

# Adventures in Emulation

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# Outline

Emulators

Stommel Model

Extremes

Emulation as Parameterisation

# Emulators

- ▶ There has been a lot of discussion at the workshop about emulators but just to recap
- ▶ We have a simulator

$$y = f(x)$$

- ▶ Treat  $f(\cdot)$  as an unknown random function and use Bayesian methods to estimate it
- ▶ Note it is possible to redo all this work in a frequentist way see book by Santner et al

# Gaussian Processes

- ▶ We model the simulator with a Gaussian Process
- ▶ This has mean

$$y = f(x) = h(x)^T \beta$$

- ▶ Variance  $\sigma^2$
- ▶ And correlation function  $c(x, x')$  Usually, but not invariably, we take

$$c(x, x') = \exp(-(x - x')^T C(x - x'))$$

$$C^{-1} = \text{diag}(\delta)$$

- ▶ so we have a set of GP parameters  $(\beta, \sigma, \delta)$  which we need to estimate

# The Prior

$$\mu(x) = h(x)^T \beta$$

$h(\cdot)$  is a known vector of regressor (or basis) functions

e.g.  $h(x)^T = (1, x, x^2)$

$\beta$  is a vector of unknown parameters

$$\rho(x_1, x_2) = \sigma^2 c(\|x_1, x_2\|)$$

$$c(x_1, x_2) = \exp\left(-\frac{\|x_1, x_2\|^2}{\delta}\right)$$

$$\pi(\beta, \sigma^2) \propto \sigma^{-2}$$

# The Posterior

$$\eta(x) \sim t_{n-q}$$

$$E(\eta(x)) = h(x)^T \beta' + t(x)^T A^{-1} (y - H\beta')$$

$$\beta' = \left( H^T A^{-1} H \right)^{-1} H^T A^{-1} y$$

H is the matrix  $\{h(x_1), \dots, h(x_n)\}^T$

*These are the regression terms at x*

$$t(x) = \{c(x, x_1), \dots, c(x, x_n)\}$$

*This is the correlation of x with the data,  $x_i$*

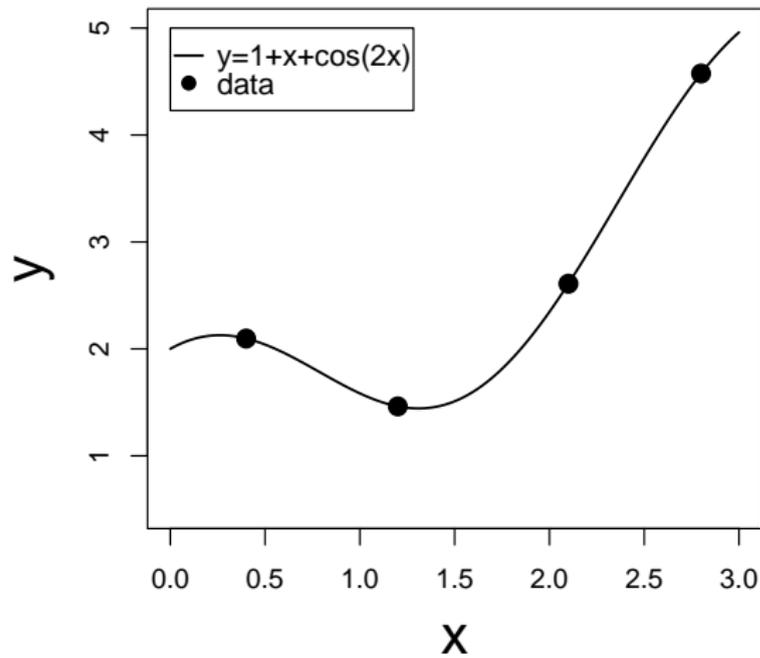
A is the matrix  $\{c(x_i, x_j)\}$

*This is the correlation matrix of the data with itself*

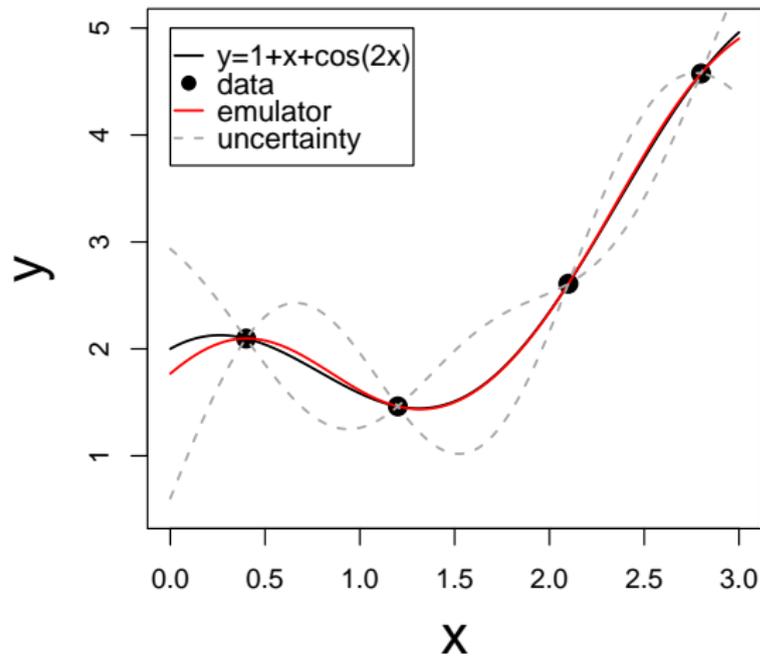
And there are similar, but more complex, expressions for the variance

We estimate  $\delta$  by maximising the marginal likelihood

# Example



# Example



# Some Adventures

- ▶ Highly non-linear models (the Stommel model)
- ▶ Extremes
- ▶ Emulation as Parameterisation

# Outline

Emulators

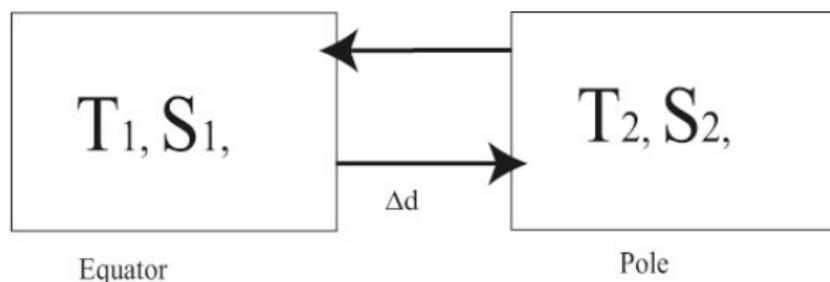
**Stommel Model**

Extremes

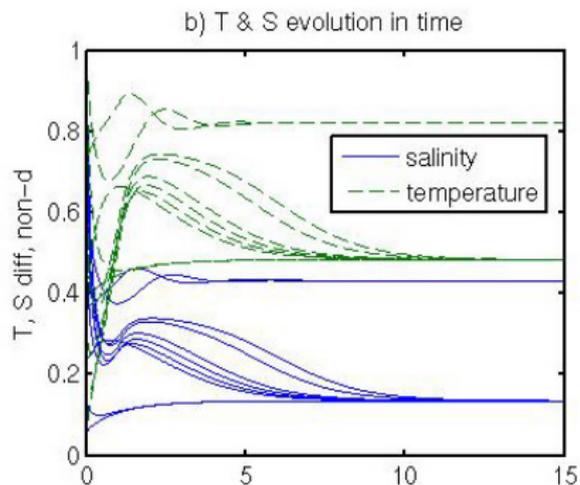
Emulation as Parameterisation

# The Stommel Model

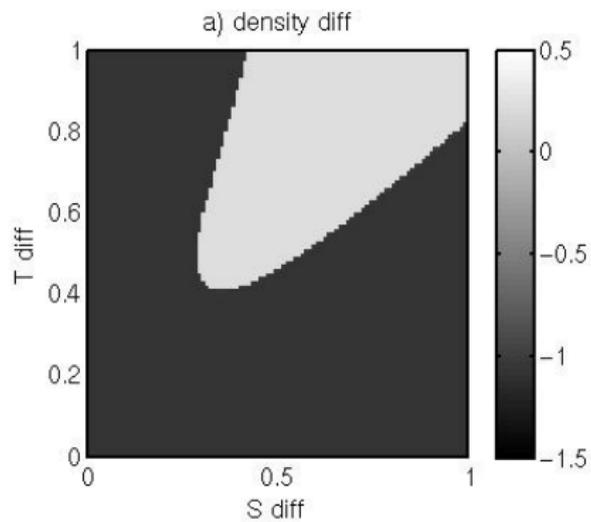
- ▶ The Stommel model for the Atlantic overturning circulation has only two states
- ▶ Our emulators assume 'smoothness'
- ▶ Can we emulate such a highly non-linear model?



# Emulating the Stommel Model

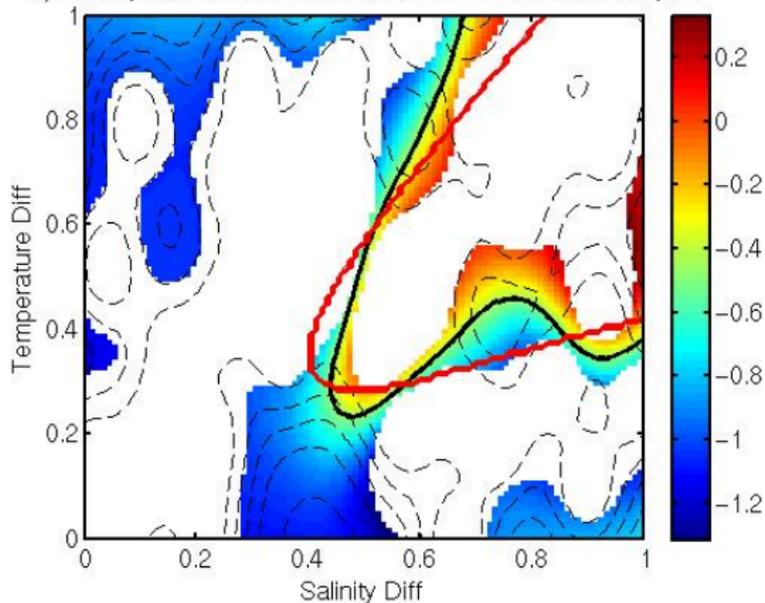


# Emulating the Stommel Model



# Emulating the Stommel Model

5) Density Dist from Emulator 40 Pts with variance overlaid



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Stommel Model

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Emulation as Parameterisation

# Extremes

- ▶ Often we are interested in future climate extremes not mean values

# The Statistics of Extremes

- ▶ In a similar way to the central limit theorem extremes have their own limits

$$\lim_{N \rightarrow \infty} F^N \left( \frac{x - a_N}{b_N} \right) = G(x)$$

- ▶ Distributions that satisfy these limits exactly are known as *max stable* distributions
- ▶ There is only one possible form: the *Generalised Extreme Value* distribution

$$P(X < x) = \exp \left\{ - \left[ 1 + \xi \left( \frac{x - \mu}{\sigma} \right) \right]^{-1/\xi} \right\}$$

- ▶ (Sometimes the limit is given as three different forms: Fréchet, Gumbel, and Weibull)

- ▶ These are obtained by performing extreme value analysis on model output via downscaling or a 'weather generator'
- ▶ These estimates don't have the simulator uncertainty included
- ▶ Can we emulate extremes directly across an ensemble of climate models?
- ▶ It is unrealistic to use GP's for this as we know that extremes have very non-Gaussian distributions

# Max stable processes

- ▶ In a similar way to Gaussian processes we can define max stable processes whose marginals are the extreme value distributions
- ▶ These are much more complex than Gaussian processes
- ▶ Brown-Resnick processes may be suitable for building extremal emulators

$$\eta(t) = \bigvee_{i=1}^{\infty} \left\{ U_i + W_i(t) - \frac{\sigma^2(t)}{2} \right\}$$

# An Alternative

- ▶ The Generalised Extreme Value (GEV) distribution has three parameters
- ▶ Extremes do not have Gaussian distributions
- ▶ But the parameters of the GEV can be assumed to do so
- ▶ Therefore we can jointly emulate the three parameters
- ▶ Since these three jointly define the extremes we have, in effect, a GP emulator for extremes
- ▶ The max stable process defined this way is less adaptable than the Brown-Resnick process

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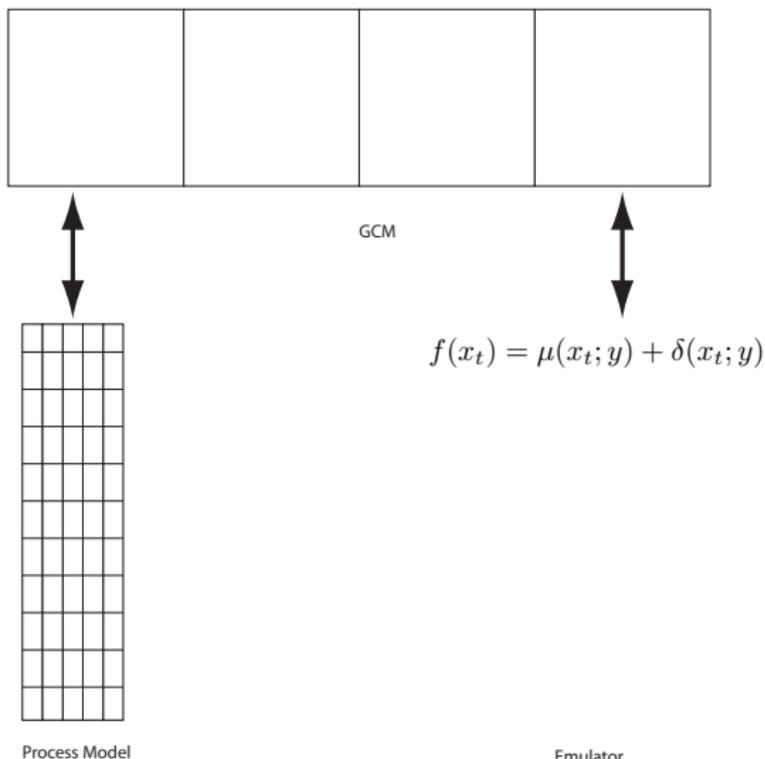
Extremes

Emulation as Parameterisation

# GCM's and Process Models

- ▶ GCM's do not model well sub-grid scale processes
- ▶ Often we have good process models
- ▶ These are too expensive to embed in the GCM
- ▶ Replace the process model with an emulator

# Emulation as parameterisation



We have a GCM represented by

$$x_{t+1} = g(x_t; \theta)$$

And a process model

$$x'_t = f(x_t; \phi, y_t)$$

where  $y_t$  are nuisance parameters We would like to calculate

$$x_{t+1} = g(f(x_t; \phi, y_t); \theta)$$

But it is too expensive

Conventionally we parameterise  $f(\cdot)$  with a simple (but possibly non-linear) parameterisation

$$f^\dagger(x_t) \approx f(x_t)$$

so we have

$$x_{t+1} = g(f^\dagger(x_t); \theta)$$

We propose to replace  $f^\dagger$  with an emulator of  $f$

$$f^* = \mu + \delta$$

where  $\mu$  is a mean function and  $\delta$  is a zero mean Gaussian process

# Nuisance Parameters

- ▶ The process model  $f(\cdot)$  is not only driven by the GCM state parameters but also by other *nuisance* parameters
- ▶ We need values for these to drive the emulator
- ▶ (unless we find them non-active during the emulation process)

# Nuisance Parameters

Encapsulate our prior knowledge about  $y$  in a prior  
(since  $y$  may be affected by the value of  $x$  we make our prior  
conditional on the value of  $x$ )

so we have  $p(y|x)$

There are two ways we can use this information

1. Deterministically - replace  $y$  by  $E(y|x)$
2. Stochastically - replace  $y$  by a sample from  $p(y|x)$

# Emulation as Parameterisation Summary

- ▶ Emulators can be used to parameterise sub-grid scale processes
- ▶ They (approximately) preserve all the physics
- ▶ Need some examples

# Conclusions

- ▶ Emulators are powerful tools for analysing climate models
- ▶ There are a lot of new exciting applications
- ▶ Look forward to many more adventures