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BAYESIAN MULTI-OBJECTIVE OPTIMIZATION FOR QUANTITATIVE RISK ASSESSMENT IN MICROBIOLOGY

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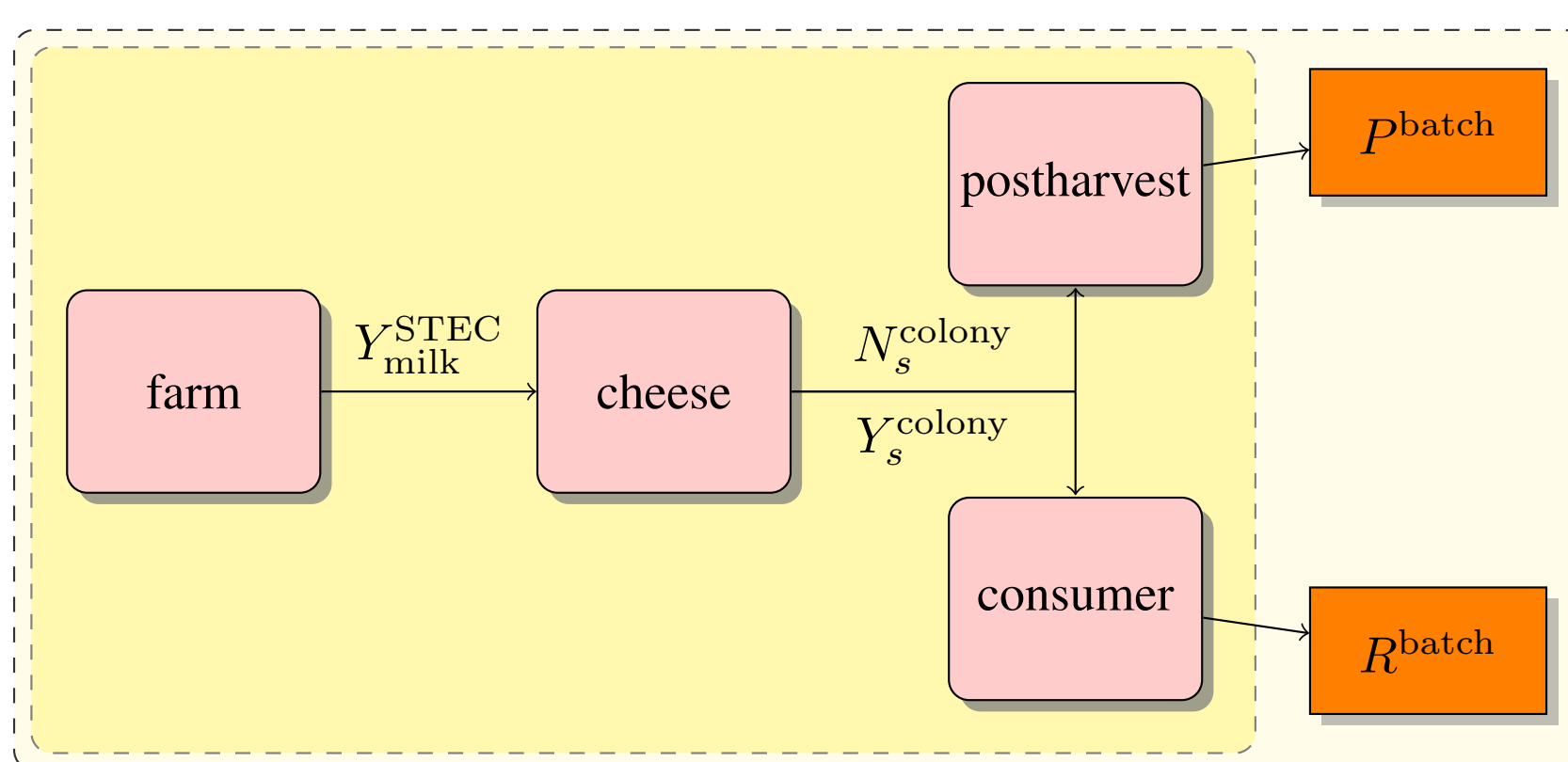
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Context

As a part of the European project [ArtiSaneFood](#), the primary goal of this collaborative work between ANSES, CNIEL and L2S is to establish efficient bio-intervention strategies for cheese producers in France, in order to “economically” reduce the risk of Haemolytic Uremic Syndrome (HUS) caused by Shiga-Toxin producing Escherichia Coli (STEC) present in raw-milk soft cheese. This translates into a multi-objective optimization problem of a stochastic simulator based on a quantitative risk assessment (QRA) model proposed by Perrin et al. (2014), to estimate the Pareto optimal solutions for the process intervention parameters.

QRA simulator



Batch level stochastic simulator

The farm-to-fork continuum for one batch

• Farm module

STEC and E.coli strains follow same fecal route!
 – A batch of milk is tested with probability $p_{\text{test}}^{\text{milk}}$
 – Farms with E.coli conc. $> I^{\text{sort}}$ are rejected
 STEC conc. $Y_{\text{milk}}^{\text{STEC}}$ in farm milk is computed

• Cheese module

STEC cells form colonies (clusters) inside cheese
 – No. of colonies (Poisson): N_s^{colony}
 – Size of colonies (LogNormal): Y_s^{colony}
 for strain s

• Consumer module

Batch risk is computed using a dose-response model:

$$\Gamma = \sum_s N_s^{\text{colony}} \cdot Y_s^{\text{colony}} \quad (1)$$

$$R^{\text{batch}} = \sum_{\text{age}} g_{\text{age}} \int_{\Gamma} P[\text{HUS}|\gamma, \text{age}] \cdot p(\gamma) d\gamma \quad (2)$$

averaging over consumer age

• Post-harvest module

Proportion of rejected batches is estimated using number of test sample n_{sample} given a test rate $p_{\text{test}}^{\text{cheese}}$

$$P^{\text{batch}} = P[\Gamma > 0] = 1 - \exp(-K \cdot n_{\text{sample}})$$

Quantities of Interest (QoI)

Several batches are simulated to estimate

- $R_{\text{avg}} = \mathbb{E}[R^{\text{batch}} \cdot (1 - P^{\text{batch}} \cdot p_{\text{test}}^{\text{cheese}})]$
- $P_{\text{avg}} = \mathbb{E}[P^{\text{batch}} \cdot p_{\text{test}}^{\text{cheese}}]$

QoIs are

- **Relative risk:** $f_1 = \frac{R_{\text{avg}}}{(1 - P_{\text{avg}}) \cdot K_1}$, (K_1 : baseline risk)
- **Batch rejection rate:** $f_2 = P_{\text{avg}}$

Multi-objective optimization

We consider the multi-objective optimization problem

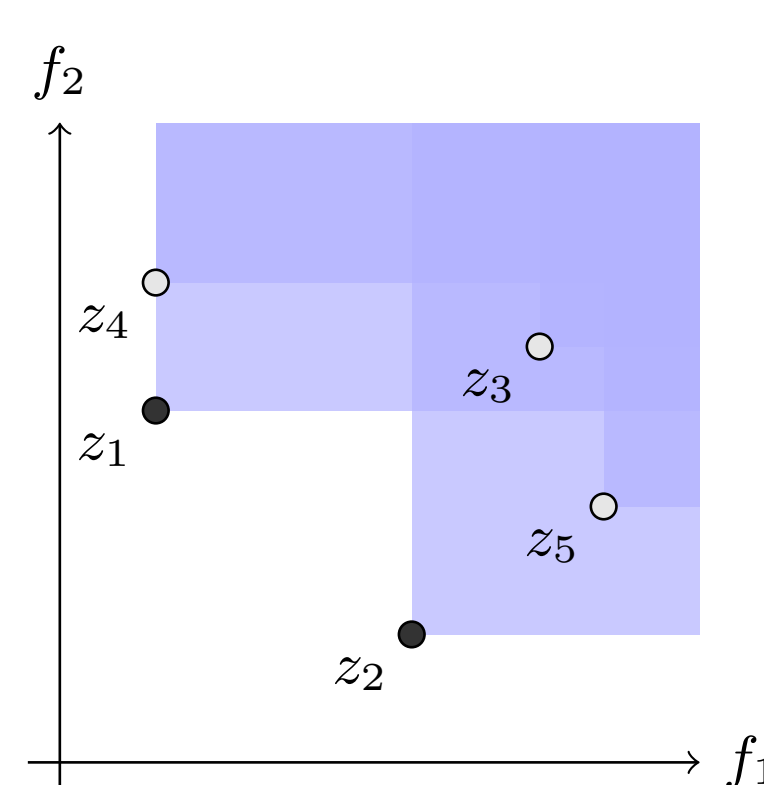
$$\min_{x \in \mathbb{X}} f(x)$$

where, $f = (f_1, f_2, \dots)$

- The solution set \mathcal{P} contains **Pareto optimal** points

$$\mathcal{P} = \{x \in \mathbb{X} : \nexists x' \in \mathbb{X}, f(x') \prec f(x)\}$$

where $f' \prec f \implies f'_i \leq f_i, \forall i$, with at least one of the inequalities being strict



Pareto optimal points z_1 and z_2

- In a stochastic setting, we assume additive noise: for a given $x_i \in \mathbb{X}$, we observe $Z_i = f(x_i) + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, \Sigma)$

PALS

Proposed by Zuluaga et al. (2013) and extended for the **stochastic** case by Barracosa et al. (2021).

- Initial design $I_0, n = 0, \beta > 0$

- **Step I** – $\forall x \in \mathbb{X}$, construct confidence rectangles

$$R_n(x) = \{z \in \mathbb{R}_+^2 : R_n^-(x) \prec z \prec R_n^+(x)\}$$

using posterior means $\mu_{n,j}(x)$ and variances $\sigma_{n,j}^2(x)$

$$R_n^\pm(x) = \mu_{n,j}(x) \pm \beta^{1/2} \sigma_{n,j}(x)$$

based on I_n (indep. GP models for $f_j, j \in \{1, 2\}$)

- **Step II** – Classify each $x \in \mathbb{X}$ into one of three classes

– **Deemed Pareto optimal** P_n :

$$P_n = \{x \in \mathbb{X} | \nexists x' \in \mathbb{X} \setminus \{x\}, R_n^-(x') \prec R_n^+(x)\}$$

– **Non Pareto optimal** N_n :

$$N_n = \{x \in \mathbb{X} | \exists x' \in \mathbb{X} \setminus \{x\}, R_n^+(x') \prec R_n^-(x)\}$$

– **Unclassified** $U_n = \mathbb{X} \setminus (P_n \cup N_n)$

- **Step III** – Sample the next point of evaluation

$$X_{n+1} = \arg \max_{x \in (U_n \cup P_n)} \|R_n^-(x) - R_n^+(x)\|_2$$

$$I_{n+1} = I_n \cup (X_{n+1}, Z_{n+1}), Z_{n+1} = f(X_{n+1}) + \varepsilon_{n+1}$$

- Increase n and **Repeat I-III** until $n \leq n_{\text{max}}$

PALS with quantiles

PALS is not directly suitable for our application:

- f_1 is **not** the expectation of a simulator output,
- we build a GP model for R_{avg} instead.

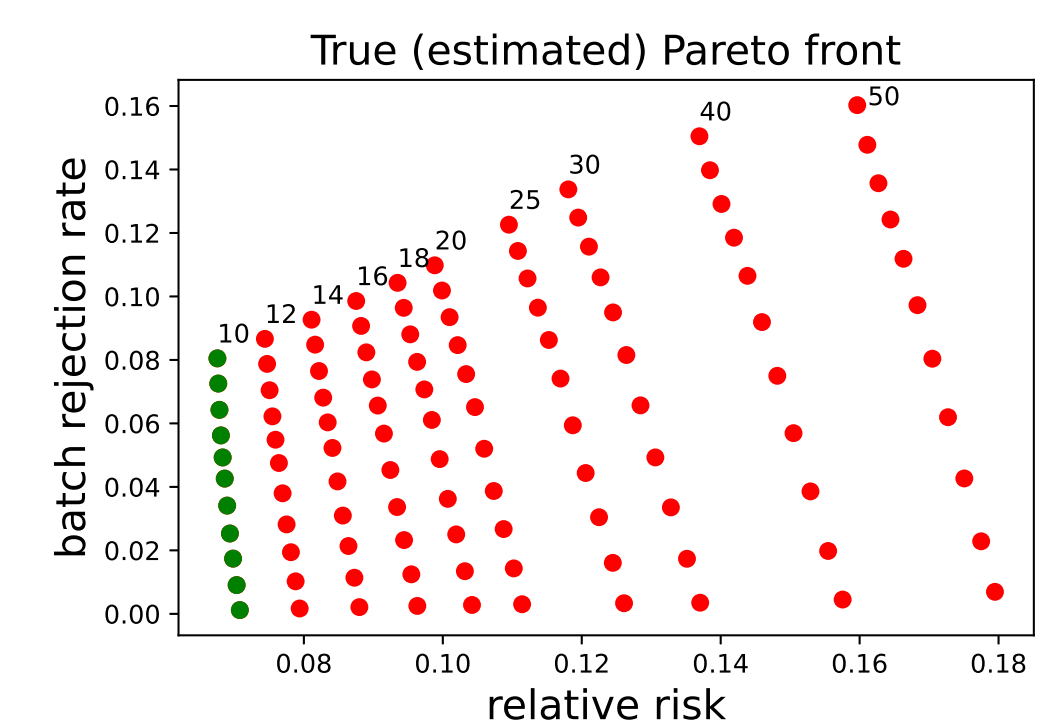
So, we propose using quantiles of QoI to construct confidence rectangles of coverage probability α

$$R_{n,j}^-(x) = q_{n,j}(\alpha/2) \text{ and } R_{n,j}^+(x) = q_{n,j}(1 - \alpha/2)$$

with $q_{n,j}(\cdot)$ being a posterior quantile of $f_j(x)$

Experimental results

- Minimizing f , given $p_{\text{test}}^{\text{milk}} = 1, p_{\text{test}}^{\text{cheese}} = 0.5$, w.r.t.
 - $n_{\text{sample}} \in \{1, 5, 10, 15, \dots, 50\}$
 - $I^{\text{sort}} \in \{10, 12, 14, 16, 18, 20, 25, 30, 40, 50\}$
- **True Pareto front:** estimated using 5000 samples for each of 11×10 input pair
 - A GP regressor is used to smooth the predictions

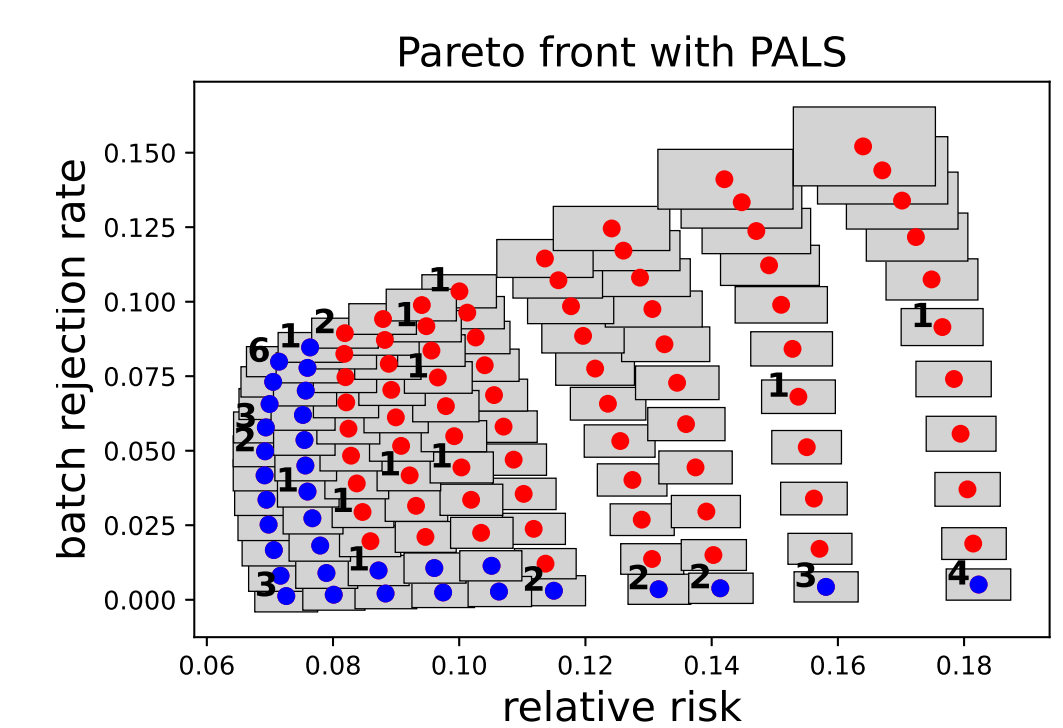


(stripes corresponding diff. values of I^{sort})

– Pareto optimal (green) and dominated points (red)

- **Pareto front estimated using PALS**

– $|I_0| = 10, n_{\text{max}} = 30, \text{samples/evaluation} = 200$



(integers denoting evaluation counts)

- With PALS using significantly less (40×200) budget, the user can provide the following insights

– Points with $I^{\text{sort}} > 12$ are dominated (red)
 – $I^{\text{sort}} \leq 12$ remain unclassified (blue)

Future work

- Integrate milk loss as objective and $p_{\text{test}}^{\text{milk}}, p_{\text{test}}^{\text{cheese}}$ as design variables
- Take the correlation between outputs into account

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