Comparing Correlation Functions and Exploring Efficiency and Identifiability Issues for the Gaussian Process

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Abstract

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2.1.1 Standard linear model

The standard linear model summises that we have some data-generating function $f(.)$ that linearly combines training data X and parameters of some model W to produce an output y:

$$\begin{aligned} y &= f(X) + \epsilon \\ f(X) &= X^T W \end{aligned} \tag{1}$$

We add a noise term ϵ because y is rarely a perfect observation of $f(X)$ (e.g. measurement error). The standard linear model assumes that ϵ is drawn from a Gaussian distribution $\epsilon \sim N(0, \sigma_n^2 I)$. We add a covariance matrix I to describe how the noise for one observation is related to the noise of another observation.

We can combine our expressions and assumptions for $f(X)$ and ϵ to produce a conditional distribution. Effectively a distribution of errors, this is the distribution from which y is drawn from after knowing perfectly X and W:

$$p(y|X, W) = \mathcal{N}(y|X^T W, \sigma_n^2 I)$$

2.1.2 Determining weights

Our first task is to find W as we typically do not know these in advance. Frequentist approaches focus on arriving at a single estimate of W ($\hat{W}$) via "maximum likelihood estimation" (MLE). $p(y|X, W)$ is at its highest density around the expected value $y|X^T W$ so we can use optimisation methods to find the $\hat{W}$ at the maximum of $p(y|X, W)$. Because we assume $E[p(y|X, W)] = 0$, the values of W at the maximum of $p(y|X, W)$ are also the values of W that pushes the squared error $||y - X^T W||^2$ closest to zero. We can communicate uncertainty surrounding $\hat{W}$ by computing "standard errors", or the ratio between the variance of our errors and the variance of X. A high variance in errors shows that $\hat{W}$ i, but a broader range of X makes it easier to estimate W.

Instead of producing point estimates for $\hat{W}$ and uncertainty, Bayesian statistics treats W as a random variable and specifies an expected value and a variance. Placing W in a probabilistic framework allows us to propagate uncertainty throughout the model and to encode beliefs (e.g. from domain experts) about the weights before observing the data.

We start with a "prior" distribution of W, which the Bayesian linear model assumes:

$$p(W) \sim N(0, \Sigma_p) \tag{2}$$

Then, we observe the data and update our beliefs about the weights using Bayes' theorem to produce a "posterior" distribution $p(W|X, y)$.

$$p(W|X, y) = \frac{p(y|X, W)p(W)}{p(y|X)}$$

$p(y|X, W)$ is the density of the residuals after applying $p(W)$ to X, W under our assumed noise model ϵ, and $p(y|X)$ is the marginal likelihood - how likely the data is given the model.

2.1.2.1 Deriving our posterior To understand the relationship between $p(W|X, y)$ and W, we can ignore terms that do not vary with W (e.g. our marginal likelihood) by absorbing them into the proportionality constant:

$$p(W|X, y) \propto p(y|X, W)p(W) \tag{3}$$

TODO fix We can get a probability density function (PDF) for our error distribution by representing $Y|X^T W$ in squared error form and substituting it into the Gaussian PDF:

$$p(y|X, W) = exp\left(-\frac{1}{2\sigma_n^2}||y - X^T W||^2\right) \tag{4}$$

Reframing $p(W)$ as a PDF:

$$p(W) = \frac{1}{[\sqrt{\sigma_p}]\sqrt{2\pi}} exp\left(-\frac{1}{2}\frac{([W] - [0])}{[\Sigma_p]}\right)$$

The first term can be absorbed into the proportionality constant. Rewriting the second term as a negative exponential:

$$p(W) \propto exp\left(-\frac{1}{2}W^T \Sigma_p^{-1} W\right) \tag{5}$$

Putting both expressions for 4 and 5 into 3:

$$p(W|X, y) \propto exp\left(-\frac{1}{2\sigma_n^2}||y - X^T W||^2\right) exp\left(-\frac{1}{2}W^T \Sigma_p^{-1} W\right)$$

Expanding $||y - X^T W||^2$ to $y^T y - 2y^T XW + W^T X^T XW$:

$$p(W|X, y) \propto exp\left(-\frac{1}{2\sigma_n^2}(y^T y - 2y^T XW + W^T X^T XW)\right) exp\left(-\frac{1}{2}W^T \Sigma_p^{-1} W\right)$$

Putting both exponentials together by adding their powers:

$$p(W|X, y) \propto exp\left(\frac{1}{\sigma_n^2}(y^T y - 2y^T XW + W^T X^T XW) + \left(-\frac{1}{2}W^T \Sigma_p^{-1} W\right)\right)$$

Rearranging the inside term to be a quadratic, linear and constant term in W:

$$p(W|X, y) \propto exp\left(\frac{1}{2}W^T\left(\frac{1}{\sigma_n^2}X^T X + \Sigma_p^{-1}\right)W - \left(\frac{1}{\sigma_n^2}y^T X\right)W + \frac{1}{2}y^T y\right)$$

We can ignore the constant final term. Introducing these terms to simplify this result:

$$\begin{aligned} A &= \Sigma_p^{-1} + \frac{1}{\sigma_n^2}X^T X \\ b &= \frac{1}{\sigma_n^2}y^T X \\ p(W|X, y) &\propto exp\left(-\frac{1}{2}W^T AW + b^T W\right) \end{aligned} \tag{6}$$

2.1.2.2 Deriving the properties of the posterior by completing the square Now we have a simplified form of the posterior's PDF, we need to get it into a Gaussian form to recover the properties of the posterior distribution.

Bringing all terms inside the exponential to a single term:

$$-\frac{1}{2}W^T AW + b^T W = \frac{1}{2}\left(-W^T AW + 2b^T W\right)$$

Completing the square on our new inner term $W^T AW - 2b^T W$

$$W^T AW - 2b^T W = (W - A^{-1}b)^T A(W - A^{-1}b) - b^T A^{-1}b p(W|X, y) \propto exp\left(-\frac{1}{2}\left((W - A^{-1}b)^T A(W - A^{-1}b) - b^T A^{-1}b\right)\right) \tag{7}$$

Looking at the Gaussian PDF:

$$N(W|\mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} exp\left(-\frac{1}{2}(W - \mu)^T \Sigma^{-1}(W - \mu)\right) \tag{8}$$

Our expression lines up with the Gaussian PDF's "kernel" term $exp\left(-\frac{1}{2}(W - \mu)^T \Sigma^{-1}(W - \mu)\right)$, where $\mu = A^{-1}b$ and $\Sigma = A^{-1}$ ($\Sigma^{-1} = A$). Therefore, 7 can be represented as a Gaussian distribution:

$$p(W|X, y) \sim N(A^{-1}b, A^{-1}) \tag{9}$$

Inside our definition of A at **??**, we are missing an expression for Σ_p. Assuming independence of noise under the linear model, our weight variance Σ_p under the Bayesian linear model is "isotropic", meaning it is the same in all directions.

$$\Sigma_p = \tau^2 I$$

Because we assume independence, I is an "identity matrix where each diagonal element is 1 and all off-diagonal elements are 0. τ^2 is a scalar variance term, chosen as a prior.

Substituting the isotropic prior Σ_p into A:

$$A = \Sigma_p^{-1} + \frac{1}{\sigma_n^2}X^T X = \left[\tau^2 I\right]^{-1} + \frac{1}{\sigma_n^2}X^T X = \frac{1}{\tau^2}I + \frac{1}{\sigma_n^2}X^T X$$

Simplifying:

$$A = \frac{1}{\sigma_n^2}\left(X^T X + \frac{\sigma_n^2}{\tau^2}I\right) \tag{10}$$

2.1.2.3 Gaussian posteriors and ridge regression So far we have worked exclusively within the Bayesian paradigm, but we can draw some value of W from our posterior distribution to relate it to a frequentist framework. For Gaussian posteriors, our expected value of W $A^{-1}b$ is also its mode. This is called the maximum a posteriori (MAP) estimate of W, and is due to symmetries in linear model and posterior and is not the case in general. Our MAP estimate does not matter within the Bayesian framework but is equivelant to our frequentist $\hat{W}$.

Substituting our full expressions for A 10 and b 6 into our MAP estimation:

$$W_{\text{MAP}} = A^{-1}b = \left[\frac{1}{\sigma_n^2}(X^TX + \frac{\sigma_n^2}{\tau^2}I\right]^{-1} \cdot \left[\frac{1}{\sigma_n^2}y^TX\right]$$

Inverting LHS term of A:

$$A^{-1} = \frac{\sigma_n^2}{X^TX + \frac{\sigma_n^2}{\tau^2}I} = \sigma_n^2\left(X^TX + \frac{\sigma_n^2}{\tau^2}I\right)^{-1}$$

Substituting this back into W_{MAP} cancels out the σ_n^2 term in A with the $\frac{1}{\sigma_n^2}$ term in B:

$$W_{\text{MAP}} = \sigma_n^2\left(X^TX + \frac{\sigma_n^2}{\tau^2}I\right)^{-1} \cdot \frac{1}{\sigma_n^2}y^TX = \left(X^TX + \frac{\sigma_n^2}{\tau^2}I\right)^{-1} \cdot y^TX$$

This is equivelant to the solution to ridge regression, where $\lambda = \frac{\sigma_n^2}{\tau^2}$.

$$W_{\text{ridge}} = \left(X^TX + \lambda I\right)^{-1} X^Ty$$

Ridge regression introduces some bias to lower the variance in a frequentist linear model by shrinking weights, where the λ term controls the amount of shrinkage applied to the weights. This is traditionally useful where variance is particularly high (e.g. multicollinearity) and can be reduced at the cost of little bias.

Our MAP estimation in Bayesian linear regression with isotropic priors is equivalent to ridge regression, where the amount of bias we introduce depends on our confidence in our priors. The more we trust our prior, the higher our λ and the more we shrink our weights towards zero. A lower τ means we are more confident in $p(W)$ and have better priors, whereas a higher σ_n means lower confidence in $p(y|X, W)$ and worse weights that should be shrunk closer to zero.

2.1.3 Predictive distribution

2.1.3.1 Deriving the predictive distribution Our second task is to make predictions y_* using new input data X_* and our previously learned weights W. Frequentist methods simply multiply $\hat{W}$ by X_*, but this does not propagate uncertainty in W. In this Bayesian framework, we form a "predictive distribution" which we sample from to get our noise-free function evaluations $f(X_*)$ (denoted f_*) and add ϵ to get our noisy predictions y_*.

$$p(f_*|X_*, X, y) = \int p(f_*|X_*, W) \cdot p(W|X, y)dW$$

$p(f_*|X_*, W)$ is what we think the function looks like after producing a prediction using X_* and perfect knowledge of W. $p(W|X, y)$ is our familiar 9 posterior distribution of weights. $p(f_*|X_*, W) \cdot p(W|X, y)$ is the joint distribution of our predictions and our posterior weights, which gets us the conditional distribution $p(f_*, W|X_*, X, y)$ by definition of conditional probability. Because $p(f_*, W|X_*, X, y)$ relies on our perfect knowledge of W, which we lack, we integrate over all possible W to get the final predictive distribution $p(f_*|X_*, X, y)$

$p(f_*|X_*, W)$ is our error distribution, which we assume to be distributed normally and independently with our I identity matrix:

$$p(f_*|X_*, W) = \mathcal{N}(f_*|W^TX_*, \sigma_n^2 I)$$

Substituting into 8 and absorbing the LHS term into the proportionality constant:

$$p(f_*|X_*, w) \propto exp\left(-\frac{1}{2}\frac{1}{\sigma_n^2}(f_* - W^TX_*)^2\right)$$

Multiplying $P(f_*|X_*, W)$ and $p(W|X, y)$ to get our conditional $p(f_*, W|X_*, X, y)$, and add the exponents:

$$p(f_*, W|X_*, X, y) \propto exp\left(\frac{1}{2}(-W^TAW + 2b^TW) + \left(-\frac{1}{2}\frac{1}{\sigma_n^2}(f_* - W^TX_*)^2\right)\right)$$

Combining the terms inside the exponent:

$$p(f_*, W|X_*, X, y) \propto exp\left(-\frac{1}{2}\left(W^TAW - 2b^TW + \frac{1}{\sigma_n^2}(f_* - W^TX_*)^2\right)\right)$$

Expanding the squared term:

$$p(f_*, W|X_*, X, y) \propto exp\left(-\frac{1}{2}\left(W^TAW - 2b^TW + \frac{1}{\sigma_n^2}(f_*^2 - 2f_*W^TX_* + W^TX_*X_*^TX_*)\right)\right)$$

Similar to our posterior, we can rearrange this to be a quadratic, linear and constant term in W:

$$p(f_*, W|X_*, X, y) \propto exp\left(-\frac{1}{2}\left(W^T\left(A + \frac{1}{\sigma_n^2}X_*X_*^T\right)W - 2\left(b + \frac{1}{\sigma_n^2}f_*X_*\right)^TW + \frac{1}{\sigma_n^2}f_*^2\right)\right) \quad (11)$$

We can define new terms A_* and b_* to simplify this expression:

$$A_* = A + \frac{1}{\sigma_n^2} X_* X_*^T$$
$$b_* = b + \frac{1}{\sigma_n^2} f_* X_*$$

Substituting into 11:

$$p(f_*, W|X_*, X, y) \propto exp\left(-\frac{1}{2}\left(W^T A_* W - 2b_*^T W + \frac{1}{\sigma_n^2} f_*^2\right)\right)$$

Integrating out W to get our predictive distribution:

$$p(f_*|X_*, X, y) = \int p(f_*, W|X_*, X, y) dW \propto \int exp\left(-\frac{1}{2}\left(W^T A_* W - 2b_*^T W + \frac{1}{\sigma_n^2} f_*^2\right)\right) dW \tag{12}$$

Factoring out $\frac{1}{\sigma_n^2} f_*^2$ as it does not depend on W (since $\int exp(X)dX = exp(X)$):

$$= exp\left(-\frac{1}{2}\frac{1}{\sigma_n^2} f_*^2\right) \times \int exp\left(-\frac{1}{2}\left(W^T A_* W - 2b_*^T W\right)\right) dW$$

Evaluating the RHS multivariate Gaussian integral:

$$\int exp\left(-\frac{1}{2}\left(W^T A_* W - 2b_*^T W\right)\right) dW = \frac{(2\pi)^{D/2}}{\sqrt{|A_*|}} exp\left(\frac{1}{2} b_*^T A_*^{-1} b_*\right)$$

Substituting back into 12:

$$p(f_*|X_*, X, y) \propto exp\left(-\frac{1}{2}\frac{1}{\sigma_n^2} f_*^2\right) + \frac{(2\pi)^{D/2}}{\sqrt{|A_*|}} \cdot exp\left(\frac{1}{2} b_*^T A_*^{-1} b_*\right)$$

Now that no part of our expression is dependent on W, we need an expression for everything that depends on f_*.

Absorbing the second term (since it does not depend on f_*) into the proportionality constant, and combining the remaining exponential terms by adding their powers:

$$p(f_*|X_*, X, y) \propto \exp\left(-\frac{1}{2}\frac{1}{\sigma_n^2} f_*^2 + \frac{1}{2} b_*^T A_*^{-1} b_*\right)$$

Similar to deriving properties from our posterior, we can rearrange this expression and complete the square to derive the properties of our predictive distribution:

$$p(f_*|X_*, W) \sim N(X_*^T A^{-1} b, X_*^T A^{-1} X_*) \tag{13}$$

The variance is quadratic in X_* with A^{-1}, showing that predictive uncertainties grow with size of X_*.

2.1.4 Projections of inputs into feature space

One problem with this model is that it assumes a linear relationship between X and y. We can project our inputs into a higher dimensional feature space and apply a linear model in this space to express non-linear relationships between X and y.

Defining $\phi(X)$ as a function that maps a D-dimensional input vector X into an N dimensional feature space, our standard linear model becomes:

$$f(X) = \phi(X)^T W$$

For example, a scalar x could be projected into the space of powers of x: $\phi(x) = [1, x, x^2, \ldots, x^d]^T$ for a polynomial basis expansion of degree d to represent a d-power relationship between x and y. . Substituting $\phi(X)$ for X in 13:

$$p(f_*|X_*, X, y) = N(\phi(X_*)^T A_\phi^{-1} b_\phi, \phi(X_*)^T A_\phi^{-1} \phi(X_*)) \tag{14}$$

Where A_ϕ and b_ϕ are now:

$$A_\phi = \Sigma_p^{-1} + \frac{1}{\sigma_n^2} \phi(X)^T \phi(X) b_\phi = \frac{1}{\sigma_n^2} \phi(X)^T y$$

2.1.5 Computational issues

2.1.5.1 Avoiding inversion of A_ϕ 14 requires inverting the $N \times N$ matrix A_ϕ, where N is dimension of feature space, to get the expected value and variance.

Typically, matrices are inverted using Gaussian elimination. We need to perform a "forward" pass which requires N pivots on every row and column, N eliminations per pivot, and up to $2N$ columns to update, resulting in an $O(N^3)$ time complexity. Then, we need to perform a backwards pass in the opposite direction which is another $O(N^3)$ operation. Finally, we need to multiply the inverse by the RHS vector b_ϕ, which is an $O(N^2)$ operation but appears trivial next to these two cubic steps.

We can mitigate this for a particular class of high-dimensional $N > n$ problems by restating the predictive distribution in terms of the number of training data points n which would require inverting an $n \times n$ matrix instead. For polynomial basis expansions, N is degree D multiplied by number of features, so N can be very large or even infinite (e.g. SE).

Substituting b_ϕ into our predictive distribution mean:

$$\mathbb{E}_{p(f_*|X_*,X,y)}[f_*] = \phi(X_*)^T \cdot A_\phi^{-1} \cdot \left[\frac{1}{\sigma_n^2}\phi(X)^T y\right]$$

Rearranging to isolate $A_\phi^{-1}\phi(X)$

$$= \frac{1}{\sigma_n^2}\left[A_\phi^{-1}\phi(X)\right]^T y$$

We can use the Sherman-Morrison identity to get an expression for A_ϕ^{-1} directly, where $K = \phi(X)^T\Sigma_p\phi(X)$

$$A_\phi^{-1} = \Sigma_p - \Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1}\phi(X)^T\Sigma_p$$

For the mean, we can use the Sherman-Morrison identity again to get an expression for $A_\phi^{-1}\phi(X)$

$$A_\phi^{-1}\phi(X) = \sigma_n^2\Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1} \tag{15}$$

Substitute in 15 into our 14:

$$\mathbb{E}_{p(f_*|X_*,X,y)}[f_*] = \phi(X_*)\frac{1}{\sigma_n^2}\left[\sigma_n^2\Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1}\right]^T y$$

$\frac{1}{\sigma_n^2}$ and σ_n^2 cancel out, leaving us with this final expression for the mean:

$$\mathbb{E}_{p(f_*|X_*,X,y)}[f_*] = \phi(X_*)^T \cdot \Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1} y \tag{16}$$

For the variance, we cannot use the Sherman-Morrison identity to arrive at an expression for $A_\phi^{-1}\phi(X_*)$ because $\phi(X_*)$ is an arbitrary N-vector, not one of the columns of $\phi(X)$. Instead, we use the A_ϕ^{-1} expression we derived earlier to get an expression for $A_\phi^{-1}\phi(X_*)$:

$$A_\phi^{-1}\phi(X_*) = \Sigma_p \cdot \phi(X_*) - \Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1}\phi(X)^T\Sigma_p \cdot \phi(X_*)$$

Substituting this into 14:

$$\mathrm{Var}_{p(f_*|X_*,X,y)}[f_*] = \phi(X_*)^T\Sigma_p\phi(X_*) - \phi(X_*)^T\Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1}\phi(X)^T\Sigma_p\phi(X_*) \tag{17}$$

With our alternative mean 16 and variance 17, we can form an alternative expression for our predictive distribution:

$$\begin{aligned} p(f_*|X_*,X,y) = \mathcal{N}(\\ \phi(X_*)^T\Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1}y, \\ \phi(X_*)^T\Sigma_p\phi(X_*) - \phi(X_*)^T\Sigma_p\phi(X)(K + \sigma_n^2 I)^{-1}\phi(X)^T\Sigma_p\phi(X_*) \\ ) \end{aligned} \tag{18}$$

With this alternative formulation, we need to invert the $n \times n$ matrix $K + \sigma_n^2 I$ only. Geometrically, n datapoints can span at most n dimensions in the feature space - if $N > n$, the data forms a subspace of the feature space.

2.1.5.2 Kernels and the kernel trick In 18, $\phi(.)$ is always an inner product of a positive definite correlation matrix Σ_p, but with different arrangements of $\phi(X)$ and $\phi(X_*)$. We can define $k(X, X') = \phi(X)^T\Sigma_p\phi(X')$ as a covariance function or kernel, where X and X' are either X or X_*. For example, in 18 the definition of $K = \phi(X)^T\Sigma_p\phi(X)$ becomes $K = k(X, X)$.

Introducing $\psi(X)$ to better represent $k(X, X')$ as an inner product:

$$\psi(X) = \phi(X)\Sigma_p^{1/2}$$
$$k(X, X') = \psi(X)^T\psi(X')$$

These inner product representations require us to compute $\phi(X)$ and $\phi(X')$ in the feature space. A higher-dimensional feature space requires more compute to evaluate $\phi(X)$ and more memory to store $\phi(X)$ and $\phi(X')$.

Instead, the representer theorem guarantees that we can find an equivelant kernel that does not require us to explicitly compute $\phi(X)$ or $\phi(X')$ in the feature space. With this "kernel trick" we avoid the associated memory and computational costs of explicitly computing $\phi(X)$ and $\phi(X')$. Since computing the kernel directly is more convenient than the feature vectors themselves, these kernels become the object of primary interest.

For example, if we had some polynomial transformation $\phi(X) = [1, x^1, ..., x^D]^T$ and Σ_p as an identity matrix, we could define $k(X, X')$ as inner products:

$$\psi(X) = [1, x^1, ..., x^D]^T k(X, X') = \psi(X)^T \psi(X')$$

This approach requires arranging ϕ and $\phi(X')$ into a D sized vector, then taking the dot product. This is trivial for small D, but as D becomes infinite (e.g. RBF kernel), arranging a D sized vector requires too much memory and the dot product becomes computationally expensive.

Instead, we can define $k(X, X')$ as an equivelant function of X and X' directly:

$$k(X, X') = (1 + X \cdot X')^D$$

This is the polynomial kernel, which is equivalent to our original polynomial basis expansion $\phi(X)$ without explicitly computing $\phi(X)$.

2.2 Function-space view [4]

2.2.1 Gaussian processes (GP)

2.2.1.1 Bayesian linear model We can define our Bayesian linear model of a real process $f(X)$ entirely in terms of mean function $m(X)$ and covariance function $k(X, X')$:

$$m(X) = \phi(X)^T \mathbb{E}[W] = \phi(X)^T [0] = 0$$
$$k(X, X') = \phi(X)^T \mathbb{E}[WW^T] \phi(X') = \phi(X)^T \Sigma_P \phi(X')$$

Our covariance function here is in inner product form. The kernel trick here uses the squared exponential (SE) covariance function, also known as the radial basis function (RBF) or Gaussian kernel:

$$k(f(X), f(X')) = \exp\left(-\frac{1}{2}\frac{|X - X'|^2}{l^2}\right)$$

It can be shown that SE corresponds to a Bayesian linear regression model with infinite basis functions.

2.2.1.2 Function evaluations to a random function We can choose a subset X_{*1} from our test data X_* and apply it to our model get some function evaluations $f(X_{*1})$. $f(X_{*1})$ can be described as a multivariate Gaussian distribution, e.g. in the Bayesian linear model $f(X_{*1}) \sim N(0, k(X_{*1}, X_{*1}))$. Each output $f(X_{\theta *1})$ in our $f(X_{*1})$ vector is a random variable with mean 0 and covariance with each other $K_{\theta\theta'} = k(X_{\theta *}, X_{\theta' *})$. There exists some random function $g(X_{*1})$ for our subsets such that $f(X_{*1}) = g(X_{*1})$. We only know the value of $g(X_{*1})$ at the points X_{*1}, so $g(X_{*1}) = X_{*1} : f(X_{*1})$. Because $g(X)$ entirely consists of random points, we can think of $g(X_{*1})$ as a random function and our distribution $f(X)$ can be seen as a distribution of these random $g(X)$ functions. We can recover our individual $g(X_{*1}$ thanks to consistency - if we marginalised out our subset from the entire distribution $f(X_*)$, we would recover the subset distribution $N(0, K_*(X_{*1}, X_{*1}))$ that describes our random function $g(X_{*1})$.

2.2.1.3 Definition of a GP A GP is a collection of random variables, any finite number of which have a joint Gaussian distribution. Ultimately, GPs describe a distribution of random functions where each drawn function is a $g(X)$ sample from the GP.

$$f(X) \sim \mathcal{GP}(m(X), k(X, X')),$$
$$m(X) = \mathbb{E}[f(X)],$$
$$k(X, X') = \mathrm{Cov}(f(X), f(X')) = \mathbb{E}[(f(X) - m(X))(f(X') - m(X'))]$$

2.2.1.4 Consistency requirement This definition implies a consistency requirement - any group of functions drawn from our GP can be described by the same distribution as our GP. For example, if our GP implies that $(f(X_1), f(X_2)) \sim \mathcal{N}(\mu, \Sigma)$, then $(f(X_1) \sim \mathcal{N}(\mu_1, \Sigma) and f(X_2) \sim \mathcal{N}(\mu_2, \Sigma))$ where $\mu_\theta = m(X_\theta)$ and $\Sigma_{\theta\theta} = k(X_\theta, X_\theta)$. This requirement is also called the marginalisation property, because to get the smaller distribution of $f(X_1)$ we marginalise out the larger distribution of $f(X_1), f(X_2)$ by integrating the larger distribution wrt $f(X_2)$. Consistency is automatically gained if our covariance function specifies entries in a covariance matrix.

2.2.2 Predictive distributions with noise-free observations

2.2.2.1 Prior distribution over functions $f(X)$ and $f(X_*)$ are jointly distributed according to the prior:

$$\begin{pmatrix} f(X) \\ f(X_*) \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K(X,X) & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{pmatrix}\right)$$

2.2.2.2 Posterior distribution of functions To get the posterior distribution of functions given the training data and our prior, we can condition the joint prior distribution on the training data. Intuitively, this is like generating random functions $g(X)$ and rejecting those that do not pass through the training data. Probabilistically, we condition our joint Gaussian prior distribution on the observations $p(f(X_*)|X_*, X, f(X))$.

Substituting $p(W)$ and our conditioning X into the Gaussian multivariate conditioning identity:

$$\begin{aligned} p(f(X_*)|X_*, X, f(X)) \sim N(\\ [0] + [K(X_*,X)][K(X,X)]^{-1}([f(X)] - [0]), \\ [K(X*,X*)] - [K(X_*,X)][K(X,X)]^{-1}[K(X,X_*)] \\ ) \end{aligned}$$

Although we condition on X_*, X, and $f(X)$, we only substitute $f(X)$ because X_* and X are known constants, but $f(X)$ is random because it is a sample from the prior. We also swap $f(X_*)$ and $f(X)$ in our prior to match the conditioning identity, such that our input vector into the conditioning identity is $(f(X_*), f(X))^T$.

Simplifying the last term in the mean:

$$\begin{aligned} p(f(X_*)|X_*, X, f(X)) \sim N(\\ K(X,X_*)K(X,X)^{-1}f(X), \\ K(X_*,X_*) - K(X_*,X)K(X,X)^{-1}K(X,X_*) \\ ) \end{aligned} \tag{19}$$

2.2.3 Predictive distributions with noisy observations

2.2.3.1 Noisy observations prior It is typical to not have the noise-free function evaluations $f(X)$ as our training data, but instead our noisy observations y. We can simply add ϵ:

$$\mathrm{Cov}(y_p, y_q) = K(X_p, X_q) + \sigma_n^2 \delta_{pq}$$

δ_{pq} represents our independence condition in 1D. This is the Kronecker delta, which returns 1 if indices (p, q) are equal and 0 otherwise. σ_n^2 is the noise variance, which is a constant for all observations.

In matrix form:

$$\mathrm{Cov}(Y) = k(X,X) + \sigma_n^2 I$$

This gives us this prior:

$$\begin{pmatrix} Y \\ f(X_*) \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} K(X,X) + \sigma_n^2 I & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) \end{pmatrix}\right)$$

2.2.3.2 Noisy observations posterior As before, we can form a predictive distribution using the Gaussian multivariate conditioning identity:

$$\begin{aligned} p(f(X_*)|X_*, X, Y) \sim N(\\ K(X_*,X)[K(X,X) + \sigma_n^2 I]^{-1}Y, \\ K(X_*,X_*) - K(X_*,X)[K(X,X) + \sigma_n^2 I]^{-1}K(X,X_*) \\ ) \end{aligned}$$

Substituting $k(X, X') = \phi(X)^T \Sigma_p \phi(X')$ into here gives us the exact same result as 18.

Our variance is independent of the targets y and only depends on our inputs X and X_*. Our variance is two terms: our prior covariance $K(X_*, X_*)$, a term representing the information the observations give us about the function. As before, we can compute the predictive distribution of y_* by adding the noise term $\sigma_n^2 I$ to the variance.

2.2.4 Marginal likelihood

We need some measure of how well our GP fits the data, which we can get by computing the marginal likelihood $p(Y|X)$:

$$p(Y|X) = \int p(Y|f, X)p(f|X)df$$

$p(y|f, X)$ is our familar predictive distribution $p(y|f, X) \sim N(f, \sigma_n^2 I)$, and represents how well f maps X to y. $p(f|X)$ is our prior distribution over weights $\sim N(0, K)$ which we use here to represent the complexity of f. Our weight's mean will always be the same under our prior, but our $K(X, X')$ tells us how "wiggly" our function is. The closer our $p(f|X)$ distribution is to the true complexity of the function, the higher our marginal likelihood. For example, for SE if our data is close together, then $|X - X'|$ becomes small and our covariance $k(X, X')$ on our function distribution prior is large. Therefore, we get a high variety of functions and a higher probability of sampling a more complex function.

We can express $p(Y|X)$ as a Gaussian integral over the joint distribution of f and Y ($p(Y, f|X)$), and marginalise out f to get this PDF:

$$logp(Y|X) = -\frac{1}{2}Y^T(K + \sigma_n^2 I)^{-1}Y - \frac{1}{2}log|K + \sigma_n^2 I| - \frac{n}{2}log(2\pi) \tag{20}$$

Alternatively, from 1 we know that y is Gaussian. Since both y and f are Gaussian, we can simply add their means and variances:

$$p(Y|X) = N(0, K + \sigma_n^2 I)$$

We can plug these mean and variances into Gaussian PDF 8 to get 20.

2.2.5 Algorithm for predictive distribution

1. Take in inputs X, outputs y, covariance function k, noise level σ_n^2, and test input X_*
2. $L = \text{cholesky}(K(X, X) + \sigma_n^2 I)$
   - Invert our $[K(X, X) + \sigma_n^2 I]$ matrix needed for mean and variance using Cholesky decomposition
3. $alpha = L^T \backslash (L \backslash y)$
   - Prepare the mean of our predictive distribution in linear combination form by computing the α vector
4. $mu = K(X_*, X)^T \cdot alpha$
   - Compute the mean
5. $v = L \backslash K(X_*, X)^T$
   - Prepare to compute variance by computing v, the form in which L is used in the variance
6. $var = K(X_*, X_*) - v^T v$
   - Compute the variance
7. $\text{log}p(Y|X) = -\frac{1}{2}y^T \cdot alpha - \frac{1}{2}log|K(X, X) + \sigma_n^2 I| - \frac{n}{2}log(2\pi)$
   - Compute the log marginal likelihood
8. Return the mean mu, variance var, and log marginal likelihood

TODO Choelsky decomposition if needed, missing background

2.3 Varying the length scale [4]

Our covariance functions has some hyperparameters, e.g. the full form of SE in one dimension contains some free parameters σ_f^2, σ_n^2, and l:

$$k_y(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2}\frac{|x - x'|^2}{l^2}\right) + \sigma_n^2 \delta_{x,x'}$$

Note that our covariance function is for k_y as it is for the noisy targets y, not the function f. σ_f^2 is the signal variance, which controls the overall scale of the function. σ_n^2 is the noise variance, which controls the amount of noise in the observations. $\delta_{X,X'}$ is the Kronecker delta which represents our independence of noise assumption.

l is a "length scale" hyperparameter that controls how sensitive our functions are - if we specify a lower l, we can "artificially" get a high $k(X, X')$. One way to determine l is by the expected number of "upcrossings" that our kernel is expected to make for a given level u. A function performs an upcrossing for u when $u = f(x)$ and $dy/dx > 0$. For example, with $u = 2$ and $y = x^2$, there exists one upcrossing at $(2, \sqrt{2})$ where $dy/dx = 4$, and a downcrossing at $(2, -\sqrt{2})$ where $dy/dx = -4$. For our zero-mean Gaussian processes, the expected number of upcrossings of our (stationary) kernel for a level $0 < u < 1$ is:

$$\mathbb{E}[N_u] = \frac{1}{2\pi}\sqrt{\frac{-k''(0)}{k(0)}} \exp\left(-\frac{u^2}{2k(0)}\right)$$

We can empirically count the number of upcrossings between 0 and 1 and set this equal to the expected number of upcrossings to get a value for l:

$$\frac{1}{2\pi}\sqrt{\frac{-k''(0)}{k(0)}} \exp\left(-\frac{u^2}{2k(0)}\right) = \hat{N}_u \tag{21}$$

A large amount of upcrossings implies our data-generating function wiggles rapidly, so our l becomes smaller to produce a covariance function that in turn produces more flexible functions.

3 Exploring Covariance Functions

3.1 Characteristics of covariance functions [4]

3.1.1 Symmetry and positive semidefiniteness

Given a vector of input points $X_i | i = 1, ..., n$, the Gram matrix K is the $n \times n$ matrix whose (i, j)-th entry is the inner product between X_i and X_j. Since our covariance matrix can be represented as inner products of our vectors of inputs, we can represent it as a Gram matrix. The Gram matrix has two key properties, symmetry and positive semidefiniteness:

$$K_{ij} = K_{ji}$$
$$X^T K X \geq 0$$

TODO prove positive semidefiniteness, background needed

3.1.2 Mean square continuity and differentiability

To understand how smooth the functions drawn from a Gaussian process are, we need to understand how differentiable and continuous they are. A more differentiable function implies that the function contains higher order polynomials which makes it smoother, and a continuous function avoids any reductions in smoothness produced by discontinuities.

Because the functions drawn from the Gaussian distribution are random functions between datapoints, there are infinitely many possible functions and determining if they are all continuous or differentiable is impossible. TODO

3.1.2.1 Continuity Let x be an infinite-length vector of inputs $x_1, x_2, ...$ whose values linearly approach some stable fixed point x_* as the sequence progresses. Formally:

$$\lim_{k \to \infty} |x_k - x_*| = 0$$

A regular function f is continuous at x_* if three conditions are met. x_* must exist in the domain of f, e.g. $f(X) = 1/x$ is not continuous at $f(0)$ because 0 is not in the domain of f. There must be a single limit the function approaches.

$$f(X) = \begin{cases} 0 & \text{if } X < 0 \\ 1 & \text{if } X > 0 \\ 2 & \text{if } X = 0 \end{cases}$$

In this example, at $f(0)$ x is not continuous at $x = 0$ since f approaches both 0 and 1. This single limit needs to be the same as the function evaluation at the limit. If we removed the 0 if $X < 0$ case to produce a single limit, it would still not be continuous at $x = 0$ since the limit would be 1 but $f(0) = 2$. Formally summarising these three ideas:

$$\lim_{x \to x_*} |f(x) - f(x_*)| = 0$$

A Gaussian process f is MS continuous at x_* if the expected function evaluations $E[f(x)]$ quadratically approach $f(x_*)$ as $x \to x_*$. Formally:

$$\lim_{x \to x_*} \mathbb{E}[(f(x) - f(x_*))^2] = 0$$

Thanks to the quadratic term, we can expand our error term directly into kernel terms. The covariance function k is defined as the expected value of the product of two function evaluations:

$$\begin{aligned} \mathbb{E}[(f(x) - f(x_*))^2] &= \mathbb{E}[f(x)^2] + \mathbb{E}[f(x_*)^2] - 2\mathbb{E}[f(x)f(x_*)] \\ &= k(x, x) + k(x_*, x_*) - 2k(x, x_*) \end{aligned}$$

Using this expansion in our definition of MS continuity:

$$\lim_{x \to x_*} |k(x, x) - 2k(x, x_*) + k(x_*, x_*)| = 0 \tag{22}$$

Because x_* is given, $k(x_*, x_*)$ is a constant. This limit requires that both $k(x, x)$ and $k(x, x_*) \to k(x_*, x_*)$ as $x \to x_*$, which is the very definition of continuity of k at x_* - they guarantee that x_* is in the domain of k, that it has a single limit, and this limit of $k(x, x_*)$ is $k(x_*, x_*)$ as $x \to x_*$. Therefore, a Gaussian process is MS continuous at x_* if and only if the covariance function k is continuous at x_*.

3.1.2.2 Differentiability f is MS differentiable at x_* in the ith direction of our input vector X if:

$$\lim_{h\to 0}\mathbb{E}\left[|\frac{(f(x_*+he_i)-f(x_*))}{h}-\frac{\partial f}{\partial x_{*i}}(x_*)|\right]^2=0$$

$e_i=(0_0,...,0_{i-1},1_i,0_{i+1},...,0_n)$ is a unit vector that constrains the change in x to only the ith dimension. We assume $m(x_*)=0$ for simplicity, but a non-zero mean does not change the structure of this proof and leads to the same result.

Expanding and creating simplifying A and B terms to represent the limit and the proposed derivative respectively:

$$\lim_{h\to 0}\mathbb{E}\left[(A_h-B)^2\right]=\mathbb{E}[A_h^2]+\mathbb{E}[B^2]-2\mathbb{E}[A_hB]=0$$
$$A_h=\frac{f(x_*+he_i)-f(x_*)}{h}$$
$$B=\frac{\partial f}{\partial x_{*i}}(x_*)$$

Similar to MS continuity, we expand A_h^2 into kernel terms:

$$\mathbb{E}[A_h^2]=\frac{1}{h^2}\left(k(x_*+he_i,x_*+he_i)+k(x_*,x_*)-2k(x_*+he_i,x_*)\right)\tag{23}$$

$k(x_*,x_*)$ is a constant, but the other terms vary with h. We can use a second-order Taylor series to approximate these terms if k is twice continuously differentiable at x_*. Starting with the univariate $k(x_*+he_i,x_*)$:

$$\begin{aligned}k(x_*+he_i,x_*)=&\\ k(x_*,x_*)&\\ +h[\partial_{u_i}k](x_*,x_*)&\\ +\frac{h^2}{2}[\partial^2_{u_iu_i}k](x_*,x_*)&\\ +O(h^3)&\end{aligned}$$

u_i and v_i denote the first x_*+he_i and second x_* arguments respectively in the ith direction. TODO explain O and why it's in terms of h^3 Then, the multivariate $k(x_*+he_i,x_*+he_i)$:

$$\begin{aligned}k(x_*+he_i,x_*+he_i)=&\\ k(x_*,x_*)&\\ +h[\partial_{u_i}k+\partial_{v_i}k](x_*,x_*)&\\ +\frac{h^2}{2}[\partial^2_{u_iu_i}k+\partial^2_{u_iv_i}k+\partial^2_{v_iv_i}k](x_*,x_*)&\\ +O(h^3)&\end{aligned}$$

Substituting these approximations into 23:

$$\begin{aligned}\mathbb{E}[A_h^2]=\frac{1}{h^2}&\\ k(x_*,x_*)+k(x_*,x_*)-2k(x_*,x_*)&\\ +h[\partial_{u_i}k+\partial_{v_i}k](x_*,x_*)-2h[\partial_{u_i}k](x_*,x_*)&\\ +\frac{h^2}{2}[\partial^2_{u_iu_i}k+\partial^2_{u_iv_i}k+\partial^2_{v_iv_i}k](x_*,x_*)-2\frac{h^2}{2}[\partial^2_{u_iu_i}k](x_*,x_*)&\\ +O(h^3)&\end{aligned}$$

The constant $k(x_*,x_*)$ terms cancel and the $O(h^3)$ remainders combine but remain the same order.

We can combine the linear partial derivatives to form a single function $[\partial_{u_i}k+\partial_{v_i}k-2\partial_{v_i}k]$. Thanks to the symmetry of the covariance matrix inherited from the Gram matrix, $k(u,v)=k(v,u)$ and $\partial_{u_i}k=\partial_{v_i}k$ and substituting in either into our linear term cancels it completely.

Similarly, we can combine the quadratic derivatives:

$$E[A^2]=\frac{1}{h^2}\frac{h^2}{2}[\partial^2_{u_iu_i}k+\partial^2_{u_iu_i}k+\partial^2_{v_iv_i}k](x_*,x_*)-h^2[\partial^2_{u_iv_i}k](x_*,x_*)$$

Cancelling $\frac{1}{h^2}$ and $\frac{h^2}{2}$ and simplifying:

$$\begin{aligned}&=[\partial^2_{u_iv_i}k+\partial^2_{u_iu_i}k+\partial^2_{v_iv_i}k-\partial^2_{u_iv_i}k](x_*,x_*)\\ &=[\partial^2_{u_iu_i}k+\partial_{u_iv_i}k-\partial^2_{v_iv_i}k](x_*,x_*)\end{aligned}$$

Similarly to the linear terms, using the symmetry of k to cancel $\partial^2_{u_iu_i}$ and $\partial^2_{v_iv_i}$ yields the final expression for $\mathbb{E}[A_h^2]$:

$$\mathbb{E}[A_h^2] = \partial^2_{u_iv_i} k(x_*, x_*) + O(h^3) \tag{24}$$

Because B is Gaussian, its square is simply its variance:

$$\begin{aligned}\mathbb{E}[B^2] &= \mathrm{Var}\left(\frac{\partial f}{\partial x_{*i}}(x_*)\right)\\ &= \mathrm{Cov}\left(\frac{\partial f}{\partial x_{*i}}(x_*), \frac{\partial f}{\partial x_{*i}}(x_*)\right)\end{aligned}$$

We can substitute our regular limit definition of differentiability outside of MS space, with different small increments h and h':

$$= \mathrm{Cov}\left(\frac{f(x_* + he_i) - f(x_*)}{h}, \frac{f(x_* + h'e_i) - f(x_*)}{h'}\right)$$

The h and h' denominators merely scale the covariance, so we can take them out of the covariance expression:

$$= \frac{1}{hh'}\mathrm{Cov}\left(f(x_* + he_i) - f(x_*), f(x_* + h'e_i) - f(x_*)\right)$$

Using additivity TODO explain:

$$\mathbb{E}[B^2] = \frac{1}{hh'}\left(k(x_* + he_i, x_* + h'e_i) - k(x_*, x_* + h'e_i) - k(x_* + he_i, x_*) + k(x_*, x_*)\right)$$

We already have $k(x_* + he_i, x_*)$ from **??** directly, and $k(x_*, x_* + he_i)$ by symmetry and substituting h' for h. Our multivariate Taylor series $k(x_* + he_i, x_* + h'e_i)$ looks similar to **??**:

$$\begin{aligned}k(x_* + he_i, x_* + h'e_i) &=\\ k(x_*, x_*)&\\ +h[\delta_{u_i}k](x_*, x_*) + h'[\delta_{v_i}k](x_*, x_*)&\\ +\frac{h^2}{2}[partial^2_{u_iu_i}k](x_*, x_*)&\\ +hh'[\partial^2_{u_iv_i}k](x_*, x_*)&\\ +\frac{h'^2}{2}[\partial^2_{v_iv_i}k](x_*, x_*)&\\ +O(||(h, h')||^3)&\end{aligned}$$

Substituting these results into $\mathbb{E}[B^2]$:

$$\begin{aligned}\mathbb{E}[B^2] = \frac{1}{hh'}&\\ k(x_*, x_*)&\\ +k(x_*, x_*) + k(x_*, x_*) - k(x_*, x_*)&\\ +h[\delta_{u_i}k](x_*, x_*) - h[\delta_{u_i}k](x_*, x_*)&\\ +h'[\delta_{v_i}k](x_*, x_*) - h'[\delta_{v_i}k](x_*, x_*)&\\ +\frac{h^2}{2}[\partial^2_{u_iu_i}k](x_*, x_*) - \frac{h^2}{2}[\partial^2_{u_iu_i}k](x_*, x_*)&\\ +hh'[\partial^2_{u_iv_i}k](x_*, x_*)&\\ +\frac{h'^2}{2}[\partial^2_{v_iv_i}k](x_*, x_*) - \frac{h'^2}{2}[\partial^2_{v_iv_i}k](x_*, x_*)&\\ +O(h^3) + O(h'^3) + O(||(h, h')||^3)&\end{aligned}$$

All constant, linear h and h', and h^2 and h'^2 terms cancel, leaving the mixed term and the remainders. $\frac{1}{hh'}$ cancel and the remainders can be combined since TODO:

$$\mathbb{E}[B^2] = \partial^2_{u_iv_i} k(x_*, x_*) + O(h^2) \tag{25}$$

For $\mathbb{E}[A_hB]$, assuming zero-mean:

$$\mathbb{E}[A_hB] = \mathrm{Cov}\left(\frac{f(x_* + he_i) - f(x_*)}{h}, \frac{\partial f}{\partial x_{*i}}(x_*)\right)$$

Similarly to B, we can remove the scaling factor $\frac{1}{h}$:

$$= \frac{1}{h}\mathrm{Cov}\left(f(x_* + he_i) - f(x_*), \frac{\partial f}{\partial x_{*i}}(x_*)\right)$$

By linearity of covariance TODO elabourate:

$$= \frac{1}{h}\left[\mathrm{Cov}(f(x_* + he_i), \frac{\partial f}{\partial x_{*i}}(x_*)) - \mathrm{Cov}(f(x_*), \frac{\partial f}{\partial x_{*i}}(x_*))\right]$$

A fundamental identities for Gaussian fields TODO elabourate is:

$$\mathrm{Cov}(f(u), \delta_{u_i} f(v)) = \delta_{u_i} k(u, v)$$

Applying it to both terms:

$$\mathrm{Cov}(f(x_* + he_i), \frac{\partial f}{\partial x_{*i}}(x_*)) = \delta_{u_i} k(x_* + he_i, x_*)$$
$$\mathrm{Cov}(f(x_*), \frac{\partial f}{\partial x_{*i}}(x_*)) = \delta_{v_i} k(x_*, x_*)$$

Taylor expanding our first term:

$$\begin{aligned} \delta_{u_i} k(x_* + he_i, x_*) = \\ \delta_{u_i} k(x_*, x_*) \\ + h\delta^2_{u_i v_i} k(x_*, x_*) \\ + \frac{h^2}{2}\delta^3_{u_i u_i u_i} k(x_*, x_*) \\ + O(h^3) \end{aligned}$$

We can take advantage of symmetry of k to cancel out the constant term using the second term in $\mathbb{E}[A_h B]$ - when $u = v$, $\delta_{v_i} k(x_*, x_*) = \delta_{u_i} k(x_*, x_*)$. Substituting this into $\mathbb{E}[A_h B]$:

$$\begin{aligned} \mathbb{E}[A_h B] = \frac{1}{h} \\ h\delta^2_{u_i v_i} k(x_*, x_*) + \frac{h^2}{2}\delta^3_{u_i u_i v_i} k(x_*, x_*) \\ + O(h^3) \end{aligned}$$

Dividing by h reduces the order of the remainder. Simplifying for a final expression:

$$\mathbb{E}[A_h B] = \delta^2_{u_i v_i} k(x_*, x_*) + \frac{h}{2}\delta^3_{u_i u_i u_i} k(x_*, x_*) + O(h^2) \tag{26}$$

Substituting 24, 25, and 26 into our original limit definition of MS differentiability:

$$\lim_{h \to 0} \delta^2_{u_i v_i} k(x_*, x_*) + O(h^3) + \delta^2_{u_i v_i} k(x_*, x_*) + O(h^2) - 2\left(\delta^2_{u_i v_i} k(x_*, x_*) + \frac{h}{2}\delta^3_{u_i u_i u_i} k(x_*, x_*) + O(h^2)\right) = 0$$

Redefining $A = \delta^2_{u_i v_i} k(x_*, x_*)$ and $B = \frac{h}{2}\delta^3_{u_i u_i v_i} k(x_*, x_*)$ for brevity:

$$\lim_{h \to 0} A + O(h^3) + A + O(h^2) - 2(A + \frac{h}{2}B + O(h^2)) = 0$$

Expanding the last term:

$$\lim_{h \to 0} A + O(h^3) + A + O(h^2) - 2A - hB - 2O(h^2) = 0$$

All A terms cancel. Combining and reducing the remainders to the lowest order:

$$\lim_{h \to 0} hB + O(h) = 0$$

We can aborsb hB into $O(h)$ since it is a linear term in h:

$$\lim_{h \to 0} O(h) = 0 \tag{27}$$

$O(h)$ approaches 0 as $h \to 0$, so our limit definition of MS differentiability is met using a second-order Taylor expansion. We can extend this to any k-th derivative in MS space by using a $2k$-th order Taylor expansion of the covariance functions, which requires the covariance function to be $2k$-times continuously differentiable at x_*.

3.2 Stationary GPs [4]

3.2.1 Stationarity and isotropicism

A stationary covariance function $k(X - X')$ is some function of $X - X'$, and is invariant to the exact locations of X and X'. An isotropic covariance function $k(|X - X'|)$ is a function of $|X - X'|$, and is is invariant to the direction of $X - X'$. For example, SE [**eq:se**] is both stationary and isotropic because it is a function of $|X - X'|$.

3.2.2 Stationary GPs in MS space

Putting the stationary kernel $k(x, x') = k(x - x')$ into 22:

$$\lim_{x \to x_*} |k(x - x) - 2k(x - x_*) + k(x_* - x_*)| = 0$$

Simplifying the terms inside the kernels and combining like terms:

$$\lim_{x \to x_*} 2|k(0) - k(x - x_*)| = 0$$

2 is a constant factor and can be ignored. Because $|k(0) - k(x - x_*)|$ is invariant to direction, we can swap them to align with the definition of continuity at 0:

$$\lim_{x \to x_*} |k(x_* - x) - k(0)| = 0$$

Thus, a stationary covariance function is MS continuous at x_* if and only if it is continuous at $x_* = 0$. Similarly, it can be shown that stationary covariance functions are MS differentiable at x_* if and only if they are MS differentiable at $x_* = 0$.

3.2.3 Squared exponential (SE)

Here is the already introduced SE:

$$k(X, X*) = \exp\left(-\frac{|X - X'|^2}{2l^2}\right)$$

This covariance function is infinitely differentiable at $x - x' = 0$ thanks to the squared difference between X and X' in the exponent, so a GP using SE is infinitely mean-squared differentiable which produces extremely smooth functions.

3.2.3.1 From feature space to SE We can derive this form by expanding X into our feature space ϕ defined by Gaussian-shaped basis functions centred densely in X. Defining this basis function:

$$\phi_c(x) = \exp\left(-\frac{|x - c|^2}{2l^2}\right)$$

c the centre of our basis functions. With our familiar isotropic Gaussian prior on the weights $W \sim \mathcal{N}(0, \sigma_p^2 I)$, we get our familiar covariance function in weight-space:

$$k(x, x') = \sigma_p^2 \sum_{c=1}^{N} \phi_c(x)\phi_c(x')$$

N represents the number of these basis functions. If $N = \infty$ with centres everywhere between some interval c_{min} and c_{max}, we can simply integrate over the interval:

$$\lim_{N \to \infty} \sigma_p^2 \sum_{c=1}^{N} \phi_c(x)\phi_c(x') = \sigma_p^2 \int_{c_{min}}^{c_{max}} \phi_c(x)\phi_c(x')dc$$

Plugging in our basis function:

$$k(x, x') = \sigma_p^2 \int_{c_{min}}^{c_{max}} \exp\left(-\frac{|x - c|^2}{2l^2}\right) \exp\left(-\frac{|x' - c|^2}{2l^2}\right) dc$$

Combining the exponentials:

$$= \sigma_p^2 \int_{c_{min}}^{c_{max}} \exp\left(-\frac{|x - c|^2 - |x' - c|^2}{2l^2}\right) dc$$

Expanding the squared terms, rearranging the fraction and simplifying:

$$= \sigma_p^2 \int_{c_{min}}^{c_{max}} \exp\left(-\frac{1}{l^2}\left[c^2 - c(x + x') + \frac{x^2 + x'^2}{2}\right]\right) dc$$

We can complete the square on the c terms to get a product of two exponentials:

$$= \sigma_p^2 \int_{c_{min}}^{c_{max}} \exp\left(-\frac{1}{l^2}\left[(c - \frac{x + x'}{2})^2 - \frac{(x + x')^2}{4}\right]\right) dc$$

Our second term in the exponential does not vary with c and can be safely factored out of the integral:

$$= \sigma_p^2 \exp\left(\frac{(x + x')^2}{4l^2}\right) \int_{c_{min}}^{c_{max}} \exp\left(-\frac{1}{l^2}(c - \frac{x + x'}{2})^2\right) dc$$

If we let our c_{min} and c_{max} approach infinity, we can use the standard Gaussian integral:

$$\int_{-\infty}^{\infty} \exp\left(-\frac{1}{l^2}(c - \frac{x+x'}{2})^2\right) dc = l\sqrt{\pi}$$

Substituting this in:

$$k(x,x') = \sigma_p^2 l\sqrt{\pi} \exp\left(-\frac{(x-x')^2}{4l^2}\right)$$

We can absorb the $l\sqrt{\pi}$ into the σ_p^2 term to produce our familiar SE with a $\sqrt{2}$ longer length scale:

$$k(x,x') = \sigma_p^2 \exp\left(-\frac{(x-x')^2}{2(\sqrt{2}l)^2}\right)$$

3.2.3.2 Length scale in SE We can observe the role l plays in SE by finding the value for l analytically and rearranging it for $\hat{N}_u$ to see its effect on smoothness.

Using 21:

$$l = \frac{1}{2\pi\hat{N}_u} \exp\left(-\frac{u^2}{2\sigma^2}\right)$$

Setting $u = 0$ makes our term inside the exponential equal to zero:

$$l = \frac{1}{2\pi\hat{N}_u}$$

Rearranging for $\hat{N}_u$:

$$\hat{N}_u = \frac{1}{2\pi l}$$

Here, l behaves as a length scale - a larger l reduces the number of upcrossings, stretching out the features over longer distances and producing smoother sample paths.

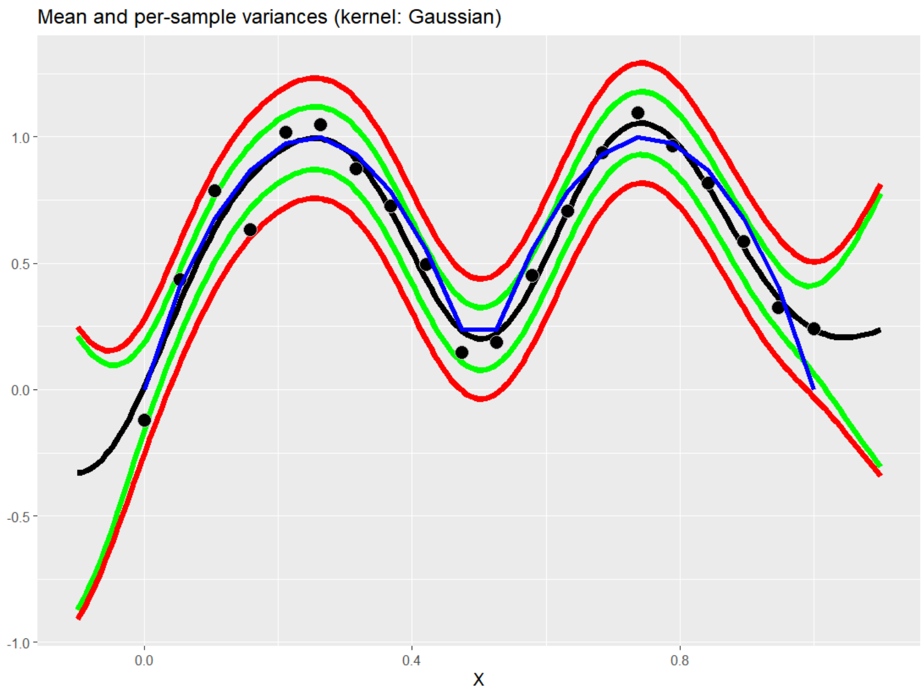


Figure 1: Plot of a Gaussian process using SE applied to a toy dataset. The toy dataset ($n = 15$) is a data-generating function in blue with some Gaussian noise applied to produce the datapoints in black. The black line represents the expected function from the Gaussian process. The green line represents the 90% confidence interval around the predictive distribution without the σ_n^2 term, representing the uncertainty surrounding predictions of the noise-free mean function $f(X)$. The red line represents the 90% confidence interval with σ_n^2, representing the uncertainty surrounding predictions of the noisy observations y.
TODO explain

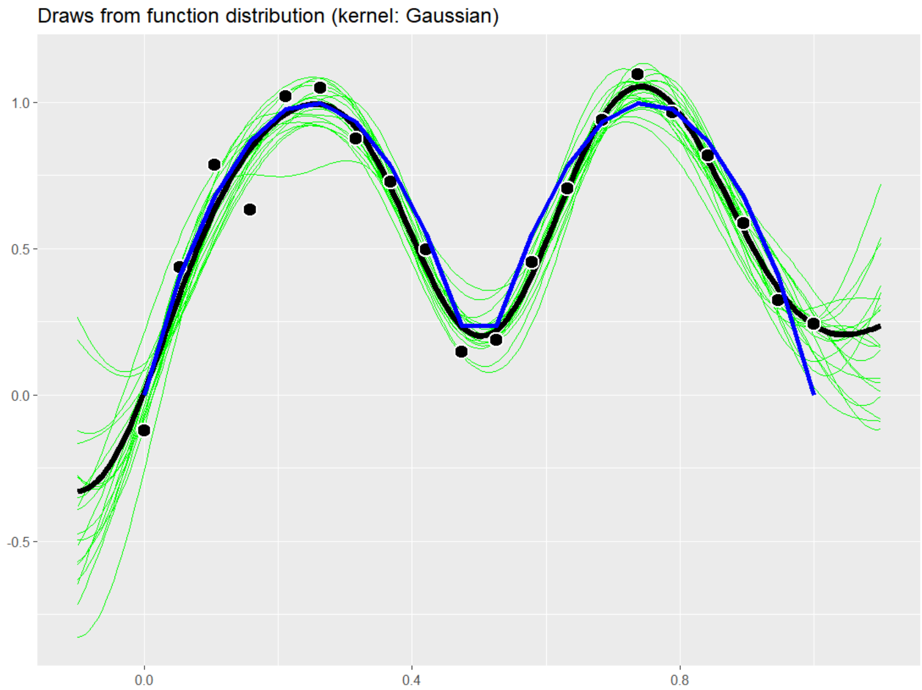


Figure 2: Plots of functions from a Gaussian process using SE applied to the same toy dataset. The blue line and black datapoints and lines are as before, but the green lines here are a sample of functions drawn from the Gaussian process. TODO explain

3.2.4 γ-exponential and exponential

SE has no parameter that controls or reduce its MS differentiability and its smoothness, rendering it a poor approximation of the less smooth functions we often encounter in the real world. We can introduce a differentiability parameter γ to control how differentiable the covariance function is:

$$k(X, X') = \exp\left(-\frac{|X - X'|^{\gamma}}{l^{\gamma}}\right)$$

where $0 < \gamma \geq 2$ controls the smoothness of the covariance function.

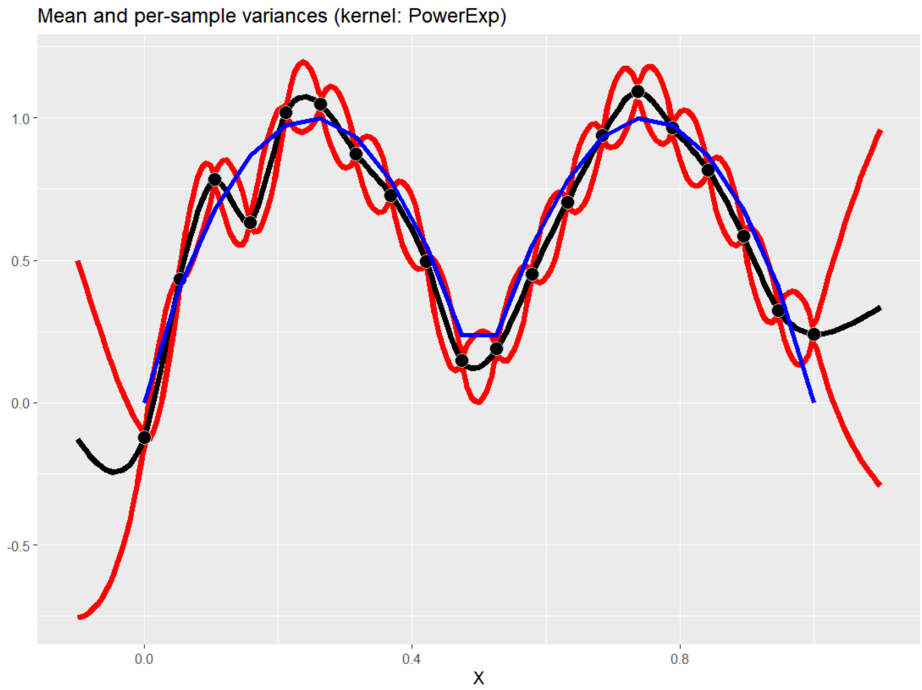


Figure 3: Plot of a Gaussian process using γ-exponential applied to the toy dataset. For this dataset, the R package GauPro [**gaopro**] has used $\gamma = 1.688043$ obtained via MLE.
There are no green lines here because TODO. γ-exponential produces much rougher functions than SE, so its expected function has a lot more wiggle and conforms to the datapoints much closer than SE. In this case, our data-generating function is smooth so SE is closer to the data-generating function than γ-exponential, but real world data-generating functions are often much rougher and would benefit from a kernel flexible enough to pass through the datapoints.

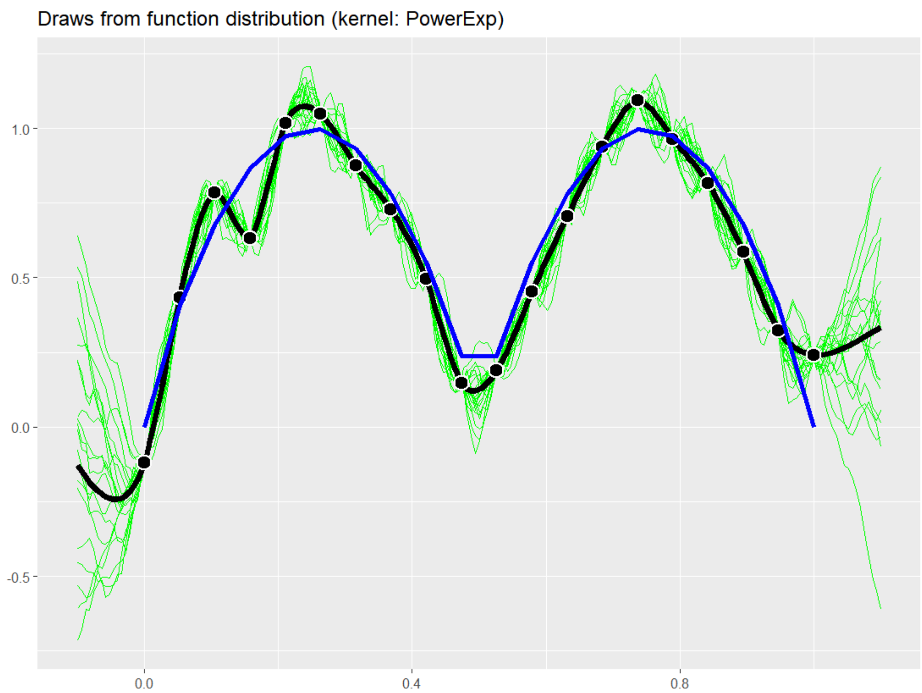


Figure 4: Plots of functions from a Gaussian process using γ-exponential applied to the same toy dataset.
These sample function draws are much rougher than SE.

$\gamma = 2$ produces SE for maximal smoothness, while $\gamma = 1$ produces the exponential covariance function:

$$k(X, X') = \exp\left(-\frac{|X - X'|}{l}\right)$$

Here, and for all other values of γ other than 2, the covariance function is continuous but not differentiable at all at $|x - x'| = 0$, which coincides with the undifferentiable turning point of the modulus function at $x - x' = 0$, and produces the roughest functions of all covariance functions we consider.

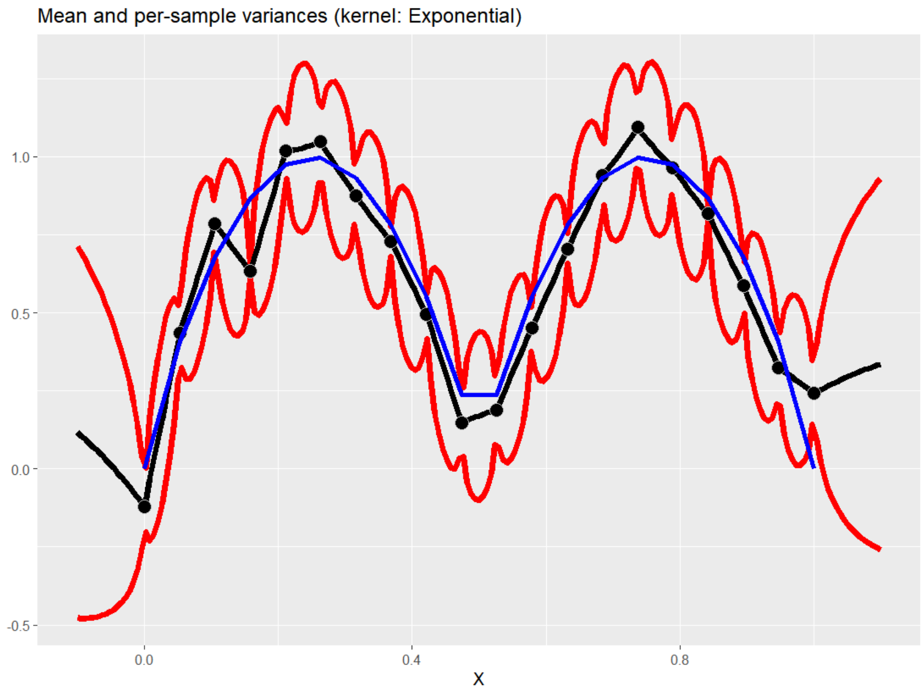


Figure 5: Plot of a Gaussian process using exponential applied to the toy dataset.TODO explain

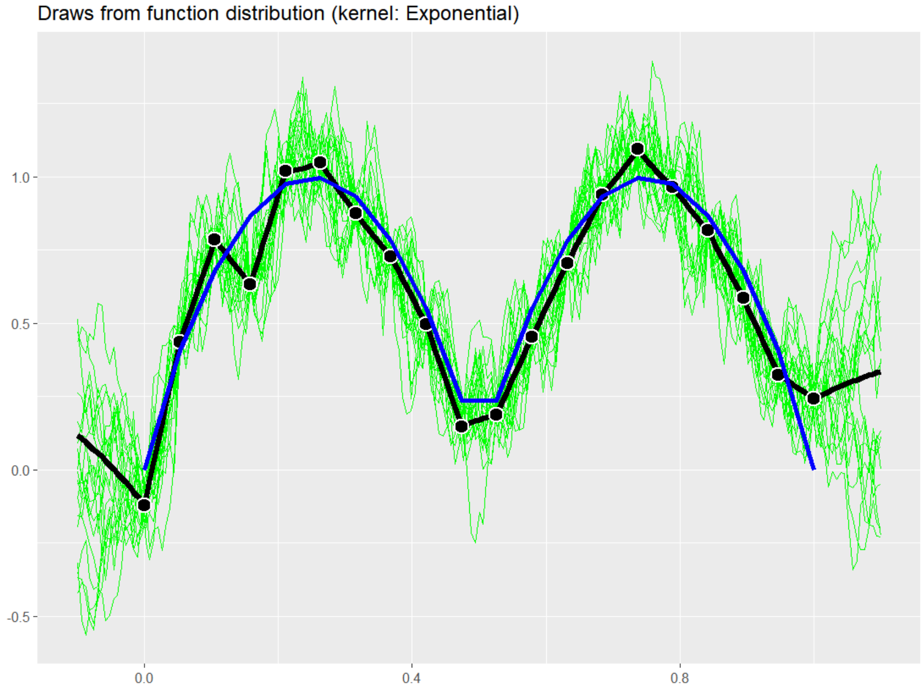


Figure 6: Plots of functions from a Gaussian process using exponential applied to the same toy dataset. These sample function draws are much rougher than SE and γ-exponential.

3.2.5 Matern-class

The γ-exponential generalisation is not useful due to its brittleness - it can only produce two covariance functions representing the extremes of the smoothness-roughness scale. The Matern class of covariance functions addresses this by introducing a parameter $\nu > 0$ that controls the smoothness of the function. The Matern class is defined as:

$$k(X, X') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}|X - X'|}{l} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu}|X - X'|}{l} \right)$$

l is our familiar length scale hyperparameter. TODO Bessel function K_ν, background needed. Therefore, a Gaussian process using a Matern class kernel is k-times MS differentiable if and only if $\nu > k$.

Using half-integers, i.e. $\nu = p + 1/2$ where p is a non-negative integer, the covariance function becomes a product of a polynomial and an exponential:

$$k_{\nu=p+1/2}(X,X') = \exp\left(-\frac{\sqrt{2\nu}|X-X'|}{l}\right)\frac{\Gamma(p+1)}{\Gamma(2p+1)}\sum_{i=0}^{p}\frac{(p+i)!}{i!(p-i)!}\left(\frac{\sqrt{8\nu r}}{l}\right)^{p-i}$$

$\nu = 1/2$ is equivelant to the exponential covariance function. As $\nu \to \infty$, the Matern covariance function approaches the SE covariance function. Practically, $\nu \geq 7/2$ produces functions that are as smooth as SE, leaving us with two cases of interest: $\nu = 3/2$ and $\nu = 5/2$.

3.2.5.1 Matern 3/2

$\nu = 3/2$ produces the following covariance function:

$$k_{3/2}(X,X') = \left(1+\frac{\sqrt{3}|X-X'|}{l}\right)\exp\left(-\frac{\sqrt{3}|X-X'|}{l}\right)$$

3/2 is one-time MS differentiable, leading to much rougher functions than SE.

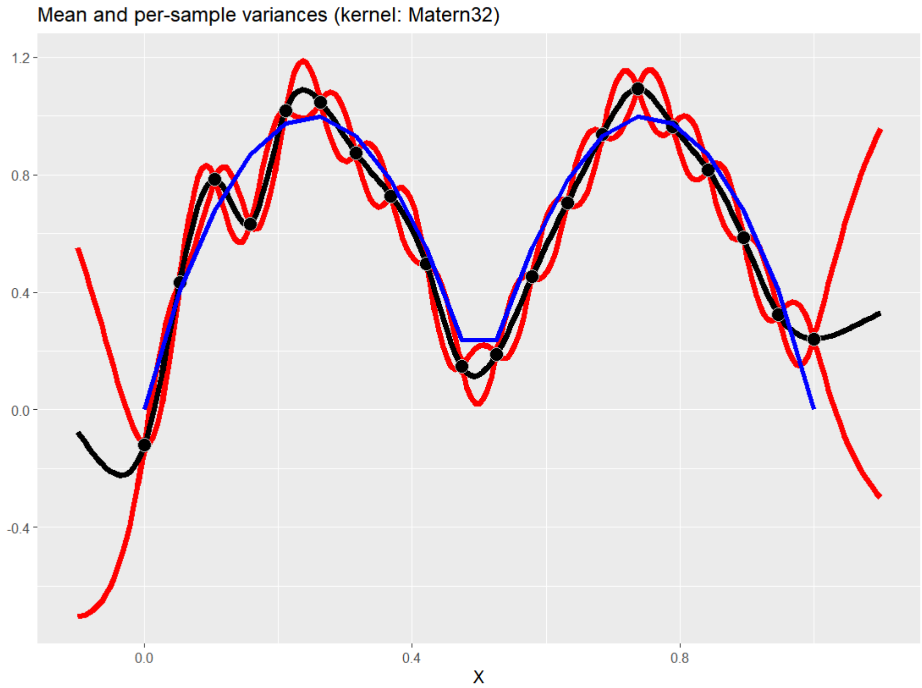


Figure 7: Plot of a Gaussian process using Matern 3/2 applied to the toy dataset.TODO explain

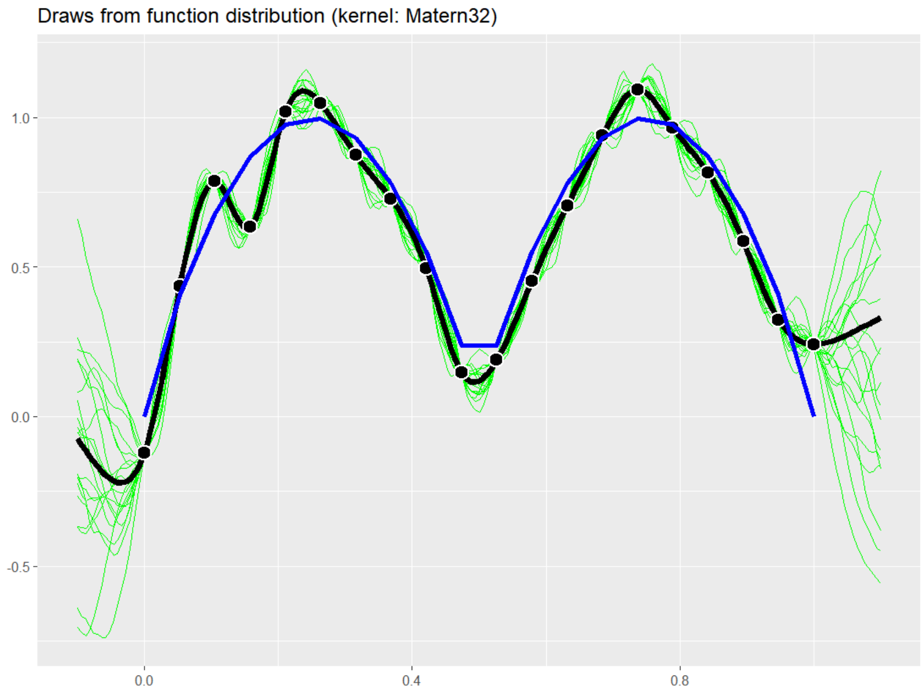


Figure 8: Plots of functions from a Gaussian process using Matern 3/2 applied to the same toy dataset. TODO explain

3.2.5.2 Matern 5/2 $\nu = 5/2$ produces the following covariance function:

$$k_{5/2}(X, X') = \left(1 + \frac{\sqrt{5}|X - X'|}{l} + \frac{5|X - X'|^2}{3l^2}\right) \exp\left(-\frac{\sqrt{5}|X - X'|}{l}\right)$$

5/2 is twice MS differentiable, producing functions that are slightly smoother than 3/2.

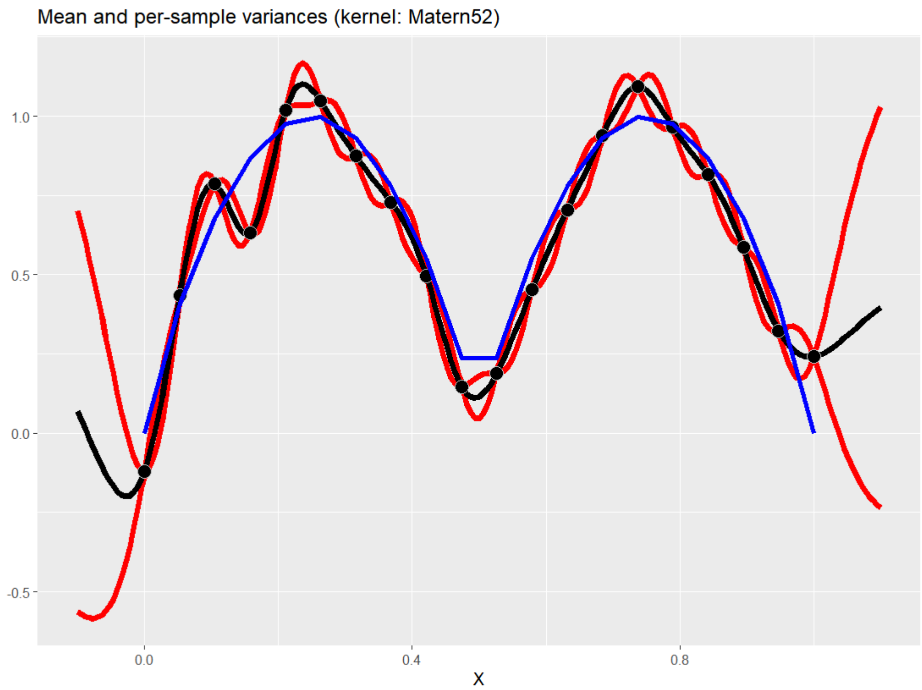


Figure 9: Plot of a Gaussian process using Matern 5/2 applied to the toy dataset.
The expected function deviates very slightly from datapoints compared to 3/2, but the big difference compared to 3/2 is in the variances. 5/2 has narrower variances than 3/2, producing smoother functions and functions that are closer to the expected function. SE is still better in this instance because it is the most smooth and our data-generating function is unusually smooth. However, 5/2 is generally the most popular covariance function because it achieves this parsimonious balance between smoothness, to still reach some reasonable approximation of the data-generating function, and flexibility, to still pass through the datapoints.

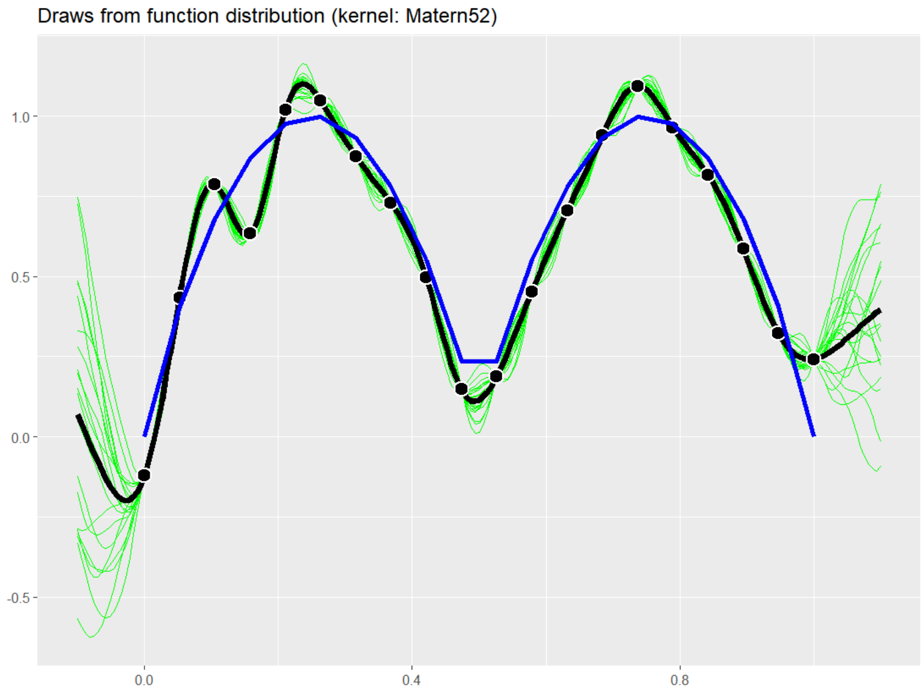
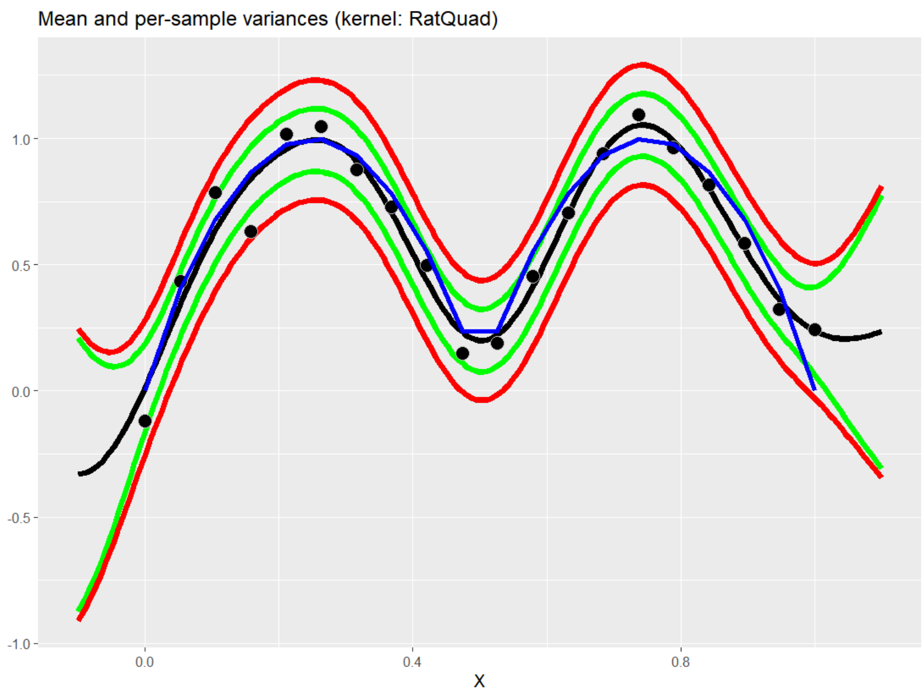


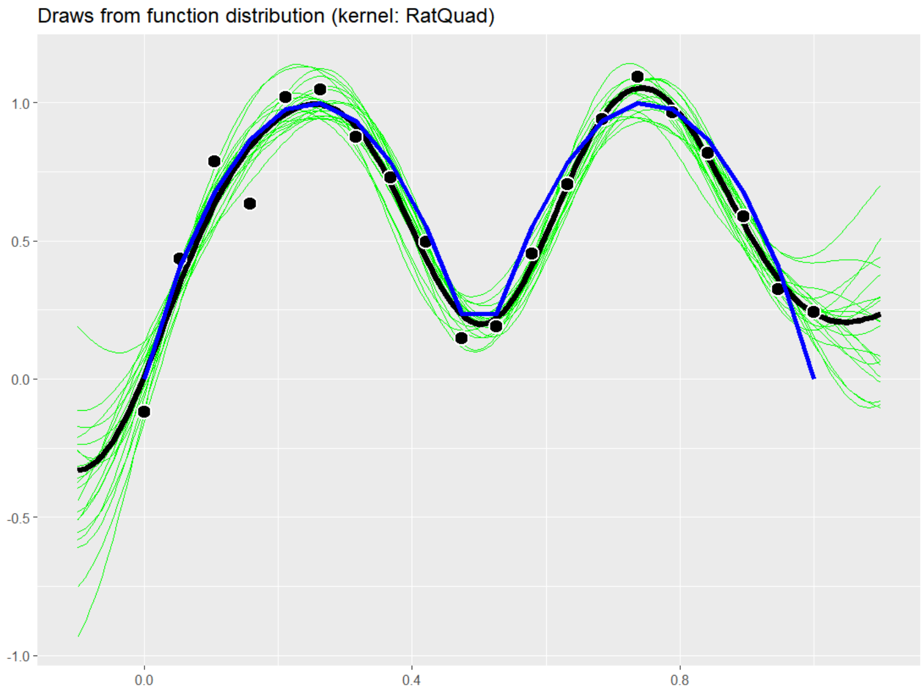
Figure 10: Plots of functions from a Gaussian process using Matern 5/2 applied to the same toy dataset. These sample function draws conform more to the expected function than 3/2 due to the narrower variances, but are still much rougher than SE and approach the data-points.

3.2.6 Rational quadratic

The rational quadratic can be seen as an infinite sum of SE with different length-scales.

TODO formulas





Draws from function distribution (kernel: RatQuad)
1.0
0.5
0.0
-0.5
-1.0
0.0
0.4
0.8

4 Computational Issues

4.1 Covariance function approximations using spectral density

4.1.1 Spectral density [4]

Bochner's theorem states that a complex-valued function is the covariance function of a

It can be shown [1] that the covariance function of a stationary process can be represented as the Fourier transform of a positive finite measure.

4.1.2 Speedups with spectral density [**foreman-mackay**]

4.2 Matrix inversion approximations [3]

Inverting the $[K(X, X) + \sigma_n^2 I]$ matrix in our predictive distribution scales poorly with the number of training data points n, as inverting the $n \times n$ matrix X that represents our training data is $O(n^3)$. Strategies to approximate the result of this inversion fall into two categories: those that produce a single approximation for the entire dataset, or those that produce several approximations that are "experts" in a particular region of the dataset and combine these local approximations to form a global approximation.

4.2.1 Global approximations

4.2.1.1 Subset-of-data The simplest strategy is to use a subset M of X to reduce the cost of inversion to $O(m^3)$, where m is the number of training points in M. Although this approach does not address the issues of matrix inversion directly,a theoretical graphon analysis proves that choosing M randomly gives an accuracy of $O(log^{-1/4}m)$ for the predictive mean and variance, which produces more accurate predictions with faster runtimes than sparse approximations as n increases. [2] Subset-of-data also requires no analytic assumptions about the kernel.

We can reduce m needed to achieve the same level of accuracy with a "greedy" approach by determining the gain in likelihood from including each data point x_i in X, adding the maximum gain in likelihood point to M and repeating until the size of M reaches m. However, computational savings from reducing m are smaller than the cost of searching X for these centroids $O(n^2m)$. Instead, we can use a "matching pursuit" approach - maintain a cache of the already precomputed kernel values, and use these to compute the gain in likelihood for each point in X in $O(nm^2)$ time. [**matching-pursuit**]

4.2.1.2 Sparse kernels A sparse kernel is a particularly designed kernel that imposes $k(X, X') = 0$ if $|X - X'|$ is larger than some threshold d to create a sparse covariance matrix. This reduces the number of calculations that need to be performed and computational complexity to $O(an^3)$, where a is the proportion of non-zero entries remaining, but the kernel needs to be carefully designed to work with zeroes and ensure all entries are positive definite to satisfy completeness. TODO sparse RBF

4.2.1.3 Sparse approximations TODO, missing background

4.2.1.3.1 Prior approximation

4.2.1.3.2 Posterior approximation

4.2.1.3.3 Structured sparse approximation

4.2.2 Local approximations

TODO

4.2.2.1 Naive-local-experts

4.2.2.2 Mixture-of-experts

4.2.2.3 Product-of-experts

4.2.3 Improvements

TODO

4.2.3.1 Scalability

4.2.3.2 Capability

5 Applying a Gaussian Process to Astrostatistics

5.1 Introduction

5.2 Methodology

5.2.1 Applying the Gaussian Process

5.2.2 Matrix inversion

5.2.3 Spectral density

5.3 Results

5.4 Discussion

5.5 Conclusion

6 Conclusion

References

[1] Iosif I Gikhman and Anatoli V Skorokhod. *The theory of stochastic processes I*. en. Classics in mathematics. Berlin, Germany: Springer, Mar. 2004.

[2] Kohei Hayashi, Masaaki Imaizumi, and Yuichi Yoshida. "On Random Subsampling of Gaussian Process Regression: A Graphon-Based Analysis". In: *Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics*. Ed. by Silvia Chiappa and Roberto Calandra. Vol. 108. Proceedings of Machine Learning Research. PMLR, 26–28 Aug 2020, pp. 2055–2065. URL: `https://proceedings.mlr.press/v108/hayashi20a.html`.

[3] Haitao Liu et al. "When Gaussian Process Meets Big Data: A Review of Scalable GPs". In: *IEEE Transactions on Neural Networks and Learning Systems* 31.11 (2020), pp. 4405–4423. DOI: `10.1109/TNNLS.2019.2957109`.

[4] Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning*. The MIT Press, Nov. 2005. ISBN: 9780262256834. DOI: `10.7551/mitpress/3206.001.0001`. eprint: `https://direct.mit.edu/book-pdf/2514321/book\_9780262256834.pdf`. URL: `https://doi.org/10.7551/mitpress/3206.001.0001`.