Explanation of Mathematical Methods Behind the First Half of the Project

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Introduction

What mathematical methods will I explain in this document?

- Gaussian processes
- Bayesian History Matching
- Kriging
- Expected Improvement
- Augmented Expected Improvement
- Knowledge Gradient
- K-Means Clustering

Context

We are building on the paper "Using history matching to speed up management strategy evaluation grid searches". This paper is looking to find the Harvest Control Rule parametrised by F_{target} and $B_{trigger}$ that maximises the catch whilst keeping the risk below 0.05 for a single-stock fishery. The paper does not consider fleet dynamics. We have an objective function in the paper which combines the risk and the catch and so this is the function we want to maximise to get our maximal catch with the constraint of keeping the risk below 0.05.

To do this, the paper takes a Bayesian History Matching (BHM) approach. Firstly, we sample our first eight points which are spaced evenly throughout the sample space to get some initial data. Then, for each round we do the following:

- We set up or update the Gaussian Process (GP) to model the risk and the GP to model the catch
- We can then use the risk as a threshold so that we only consider the values of F_{target} and $B_{trigger}$ that have risk below 0.05
- We use the GP which is modelling the catch to get the value for the catch at every point in the sample space, which will have some uncertainty
- We use BHM to remove any points that are implausible (that have a low probability of being higher than the current best catch)
- We select 8 plausible points to sample in the next round

We repeat this process until there is only one plausible point left and then we will accept this as being the F_{target} and $B_{trigger}$ that maximise the catch whilst keeping the risk below 0.05.

Now, we will look at the mathematics behind the methods above and also at the acquisition functions of Expected Improvement, Augmented Expected Improvement and Knowledge Gradient which I added to the original code.

General theory

Gaussian Processes

A Gaussian Process F has a mean function μ_0 and a covariance function $\text{cov}_0(x_i, x_j)$. We can then evaluate the covariance function $\text{cov}_0(x_i, x_j)$ for every pair x_i, x_j where $i, j \in \{1, \ldots, n\}$ to find the covariance matrix $\Sigma_{1:n}$. Then, F is a probability distribution over our objective function f with the property that, for any given collection of points $x_1, \ldots x_n$, the marginal probability distribution on $F(x_{1:n}) = (F(x_1), \ldots, F(x_n))$ is given by (Frazier 2018):

$$F(x_{1:n}) \sim N((\mu_0(x_{1:n}), \Sigma_{1:n}) \tag{1}$$

where

$$\mu_0(x_{1:n}) = (\mu_0(x_1), \ldots, \mu_0(x_n))$$

We choose a covariance function such that inputs that have nearby points that have been evaluated have a more certain output than points that are further away from the points that have been evaluated (Spence 2025). This is equivalent to saying that if for some x, x', x'' in the design space we have $\|x - x'\| < \|x - x''\|$ for some norm $\|\cdot\|$, then $\text{cov}_0(x, x') > \text{cov}_0(x, x'')$ (Frazier 2018).

We use a GP to emulate the objective function because it is much cheaper to evaluate than our objective function. We can calculate $F(x)$ for any x in the design space as our estimate of $f(x)$ based on our current beliefs. This is true even for the evaluated points $x_1, \ldots, x_m$ as the emulator is fitted to these points (Spence 2025).

Maximum Likelihood Estimation

When using GPs to emulate our objective function, we need to be able to estimate the coefficients of the objective function using the data we gain from evaluating our points $x_1, \ldots, x_n$ (Frazier 2018).

We can do this as follows. Firstly, we let the vector η represent the hyperparameters that give us μ_0 and cov_0. Then, given the observations $f(x_{1:n}) = (f(x_1), \ldots, f(x_n))$, we calculate the likelihood of these observations under the prior given η which is denoted as $p(f(x_{1:n})|\eta)$ which is modelled by Equation 1 . Lastly, we set $\hat{\eta}$ to the value that maximizes this likelihood Frazier (2018)]:

$$\hat{\eta} = argmax_\eta p(f(x_{1:n})|\eta)$$

Kriging

Kriging is a Bayesian statistical method for modelling functions (Frazier 2018). Again, let f be the objective function and we focus on the design space $X := \{x_1, \ldots, x_n\}$. Now, if we have evaluated n points such that we have $f(x_{1:n})$ and want to evaluate x_{n+1} we let $k = n + 1$ in Equation 1 . Then, we can compute the conditional distribution of $F(x_{n+1})$ given $f(x_{1:n})$ using Bayes' rule:

$$F(x_{n+1})|f(x_{1:n}) \sim N(\mu_n(x_{n+1}), \sigma_n^2(x_{n+1})) \tag{2}$$

where:

$$\mu_n(x_{n+1}) = \text{cov}_0(x_{n+1}, x_{1:n})(\Sigma_{1:n})^{-1}(f(x_{1:n}) - \mu_0(x_{1:n})) + \mu_0(x_{n+1})$$

$$\sigma_n^2(x_{n+1}) = \text{cov}_0(x_{n+1}, x_{n+1}) - \text{cov}_0(x_{n+1}, x_{1:n})(\Sigma_{1:n})^{-1}\,\text{cov}_0(x_{1:n}, x_{n+1})$$

where:

$$\text{cov}_0(x_{n+1}, x_{1:n}) = (\text{cov}_0(x_{n+1}, x_1), \ldots, \text{cov}_0(x_{n+1}, x_n))$$

This conditional distribution $F(x_{n+1})|f(x_{1:n})$ is called the posterior probability distribution for x_{n+1}. We can calculate this distribution for every point in the design space X. This results in a new GP F_n with a mean vector and covariance kernel that depend on the location of the unevaluated points, the locations of the evaluated points $x_{1:n}$ and their values $f(x_{1:n})$(Frazier 2018). So, we can update our GP every round based on the new

points $x_{1:n}$, and their values $f(x_{1:n})$(Frazier 2018). So, we can update our GP every round based on the new points we have evaluated.

Bayesian History Matching

Let x be a point in the sample space. We begin with some uncertainty about our objective function $f(x)$ (Spence 2025). However, we can make probabilistic statements such as:

$$P(f(x) > a) = \int_a^\infty P(f(x))df(x)$$

Once we evaluate another point x' where $x' \neq x$, we are able to use Bayes' Theorem improve our integral to:

$$P(f(x) > a|f(x')) = \int_a^\infty P(f(x)|f(x'))df(x)$$

We now let $a = max\{f(x_1), \ldots, f(x_n)\}$ where n is the number of points we have evaluated so far. For the first round, $n = 8$ but as the rounds increase we make sure to include all previous points of the objective function that have been evaluated.(Spence 2025) We remove the point x if:

$$P(f(x) > a|f(x_{1:n}) = \int_a^\infty P(f(x)|f(x_{1:n})df(x) < \varepsilon \tag{3}$$

for a small $\varepsilon > 0$ until no plausible points remain. Then, the optimum will be x^* such that:

$$f(x^*) = max\{f(x_{1:n})\}$$

as our index n counts the number of points we have evaluated throughout the whole simulation.

Expected Improvement

The first type of acquisition function we will look at is Expected Improvement (EI). Suppose we have sampled the points $x_1, \ldots, x_n$ and observe the values $f(x_{1:n})$. Then, if we were to return a solution at this point, bearing in mind we observe the objective function f without noise and we can only return points we have already evaluated, we would return $f_n^* = max\{f(x_1), \ldots, f(x_n)\}$ (Frazier 2018). Imagine we then consider evaluating another point x_{n+1} to get $f(x_{n+1})$. We can then define the Expected Improvement as:

$$EI_n(x_{n+1}) := E[F(x_{n+1})|f(x_{1:n}) - f_n^*]^+$$

where $[F(x_{n+1}) - f_n^*]^+$ is the positive part of $[F(x_{n+1}) - f_n^*]$. This acquisition function is relatively easy to optimise and many different methods have been developed for doing this (Frazier 2018).

There is another expression for $EI_n(x_{n+1})$:

$$EI_n(x_{n+1}) = [(\mu_n(x_{n+1}) - f_n^* \cdot \Phi(Z)) + (\sigma_n(x_{n+1}) \cdot \phi(Z))]^+ \tag{4}$$

where again the notation $[\cdot]^+$ means the positive part and where:

$$Z = \frac{\mu_n(x_{n+1}) - f_n^*}{\sigma_n(x_{n+1})}$$

Equation 4 can be gained from Equation 1 by setting $k = n + 1$ and then studying the distribution of $F(x_{n+1}) - f_n^*$. However, we can also consider it as a version of Equation (15) from (Jones, Schonlau, and Welch 1998) where we first flip the signs as we are focused on the maximisation case and then set $f_{min} = f_n^*$, $\hat{y} = \mu_n(x)$ and $s = \sigma_n(x)$.

Augmented Expected Improvement

This was included to help make the method perform better for noisy functions which will make it more generally applicable (Huang et al. 2006). To deal with these noisy observations, a change was proposed to standard EI function as detailed below. This change seems mostly to have been justified by empirical performance (Letham et al. 2018).

By adjusting Equation (12) found in (Huang et al. 2006) to our own notation, we get that:

$$AEI_n(x_{n+1}) = E_n[F(x_{n+1})|f(x_{1:n}) - f^*_{eb}]^+ \left(1 - \frac{\sigma_{obs}}{\sqrt{\sigma^2_n(x_{n+1}) + \sigma^2_{obs}}}\right)$$

where σ_{obs} is the standard deviation of the noise variable set by the user and $\sigma_n(x)$ is the standard deviation of GP F at the n^{th} iteration, as used beforehand. We have also changed f^*_n to f^*_{eb} which is the highest predicted mean at any sampled point so far so that we take into account that the uncertainty in our observations could cause a large spike (Huang et al. 2006).

Knowledge Gradient

We remove the assumption of EI that we have to return a pre-evaluated point as our best point (Frazier 2018). This allows us to do some different computations to the ones in EI. We also now start by saying that the solution we would choose if we have to stop sampling after n points would be the point in the design space with the largest $\mu_n(\cdot)$ value, where $\mu_n(\cdot)$ is the mean vector of the posterior probability distribution after n iterations. We call this maximum x^*_n and then can say that $F(x^*_n)$ is random under the posterior distribution and has the mean vector after sampling $f(x_{1:n})$ of:

$$\mu^*_n := \mu_n(x^*_n) = max_x \mu_n(x)$$

where x is any point in the sample space (Frazier 2018).

Then, we imagine that we are now allowed to sample a new point x_{n+1}. We get a new posterior distribution at the point x which we can calculate using Equation 2 by replacing x_{n+1} with x and $x_{1:n}$ with $x_{1:n+1}$ to include our new observation. This will have the posterior mean function $\mu_{n+1}(\cdot)$ and the conditional expected value for $F(x^*_n)$ changes to be:

$$\mu^*_{n+1} := max_x \mu_{n+1}(x)$$

So, we can see that the increase in the conditional expected value of $F(x^*_n)$ by sampling the new point x_{n+1} is (Frazier 2018):

$$\mu^*_{n+1} - \mu^*_n$$

While this quantity is unknown before we sample x_{n+1} we can calculate it's expected value given our observations $x_1, \ldots, x_n$. The Knowledge Gradient for sampling at a new point x in the design space is defined as (Frazier 2018):

$$KG_n(x) := E_n[\mu^*_{n+1} - \mu^*_n | x_{n+1} = x] \tag{5}$$

where again E_n indicates the expectation taken under the posterior distribution at the n^{th} iteration. We would sample the point x with the largest $KG_n(x)$ as our next point (Frazier 2018).

The easiest way to calculate the KG is via simulation. This can be done by simulating one possible value for $f(x_{n+1})$. Then, we calculate μ^*_{n+1} and subtract μ^*_n. We iterate this process many times so that we can find the average of $\mu^*_{n+1} - \mu^*_n$ and this allows us to estimate $KG_n(x)$ (Frazier 2018). This process, or calculating Equation 5 directly from the properties of the normal distribution, both work well in discrete, low dimensional problems which is the situation we are in for the first half of the project (Frazier 2018).

Alternatively, we can calculate μ_{n+1} using the formula below (Ungredda, Pearce, and Branke 2022):

$$\mu_{n+1}(x) = \mu_n(x) + \frac{\mathrm{cov}_n(x_{n+1}, x)}{\mathrm{var}_n(x_{n+1}) + \sigma^2_{\mathrm{obs}}}(F(x_{n+1}) - \mu_n(x_{n+1})) \tag{6}$$

where σ_{obs} is a noise variable which can be determined by the user (Ungredda, Pearce, and Branke 2022). From the GP for catch, we get $\mathrm{cov}_n(x_{n+1}, x)$ and the standard deviation σ^2_{obs}.

Kmeans process for selecting multiple points

HIGHLIGHT THAT COMBINING THIS WITH AN ACQUISITION FUNCTION WAS AN IDEA I HAD BEFORE READING ANY LITERATURE ON IT (AS I THINK THERE IS SOME). - NOT QUITE SURE HOW TO DO THIS, ASK GUSTAV ON TUES

We have now been able to determine which points are possible based on the probability that their catch is higher than the current maximum catch (using Bayesian History Matching) and the probability that their risk is less than 0.05. These points will be called the Possible Space, PS. We have then assigned a value to each point in PS using one of the acquistion functions above. Now, we want to decide which 8 points are best to evaluate next.

For sampling only one point next, this would be very simple as you would take the point with the highest value assigned by the acquisition function (Frazier 2018). However, we want to sample 8 points next so that we continue the pattern set up in the original paper and we want a good trade-off between exploration and exploitation (Spence 2025),(**batchspreadinoutjustification?**).

So, we use the `kmeans` function which is part of the stats package in R (which is automatically loaded into an R session). This function uses the algorithm from Hartigan and Wong, 1979 by default(Hartigan and Wong 2018), (RDocumentation 2025). The k-means clustering method is the most commonly used due to its simplicity compared to other clustering algorithms(Kodinariya, Makwana, et al. 2013.)

This algoritm creates k clusters (groups of points) such that the points within each cluster have the sum of squares to the centre of their cluster smaller than it would be to the centre of any other cluster (RDocumentation 2025). It starts by defining k centroids which should be placed as much as possible far away from each other (Kodinariya, Makwana, et al. 2013). Then, we take each point in the space and associate it to the nearest centroid. We stop when every point has been assigned to a centroid (Kodinariya, Makwana, et al. 2013). At this point, we re-calculate k new centroids as the centers of the clusters created by the previous step. This may result in some points changing clusters (Hartigan and Wong 2018). We repeat this process until no points change clusters (Hartigan and Wong 2018),(Kodinariya, Makwana, et al. 2013).

However, before the algorithm can start, we must specify how many clusters we want (Kodinariya, Makwana, et al. 2013). This can be difficult in many cases (Kodinariya, Makwana, et al. 2013). In our case, it is relatively simple as we know how many points we want to sample next and so we set this to be the number of clusters. We then run the algorithm on PS to form the clusters. Then, we pick the point with the highest value of the acquisition function from each cluster to sample in our next round. This allows us to search for viable points by looking in the Possible Space but also to keep the points we are going to sample spread out so that we can balance exploitation and exploration more effectively (Azimi, Fern, and Fern 2010).

Application of theory in my project

Set up the Gaussian Processes

We are focusing on maximising the objective function from the paper which is given below (Spence 2025):

$$f(\theta) = I_{[0.95,1]}(P(B(\theta) > B_{lim})) \times C(\theta)$$

where $C(\theta)$ is median long term catch, $B(\theta)$ is long-term SSB and:

$$I_{[0.95,1]}(x) = \begin{cases} 1 & \text{if } x \in [0.95, 1] \\ 0 & \text{otherwise} \end{cases}$$

is an indicator function.

To do this, Spence uses two GPs where the risk GP models $ln(risk)$ and the catch GP models $ln(catch)$ (Spence 2025). Maintaining the notation from the Spence 2025 paper, we use m_1 for the mean function of the catch GP and m_2 for the mean function of the risk GP (Spence 2025):

$$m_1(\phi) = \beta_{1,0} + \beta_{1,1}(\ln(\phi_1 + 0.1)) + \beta_{1,2}(\ln(\phi_1 + 0.1))^2 + \beta_{1,3}(\ln(\phi_1 + 0.1))^3 + \beta_{1,4}(\phi_2 \ln(\phi_1 + 0.1)) + \beta_{1,5}\phi_2$$

$$m_2(\phi) = \beta_{2,0} + \beta_{2,1}\phi_1 + \beta_{2,2}\phi_2 + \beta_{2,3}\phi_1\phi_2$$

where all of the above $\beta_{s,t}$ for $s \in \{1, 2\}$ and $t \in \{1, 2, 3, 4, 5\}$ are coefficients to be found through maximum likelihood estimation and:

$$\phi_1 = \frac{F_{target} - 0.1}{0.4} \quad \text{and} \quad \phi_2 = \frac{B_{trigger} - 110000}{90000}$$

where we rescale for numerical stability in the GP (Spence 2025).

Our covariance function c for both GPs is the variance σ_i^2 (which is acting as a scalar) times the Ornstein-Uhlenbeck correlation function (Spence 2025):

$$r_i(\phi, \phi', \delta_i) = \exp\left(-\frac{|\phi_1 - \phi_1'|}{\delta_{i,1}} - \frac{|\phi_2 - \phi_2'|}{\delta_{i,2}}\right)$$

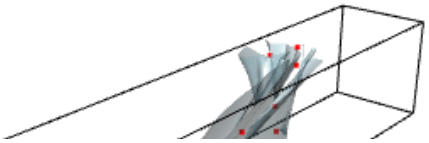
where $\delta_{i,1}$ and $\delta_{i,2}$ are the length scales for each of the ϕ_1 and ϕ_2 terms respectively (**williams2006gaussian?**).

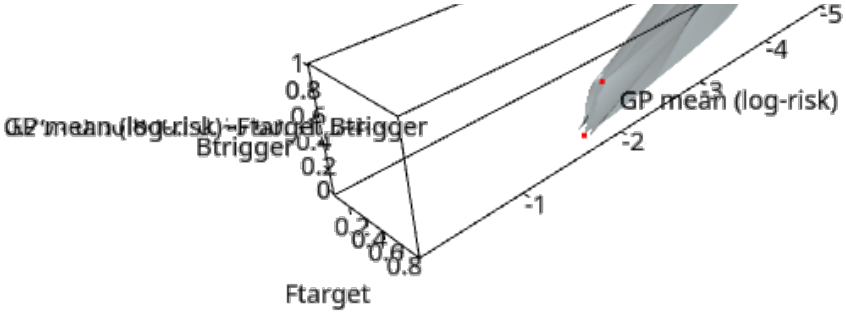
We need to sample our first round of eight points before setting up the GPs so that we have enough data to estimate all of the coefficients in our GPs (Jones, Schonlau, and Welch 1998). Note that until we have sampled sixteen points, we set the prior of the catch GP to be the same as the risk GP, $m_2(\phi)$ (Spence 2025). This is because we need to estimate the coefficients for the mean function for the catch, risk and the length scales for the covariance function c (Jones, Schonlau, and Welch 1998),(Roustant, Ginsbourger, and Deville 2012). For mathematical stability, these functions cannot have more than eight coefficients between them in our first round as we are only sampling eight points per round due to computation limitations encountered at the time of the Spence 2025 paper (Jones, Schonlau, and Welch 1998),(Spence 2025). However, after our first round we reset the mean function for the catch GP to $m_1(\phi)$ (Spence 2025).

We can set up Gaussian Processes (GPs) as described above in R using the DiceKriging package and use maximum likelihood estimate to get the hyperparameters of $m_1(\phi), m_2(\phi)$ and c for our GPs (Roustant 2025), (Roustant, Ginsbourger, and Deville 2012). Then, we use them to predict the $ln(catch)$ and $ln(risk)$ at every point in the design space. We can then exponentiate these results where needed. We are building our GPs with ln of the values we want because this helps us generate better predictions (Huang et al. 2006).

We have been able to visualise the GPs after the first round in 3D:

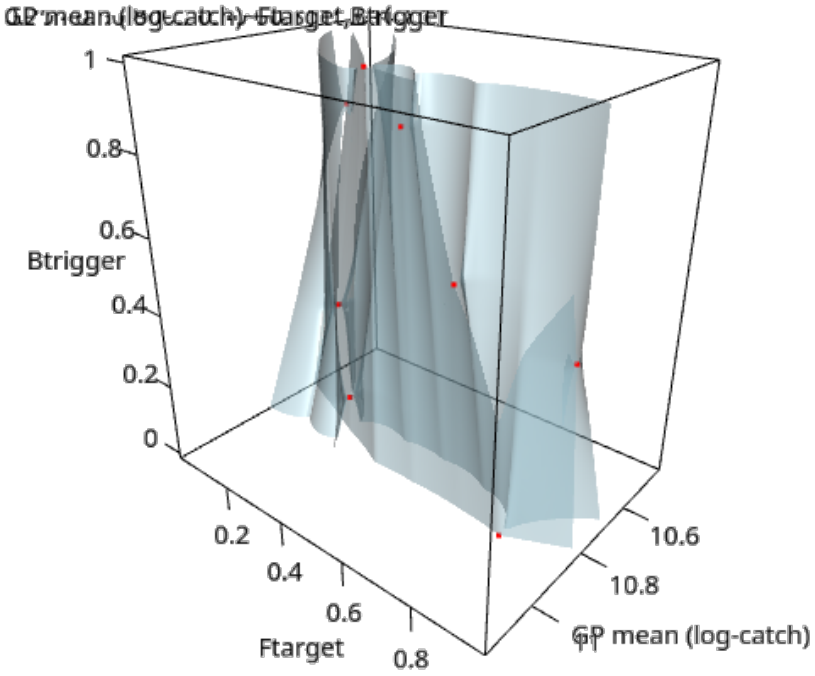
```
This build of rgl does not include OpenGL functions.  Use
 rglwidget() to display results, e.g. via options(rgl.printRglwidget = TRUE).
```





The middle plane is the mean of the GP, whereas the bottom and top planes represent the lower and upper bounds of the 95% confidence interval respectively. The planes meet at the evaluated points, which are the red dots on the diagram. The scales are odd due to the re-scaling of F_{target} and $B_{trigger}$ and fitting our GPs to log of the values we want throughout the code which helps to keep the GP stable (Huang et al. 2006).

We can then also do this for the GP for catch:



Excluding implausible points

Firstly, we enforce the precautionary threshold by calculating $P(ln(risk) \leq 0.05)$. We exclude these points by setting their value of the acquisition function to 0 so that they will not be chosen as a point to sample in the next round.

Then, we use Bayesian history matching to speed up the process by removing any points that are implausible according to Equation 3. In our case, x^* is the F_{target} and $B_{trigger}$ that will give the highest catch whilst following the precautionary principle (Spence 2025).

Deciding on next point to sample

We have three different acquisition functions we have investigated using here..

Expected Improvement

We use the Equation 4 expression and calculate the EI for every point in the sample space, setting those that don't meet the precautionary threshold to zero as explained above.

Augmented Expected Improvement

As our situation has no noise, in our code we are still using f_n^* (Spence 2025). Thus, we use the equation:

$$AEI_n(x_{n+1}) = EI_n(x_{n+1}) \left(1 - \frac{\sigma_{obs}}{\sqrt{\sigma_n^2(x_{n+1}) + \sigma_{obs}^2}}\right)$$

calculate the AEI for every point in the sample space. We again make sure to set any points not meeting the precautionary threshold to have AEI = 0.

Knowledge Gradient

We estimate the KG from 100 simulations and update the KG each round using Equation 6 . As in the other acquisition functions, we make sure to set the value to zero for any point in the sample space not meeting the precautionary threshold.

Kmeans process

To then make sure that the next points we sample are spread out across the sample space, we use the Kmeans process (Azimi, Fern, and Fern 2010). We create eight clusters and note the point with the highest value of the acquisition function in each cluster. These are the points we will sample in the next round.

Updating our GPS

In our second round, we need to update our GPs with new data (Spence 2025). We do this by adding in the data for the points that have been newly evaluated this round. Hence, we can do the calculations from the Kriging section to update the GP with a new mean vector and covariance kernel for our next round. - CHECK SITLL IN KRIGING SECTION For the catch GP, we move on to using $m_1(\phi)$ from the second round onwards because by the time we create this GP we have sampled 16 points(Spence 2025).

Now, we repeat the full process described in the Application of theory in my project section until there are no points with a positive KG. Then, the optimal point is the x^* that has the highest catch out of the precautionary points.

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