Emulating computer experiments of rail infrastructure slope stability using Gaussian processes and Bayesian inference

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Deterioration of infrastructure slopes[1]

- Many rail slopes ≈ 200 years old[2]
- Built in high-plasticity clay (London Clay)
- Wet weather and weather extremes increase deterioration
- Highways suffer similar problems
  - Though they're younger
- Our focus: Great Western Main Line

[1] https://www.achilles-grant.org.uk/
[2] Skempton AW. *Construction History*. 1996;11:33-49.

Computer experiments of deterioration

- Modelling strain softening of over-consolidated clays in cutting slopes[3,4]
  - Influence of weather and seasonal cycles
  - Seasonal shrink-swell cycles impact strength
- Model informed by previous studies
- Latin hypercube design of 76 experiments
  - Geometry (height and angle cotangent)
  - Soil strength (peak cohesion)
  - Soil strength (peak friction angle)
  - Permeability
- **Monitor time to slope failure (years)- completed**
- **Monitor factor of safety- ongoing**

[3] Rouainia M, Helm P, Davies O, Glendinning S. *Acta Geotechnica*. 2020;15:2997-3016.
[4] Postill H, Helm P, Dixon N, *et al*. *Engineering Geology*. 2021;280;1-19.

Superficial cut slope failure on the GWML between London and S Wales

https://theconversation.com/britain-needs-infrastructure-ready-for-climate-change-before-its-too-late-62375

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Emulating computer experiments

- Numerical models are very time-consuming

Numerical model*	Emulator*[5]
76 models	900 models
40 days	5 hours
10 machines	1 machine

* Once trained

[5] Svalova A, Helm P, Prangle D, Rouainia M, Glendinning S, Wilkinson DJ. *Data-Centric Engineering*. 2021.

Emulating computer experiments

- Consider a simulator f evaluated at inputs $\boldsymbol{x}$ (e.g. geometry, strength, permeability) to produce outputs $\boldsymbol{y} = f(\boldsymbol{x})$[6]
- Require η s.t. $\eta(\boldsymbol{x}) \approx f(\boldsymbol{x})$
  - Use **Gaussian processes**
- Need f to be smooth and continuous
- Assume f can be approximated by a multivariate normal distribution

[6] Bastos LS, O'Hagan A. *Technometrics*. 2009;51:425-438.

Gaussian processes for emulation

- Gaussian processes- infinite-dimensional distributions for functions
- Assume $\eta(\cdot)$ takes input $\boldsymbol{x} = (x_1, x_2, \dots, x_p)$ where $x_i \in \chi_i \subset \mathbb{R}$
- A scalar-valued Gaussian process is fully defined by its mean and covariance functions m and V:

$$\eta(\cdot)|\boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta}, \tau \sim \mathrm{GP}\big(m(\cdot), V(\cdot,\cdot)\big),$$

$$m: \mathbb{R}^{\mathrm{p}} \to \mathbb{R}, \qquad V: \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$$

[6] Bastos LS, O'Hagan A. *Technometrics*. 2009;51:425-438.

Gaussian processes for emulation

- m is often a linear transformation of the input variables

$$m(\boldsymbol{x}) = h(\boldsymbol{x})^T \boldsymbol{\beta}, \qquad h(\cdot): \mathbb{R}^p \to \mathbb{R}^q,$$

$$e.g.\, h(\boldsymbol{x}) = \left(1, x_1, \dots, x_p\right), \qquad \boldsymbol{\beta} = \left(\beta_0, \beta_1, \dots, \beta_{p+1=q}\right)$$

- V has the form $V(\boldsymbol{x}, \boldsymbol{x}') = \sigma^2 \left[C(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{\theta}) + \tau \mathbb{I}(\boldsymbol{x}, \boldsymbol{x}')\right]$
  - σ^2- marginal variance
  - $C(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{\theta})$- is a correlation function (cts and psd)
  - $\boldsymbol{\theta}$- vector of correlation lengths
  - τ- nugget[7,8]
  - $\mathbb{I}(\boldsymbol{x}, \boldsymbol{x}')$ is an indicator function

[7] Andrianakis I, Challenor PG. *Computational Statistics and Data Analysis*. 2012;56:4215-4228.

Types of the correlation functions

- Gaussian correlation function[6]

$$C_G(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{\theta}) = \exp\left\{-\sum_{(i=1)}^{p} \frac{(x_i - x_i')^2}{\theta_i^2}\right\}$$

- Matern correlation function family[9]

$$C_M(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{\theta}, \nu) = \prod_{(i=1)}^{p} \frac{1}{\Gamma(\nu)2^{\nu-1}} \left(\frac{\sqrt{2\nu}|x_i - x_i'|}{\theta_i}\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}|x_i - x_i'|}{\theta_i}\right)$$

K_ν- modified Bessel function of second kind of order ν

[6] Bastos LS, O'Hagan A. *Technometrics*. 2009;51:425-438.
[9] Rasmussen CE, Williams CKI. *Gaussian processes for machine learning*. 2006. The MIT Press: Cambridge, Massachusetts.

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GPE conditional on observations

- GPs are closed under conditioning- can derive an analytical expression for the GPE conditioned on a set of computer experiments.
- Assume a collection of n outputs $\boldsymbol{y} = \left(f(\boldsymbol{x}_1), f(\boldsymbol{x}_2), \ldots, f(\boldsymbol{x}_n)\right)$ performed on $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$
  - $\boldsymbol{y} | \boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta}, \tau \sim \mathrm{N}(H_x \boldsymbol{\beta}, \sigma^2\, \Sigma_x)$
  - H_x- regressor matrix, $H_{x,i} = h(\boldsymbol{x}_i)$
  - $\Sigma_{x(i,j)} = C\left(\boldsymbol{x}_i, \boldsymbol{x}_j, \boldsymbol{\theta}\right) + \tau \mathbb{I}(i,j)$- correlation matrix

$$\eta(\cdot) | \boldsymbol{y}, \boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta}, \tau \sim \mathrm{GP}\left(m^*(\cdot), V^*(\cdot,\cdot)\right),$$

$$m^*(\boldsymbol{x}) \;=\; h(\boldsymbol{x})^T \boldsymbol{\beta} + t(\boldsymbol{x})^T\, \Sigma_x^{-1}\, (\boldsymbol{y} - H_x \boldsymbol{\beta}),$$

$$V^*(\boldsymbol{x}, \boldsymbol{x}') = \sigma^2 \left(C(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{\theta}) - t(\boldsymbol{x})^T\, \Sigma_x^{-1} t(\boldsymbol{x}')\right),$$

$$t(\boldsymbol{x}) \;=\; \left(C(\boldsymbol{x}, \boldsymbol{x}_1, \boldsymbol{\theta}), C(\boldsymbol{x}, \boldsymbol{x}_2, \boldsymbol{\theta}), \ldots, C(\boldsymbol{x}, \boldsymbol{x}_n, \boldsymbol{\theta})\right)^T$$

[6] Bastos LS, O'Hagan A. *Technometrics*. 2009;51:425-438.

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Censored computer output

- For some models, failure not reached within 184 years
  - n experiments at $\boldsymbol{x}_o = \left(\boldsymbol{x}_{o,1}, \boldsymbol{x}_{o,2}, \dots, \boldsymbol{x}_{o,n}\right)$ produced uncensored observations $\boldsymbol{y}_o$
  - n_c experiments at $\boldsymbol{x}_c = \left(\boldsymbol{x}_{c,1}, \dots, \boldsymbol{x}_{c,n_c}\right)$ produced censored "observations" $\boldsymbol{y}_c$
- Define a new process $\eta_c(\cdot)$ where[10]

$$\eta_c(x) = \begin{cases} \eta(x), & \text{if } \eta(x) < c, \\ c, & \text{otherwise} \end{cases}$$

- The distribution of $\eta_c(\boldsymbol{X})$ at design points $\boldsymbol{X} = (\boldsymbol{x}_c, \boldsymbol{x}_o)$ is:

$$\eta(\boldsymbol{x}_o) \mid \boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta}, \tau \sim \mathrm{N}(H_o\boldsymbol{\beta}, \sigma^2\Sigma_o),$$

$$\eta_c(\boldsymbol{x}_c) | \eta(\boldsymbol{x}_o), \boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta} \sim \mathrm{TN}_{(c,\infty)}(m_c, V_c),$$

$$m_c = H_c\boldsymbol{\beta} + \Sigma_{c,o}\Sigma_o^{-1}(\eta(\boldsymbol{x}) - H_o\boldsymbol{\beta}) \text{ and } V_c = \sigma^2\left(\Sigma_c - \Sigma_{c,o}\Sigma_o^{-1}\Sigma_{o,c}\right)$$

  - H_o and Σ_o are equivalent to H_x and Σ_x
  - H_c is a matrix of regressors associated with $\boldsymbol{x}_c$, $\Sigma_{c(i,j)} = C(\boldsymbol{x}_{c,i}, \boldsymbol{x}_{c,j}, \boldsymbol{\theta}) + \tau\, \mathbb{I}(i,j)$
  - $\Sigma_{c,o(i,j)} = C\left(\boldsymbol{x}_{c,i}, \boldsymbol{x}_{o,j}, \boldsymbol{\theta}\right)$ and $\Sigma_{o,c} = \Sigma_{c,o}^T$

[10] Kyzyurova KN. PhD. *On uncertainty quantification for systems of computer models*. 2014. Duke University.

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Bayesian inference

- Values of $\boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta}$ and τ unknown
- The priors are as follows:

$$\beta_0 \sim \mathrm{N}(0,10^2), \quad \beta_i \sim \mathrm{N}(0,4^2), \quad \sigma^2 \sim \mathrm{IGa}(3,0.5),$$
$$\theta_i \sim \mathrm{Exp}(0.2), \quad \tau \sim \mathrm{IGa}(3,1), \quad i = 1,2,\dots,5$$

- The resulting posterior of $\eta(\cdot)|$ ... also unknown
- Use MCMC
  - Met+Gibbs
  - Impute $\boldsymbol{y}_{censored}$ (data augmentation)
- Most optimal:
  - Regressor function mean
  - Matern correlation function with $\nu = 5/2$
  - Square root of output

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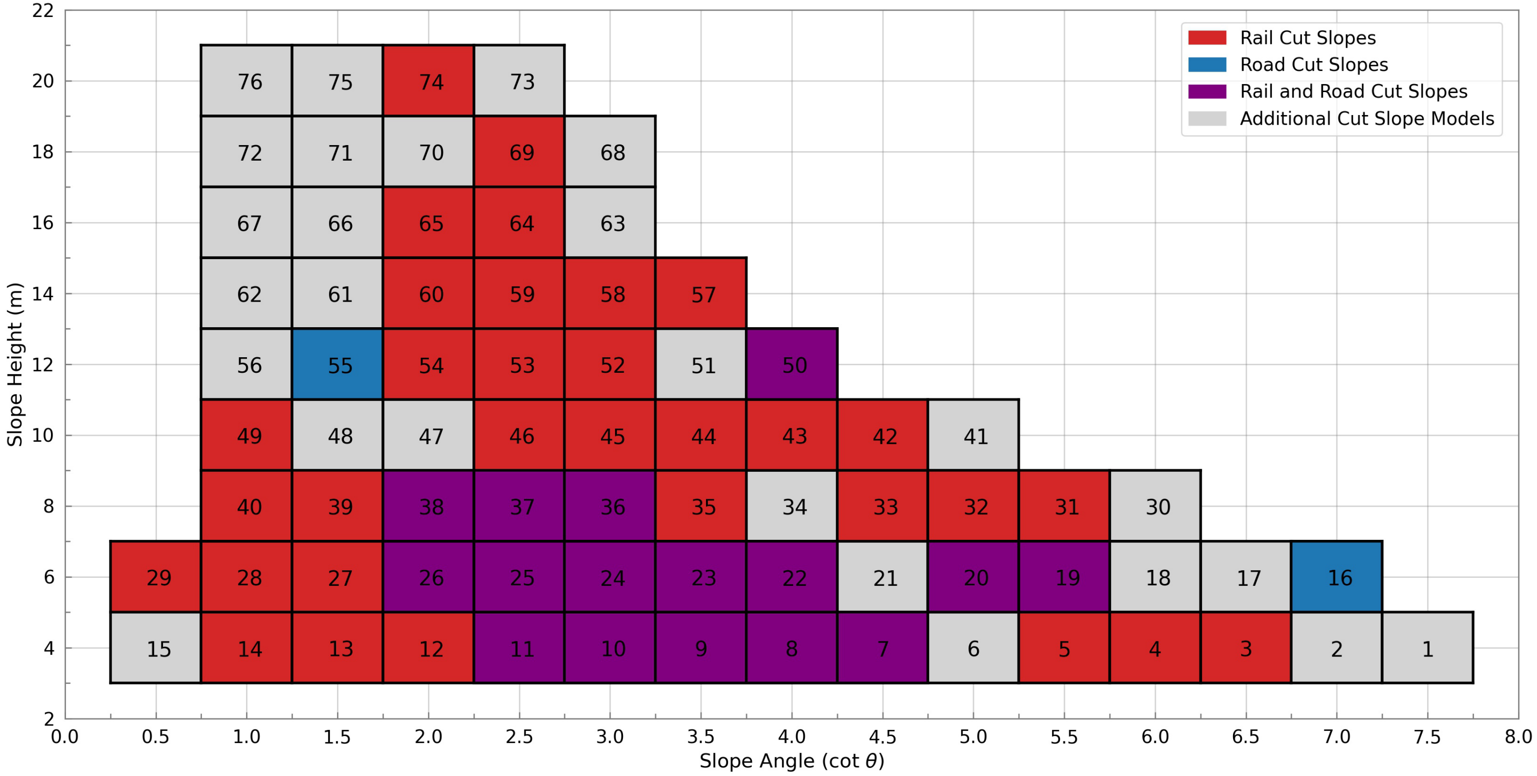
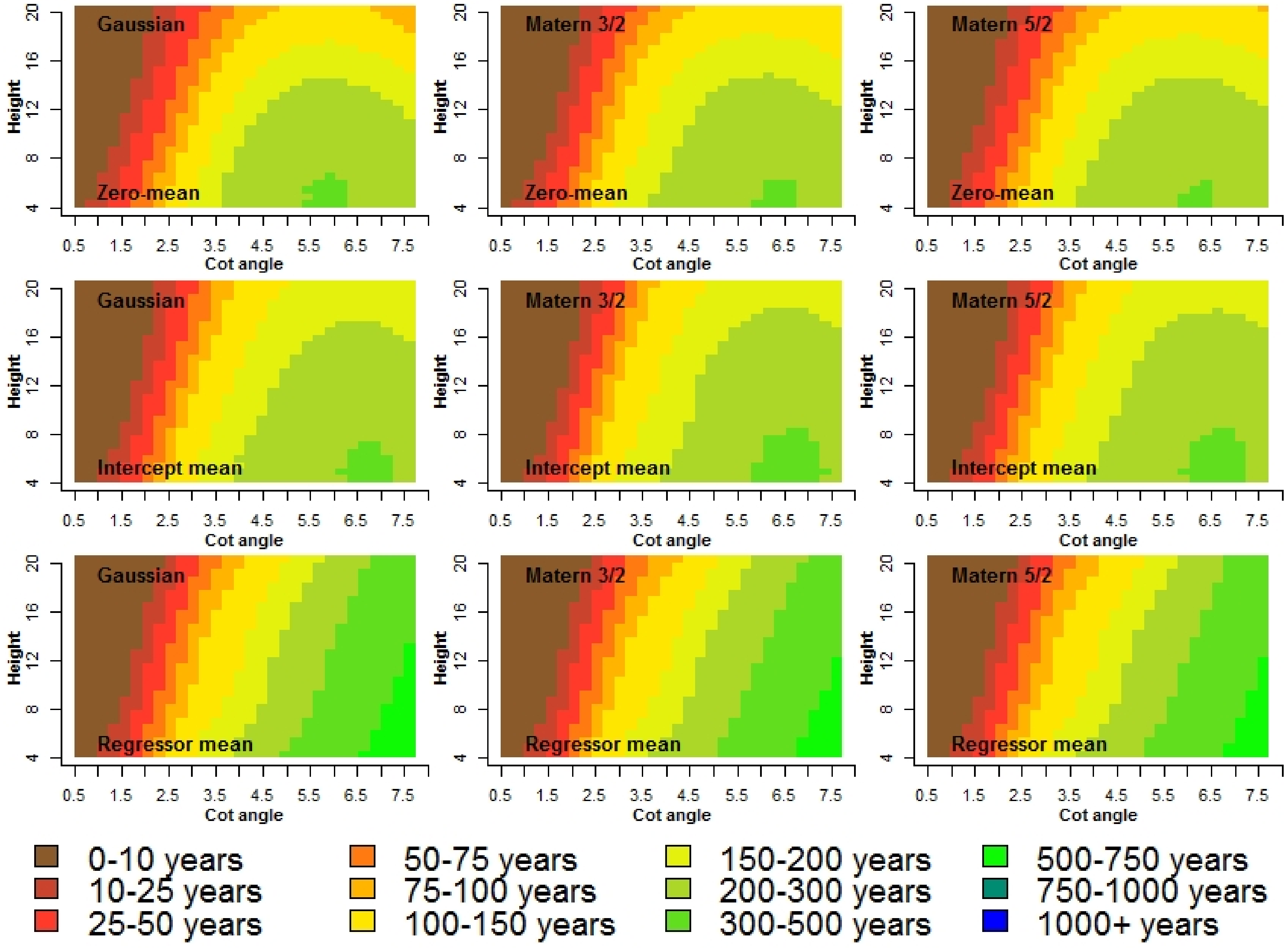
Latin hypercube design



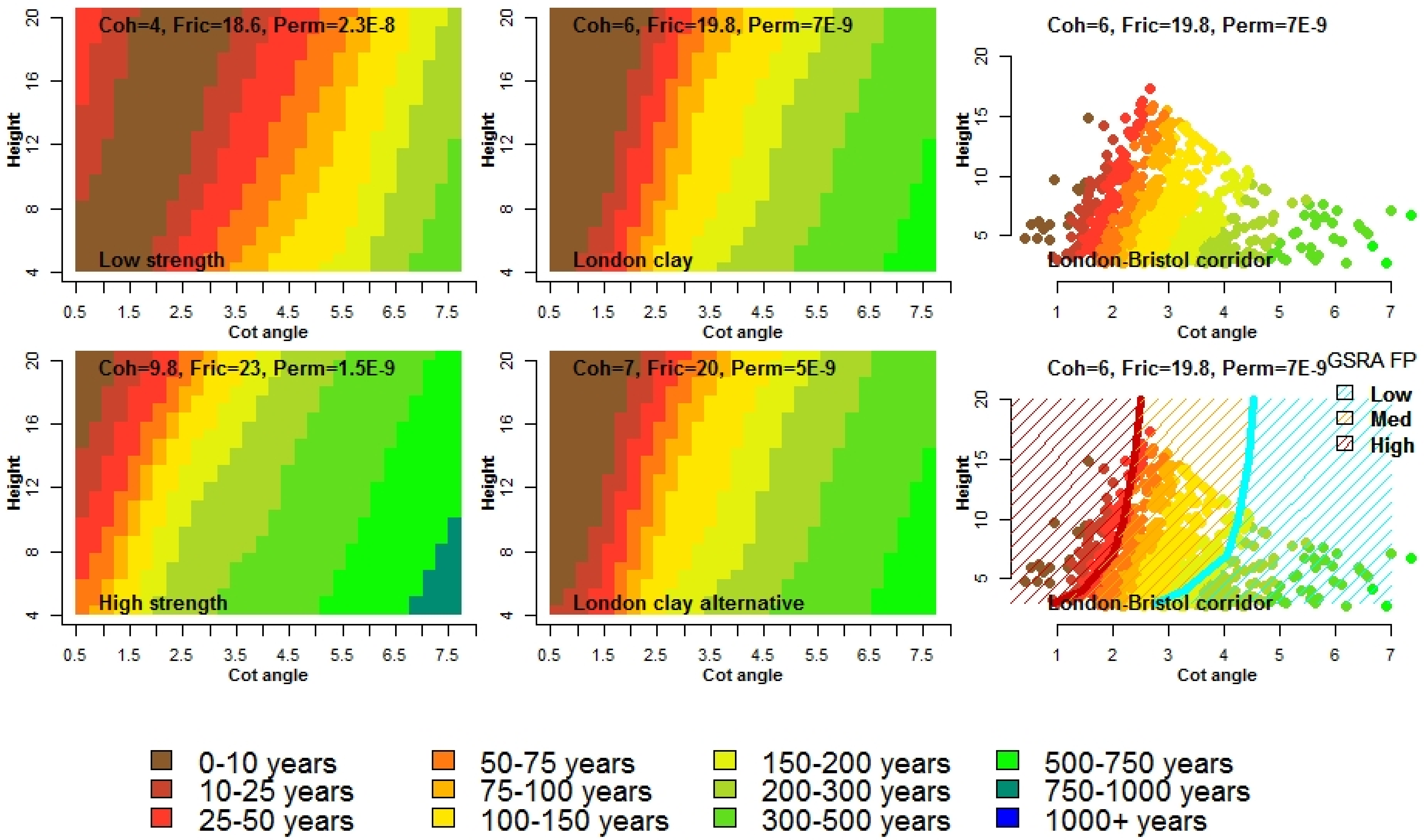
Variable	Height m	Cot angle $degrees$	Cohesion kPa	Friction $degrees$	Permeability ms^{-1}
Range	[4, 20]	[0.5, 7.5]	[3, 10]	[18.5, 25]	[1.45E-9, 2.5E-8]

TTF BPD using different mean and correlation functions

Cohesion = 7 kPa
Friction = 19.8 deg
Perm = 7E-9 ms^{-1}



Results: TTF



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Sensitivity analysis

- Explain the variation in the mean response of the emulator due to an individual or a combination of input variable(s)[11]
- Fully-Bayesian
- For independent input variables $x_i, U(x) = \prod_{i=1}^{p} u_i(x_i)$
- Main effects[11]:

$$me(x_i) \equiv E_{U_{-i}}(\eta|x_i)$$
$$= \int\int_{-\chi_{-i}} \eta p(\eta|x_1, x_2, \ldots, x_p) \cdot u_{-i}(x_{-i}) dx_{-i} d\eta$$

[11] Gramacy R. *Surrogates*. 2020. CRC Press: Boca Raton.

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Sensitivity indices[12,13]

- The first-order sensitivity index $S_{1,i}, i = 1,2, \ldots, p$ evaluates the fractional contribution of x_i to the variance of the output

$$S_{1,i} = \frac{\mathrm{E}\left[\mathrm{E}^2[\eta|x_i]\right] - \mathrm{E}^2[\eta]}{\mathrm{Var}(\eta)}$$

- The total sensitivity index $S_{T,i}$ is a measure of the entire influence attributable to a given variable

$$S_{T,i} = 1 - \frac{\mathrm{E}\left[\mathrm{E}^2[\eta|x_{-i}] - \mathrm{E}^2[\eta]\right]}{\mathrm{Var}(\eta)}$$

- A large difference between the distributions of $S_{1,i}$ and $S_{T,i}$ would indicate that the interactions between the x_i and the remaining input variables are important to explaining the output variation

[12] Homma T, Saltelli A. *Reliability Engineering and System Safety*. 1996;35;1-17.
[13] Farah M, Kottas A. *Technometrics*. 2014;56:159-173.

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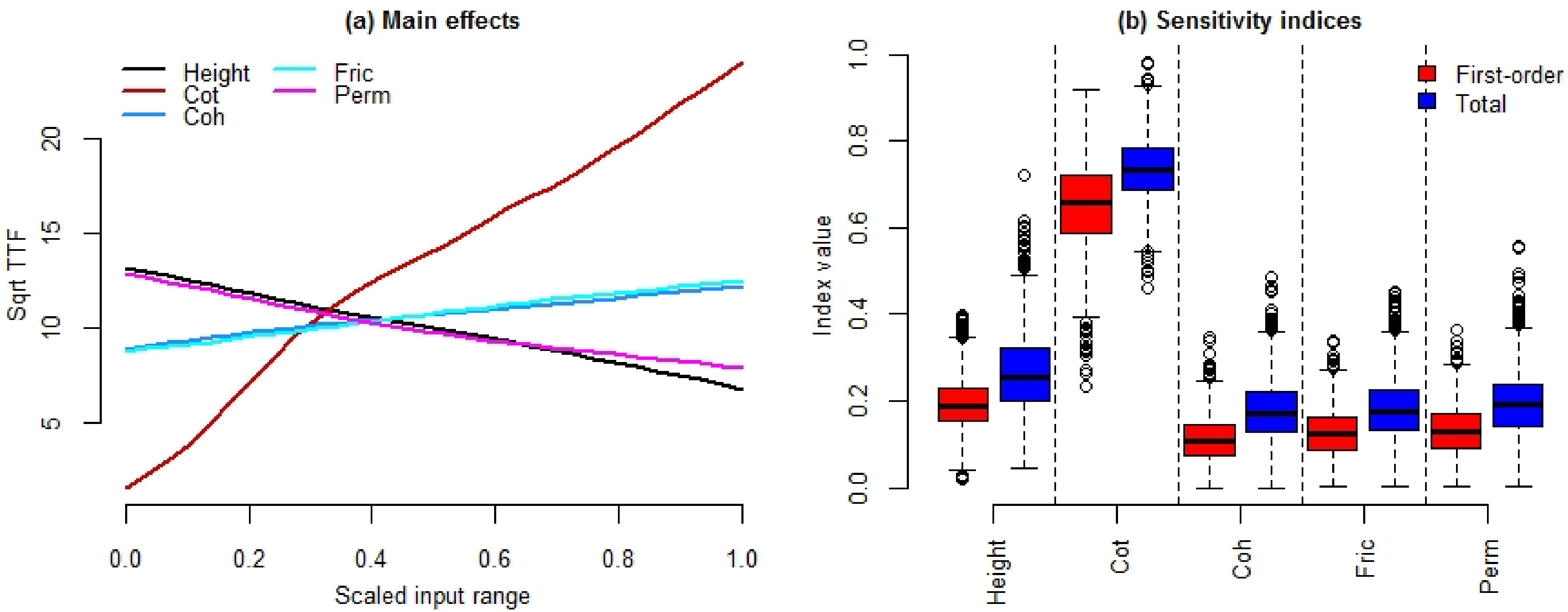
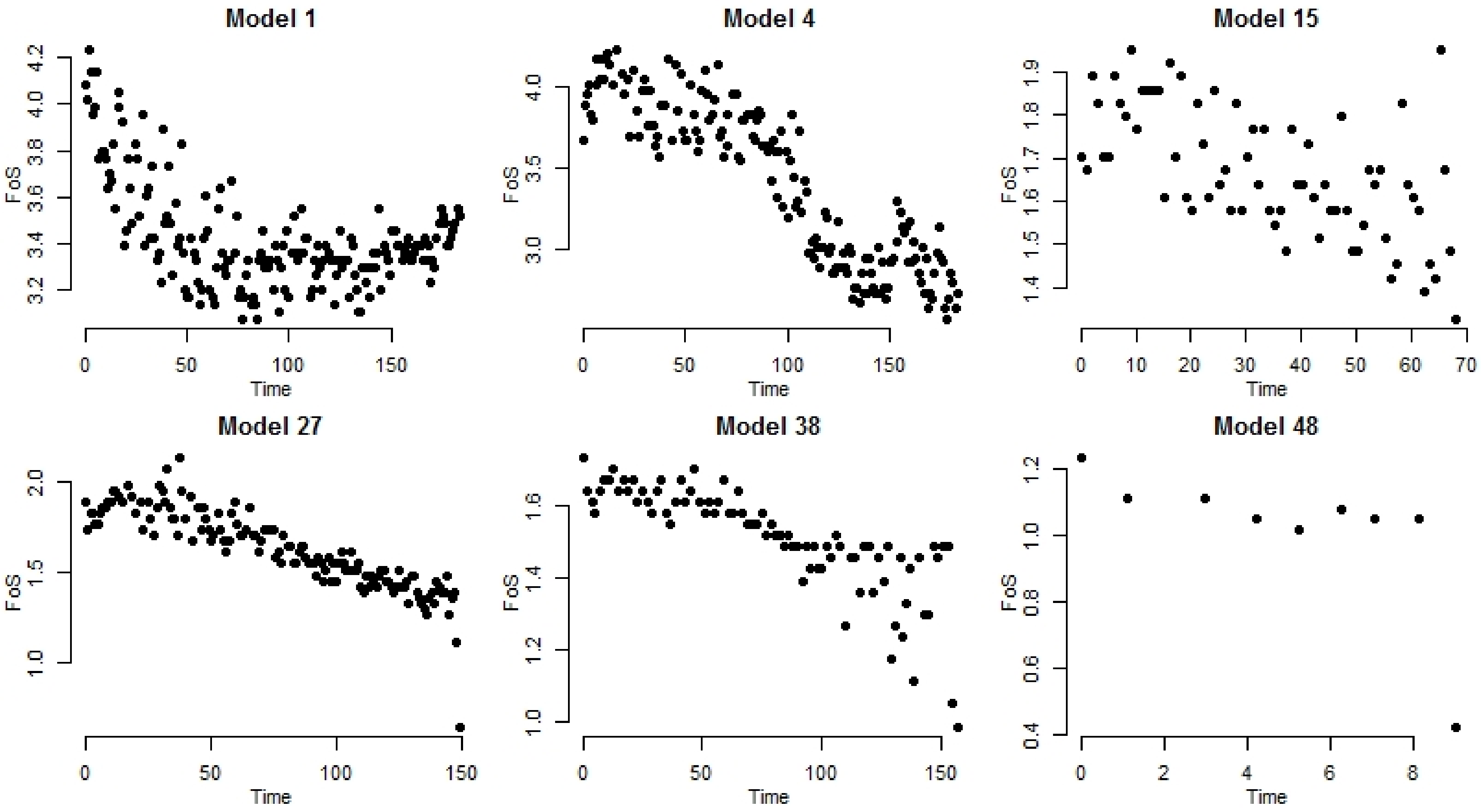
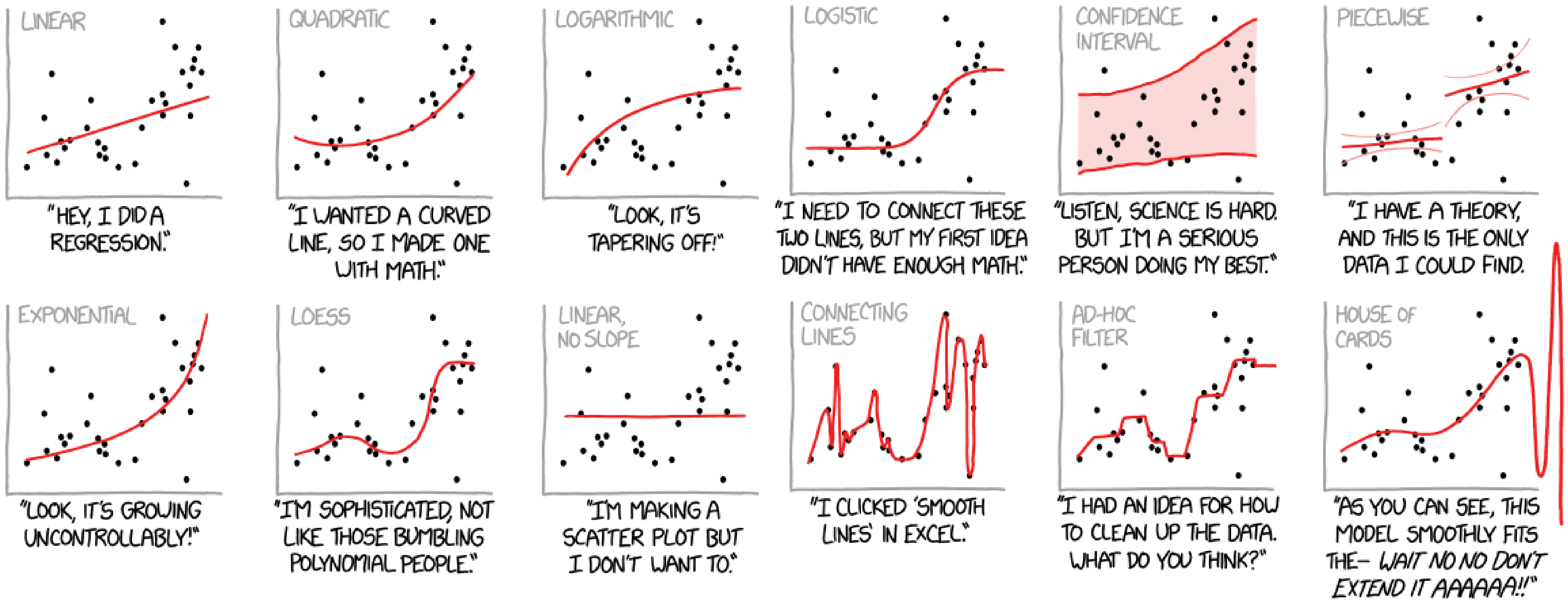
Sensitivity analysis



FoS modelling



FoS modelling- approximation with a simple model



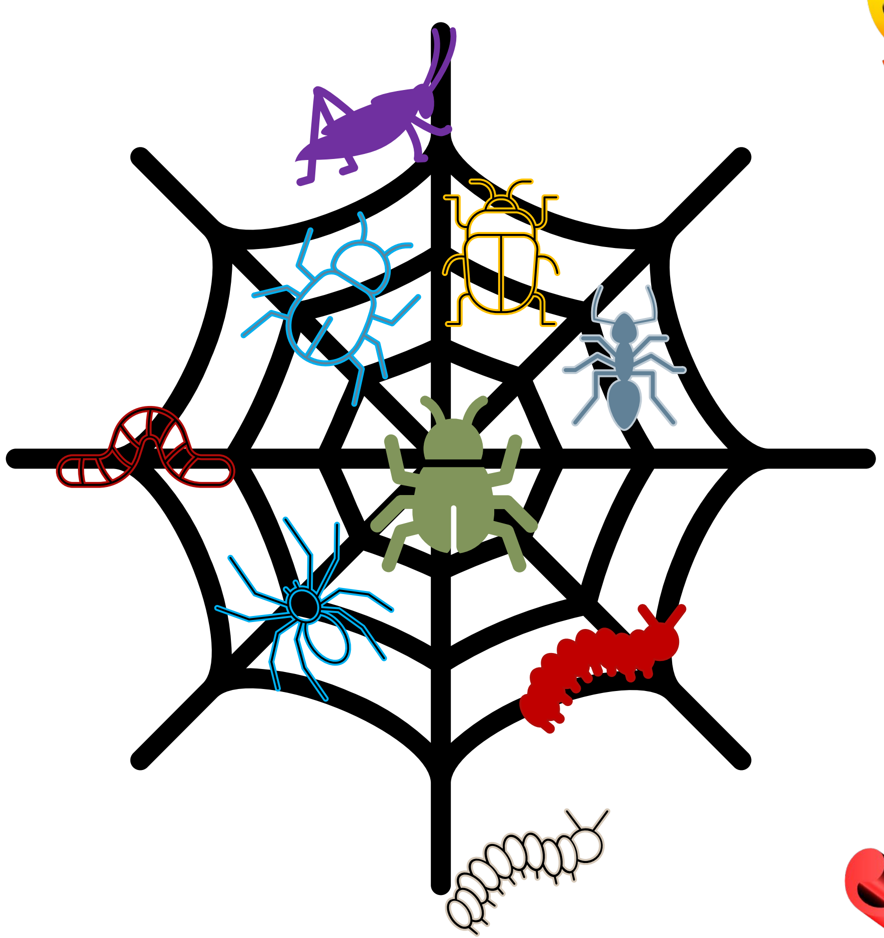
Quadratic model of FoS

- Put a GP prior on the polynomial coefficients
- Let $y_{i,j} = \mathrm{FoS}_{i,j} - 1$

$$y_{i,j} = \alpha_{0,i} + \alpha_{1,i} t_{i,j} + \alpha_{2,i}\, t_{i,j}^2 + \varepsilon_{i,j}, \qquad \varepsilon_{i,j} \sim N(0, \sigma_i^2)$$

- Can also re-formulate $y_{i,j}$ to include failure time
- Constrain the quadratic coefficients to avoid convex curves
  - Failure is defined by $y_{i,j}$ reaching zero for the first time

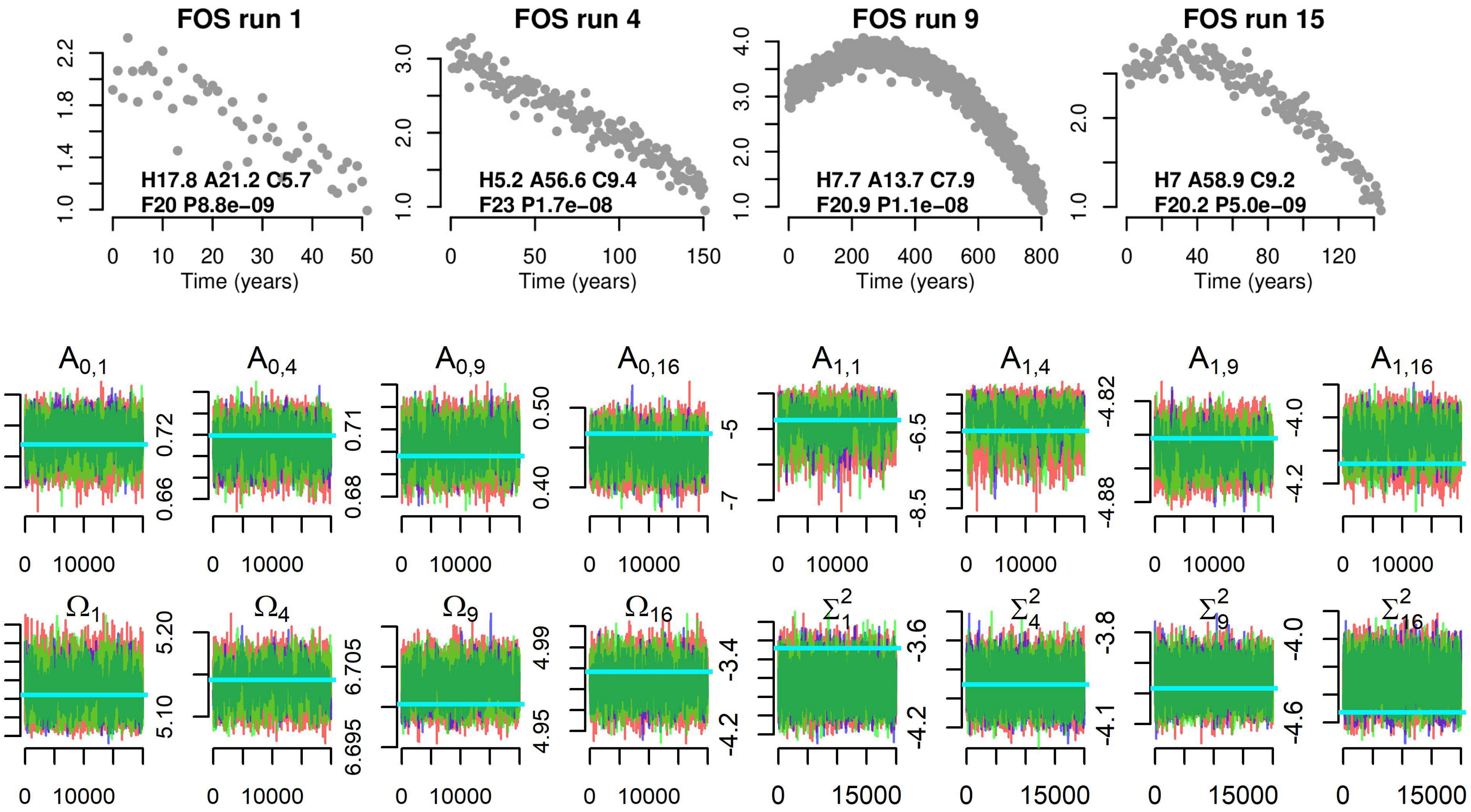
Quadratic model of FoS- debugging



STAN

R

JAGS


FOS run 1
FOS run 4
FOS run 9
FOS run 15
H17.8 A21.2 C5.7
F20 P8.8e−09
H5.2 A56.6 C9.4
F23 P1.7e−08
H7.7 A13.7 C7.9
F20.9 P1.1e−08
H7 A58.9 C9.2
F20.2 P5.0e−09
Time (years)
Time (years)
Time (years)
Time (years)
A0,1
A0,4
A0,9
A0,16
A1,1
A1,4
A1,9
A1,16
Ω1
Ω4
Ω9
Ω16
Σ1 2
Σ4 2
Σ9 2
Σ16 2

Summary

- A GPE estimates the relationship between slope TTF and geometry, soil strength, and permeability
- Strong computational advantage
- Current work
  - FoS curves
  - Residual factor