Durham University

# EXAMINATION PAPER

| Examination Session: | Year: | Exam Code: |
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| May/June | 2026 | MATH4337-WE01 |

| Title: |
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| Uncertainty Quantification IV |

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| Time: | 2 hours | |
| Additional Material provided: | None | |
| Materials Permitted: | None | |
| Calculators Permitted: | No | Models Permitted: Use of electronic calculators is forbidden. |

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| Instructions to Candidates: | Answer all questions.<br>The indicative marks shown in brackets for the main parts of each question are given as a guide to the weighting the markers expect to apply.<br>Write your answer in the white-covered answer booklet with barcodes.<br>Begin your answer to each question on a new page. |

| Revision: | |
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ED01/2026

## SECTION A

**1.** We wish to emulate an expensive 1D computer model $f(x)$ over the input range $x \in [0, 1]$. We set up a standard Bayes Linear emulator, specifying a squared exponential prior covariance structure, with $\sigma^2 = 4$, $\theta = 1/3$, and prior expectation $\mathrm{E}[f(x)] = 2$. A single run is performed at the location $x^{(1)} = 0.6$, yielding the output $D = f(x^{(1)}) = 5$.

(a) Find an expression for the emulator adjusted expectation $\mathrm{E}_D[f(x)]$. **[3]**

(b) Find an expression for the emulator adjusted variance $\mathrm{Var}_D[f(x)]$. **[2]**

(c) Find an expression for the emulator adjusted covariance $\mathrm{Cov}_D[f(x), f(x')]$. **[3]**

(d) After we have evaluated the run at $x^{(1)}$, is the resulting adjusted covariance structure stationary? **[2]**

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**2.** We wish to emulate an expensive computer model $f(x)$ with 1D input $x \in \mathbb{R}$ and scalar output $f \in \mathbb{R}$. We use a Bayes Linear emulator with prior expectation $\mathrm{E}[f(x)] = 0$, and specify covariance structure

$$\mathrm{Cov}[f(x), f(x')] \;=\; \sigma^2 c(x - x')$$

where $c(x - x')$ represents a standard correlation function of a weakly stationary process. Two runs have been performed and these are at locations $x^{(1)}$ yielding $D_1 = f(x^{(1)})$ and at $x^{(2)}$ yielding $D_2 = f(x^{(2)})$, where $x^{(1)} \neq x^{(2)}$. The vector of run outputs is denoted $D = (D_1, D_2)^T$.

(a) By explicitly constructing $\mathrm{Var}[D]$, show that its inverse is given by

$$\mathrm{Var}[D]^{-1} \;=\; \frac{1}{\sigma^2(1 - v^2)} \begin{pmatrix} 1 & -v \\ -v & 1 \end{pmatrix}$$

where $v = c(x^{(1)} - x^{(2)})$. **[2]**

(b) Hence show that the emulator expectation $\mathrm{E}_D[f(x)]$ is given by:

$$\mathrm{E}_D[f(x)] \;=\; \frac{1}{1 - v^2}\left\{ \Big[w_1(x) - v\, w_2(x)\Big] D_1 \;+\; \Big[w_2(x) - v\, w_1(x)\Big] D_2 \right\}$$

where $w_1(x) = c(x - x^{(1)})$ and $w_2(x) = c(x - x^{(2)})$. **[3]**

(c) Show that the emulator variance $\mathrm{Var}_D[f(x)]$ is given by:

$$\mathrm{Var}_D[f(x)] \;=\; \frac{\sigma^2}{1 - v^2}\left\{ 1 - v^2 - w_1(x)^2 - w_2(x)^2 \;+\; 2v\, w_1(x) w_2(x) \right\}$$ **[3]**

(d) Examine the limits of $\mathrm{E}_D[f(x)]$ and $\mathrm{Var}_D[f(x)]$ as $x \to \infty$ and comment. **[2]**

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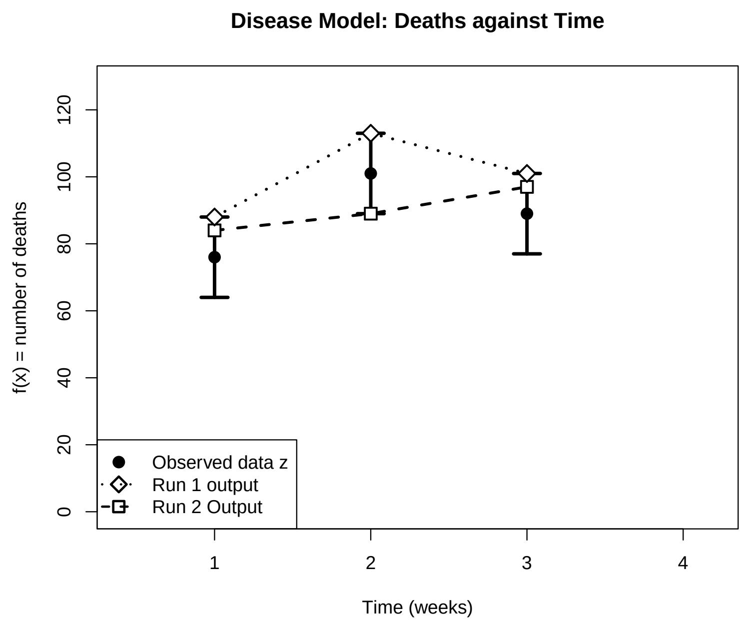
## SECTION B

**3.** An outbreak of Ebola occurs in a network of towns in sub-Saharan Africa. Three observations $z = (76, 101, 89)$ are available around the peak of the outbreak, giving the number of deaths in weeks $t = 1, 2$ and 3. These are shown in the figure below along with error bars $z_i \pm 3\sqrt{\mathrm{Var}[e_i] + \mathrm{Var}[\epsilon_i]}$ for weeks $t = i = 1, 2, 3$, representing a possible combination of observation errors $e$ and model discrepancy $\epsilon$, where $\mathrm{Var}[e_i] + \mathrm{Var}[\epsilon_i] = \sigma_{tot}^2$ and where $\sigma_{tot}$ is judged to be 4 throughout this question. A deterministic epidemiological computer model $f(x)$ is constructed to mimic the outbreak where $f_i(x)$ gives the model prediction for the number of deaths at week $t = i$. Output from two runs of the model $f(x^{(1)})$ and $f(x^{(2)})$ are shown as diamond points (run 1) and square points (run 2) respectively, where the three outputs $f_1(x^{(j)}), f_2(x^{(j)}), f_3(x^{(j)})$ have been connected by dotted lines for run 1 and dashed lines for run 2, to highlight the shape of each run over time.




(a) Find the maximum implausibility $I_M(x^{(j)})$ and second maximum implausibility $I_{2M}(x^{(j)})$ for each run (so no emulation is required) where the run outputs are given by:

$$f(x^{(1)}) = \begin{pmatrix} f_1(x^{(1)}) \\ f_2(x^{(1)}) \\ f_3(x^{(1)}) \end{pmatrix} = \begin{pmatrix} 88 \\ 113 \\ 101 \end{pmatrix}, \quad f(x^{(2)}) = \begin{pmatrix} f_1(x^{(2)}) \\ f_2(x^{(2)}) \\ f_3(x^{(2)}) \end{pmatrix} = \begin{pmatrix} 84 \\ 89 \\ 97 \end{pmatrix}$$

**[3]**

(b) Initially all the errors $\sigma_{tot}$ are assumed to come from observation error, so $\mathrm{Var}[e_i] = \sigma_e^2 = \sigma_{tot}^2$ and $\mathrm{Var}[\epsilon_i] = 0$. The observation errors are assumed to be uncorrelated so $\mathrm{Cov}[e_i, e_j] = 0$ for $i \neq j$. Construct the $3 \times 3$ covariance matrix $\mathrm{Var}[\epsilon + e]$ and hence evaluate the multivariate implausibility $I_{MV}(x^{(j)})$ at each of the two runs:

$$I_{MV}(x^{(j)}) = (f(x^{(j)}) - z)^T (\mathrm{Var}[\epsilon] + \mathrm{Var}[e])^{-1} (f(x^{(j)}) - z)$$

Compare values of $I_{MV}(x^{(j)})$ for each run and comment. **[2]**

(c) An alternative specification is made, where all the errors $\sigma_{tot}$ are assumed to come solely from the model discrepancy, so $\text{Var}[e_i] = 0$ and $\text{Var}[\epsilon_i] = \sigma_\epsilon^2 = \sigma_{tot}^2$. The model discrepancy is judged to be highly correlated, with $\text{Cov}[\epsilon_i, \epsilon_j] = \sigma_\epsilon^2 \rho$ for $i \neq j$, with correlation $\rho \lesssim 1$. Show that the $3 \times 3$ inverse covariance matrix $\text{Var}[\epsilon + e]^{-1}$ can now be written in the form:

$$\text{Var}[\epsilon + e]^{-1} \;=\; aI \;+ bJ$$

where $I$ is the $3 \times 3$ identity matrix, $J$ is the $3 \times 3$ matrix with every element equal to 1 and where you must find explicit expressions for both $a$ and $b$. **[6]**

(d) Hence evaluate $I_{MV}(x^{(j)})$ for each run, state which run is preferred by this measure and discuss why. **[3]**

(e) Which run would you prefer to use to predict deaths in week 4? **[1]**

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**4.** We wish to optimise an expensive function $f(x)$ over the region $\mathcal{X} \subset \mathbb{R}^m$ using a Bayesian Optimisation approach. We have performed a set of $n$ runs giving model output values $D = (f(x^{(1)}), \ldots, f(x^{(n)}))^T$. We denote the highest run output so far found as $f^+ = f(x^+)$ with $x^+ \in \{x^{(1)}, \ldots, x^{(n)}\}$ the corresponding best input so far.

(a) Define the Probability of Improvement $PI(x)$ and the Expected Improvement $EI(x)$ acquisition functions. **[2]**

(b) By re-expressing both acquisition functions in terms of utilities, discuss why $EI(x)$ is generally considered superior to $PI(x)$. **[2]**

(c) The Expected Improvement Squared acquisition function has utility:

$$U_{EI_2}(x) \;=\; \mathcal{I}(x)^2$$

where $\mathcal{I}(x)$ is the usual improvement function. Show that, when using a Gaussian Process emulator, the Expected Improvement Squared acquisition function becomes:

$$EI_2(x) \;=\; \sigma_D(x)c(x)\phi(z^*) + (\sigma_D^2(x) + c^2(x))\Phi(z^*)$$

where $z^* = (\mu_D(x) - f^+)/\sigma_D(x)$; $\mu_D(x)$ and $\sigma_D(x)$ denote the emulator mean and standard deviation updated by the runs $D$; $\phi(\cdot)$ and $\Phi(\cdot)$ denote the p.d.f. and c.d.f. of the standard normal distribution respectively; and the deviation is defined as $c(x) = \mu_D(x) - f^+$. **[6]**

(d) When using a Gaussian Process emulator, the Expected Improvement acquisition function is given by:

$$EI(x) \;=\; \sigma_D(x)\phi(z^*) + c(x)\Phi(z^*),$$

(you do not need to prove this). Compare the behaviour of the Expected Improvement and the Expected Improvement Squared acquisition functions. Your answer should include discussion of the cases where $z^* \simeq 0$ and $z^* \gg 1$. **[3]**

(e) What fundamental weakness do all three acquisition functions, $PI(x)$, $EI(x)$ and $EI_2(x)$, possess? **[2]**

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