# Untitled EnKF paper

Keiran Suchak

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**Abstract**

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## 1 Introduction

Write introduction

Contents:

- Provide context and motivation for investigation.
- Outline aims and objectives.

Main aim: show that an Ensemble Kalman Filter (EnKF) can improve the accuracy with which an agent-based model simulates a system of pedestrians.

Points of distinction to highlight:

- Comprehensive assessment of efficacy of an EnKF for an ABM.
- Defining an approach for defining whether an agent is active or inactive in an ensemble of models.
- Comparing error in ensemble mean with mean of errors of ensemble-member models.
- Explaining the importance of an appropriate summary statistic (median instead of mean) when calculating the average error over time.
- Explaining the importance of considering time-steps when a sufficient number of filters are still running when collecting summary statistics of multiple filter runs.
- Using EnKF to improve the accuracy with which an ABM simulates a pedestrian system.

Other things to mention in the introduction:

- Pseudo-truth data. "The purpose of the base model for these experiments is simply to provide a state against which to compare the performance of filters."
- Broad overview of the experimental approach (how do the experiments show that the EnKF is/isn't working?)

# 2 Background

Write background

- Discuss previous relevant work:
  - Ward et al. (2016)
  - Malleson et al. (2020)
  - Clay et al. (2020)

# 3 Methods

Write methods

## 3.1 Model

Explain about `StationSim_GCS`.

Things to note:

- What an 'active' agent is
- Which model variables are known to the ensemble models (start gate and exit gates?)
- 'side stepping' behaviour the agents use to avoid each other and obstacles.

## 3.2 Ensemble Kalman Filter

- Explain about the Ensemble Kalman Filter (Evensen, 2003), which is based on the Kalman Filter (Kalman, 1960).
- Point to previous experiments in the thesis. E.g. "Results: The data assimilation scheme was tested for a range of different filter parameter values, and it was found that improvements in filter performance resulted from increases in the ensemble size, reductions in the standard deviation of the observation error and reductions in the number of time-steps between successive attempts to assimilate observational data into the system." (p113)

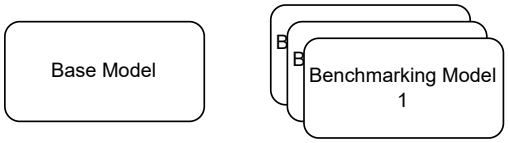
# 4 Experiments

The experiments, outlined visually in Figure 1, aim to demonstrate that the EnFK can improve the accuracy of a pedestrian system in comparison to a baseline scenario with no data assimilation. In order to better understand the impact of data assimilation on an agent-based model, rather assess the realism of the model itself, we use the "identical twin" approach **?**. In this approach, a 'Base Model' is used. A Base Model is an instance of `StationSim_GCS` that is used to generate 'pseudo-true' data that are taken as the real-world observations in the experiments (in lieu of data from a real crowd).

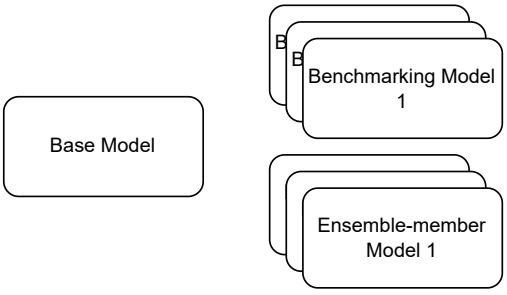
The initial experiment, ('benchmarking', Figure 1a) seeks to establish a benchmark against which to compare subsequent implementations of the EnKF. This is achieved by running an ensemble of models, each initialised as duplicates of a base model which is used to generate pseudo-truth values for the system state.

The second experiment (Figure 1b) seeks to XXXX. It does this by exploring the

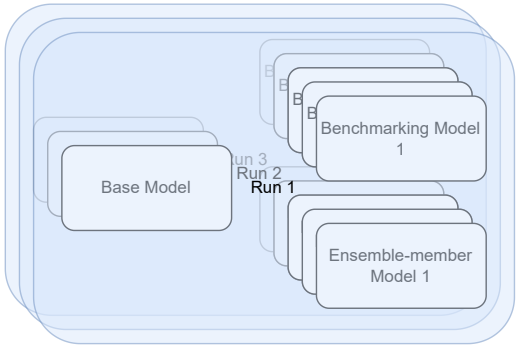
Keiran what is the higher-level purpose of this experiment?




(a) Experiment 1: Benchmarking




(b) Experiment 2: Exploring Ensemble-Member Models




(c) Experiment 3: Implementing the Ensemble Kalman Filter

Figure 1: Graphical outline of the three experiments. Note that the 'base model' is use to generate pseudo-true observation data

variation in the accuracy of individual ensemble members. This is achieved by running a single EnKF which maintains a benchmarking ensemble of models, providing a baseline against which to compare results, along with and ensemble of models that are periodically updated by the EnKF assimilation process. In such a situation, we are able to compare the average error per agent in each of the ensemble member models at each assimilation time-step.

The final experiment (Figure 1c) takes this exploration a step further by seeking to capture the variation in error at an ensemble level. This involves running a collection of EnKFs for the same set of model and filter parameters, and in each case gathering data regarding the variation in the error in the ensemble mean state over time, comparing this with the variation in the corresponding collection of benchmark errors.

Again, why?

## 4.1 Measuring Error

- Talk about measures used when running experiments with multiple EnKFs to ensure that outliers don't skew results:
  - Median instead of mean error.
  - Only considering time-steps when a sufficient number of models are active.

## 4.2 Active and inactive agents

As the following sections will discuss, error is calculated by comparing the positions of agents in the simulation with the positions of corresponding agents in the base model (i.e. the pseudo-truth data, discussed in Section 4). To do this, it is necessary to consider whether an agent is 'active' or 'inactive' as once an agent has left the simulation they should not be included in an error calculation. However, an agent might be active in the base (pseudo-truth) model and inactive in some or all of the EnKF ensemble members, or vice versa. Here we assume that an agent is active only while it is active in the EnKF ensemble because in a real situation we would not necessarily have access to the true positions of the individuals in the crowd, so could only assess an agent's status from the information available in the ensemble of models. Hence an agent is considered active if its most common (i.e. modal) status across the ensemble is active.

### 4.2.1 Agent-level error

Error at the level of the individual agents is quantified by calculating the distance between the position of an agent estimated by the ensemble of models in the EnKF (the 'ensemble mean state') and the position of the corresponding agent in the base model, $d_i$:

$$d_i = \begin{cases} |\hat{\mathbf{x}}_i - \mathbf{x}_i| & \text{if } i\text{th agent is active;} \\ 0 & \text{otherwise,} \end{cases} \tag{1}$$

where $\hat{\mathbf{x}}_i$ is the $x$-$y$ position of the $i$th agent estimated by the ensemble of models and $\mathbf{x}_i$ is the $x$-$y$ position of the $i$th agent in the base model. The distance between the $\hat{\mathbf{x}}_i$ and $\mathbf{x}_i$ agent is calculated using the Euclidean distance.

### 4.2.2 Model-level error

To calculate the error across the whole system, we calculate the average distance over all active agents in the system, $\bar{d}$:

$$\bar{d} = \frac{1}{N} \sum_{i=1}^{N} d_i, \tag{2}$$

where $N$ is the number of *active* agents. This average distance, $\bar{d}$, can then be used to measure the error in an ensemble of models given the ensemble mean state for a given time-step and the base model state at the same time-step. In this way, we create a base model which is used to generate a ground truth and an ensemble of models from which we can obtain the average behaviour behaviour by averaging across the ensemble. The accuracy with which this average behaviour simulates the ground truth generated by the base model is assessed by considering the error between the base model and the average of the ensemble.

### 4.3 Experiment 1: Benchmarking

The initial experiment to be performed is to develop a model baseline, establishing the effectiveness of `StationSim_GCS` in modelling a system in the absence of any information whilst running.

Is this what the experiment actually does, or is it more about quantifying the uncertainty in the simulation? Aka "ensemble variance"?

This is applied to ensembles with increasing population sizes (as per Table 1) to explore how this behaviour varies with population size.

Should we remove the last four rows in the table because these are fixed?

| Parameter | Value |
|---|---|
| Population size | $[10, 20, 50, 100]$ |
| Ensemble size | 100 |
| Number of entrances | 11 |
| Number of exits | 11 |
| Environment height | 700 |
| Environment width | 740 |

Table 1: Table of model parameters used for estimating the baseline level of error.

In the benchmarking experiments, the following approach is taken:

1. Create an instance of the model to be considered the base model which provides pseudo-truth states of the pedestrian system.

2. Create an ensemble of 100 models, each of which is a copy of the base model; this means that each of the duplicates in the ensemble contain the same information regarding which exits each of the agents will enter and exit through, as well as at what time they will be activated within the model. These models, however, are liable to diverge from the base model due to the collisions that occur between pedestrian agents.

3. Iterate each of the base model and the ensemble of models forward for each time-step. At each time-step, calculate average model state for each agent in the system population, and calculate the average error per agent between this average model state and the pseudo-truth state generated from the base model for this time-step.

### 4.4 Experiment 2: Exploring Ensemble Members

Better word than 'exploring' above? Something more specific?

After having established a benchmark for the accuracy with which the `StationSim_GCS` model can simulate the trajectories of pedestrians moving around the concourse of Grand

Central Station in New York), the next experiment aims to explore the variation amongst the models *within* the ensemble of an EnKF whilst observations are being assimilated into the ensemble. In order to achieve this, rather than calculating the distance between the ensemble mean state and the base model state (as per (1)), the error is calculated by the distance between each of the ensemble member model states and the base model state. If we consider $d_{ij}$ to represent the distance error of the $j$th model's state for the $i$th agent compared to the $i$th agent in the base model, this can be calculated as follows:

(earlier point about

Explain why this is important

$$d_{ij} = \begin{cases} |\hat{\mathbf{x}}_{ij} - \mathbf{x}_i| & \text{if } i\text{th agent is active;} \\ 0 & \text{otherwise,} \end{cases} \tag{3}$$

where $\hat{\mathbf{x}}_{ij}$ is the $x$-$y$ position of the $i$th agent in the $j$th model and $\mathbf{x}_i$ is the $x$-$y$ position of the $i$th agent in the ground state system, i.e. the base model. Given this expression, we adapt (2) slightly to calculate the mean error per agent for each ensemble member model, $\bar{d}_j$, at a given time-step as:

$$\bar{d}_j = \frac{1}{N} \sum_{i=1}^{N} d_{ij}. \tag{4}$$

Based on this, we can construct a vector containing all of the mean errors per agent for each of the ensemble member models:

$$\bar{\mathbf{d}} = \left[\bar{d}_1, \ldots, \bar{d}_M\right] \tag{5}$$

$$= \left[\bar{d}_j\right], \forall j \in (1, M), \tag{6}$$

where $M$ is the ensemble size. A vector of average errors per agent for each ensemble member models can then be calculated for each time-step.

Based on this error calculation process, we can explore the variation of error across the ensemble using the following steps:

1. Create an EnKF with a population size of 20 pedestrians, containing a base model and an ensemble of 20 duplicates (prior experimentation showed only marginal performance improvements above an ensemble size of 20 members.

   ref Keiran thesis

2. Iterate each of the base model and ensemble of models forward for each time-step. If the time-step is an assimilation time-step, i.e. a time-step in which synthetic data are produced from the base model, the ensemble of models are updated using the update procedure outlined in Section 3.2. Assimilation time-steps occur with a fixed period of 20 time-steps. At each assimilation time-step, errors are calculated between the following pairs:

   - The base model state and each of the ensemble member models, as per (**??**) , after updating with observations.
   - The base model state and the mean state of the ensemble of models, as per (**??**), after updating with observations.
   - The base model state and the mean state of the benchmarking ensemble (i.e. the baseline error), as per (**??**).

   Keiran could you refer to the specific equations here?

Need a table of parameters like Table 2?

### 4.5 Experiment 3: Assessing the EnKF

The previous experiments will show that, as expected, the error in the ensemble mean state accurately reflects the variation in error over time, and that it does not differ greatly from the error in each of the ensemble member models. On this basis, this final experiment focusses on comparing the variation in the ensemble mean state error over time with the error in the benchmarking ensemble as well as with the error in the observations of the pedestrians' locations on the station concourse. This considers both the ensemble mean state before and after assimilating observations, i.e. the forecast error and the analysis error. The experiment will make use of the parameters outlined in Table 2.

| Parameter | Value |
|---|---|
| Population size | 20 |
| Ensemble size | 100 |
| Assimilation period | 20 |
| Observation noise standard deviation | 1.0 |

Table 2: Table of filter parameters used for the EnKF.

As with the benchmarking experiment, errors are calculated as the distance between the 'estimated' agent location and the agent's location in the pseudo-truth base model; see (1). Note that in this case, there are different ways to 'estimate' an agent's location and hence calculate error. We calculate the following errors:

- the base model state compared to the forecast ensemble mean state (i.e. the prior error);
- the base model state compared the analysis ensemble mean state (i.e. the posterior error);
- the base model state compared to the observations provided to the ensemble for updating (i.e. the observation error);
- the base model state compared to the mean state of the benchmarking ensemble (i.e. the baseline error)

We use all of these methods and in each case the distance is calculated in the same manner. Consequently, an average error in each of the four state estimates across all pedestrians can also be calculated in the same manner as per (2).

We explore the variation of error across the ensemble using the following steps:

1. Create an EnKF containing a base model and an ensemble of 20 duplicates of the base model.
2. Iterate each of the base model and ensemble of models forward for each time-step, updating the ensemble using the data assimilation outlined in Section 3.2 every 20 time-steps, calculating the errors using the four methods above.

This process is repeated 20 times for the same model and filter parameter values.

## 5 Results

### 5.1 Experiment 1: Benchmarking

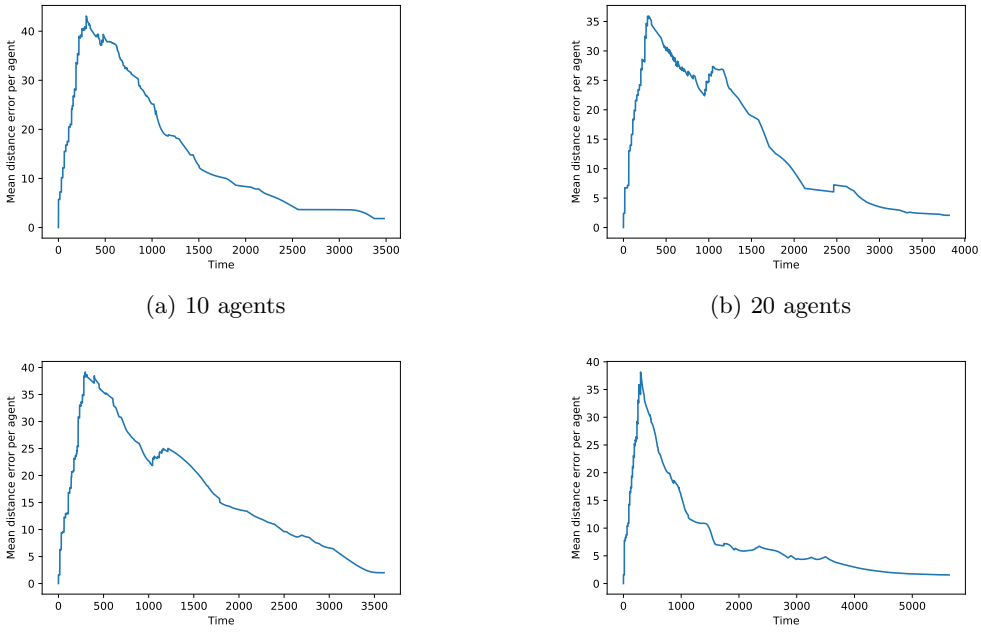
The results of Experiment 1 are shown in Figure 2, illustrating how the error varies between a benchmark model (i.e. pseudo-truth data) and an ensemble of 100 models

(without data assimilation) as the population size increases. Each of the time-series follows a similar trajectory. The initial error per agent is very low as the starting locations of the agents are known to the ensemble, but it rises sharply as agents begin to move across the environment towards their respective exit gates. The common peak in error is a consequence of the *activation rate* parameter that controls the rate at which agents enter the environment and effectively places an upper limit on the number of agents that can be present in the model at any one time. The peak in error simply at the point in time when the environment contains the largest number of agents.

The error itself is largely attributed to two factors: variations in the precise location along a gate at which an agent enters (although the entrance gate for each agent is known, the exact position within a gate is random) and the number of agent-agent interactions. At lower agent population sizes, the latter is likely to contribute less towards the error with fewer interactions occurring.

Note: have some commented text about how to contextualise the error if we think we need it (I don't think so).

Kieran can you reproduce Figure 2 so that the y axes are the same in each sub-figure? (If it's a pain don't worry, we'll see if the reviewers pick up on it.)




(a) 10 agents

(b) 20 agents

(c) 50 agents

(d) 100 agents

Figure 2: Variation in average error per agent with model time for different population sizes.

In summary, the aim of Experiment 1 has been to create a benchmark estimate for the level of error that might be exhibited *without* data assimilation. Having established this benchmark, the following experiment explores how error varies when data assimilation is implemented.

## 5.2 Results 2: Exploring Ensemble Members

Experiment 2 consists of running a filter that contains an ensemble of models (the 'filter ensemble') that undergo data assimilation alongside a benchmarking ensemble of models (the 'benchmark ensemble') that have no data assimilation. Both of these ensembles are compared to observations generated by a single base model (the 'pseudo-truth' data). This allows us to compare the performance of the filter ensemble against a similar ensemble that has no data assimilation and, importantly, allows us to compare the distribution of errors *within* the filter ensemble by examining the errors in the individual ensemble models.

### Overall Filter Performance

Figure 3 demonstrates that, as expected, the benchmarking error is much larger than the average error per agent calculated from the filter ensemble mean state. As with previous experiments, the benchmarking error is high at beginning of the experiment and declines over the course of the filter run.

Keiran why in Figure 3 does the error start high (60+) whereas in the previous experiment, Figure 2 it starts at 0?

This shows us that the Ensemble Kalman Filter is extremely effective at using observations to reduce the error in the ensemble.

Keiran please check this last sentence is right.

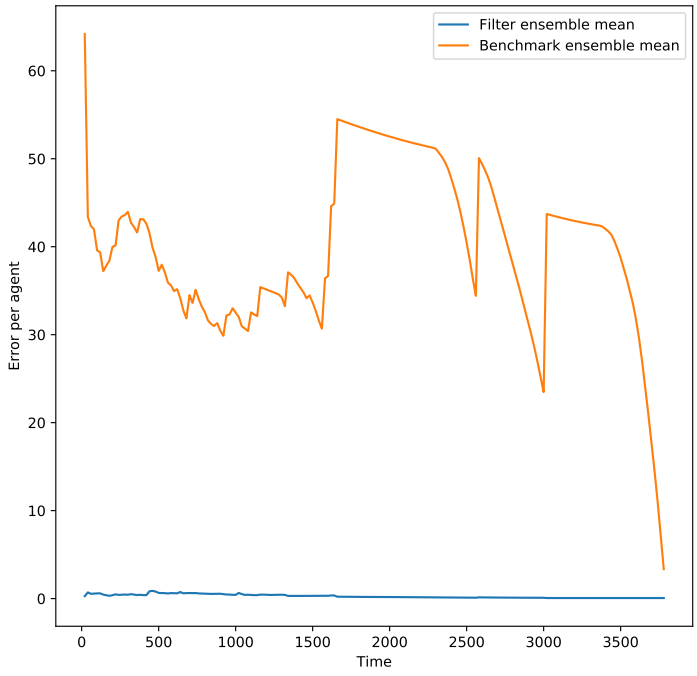
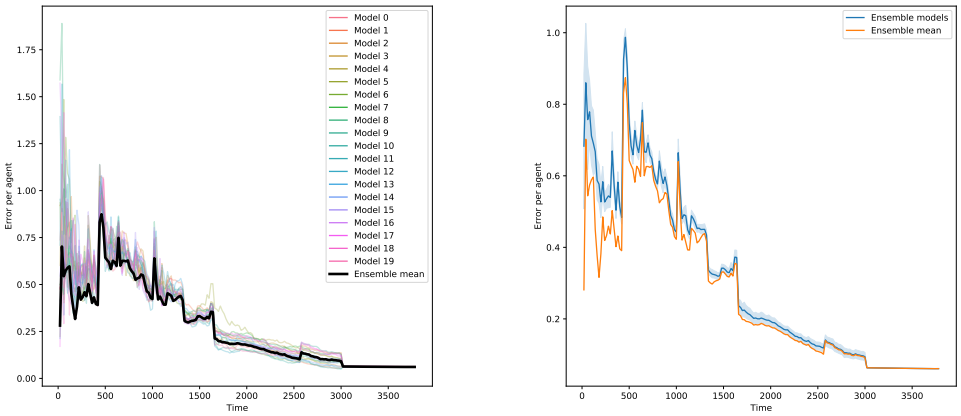



Figure 3: Line plot of the average error per agent based on the mean state of the benchmarking ensemble and the mean state of the filter ensemble.

**Within-Filter Performance**

We can now explore how the average error per agent varies across the filter ensemble member models and how this compares to the ensemble mean state. This is shown in Figures 4a and 4b respectively. In Figure 4a, the average error per agent is plotted for each ensemble member model as well for the ensemble mean state (plotted in bold black). We can see that the variations in the error in the individual models largely mirror those seen in the ensemble mean state error. Importantly, we see that the error per agent is considerably lower when the filter is used in comparison to the benchmark.

Keiran why is this important?




(a) Error per agent based of each ensemble member.

(b) Average error per agent from all ensemble member models, with confidence intervals.

Figure 4: Comparing the ensemble mean error with the errors of the filter ensemble members.

It is worth nothing that the error in the ensemble mean state appears to typically be lower than the errors in the majority of the individual models. This is further supported by Figure 4b which, rather than showing the error of the individual models, plots the mean of the model errors and the 95% confidence interval around it. Whilst we may have expected that these two sets of errors would be identical, this is not the case. However, this is not surprising with hindsight if we consider the hypothetical example illustrated in Figure 5. It immediately becomes clear that the mean agent location (the 'ensemble mean') is likely to have a lower error than the mean of the errors of the individual ensemble members.

In summary, this experiment has demonstrated ...

Keiran what do you think are the main takeaway messages from this section? Other than the Filter is good!

## 5.3 Results 3: Assessing the EnKF

Having established a model baseline level of error and undertaken some exploration of the variation in error across the ensemble-member models within an EnKF, this section completes the experiments by assessing the success of the EnKF as a means of updating an ABM in real time and explores some of the emerging challenges.

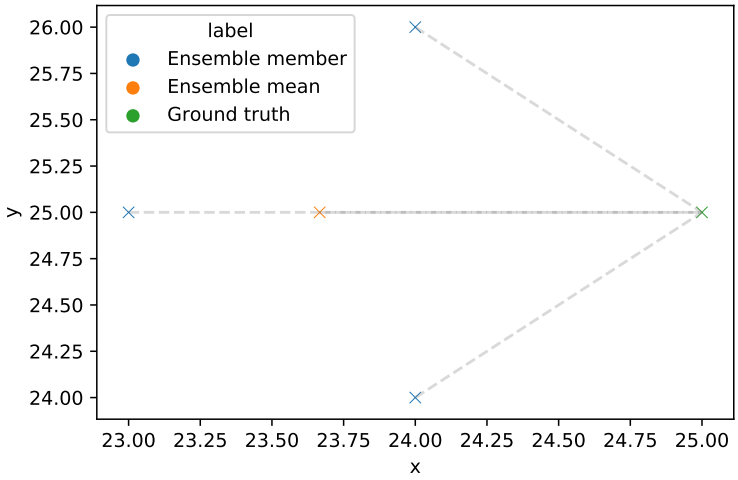



Figure 5: Working example — calculating error based on the ensemble mean compared to the mean error of each individual member models.

NM: is it clear that this section is all about error per agent, not aggregate performance?

### Agent Behaviour under EnKF

It is illuminating to explore the behaviour of the individual agents as their state variables are manipulated by the EnKF. To this end, Figure 6 illustrates the prior and posterior positions of two individual agents ('agent A' and 'agent B'). When comparing the prior and posterior for both agents, we see that the introduction of observations through data assimilation has resulted in the reduction in the spread of the ensemble-member model representations of the agents, i.e. the uncertainty in the model estimate of the positions has been reduced. This pattern is observed across the other agents in the system.

Having established the ability of the EnKF to reduced the uncertainty in the estimates of pedestrians' positions in the environment, we see to tackle a number of additional challenges.

It's great to see that actual impact of the filter on the estimated positions. Any room to elaborate further on this result? Maybe a comparison with the baseline? It just feels as though the section ends a bit abruptly.

### Managing Outliers

When running a large number of filters with the same filter and model parameters, there is inevitably some variation in the results. This pertains to both the way in which the average error per agent varies over time, and the length of time a filter takes to reach completion. Whilst the majority of the filters reach completion within the first 4500 time-steps, which is consistent with the baseline, some do not until approximately 10000 time-steps. This is evidenced in Figure 7. These outliers must be removed as they artificially increase the apparent error of the filter. Hence when calculating error, time-steps after which 90% of the models have completed (typically around 5000 time-steps

Briefly, why does this happen? I'd query this if I were a reviewer.

Is 5000 correct?

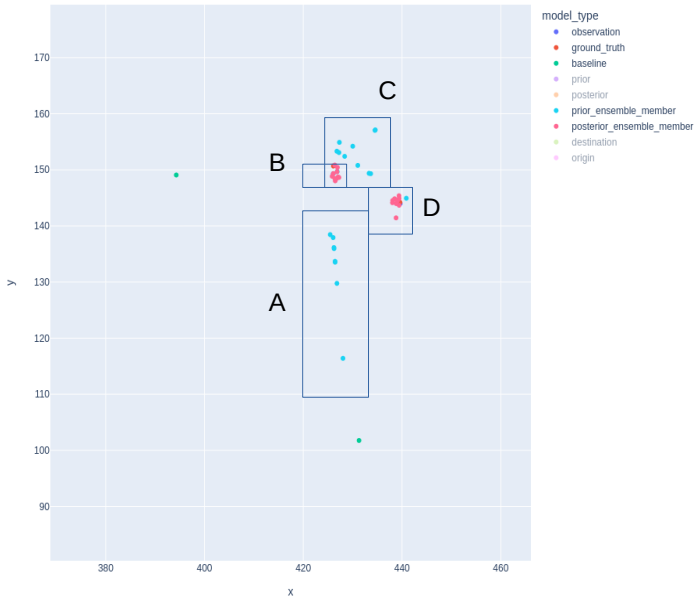



Figure 6: Comparison of prior and posterior positions (in blue and pink, respectively) of two agents ('A' and 'B') in all ensemble member models. Boxes A and B: the prior and posterior positions of agent A. Boxes C and D: the prior and posterior positions of agent B.

are disregarded. In addition, the median, rather than the mean, is used to summarise the overall error per agent.

### Filter Performance

When assessing the average error per agent, three comparisons need to be drawn: (i) benchmarking ensembles against the analysis of the filter ensembles; (ii) the forecast of the filter ensembles against the analysis of the filter ensembles; (iii) and the observations against the analysis of the filter ensembles. This section goes on to explore each of these comparison. In each case, the comparison is aided by the use of two figures:

- a line plot of the average error per agent over time where the line represents the median of the collection of filters at each time-step and the shaded area represents the 95% confidence interval around the line;
- a boxplot showing the distribution of these errors when aggregated over time (logged to reduce the visual impact of the skewed distributions);

Figure 8 plots the median error per agent by comparing the benchmarking ensembles to the analysis of the filter ensembles. In Figure 8a, we can see that the average error per agent in the filter analysis states is much lower throughout. This is echoed by the logged boxplot in Figure 8b. The majority of the logged data pertaining to the analysis error lie below 0, indicating that the average error per agent for the analysis is often below 1. In the case of the benchmarking data, however, the majority of the data lie above 0, indicating that in most cases, the average error per agent for the benchmarking ensembles is much higher.

why does it increase at the end?

Figure 9 compares the average error per agent in the forecast and analysis states of the filter model ensembles, i.e. the error before and after assimilating data at each time-step.

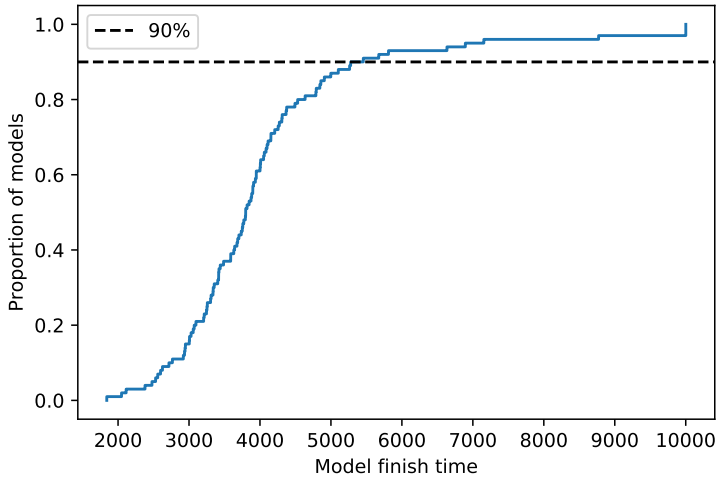
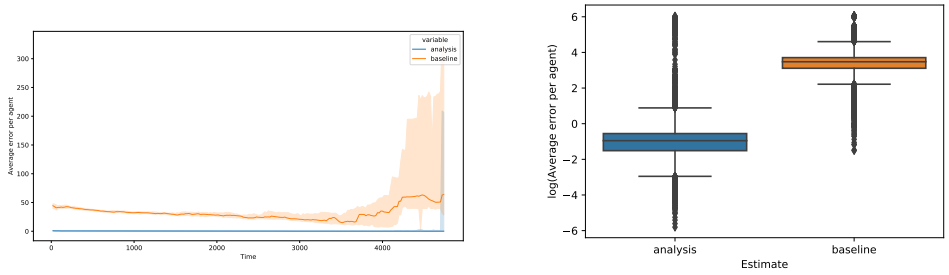



Figure 7: Empirical cumulative distribution function (eCDF) plot of filter finish times; dotted line represents a cumulative level of 90%.

We see that the error in the analysis state is typically an improvement on the error in the forecast state, with the improvements being most noticeable at the beginning of the set of time-steps and at the end of the time-steps (Figure 9a). The difference at the beginning is due to the reasoning outlined in Section **??** — the entrance of multiple agents at the beginning of the filter run time and the entry of agents at points on the gates that do not match the exact entry point of corresponding agents in the base model lead to an initial growth in error. The error in the analysis state does not suffer from this growth as it is updated by the provided observations. The increase in the variance of the errors towards the end of the experiment is a consequence of many filters reaching completion and hence the summary statistics being drawn over a decreasing number of filters. Furthermore, Figure 9b illustrates that, again, the majority of the data lie below 0, indicating that the average error per agent in each case often lies below 1.

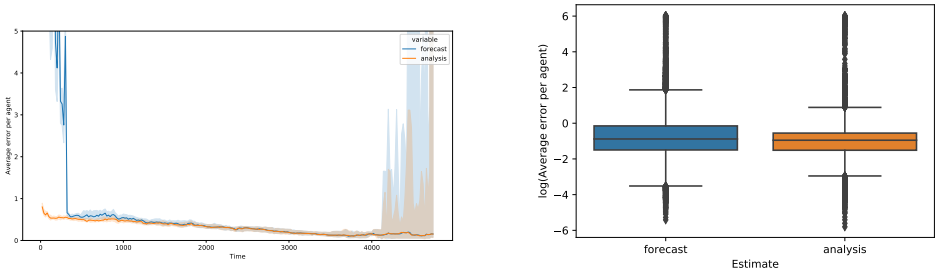
fix ref

Finally, Figure 10 compares the variation of the average error per agent in the (pseudo-




(a) Line plot of average error per agent over time. (b) Box plot of log of average error per agent.

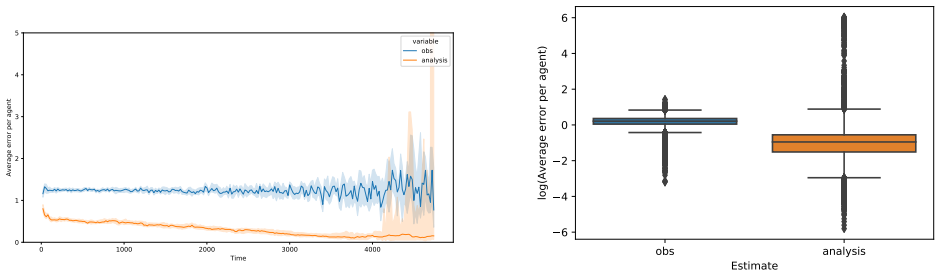
Figure 8: Comparison of average error per agent between analysis and benchmarking filters




(a) Line plot of average error per agent over time. (b) Box plot of log of average error per agent.

Figure 9: Comparison of average error per agent between analysis and forecast.

true) observations and the analysis states of the filter model ensembles. The average observation error is largely constant throughout the experiment (Figure 10a). The increase in error variance is again caused by averaging over a decreasing number of filters. In comparison to the observation error, the analysis error is typically lower for the majority of the time-steps for which the filters are running. This is not always the case, however, as highlighted in Figure 10b. In each case, the errors appear to be low; however, there are substantial outliers pertaining to the analysis error. The observation error, on the other hand, contains relatively few outliers. This is a consequence of how the observations are produced; by adding normally distributed random noise to the base model state.




(a) Line plot of average error per agent over time. (b) Box plot of log of average error per agent.

Figure 10: Comparison of average error per agent between analysis and observations.

# 6 Conclusion

Write conclusions

# References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