

# TIF345/FYM345 Project3: A Galton board on a rocking ship

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# Introduction

The Galton board, or “bean machine,” is a classic demonstration of the central limit theorem, traditionally producing a binomial-like distribution of beads as they fall through a grid of pegs [1][2]. In this project, the problem is extended by introducing two additional parameters that influence the bead trajectories: an inertia parameter  $\alpha$ , which makes it more likely for a bead to continue falling in the same direction as its previous step, and a slope parameter  $s$ , modeling a rocking base that tilts the board slightly and biases the bead distribution. Estimating these hidden parameters from observed distributions is challenging because the likelihood function  $p(y_m|\alpha, s)$  is analytically intractable. Thus, we employ Approximate Bayesian Computation (ABC), a likelihood-free inference method, to infer  $\alpha$  and  $s$  by simulating outcomes under various parameter guesses and comparing them to experimental results. To improve both the efficiency and the precision of this inference, we further integrate a neural network, trained to map observed bead distributions to parameters, thereby providing better proposals for the ABC routine. By combining simulation, Bayesian inference, and machine learning, we seek a robust and computationally tractable approach to uncovering these hidden parameters in a complex physical system.

## Background, Data Generation and Simulation

A Galton board simulator was constructed to generate synthetic data. At each peg, the bead falls to the left or right with probability:

$$P_{\pm} = 0.5 \pm (\alpha M + s), \quad (1)$$

where  $\alpha$  controls the inertial bias and  $s$  the slope-induced bias. The parameter  $M$  encodes the previous bead’s direction, set to 0.5 if the bead last fell to the right and  $-0.5$  if it fell to the left. Initially,  $M = 0$  for the first peg.

We sampled  $\alpha$  from  $[0, 0.5]$  and  $s$  from  $[-0.25, 0.25]$ , ensuring a reasonable range that introduces noticeable biases without degenerating the distribution. For each  $(\alpha, s)$  pair, multiple simulations of 1000 beads passing through 31 rows of pegs were conducted. The final positions of these beads were recorded, producing a variety of outcome distributions that reflect different underlying parameters. All simulations were performed in a Linux environment, orchestrated by Python scripts and shell commands. The output was stored as NumPy arrays for convenient retrieval and subsequent analysis, ensuring a reproducible data-generation pipeline [3].

Figure 1 presents three plots demonstrating the effect that  $s$  and also  $\alpha$  has on the shape of the distribution. The  $s$  introduces a skewness in the distribution, a high  $s$ -value shifts the distribution to more often fall to the right.  $\alpha$  affects how narrow the distribution is, a higher value indicates that the beads are more spread out than other ones. Using more beads would create a smoother distribution as it is now rough.

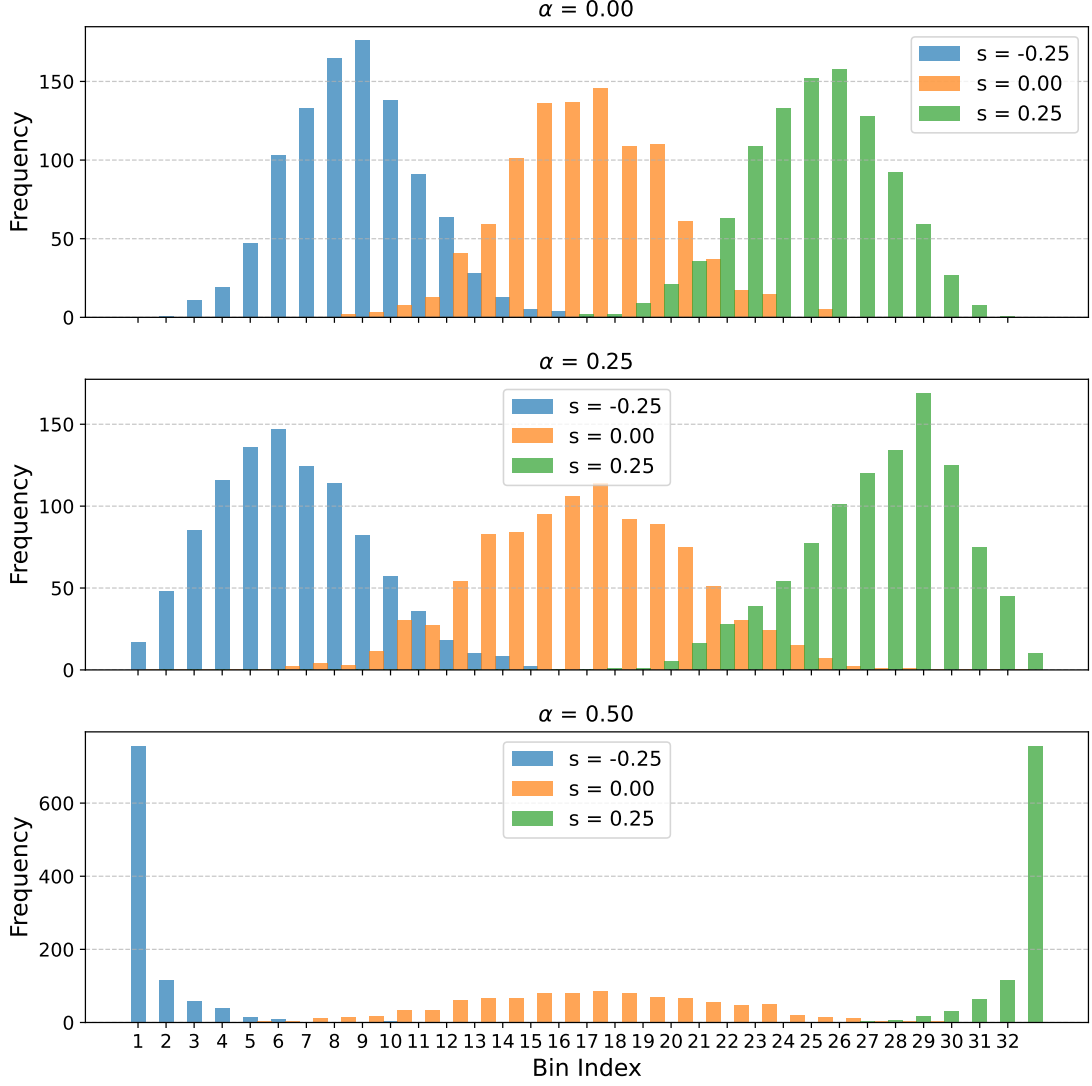


Figure 1: Simulation of 1000 beads for three different  $\alpha$ -values and three different values of  $s$ .

## Approximate Bayesian Computation (ABC) Framework

In implementing the ABC framework for this problem, the objective was to infer the most probable values of  $\alpha$  and  $s$  by simulating synthetic data and comparing it against observed outcomes. Since directly evaluating the likelihood function  $p(y_m|\alpha, s)$  is not feasible, ABC provides a likelihood-free inference method. To initialize ABC, appropriate summary statistics  $s(y)$  and a kernel function  $K(0)$  were selected. Based on the observation that the final bead distribution, though discrete and influenced by binomial dynamics, can be approximated by a normal distribution, the mean and variance of the normalized distribution were employed as summary statistics [4].

A Gaussian kernel was chosen to measure the distance between the observed and simulated summary statistics. The kernel bandwidth  $h$  was determined through experimentation, aiming for a balance between computational efficiency and the quality of the posterior approximation. Here,  $h$  was tuned to achieve an acceptance probability of ap-

proximately 5%. The chosen kernel has the form:

$$K((s(y^*) - s(y_{obs}))/h) = \exp\left(-\frac{|s(y^*) - s(y_{obs})|^2}{2h^2}\right). \quad (2)$$

Within the implemented code,  $\alpha$  and  $s$  are drawn uniformly from their respective prior ranges, a Galton board simulation is run to produce a candidate dataset  $y^*$ , and  $s(y^*)$  is then computed and compared with  $s(y_{obs})$ . The kernel value derived from this comparison serves as the acceptance probability in a rejection sampling scheme, progressively building an approximate posterior distribution for  $\alpha$ . Concretely,  $\alpha$  and  $s$  are sampled from uniform distributions, a simulation is generated, and its summary statistics are computed alongside those from a randomly chosen experiment  $y_{obs}$ . The Gaussian kernel, which does not require a normalization coefficient since  $K(0) = 1$ , determines whether the simulated result is accepted. This process repeats until a sufficient number of samples are collected to form a histogram of the posterior estimates.

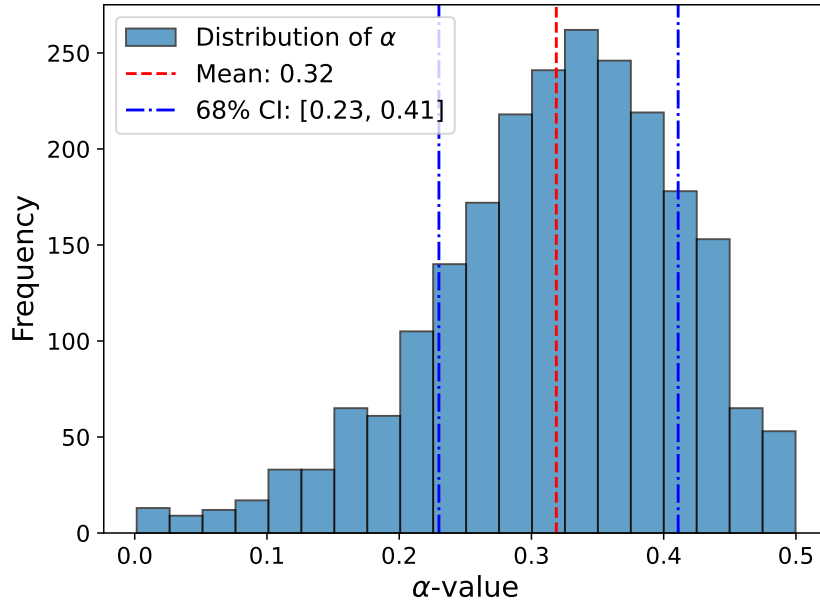


Figure 2: Histogram of sampled  $\alpha$  values from the posterior distribution using the ABC framework.

Although this initial ABC routine successfully produces posterior estimates, it often yields wide credible intervals. This is due in part to the simultaneous inference of two parameters ( $\alpha$  and the latent slope  $s$ ) and the relatively simple summary statistics, which may not fully capture the underlying dynamics. To improve upon this approach, one can integrate a neural network to provide more informed initial guesses or use importance sampling and sequential Monte Carlo (SMC) methods to refine the posterior. However, as illustrated in Figure 2, these initial attempts without additional refinements do not strongly constrain the value of  $\alpha$ , highlighting the need for further methodological enhancements.

## Neural Network-Based Parameter Estimation

To counter the effect that the bias  $s$  has on the simulation and experimental values, a neural network is trained on 100000 simulations. The simulations was split into a training set with 80% of the data and the rest as validation data. The data was standardized as the output neurons are of different scales and it is good practice to scale data for Neural networks. The network that was used has then 32 input neurons, then two layers with first 128 and 64 neurons and finally the two output neurons. The activation function is ReLU. As  $\alpha$  and  $s$  are on different scales, all data has been standardized for better performance of the network.

The training process is illustrated in Figure 3, which shows both training and validation root-mean-square error (RMSE) decreasing over 100 epochs, indicating stable convergence. For the validation set, the RMSE was approximately 0.0220 for  $\alpha$  and 0.0051 for  $s$ , suggesting that the NN learned a reasonably accurate mapping from final distributions to parameters.

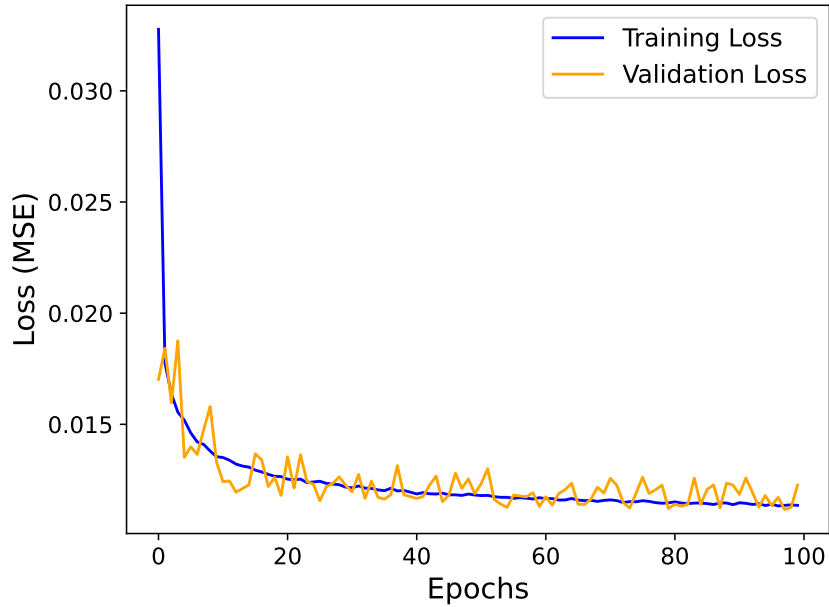


Figure 3: Training and validation loss (RMSE) over 100 epochs, showing model convergence during training.

The accuracy of the NN predictions is further demonstrated in Figure 4, where predicted versus true values are plotted for both parameters. The dashed red line represents the ideal scenario where predictions match true values exactly. While the NN performs well on both parameters, it shows notably higher accuracy for  $s$ . This is likely because changes in the slope  $s$  produce more symmetric or asymmetric shifts in the bead distribution, making  $s$  easier to identify. In contrast, the inertial bias  $\alpha$  affects the beads' trajectories more subtly, resulting in slightly less precise estimates.

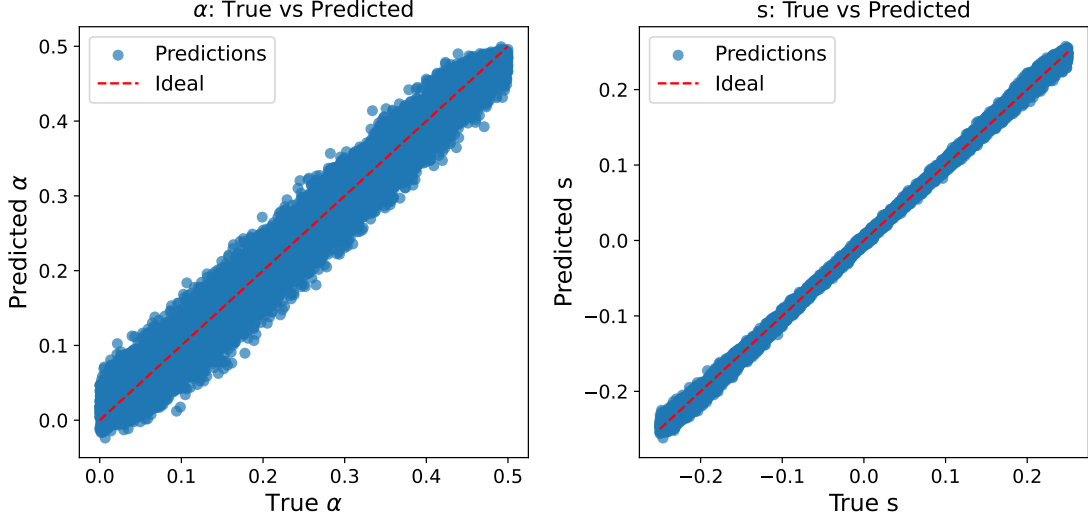


Figure 4: True vs. predicted values for  $\alpha$  (left) and  $s$  (right), demonstrating the accuracy of the ABC model.

By providing a more accurate initial estimate for  $s$  (and a reasonable guess for  $\alpha$ ), the NN can serve as a valuable tool to guide the ABC routine. Rather than starting from a broad uniform prior, ABC can be initiated with proposals informed by the NN’s predictions. This approach reduces the effective dimensionality of the search and may lead to more efficient posterior refinement, especially when combined with iterative ABC techniques.

## Integrating the Neural Network into ABC

Having established that the neural network (NN) can provide accurate estimates of  $s$  and a reasonable guess for  $\alpha$ , we now integrate these predictions into the ABC framework. The key idea is to use the NN’s output to concentrate our parameter search around the predicted value for  $s$ . By replacing the broad uniform prior on  $s$  with a localized proposal distribution centered on the NN estimate, we effectively reduce the complexity introduced by the latent slope parameter.

Concretely, given an observed experiment  $y_{obs}$ , we pass it through the NN to obtain a predicted slope  $\hat{s}$ . To acknowledge the uncertainty in this prediction, we perturb  $\hat{s}$  by drawing from an error model  $g(|z - z^{ML}|)$ , where  $z$  represents a candidate slope and  $z^{ML}$  could be the NN’s maximum likelihood estimate for  $s$ . This ensures that we still explore a neighborhood around the NN prediction rather than treating  $\hat{s}$  as fixed. The prior for  $s$ , denoted as  $\pi_z(z^*)$ , now reflects this localized approach, shifting from a uniform range to a distribution concentrated around  $\hat{s}$ .

The acceptance probability in the modified ABC step remains governed by the kernel  $K$ , but now incorporates these adjusted priors and the error model. Specifically, the acceptance probability can be written as:

$$p_{\text{acceptance}} = \frac{K((s(y^*) - s(y_{obs}))/h)\pi_z(z^*)}{g(|z - z^{ML}|)m}, \quad (3)$$

where  $m = \max_{\alpha, z} (K(0)\pi_z(z^*)/g(|z - z^{ML}|))$  is a normalizing constant. Since  $m$  is independent of individual draws, it effectively cancels out as a scaling factor. This formulation

emphasizes that parameter draws closer to the NN-predicted  $s$  and consistent with the observed data  $y_{\text{obs}}$  are more likely to be accepted.

By incorporating the NN predictions, the ABC routine focuses on parameter values that yield bead distributions similar to the observed data. This informed search reduces the need to explore the entire parameter space blindly, thereby increasing efficiency and narrowing the resulting posterior distribution. As shown in Figure 5, the posterior distribution for  $\alpha$  is notably more concentrated than in the initial ABC approach, illustrating a visibly narrower credible interval.

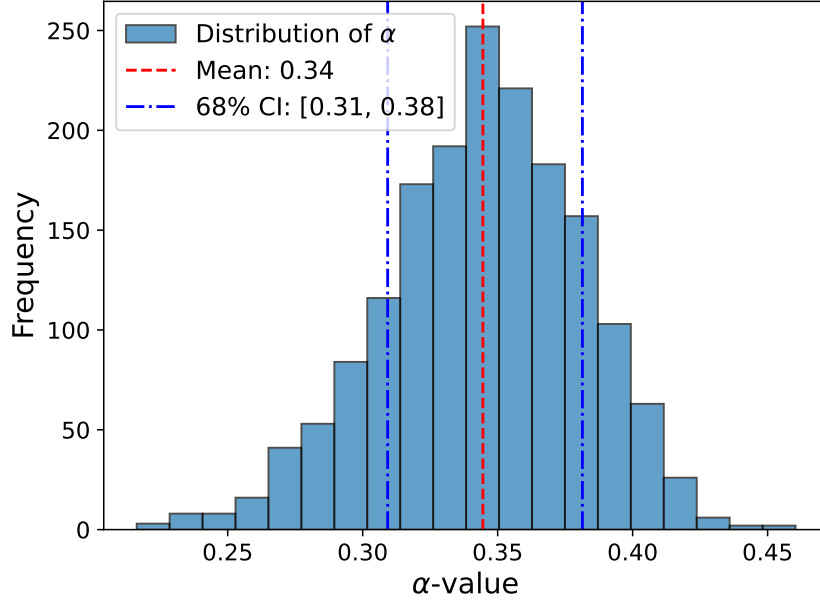


Figure 5: Posterior distribution of  $\alpha$  after NN-guided ABC, showing a narrower 68% credible interval.

## Iterative ABC

In this task, the ABC framework, combined with the neural network's predictions, is run iteratively to achieve a more refined posterior distribution for  $\alpha$ . Instead of starting with a uniform prior, the posterior distribution from the previous iteration is sampled and used as the prior for the next. This iterative process narrows the confidence interval for  $\alpha$ , as illustrated in Figure 6.

This iterative ABC approach effectively "zooms in" on the most likely values of  $\alpha$ . By using the posterior from one iteration as the prior for the next, the parameter space becomes increasingly concentrated around regions of higher probability. This not only improves the acceptance rate but also significantly reduces the range of plausible parameter values that need to be explored, yielding tighter credible intervals.

Figure 6 demonstrates the results after one additional iteration of ABC. Compared to the posterior distribution shown in Figure 5, the credible interval for  $\alpha$  is significantly narrower, reflecting the improved precision of the iterative process.

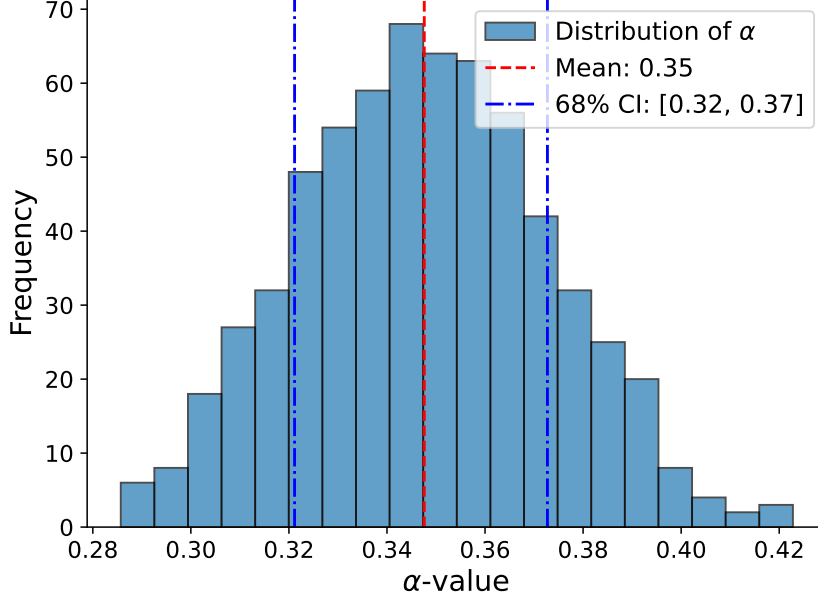


Figure 6: Posterior distribution of  $\alpha$  after iterative ABC with a narrower credible interval.

## Improvements for the ABC

There are several areas where improvements to the ABC routine could be implemented. One improvements is to increase the number of beads in the experiment, that would improve the currently used summary statistics as the central limit theorem is applied. Furthermore, different summary statistics could be tested more thoroughly to get a better understanding of the ABC method. In the basic approach that this project has been approached, this has not been explored.

The prediction for  $\alpha$  by the NN can be implemented into the ABC with latent variable elimination. It could serve as a prior for the  $\alpha$  values. The error associated with the NN can be included in the acceptance probability in the same manner as the  $s$ -variable.

Moreover, another methods like ABC-SMC (Sequential Monte Carlo) or ABC-MCMC (Markov Chain Monte Carlo) could be explored to adaptively refine proposals and thresholds during inference. By systematically reducing the bandwidth  $h$ , these methods focus sampling around the most plausible parameter values, accelerating convergence and improving posterior precision. These enhancements would make the ABC framework more robust, efficient, and accurate for complex parameter inference problems.



## References

- [1] Wikipedia contributors. The galton board. [https://en.wikipedia.org/wiki/Bean\\_machine](https://en.wikipedia.org/wiki/Bean_machine), 2024. Accessed: 2024-12-19.
- [2] Paul Erhart, Andreas Ekström, and Arkady Gonoskov. *Advanced Simulation and Machine Learning*. Lecture notes, 2024. Chapter 10.
- [3] Real Python Team. Introduction to pyenv: Manage multiple python versions and environments. <https://realpython.com/intro-to-pyenv/#virtual-environments-and-pyenv>, 2024. Accessed: 2024-12-19.
- [4] Scott A. Sisson, Yanan Fan, and Mark Beaumont. *Handbook of Approximate Bayesian Computation*. Chapman & Hall/CRC, Boca Raton, FL, 2019.

## Code

```
1  # %%
2  import numpy as np
3  import matplotlib.pyplot as plt
4  import scipy.stats as stats
5
6  # Set some default plotting parameters
7
8  plt.rcParams['font.size'] = 15
9  plt.rcParams['axes.titlesize'] = 14
10 plt.rcParams['axes.labelsize'] = 15
11 plt.rcParams['xtick.labelsize'] = 12
12 plt.rcParams['ytick.labelsize'] = 12
13 plt.rcParams['legend.fontsize'] = 13
14
15 # %%
16 # Step 1: Simulator for the Galton Board
17
18 def galton_simulator(alpha, s, num_rows=31, num_beads=1000):
19     """
20     Simulates the Galton board experiment for given \u03b1 (inertia) and s (
21         slope).
22
23     Args:
24         alpha (float): Inertia parameter.
25         s (float): Slope parameter.
26         num_rows (int): Number of rows in the Galton board.
27         num_beads (int): Number of beads to simulate.
28
29     Returns:
30         np.ndarray: Distribution of beads in the bottom cells (32,).
31     """
32     positions = np.zeros(num_beads, dtype=int)
33     for bead in range(num_beads):
34         M = 0 # No bias at the first peg
35         num_right = 0
36
37         for _ in range(num_rows):
38             prob_plus = 0.5 + (alpha * M + s)
39
40             # Randomly choose between 0 and 1 based on the probabilities
```

```

40         choice = 1 if np.random.rand() < probb_plus else 0
41
42         if choice == 1:
43             M = 0.5
44             num_right += 1
45         else:
46             M = -0.5
47         positions[bead] = num_right
48     return positions
49
50 def reshape_bin_array(data):
51     unique_positions, counts = np.unique(data, return_counts=True)
52     final_observed_data = np.zeros(32, dtype=int)
53     # Map the counts to their corresponding bins
54     for pos, count in zip(unique_positions, counts):
55         final_observed_data[pos] = count
56     return final_observed_data
57
58
59 # %%
60 alphas = np.linspace(0, 0.5, 3)
61 ss = np.linspace(-0.25, 0.25, 3)
62
63 # Create subplots for all alpha values
64
65 fig, axes = plt.subplots(len(alphas), 1, figsize=(10,10), sharex=True)
66
67 bar_width = 0.5
68
69 for ax, alpha in zip(axes, alphas):
70     all_observed_data = np.zeros((len(ss), 32), dtype=int)
71     i = 0
72     for s in ss:
73         observed_data = galton_simulator(alpha, s)
74         final_observed_data = reshape_bin_array(observed_data)
75         all_observed_data[i] = final_observed_data
76         i += 1
77
78     # Plot overlapping bar plots for each alpha
79     for idx, final_observed_data in enumerate(all_observed_data):
80         x_positions = np.arange(32) + idx * bar_width # Adjust x positions
81         # for overlapping
82         ax.bar(x_positions, final_observed_data, width=bar_width, label=f"s_{idx} = {ss[idx]:.2f}", alpha=0.7)
83
84     ax.set_ylabel('Frequency')
85     ax.set_title(rf'$\alpha$ = {alpha:.2f}')
86     ax.grid(axis='y', linestyle='--', alpha=0.7)
87     ax.legend()
88
89 # Add shared x-label for all subplots
90 plt.subplots_adjust(wspace=0, hspace=0)
91 plt.xlabel('Bin_Index')
92 plt.xticks(range(32), labels=range(1, 33)) # Set x-ticks for bin indices
93 plt.tight_layout()
94 plt.savefig('example_plots.pdf')
95 fig.suptitle
96
97

```

```

98 # %%
99 observed_data = galton_simulator(alpha=0.2, s=0.1)
100 unique_positions, counts = np.unique(observed_data, return_counts=True)
101
102 final_observed_data = np.zeros(32, dtype=int)
103
104 # Map the counts to their corresponding bins
105 for pos, count in zip(unique_positions, counts):
106     final_observed_data[pos] = count
107
108 print(final_observed_data)
109
110 plt.figure(figsize=(12, 6))
111 plt.bar(range(1, 33), final_observed_data, alpha=0.8)
112 plt.xlabel('Feature_Index')
113 plt.ylabel('Average_Value')
114 plt.xticks(range(1, 33)) # Set x-ticks for each column index
115 plt.grid(axis='y', linestyle='--', alpha=0.7)
116 plt.show()
117
118
119 # %%
120 def summary_statistics(data, arr_bin_index):
121     mean_bin_index = np.sum(data * arr_bin_index) / np.sum(data)
122     variance = np.sum(data * (arr_bin_index - mean_bin_index)**2) / np.sum(data)
123     #skewness = skew(data)
124     return np.array([mean_bin_index, variance])
125
126 def gauss_kernel(distance, h):
127     return np.exp(-0.5 / (h*h) * distance**2)
128
129 def abc_routine(experiment_data, num_samples, simulator, summary_func,
130                 num_rows, num_beads, h):
131     """
132     Approximate Bayesian Computation (ABC) routine.
133
134     Args:
135         experiment_data (np.ndarray): Observed data.
136         num_samples (int): Number of prior samples.
137         simulator (function): Simulator function.
138         summary_func (function): Function to compute summary statistics.
139         num_rows (int): Number of rows in the Galton board.
140         num_beads (int): Number of beads to simulate.
141         h (float): Bandwidth for the Gaussian kernel.
142
143     Returns:
144         np.ndarray: Accepted alpha parameters.
145         float: Acceptance rate.
146     """
147     alpha_prior = np.random.uniform(0, 0.5, num_samples)
148     s_prior = np.random.uniform(-0.25, 0.25, num_samples)
149     accepted_params = []
150     arr_bin_index = np.arange(1, 33, 1)
151     accepted_count = 0
152
153     for alpha, s in zip(alpha_prior, s_prior):
154         i = np.random.randint(0, len(experiment_data))
155         simulated_data = simulator(alpha, s, num_rows, num_beads)
156         simulated_data = reshape_bin_array(simulated_data)

```

```

157     # normalize the data
158     simulated_data = simulated_data/np.sum(simulated_data)
159     experiment_data[i] = experiment_data[i] / np.sum(experiment_data[i])
160
161     simulated_stat = summary_func(simulated_data, arr_bin_index)
162     observed_stat = summary_func(experiment_data[i], arr_bin_index)
163
164     #print(simulated_stat)
165     distance = np.linalg.norm(simulated_stat - observed_stat)
166     kernel_prob = gauss_kernel(distance, h)
167
168     #print(alpha, s, kernel_prob, simulated_stat, observed_stat)
169
170     if kernel_prob > np.random.uniform(0, 1):
171         accepted_params.append((alpha))
172         accepted_count += 1
173
174     return np.array(accepted_params), accepted_count/num_samples
175
176 experiment_data = np.load("board_data_.npz")
177
178 num_rows = 31
179 num_beads = 1000
180 num_samples = 40000
181 h = 1.8 # Bandwidth for the Gaussian kernel, about 5% acceptance rate
182
183 accepted_params, acceptance_rate = abc_routine(experiment_data, num_samples,
184         galton_simulator, summary_statistics, num_rows, num_beads, h)
185 #print(accepted_params)
186 #print(acceptance_rate)
187 np.save('accepted_params.npy', accepted_params)
188
189
190 # %%
191 acceptance_probs = {}
192
193 h_values = [0.1, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0]
194 for h in h_values:
195     accepted_params, acceptance_prob = abc_routine(experiment_data,
196         num_samples, galton_simulator, summary_statistics, num_rows, num_beads,
197         h)
198     acceptance_probs[h] = acceptance_prob
199     print(f"h={h}, Acceptance_Probability={acceptance_prob}")
200
201 # %%
202 accepted_params = np.load('accepted_params.npy')
203
204 mean_alpha = np.mean(accepted_params)
205 ci_lower, ci_upper = np.percentile(accepted_params, [16, 84]) # 68% CI
206     corresponds to 16th and 84th percentiles
207
208 print(accepted_params)
209 # Need to redo
210 plt.hist(accepted_params, bins=20, edgecolor='black', alpha=0.7, label = r'
211     Distribution of  $\alpha$ )
212 plt.axvline(mean_alpha, color='red', linestyle='--', label=f'Mean: {mean_alpha
213     :.2f}')

```

```

211 plt.axvline(ci_lower, color='blue', linestyle='-.', label=f'68%_CI:_{ci_lower
    :.2f},_{ci_upper:.2f}'])
212 plt.axvline(ci_upper, color='blue', linestyle='-.')
213
214 plt.xlabel(r'$\alpha$-value')
215 plt.ylabel('Frequency')
216 plt.legend()
217 plt.tight_layout()
218 plt.savefig('abc.pdf')
219 # Show plot
220 plt.show()
221
222 print("acceptance_rate:", len(accepted_params)/num_samples)
223
224
225 # %%
226 # Create simulation data for NN
227 num_samples = 100000
228 simulated_data = np.zeros((num_samples, 32), dtype=int)
229 alpha = np.random.uniform(0, 0.5, num_samples)
230 s = np.random.uniform(-0.25, 0.25, num_samples)
231
232 for i in range(num_samples):
233     print(i)
234     observed_data = galton_simulator(alpha[i], s[i], 31, 1000)
235     final_observed_data = reshape_bin_array(observed_data)
236     simulated_data[i] = final_observed_data
237
238
239 np.save("simulated_data1.npy", simulated_data)
240 np.save("simulated_params1.npy", np.vstack((alpha, s)).T)
241
242 # %%
243 import tensorflow as tf
244 from sklearn.preprocessing import StandardScaler
245 from sklearn.model_selection import train_test_split
246 from sklearn.metrics import mean_squared_error
247
248 # Load the data
249 X = np.load("simulated_data.npy")
250 y = np.load("simulated_params.npy")
251
252 # Split data into training and testing sets
253 X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2,
    random_state=42)
254
255 # Standardize the input features
256 scaler = StandardScaler()
257 X_train_scaled = scaler.fit_transform(X_train)
258 X_val_scaled = scaler.transform(X_val) # Use the same scaler for the
    validation set
259
260 # Optionally, standardize the target variables (if necessary)
261 y_scaler = StandardScaler()
262 y_train_scaled = y_scaler.fit_transform(y_train)
263 y_val_scaled = y_scaler.transform(y_val)
264
265
266 # %%
267 # Define a simple neural network model using TensorFlow/Keras

```

```

268 model = tf.keras.Sequential([
269     tf.keras.layers.Dense(128, activation='relu', input_dim=X_train_scaled.
        shape[1]),
270     tf.keras.layers.Dense(64, activation='relu'),
271     tf.keras.layers.Dense(2) # Output layer for two target variables (alpha
        and s)
272 ])
273
274 # Compile the model
275 model.compile(optimizer='adam', loss='mean_squared_error')
276
277 # Train the model
278 history = model.fit(X_train_scaled, y_train_scaled, epochs=100, batch_size=32,
        validation_data=(X_val_scaled, y_val_scaled))
279
280 # Make predictions
281 y_pred_scaled = model.predict(X_val_scaled)
282
283 # Inverse transform predictions
284 y_pred = y_scaler.inverse_transform(y_pred_scaled)
285
286 # Calculate the Mean Squared Error (MSE)
287 mse = mean_squared_error(y_val, y_pred)
288 print(f'Mean_Squared_Error_(TensorFlow):_{mse}')
289
290 # %%
291 #model.save('regression_model.h5')
292 # To load it:
293 model = tf.keras.models.load_model('regression_model.h5')
294
295 # %%
296 plt.figure()
297 plt.plot(history.history['loss'], label='Training_Loss', color='blue')
298 plt.plot(history.history['val_loss'], label='Validation_Loss', color='orange')
299 #plt.title('Model Loss during Training')
300 plt.xlabel('Epochs')
301 plt.ylabel('Loss_(RMSE)')
302 plt.legend()
303 plt.tight_layout()
304 plt.savefig('NN_training.pdf')
305 plt.show()
306
307 print(history.history.keys())
308
309 # %%
310 from sklearn.metrics import mean_absolute_error, r2_score
311
312 # Predictions on the validation set
313 y_pred_scaled = model.predict(X_val_scaled)
314
315 # Inverse transform predictions
316 y_pred = y_scaler.inverse_transform(y_pred_scaled)
317
318 # Separate true and predicted values for alpha and s
319 alpha_true, s_true = y_val[:, 0], y_val[:, 1]
320 alpha_pred, s_pred = y_pred[:, 0], y_pred[:, 1]
321
322 # Calculate errors for alpha
323 alpha_mse = mean_squared_error(alpha_true, alpha_pred)
324 alpha_mae = mean_absolute_error(alpha_true, alpha_pred)

```

```

325 alpha_r2 = r2_score(alpha_true, alpha_pred)
326
327 # Calculate errors for s
328 s_mse = mean_squared_error(s_true, s_pred)
329 s_mae = mean_absolute_error(s_true, s_pred)
330 s_r2 = r2_score(s_true, s_pred)
331
332 # RMSE
333 alpha_rmse = np.sqrt(alpha_mse)
334 s_rmse = np.sqrt(s_mse)
335
336 # Create error model for latent variable s
337 s_residuals = s_true - s_pred
338 s_residuals_mean = np.mean(s_residuals)
339 s_residuals_std = np.std(s_residuals)
340 s_residuals_gaussian = stats.norm(s_residuals_mean, s_residuals_std)
341
342 # Print error metrics
343 print(f"Alpha_MSE: {alpha_mse:.4f}, MAE: {alpha_mae:.4f}, RMSE: {alpha_rmse:.4f}, R2: {alpha_r2:.4f}")
344 print(f"S_MSE: {s_mse:.4f}, MAE: {s_mae:.4f}, RMSE: {s_rmse:.4f}, R2: {s_r2:.4f}")
345
346 plt.figure(figsize=(10, 5))
347
348 # Alpha
349 plt.subplot(1, 2, 1)
350 plt.scatter(alpha_true, alpha_pred, alpha=0.7, label='Predictions')
351 plt.plot([min(alpha_true), max(alpha_true)], [min(alpha_true), max(alpha_true)], color='red', linestyle='--', label='Ideal')
352 plt.title(r'$\alpha$ True vs Predicted')
353 plt.xlabel(r'True $\alpha$')
354 plt.ylabel(r'Predicted $\alpha$')
355 plt.legend()
356
357 # S
358 plt.subplot(1, 2, 2)
359 plt.scatter(s_true, s_pred, alpha=0.7, label='Predictions')
360 plt.plot([min(s_true), max(s_true)], [min(s_true), max(s_true)], color='red', linestyle='--', label='Ideal')
361 plt.title(r'$s$ True vs Predicted')
362 plt.xlabel(r'True $s$')
363 plt.ylabel(r'Predicted $s$')
364 plt.legend()
365
366 plt.tight_layout()
367 plt.savefig('NN_true_pred.pdf')
368 plt.show()
369
370
371 # %%
372 # ABC routine with neural network
373
374 def NN_predictor(data, model):
375     # Preprocess the input distribution
376     input_scaled = scaler.transform(data.reshape(1, -1))
377     predicted_scaled_params = model.predict(input_scaled)
378     predicted_params = y_scaler.inverse_transform(predicted_scaled_params)
379     return predicted_params
380

```

```

381
382 def abc_routine_nn(experiment_data, num_samples,model,error_values):
383     """
384     Approximate Bayesian Computation (ABC) routine with Neural network.
385
386     Args:
387         experiment_data (np.ndarray): Observed data.
388         num_samples (int): Number of samples.
389         model (tf.keras.Model): Neural network model.
390         error_values (np.ndarray): Error values for the latent variable s.
391     Returns:
392         np.ndarray: Accepted alpha parameters.
393     """
394     alphas = np.random.uniform(0, 0.5, num_samples)
395     h = 0.5
396     accepted_params = []
397     arr_bin_index = np.arange(1, 33, 1)
398
399     # Error model RMSE?
400
401     for alpha in alphas:
402         i = np.random.randint(0, len(experiment_data))
403         y_obs = experiment_data[i]
404
405         # Predict the parameters using the neural network
406         predicted_params = NN_predictor(y_obs, model)
407         s_pred = predicted_params[0][1]
408
409         s_pred += error_values[i]
410         #print(error_model)
411
412         simulation = galton_simulator(alpha, s_pred)
413         simulation = reshape_bin_array(simulation)
414
415         # normalize the data
416         simulation = simulation/np.sum(simulation)
417         y_obs= y_obs / np.sum(y_obs)
418
419         summary_sim = summary_statistics(simulation,arr_bin_index)
420         summary_exp = summary_statistics(y_obs,arr_bin_index)
421
422         g = np.linalg.norm(summary_sim - summary_exp)
423         kernel_prob = gauss_kernel(g, h)
424
425         p_accept = kernel_prob
426         print(alpha,p_accept)
427
428         if p_accept > np.random.uniform(0, 1):
429             accepted_params.append(alpha)
430             #print("Accepted")
431
432     return np.array(accepted_params)
433
434 model = tf.keras.models.load_model('regression_model.h5')
435 experiment_data = np.load("board_data_.npz")
436 error_values = s_residuals_gaussian.rvs(len(experiment_data))
437 num_samples = 20000
438 accepted_params_nn1 = abc_routine_nn(experiment_data, num_samples, model,
439                                     error_values)

```



```

440 print(accepted_params_nn1/num_samples)
441
442 # %%
443 # Plot the histogram of accepted parameters for ABC with NN
444 #np.save("accepted_params_nn.npy", accepted_params_nn)
445
446 print(accepted_params_nn1)
447
448 mean_alpha = np.mean(accepted_params_nn1)
449 ci_lower, ci_upper = np.percentile(accepted_params_nn1, [16, 84]) # 68% CI
    corresponds to 16th and 84th percentiles
450
451 plt.hist(accepted_params_nn1, bins=20, edgecolor='black', alpha=0.7, label = r
    'Distribution_of_$\alpha$')
452 plt.axvline(mean_alpha, color='red', linestyle='--', label=f'Mean:_{mean_alpha
    :.2f}')
453 plt.axvline(ci_lower, color='blue', linestyle='-.', label=f'68%_CI:_{ci_lower
    :.2f},_{ci_upper:.2f}'])
454 plt.axvline(ci_upper, color='blue', linestyle='-.')
455
456 plt.xlabel(r'$\alpha$-value')
457 plt.ylabel('Frequency')
458
459 plt.legend()
460 plt.tight_layout()
461 plt.savefig('abc_nn.pdf')
462 # Show plot
463 plt.show()
464
465 print("acceptance_rate:", len(accepted_params_nn1)/num_samples)
466
467 # %%
468 # ABC routine with neural network
469
470
471 def get_prior_samples(params):
472     mean = np.mean(params)
473     std = np.std(params)
474     return np.random.normal(mean, std, len(params))
475
476 def seq_abc_routine_nn(experiment_data,error_values,model,accepted_params_nn):
477     """
478     Approximate Bayesian Computation (ABC) routine with Neural network.
479
480     Args:
481         experiment_data (np.ndarray): Observed data.
482         error_values (np.ndarray): Error values for the latent variable s.
483         model (tf.keras.Model): Neural network model.
484         accepted_params_nn (np.ndarray): Accepted parameters from the previous
            ABC run.
485
486     Returns:
487         np.ndarray: Accepted (alpha) parameters.
488     """
489     alphas = get_prior_samples(accepted_params_nn)
490     h = 0.6
491     accepted_params = []
492     arr_bin_index = np.arange(1, 33, 1)
493
494     for alpha in alphas:
495         i = np.random.randint(0, len(accepted_params_nn))

```

```

495     y_obs = experiment_data[i]
496
497     # Predict the parameters using the neural network
498     predicted_params = NN_predictor(y_obs, model)
499     s_pred = predicted_params[0][1]
500
501     s_pred += error_values[i]
502
503     simulation = galton_simulator(alpha, s_pred)
504     simulation = reshape_bin_array(simulation)
505
506     simulation = simulation/np.sum(simulation)
507     y_obs= y_obs / np.sum(y_obs)
508
509     summary_sim = summary_statistics(simulation,arr_bin_index)
510     summary_exp = summary_statistics(y_obs,arr_bin_index)
511
512     g = np.linalg.norm(summary_sim - summary_exp)
513     kernel_prob = gauss_kernel(g, h)
514
515     p_accept = kernel_prob
516     print(alpha,p_accept)
517
518     if p_accept > np.random.uniform(0, 1):
519         accepted_params.append((alpha))
520         #print("Accepted")
521
522     return np.array(accepted_params)
523
524 model = tf.keras.models.load_model('regression_model.h5')
525 experiment_data = np.load("board_data_.npz")
526 #num_samples = 4000
527 error_values = s_residuals_gaussian.rvs(len(accepted_params_nn1))
528 seq_accepted_params_nn = seq_abc_routine_nn(experiment_data, error_values,
529                                             model, accepted_params_nn1)
530
531 # %%
532 # Plot the histogram of accepted parameters for ABC with NN
533 #np.save('seq_accepted_params_nn.npy', seq_accepted_params_nn)
534 print(seq_accepted_params_nn)
535
536 mean_alpha = np.mean(seq_accepted_params_nn)
537 ci_lower, ci_upper = np.percentile(seq_accepted_params_nn, [16, 84]) # 68% CI
538                                     corresponds to 16th and 84th percentiles
539
540 plt.hist(seq_accepted_params_nn, bins=20, edgecolor='black', alpha=0.7, label
541         = r'Distribution_of_{$\alpha$'})
542 plt.axvline(mean_alpha, color='red', linestyle='--', label=f'Mean:_{mean_alpha
543 :.2f}')
544 plt.axvline(ci_lower, color='blue', linestyle='-.', label=f'68%CI:_{ci_lower
545 :.2f},_{ci_upper:.2f}'])
546 plt.axvline(ci_upper, color='blue', linestyle='-.')
547 plt.xlabel(r'$\alpha$-value')
548 plt.ylabel('Frequency')
549 plt.legend()
550 plt.tight_layout()
551 plt.savefig('seq_abc_nn.pdf')
552 plt.show()
553
554 print("acceptance_rate:_", len(seq_accepted_params_nn)/num_samples)

```

```
550
551
552 # %%
553 x = np.linspace(-1, 1, 1000)
554 print(s_residuals_gaussian.pdf(x))
```