# An S4 Object structure for emulation

## The approximation of complex functions

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# Emulation

## A brief introduction

Computer models are examples of
**complex functions**
over **high dimensions**
that are **slow** to evaluate.

We would like to **predict** a model's behaviour
**without running the model**.

**An emulator is a statistical representation of a complex function**

> An emulator is a statistical representation of a complex function

For a collection $\tilde{\mathbf{x}}$ of input points it gives us

- a **probability distribution** for the function's value, $s\left(\tilde{\mathbf{x}}\right)$
- conditional on some known function values, $(\mathbf{x}, s(\mathbf{x}))$

We stipulate that

- at 'training points', where we know $s(x)$, the emulator gives the same value, with certainty
- at other points, the approximation should be 'plausible', and reflect our uncertainty.

We represent the function's value for input $\mathbf{x}$ as

$$s(\mathbf{x}) = \underbrace{\sum_{i=1}^{p} g_i(\mathbf{x})\beta_i}_{\text{Regression surface}} + \underbrace{\epsilon(\mathbf{x})}_{\text{Correlated error}} .$$

- The regression surface captures the general trend
- The correlated error term forces the emulator to interpolate the training data

# Emulation

## Why objects?

- **Encapsulation** - information that belongs together is collected as one object
- **Efficiency** - time-consuming computations can be performed just once
- **Tidiness** - changes and additions to code are simpler to make
- **Methods** - objects can be created from various beginnings using multiple dispatch

# Structure

## How it works (or how it *should* work. . . )

Crudely, there are three stages to emulation

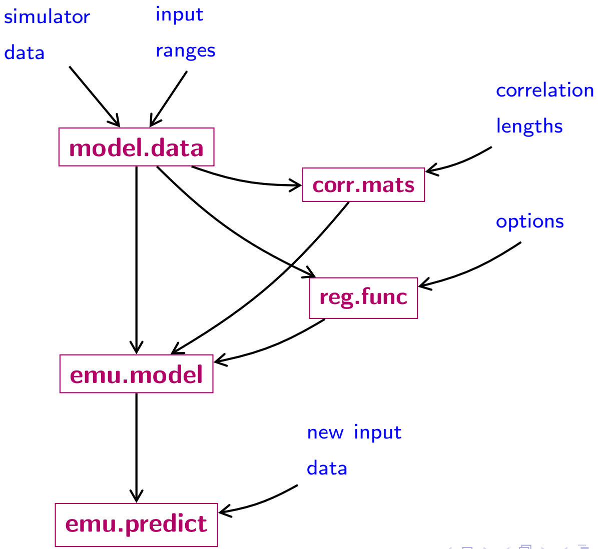
1. **Collect function data**, with which to train the emulator
2. **Make choices** about the emulator: regression functions, correlated error behaviour
3. Use the emulator to **predict** new function values.

This leads to three stages in the code:

1. **data.object** <-
   model.data(input and output data, function information)
2. **emulator.object** <-
   emu.model(**data.object**, regression and correlation choices)
3. **prediction.object** <-
   emu.predict(**emulator.object,** new input points)

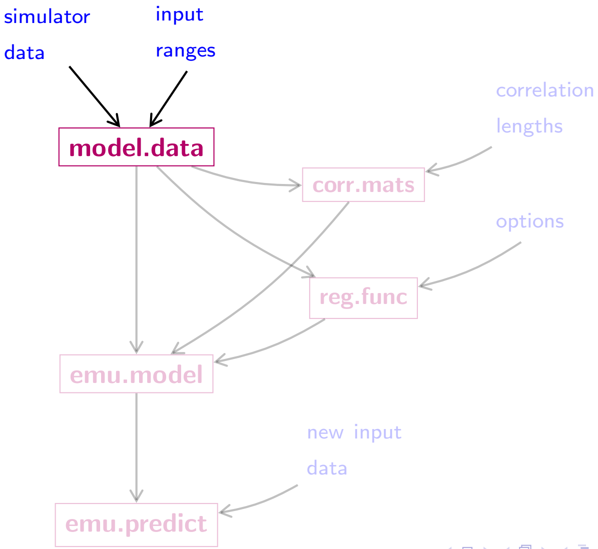
# Structure

## An overview



# Structure

## Organising model data



# Classes

## "model.data"

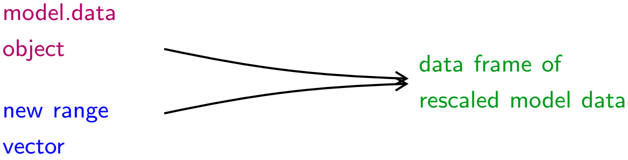
Ingredients :

- function data (possibly containing output values too)
- ranges for input variables

Slots:

- input: a data frame of input values
- oldrange: a data.frame of input ranges
- (optional) outvec and outname: output data

**"rescale"** - a method for "model.data"



# Classes

## How the data fits into the structure

Simulator output

Correlated error

$$s(\mathbf{x}) = \sum_{i=1}^{p} g_i(\mathbf{x})\beta_i + \epsilon(\mathbf{x})$$

Regression surface

# Classes

## "reg.func" - regression functions

- How many inputs should be active?
- Should the inputs be transformed?
- What order polynomial?
- How would we like to choose terms?
- Do we already know what functions

we'd like?

→

- Functions
- Active variables

$$s(\mathbf{x}) = \sum_{i=1}^{p} g_i(\mathbf{x})\beta_i + \epsilon(\mathbf{x})$$

↑

Regression surface

# Classes

## "corr.mats" - correlation matrix

Correlation is determined by **correlation lengths**

- Same values in each dimension?
- "optimise" them using the data?
- Add 'nugget' onto the diagonal?

→

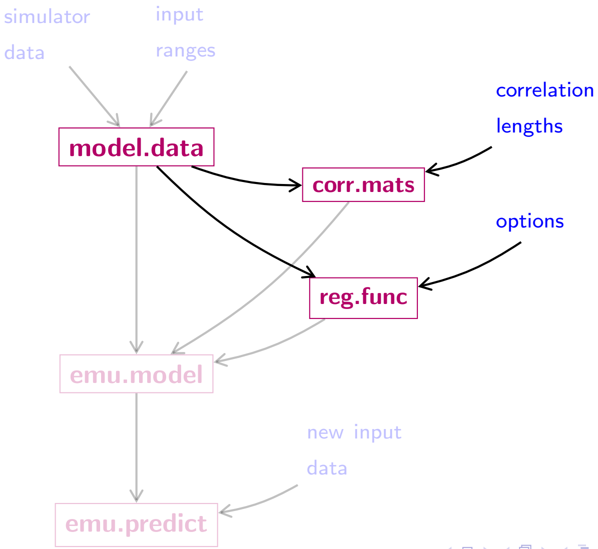
- Correlation matrix
- Cholesky factorisation of correlation matrix

$$s(\mathbf{x}) = \sum_{i=1}^{p} g_i(\mathbf{x})\beta_i + \epsilon(\mathbf{x})$$

Correlated error

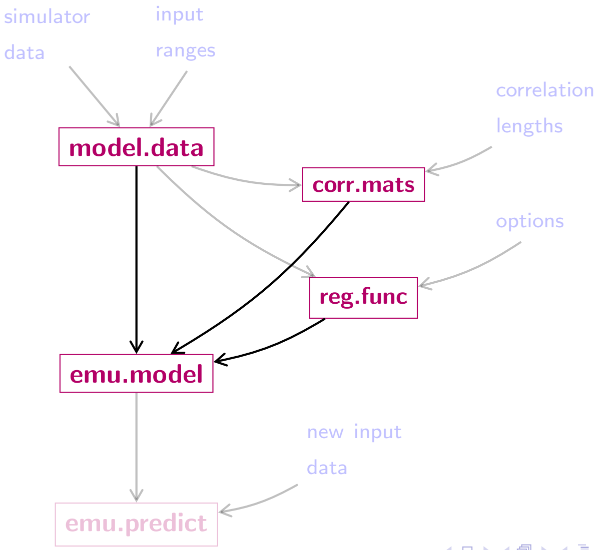
# Structure

## Creating correlation and regression objects



# Structure

## Collecting information together



# Classes

## "emu.model" - everything ready to predict

The data, regression and correlation objects together can make an "emu.model" object, containing

- data.obj ("model.data")
- func.obj ("reg.func")
- cm.obj ("corr.mats")

} Objects we've seen

- HcmH ("matrix")
- chol.HcmH ("matrix")

} Stored for computations

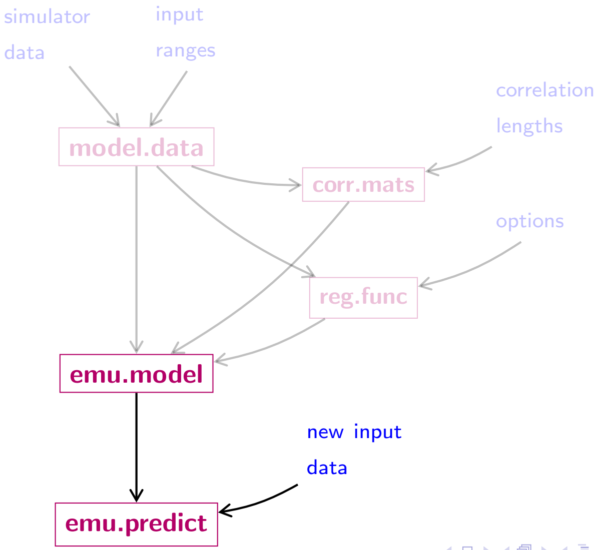
- sig.hat.sq ("numeric")
- beta.hat ("vector")

} Estimated residual variance and regression coefficients

This contains all the information we need to evaluate the probability distribution of output at new input points

# Structure

## Predicting new model output



## "emu.predict" - predicting new function values

Given model data $s(\mathbf{x})$, and new inputs $\tilde{\mathbf{x}}$,
$s\left(\tilde{\mathbf{x}}\right) \mid s\left(\mathbf{x}\right)$ has a **location-scale multivariate t-distribution**.

An "emu.predict" object contains

- **mod** - the "emu.model" used
- **xnew** - the new input points
- **loc** - vector of expected outputs (the location of the $t$-distribution)
- **scale** - the scale matrix (linked to variance)
- **deg.f** - the degrees of freedom of the $t$-distribution

One method, "**change.obj**", which requires

- **object** - an object (from this emulation structure)
- **changes** - a list of arguments to change

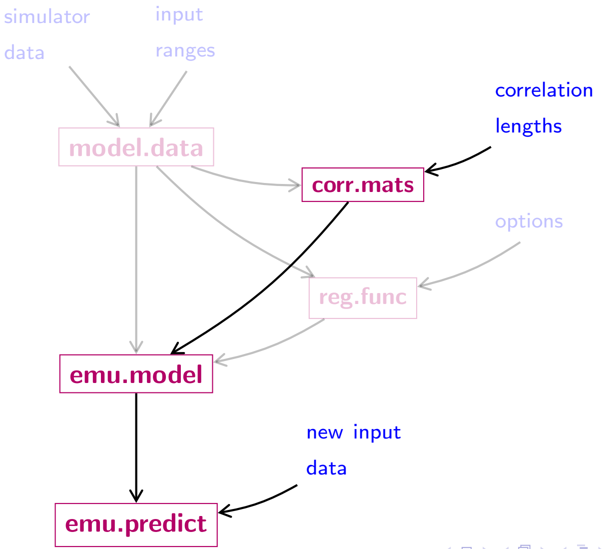
and creates a **new object** of the **same class**.

Advantages of this method:

- **quicker** - one command to remake the object
- **more transparent** - what's changed is clear
- **less error prone** - prevents use of wrong data (or deletion)

# Structure

## Using “change.obj” to change correlation length, from an “emu.predict” object



# Summary

S4 objects are an effective approach to emulation:

- **administration** - vital information for an emulator is held together (helpful for **reproducibility**)
- **efficiency** - costly calculations needn't be repeated
- **transparency** - class descriptions enforce structure
- **adaptability** - methods can be added / changed without upsetting the wider structure