Efficient Likelihood Approximation via Gaussian Processes

With an Application to a *P. Vivax* Malaria Model

Jacob Cumming

University of Melbourne, Walter and Eliza Hall Institute

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Malaria

- 600,000 deaths/year, 75% children under 5
- Two main species *P. vivax* and *P. falciparum*
- *P. falciparum* main cause of death, but *P. vivax* traditionally underestimated.
- Proportion of *P. vivax* cases increased over last 50 years.

P. vivax has Dormant Stage

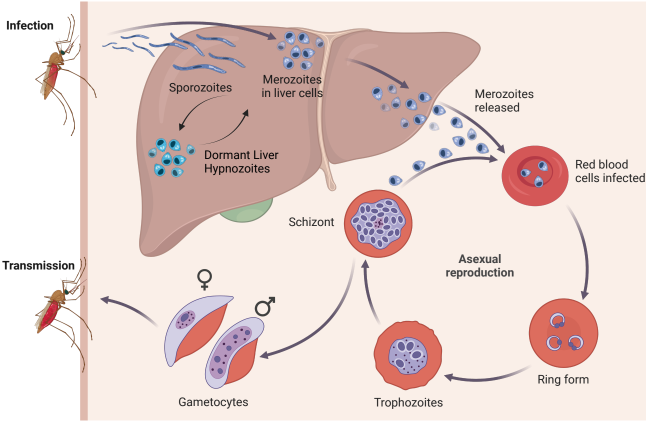

Figure: *P. vivax* lifecycle. Created with BioRender.com

Vivax Model - Champagne et. al

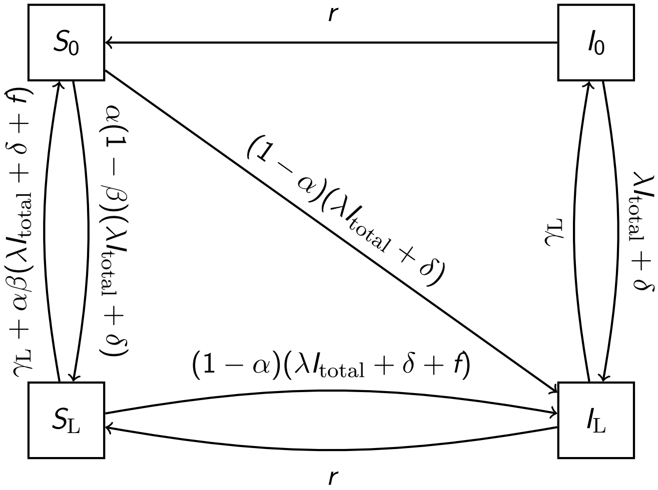

Figure: Champagne et al. 2022 *P. vivax* model

Champagne Model Parameters

- α : proportion of those infected who clear blood stage infections through treatment
- β : proportion of those cleared of blood stage infection who are also cleared of liver stage parasites (radical cure)
- λ : rate of infection
- γ_L : rate of liver stage disease clearance
- f : rate of relapse
- r : rate of blood stage clearance
- $\delta = 0$ importation rate (fixed)

Ordinary Differential Equations - Champagne et. al

$$
\begin{aligned}
\frac{\mathrm{d} I_{\mathrm{L}}}{\mathrm{d} t} =& (1-\alpha)(\lambda I_{\mathrm{total}}+\delta)(S_0+S_{\mathrm{L}})+(\lambda I_{\mathrm{total}}+\delta)I_0 \\
&+(1-\alpha)fS_{\mathrm{L}}-\gamma_{\mathrm{L}} I_{\mathrm{L}}-rI_{\mathrm{L}} \\
\frac{\mathrm{d} I_0}{\mathrm{d} t} =& -(\lambda I_{\mathrm{total}}+\delta)I_0+\gamma_{\mathrm{L}} I_{\mathrm{L}}-rI_0 \\
\frac{\mathrm{d} S_{\mathrm{L}}}{\mathrm{d} t} =& -(1-\alpha(1-\beta))(\lambda I_{\mathrm{total}}+\delta+f)S_{\mathrm{L}} \\
&+\alpha(1-\beta)(\lambda I_{\mathrm{total}}+\delta)S_0-\gamma_{\mathrm{L}} S_{\mathrm{L}}+rI_{\mathrm{L}} \\
\frac{\mathrm{d} S_0}{\mathrm{d} t} =& -(1-\alpha\beta)(\lambda I_{\mathrm{total}}+\delta)S_0+(\lambda I_{\mathrm{total}}+\delta)\alpha\beta S_{\mathrm{L}} \\
&+\alpha\beta fS_{\mathrm{L}}+\gamma_{\mathrm{L}} S_{\mathrm{L}}+rI_0
\end{aligned}
$$

The Problem

- How to calibrate model parameters?

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- Simulations take long time (and models get a lot more complicated)

Notation

- $\boldsymbol{\theta}$ vector of parameters - e.g. $[\alpha, \beta, \gamma_L, \lambda, f, r]^T$
- $\mathbf{Y}_{\text{obs}}$: a (summary) vector of observed data e.g. (weekly) incidence, prevalence, (monthly) hospitalisations

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- $\mathbf{Y}_{\text{obs}}$: a (summary) vector of observed data e.g. (weekly) incidence, prevalence, (monthly) hospitalisations
- $\mathbf{Y}_{\boldsymbol{\theta}}$: a random vector of model statistics for given $\boldsymbol{\theta}$.

In an ideal world...

- There would be an explicit form for the likelihood:

$$\mathcal{L}(\boldsymbol{\theta}|\mathbf{Y}_{\text{obs}}) := \Pr(\mathbf{Y}_{\text{obs}}|\boldsymbol{\theta})$$

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- Off to the pub

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Or not...

- Explicit likelihoods often don't exist/are intractible
  - Champagne model
  - Agent based models.

A Standard Bayesian Solution

- Approximate Bayesian Computation (ABC)
  1. Sample $\boldsymbol{\theta}_i$ from prior
  2. Run model and observe $\mathbf{Y}_{\boldsymbol{\theta}_i}$
  3. Accept or reject $\boldsymbol{\theta}_i$ run based on how well $\mathbf{Y}_{\boldsymbol{\theta}_i}$ 'matches' $\mathbf{Y}_{\text{obs}}$.

What is ‘matches’?

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1. $\mathbf{Y}_{\boldsymbol{\theta}_i} = \mathbf{Y}_{\text{obs}}$
   - Good luck...
2. Rescale $\mathbf{Y}$s, and use discrepency function $D : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ e.g. p-norm

$$D(\mathbf{Y}_{\boldsymbol{\theta}_i}, \mathbf{Y}_{\text{obs}}) := \left(\sum_{j=1}^{d} |\{\mathbf{Y}_{\boldsymbol{\theta}_i}\}_j - \{\mathbf{Y}_{\text{obs}}\}_j|^p \right)^{1/p}$$

Discrepency Function

$\mathcal{D}(\boldsymbol{\theta}) := D(\mathbf{Y}_{\boldsymbol{\theta}}, \mathbf{Y}_{\text{obs}})$ how 'close' our model is to the observed data using parameters $\boldsymbol{\theta}$

ABC

1. Sample $\boldsymbol{\theta}_i$ from prior
2. Run model
3. Accept $\boldsymbol{\theta}_i$ if $\mathcal{D}(\boldsymbol{\theta}_i) < \varepsilon$.

Overall Idea of my Research

- ABC fixes one problem but leaves another:
  - Don't need $\mathcal{L}(\boldsymbol{\theta})$.
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- ABC fixes one problem but leaves another:
  - Don't need $\mathcal{L}(\boldsymbol{\theta})$.
  - Evaluating $\mathcal{D}(\boldsymbol{\theta})$ takes as long as a model run.
- $\mathcal{D}(\boldsymbol{\theta}), \mathcal{D}(\boldsymbol{\theta}')$ will be highly correlated when $\boldsymbol{\theta}$ is near $\boldsymbol{\theta}'$.
  - Gaussian Processes

Gaussian Process Setup

A common assumption is that

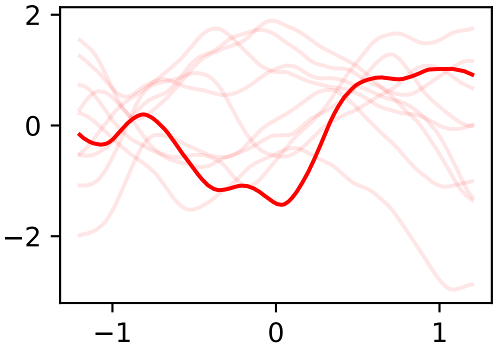
$$\begin{bmatrix} \mathbb{E}(\mathcal{D}(\boldsymbol{\theta}_1)) \\ \vdots \\ \mathbb{E}(\mathcal{D}(\boldsymbol{\theta}_n)) \end{bmatrix} \sim \text{MVN}\left(\mathbf{0},\ \mathbf{K}\right)$$

where $\mathbf{K}_{ij} = k(\boldsymbol{\theta}_i, \boldsymbol{\theta}_j)$ for some covariance kernel k that decays to 0 as $\boldsymbol{\theta}_i$ is further away than $\boldsymbol{\theta}_j$.

Gaussian Processes on $\mathbb{R}^d$

Definition (Gaussian Process)

A collection of random variables $\{f(\mathbf{x})\}_{\mathbf{x}\in\mathbb{R}^d}$ *is a Gaussian process if all finite dimensional distributions are multivariate normal distributed.*



Equivalent GP definition

Definition (Gaussian Process)

A collection of random variables $\{f(\mathbf{x})\}_{\mathbf{x}\in\mathbb{R}^d}$ *is a Gaussian process if there is a function* $m : \mathbf{x} \to \mathbb{R}$ *and covariance kernel* $k : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ *such that for all* $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$,

$$\begin{bmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ f(\mathbf{x}_n) \end{bmatrix} \sim \mathrm{MVN}\left(\begin{bmatrix} m(\mathbf{x}_1) \\ m(\mathbf{x}_2) \\ \vdots \\ m(\mathbf{x}_n) \end{bmatrix}, \mathbf{K} \right)$$

where $\mathbf{K}_{ij} := k(\mathbf{x}_i, \mathbf{x}_j)$.

k Determines Smoothness

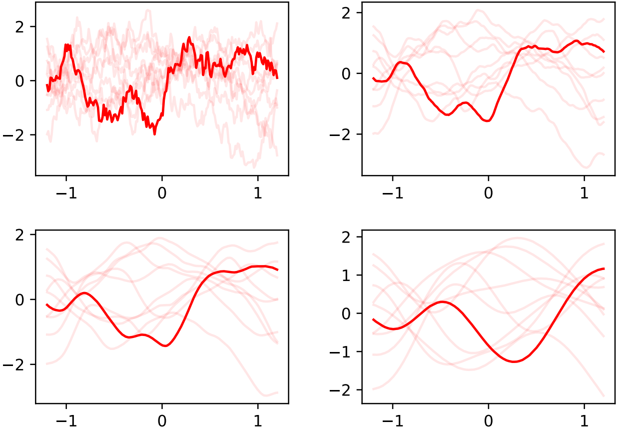


Figure: Matérn 1/2, 3/2, 5/2, and squared exponential kernels.

Gaussian Process Continuity

- Induce continuity by forcing $k(\mathbf{x}, \mathbf{x}') \rightarrow \mathrm{Var}(f(\mathbf{x}))$ (hence $\mathrm{Cor}(f(\mathbf{x}), f(\mathbf{x}')) \rightarrow 1$) as $\mathbf{x} \rightarrow \mathbf{x}'$.

Common Covariance Kernels

- Matérn Kernel with hyperparameter ν : $\lfloor \nu \rfloor$ times mean square differentiable.
- $\nu \to \infty$: infinitely mean square differentiable squared exponential covariance kernel (strong assumption)

$$k(x, x') = \sigma_k^2 \exp(-\frac{||x - x'||^2}{2\ell^2})$$

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k Determines Class of Functions

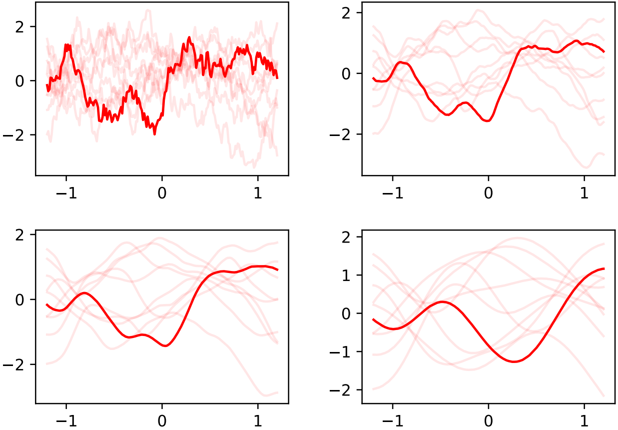
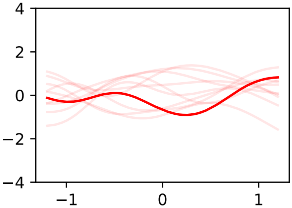


Figure: Matérn 1/2, 3/2, 5/2, and squared exponential kernels.

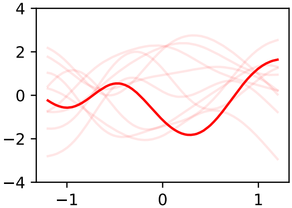
Kernel Hyperparameters

- Matérn and squared exponential kernel can both be written in the form $k(\mathbf{x}, \mathbf{x}') = \sigma_k^2 \kappa(||\mathbf{x}, \mathbf{x}'||/\ell)$
- $1/\ell$ rate of covariance decay
- $\sigma_k^2 = \mathrm{Var}(f(\mathbf{x}))$

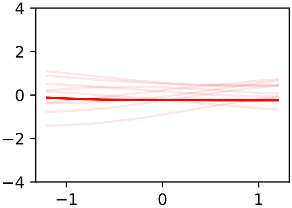
Kernel Hyperparameters



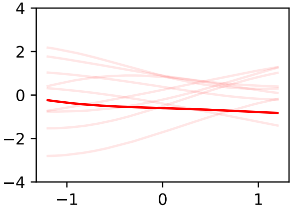
(a) $\ell = 1/2 \quad \sigma_k^2 = 1/2$



(b) $\ell = 1/2 \quad \sigma_k^2 = 2$



(c) $\ell = 2 \quad \sigma_k^2 = 1/2$



(d) $\ell = 2 \quad \sigma_k^2 = 2$

Discrepency Function Context

- Long term play: use a Gaussian process as a surrogate model for $\mathbb{E}[\mathcal{D}(\boldsymbol{\theta})]$

Discrepency Function Context

- Long term play: use a Gaussian process as a surrogate model for $\mathbb{E}[\mathcal{D}(\boldsymbol{\theta})]$
- What if we have observations already?

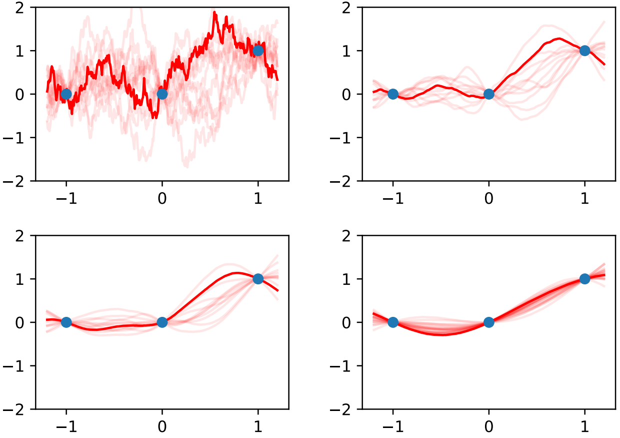
Gaussian Process Regression

$$\begin{bmatrix} f(\mathbf{x}) \\ f(\mathbf{x}_*) \end{bmatrix} \sim \text{MVN}\left(\begin{bmatrix} m(\mathbf{x}) \\ m(\mathbf{x}_*) \end{bmatrix}, \begin{bmatrix} K & K_* \\ K_*^T & K_{**} \end{bmatrix} \right)$$

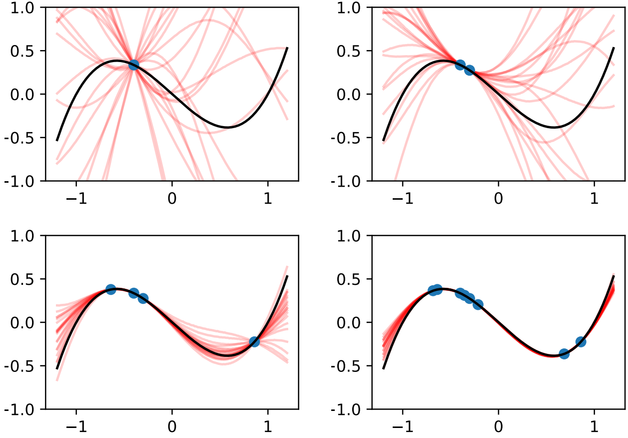
implies

$$f(\mathbf{x}) | f(\mathbf{x}_*) \sim \text{MVN}\left(m(\mathbf{x}) + K_* K_{**}^{-1}(f(\mathbf{x}_*) - m(\mathbf{x}_*)),\ K - K_* K_{**}^{-1} K_*^T \right).$$

Conditioning Gaussian Processes



GP regression on $x(x-1)(x+1)$

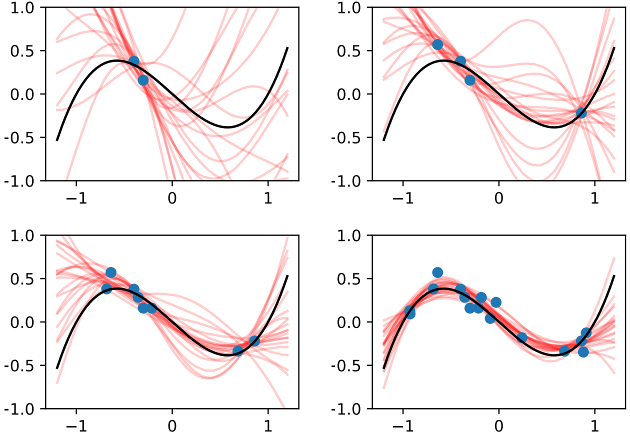


Normal observation noise

If observations actually $f(\mathbf{x}_i) + \varepsilon_i$, with $\varepsilon_i \sim N(0, \sigma_o^2)$ i.i.d., then

$$\begin{bmatrix} f(\mathbf{x}_1) + \varepsilon_1 \\ \vdots \\ f(\mathbf{x}_n) + \varepsilon_n \end{bmatrix} \sim \mathrm{MVN}\left(\begin{bmatrix} m(\mathbf{x}_1) \\ \vdots \\ m(\mathbf{x}_n) \end{bmatrix}, \mathbf{K} + \sigma_o^2 \mathbf{I}_n \right)$$

GP regression on $x(x-1)(x+1)+\varepsilon$, $\varepsilon \sim N(0, \sigma_o^2)$



Key Assumptions

- $\mathcal{D}(\boldsymbol{\theta}) \overset{d}{\approx} \mathcal{D}(\boldsymbol{\theta}')$ for $\boldsymbol{\theta}$, $\boldsymbol{\theta}'$ close.
- $\mathcal{D}(\boldsymbol{\theta})$ approximately distributed $N(\cdot, \sigma_0^2)$ with σ_o^2 independent of $\boldsymbol{\theta}$.
- $\mathbb{E}[\mathcal{D}(\boldsymbol{\theta})]$ can be well approximated by a Gaussian process.

Key Idea

Approximate $\mathcal{D}(\boldsymbol{\theta})$ with $\mathcal{D}_{\mathcal{GP}}(\boldsymbol{\theta})$, a Gaussian process with observation noise.

ABC

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2. Run model
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Approximate ABC...??

1. Sample $\boldsymbol{\theta}_i$ from prior
2. Run model
3. Accept $\boldsymbol{\theta}_i$ if $\underline{\ \mathcal{D}_{\mathcal{GP}}(\boldsymbol{\theta}_i) < \varepsilon.\ }$

Synthetic Likelihood

The probability of drawing and accepting $\boldsymbol{\theta}$ under the ABC is

$$\Pr(\mathcal{D}_{\mathcal{GP}}(\boldsymbol{\theta}) < \varepsilon) \Pr(\boldsymbol{\theta})$$

and hence we consider $L(\boldsymbol{\theta}|\mathbf{Y}_{\text{obs}}) := \Pr(\mathcal{D}_{\mathcal{GP}}(\boldsymbol{\theta}) < \varepsilon)$ a synthetic likelihood - an approximation of the true likelihood $\mathcal{L}(\boldsymbol{\theta}|\mathbf{Y}_{\text{obs}})$

Log Gaussian Process

- Alternatively we can model $\ln \mathcal{D}(\boldsymbol{\theta})$ as a Gaussian process $d_{\mathcal{GP}}(\boldsymbol{\theta})$.

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  - $\mathcal{D}(\boldsymbol{\theta})$ approximately distributed $LN(\cdot, \sigma_0^2)$ with σ_o^2 independent of $\boldsymbol{\theta}$.
  - $\mathbb{E}[\ln \mathcal{D}(\boldsymbol{\theta})]$ can be well approximated by a Gaussian process.
- $$\Pr(\mathcal{D}(\boldsymbol{\theta}_i) < \varepsilon) \approx \Pr(d_{\mathcal{GP}}(\boldsymbol{\theta}_i) < \ln \varepsilon)$$

Where to sample $\mathcal{D}(\boldsymbol{\theta})$

- To generate a reliable $\mathcal{D}_{\mathcal{GP}}$, we need to sample widely
- Generating $\mathcal{D}(\boldsymbol{\theta})$ still costly...
- Therefore sample where:

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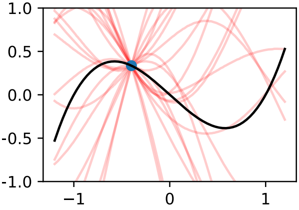
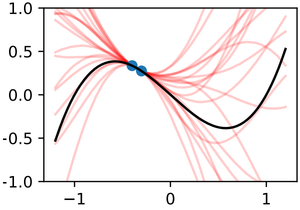




Bayesian Acquisition Functions

- Quantify where we expect $\mathcal{D}(\boldsymbol{\theta})$ small and highly unknown with Bayesian acquisition function A, and choose $\arg\min_{\boldsymbol{\theta}} A(\boldsymbol{\theta})$

Bayesian Acquisition Functions

- Gutmann and Cor 2016 use lower confidence bound

$$A_{\mathsf{LCB}}(\boldsymbol{\theta}) := \mu(\boldsymbol{\theta}) - \eta_t \sqrt{\mathrm{v}(\boldsymbol{\theta})}$$

  - $\mu(\boldsymbol{\theta})$, $\mathrm{v}(\boldsymbol{\theta})$ are posterior mean and variance of $D_{\mathcal{GP}}(\boldsymbol{\theta})$
  - η_t a slowly increasing function in t, the number of previous samples

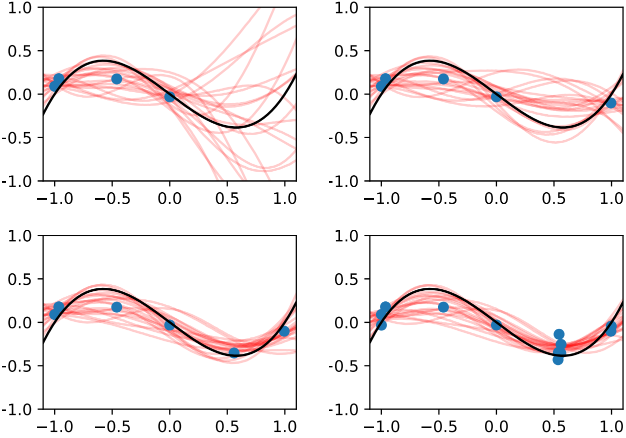
Bayesian Acquisition Functions

- Expected information

$$A_{\mathsf{EI}}(\boldsymbol{\theta}) := \mathbb{E}[\min(\mu_{\min} - \mathcal{D}_{\mathcal{GP}}(\boldsymbol{\theta}), 0)]$$

  - $\mu_{\min} := \min_{\boldsymbol{\theta}} \mu(\boldsymbol{\theta})$

Lower Confidence Bound



Vivax Model - Champagne et. al

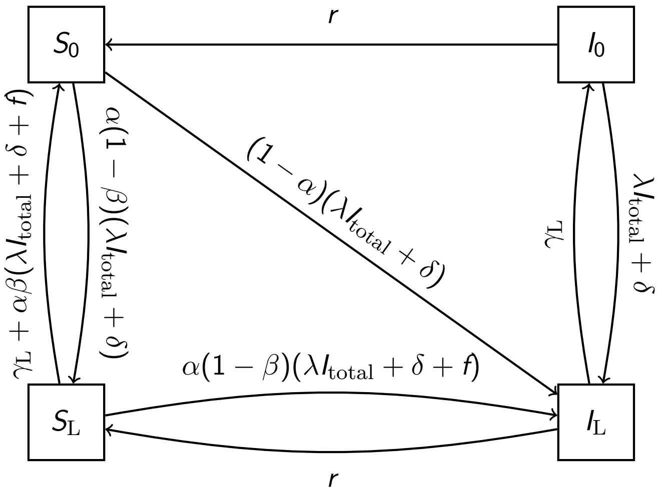


Figure: Champagne et al. 2022 *P. vivax* model

Champagne Model Parameters

- α : proportion of those infected but cleared of blood stage infections (through treatment)
- β : a further proportion that are also cleared of liver stage parasites, given that they were also cleared of blood stage infection (radical cure)
- λ : the rate of infection
- γ_L : rate of clearance of liver stage disease
- f : rate of relapse
- r : rate of blood stage clearance

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Model Simulation

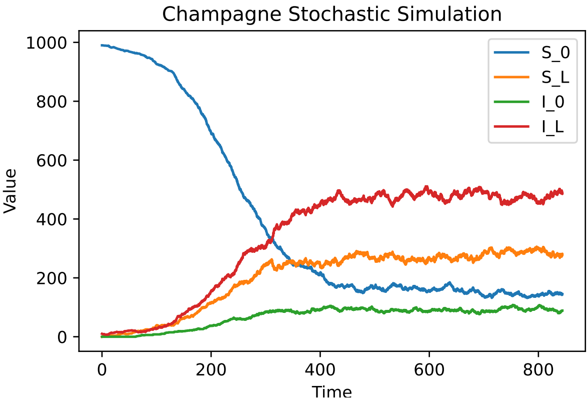

Figure: Exact stochastic simulation using parameters reported in Champagne et al. 2022.

'Observed' Data

- 'Observed' data from the model simulation 10 initial infections, in a population of 1000 people using the parameters reported in Champagne et al. 2022.
- $\mathbf{Y}_{\text{obs}} := \{w_{\text{obs}}, p_{\text{obs}}, m_{\text{obs}}\}$
  - w_{obs} : weekly incidence around (stochastic) equilibrium
  - p_{obs} : prevalence around (stochastic) equilibrium
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  - w_{obs} : weekly incidence around (stochastic) equilibrium
  - p_{obs} : prevalence around (stochastic) equilibrium
  - m_{obs} : incidence in the first month of the epidemic
- $\mathcal{D}(\alpha, \beta, \gamma_L, \lambda, f, r)$ is the L_2 norm of the relative differences

$$\sqrt{\left(\frac{p - p_{\text{obs}}}{p_{\text{obs}}}\right)^2 + \left(\frac{m - m_{\text{obs}}}{m_{\text{obs}}}\right)^2 + \left(\frac{w - w_{\text{obs}}}{w_{\text{obs}}}\right)^2}$$

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GP choices

- $\mathcal{D}(\alpha, \beta, \gamma_L, \lambda, f, r)$ is the L_2 norm of the relative differences

$$\sqrt{\left(\frac{p - p_{\text{obs}}}{p_{\text{obs}}}\right)^2 + \left(\frac{m - m_{\text{obs}}}{m_{\text{obs}}}\right)^2 + \left(\frac{w - w_{\text{obs}}}{w_{\text{obs}}}\right)^2}$$

- $\mathcal{GP}$ choices
  - Modelled $\ln \mathcal{D}$ as a Gaussian process
  - Matern kernel with $\nu = 5/2$
  - $\ell, \sigma_k^2, \sigma_o^2$ selected by leave one out cross validation.

How did it go?

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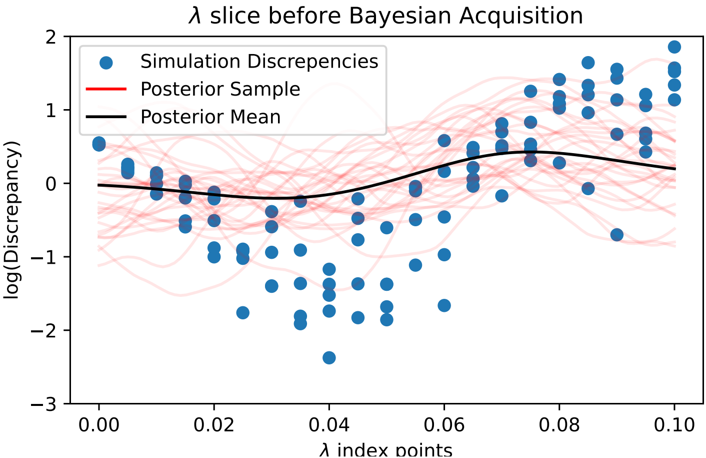
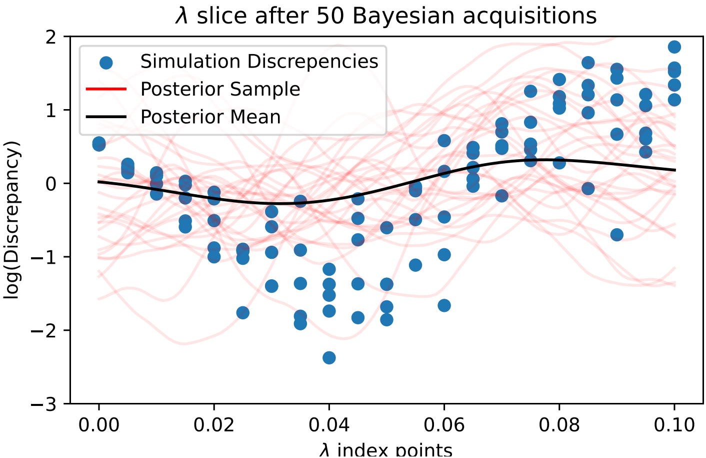
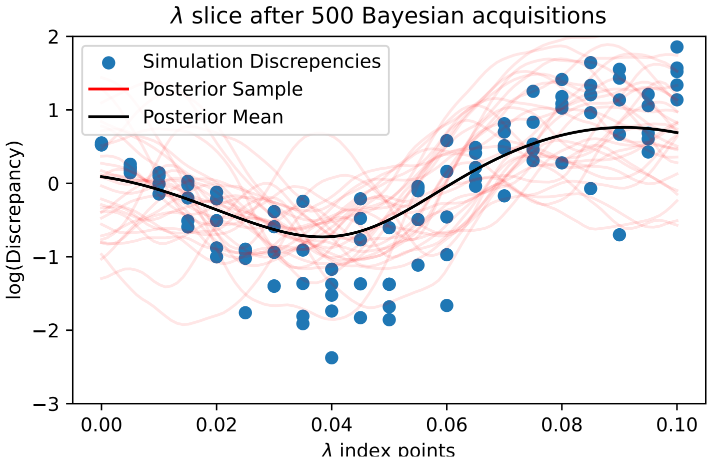

λ slice before Bayesian Acquisition
Simulation Discrepencies
Posterior Sample
Posterior Mean
log(Discrepancy)
2
1
0
−1
−2
−3
0.00
0.02
0.04
0.06
0.08
0.10
λ index points

How did it go?



λ slice after 50 Bayesian acquisitions
Simulation Discrepencies
Posterior Sample
Posterior Mean
log(Discrepancy)
λ index points
2
1
0
−1
−2
−3
0.00
0.02
0.04
0.06
0.08
0.10

How did it go?


λ slice after 500 Bayesian acquisitions
Simulation Discrepencies
Posterior Sample
Posterior Mean
log(Discrepancy)
2
1
0
−1
−2
−3
0.00
0.02
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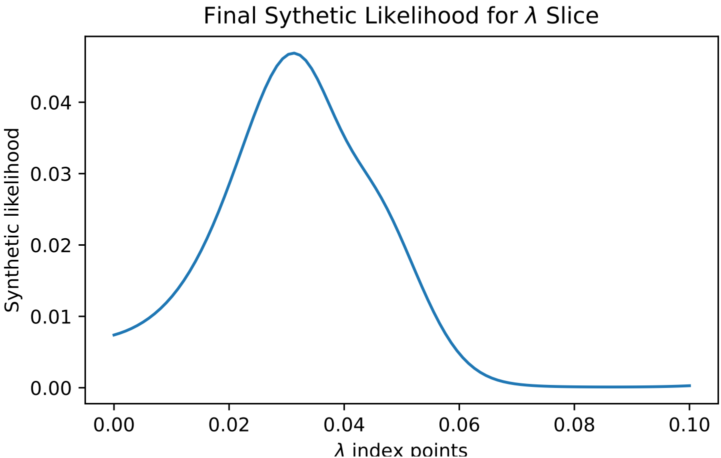
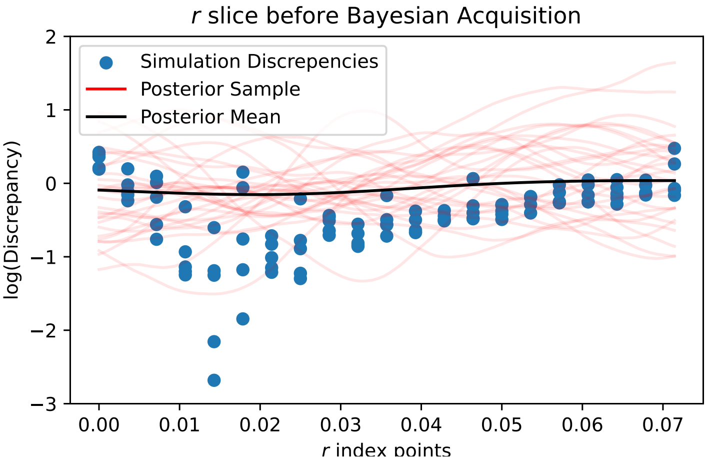
How did it go?



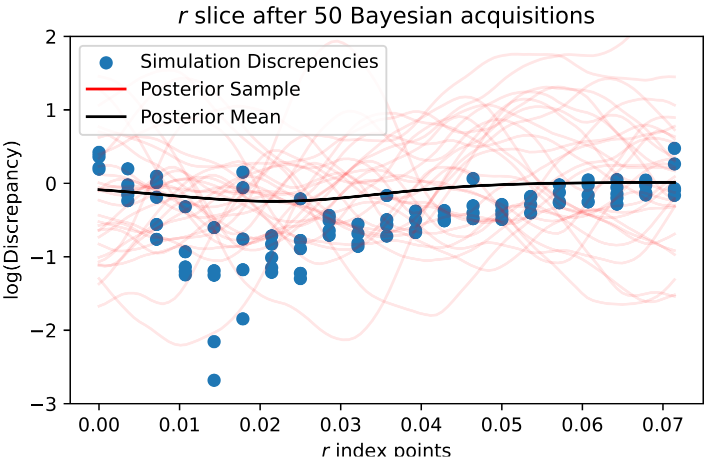
Final Sythetic Likelihood for λ Slice
Synthetic likelihood
0.04
0.03
0.02
0.01
0.00
0.00
0.02
0.04
0.06
0.08
0.10
λ index points

How did it go?



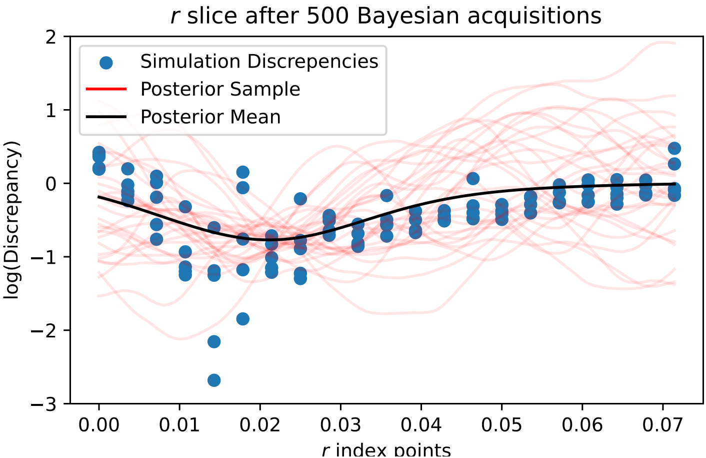
r slice before Bayesian Acquisition
Simulation Discrepencies
Posterior Sample
Posterior Mean
log(Discrepancy)
2
1
0
−1
−2
−3
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
r index points

How did it go?



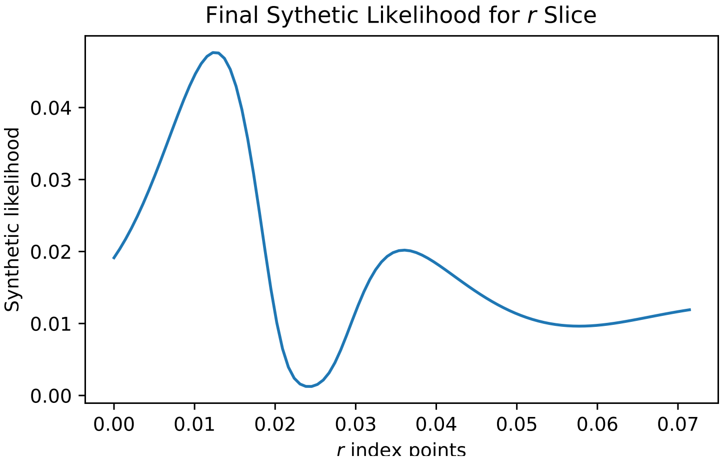
r slice after 50 Bayesian acquisitions
Simulation Discrepencies
Posterior Sample
Posterior Mean
log(Discrepancy)
2
1
0
−1
−2
−3
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
r index points

How did it go?



r slice after 500 Bayesian acquisitions
Simulation Discrepencies
Posterior Sample
Posterior Mean
log(Discrepancy)
r index points
2
1
0
−1
−2
−3
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07

How did it go?



Final Sythetic Likelihood for r Slice
Synthetic likelihood
0.00
0.01
0.02
0.03
0.04
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
r index points

Discussion

- Observation variance is considered constant across the GP (or log GP)
  - Particularly a problem at the threshold
- Assumes that normal/log-normal distribution approximates $\mathcal{D}(\boldsymbol{\theta})$
- Jumps where there is threshold/bifurcation behaviour
  - Student $t-$Process?

Thanks to

- Eamon Conway
- Jennifer Flegg

Bibliography

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