matrix $\mathcal{X} \in \mathbb{R}^{\ell \times d}$ where the ith row stores the ith datapoint $x^{(i)}$. Similarly we have $\mathcal{Y} \in \{0,1\}^N$ as a vector storing the labels $y^{(i)}$. We can rewrite the likelihood in this notation and

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{\ell} p(y^{(i)}|x^{(i)},\theta) = p(\mathcal{Y}|\mathcal{X},\theta) = \mathcal{N}(\mathcal{Y}; \mathcal{X}\theta, \sigma_y^2 I_N) \tag{52}$$

is a multivariate normal distribution.

To compute the posterior likelihood $p(\theta|\mathcal{D})$ (or $p(\theta|\mathcal{Y},\mathcal{X})$), we first need to compute $p(\mathcal{D},\theta)$. This means we need to compute the joint distribution of $p(\mathcal{Y}|\mathcal{X},\theta)$ and $p(\theta)$. Since both distributions are normal by our assumption and the conditional distribution (52) depends on the prior only in terms of a mean-shift, we can look up the property for the joint distribution from two dependent normal distributions, given in equation (31):

$$\left[\begin{array}{c} \theta \\ \hline \mathcal{Y} \end{array}\right] \sim \mathcal{N}\left(\left[\begin{array}{c} 0 \\ \hline 0 \end{array}\right], \left[\begin{array}{c|c} \Sigma_\theta & \Sigma_\theta \mathcal{X}^T \\ \hline \mathcal{X}\Sigma_\theta & \sigma_y^2 I_N + \mathcal{X}\Sigma_\theta \mathcal{X}^T \end{array}\right]\right) \ . \tag{53}$$

Next, we want to condition $p(\theta, \mathcal{Y}|\mathcal{X})$ on $\mathcal{Y}$ using (29). To do this, we first reorder the random variables:

$$\left[\begin{array}{c} \mathcal{Y} \\ \hline \theta \end{array}\right] \sim \mathcal{N}\left(\left[\begin{array}{c} 0 \\ \hline 0 \end{array}\right], \left[\begin{array}{c|c} \sigma_y^2 I_N + \mathcal{X}\Sigma_\theta \mathcal{X}^T & \mathcal{X}\Sigma_\theta \\ \hline \Sigma_\theta \mathcal{X}^T & \Sigma_\theta \end{array}\right]\right) \quad . \tag{54}$$

And then conditioning leads to $p(\theta|\mathcal{D}) = p(\theta|\mathcal{X}, \mathcal{Y}) = \mathcal{N}(\theta; \mu_{\theta|\mathcal{D}}, \Sigma_{\theta|\mathcal{D}})$ with mean and variance

$$\mu_{\theta|\mathcal{D}} = \Sigma_\theta X^T (\sigma_y^2 I_N + \mathcal{X}\Sigma_\theta \mathcal{X}^T)^{-1} \mathcal{Y} \tag{55}$$

$$\Sigma_{\theta|\mathcal{D}} = \Sigma_\theta - \Sigma_\theta X^T (\sigma_y^2 I_N + \mathcal{X}\Sigma_\theta \mathcal{X}^T)^{-1} X \Sigma_\theta \quad . \tag{56}$$

Remark: This result differs from the results presented in Bishop, section 3.3, equations 3.53 and 3.54. Numerically both results lead to the same values of mean and covariance, but the form we derived here is more useful for Gaussian Processes which we introduce later in the course.

For the normal distribution, the mode and mean are the same, so both the MAP and Mean model parameters are $\mu_{\theta|\mathcal{D}}$. For the posterior predictive distribution, we have to compute (38). We again need to apply (31) and obtain

$$p(y|x, \mathcal{D}) = \mathcal{N}(y; x^T \mu_{\theta|\mathcal{D}}, \sigma_y^2 + x^T \Sigma_{\theta|\mathcal{D}} x) \quad . \tag{57}$$

With this model, we can not only give an estimate of the y but also a measure of uncertainty based on our prior and the inherent variance of the noise.

5 From Random Functions to Random Processes

In Bayesian linear regression, we chose a parameterized family of functions, and then used probability theory to find the posterior probability of parameters given the data. This is an indirect process, insofar as our goal was to find the function that fits the data best. Defining a parameterisation was only a means to an end. But can we get around this step and directly define a probability distribution on some space of functions?

We will first start with an example, showing that random functions are more difficult to discuss than the random variables we have looked at before. Then, we introduce the notion of random processes. A word of warning: random processes are a difficult area of math and require substantial amounts of measure theory to define correctly. We will not go this route and instead try to give an intuition about, what random processes are and how to work with them.

To begin, consider a set of functions $f : \mathbb{N} \to \mathbb{R}$. As the argument is a natural number, these functions are equivalent to sequences $f(i) = f_i$, $i = 1, 2, \dots$. We can define a random function belonging to this family by picking a distribution for each f_i, for example

$$f_i \sim \mathcal{N}(0, 0.01) \ .$$

This gives us an immediate way to compute the probability of the function f, via the probability of the sequence $p(f_1, f_2, \dots)$. If we only consider sequences of length ℓ, we know how to compute the probability, as

$$p(f_1, f_2, \dots, f_\ell) = \prod_{i=1}^{\ell} \mathcal{N}(f_i; 0, 0.01) \ .$$

But what happens as $\ell \to \infty$? Let us look at two cases, $f_i = 0$, $i = 1, \dots, \ell$ and $f_i = 1$, $i = 1, \dots, \ell$. For $f_i = 1$, we obtain

$$p(1, 1, \dots) = \lim_{\ell \to \infty} \prod_{i=1}^{\ell} \underbrace{\mathcal{N}(1; 0, 0.01)}_{<1} = 0 \ ,$$

while for $f_i = 0$, we get

$$p(0, 0, \dots) = \lim_{\ell \to \infty} \prod_{i=1}^{\ell} \mathcal{N}(0; 0, 0.01) = \lim_{\ell \to \infty} \left(\underbrace{\frac{10}{\sqrt{2\pi}}}_{>1} \right)^{\ell} = \infty \ .$$

The first case is still rather benign, as probability 0 just means that we will never draw this sample. In the second case, we obtain a pdf of infinity, which will hold true when slightly varying the values of f_i around 0. However, if we compute the cdf

$$P(F_1 < u_i, F_2 < u_2, \dots) = \lim_{\ell \to \infty} \prod_{i=1}^{\ell} \underbrace{\int_{-\infty}^{u_i} \mathcal{N}(f_i; 0, 0.01) \, df_i}_{<1} = 0 \ .$$

which means that even though we integrate over volumes with infinite pdf, the resulting integrals are 0 everywhere. Thus, we can conclude that our notion of integral and probability does not make sense in these spaces. We need to find a different way to work with these objects.

5.1 Random Fields & Random Processes

As a way around the problems of defining the probability of a random function, the notion of a random field was developed.

Let Ω be an event space and let $\mathcal{X}$ be an index set (e.g. $\mathbb{N}$ or $\mathbb{R}^d$). A random field is a collection of random variables

$$F_x \in \Omega, \ \forall x \in \mathcal{X} \ .$$

Intuitively, a random field is a function that assigns a random variable to each point $x \in \mathcal{X}$. An alternative intuition is to see a random field as a (potentially infinite) set of dependent random variables, and the index set allows us to identify and select them. In the literature, if the index set is $\mathbb{R}^d$, a field is also called a random process.

The notion of a random field is very broad. For example, if we take a n-dimensional multivariate normal distributed random variable $g \in \mathbb{R}^d \sim \mathcal{N}(\mu, \Sigma)$, then, if we pick an index-set $\mathcal{X} = \{1, 2, \ldots, d\}$, the elements of the vectors g_i form a random field.

As a real world example, we can measure the height of the ocean at a set of chosen points on earth. In this example, the index set could be the longitude and latitude of the measurement position, and the measured ocean height at a given point is a random variable. when measuring at two points close to each other, the result will be highly correlated, as the same wave tends to pass through both points, while for far away points, the correlation will become less and less strong (but once you measure on opposite sides of the earth, you will be able to measure a new correlation due to the gravitational pull of the moon!). This application also introduces a new type of question that we could not ask previously: given a set of measurements, what is the distribution of ocean height at a point we have not measured yet? And where can we add a measurement position such, that it minimizes the uncertainty over all points of the ocean?

As a final example, as we can pick $\mathbb{N}$ as index set, the sequence example we discussed at the beginning of the chapter is also a random field. Thus, random fields can not solve our problems of assigning probabilities to the full collection of random variables. We must accept that even if we have an infinite set of random variables, we can only look at a finite subset $S_\ell = \{x_1, \ldots, x_\ell\} \subseteq \mathcal{X}$, $\ell \in \mathbb{N}$ at a time. This means that at any point, we can only reason about the random process F_x via its marginals

$$p(f_{x_1}, f_{x_2}, \ldots, f_{x_\ell}) \ .$$

Notation: Given a set $S = \{x_1, \dots, x_\ell\}$, $\ell \in \mathcal{N}$, we use the following shorthand notation for the marginals:

$$p(f_1, \dots, f_\ell | S) = p(f_{x_1}, f_{x_2}, \dots, f_{x_\ell}) \ .$$

We sometimes write $p(f_S|S)$, or $p(f|S)$ as shorthand if it is clear that we mean an f of size ℓ

By only looking at marginals, we no longer compute probabilities of functions, but probabilities of point-observations: the probability $p(f|S)$ measures the probability of drawing a function that has value f on the observed subset S and for any S and f, there could be infinitely many functions that could have lead to this value.

The question arises, whether we loose anything, if we discuss a random process only in terms of its marginal distributions with finite number of variables. This is answered by Kolmogorovs Consistency Theorem. We will only paraphrase it in the following as its full statement requires proper handling of measures and topology. Kolmogorovs Consistency Theorem states that we can indeed represent a random process fully via a family of marginal distributions $p(f_1, \dots, f_\ell|S)$, $S_\ell \subseteq X$, $\ell \in \mathcal{N}$. Likewise, if two random fields have the same marginal distributions, they are the same. The result is called a consistency theorem as it implies a consistency property between the marginal distribution of different subsets and it can be used to test, whether a family of marginal distributions $p(f|S)$ indeed represents a random field.

Let $T \subset S_\ell$. We can partition the vector of selected random variables $f = (f_1, \dots, f_\ell)$ as $f = (f_T, f_C)$, where f_T are the variables indexed by T and f_C are the variables indexed by S but not T. Then, Kolmogorovs consistency theorem requires

$$p(f_T|T) = \underbrace{\int p(f_T, f_C|S) \, df_C}_{p(f_T|S)} \ . \tag{58}$$

Thus, marginalizing variables in $p(f|S)$ must lead to the same result as picking the function $p(f_T|T)$ from the family of marginals. Intuitively, this makes sense: including an unobserved random variable in the model must not affect the distribution of the observed variables, as otherwise we are forced to include all unobserved random variables which makes computing probabilities impossible.

With this property, we can check, whether the given family of marginals forms a random field simply by testing, whether this property holds for all S_ℓ and T. Of course, this does not give us a way to define random fields, only to check that what we came up with is correct.

5.2 Example: Wiener Process

Let us introduce the Wiener Process as a non-trivial example for a random process. We will first give its construction, then compute the marginals and

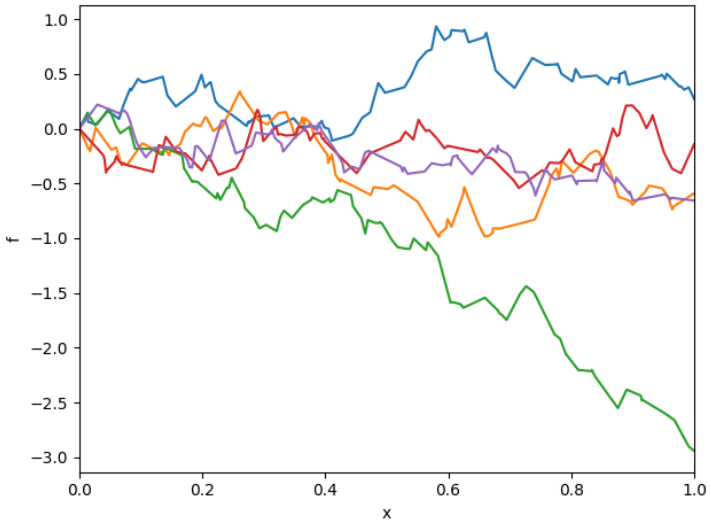


Figure 4: Samples from the Wiener process with S being a set of 100 equally spaced points

finally show that it fulfills Kolmogorovs consistency theorem.

As index set, we take an ordered set of points $S = \{x_1, \ldots, x_\ell\} \subseteq [0, 1]$, $0 = x_0 \leq x_1 < x_2 < \cdots < x_\ell$. The ordering is no limitation as we can pick any subset of points and assign their indices via their order. We then sample a set of random variables $f_1, \ldots, f_\ell$ using the following relation:

$$\begin{aligned} f_0 &= 0 \\ f_{i+1} &= f_i + W_{i+1},\ W_{i+1} \sim \mathcal{N}(0, x_{i+1} - x_i) \end{aligned}$$

Thus, the samples are created via a Markov chain with conditional distributions

$$p(f_{i+1}|f_i, S) = \mathcal{N}(f_{i+1}; f_i, x_{i+1} - x_i)$$

and marginal

$$p(f_0, \ldots, f_\ell|S) = \prod_{i=0}^{\ell-1} p(f_{i+1}|f_i, S) \ .$$

the resulting samples drawn for $\ell = 100$ are shown in Figure 4. All samples start at 0 by construction and then fan out in different directions with a larger spread the larger x is. Further, all samples are very rough and form a zick-zack path.

To check whether this definition of marginal forms a random process, we have to find a better formulation of the marginal first and then show that it fulfills the consistency theorem.

The first thing we note is that we can write the random variable f_i solely as a sum of W_i:

$$f_{i+1} = f_i + W_{i+1} = f_{i-1} + W_{i+1} + W_i = \cdots = \underbrace{f_0}_{0} + \sum_{j=1}^{i+1} W_j$$

By writing out the set of all $f_1 \ldots, f_\ell$ in matrix form, we can see that they are related by a linear transformation of W_i:

$$\underbrace{\begin{bmatrix} f_1 \\ f_2 \\ \cdots \\ f_\ell \end{bmatrix}}_{f} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ 1 & 1 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & 0 \\ 1 & 1 & 1 & \ldots & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} W_1 \\ W_2 \\ \cdots \\ W_\ell \end{bmatrix}}_{W} ,$$

where W is a multivariate normal random variable

$$W \sim \mathcal{N}\left(0, \underbrace{\begin{bmatrix} x_1 - x_0 & 0 & 0 & \ldots & 0 \\ 0 & x_2 - x_1 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & 0 \\ 0 & 0 & 0 & \ldots & x_\ell - x_{\ell-1} \end{bmatrix}}_{D}\right) .$$

This means that f is a linear transformation of a multivariate normal distributed random variable and thus it itself is multivariate random variable (property: closed under linear transformations) that follows:

$$f \sim \mathcal{N}(0, \underbrace{ADA^T}_{K(S)}) . \tag{59}$$

Next, we will compute the values of single entries of $K(S)$. Using that W is a diagonal matrix, we can write a single element is

$$K(S)_{ij} = \sum_{k=1}^{\ell} A_{ik} W_{kk} A_{jk}$$

Since A is a lower triangular matrix, in row A_i only the first i elements are non-zero and the same holds for the first j element of A_j. Thus we can limit the sum to

$$K(S)_{ij} = \sum_{k=1}^{\min\{i,j\}} A_{ik} W_{kk} A_{jk}$$

as for all other cases one of the factors will be zero. Next, we use that in the definition of A all non-zero elements are 1 and thus we can simplify further to

$$K(S)_{ij} = \sum_{k=1}^{\min\{i,j\}} W_{kk} = \sum_{k=1}^{\min\{i,j\}} (x_k - x_{k-1}) = x_{\min\{i,j\}} - x_0$$

Finally, we can simplify this further as we have defined $x_0 = 0$ and ordered the elements in S such $x_1 < x_2 < \dots$. Thus if $i < j$, $x_i < x_j$. With this we arrive at

$$K(S)_{ij} = \min\{x_i, x_j\} \tag{60}$$

With this and using the known ordering, we can write the matrix $K(S)$ simply as

$$K(S) = ADA^T = \begin{bmatrix} x_1 & x_1 & x_1 & \dots & x_1 \\ x_1 & x_2 & x_2 & \dots & x_2 \\ x_1 & x_2 & x_3 & \dots & x_3 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ x_1 & x_2 & x_3 & \dots & x_\ell \end{bmatrix} . \tag{61}$$

We now have all the tools needed, to check whether our marginals $p(S|f)$ are consistent as required by (58). For this, we must take a subset of T of any S and show that marginalizing $p(f_S|S)$ leads to the same distribution as $p(f_T|T)$. i.e., $p(f_T|S) = p(f_T|T)$. Since we have shown that the marginals are multivariate normal distributions with mean 0, the only thing we have to show is that the covariance matrices match.

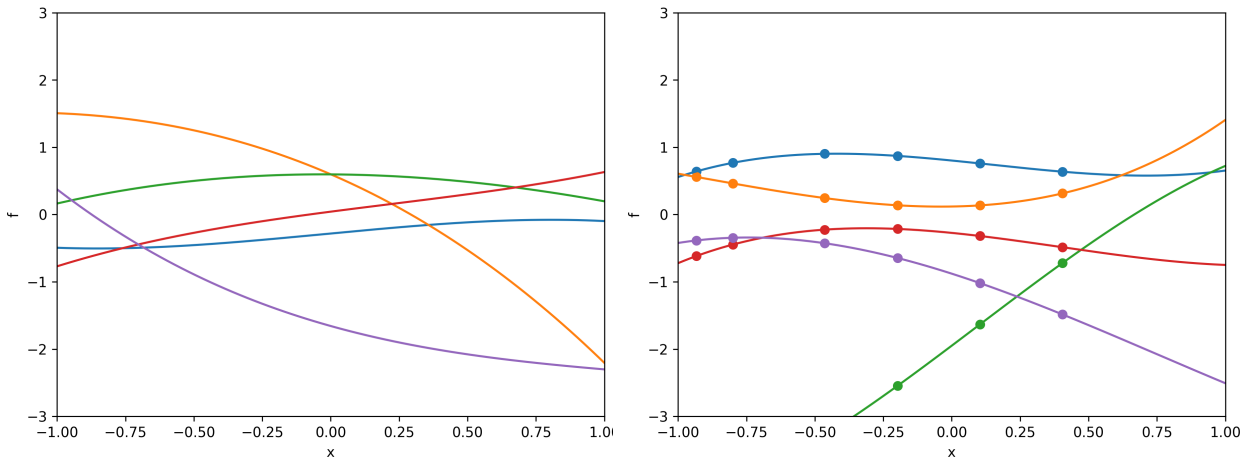
First, take T as a subset of S with one element less, for example by removing x_2. Then, marginalizing means to remove the second row and column from $K(S)$ in (61). The resulting matrix is exactly $K(T)$. Now, we can iteratively apply this process for any T by crossing out rows and columns one-by-one. This shows that the marginals are consistent, and the Wiener Process is indeed a random process.

5.3 Bayesian Linear Regression as Random Process

In this section, our aim is to view Bayesian Linear Regression through the lens of random processes. We will not focus on the prediction, but purely on a different interpretation of prior. In Bayesian linear regression, we first choose a linear regression function

$$f_\theta(x) = \theta^T \phi(x)$$

and then add a prior distribution on θ, which we choose here as some multivariate normal distribution, $\theta \sim \mathcal{N}(0, \Sigma_\theta)$. We will now change our point of view by considering that each observed value of θ leads to a function f_θ and we can thus reinterpret our prior not as a prior over the parameters of the function, but the compound of prior and basis function as a prior over a chosen set of functions.



(a) Random Function view

(b) Random Field View

Figure 5: Bayesian linear regression: Sampled functions from the function prior over third degree polynomials. Left: Just the polynomials. Right: in random processes only a few points are observed.

Example: In a 1-dimensional regression problem, we can pick ϕ as a set of polynomial basis functions, $\phi(x) = (1, x, x^2, x^3, \ldots, x^N)$. We can now assign a prior probability distribution to each θ_i, for example $\theta_1 \sim \mathcal{N}(0, 1)$ and $\theta_i \sim \mathcal{N}\left(0, \frac{1}{(i-1)^2}\right)$, for $i > 1$.
Now, sampling a θ from our prior gives rise to a polynomial function $f_\theta(x) = \theta_1 + \theta_2 x + \theta_3 x^3, \ldots$, which we can plot instead of plotting θ. An example for this for $N = 3$ is given in Figure 5a.

In reality we can not plot a function at each point, but we can only do so at a certain set of chosen locations, while for all values in-between we can only make educated guesses. To visualize this better, we give another example (Figure 5b) where we chose a set of points $S = \{x_1, \ldots x_\ell\}$ and marked the value of $f_i = f_\theta(x_i)$.

Seeing S as a subset of an index set of evaluation locations, for example $x \in [-1, 1]$ turns the observations into a random field: depending on the evaluated positions, we get a different set of random variables f_x with values given by the function values of the underlying drawn function. The marginals of this random process can be directly computed from our given prior process. As first step,

we write f for the vector of observations at points in S for some f_θ:

$$f = \begin{bmatrix} f_1 \\ f_2 \\ \dots \\ f_\ell \end{bmatrix} = \begin{bmatrix} \phi(x_1)^T\theta \\ \phi(x_2)^T\theta \\ \dots \\ \phi(x_\ell)^T\theta \end{bmatrix} = \underbrace{\begin{bmatrix} \phi(x_1)^T \\ \phi(x_2)^T \\ \dots \\ \phi(x_\ell)^T \end{bmatrix}}_{\Phi(S)\in\mathbb{R}^{\ell\times N}} \theta = \Phi(S)\theta$$

Each row of $\Phi(S)$ contains the values of the different feature maps at the evaluated points and thus the value of f can be computed as a matrix-vector product. As θ is a multivariate normal distributed random variable, we can use the property that multivariate normal distributions are closed under linear transformations, and the distribution of f can be directly written as

$$f \sim \mathcal{N}(0, \Phi(S)\Sigma_\theta\Phi(S)^T) \ .$$

Consistency can be easily shown via the same argument as for the Wiener process. Importantly, at the end of these calculations, θ itself does not appear anymore and all our information of the underlying basis functions and prior parameter distribution are contained within the covariance matrix $K(S) = \Phi(S)\Sigma_\theta\Phi(S)^T$.

6 Gaussian Processes

In the last chapter we have seen two examples of random processes in which the marginals were normal distributions, $\mathcal{N}(m(S), K(S))$, where S is a finite subset of some index set $\mathcal{X}$. In this section we will introduce a generalization of this, the family of Gaussian Processes. But before we can introduce them, we have to introduce the concept of a Hilbert-space kernel (or in short, kernel)

Definition (Kernel): Let $\mathcal{X}$ be some set. Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. If for all $S = \{x_1, \dots, x_\ell\} \subset \mathcal{X}$ and any $\ell \in \mathbb{N}$ it holds

$$K(S) = \begin{bmatrix} k(x_1, x_1) & \dots & k(x_1, x_\ell) \\ \vdots & \ddots & \vdots \\ k(x_\ell, x_1) & \dots & k(x_\ell, x_\ell) \end{bmatrix} \text{ is symmetric positive semi-definite}$$

We call k a kernel.

As a reminder, a matrix is positive semi-definite, if all its eigenvalues are bigger or equal to zero. We will refer to a matrix $K(S)$ defined as above as kernel matrix. The definition of a kernel is to this point purely abstract and the goal in the remainder of the chapter is to fill this definition with meaning and to provide an intuition into what a kernel is doing. For now, we will just use the kernel to define Gaussian Processes:

Definition (Gaussian Process): Let $\mathcal{X}$ be an index set

A random field $F_x \in \mathbb{R}$ whose marginals $p(f|S)$ are Multivariate Normal distributions, is called a Gaussian Process.

Moreover, there exists a kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and a function $m : \mathcal{X} \to \mathbb{R}$ such, that

$$p(f|S) = \mathcal{N}(m(S), K(S)), \forall S = \{x_1, \dots, x_\ell\} \subset \mathcal{X}, \forall \ell \in \mathbb{N}$$

with $m(S) = (m(x_1), \dots, m(x_\ell))$ and $K(S)_{ij} = k(x_i, x_j)$. If m and k are known, we write

$$f \sim \mathcal{GP}(m(\cdot), k(\cdot, \cdot))$$

This relation also holds in reverse: every choice of m and k leads to a random process. In the following, we will first shed light on how kernels affect the Gaussian process as a prior, and we will then use Gaussian processes in a machine-learning task. We end this chapter by discussing how to combine and select kernels.

6.1 Kernels and Gaussian Process Priors

As said, the two processes we have investigated before are examples of Gaussian processes:

- The Wiener process is a Gaussian Process with $m(x) = 0$ and

$$k(x, x') = \min\{x, x'\}$$

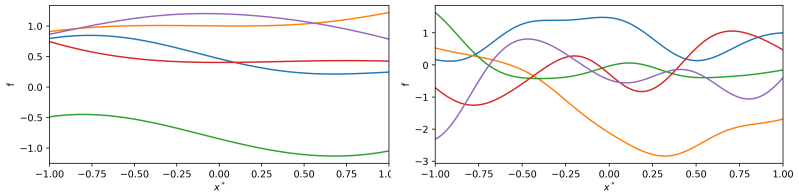
- Bayesian Linear Regression as random process also leads to normal distributed marginals with $m(x) = 0$ and $k(x, x') = \phi(x)\Sigma_\theta\phi(x')$

In both cases we did not have to show the kernel property, because we have derived the kernel from the underlying distribution. Of course, if we are given an arbitrary function k one would need to show first that it is a proper kernel, which means that the matrices $K(S)$ must positive semi-definite, independent of choice of the set S. Showing that an arbitrary function is a kernel can be difficult and in practice kernels are often created from a set of known kernels and are then combined in a way that keeps the kernel property.

From a practitioners point of view, $K(S)$ just being positive *semi*-definite is not enough, as semi-definiteness implies that the marginal distributions might not have a pdf which makes it difficult to calculate probabilities. At first, it is not intuitively clear why this should happen, but already in the case of Bayesian Linear Regression from the last section, one can observe this:

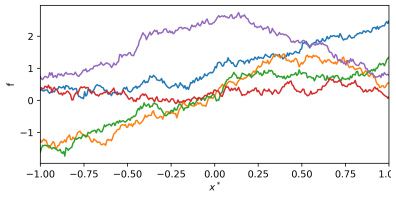
Example (continued): In the previous example we visualized a set of polynomial random functions $\phi(x) = (1, x, x^2, x^3)$, forming a third degree polynomial. A third degree polynomial has 4 parameters, $\theta_1, \dots, \theta_4$. Given 4 pairs of (x_i, f_i) it is possible to uniquely define a polynomial $f(x)$. What happens if we add a fifth pair (x_5, f_5)? Either, it is on the graph of f, that is $f(x_5) = f_5$ or there does not exist a third degree polynomial passing through all 5 points. Similarly, if we use the kernel $k(x, x') = \phi(x)\Sigma_\theta\phi(x')$ that is derived from third degree polynomials, our underlying sampled functions will have third degree. While we can observe the functions at any number of locations $S = \{x_1, x_2, \dots, x_\ell\}$, any set of 4 observations will be enough to fully predict the remaining observations - there is no randomness left as all underlying parameters are fully defined. Thus, the kernel derived from polynomial linear regression is only semi-definite.

While the problems of semi-definiteness can be overcome, there exists a subset of kernels which guarantee that the covariance matrix is positive definite

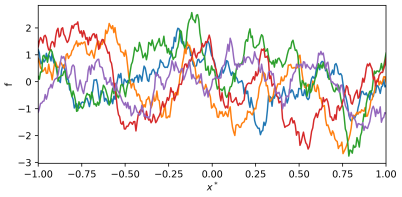


(a) Gaussian Kernel, $\gamma = 0.5$

(b) Gaussian Kernel, $\gamma = 5$



(c) Matern Kernel, $\gamma = 0.5$



(d) Matern Kernel, $\gamma = 5$

Figure 6: Samples taken from a Gaussian Process with $m(x) = 0$ and different choice of kernels and parameters. 300 points are sampled evenly spaced in $[-1, 1]$.

Definition (Universal Kernel): If k is a kernel and for all $S = \{x_1, \ldots, x_\ell\} \subset \mathcal{X}$ with $x_i \neq x_j, i \neq j$ additionally holds

$$K(S) \text{ is positive definite}$$

Then, we call k universal.

Showing that a kernel is universal is no easy feat and there are very general theorems stating under which conditions a kernel is universal. Two commonly used universal kernels are

1. Gaussian kernel
$$k(x, y) = \exp(-\gamma \|x - y\|^2)$$
2. Matern 3/2 kernel
$$k(x, y) = \left(1 + \gamma\sqrt{3}\|x - y\|\right) \exp\left(-\gamma\sqrt{5}\|x - y\|\right)$$

The choice of kernel has a huge impact on the functions sampled from the Gaussian Process. We can get a better idea of what types of functions the kernel generates by taking S as 300 points on an evenly spaced grid in [-1,1] and plotting the resulting function values, which we show in Figure 6. As we can see, the functions sampled from the Gaussian processes vary a lot. While the Gaussian Kernel generates functions with several smooth hills and valleys, the

Matern 3/2 kernel generates much more rugged landscapes. For both kernels the choice of γ affects the width of the valleys.

It is not directly obvious to what degree the choice of kernel matters for the Gaussian process, but we already know that if we sample a set of observations according to $p(f|S)$ of a GP using the Matern kernel, then evaluating its probability under a Gaussian process using a Gaussian kernel — or a Matern kernel with different choice of γ — will lead to a small value. It will turn out that both the choice of kernel and its hyper parameters — here γ— are important for the performance of Gaussian Processes in practice. We will discuss this more in the next sections.

As an end to this section, we introduce two important theorems that bind Gaussian processes, kernels, and Bayesian Linear Regression tightly together. Due to their complexity and reliance on additional abstract concepts of function theory (Reproducing Kernel Hilbert Spaces), we show them in a simplified version and without proof.

The first is a characterisation of what a kernel is called Mercer's Theorem

Theorem (Mercer's, simplified): Let $\mathcal{X} \subset \mathbb{R}^d$ be compact and bounded. Let $k : \mathcal{X} \times \mathcal{X}$ be a kernel. Then, there exists a sequence of features $\phi_1, \phi_2, \dots$ such, that

$$k(x, x') = \sum_{i=1}^{\infty} \phi_i(x)\phi_i(x')$$

For universal kernels the sequence is infinite.

Mercers theorem is a generalization of the result we obtained with Bayesian linear regression. The kernel we obtained there, $k(x, x') = \phi(x)\Sigma_\theta\phi(x')$ can be rewritten in the form of Mercer's theorem. We can write $\Sigma_\theta = AA^T$ and thus $k(x, x') = \phi'(x)\phi'(x') = \sum_{i=1}^{N} \phi'_i(x)\phi'_i(x')$ with $\phi'(x) = A^T\phi(x)$. With this we have established that each kernel can be reinterpreted as an advanced form of Bayesian linear regression, with the additional bonus that for some kernels the corresponding feature map would be infinite dimensional. This connection can be made stronger using the following theorem:

Theorem (Karhunen-Lowe, simplified): Let $f \sim \mathcal{GP}(0, k(\cdot, \cdot))$, ϕ_i given by Mercer's theorem and $x \in \mathcal{X}$, then the random variable

$$\tilde{f}_N = \sum_{i=1}^{N} \theta_i\phi_i(x),\ \theta_i \sim \mathcal{N}(0, 1)$$

converges to f_x as $N \to \infty$, where convergence is measured in squared norm.

This theorem represents the other direction: sampling from a Gaussian Pro-

cess can be modeled as a prior on some hidden set of parameters θ_i that are used to scale the features $\phi_i(x)$, just that in the case of a universal kernel, we might have an infinite number of parameters in our model.

6.2 Machine-Learning using Gaussian Processes

In the previous section, we have seen an equivalence between the prior of Bayesian linear regression and Gaussian Processes, with the advantage for Gaussian Processes that they can represent functions with possibly infinitely many parameters. What we are missing so far is any practical use of this tool.

For this section, we assume a similar setup as in Bayesian linear regression. We are given a set of data points $\mathcal{D} = \{(x^{(1)}, y^{(1)}), \dots, (x^{(\ell)}, y^{(\ell)})\}$. The labels are given by a noisy observation $y = g(x) + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma_y^2)$. Our goal is to learn a likely set of functions that approximate $g(x)$ and we aim to predict a function value f^* at location x^* with $f^* \approx g(x^*)$. Unlike Bayesian linear regression, we do not assume a set of features and prior parameter values, but instead that $f \sim \mathcal{GP}(0, k(\cdot, \cdot))$, where k is some kernel[1]. We will refer to the set of known data point locations as $S = \{x^{(1)}, \dots, x^{(\ell)}\}$. With this, we can write the likelihood of the posterior function of y^* after observing $\mathcal{D}$ as

$$p(f^*|x^*, \mathcal{D}) = \frac{\int p(y|f_S)p(f^*, f_S|S \cup x^*)df_S}{p(y|S)} \tag{62}$$

To understand this, we have to understand and derive the different parts. The distribution $p(f^*, f_S|S \cup x^*) = p(f_{x^*}, f_{x^{(1)}}, \dots, f_{x^{(\ell)}})$ is the marginal of the Gaussian process of function values observed at locations in S and x^*. This is the prior distribution of function values we expect to observe. The distribution $p(y|f_S)$ is then the probability of observing the vector of y-values given a chosen set of function-values f_S at the observed locations in S, which is the difference produced by the random noise. Thus $p(y|f_S) = \mathcal{N}(y; f_S, \sigma_y^2 I_\ell)$.

In equation (62) we then integrate over f because we never observed the true function values at S, but only the noisy labels. This gives us the distribution

$$p(y, f^*|S \cup x^*) = \int p(y|f_S)p(f^*, f_S|S \cup x^*)df_S$$

and the last step is to condition on the observations y

$$\begin{aligned} p(f^*|y, S \cup x^*) &= \frac{p(y, f^*|S \cup x^*)}{\int p(y|S \cup x^*)} \\ &= \frac{\int p(y|f_S)p(f^*, f_S|S \cup x^*)df_s}{p(y|S \cup x^*)} \quad . \end{aligned}$$

[1] The mean function $m(x)$ can also be included here, but in most applications this is just 0 or some other constant and we ignore it for simplicity. Choosing a mean function is equivalent to fitting a Gaussian Process with 0-mean to $y^{(i)} - m(x^{(i)})$.

This leads to equation (62), except the normalization constant, which we can show does not depend on x^* when performing the integration over f^* carefully:

$$\begin{aligned} p(y|S \cup x^*) &= \int p(y, f^*|S \cup x^*) df^* \\ &= \int \int p(y|f_S) p(f^*, f_S|S \cup x^*) df_S df^* \\ &= \int p(y|f_S) \underbrace{\int p(f^*, f_S|S \cup x^*) df^*}_{p(f_S|S)} df_S \\ &= \int p(y|f) p(f_S|S) df = p(y|S) \ . \end{aligned} \tag{63}$$

In the third step we reordered the integrals in order to integrate over f^* and the result is due to Kolmogorovs consistency theorem. In itself, this quantity is the probability that our observations are generated from the Gaussian process with added noise, and is called the evidence.

Computing the actual pdf $p(f^*|x^*, \mathcal{D})$ by computing the integrals directly is cumbersome. Moreover, if the kernel is not universal, we run the risk of computing densities of normal distributions that do not have positive definite covariance. Instead we again use the generating model to quickly compute the distribution using the rules we have established in Section 2.

We first begin by writing the distribution of $p(f^*, f|S \cup x^*)$ in block-form:

$$\left[\begin{array}{c} f \\ \hline f^* \end{array}\right] \sim \mathcal{N}\left(0, \left[\begin{array}{c|c} K(S) & k(S, x^*) \\ \hline k(S, x^*)^T & k(x^*, x^*) \end{array}\right]\right)$$

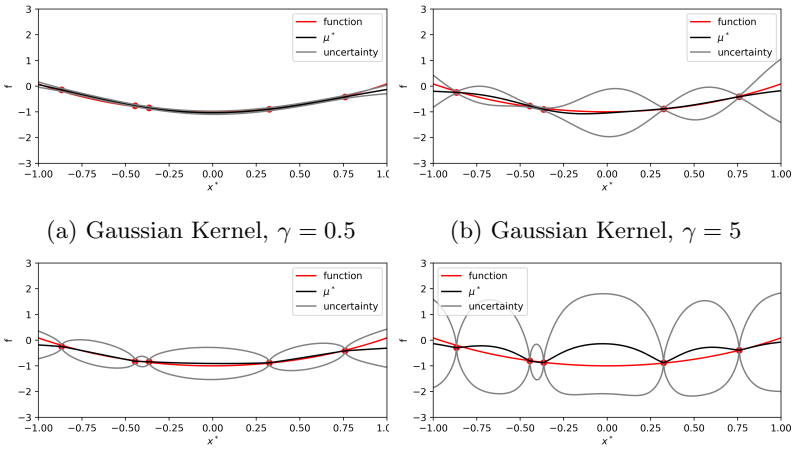
The matrix can directly be obtained by insertion into the definition of a Gaussian process where the new position x^* is added as last element to S. In block-notation we added the following quantities: The matrix $K(S)$ is the previously introduced kernel-matrix, $K(S)_{ij} = k(x^{(i)}, x^{(j)})$. We further introduced $k(S, x^*)$ which is a vector with elements $k(S, x^*)_i = k(x^{(i)}, x^*)$ and $k(x^*, x^*)$ is the kernel applied to x^* at both arguments.

Next, in our generative model, the noise variable $\epsilon \sim \mathcal{N}(y; 0, \sigma_y^2 I_\ell)$ is added to the values of f — but not f^* as we are interested in predicting the most likely true function value, and not the value that is disturbed by measurement noise. In block notation, this means:

$$\left[\begin{array}{c} y \\ \hline f^* \end{array}\right] = \left[\begin{array}{c} f \\ \hline f^* \end{array}\right] + \left[\begin{array}{c} \epsilon \\ \hline 0 \end{array}\right] \tag{64}$$

Even though the last element of the second vector is 0, it is still a sample of a multivariate normal distribution (even though it does not have a pdf), with distribution

$$\left[\begin{array}{c} \epsilon \\ \hline 0 \end{array}\right] \sim \mathcal{N}\left(0, \left[\begin{array}{c|c} \sigma_y^2 I_\ell & 0 \\ \hline 0 & 0 \end{array}\right]\right) \ .$$



(a) Gaussian Kernel, $\gamma = 0.5$

(b) Gaussian Kernel, $\gamma = 5$

(c) Matern Kernel, $\gamma = 0.5$

(d) Matern Kernel, $\gamma = 5$

Figure 7: Visualisation of the posterior $p(f^*|x^*, \mathcal{D})$ and different choice of kernels and parameters. Points and underlying true function $f(x) = e^x + e^{-x} - 3$ in red, $x^* \in [-1, 1]$. The black line visualizes the mean μ^* for chosen x^*. Grey lines mark the 95% confidence interval, $\mu^* \pm 1.96\sigma^*$.

Thus, the distribution of the left hand side of equation (64) is a normal distribution with density of a sum of two normal distributions, and we can use rule (32) and obtain

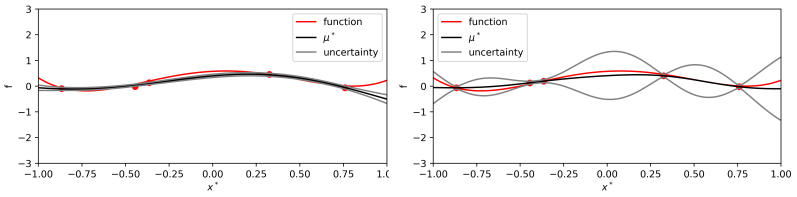
$$\begin{bmatrix} y \\ \hline f^* \end{bmatrix} \sim \mathcal{N}\left(0, \left[\begin{array}{c|c} K(S) + \sigma_y^2 I_\ell & k(S, x^*) \\ \hline k(S, x^*)^T & k(x^*, x^*) \end{array}\right]\right) \quad . \tag{65}$$

The last step is obtained by conditioning on the observed values of y using (29). This results in an equation very similar to Bayesian linear regression

$$\begin{aligned} f^*|y &\sim \mathcal{N}(\mu^*, \sigma^*) \\ \mu^* &= k(S, x^*)^T((S) + \sigma_y^2 I_\ell)^{-1} y \\ (\sigma^*)^2 &= k(x^*, x^*) - k(S, x^*)^T((S) + \sigma_y^2 I_\ell)^{-1} k(S, x^*) \end{aligned} \tag{66}$$

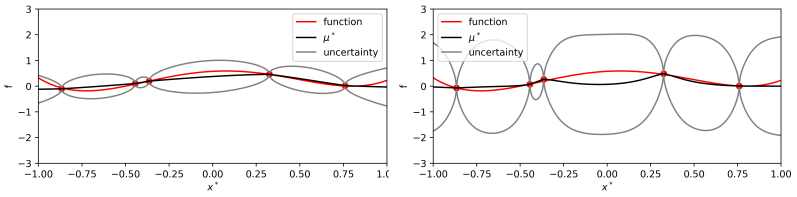
As in the normal distribution mean and mode are identical, μ_* is the maximum likelihood estimate and the mean for f^*, and thus a good candidate for prediction of the function value. However, the Gaussian Process also provides us with an uncertainty estimate of this prediction, that we can use to quantify uncertainty further, for example by reporting a confidence interval $\mu^* \pm 1.96\sigma^*$, which is the 95% confidence interval for location of f^*, i.e., 95% of sampled values from $p(f^*|x^*, \mathcal{D})$ lie within this interval.

This suggests a very simple algorithm to train and apply a Gaussian Process model:



(a) Gaussian Kernel, $\gamma = 0.5$

(b) Gaussian Kernel, $\gamma = 5$



(c) Matern Kernel, $\gamma = 0.5$

(d) Matern Kernel, $\gamma = 5$

Figure 8: Visualisation of the posterior $p(f^*|x^*, \mathcal{D})$ and different choice of kernels and parameters. Points and underlying true function $f(x) = 2(x + 0.9)(x + 0.5)(x - 0.8)^2$ in red, $x^* \in [-1, 1]$. The black line visualizes the mean μ^* for chosen x^*. Grey lines mark the 95% confidence interval, $\mu^* \pm 1.96\sigma^*$.

Algorithm (GP, simple):

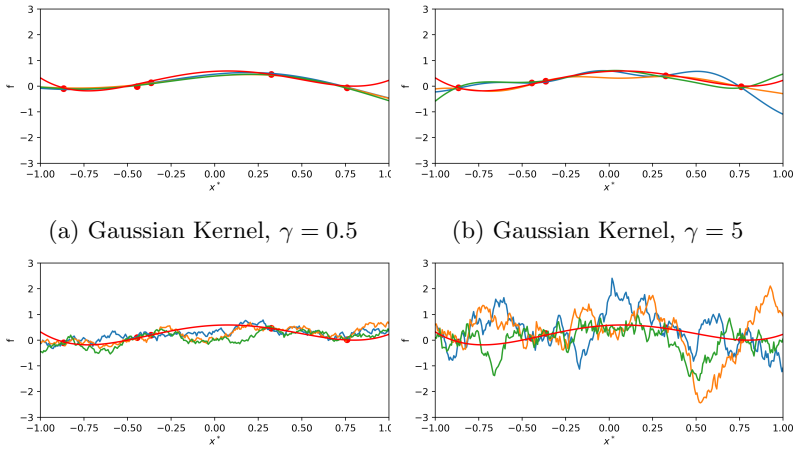
- Pick kernel $k(\cdot, \cdot)$ and noise variance $\sigma_y > 0$
- Get data $(x_1, y_1), \ldots, (x_1, y_1)$, $S = \{x_1, \ldots x_\ell\}$
- Compute $G = (\sigma_y^2 I_N + K(S))^{-1}$ and $\alpha = Gy$

For a new point x^* to predict:

- Compute $\mu_* = k(S, x^*)^T \alpha$
- Compute $(\sigma^*)^2 = k(x^*, x^*) - k(S, x^*)^T G k(S, x^*)$

We can use this algorithm to visualize the behaviour of the GP model for different choices of functions and kernels in a one-dimensional problem (Figures 7& 8). We can see that for different choices of function the prediction for μ^* vary a lot and also the uncertainties vary by a large amount. This is because Gaussian Processes are a Bayesian model: we chose a prior distribution of f and then predict posterior means and uncertainty. Thus, depending on the kernel our prediction for how the function could continue between observed points will be purely guided by this choice of prior and the uncertainties will follow roughly the behaviour of what we have seen in the prior samples (Figure 6).

The Matern 3/2 kernel shows very sudden changes between points in the prior. In the posterior, this is reflected by the uncertainty rising quickly around



(a) Gaussian Kernel, $\gamma = 0.5$

(b) Gaussian Kernel, $\gamma = 5$

(c) Matern Kernel, $\gamma = 0.5$

(d) Matern Kernel, $\gamma = 5$

Figure 9: Visualisation of the posterior samples and different choice of kernels and parameters. Points and underlying true function $f(x) = 2(x + 0.9)(x + 0.5)(x - 0.8)^2$ in red. Samples are taken by evenly sampling 300 points between $[-1, 1]$ from the posterior.

an observed point. Similarly, the Gaussian kernel for $\gamma = 0.5$ showed very smooth curves, which are perfect for prediction the first function, with tight mean and variance estimates. In contrast, the same kernel for $\gamma = 5$ produces much smaller valleys and thus the uncertainties become larger for the first function. However, when we look at the polynomial function in Figure 8, the $\gamma = 0.5$ kernel does not model this vary well and predicts the variability of the function poorly, while now the $\gamma = 5$ kernel works comparatively well.

A better way to understand this is to use the GP model not to predict a single point, but several points simultaneously. This amounts to a slight change of derivation where instead of prediction for a single x^*, we predict for a whole second set of points $S^* = \{(x^*)^{(1)}, \ldots, (x^*)^{(T)}\}$ use as prior $p(f_{S^*}, f_S | S^* \cup S)$ which introduces additional dependencies between points contained in S^*. We skip the derivation for sake of shortness of the script, but the same steps apply as in the previous derivations and the reader is invited to produce the equations themselves!

Visualizing this using S^* as the same 300 points as for the priors on the polynomial function, we obtain Figure 9. This visualisation confirms the explanation we have found for the previous two figures: samples from the posterior using the Gaussian kernel tend to be smooth functions, with neighbouring function values being close to each other. We also see that again for $\gamma = 0.5$ the function tends to be overly smooth, while samples from $\gamma = 5$ look like possible extensions that closely align with the change of curvature of the real function. While the samples do not follow the true shapes, this indicates that this kernel

gives approximately correct uncertainty estimates. In contrast, the Matern kernel predicts completely different function shapes and is only bound by passing nearby the observed function values. Thus, this kernel would be a bad choice for this type of function.

6.3 Kernel combination & Kernel selection

As we have seen, the choice of kernel has a major effect on the predictions of mean and variance of a Gaussian Process. The question arises, how to pick a kernel? Without any tools, we have to guess which shape of kernel works best and use expert knowledge about the task to choose the kernel. Of course, we can remain with our pick of two kernels with parameters, but often we might guess that a function behaves mostly smooth, but also has slightly rugged features. How can we represent that? We can use rules that combine kernels while ensuring that the result is a kernel, for example:

- Let k_1 be a kernel and $\sigma^2 > 0$ a positive constant. Then $k(x, x') = \sigma^2 k_1(x, x')$ is a kernel
- Let k_1 and k_2 be kernel functions. Then, $k(x, x') = k_1(x, x') + k_2(x, x')$ is a kernel
- Let k_1 be a kernel and $a > 0$ a positive constant. Then $k(x, x') = k_1(x, x') + a$ is a kernel

The first rule allows to scale a kernel. This is very important in Gaussian Processes. To understand it, let $K_1(S)$ be the kernel matrix produced by kernel k_1 when applied to set S. Then for the scaled kernel k, we have $p(f|S) = \mathcal{N}(0, \sigma^2 K_1(S))$. In this case, the scaling value takes the role of scaling the variance of the normal distribution. This is important for example for the Gaussian kernel as for it the diagonal $K(S)_{ii} = 1$ and thus it can not model functions with large values very well. The third rule finally is a special case of the second rule. adding a constant is the same as adding the constant kernel $k(x, x') = a$. Its effect is adding a constant to the predicted function values. The three rules together allow to learn arbitrary scale and shifts of function values. (e.g., when learning a function with values between -10 and 100 with most values centered around 40, the standard Gaussian kernel is a bad fit).

Further, the rules allow to combine different kernels with different scales in order to produce kernels which have properties of both. Still, in many cases, we don't have a good idea for the values of the kernel parameters, their scaling values and the added measurement noise σ_y^2. How can we select these values in a systematic manner?

For this, let $p(f|S, \eta)$ be the marginal of the GP with the chosen hyperparameters, where η is a vector representing all parameters of the chosen kernel $k_\eta(x, x')$. A popular approach is to find the choice of η, σ_y^2 that maximizes the evidence (63).

The evidence, depending on the parameters is

$$p(y|S,\eta,\sigma_y^2) = \int p(y|f,\sigma_y^2)p(f|S,\eta)df$$

And the noisy observations have distribution

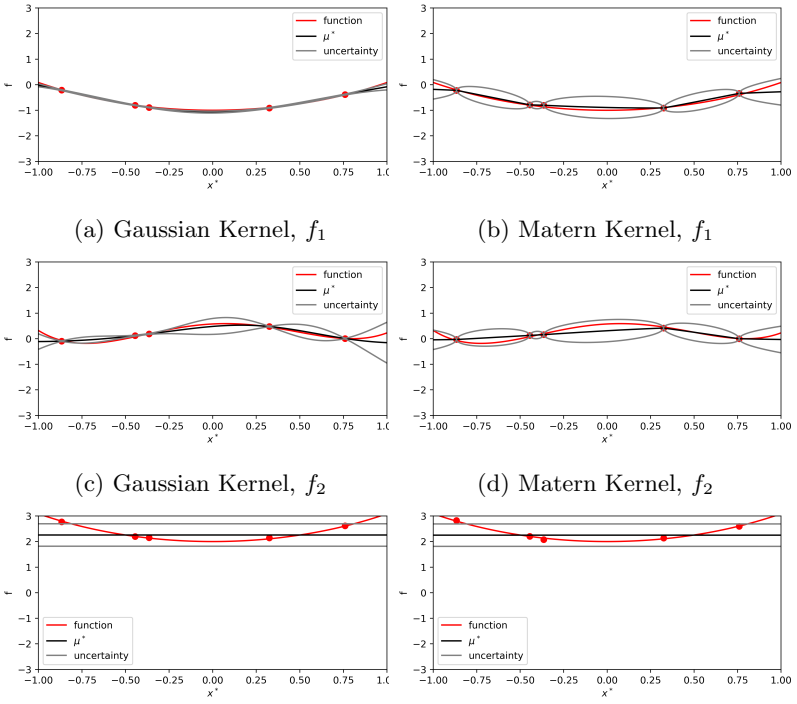
$$y \sim \mathcal{N}\left(0, \sigma_y^2 I_\ell + K_\eta(S)\right) \quad .$$

Here, $K_\eta(S)$ is the kernel matrix of kernel k_η. The pdf of the distribution (equation (26)) computes the likelihood that the Gaussian process with added noise would produce the observation y and thus, finding the parameters that maximize the log-likelihood looks like a good solution. The log-likelihood of the evidence is:

$$\log p(y|S,\eta,\sigma_y^2) = -\frac{1}{2}y^T(\sigma_y^2 I_\ell + K_\eta(S))^{-1}y - \frac{1}{2}\log\det(\sigma_y^2 I_\ell + K_\eta(S)) - \frac{d}{2}\log\sqrt{2\pi}$$

Finding the maximum of this function in terms of η and σ_y^2 is surprisingly difficult as it has several local optima and gradient-descent algorithm often get stuck at a poor local minimum. A good strategy is to use grid-search or random-search to obtain a good starting point. Further, because we optimize the log-likelihood, we have to ensure that the obtained covariance matrices are positive definite, and sufficiently so to not suffer from numerical difficulties. Thus, universal kernels should be favoured or lower bounds put in place that prevent σ_y^2 is chosen too small.

We again visualize the effects of tuning the parameters. This time, we will pick three different functions, $f_1(x) = e^x + e^{-x} - 3$, $f_2(x) = 2(x+0.9)(x+0.5)(x-0.8)^2$ and $f_3(x) = f_1(x)+3$. The added function is here to visualize the effect of a mean-shift if the underlying kernel can not handle arbitrary means. We visualize both the Gaussian and Matern Kernel with their single parameters as well as optimized σ_y^2, without using the additional scaling parameters of the rule introduced before. As grid we use 20 evenly spaced points in $[10^{-4}, 5]$ on both parameters, leading to 400 points evaluated in total. The results are given in Figure 10. The optimized Gaussian Process parameter for f_1 and f_2 in a)-d) make sense and closely follow the function shapes. While the Matern Kernel still shows a much quicker increase of the variance, it does not vastly under or overestimate the uncertainty and the true function is within the learned 95% confidence intervals. For the third function, e)+f), both approaches do not provide reasonable estimates. This is because both kernels can not learn mean-shifts of function values and instead prefer functions with mean close to 0. The result is that after observing a large value at a location, the Gaussian Process with these kernels tends to predict lower values, to get back to the assumed prior assumption of values having 0 mean (an example for this can be seen for the Matern Kernel in Figure 7d)). The only way to prevent this is to choose $\gamma \approx 0$ as this makes the kernels wide, allowing it to predict an almost constant function. And indeed, the result for γ is the smallest value of the grid, 10^{-4}. To model the variations in function values, the noise variance σ_y^2 is increased, modeling all deviations from the mean as noise.



(a) Gaussian Kernel, f_1

(b) Matern Kernel, f_1

(c) Gaussian Kernel, f_2

(d) Matern Kernel, f_2

(e) Gaussian Kernel, f_3

(f) Matern Kernel, f_3

Figure 10: Visualisation of the posterior $p(f^*|x^*, \mathcal{D})$ for different functions and optimized parameters for Gaussian and Matern 3/2 kernels. Points and underlying true functions in red, $x^* \in [-1, 1]$. The black line visualizes the mean μ^* for chosen x^*. Grey lines mark the 95% confidence interval, $\mu^* \pm 1.96\sigma^*$.

While this explanation sounds hand-wavy, the observation can also be predicted from the math. The mean prediction in our algorithm is written as $\mu^* = k(S, x^*)^T \alpha = \sum_{i=1}^{\ell} \alpha_i k(x^{(i)}, x')\alpha_i$. The mean prediction function is a linear combination of kernel functions. With the Gaussian kernel the function is a linear combination of Gaussian bell functions, each converging to 0 on their tails. This creates the aforementioned trend of converging back to 0 and this is alleviated as the Gaussian kernel becomes wider, and thus locally more constant.

While this is a poor solution, it is the only one that the kernels have available that makes the data likely, thus if the function modeled does not align with the underlying kernel assumptions, the predicted means, variances and learned noise-levels do not necessarily make sense anymore. Does this mean we have to include the scaling and shift parameter mentioned earlier? Not necessarily. In many cases, we can just get by by normalising the observations y to something that fits the kernel. In our case we can scale the labels to have zero mean, unit variance. Then we can learn a Gaussian Process on the normalized data and during prediction undo the normalization for the predicted values. This is standard practice in many applications.