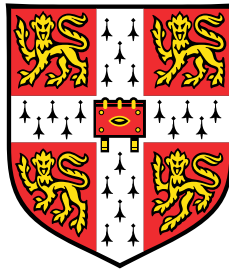


# **Analysing and Maximising the Effectiveness of Test, Trace, and Isolate Strategies**

Machine Learning and the Physical World - **Group Project**



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## Abstract

The Test, Trace, and Isolate (TTI) explorer (`tti-explorer`) is a model used to simulate the spread of COVID-19 infection in the UK, given various TTI strategies and non-pharmaceutical interventions (NPIs). This report seeks to analyse the magnitude of effect of various TTI strategies and NPIs on the effective reproduction number (effective  $R$ ) of the disease and to derive optimal policies for containing the outbreak. These objectives were achieved by employing sensitivity analysis and optimisation methods on the `tti-explorer` simulator. Specifically, we used global sensitivity analysis methods, amounting to grid and axis variations, to analyse the impact of each factor in isolation; and the analysis of variance (ANOVA) decomposition using the Gaussian process emulator, to examine the overall impact of all factors, considering the interactions between them. We show that the Gaussian process emulator enables rapid computation of ANOVA decomposition, thus allowing us to present a more complete sensitivity analysis result that complement prior work in the COVID-19 domain. Subsequently, we used random search, unconstrained Bayesian optimisation, and constrained Bayesian optimisation to derive an optimal policy for slowing the spread of the virus. We demonstrate the superiority of Bayesian optimisation-based approaches over the random search, as they obtained more optimal and sensible policies much faster.

## Codes

The codes written in Python is available at: <https://github.com/maleakhiw/gaussian-processes-tti-explorer>.

# Contents

<b>1</b>	<b>Introduction</b>	<b>4</b>
<b>2</b>	<b>Experimental Setup and Design Choices</b>	<b>4</b>
2.1	Simulator . . . . .	4
2.2	Sensitivity Analysis Factors . . . . .	5
2.3	Policy Optimisation Factors . . . . .	6
<b>3</b>	<b>Sensitivity Analysis</b>	<b>7</b>
3.1	Grid and Axis Variation . . . . .	7
3.2	Analysis of Variance Decomposition . . . . .	13
3.2.1	Background . . . . .	13
3.2.2	Experiment Results . . . . .	13
3.3	Causal Analysis . . . . .	16
<b>4</b>	<b>Policy Optimisation</b>	<b>17</b>
4.1	Unconstrained Optimisation . . . . .	18
4.1.1	Random Search . . . . .	18
4.1.2	Bayesian Optimisation . . . . .	19
4.2	Ablation Studies . . . . .	21
4.3	Constrained Optimisation . . . . .	23
<b>5</b>	<b>Conclusion</b>	<b>24</b>
<b>6</b>	<b>Appendices</b>	<b>25</b>

# 1 Introduction

The COVID-19 pandemic has presented a significant challenge to policymakers. The SARS-CoV-2 virus is difficult to control due to its high reproduction rate, high asymptomatic rate, and frequent unavoidable occurrences of super-spreading events [3, 8, 18]. During the initial stages of the outbreak, policymakers could rely on standard, less strict strategies, such as test-trace-isolate (TTI) strategies and COVID-19 health protocols [19, 27]. Nevertheless, the epidemic continues to escalate, necessitating other strict non-pharmaceutical interventions (NPIs), such as school closures and working from home. Studies have shown that despite the need for a strict policy to slow the spread of the virus, such a policy may cause significant disruption to societies (e.g., psychological distress and mental health problems [6, 13, 26]) and to the country’s economy [1]. Therefore, it is crucial for policymakers to develop policies that balance effectiveness and strictness.

This report has two primary objectives. Firstly, to evaluate the magnitude of effect of various TTI strategies and NPIs on the effective reproduction number (effective  $R$ ) of the disease – that is, the average number of secondary cases per infectious case in a population comprising both susceptible and non-susceptible hosts [14]. Secondly, it aims to derive an optimal policy that has the greatest effect on the reduction of effective  $R$ , while considering available resources and restrictions (e.g., number of tests needed [7], the inability of essential workers to work from home [4]). We implemented various global sensitivity analysis methods, amounting to grid and axis variations that analyse factors in isolation, and analysis of variance (ANOVA) decomposition, which analyses factors while considering the interactions between them. Subsequently, we implemented random search, unconstrained Bayesian optimisation, and constrained Bayesian optimisation for the policy optimisation problem. Both sensitivity analysis and policy optimisation methods are applied on the simulator, `tti-explorer` [12, 27], a model used to simulate the spread of COVID-19 infection in the UK given various TTI strategies and NPIs as parameters.

The remainder of the report is organised as follows. Section 2 describes the assumptions and setup of the experiments. Section 3 discusses global sensitivity analysis and causal analysis results. Section 4 presents optimal policies obtained by various optimisation methods. It then compares the performance of different optimisation methods, identifying their strengths and weaknesses. Finally, Section 5 summarises the main findings of the study.

## 2 Experimental Setup and Design Choices

This section describes `tti-explorer` and how it was adapted for the experiments. Subsequently, it lists and defines important factors considered in both the sensitivity analysis and policy optimisation experiments.

### 2.1 Simulator

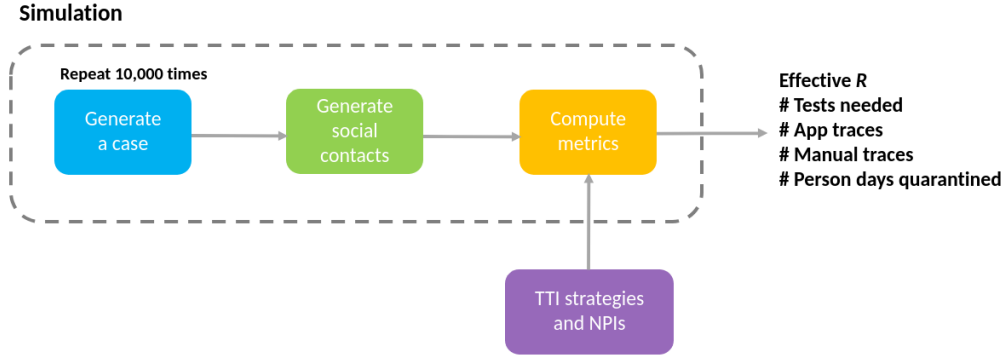
The simulator, `tti-explorer` was developed by Kucharski et al. [12] and He et al. [27] to simulate the spread of COVID-19 in the UK, given various parameter configurations related to different TTI strategies and NPIs as inputs. Each time a simulation is run, the simulator performs three main steps, visualised in Figure 1.

1. The first step involves generating initial cases. Each case describes an individual that can be under or over 18, COVID positive or negative, and with or without symptoms, based

on configured probability distributions. In the experiments, we generated 10,000 initial cases.

2. The next step generates social contacts for each initial case. To select the number of contacts, the simulator samples the BBC Pandemic dataset [11], which contains the number of daily contacts in different situations collected from UK volunteers.
3. Finally, given a particular strategy (e.g. test-based TTI with NPI of stringency level S3), each case is passed through the simulator, which computes various metrics, including the effective  $R$ , number of tests needed, number of app traces, number of manual traces, and number of person days quarantined<sup>1</sup>. The results of each case are then collected and averaged to return the output of the simulator.

The simulator is treated as a function that maps strategy inputs to the aforementioned output metrics. These functions are then approximated using Gaussian process surrogate models for several experiments described in Sections 3 and 4.



**Figure 1:** The three main steps of the simulation: generate cases, generate social contacts, and compute required metrics given a particular strategy.

## 2.2 Sensitivity Analysis Factors

We identified 13 parameters that strongly influence the effective  $R$  and can be used to influence decision-making and inform policies [9]. The parameters are grouped into **general factors**, **policy factors**, and **compliance factors** (listed in Table 1).

**General factors** The general factors contain variables that provide an overarching view of the simulation. These include the probability of being under 18 ( $p_{\text{under18}}$ ) and secondary attack rates (SARs) ( $\text{home\_sar}$ ,  $\text{work\_sar}$ ,  $\text{other\_sar}$ ). These provide insights into how the general properties of a population affect the effective  $R$ .

**Policy factors** The policy factors are variables that can be influenced through policy-making. They include the proportion of adults working from home ( $\text{wfh\_prob}$ ), maximum social contacts ( $\text{max\_contacts}$ ), and quarantine length ( $\text{quarantine\_length}$ ). Policy factors provide insights into the success of different policies at preventing the spread of the virus.

<sup>1</sup>Full list of output metrics are described in [27].

**Compliance factors** Finally, compliance factors are proxy variables that capture human behaviour, such as the level of compliance (`compliance`) and tracing application coverage (`app_cov`). They provide an insight of policy limitations due to human behaviour.

	Variables
<b>General Factors</b>	<code>p_under18</code>
	<code>home_sar</code>
	<code>work_sar</code>
	<code>other_sar</code>
<b>Policy Factors</b>	<code>wfh_prob</code>
	<code>go_to_school_prob</code>
	<code>max_contacts</code>
	<code>quarantine_length</code>
	<code>testing_delay</code>
	<code>manual_trace_delay</code>
	<code>app_trace_delay</code>
<b>Compliance Factors</b>	<code>compliance</code>
	<code>app_cov</code>

**Table 1:** Grouping of factors into three different groups: general, policy, and compliance factors. A detailed description of each parameter is presented in Table 6.

### 2.3 Policy Optimisation Factors

For the optimisation task we selected all parameters influenceable through policymaking. In total this was 14 policy parameters (set out in Table 2) that capture the functional essence of the variable groups set out in Section 2.2. Notably, there are several parameters which cannot be affected via policies. For example, SARs are more related to the infectiousness of a viral strain. Consequently, these parameters are excluded.

Variables	Type
<code>go_to_school_prob</code>	<i>Float</i> , range:[0,1]
<code>wfh_prob</code>	<i>Float</i> , range:[0,1]
<code>isolate_individual_on_symptoms</code>	<i>Boolean</i> , range: [True, False]
<code>isolate_individual_on_positive</code>	<i>Boolean</i> , range: [True, False]
<code>isolate_household_on_symptoms</code>	<i>Boolean</i> , range: [True, False]
<code>isolate_household_on_positive</code>	<i>Boolean</i> , range: [True, False]
<code>isolate_contacts_on_symptoms</code>	<i>Boolean</i> , range: [True, False]
<code>isolate_contacts_on_positive</code>	<i>Boolean</i> , range: [True, False]
<code>test_contacts_on_positive</code>	<i>Boolean</i> , range: [True, False]
<code>do_symptom_testing</code>	<i>Boolean</i> , range: [True, False]
<code>do_manual_tracing</code>	<i>Boolean</i> , range: [True, False]
<code>do_app_tracing</code>	<i>Boolean</i> , range: [True, False]
<code>max_contacts</code>	<i>Integer</i> , range: [1,20]

quarantine_length	<i>Integer</i> , range: [0,14]
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**Table 2:** List of variables used for optimisation in Section 4. A detailed description of each parameter is presented in Table 7.

### 3 Sensitivity Analysis

This section details the global sensitivity analyses conducted to evaluate the magnitude of each parameter effect on the effective  $R$ . We performed two sets of analysis: one analysing the effect of each variable in isolation and another that included the interactions between them. In addition to effective  $R$ , we measured the variables’ impacts on the number of tests needed, number of app traces, number of manual traces, and number of person days quarantined. These analyses serve as a basis for determining resources that could be limited in practice, thus helping to identify factors to target during policy optimisation in Section 4. We also performed causal analysis by intervening directly in the simulator to understand the causal relationships between variables.

#### 3.1 Grid and Axis Variation

The grid and axis variation are two simple strategies that can be used to perform global sensitivity analysis [17]. Grid variation refers to trying all possible combinations of parameters in the group to determine their contributions. Conversely, axis variation refers to trying one parameter at a time, while keeping all remaining parameters fixed. Both methods are used to measure the impact of a parameter on a function in isolation, as they cannot detect interactions between parameters [2]. Section 3.2 extends the experiments by considering more parameters, while also considering the interactions between them.

We selected several parameters to conduct sensitivity analysis, following the grouping and reasoning discussed in Section 2. From Table 1, we selected nine parameters to vary in order to analyse their impacts on the effective  $R$ : `p_under18`, `home_sar`, `work_sar`, `other_sar`, `wfh_prob`, `go_to_school_prob`, `max_contacts`, `compliance`, and `app_cov`. The simulations were conducted five times for each experiment and we reported the mean and 95% confidence interval.

**Age** We varied `p_under18` from 0.0 (all working adults) to 1.0 (all school-going children) to investigate how age affects the effective  $R$ . The results are plotted in Figure 2. Generally, we observed that age plays an important role in influencing the disease’ effective  $R$ . Specifically, the higher the `p_under18` (higher population of school-going children), the lower the effective  $R$ . Further observation on the BBC Pandemic dataset suggests that this phenomenon is caused by the vast difference in the number of social interactions of under 18 individuals compared to working adults. Social interaction of individuals under 18 is primarily restricted to household members and schoolmates, while working adults come into contact with more individuals, for example when meeting clients, travelling for work, and socialising with friends. This relationship holds for different strictness environments, suggesting that age is an important parameter.

**Work from home** We varied `wfh_prob` from 0.0 (all working adults work from the office) to 1.0 (all working adults work from home) to evaluate how a work from home policy impacts the

spread of COVID-19. Figure 2 shows a strong negative linear relationship between `wfh_prob` and effective  $R$  at all five strictness levels of NPIs (S1-S5). Particularly, we observed a maximum reduction of 44% in the effective  $R$ , suggesting that a strict work-from-home policy is effective at containing the pandemic.

**Go to school** Considering the previous result, it is unsurprising that `go_to_school_prob` also affects the effective  $R$ . Indeed, Figure 2 depicts a positive linear relationship between `go_to_school_prob` and the effective  $R$ . We observed a maximum increase of 17% in the effective  $R$ . In Section 3.2, we observed that the hidden variable is the number of contacts with which each individual comes into contact. Going to school increases the number of contacts, which in turn results in a more drastic rise in the effective  $R$ .

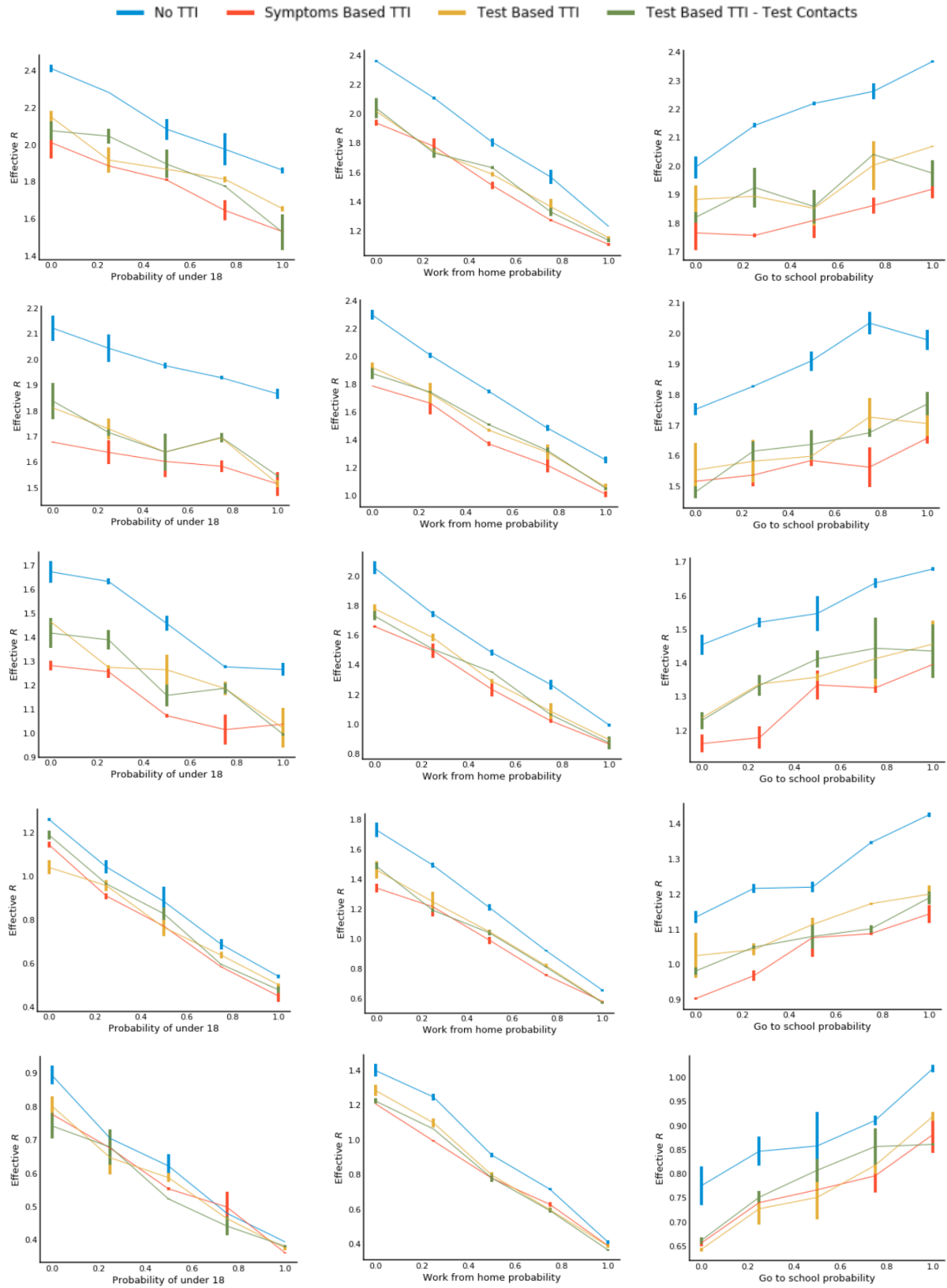
**Secondary attack rates** We varied `home_sar`, `work_sar`, and `other_sar` from 0.0 (no secondary attack) to 0.5 (50% probability of secondary attacks given a positive case). Figure 3 shows a positive linear relationship between all SARs variables and the effective  $R$  for all five levels of governmental measures (S1-S5). We observed that `work_sar` had the greatest effect, followed by `other_sar`, and `home_sar`. The phenomenon makes sense as there are more social contacts at work than at home or in other places.

**Maximum contacts** Since the previous analyses suggest that the number of social contacts plays a large role in containing the virus, we varied the `max_contacts` from 2 to 20. We observed a positive linear trend between it and the effective  $R$ , thus agreeing with the previous analyses, as shown in Figure 4. Further analysis showing the importance of limiting contacts is presented in Section 3.2.

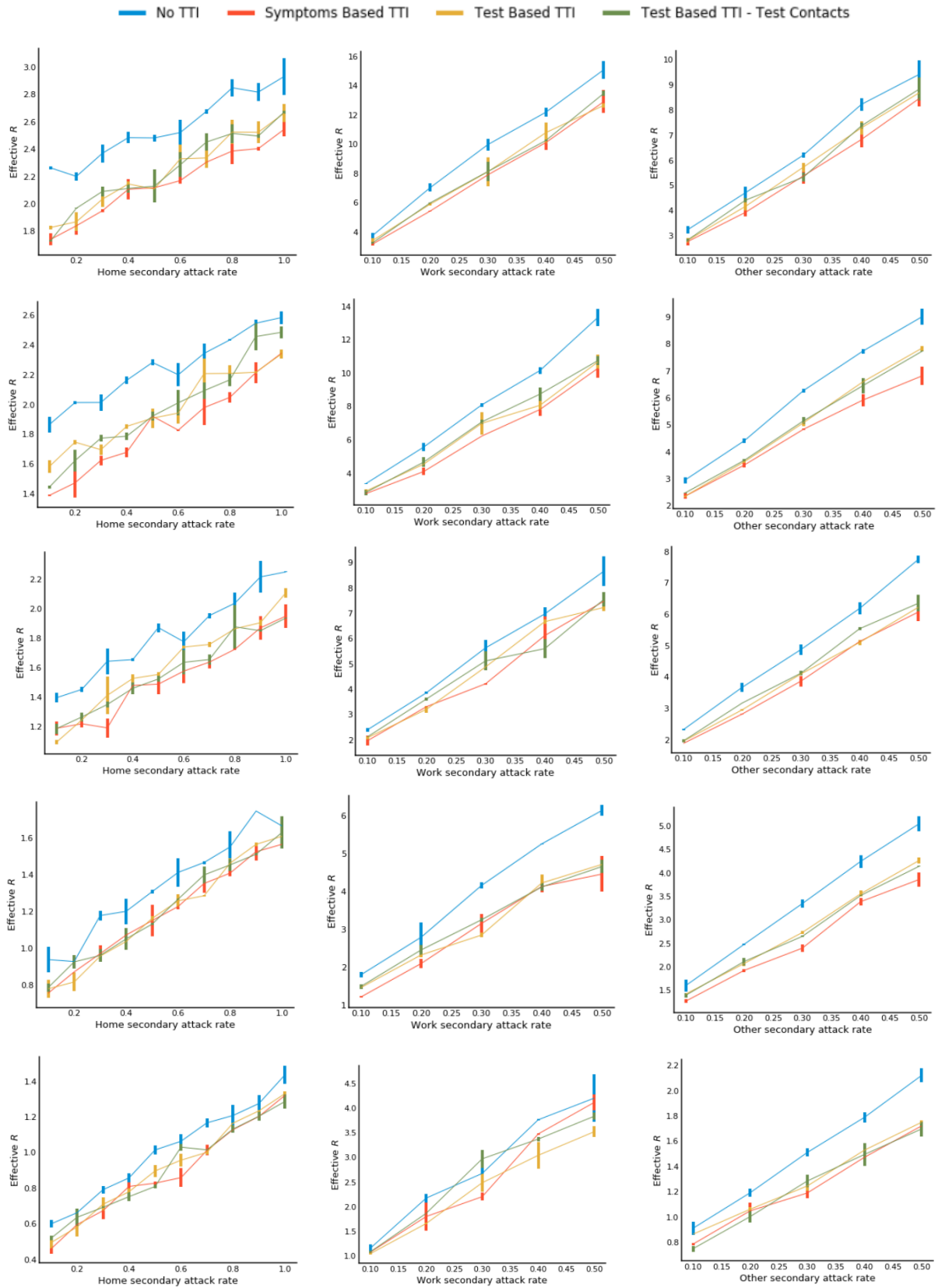
**Compliance** Naturally, the more likely a person is to comply with rules and regulations, the lower the effective  $R$ . Even in the least strict policy scenario (S1), we see that a 90% compliance level helps reduce effective  $R$  by 25% in the absence of testing and tracing, as visualised in Figure 4. This suggests that enacting fines and penalties to enforce compliance can significantly help to reduce the effective  $R$ .

**Application coverage** We varied the `app_coverage` from 0.0 to 1.0, shown in Figure 4. We observed that increasing application uptake slightly reduces the effective  $R$ , as tracing can be carried out more quickly without delay. However, we noted that the difference between 0.0 and 1.0 `app_coverage` is minor, so this parameter is less significant than other parameters.

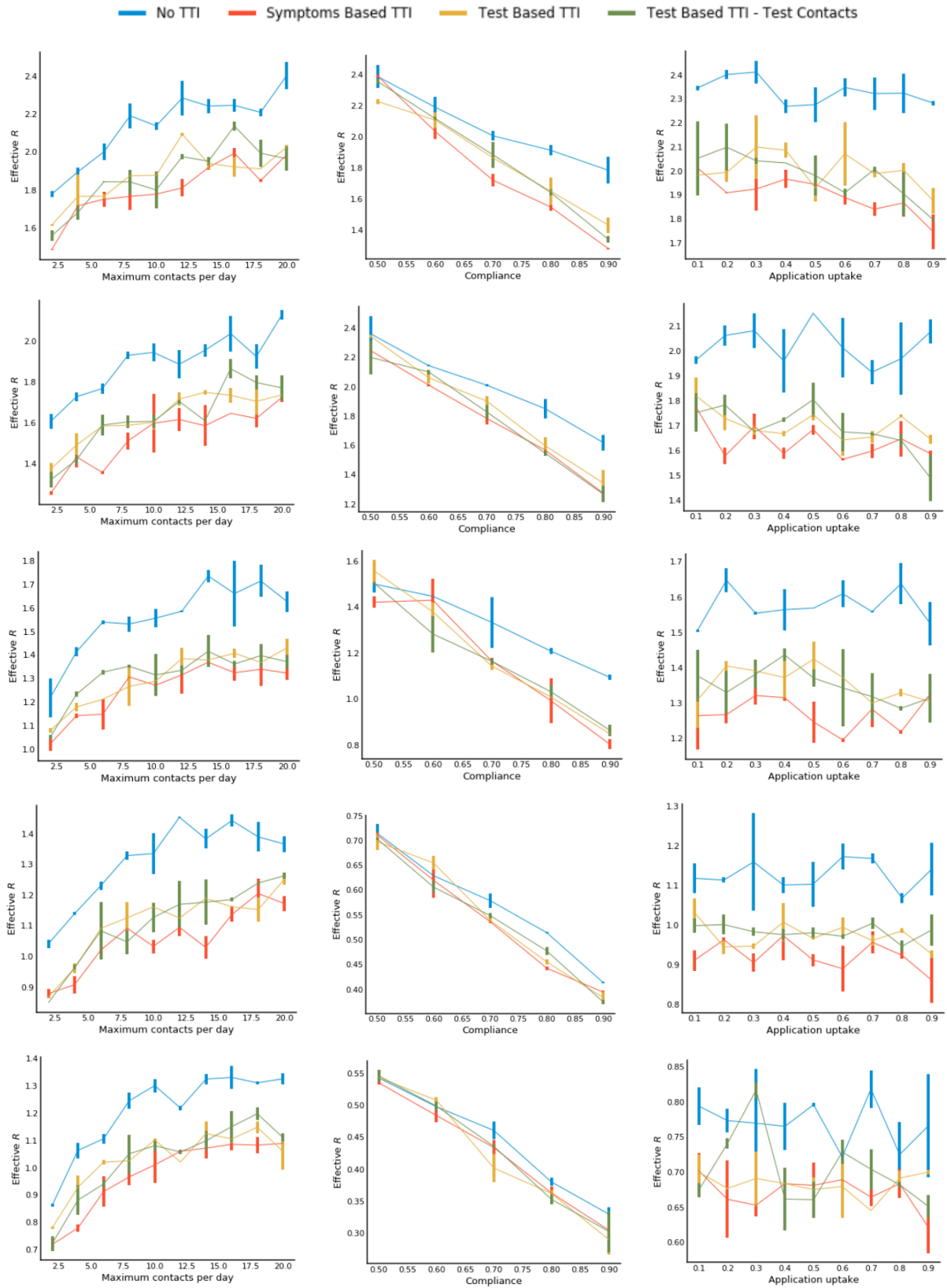




**Figure 2: Left:** Effect of varying the probability of under 18 on effective  $R$ . **Middle:** Effect of varying work from home proportion on effective  $R$ . **Right:** Effect of varying go to school probability on effective  $R$ . **Top to Bottom:** 5 levels of governmental measures: S1-S5. The error bars are 95% confidence intervals.

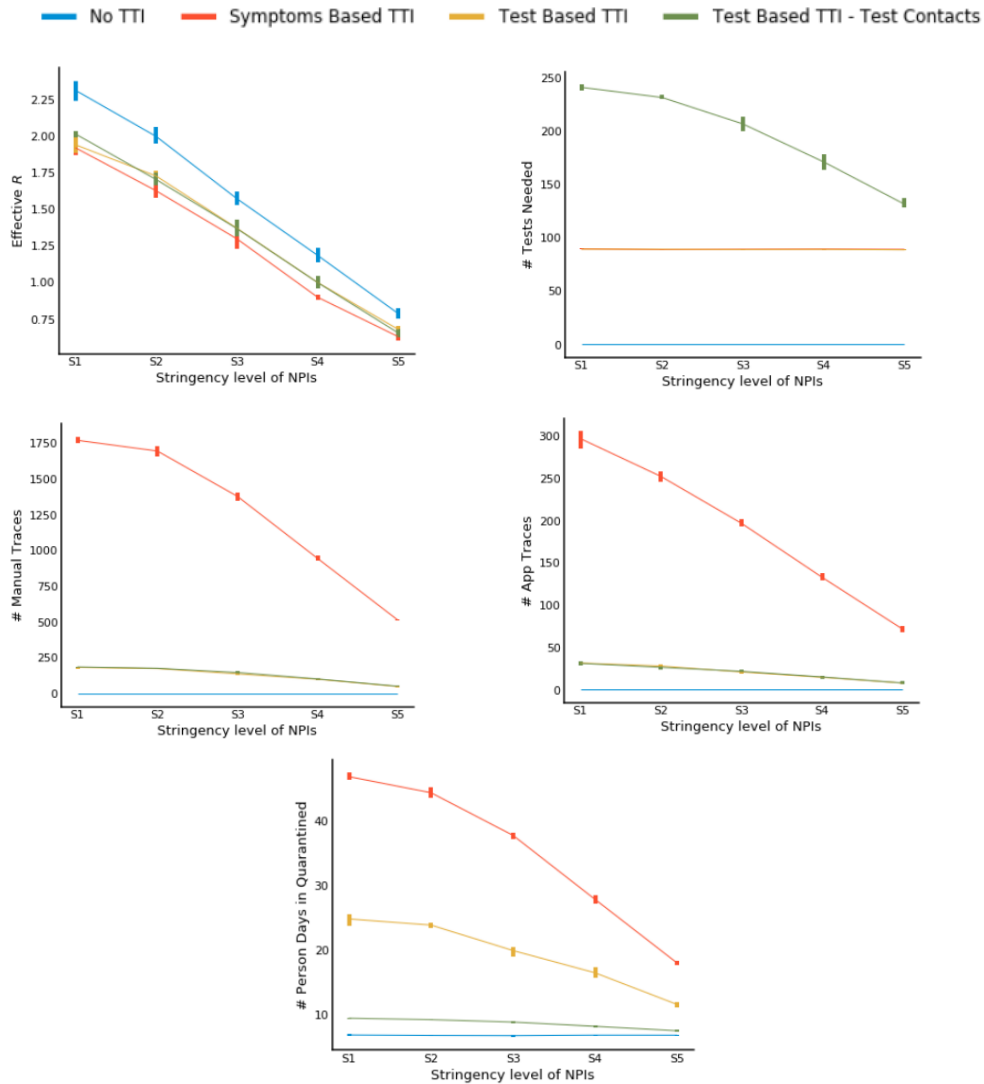


**Figure 3:** **Left:** Effect of varying the home secondary attack rate on effective  $R$ . **Middle:** Effect of varying the work secondary attack rate on effective  $R$ . **Right:** Effect of varying the other secondary attack rate on effective  $R$ . **Top to Bottom:** 5 levels of governmental measures: S1-S5. The error bars are 95% confidence intervals.



**Figure 4:** Left: Effect of varying the number of maximum contacts per day on effective  $R$ . Middle: Effect of varying the compliance level on effective  $R$ . Right: Effect of varying the application coverage on effective  $R$ . Top to Bottom: 5 levels of governmental measures: S1-S5. The error bars are 95% confidence intervals.

We employed grid variation, varying the five levels of governmental measures (S1-S5) and four TTI strategies: no TTI, trace on symptoms, trace on positive test and trace on positive test with contacts testing. We observed their overall effects on the effective  $R$ , number of tests needed, number of manual traces, number of app traces and number of total days quarantined. The results are shown in Figure 5. The effective  $R$  plot demonstrates the benefits of TTI, through a lower effective  $R$  compared to no TTI. Interestingly, the lowest effective  $R$  was achieved using symptoms- and test-based TTI strategies, suggesting that trace on positive test with contacts testing is not beneficial, despite its expense. From the other plots, we observed that the number of traces and person days quarantined are significantly higher for the symptoms-based TTI strategy than for other strategies. The overall high-level overview suggests that the test-based TTI strategy is the most beneficial as it attains the minimum effective  $R$  with reasonable resource requirements.



**Figure 5:** Impact on effective  $R$  and resource requirement of various TTI strategies across the five sets of governmental measures, for 10,000 primary cases. The number of tests, manual traces, app traces, and person days quarantined are in thousands.

## 3.2 Analysis of Variance Decomposition

### 3.2.1 Background

Due to their simplicity, axis and grid variations cannot capture the interactions between variables. Consequently, we used the ANOVA decomposition method for a complete global sensitivity analysis that can fully explore the input spaces, while considering the interactions between parameters and nonlinear responses [24]. The ANOVA decomposition performs sensitivity analysis by decomposing the variance of a target function into parts attributable to input parameters and their interactions. The magnitude of the effect of input to output is then calculated relative to the variance in output caused by that input. More formally, the following equation defines the ANOVA decomposition of the total variance into a combination of the variances of the smaller functions, each representing the interactions between different inputs:

$$\begin{aligned}\text{Var}[g] &= \langle g(\mathbf{x})^2 \rangle_{p(\mathbf{x})} - \langle g(\mathbf{x}) \rangle_{p(\mathbf{x})}^2 \\ &= \langle g(\mathbf{x})^2 \rangle_{p(\mathbf{x})} - g_0^2 \\ &= \sum_{i=1}^p \text{Var}[g_i(x_i)] + \sum_{i < j}^p \text{Var}[g_{ij}(x_i, x_j)] + \cdots + \text{Var}[g_{1,2,\dots,p}(x_1, x_2, \dots, x_p)]\end{aligned}$$

The  $\langle g(\mathbf{x}) \rangle_{p(\mathbf{x})}$  is the expectation of the function  $g(\mathbf{x})$  under the density  $p(\mathbf{x})$ , which represents the probability distribution of inputs we're interested in. While  $g_i(x_i)$  represent the impact of a single variable,  $g_{i,j}(x_i, x_j)$  measures the effect of two variables interacting. It is common to rescale the components with the total variance of the function; these rescaled components are known as the *Sobol indices*:

$$S_\ell = \frac{\text{var}(g(\mathbf{x}_\ell))}{\text{var}(g(\mathbf{x}))}$$

Using the Sobol indices, we can evaluate the effect of each set of inputs on the output. There are two metrics for quantifying these effects: *main effects* and *total effects*. The main effects consider only summing the first-order Sobol indices to measure the magnitude of each input. Conversely, the total effects also consider higher-order interaction terms of any order. To compute both the main and total effects, we used `Emukit` [20]. We estimated the Sobol indices using two methods: *model-free Monte Carlo*, which calculates these indices by sampling the simulator directly [23], and *model-based Monte Carlo*, which calculates indices by sampling a Gaussian process emulator [15]. For the experiments (see Section 3.2.2), we computed 10,000 evaluations for the model-free and model-based Monte Carlo approaches to estimate the indices. Model-free Monte Carlo requires lengthy computation time, as each simulation run takes around 1 second to complete, in total demanding over 10 hours of computation to estimate the Sobol indices. Conversely, model-based Monte Carlo achieved comparable results within a significantly shorter time of 15 minutes. This highlights the benefits of employing Gaussian process emulator, which makes it feasible to employ variable-based sensitivity analysis methods.

### 3.2.2 Experiment Results

The ANOVA decomposition approach provided a nuanced understanding of the interaction between factors. We first included all 13 variables and analysed the variances. This provided a

general insight into which variables play essential roles in influencing the effective  $R$ . We then conducted further analysis to understand how variables in the three groups (Table 1) affect the effective  $R$ .

**All factors** Figure 6 presents the results of the analysis of all variables. With everything allowed to be varied, the maximum number of contacts of an individual has the greatest effect on the effective  $R$ . Given that the effective  $R$  measures the spread of the pandemic throughout a population, it makes sense that restricting the number of contacts each individual can have may greatly limit the spread of the pandemic. Other important factors are quarantine\_length and testing\_delay. Quarantine length limits the amount of time for which an individual exposes themselves to the general population. Testing delay controls how quickly an individual with symptoms is identified, thus affecting how quickly they can be quarantined. The analysis suggests that while testing affects the effective  $R$  to a certain extent, the most effective solution is to limit social contacts.

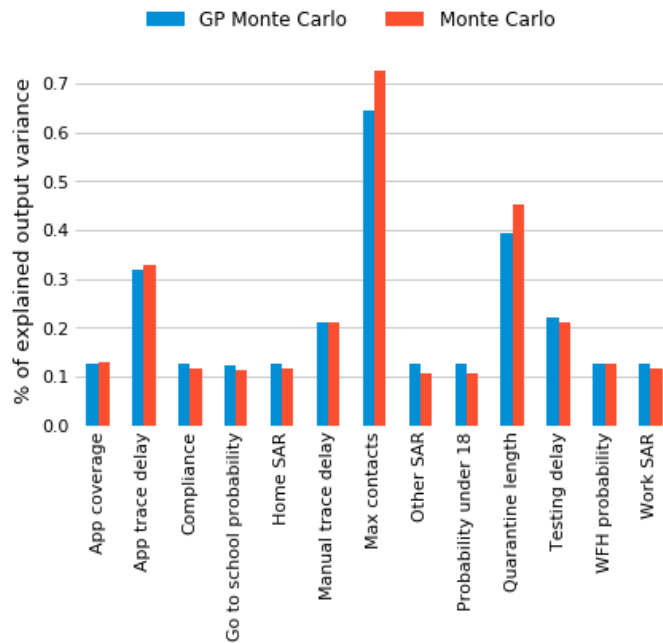
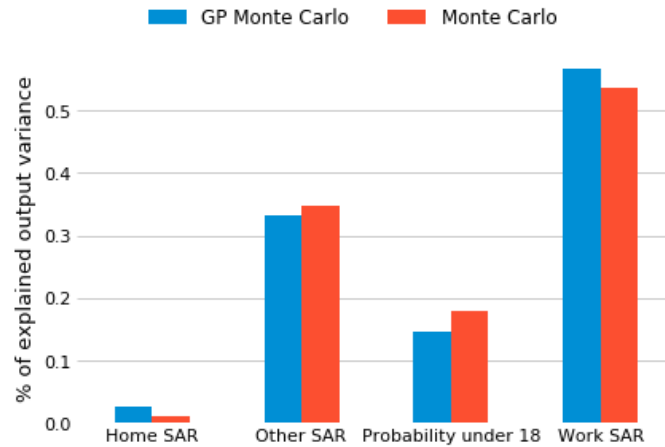


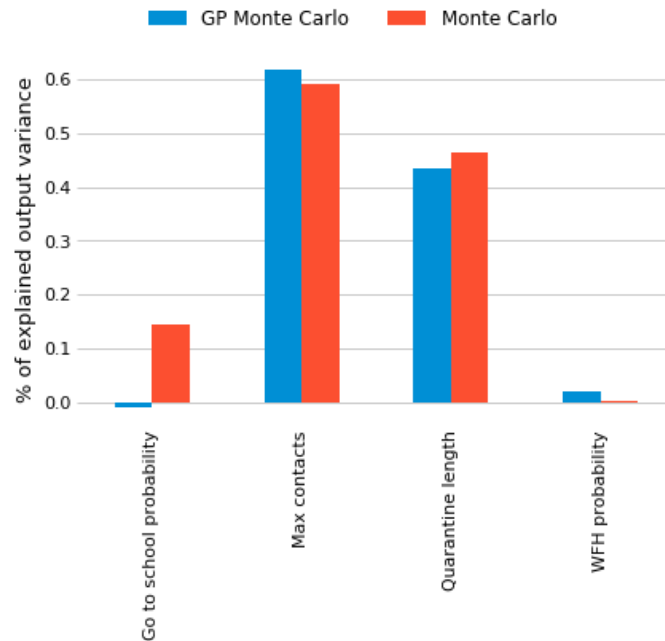
Figure 6: Total effects of all 13 variables on the effective  $R$ .

**General factors** Further analysis was conducted on the general factors. The results are shown in Figure 7. We observed that work\_sar makes the greatest contribution to the effective  $R$  variance, followed by other\_sar, p\_under18, and home\_sar. This is consistent with the analysis detailed in Section 3.1.



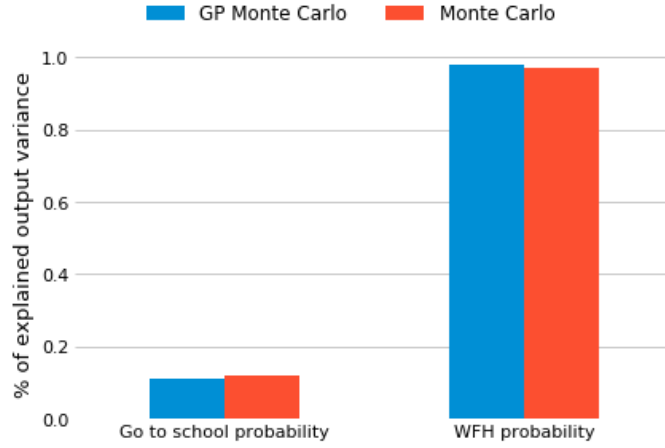
**Figure 7:** Total effects of all general factor variables on the effective  $R$ .

**Policy factors** We then analysed how different policy factors influence the effective  $R$ . The results are shown in Figure 8. This confirms previous findings that limiting social contacts would have the greatest impact on reducing the infection spread.



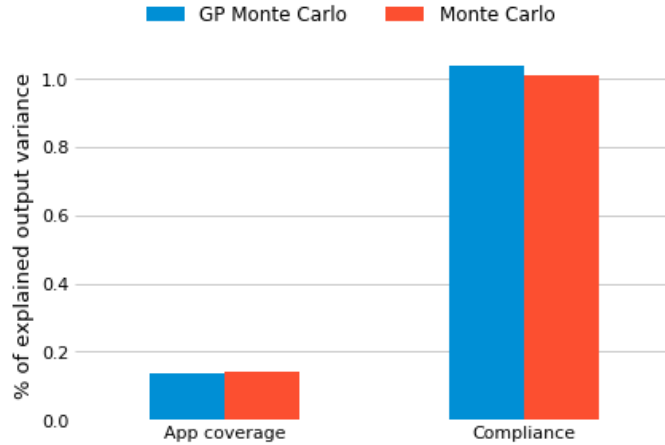
**Figure 8:** Total effects of all policy factor variables on the effective  $R$ .

Limiting the number of social contacts and increasing quarantine length are disruptive measures and difficult to enforce. Consequently, we investigated other measures that policymakers can control in the absence of the aforementioned variables. This was done by removing `max_contacts` and `quarantine_length`, and conducting sensitivity analysis on the remaining variables. The results shown in Figure 9 show that in the absence of strict social distancing and quarantine, the most influential variable for the effective  $R$  variance was `wfh_prob`. This suggests that working from home is a viable strategy to implement for reducing the effective  $R$ .



**Figure 9:** Total effects of go\_to\_school\_prob and wfh\_prob on the effective  $R$ .

**Compliance factors** Figure 10 illustrates the total effects of compliance variables on the effective  $R$ . We observed that the compliance level has a greater effect than app coverage. This suggests the greater importance for individuals to comply with government policies than to download the TTI app, a finding, which is consistent with the results of Section 3.1.



**Figure 10:** Total effects of compliance factor variables on the effective  $R$ .

### 3.3 Causal Analysis

Further extending sensitivity analysis, we conducted causal analysis to find direct causal variables of the effective  $R$ . This was done by directly intervening in the simulator and observing any distribution changes in the value of effective  $R$  – a method proposed by Pearl and Mackenzie [21]. We state that a variable  $T$  causally affects  $Y$  if intervening on  $T$  changes the distribution of  $Y$ . Mathematically, this is captured by the following formula:

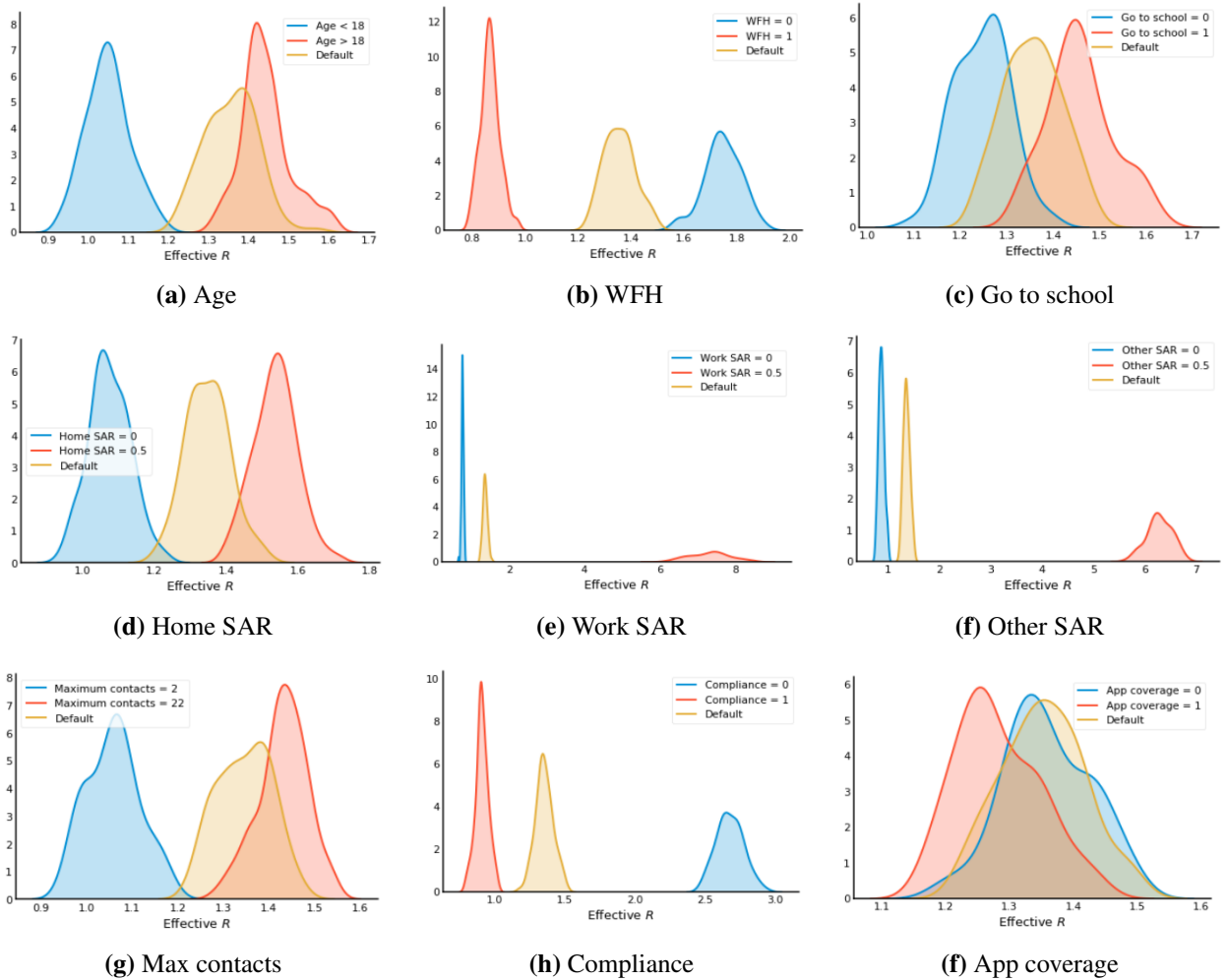
$$\Pr(Y) \neq \Pr(Y|do(T))$$

We selected the following nine parameters to vary from Table 1 based on the previous sensitivity analyses: p\_under18, home\_sar, work\_sar, other\_sar, wfh\_prob, go\_to\_school\_prob,



max\_contacts, compliance, and app\_cov. We intervened on a parameter, then conducted the simulations 100 times to obtain the distribution of the effective  $R$ . To determine whether their distribution differs, we applied the Kolmogorov-Smirnov statistical test [16] to compare the original effective  $R$  distribution against the intervened distribution.

Figure 11 presents the distribution results for the nine considered variables. Overall, we observed that with a 5% significance level ( $\alpha = 0.05$ ), we rejected the null hypothesis for all variables, except for app\_cov, suggesting that their distributions differ – implying causality for all variables, except for the app\_cov, under the definition provided by Pearl and Mackenzie [21]. This is consistent with previous analyses, as the sensitivity analysis indicates that the app\_cov does not strongly impact the effective  $R$ .



**Figure 11:** Kernel density estimate of the effective  $R$  distribution on the original and do-intervention settings for all variables. We rejected the null hypothesis for all variables, except for the app\_cov.

## 4 Policy Optimisation

This section discusses various optimal policies found by different optimisation methods, including random search and Bayesian optimisation. It comprises two main sections: the uncon-

strained optimisation and constrained optimisation further detailed below.

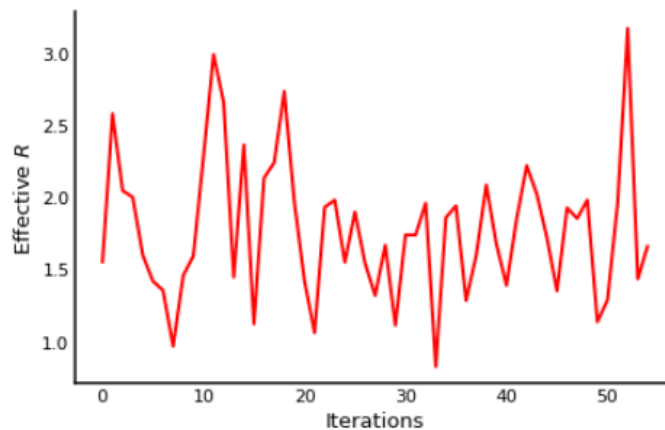
## 4.1 Unconstrained Optimisation

The unconstrained optimisation problem aims to find the optimal set of parameters to minimise the effective  $R$ , without any resource constraints. For this section, we implemented random search and Bayesian optimisation methods on 14 input parameters (Table 2). These are all parameters that can be influenced through policy, whether directly like `quarantine_length` or indirectly like `max_contacts`.

Both random search and Bayesian optimisation methods were run for 50 iterations. We used Emukit [20] and GPy [5] libraries for experimentation in this section.

### 4.1.1 Random Search

Random search explores different sets of possible policy parameters at random. The performance of this algorithm is thus expected to be poorer than that of Bayesian optimisation, as it does not learn from past searches to guide future searches. The random search is used as a comparison baseline in the experiments; the comparison between methods is further discussed in Section 4.1.2. Overall, the experiment results were erratic, with the effective  $R$  varying between 1.0 and 3.5, shown in Figure 12.



**Figure 12:** The effective  $R$  across iterations for random search.

Random search was able to find a minimum effective  $R$  of 0.78, with the set of policy parameters shown in Table 3. Several other policies found by the random search are displayed in Table 8.

Policy Parameter	Optimal Value
<code>go_to_school_prob</code>	0.440
<code>wfh_prob</code>	0.830
<code>isolate_individual_on_symptoms</code>	True
<code>isolate_individual_on_positive</code>	True
<code>isolate_household_on_symptoms</code>	True
<code>isolate_household_on_positive</code>	True
<code>isolate_contacts_on_symptoms</code>	False

isolate_contacts_on_positive	False
test_contacts_on_positive	True
do_symptom_testing	False
do_manual_tracing	True
do_app_tracing	False
max_contacts	1
quarantine_length	7

**Table 3:** Set of optimal policy parameters found by random search.

#### 4.1.2 Bayesian Optimisation

Bayesian optimisation [22] is a sequential decision-making approach to finding the optimum value of an objective function that is expensive to evaluate. This approach is appropriate for our task, as the simulator does not have an explicit functional form and is expensive to compute.

The main part of a Bayesian optimisation system is a loop that iteratively decides on new locations for which the objective function should be evaluated. It comprises two main components: the *surrogate model* and the *acquisition function*. The surrogate model approximates the underlying objective function and is used to guide the search. The acquisition function then decides where to sample next, balancing the exploration of regions where the model is uncertain, and the exploitation of the model’s confidence about good areas of the input space.

We first built a surrogate model for approximating the simulator – multi-argument function for computing the effective  $R$  (see Section 2). We adopted the *expected improvement* (EI) function in the experiment, detailed in Section 4.2. After building the initial surrogate model, the algorithm iterates the following steps 50 times:

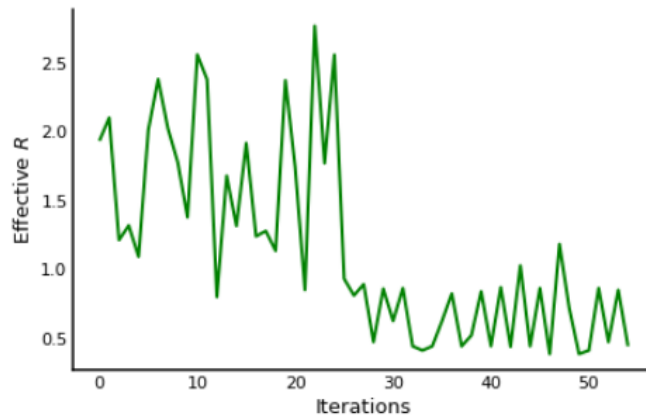
1. Find the next point to evaluate the effective  $R$  using a numerical solver to optimise the acquisition function.
2. Evaluate the effective  $R$  at that point.
3. Update the surrogate model using the new information gained.

Figure 13 shows the effective  $R$  found by the Bayesian optimisation over the iterations. Comparing the results of Bayesian optimisation and random search (Figure 12) we observed the superiority of Bayesian optimisation, as it obtained a 44% lower minimum, in a smaller number of steps, than random search. We also noted the robustness of the method as it converges to the optimum, while random search does not.

Policy Parameter	Optimal Value
go_to_school_prob	0.0166
wfh_prob	0.996
isolate_individual_on_symptoms	True
isolate_individual_on_positive	True
isolate_household_on_symptoms	True
isolate_household_on_positive	False
isolate_contacts_on_symptoms	False

isolate_contacts_on_positive	False
test_contacts_on_positive	True
do_symptom_testing	False
do_manual_tracing	False
do_app_tracing	False
max_contacts	2
quarantine_length	2

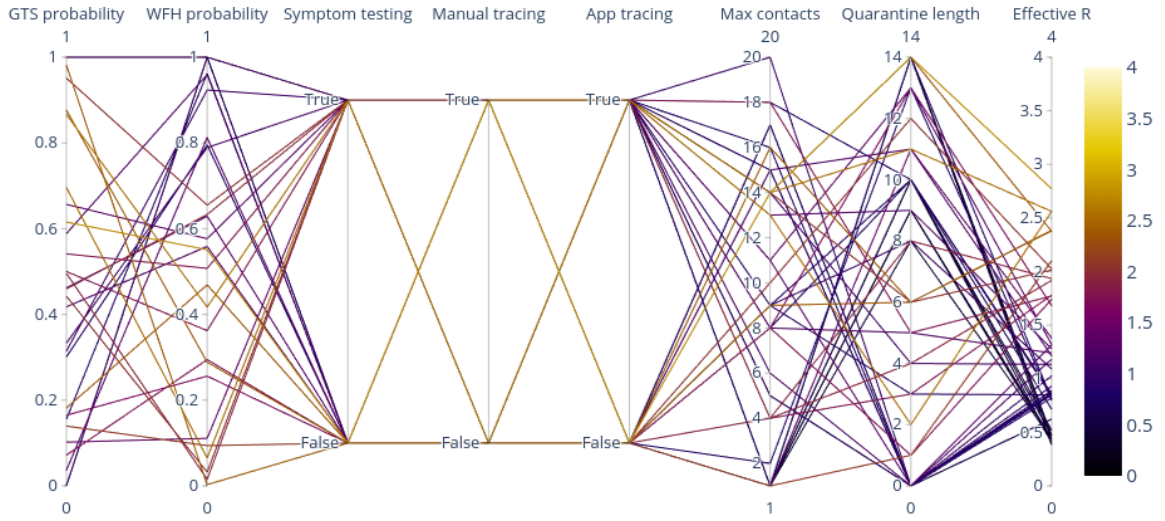
**Table 4:** Set of optimal policy parameters found by Bayesian optimisation.



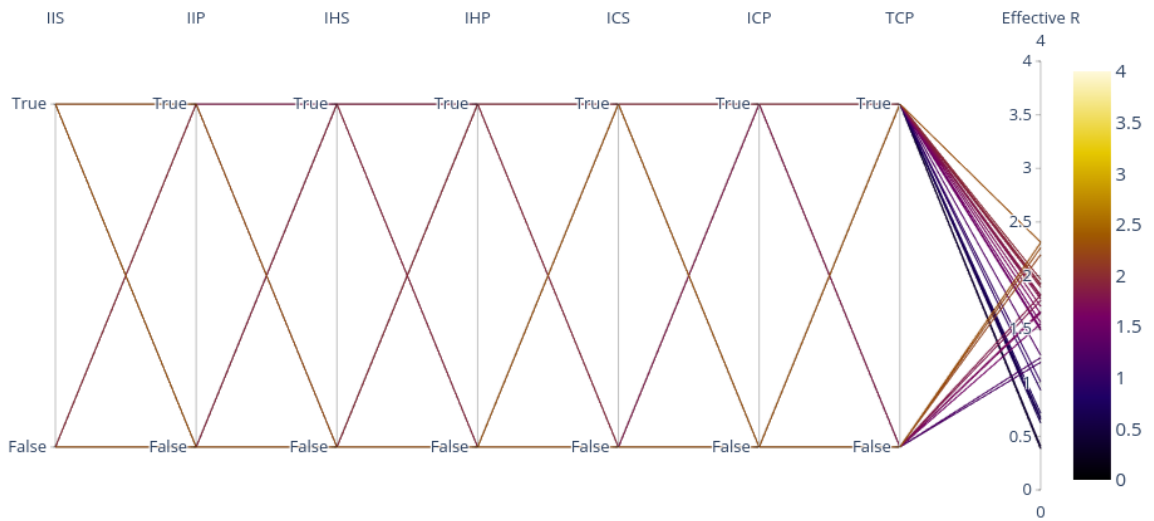
**Figure 13:** The effective  $R$  across iterations for Bayesian optimisation with the expected improvement acquisition function.

Bayesian optimisation was able to achieve a policy with an effective  $R$  of **0.38**, as listed in Table 4. The optimal policy agrees with the analyses discussed in Section 3, indicating that limiting the amount of social contact is the most effective way to suppress the effective  $R$ , followed by enforcing working from home. Several other policies evaluated by the Bayesian optimisation are displayed in Table 9.

To gain an understanding of how different policy parameters affect the effective  $R$ , we plotted the overall search results on a parallel coordinate plot, shown in Figure 14. Generally, we observed that policies with lower effective  $R$  tend to enforce longer quarantine length, limit the number of contacts, and advocate a work from home policy. We also plotted the overall search results of isolation decision-related variables, showing that isolating individuals as soon as they develop symptoms should be advocated for, rather than waiting for positive test results (Figure 15).



**Figure 14:** Policy parameter search results on the effective  $R$ . Each line in the plots represents a single policy configuration.



**Figure 15:** Isolation decision-related variables search results on the effective  $R$ . Each line in the plots represents a single configuration. The columns are variables in the order presented in Table 2

## 4.2 Ablation Studies

This section discusses ablation test results on both the choice of acquisition functions and surrogate models for the Bayesian optimisation routines.

**Acquisition functions** To investigate how different acquisition functions perform we selected three of them, namely the EI, the *negative lower confidence bound* (NLCB), and the *probability of improvement* (PI). The definition of each function is as follows:

- **Expected improvement:** the EI [10], computes for each data point, how much it can improve with respect to the current best observed location  $f(x^*)$ . Then, it computes the following equation:

$$E_{p(f|D)}[\max(f(x^*) - f(x), 0)].$$

where  $f(x^*) \in \arg \min\{f(x_0), \dots, f(x_n)\}$ . Assuming  $p(f|D)$  to be a Gaussian, we can compute EI in closed form by:

$$\sigma(x)(\gamma(x)\Phi(\gamma(x)) + \phi(\gamma(x)))$$

where  $\gamma(x) = \frac{f(x^*) - \mu(x)}{\sigma(x)}$ ,  $\Phi$  is the cumulative distribution function (CDF), and  $\phi$  is the probability density function (PDF) of a standard normal distribution.

- **Negative lower confidence bound:** Based on the upper confidence bound bandit strategy, the NLCB [25] maximised the following equation:

$$a_{LCB} = -(\mu(x) - \beta\sigma(x))$$

where  $\beta$  is a user-defined hyperparameter that controls exploitation and exploration.

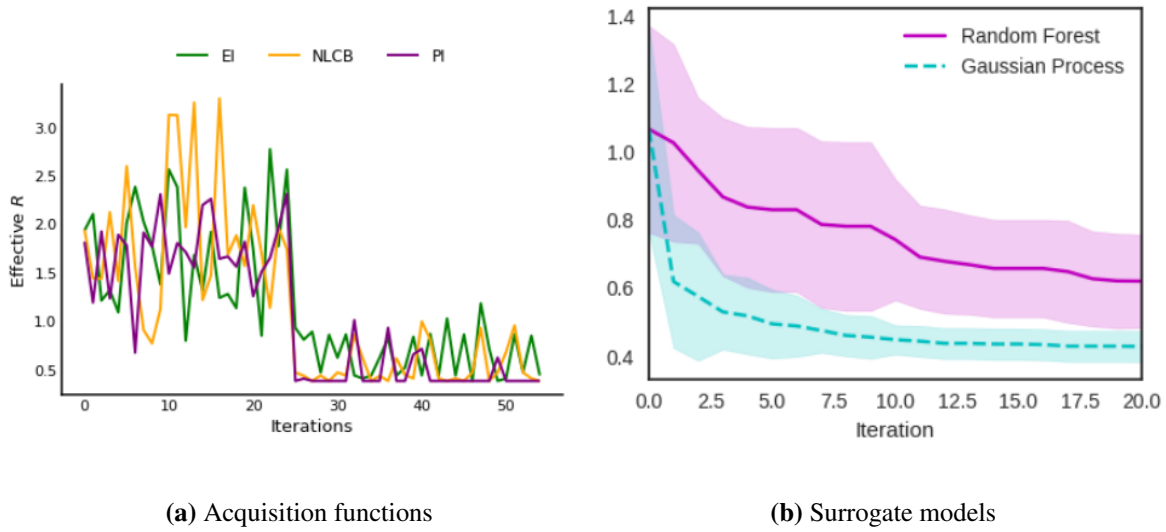
- **Probability of improvement:** Finally, the PI [10] selects a data point with the highest probability of improvement over the current best observed location  $f(x^*)$ , following the equation:

$$a_{PI}(x) = \Phi(\gamma(x))$$

where  $\gamma(x) = \frac{f(x^*) - \mu(x)}{\sigma(x)}$  and  $\Phi$  is the CDF of a standard normal distribution.

Figure 16(a) illustrates the behaviour of different acquisition functions over iterations. Generally, all three acquisition functions converged and obtained similar minima. The choice of acquisition function did not have a large impact on the convergence of the optimisation routine.

**Surrogate models** We conducted an ablation study on the choice of surrogate models for the Bayesian optimisation routine. We chose two different models to test, the Gaussian process and random forest. Each model was tested similarly, with 50 epochs, 10 random initial data points, and EI as the acquisition function. The result is shown in Figure 16(b), demonstrating the superiority of the Gaussian process over random forest as a surrogate model.



**Figure 16:** Left: The effective  $R$  across iterations for Bayesian optimisation with different acquisition functions. Right: The effective  $R$  across iterations for Bayesian optimisation with different surrogate models.

### 4.3 Constrained Optimisation

The constrained optimisation problem aims to find the best set of parameters to minimise the infection spread, with constraints, such as the number of tests and manual traces [7] reflecting real-world resource constraints.

Correctly estimating the trade-off between saving lives and minimising disruption lies outside the scope of this report. Therefore, we describe two parameterized methods for taking constraints into account, which can be tuned for practical use based on further research.

The first method is to constrain directly the sampled space, which we did by limiting the number of testing kits used per day, with the results shown in Table 5. This set of policy parameters yields an effective  $R$  of 0.56 with 0 testing kits. Intuitively, this policy suggests to not test anyone, and instead enforce everyone to stay at home. This is because, while we have limited the number of tests, we have not placed any limitations on social distancing or working from home. To make this approach more practical, it is necessary to add a limit for each of these measures.

Policy Parameter	Optimal Value
go_to_school_prob	0.0166
wfh_prob	0.996
isolate_individual_on_symptoms	True
isolate_individual_on_positive	True
isolate_household_on_symptoms	True
isolate_household_on_positive	False
isolate_contacts_on_symptoms	False
isolate_contacts_on_positive	False
test_contacts_on_positive	True
do_symptom_testing	False
do_manual_tracing	False
do_app_tracing	False

max_contacts	2
quarantine_length	2

**Table 5:** Set of optimal policy parameters found by Bayesian optimisation, constrained on the number of testing kits limited to 25k per day.

The second method consists of constructing a different loss function by combining the original objective function with penalty terms. We used a linear combination of effective  $R$  and all quantities that increase cost or disruption.

$$L(\mathbf{x}) = \lambda_1 R + \lambda_2 T + \lambda_3 M$$

where  $L(\mathbf{x})$  represents the total loss function arising from the set of policy parameters  $\mathbf{x}$ ,  $R$  is the effective  $R$ ,  $T$  is the number of tests, and  $M$  is the number of manual traces.  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are weights, which we empirically set as  $\lambda_1 = 0.6$ ,  $\lambda_2 = 0.2$ , and  $\lambda_3 = 0.2$ . Intuitively, we aim to minimise the effective  $R$  as much as possible, while considering the available resources – the number of tests and manual traces.

The resulting optimal policy parameters are shown in Table 11. The minimum effective  $R$  found was 1.19. This optimal policy corresponds to 0 manual traces, but 90,000 tests a day. This policy seems to be rather lax, as it only requires 80% of the population to work from home and students are required to attend school. Compared to the policy found by strictly constraining the number of test kits per day, it seems that this policy might be better, as it demonstrates the possibility to achieve a lower effective  $R$  with a lower number of test kits per day.

## 5 Conclusion

This report presents the results of comprehensive sensitivity analyses that investigate the effects of various TTI strategies and NPIs factors on the effective  $R$  of COVID-19. On the bases of these insights, optimisation methods were conducted to find optimal policies that can be used to help policymakers contain the pandemic. Overall, sensitivity analyses, using axis and grid variations, and ANOVA decomposition found that work from home, maximum contacts, and quarantine length factors had the greatest impact on the effective  $R$ . Further causal analysis indicated that these factors indeed directly influence the metric, suggesting that controlling these factors is key to containing the outbreak. From a technical perspective, we observed the benefits of employing the Gaussian process emulator, which enabled the fast computation of ANOVA decomposition, thus allowing the presentation of a more complete sensitivity analysis result that complement prior work in the COVID-19 domain.

In addition to analysing the effect of various variables on the effective  $R$ , we conducted policy optimisation by using random search, unconstrained Bayesian optimisation, and constrained Bayesian optimisation to search for sensible optimal policies. We observed that the optimal policies derived from all methods agreed with the sensitivity analysis results; that is they include a strict working from home routine, limit the number of social contacts, and advocate for long quarantine lengths. While these measures may sound draconian, we have seen that they effectively reduce the effective  $R$ . We also demonstrated the superiority of Bayesian optimisation-based approaches over the random search, as they obtain better and more sensible policy significantly faster.



## 6 Appendices

	Variables	Description
<b>General Factors</b>	p_under18	Probability that a person is under 18. A person that is under 18 has a very different social profile to a person over 18. A person under 18 is likely to be in school, and a person over 18 is likely to be a working adult.
	home_sar	Probability that home contact is infected, given that the current individual is infected and interacts with the home contact (e.g. family members).
	work_sar	Probability that work associate is infected, given that the current individual is infected and interacts with the work associate.
	other_sar	Probability that a person other than work associate or home family members is infected, given that the current individual is infected and interacts with that person.
<b>Policy Factors</b>	wfh_prob	Proportion of people working from home.
	go_to_school_prob	Proportion of school-aged children not going into schools.
	max_contacts	A hard limit placed on the number of non-home, non-work contacts a person has per day.
	quarantine_length	How long someone has to quarantine if they have COVID-19.
	testing_delay	Delay between test and result (in days).
	manual_trace_delay	Delay between a test result and notifying contacts manually (in days).
	app_trace_delay	Delay between a test result and notifying contacts via app (in days).
<b>Compliance Factors</b>	compliance	Probability that each person complies with the regulations set out in the policy, such as work from home, quarantine, and limit social contact.
	app_cov	Percentage of a population using the app to track and trace, and submitting locations.

**Table 6:** Descriptions of each factor in the groupings discussed in Section 2.

<b>Variables</b>	<b>Description</b>	<b>Type</b>
go_to_school_prob	Fraction of school children attending school.	<i>Float</i> , range:[0,1]
wfh_prob	Proportion of the population working from home.	<i>Float</i> , range:[0,1]
isolate_individual_on_symptoms	Isolate the individual after they present with symptoms.	<i>Boolean</i> , range: [True, False]
isolate_individual_on_positive	Isolate the individual after they test positive.	<i>Boolean</i> , range: [True, False]
isolate_household_on_symptoms	Isolate the household after individual present with symptoms.	<i>Boolean</i> , range: [True, False]
isolate_household_on_positive	Isolate the household after individual test positive.	<i>Boolean</i> , range: [True, False]
isolate_contacts_on_symptoms	Isolate the contacts after individual presents with symptoms.	<i>Boolean</i> , range: [True, False]
isolate_contacts_on_positive	Isolate the contacts after an individual tests positive.	<i>Boolean</i> , range: [True, False]
test_contacts_on_positive	Test contacts of a positive case immediately, or wait for them to develop symptoms.	<i>Boolean</i> , range: [True, False]
do_symptom_testing	Test symptomatic individuals.	<i>Boolean</i> , range: [True, False]
do_manual_tracing	Perform manual tracing of contacts.	<i>Boolean</i> , range: [True, False]
do_app_tracing	Perform app tracing of contacts.	<i>Boolean</i> , range: [True, False]
max_contacts	Limit on the number of contacts per day.	<i>Integer</i> , range: [1,20]
quarantine_length	Length of quarantine imposed on COVID cases (and household).	<i>Integer</i> , range: [0,14]

**Table 7:** Policy optimisation variables, their descriptions and types.

<b>GTS Probability</b>	<b>WFH Probability</b>	<b>IIS</b>	<b>IIP</b>	<b>IHS</b>	<b>IHP</b>	<b>ICS</b>	<b>ICP</b>	<b>TCP</b>	<b>Symptom Testing</b>	<b>Manual Tracing</b>	<b>App Tracing</b>	<b>Max Contacts</b>	<b>Quarantine Length</b>	<b>Effective R</b>
0.440	0.830	True	True	True	True	False	False	True	False	True	False	1.0	7.0	0.767
0.146	0.842	True	True	False	True	False	False	False	False	False	True	2.0	3.0	0.771
0.295	0.644	True	False	False	True	False	True	True	False	False	True	3.0	3.0	1.044
0.779	0.331	False	True	True	True	True	False	False	True	True	False	17.0	2.0	1.739
0.288	0.453	False	False	False	False	True	True	True	False	True	True	20.0	13.0	1.921

**Table 8:** Five selected policy parameters obtained by random search. The columns are variables in the order go\_to\_school\_prob, wfh\_prob, isolate\_individual\_on\_symptoms, isolate\_individual\_on\_positive, isolate\_household\_on\_symptoms, isolate\_household\_on\_positive, isolate\_contacts\_on\_symptoms, isolate\_individual\_on\_positive, do\_symptoms\_testing, do\_manual\_tracing, do\_app\_tracing, max\_contacts, quarantine\_length, and effective  $R$ .

<b>GTS Probability</b>	<b>WFH Probability</b>	<b>IIS</b>	<b>IIP</b>	<b>IHS</b>	<b>IHP</b>	<b>ICS</b>	<b>ICP</b>	<b>TCP</b>	<b>Symptom Testing</b>	<b>Manual Tracing</b>	<b>App Tracing</b>	<b>Max Contacts</b>	<b>Quarantine Length</b>	<b>Effective R</b>
0.0	1.0	True	True	True	False	True	False	True	False	True	True	1.0	14.0	0.383
0.0	1.0	True	True	True	True	True	True	False	True	True	False	1.0	8.0	0.44
0.0	1.0	True	False	False	False	True	True	True	True	True	True	9.0	10.0	0.838
0.0	1.0	True	True	True	False	False	False	True	True	False	True	20.0	0.0	1.027
0.165	0.256	True	True	False	True	False	False	False	False	False	False	8.0	13.0	1.68

**Table 9:** Five selected policy parameters obtained by unconstrained Bayesian optimisation. The columns are variables in the order go\_to\_school\_prob, wfh\_prob, isolate\_individual\_on\_symptoms, isolate\_individual\_on\_positive, isolate\_household\_on\_symptoms, isolate\_household\_on\_positive, isolate\_contacts\_on\_symptoms, isolate\_individual\_on\_positive, do\_symptoms\_testing, do\_manual\_tracing, do\_app\_tracing, max\_contacts, quarantine\_length, and effective  $R$ .

GTS Probability	WFH Probability	IIS	IIP	IHS	IHP	ICS	ICP	TCP	Symptom Testing	Manual Tracing	App Tracing	Max Contacts	Quarantine Length	Days Quarantined
0.264	0.095	False	False	False	True	False	False	True	False	False	False	15.0	0.0	0.000
0.278	0.338	False	False	False	True	False	False	True	False	False	True	14.0	3.0	51.048
0.926	0.992	False	True	False	True	False	False	False	True	False	True	20.0	2.0	53.112
0.247	0.477	False	True	False	False	False	True	True	True	False	True	20.0	2.0	68.496
0.144	0.401	False	False	False	True	True	True	False	False	False	False	6.0	6.0	110.088

**Table 10:** Five selected policy parameters obtained by unconstrained Bayesian optimisation optimising on person days quarantined. The columns are variables in the order go\_to\_school\_prob, wfh\_prob, isolate\_individual\_on\_symptoms, isolate\_individual\_on\_positive, isolate\_household\_on\_symptoms, isolate\_household\_on\_positive, isolate\_contacts\_on\_symptoms, isolate\_individual\_on\_positive, do\_symptoms\_testing, do\_manual\_tracing, do\_app\_tracing, max\_contacts, quarantine\_length, and person days quarantined (in thousands).

GTS Probability	WFH Probability	IIS	IIP	IHS	IHP	ICS	ICP	TCP	Symptom Testing	Manual Tracing	App Tracing	Max Contacts	Quarantine Length	Weighted Combination	Effective R
1.0	0.8	True	False	True	False	False	False	False	False	False	True	1.0	14.0	1.154	1.187
1.0	0.8	True	False	True	False	False	False	False	False	False	True	1.0	14.0	0.718	1.197
1.0	0.8	True	False	True	False	False	False	False	False	False	True	1.0	14.0	1.055	1.508
0.279	0.154	False	True	False	False	True	True	True	True	False	True	7.0	7.0	1.17	1.702
0.945	0.671	True	True	False	True	False	True	True	True	False	True	9.0	8.0	1.424	2.127

**Table 11:** Five selected policy parameters obtained by constrained Bayesian optimisation optimising the weighted loss function. The columns are variables in the order go\_to\_school\_prob, wfh\_prob, isolate\_individual\_on\_symptoms, isolate\_individual\_on\_positive, isolate\_household\_on\_symptoms, isolate\_household\_on\_positive, isolate\_contacts\_on\_symptoms, isolate\_individual\_on\_positive, do\_symptoms\_testing, do\_manual\_tracing, do\_app\_tracing, max\_contacts, quarantine\_length, weighted combination, and effective  $R$ .

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