Another introduction to Gaussian Processes

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Why would we want to use this very restricted class of model?

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So sums of Gaussians are Gaussian, and marginal distributions of multivariate Gaussians are still Gaussian.

Property 2: Conditional distributions are still Gaussian

Suppose

$$X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N(\mu, \Sigma)$$

where

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma 22 \end{pmatrix}$$

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So $X_2|X_1 = x_1$ is Gaussian.

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Conditional updates of Gaussian processes

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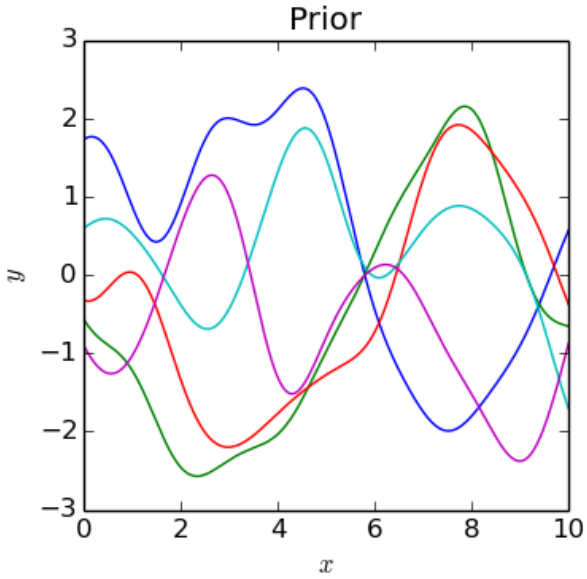
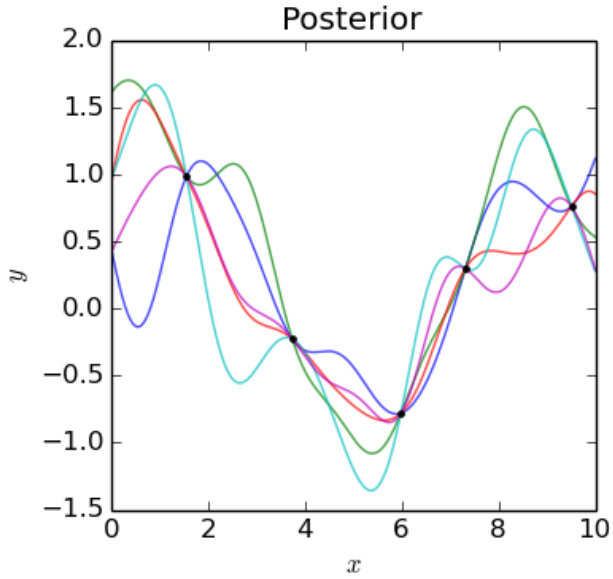
If we observe its value at $x_1, \ldots, x_n$ then

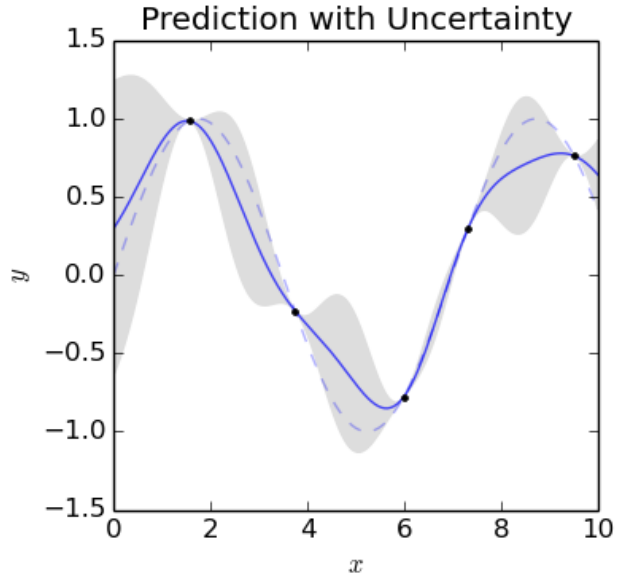
$$f(x)|f(x_1), \ldots, f(x_n) \sim N(\mu^*, \sigma^*)$$

where μ^* and σ^* are as on the previous slide.

Note that we still believe f is a GP even though we've observed its value at a number of locations.







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- Closed under any linear operation. If $f \sim GP(m(\cdot), k(\cdot, \cdot))$, then if $\mathcal{L}$ is a linear operator

$$\mathcal{L} \circ f \sim GP(\mathcal{L} \circ m, \mathcal{L}^2 \circ k)$$

e.g. $\frac{df}{dx}$, $\int f(x)dx$, Af are all GPs

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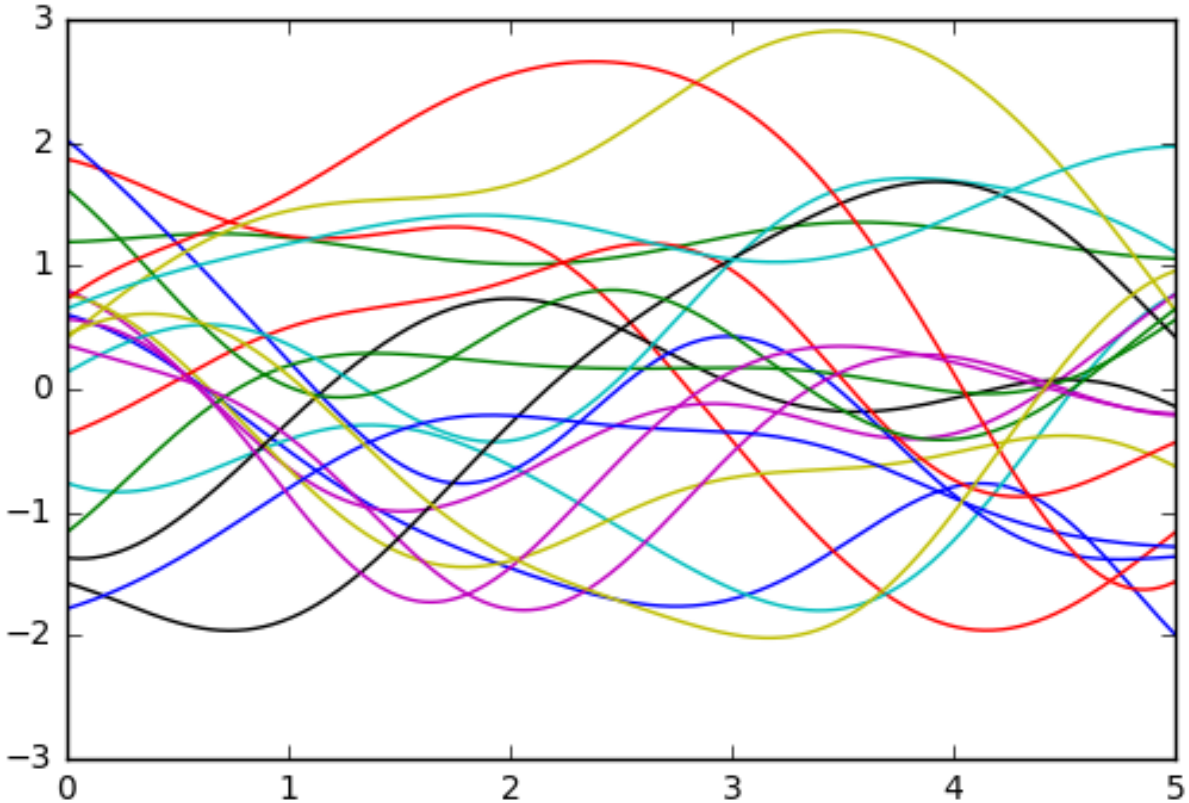
  - This can be problematic (see Nicolas' talk)

Examples

RBF/Squared-exponential/exponentiated quadratic

$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$



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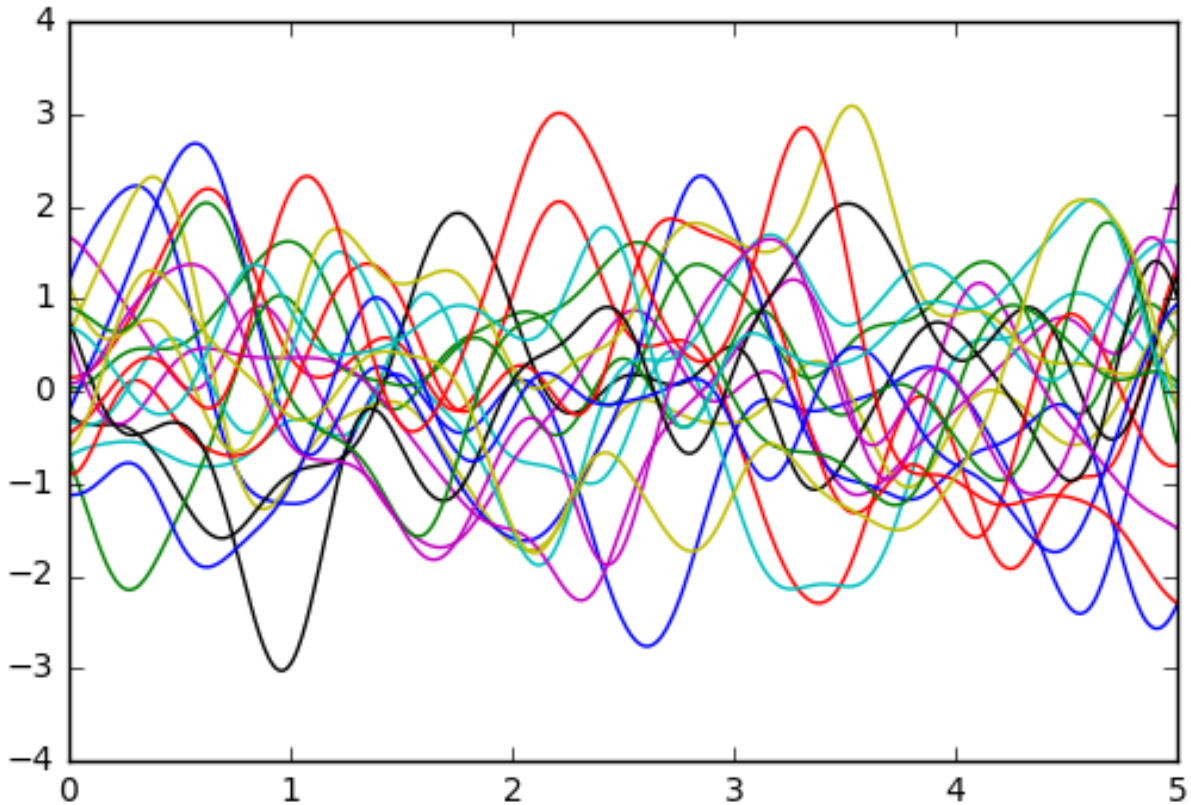
RBF/Squared-exponential/exponentiated quadratic

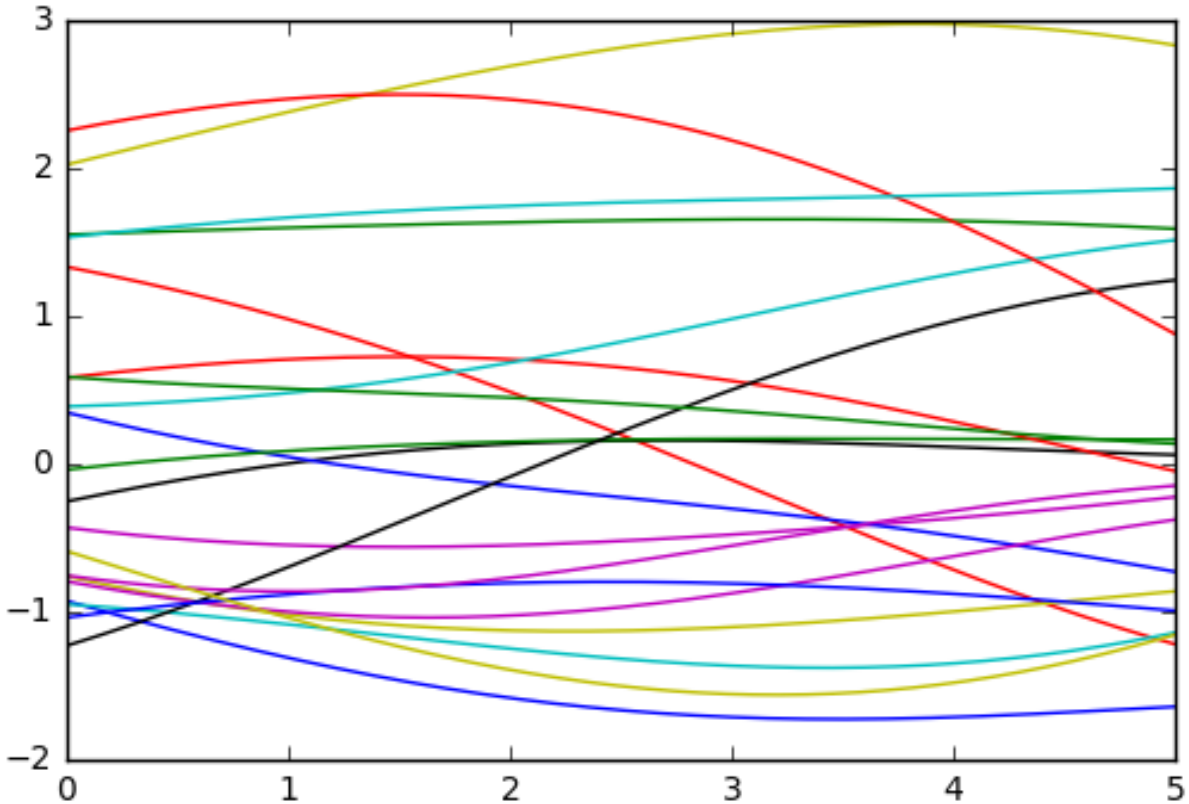
$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{0.25^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

$$k(x, x') = \exp\left(-\frac{1}{2}\frac{(x - x')^2}{4^2}\right)$$



Examples

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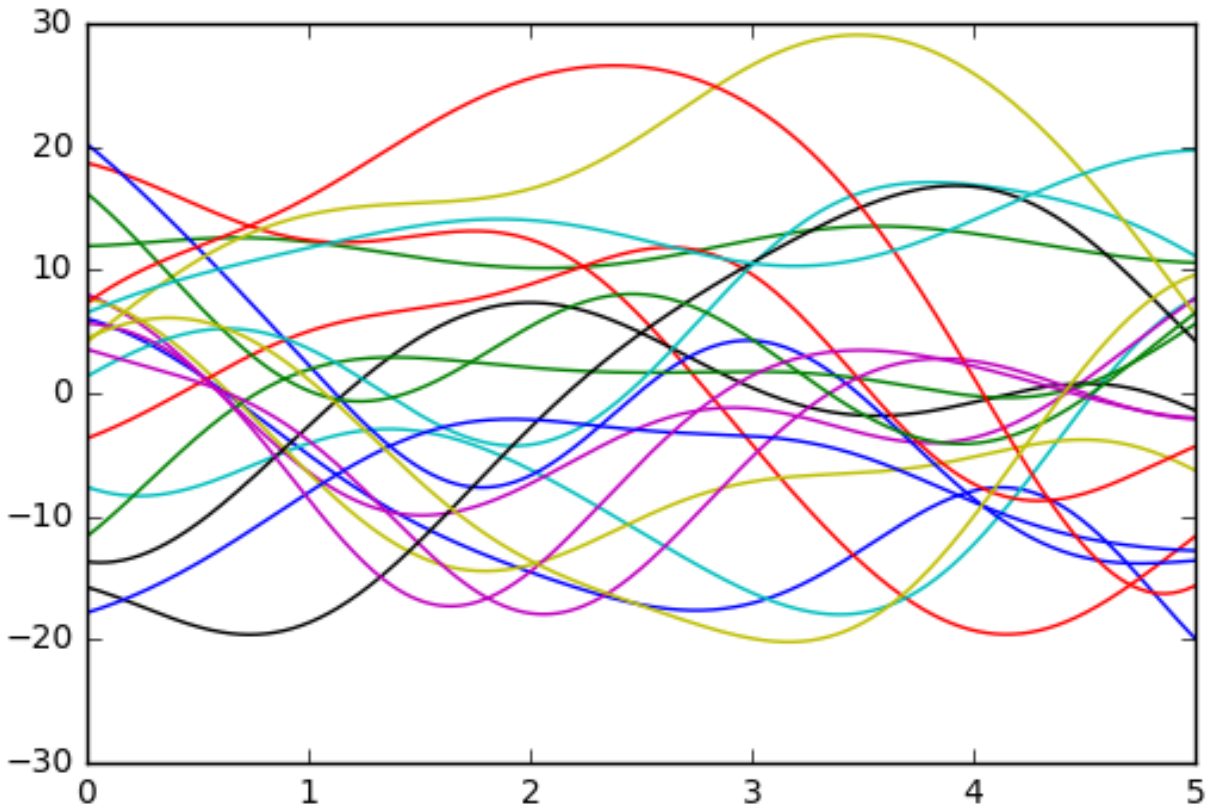
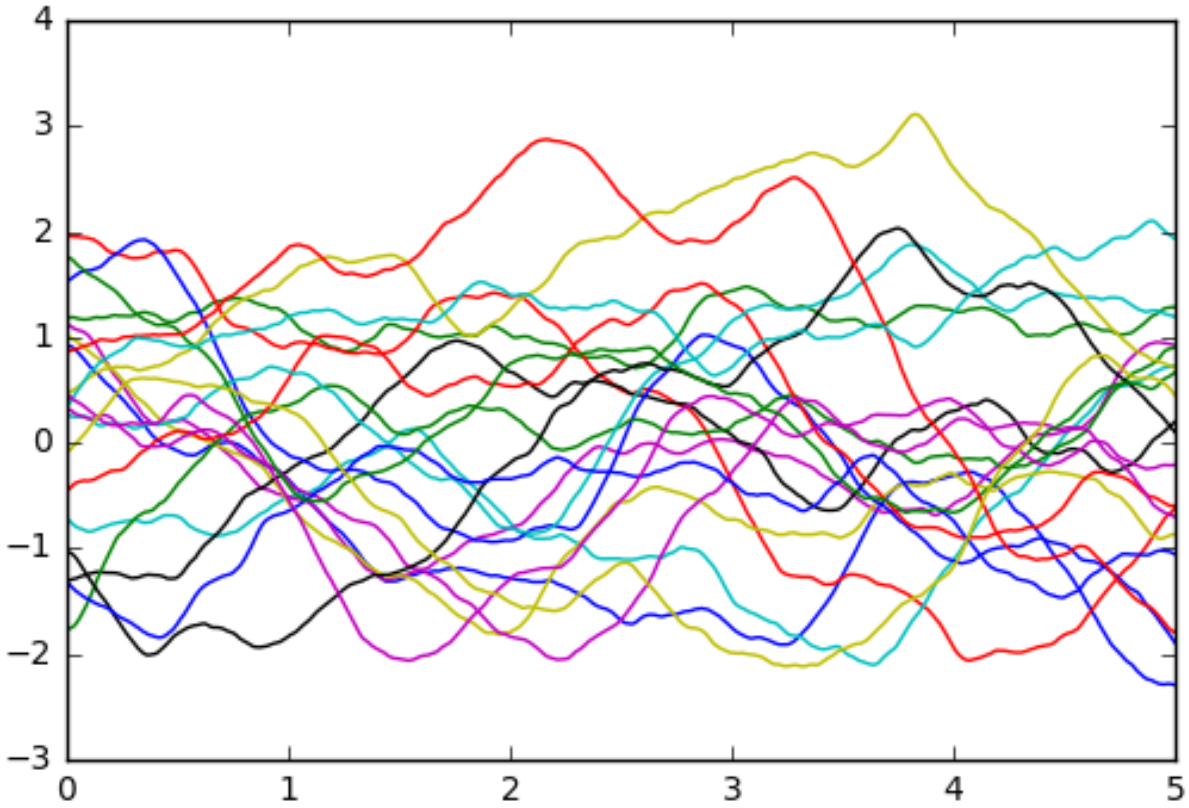
$$k(x, x') = 100 \exp\left(-\frac{1}{2}(x - x')^2\right)$$



Examples

Matern 3/2

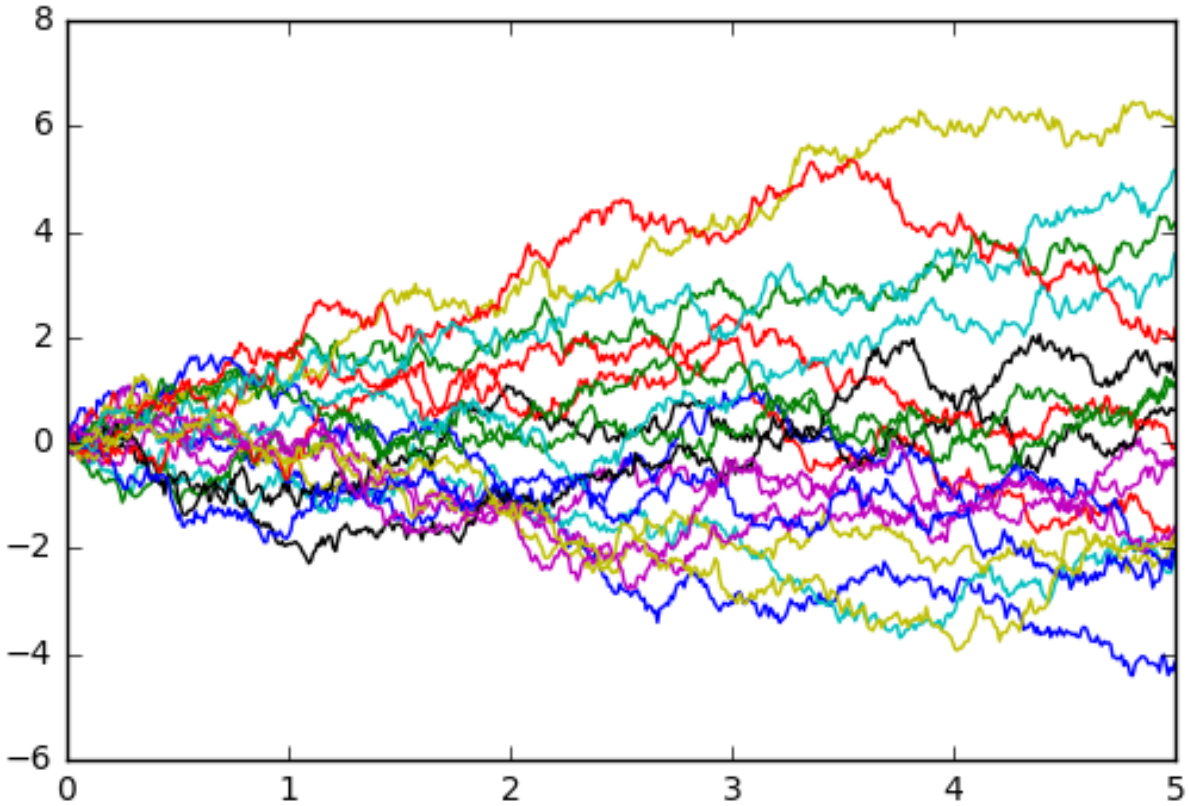
$$k(x, x') \sim (1 + |x - x'|) \exp\left(-|x - x'|\right)$$



Examples

Brownian motion

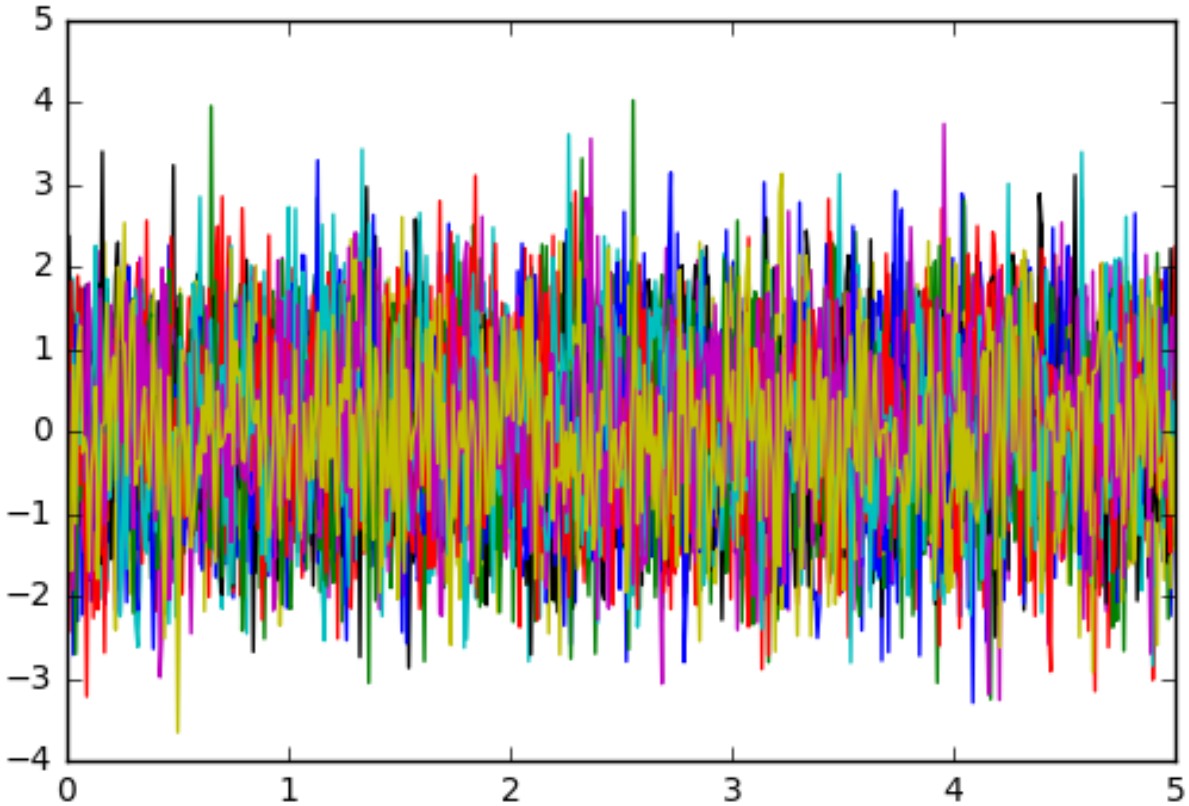
$$k(x, x') = \min(x, x')$$



Examples

White noise

$$k(x, x') = \begin{cases} 1 \text{ if } x = x' \\ 0 \text{ otherwise} \end{cases}$$



Examples

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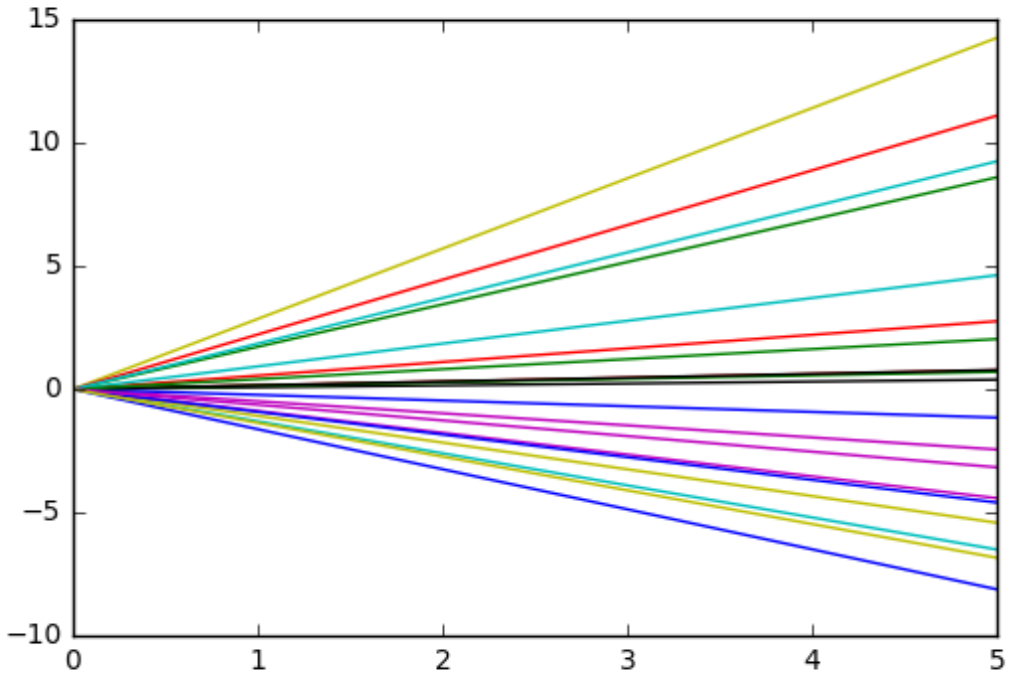
A final example

$$k(x, x') = x^\top x'$$



What is happening?

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Let's now motivate the use of GPs as a non-parametric extension to linear regression. We'll also show that k determines the space of functions that sample paths live in.

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Linear regression $y = x^\top \beta + \epsilon$ can be written solely in terms of inner products $x^\top x$.

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But the dual form makes clear that linear regression only uses inner products.

— This is useful!

Prediction

The best prediction of y at a new location x' is

$$\begin{aligned}\hat{y}' &= x'^{\top}\hat{\beta} \\ &= x'^{\top}X^{\top}(XX^{\top}+\sigma^2 I)^{-1}y \\ &= k(x')(K+\sigma^2 I)^{-1}y\end{aligned}$$

where $k(x') := (x'^{\top}x_1, \ldots, x'^{\top}x_n)$ and $K_{ij} := x_i^{\top}x_j$

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K and $k(x)$ are kernel matrices. Every element is the inner product between two rows of training points.

Prediction

The best prediction of y at a new location x' is

$$\begin{aligned}\hat{y}' &= x'^{\top}\hat{\beta} \\ &= x'^{\top}X^{\top}(XX^{\top}+\sigma^2 I)^{-1}y \\ &= k(x')(K+\sigma^2 I)^{-1}y\end{aligned}$$

where $k(x') := (x'^{\top}x_1, \ldots, x'^{\top}x_n)$ and $K_{ij} := x_i^{\top}x_j$
K and $k(x)$ are kernel matrices. Every element is the inner product between two rows of training points.
Note the similarity to the GP conditional mean we derived before. If

$$\begin{pmatrix} y \\ y' \end{pmatrix} \sim N\left(0, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}\right)$$

$$\text{then } \mathbb{E}(y'|y) = \Sigma_{21}\Sigma_{11}^{-1}y$$

where $\Sigma_{11} = K + \sigma^2 I$, and $\Sigma_{12} = \mathbb{C}\text{ov}(y, y')$ then we can see that linear regression and GP regression are equivalent for the kernel/covariance function $k(x, x') = x^{\top}x'$.

- We know that we can replace x by a feature vector in linear regression, e.g., $\phi(x) = (1\ x\ x^2)$ etc.
  Then
$$K_{ij} = \phi(x_i)^\top \phi(x_j) \qquad \text{etc}$$

- For some sets of features, the inner product is equivalent to evaluating a kernel function

$$\phi(x)^\top \phi(x') \equiv k(x, x')$$

where

$$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

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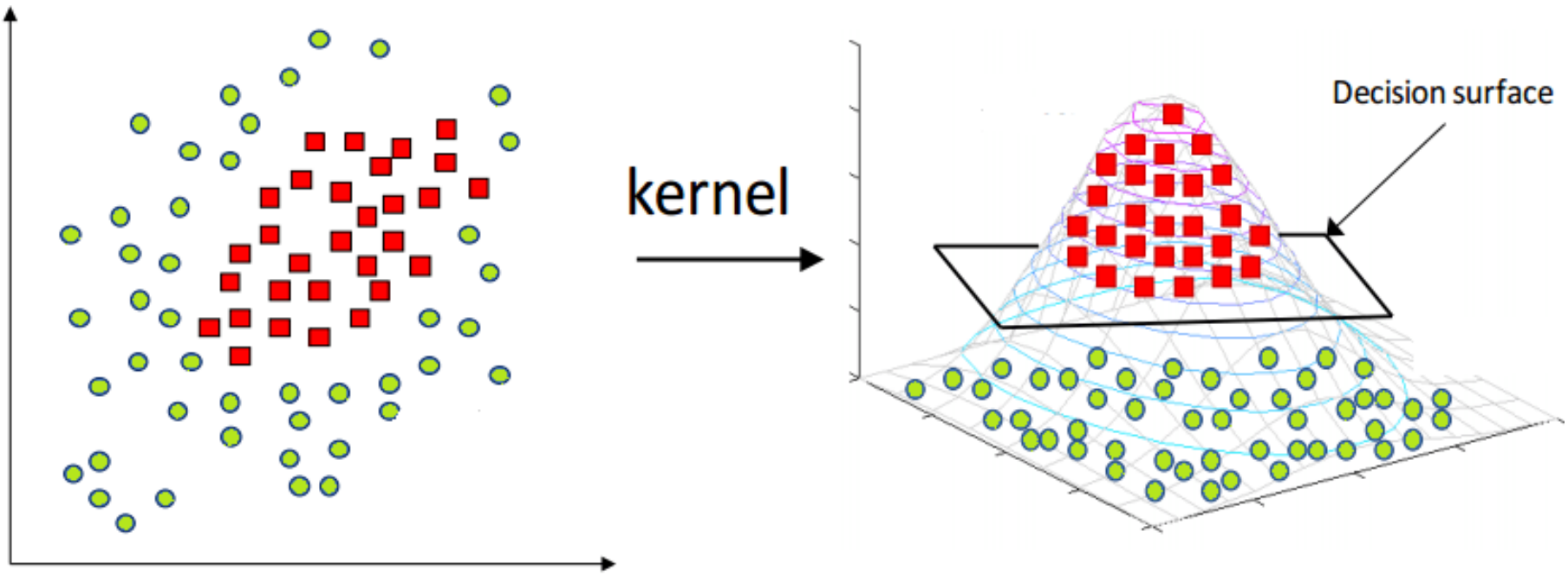
is a semi-positive definite function.

- We can use an infinite dimensional feature vector $\phi(x)$, and because linear regression can be done solely in terms of inner-products (inverting a $n \times n$ matrix in the dual form) we never need evaluate the feature vector, only the kernel.

Kernel trick:

lift x into feature space by replacing inner products $x^\top x'$ by $k(x, x')$



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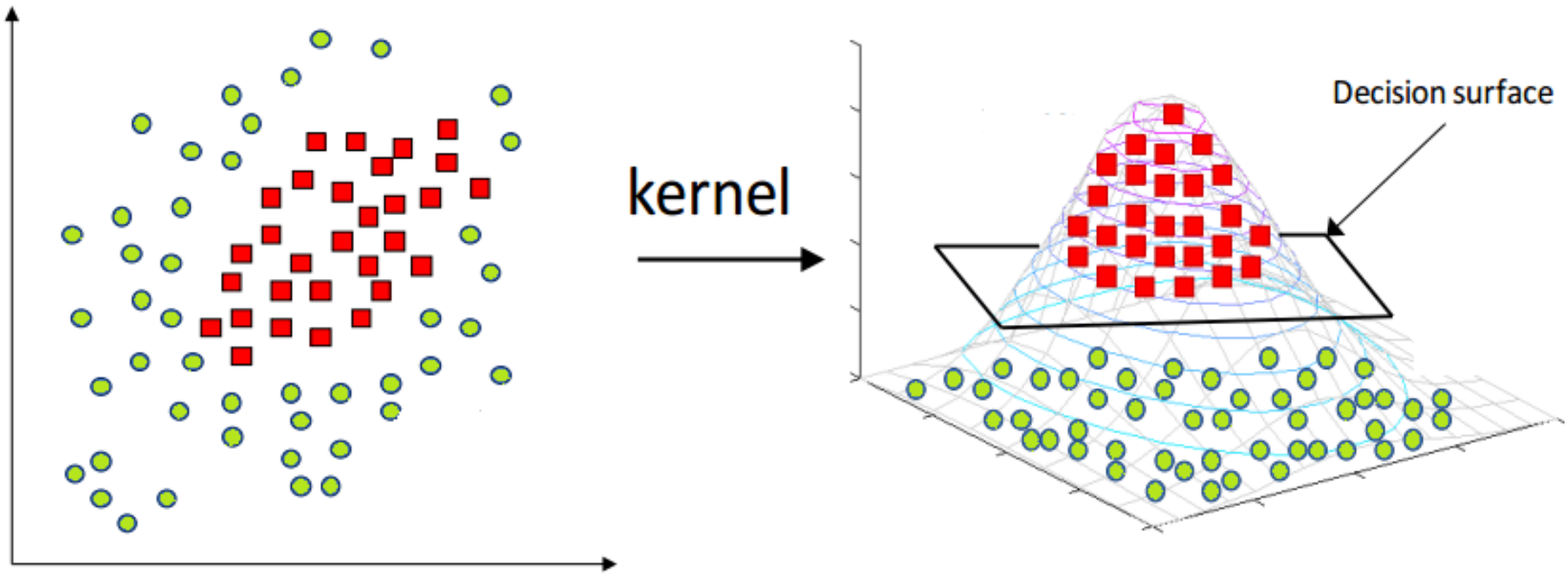

Kernel regression/non-parametric regression/GP regression all closely related:

$$\hat{y}' = m(x') = \sum_{i=1}^{n} \alpha_i k(x, x_i)$$

Generally, we don't think about these features, we just choose a kernel. But any kernel is implicitly choosing a set of features, and our model only includes functions that are linear combinations of this set of features (this space is called the Reproducing Kernel Hilbert Space (RKHS) of k).

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Example: If (modulo some detail)

$$\phi(x) = (e^{-\frac{(x-c_1)^2}{2\lambda^2}}, \ldots, e^{-\frac{(x-c_N)^2}{2\lambda^2}})$$

then as $N \to \infty$ then

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Although our simulator may not lie in the RKHS defined by k, this space is much richer than any parametric regression model (and can be dense in some sets of continuous bounded functions), and is thus more likely to contain an element close to the true functional form than any class of models that contains only a finite number of features.

This is the motivation for non-parametric methods.

Why use GPs? Answer 3: Naturalness of GP framework

Why use **Gaussian** processes as non-parametric models?

1

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One answer might come from Bayes linear methods[1].
If we only knew the expectation and variance of some random variables, X and Y, then how should we best do statistics?

[1] Statistics without probability!

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Why use **Gaussian** processes as non-parametric models?

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If we only knew the expectation and variance of some random variables, X and Y, then how should we best do statistics?

It has been shown, using coherency arguments, or geometric arguments, or..., that the best second-order inference we can do to update our beliefs about X given Y is

$$\mathbb{E}(X|Y) = \mathbb{E}(X) + \mathbb{C}\text{ov}(X, Y)\mathbb{V}\text{ar}(Y)^{-1}(Y - \mathbb{E}(Y))$$

i.e., exactly the Gaussian process update for the posterior mean.
So GPs are in some sense second-order optimal.

[1] Statistics without probability!

Why use GPs? Answer 4: Uncertainty estimates from emulators

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- point estimate
- uncertainty in that estimate

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Warning: the uncertainty estimates from a GP can be flawed. Note that given data $D = X, y$

$$\mathbb{V}\text{ar}(f(x)|X, y) = k(x, x) - k(x, X)k(X, X)^{-1}k(X, x)$$

so that the posterior variance of $f(x)$ does not depend upon y!

The variance estimates are particularly sensitive to the hyper-parameter estimates.

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- We pick a covariance function from a small set, based usually on differentiability considerations.
- Possibly try a few (plus combinations of a few) covariance functions, and attempt to make a good choice using some sort of empirical evaluation.
- Covariance functions often contain hyper-parameters. E.g
  - RBF kernel

$$k(x, x') = \sigma^2 \exp\left(-\frac{1}{2}\frac{(x - x')^2}{\lambda^2}\right)$$

  Estimate these using some standard procedure (maximum likelihood, cross-validation, Bayes etc)

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Gelman *et al.* 2017

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So the posterior can concentrate not on a point, but on some submanifold of parameter space, and the projection of the prior on this space continues to impact the posterior even as more and more data are collected.

E.g. consider a zero mean GP on $[0, 1]$ with covariance function

$$k(x, x') = \sigma^2 \exp(-\kappa^2 |x - x|)$$

We can consistently estimate $\sigma^2\kappa$, but not σ^2 or κ, even as $n \to \infty$.

Problems with hyper-parameter optimization

As well as problems of identifiability, the likelihood surface that is being maximized is often flat and multi-modal, and thus the optimizer can sometimes fail to converge, or gets stuck in local-maxima.

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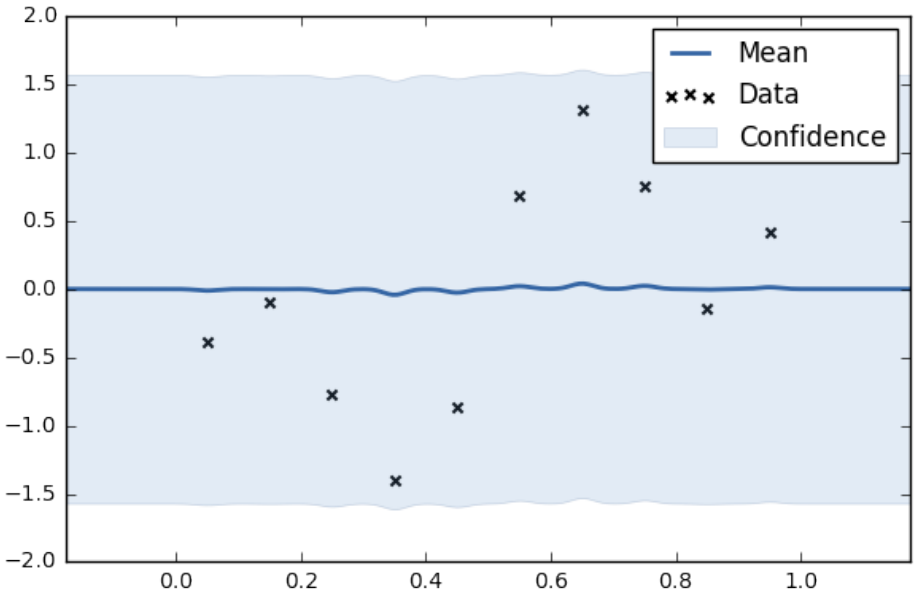
In practice, it is not uncommon to optimize hyper parameters and find solutions such as



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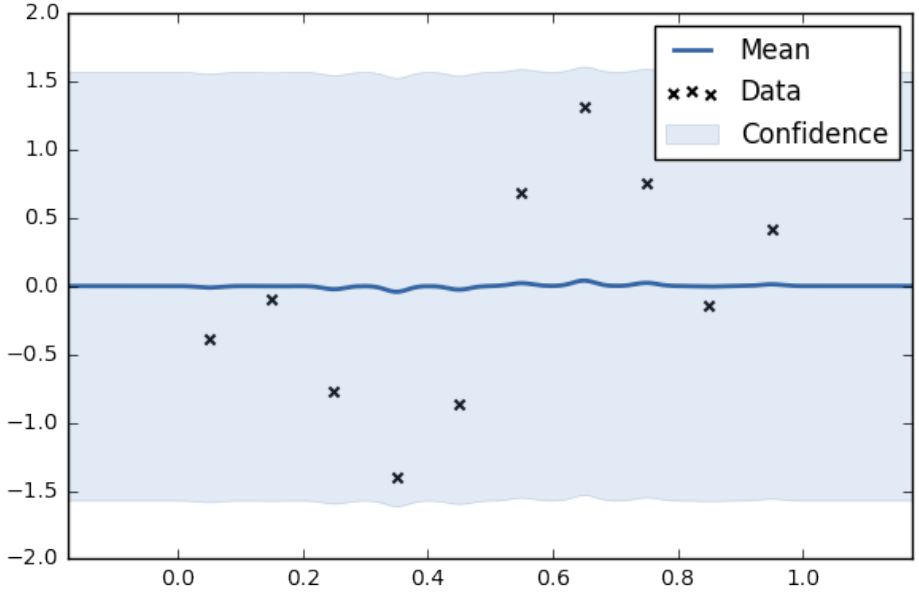

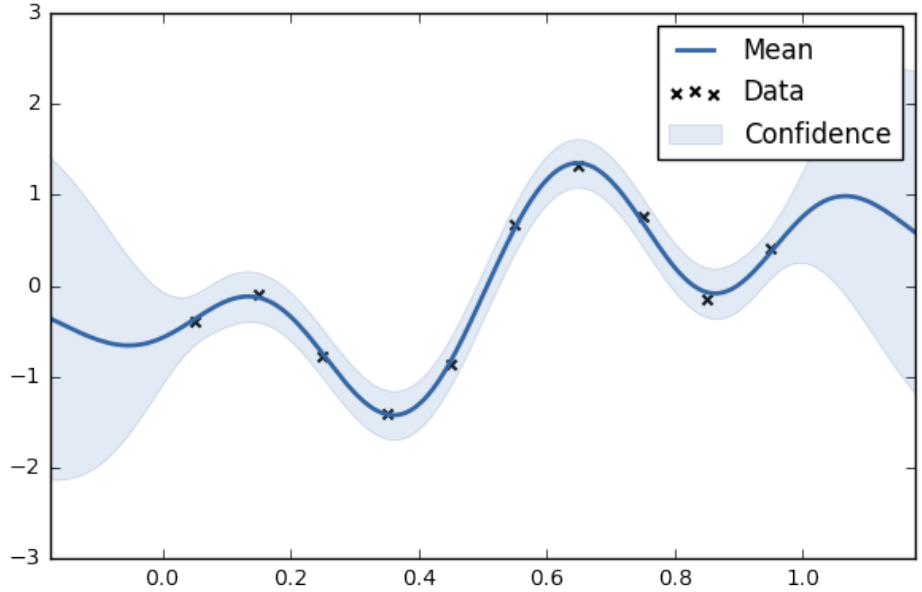

We often work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.

GPs in Uncertainty Quantification

Baker 1977 (Science):

> *'Computerese is the new lingua franca of science'*

Rohrlich (1991): Computer simulation is

> *'a key milestone somewhat comparable to the milestone that started the empirical approach (Galileo) and the deterministic mathematical approach to dynamics (Newton and Laplace)'*

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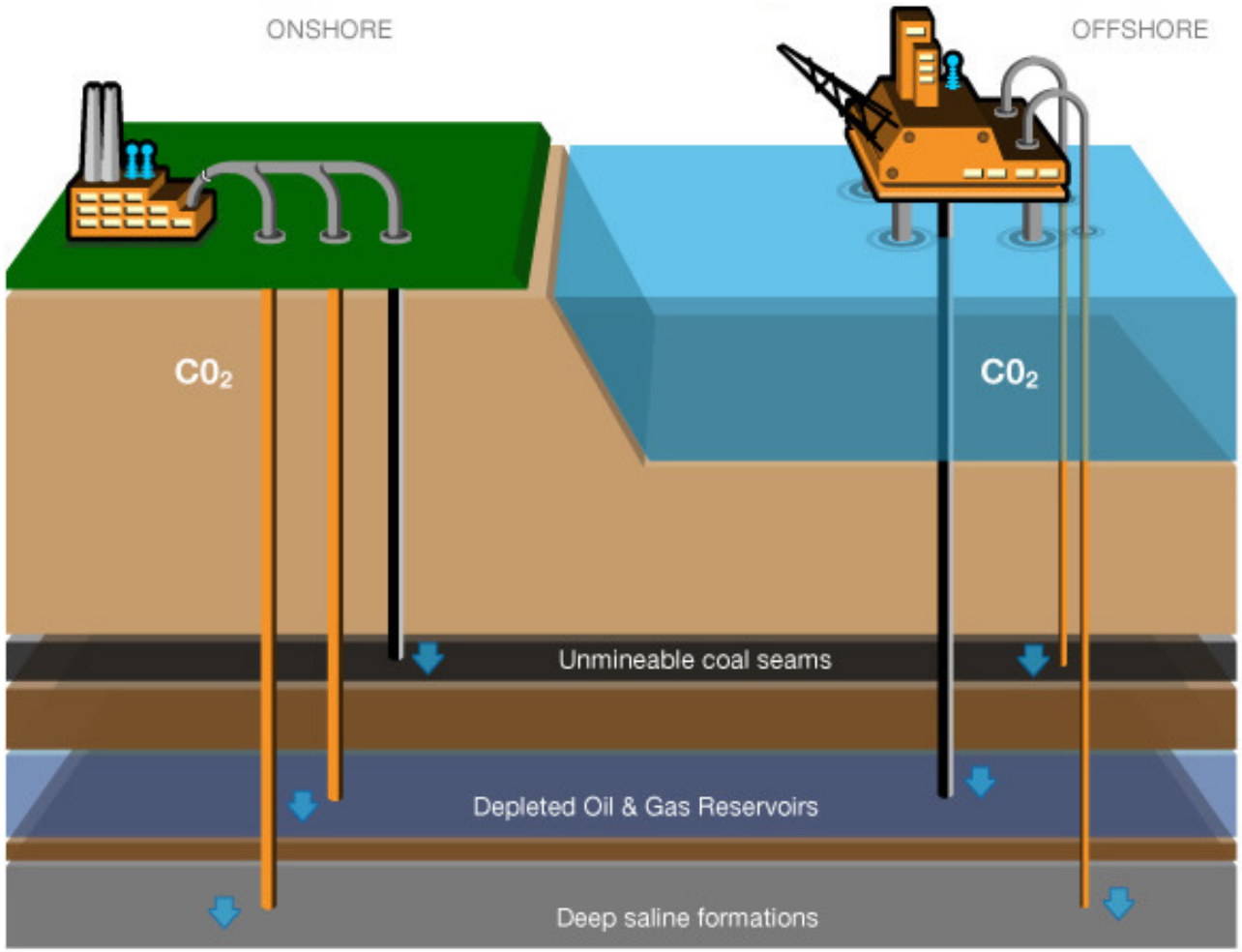
The gold-standard of empirical research is the designed experiment, which usually involves concepts such as replication, blocking, and randomization.

However, in the past three decades computer experiments (*in silico* experiments) have become commonplace in nearly all fields.

Engineering

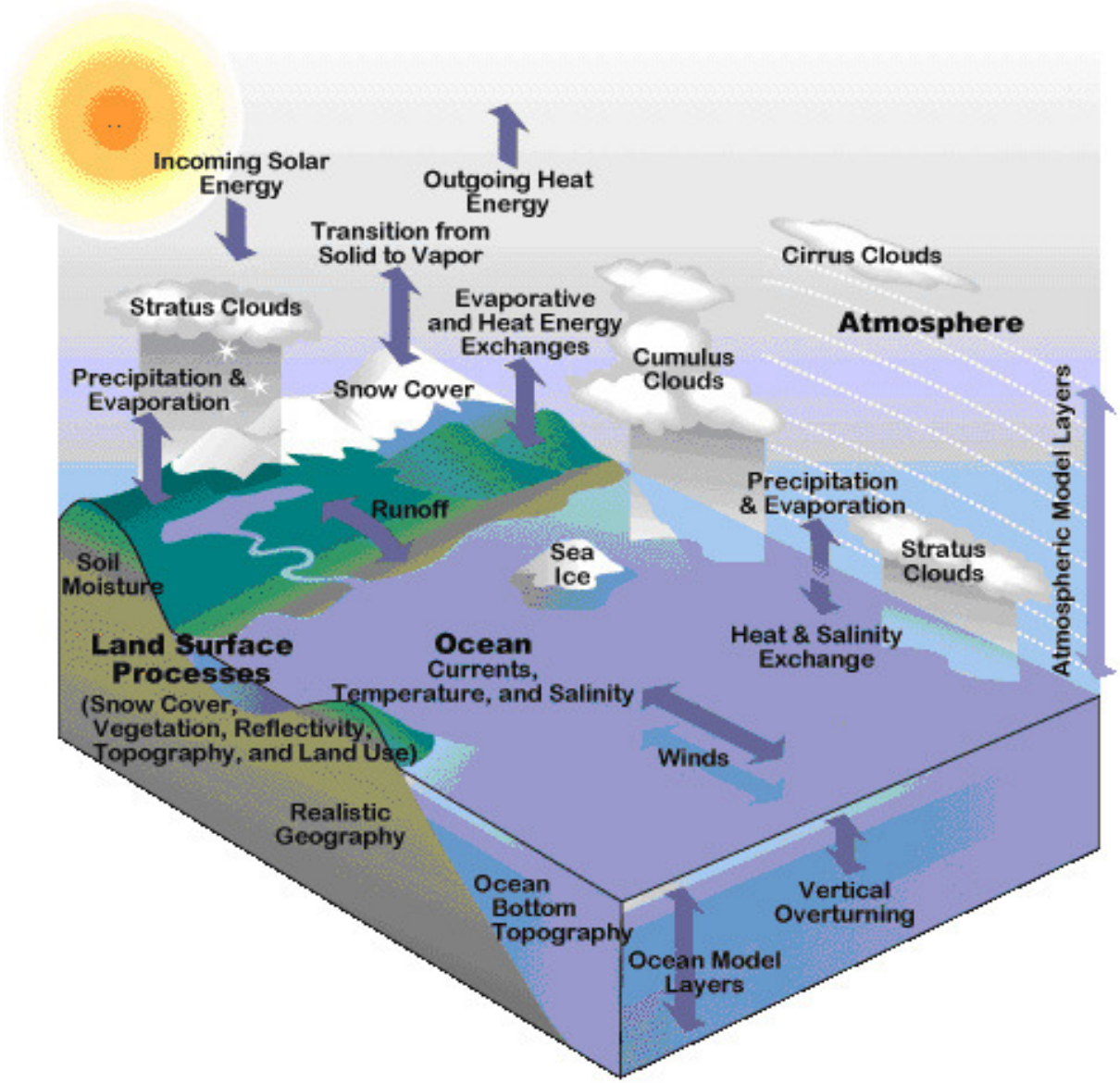
Carbon capture and storage technology - PANACEA project



Knowledge about the geology of the wells is uncertain.

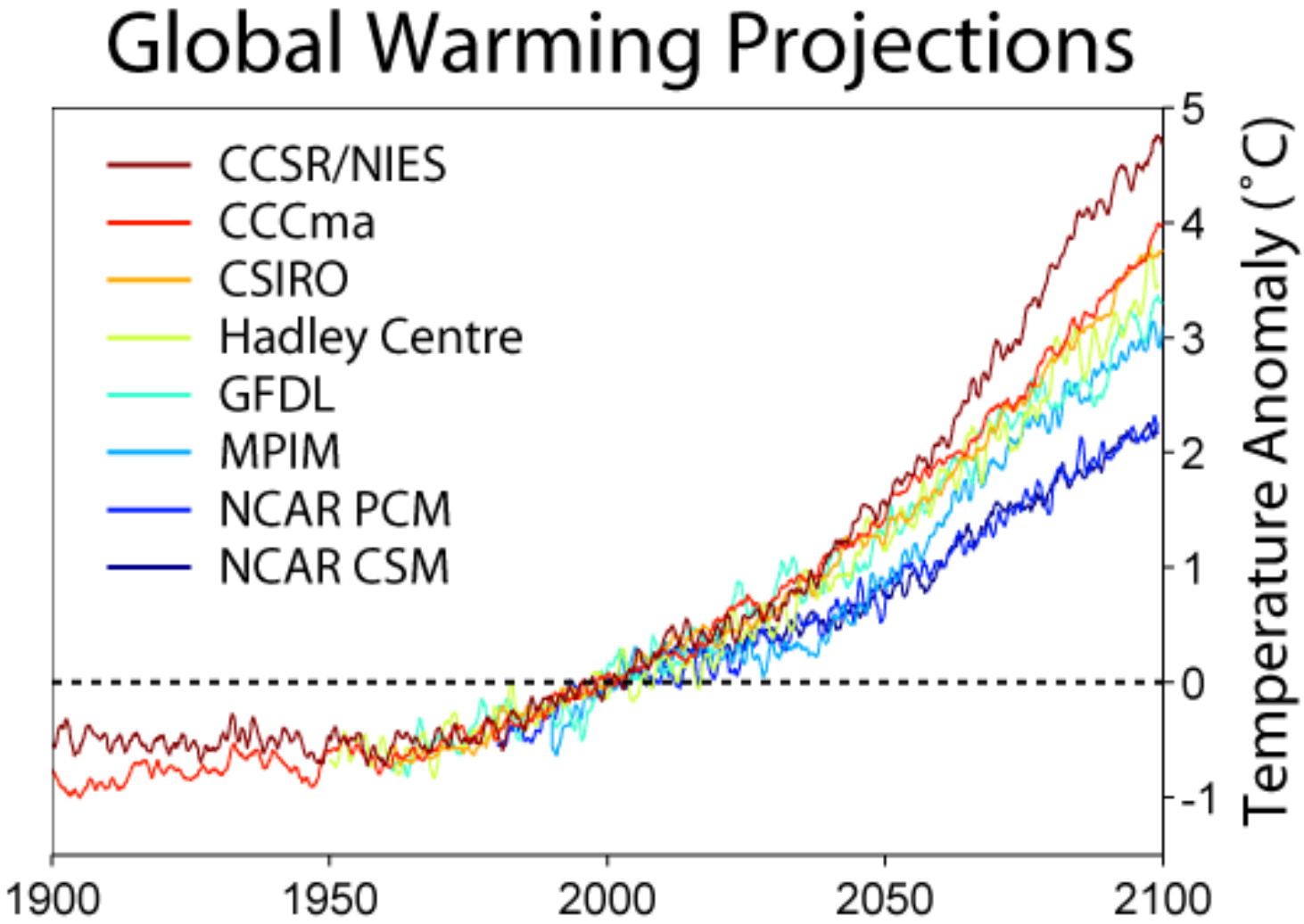
Climate Science

Predicting future climate



Challenges of computer experiments

Climate Predictions



Challenges for statistics

The statistical challenges posed by computer experiments are somewhat different to physical experiments and have only recently begun to be tackled by statisticians.

For example, replication, randomization and blocking are irrelevant because a computer model will give identical answers if run multiple times.

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Key questions: How do we make inferences about the world from a simulation of it?

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The statistical challenges posed by computer experiments are somewhat different to physical experiments and have only recently begun to be tackled by statisticians.

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Key questions: How do we make inferences about the world from a simulation of it?

- how do we relate simulators to reality? (model error)
- how do we estimate tunable parameters? (calibration)
- how do we deal with computational constraints? (stat. comp.)
- how do we make uncertainty statements about the world that combine models, data and their corresponding errors? (UQ)

There is an inherent a lack of quantitative information on the uncertainty surrounding a simulation - unlike in physical experiments.

Incorporating and accounting for uncertainty

Perhaps the biggest challenge faced is incorporating uncertainty in computer experiments.

We are used to dealing with uncertainty in physical experiments. But if your computer model is deterministic, there is no natural source of variation and so the experimenter must carefully assess where errors might arise.

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Types of uncertainty:

- Parametric uncertainty
- Model inadequacy
- Observation errors
- Code uncertainty

Code uncertainty

We think of the simulator as a function

$$\eta : \mathcal{X} \to \mathcal{Y}$$

Typically both the input and output space will be subsets of $\mathbb{R}^n$ for some n.

Monte Carlo (brute force) methods can be used for most tasks if sufficient computational resource is available.

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For example, uncertainty analysis is finding the distribution of $\eta(\theta)$ when $\theta \sim \pi(\cdot)$:

- draw a sample of parameter values from the prior $\theta_1, \ldots, \theta_N \sim \pi(\theta)$,
- Look at $\eta(\theta_1), \ldots, \eta(\theta_N)$ to find the distribution $\pi(\eta(\theta))$.

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However, for complex simulators, run times might be long.
Consequently, we will only know the simulator output at a finite number of points:

code uncertainty

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If θ is multidimensional, then even short run times can rule out brute force approaches

- $\theta \in \mathbb{R}^{10}$ then 1000 simulator runs is only enough for one point in each corner of the design space.

Meta-modelling

Idea: If the simulator is expensive, build a cheap model of it and use this in any analysis.

'a model of the model'

We call this meta-model an *emulator* of our simulator.

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We call this meta-model an *emulator* of our simulator.

We use the emulator as a cheap approximation to the simulator.

- ideally an emulator should come with an assessment of its accuracy
- rather just predict $\eta(\theta)$ it should predict $\pi(\eta(\theta)|\mathcal{D}_{sim})$ - our uncertainty about the simulator value given the ensemble $\mathcal{D}_{sim}$.

Meta-modelling

Gaussian Process Emulators

Gaussian processes provide a flexible nonparametric distributions for our prior beliefs about the functional form of the simulator:

$$\eta(\cdot) \sim GP(m(\cdot), \sigma^2 c(\cdot, \cdot))$$

where $m(\cdot)$ is the prior mean function, and $c(\cdot, \cdot)$ is the prior covariance function (semi-definite).

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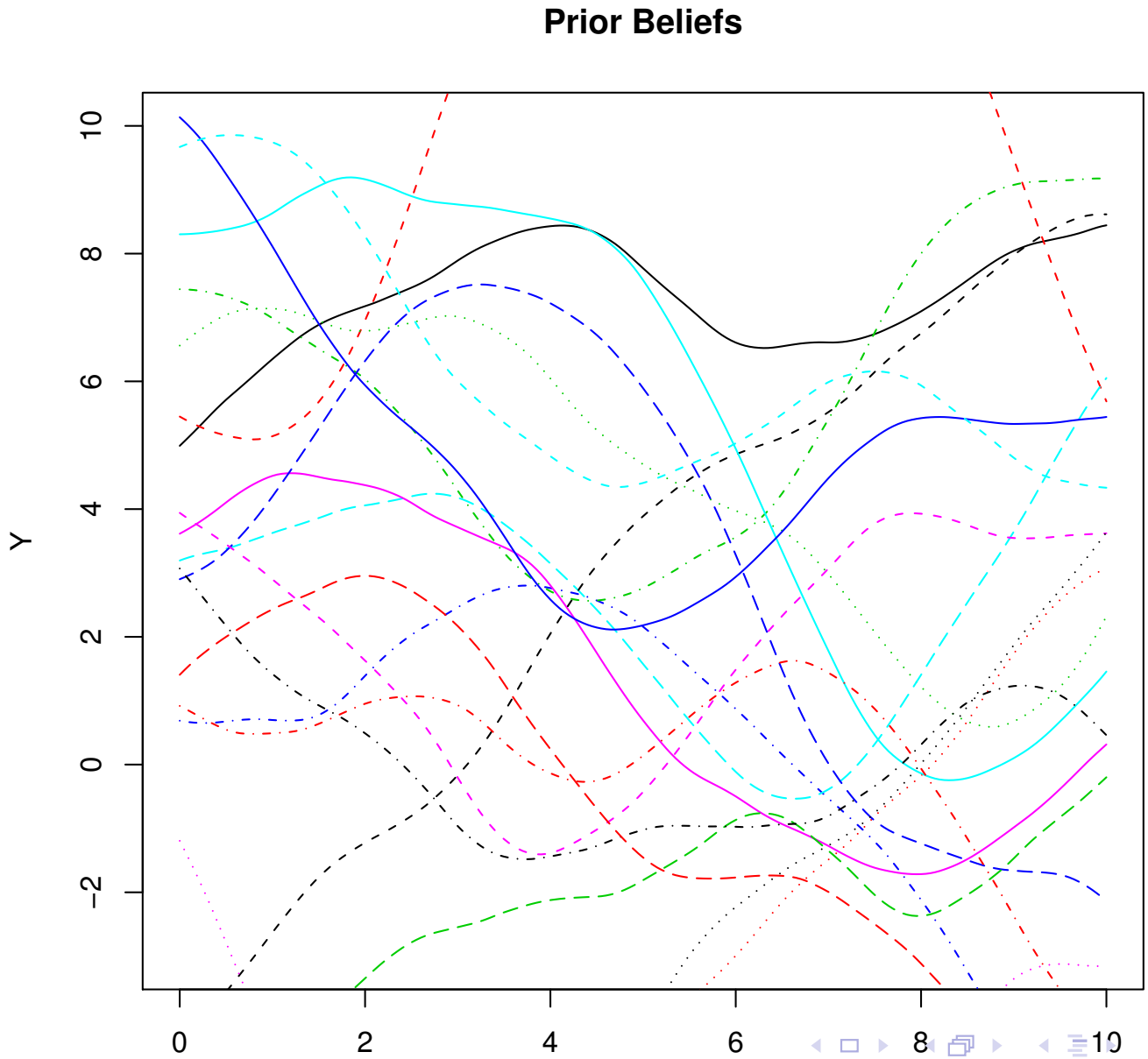
If we observe the ensemble of model runs $\mathcal{D}_{\text{sim}}$, then update our prior belief about η in light of the ensemble of model runs:

$$\eta(\cdot)|\mathcal{D}_{sim} \sim GP(m^*(\cdot), \sigma^2 c^*(\cdot, \cdot))$$

where m^* and c^* are the posterior mean and covariance functions (simple functions of $\mathcal{D}_{\text{sim}}$, m and c).

Gaussian Process Illustration

Zero mean



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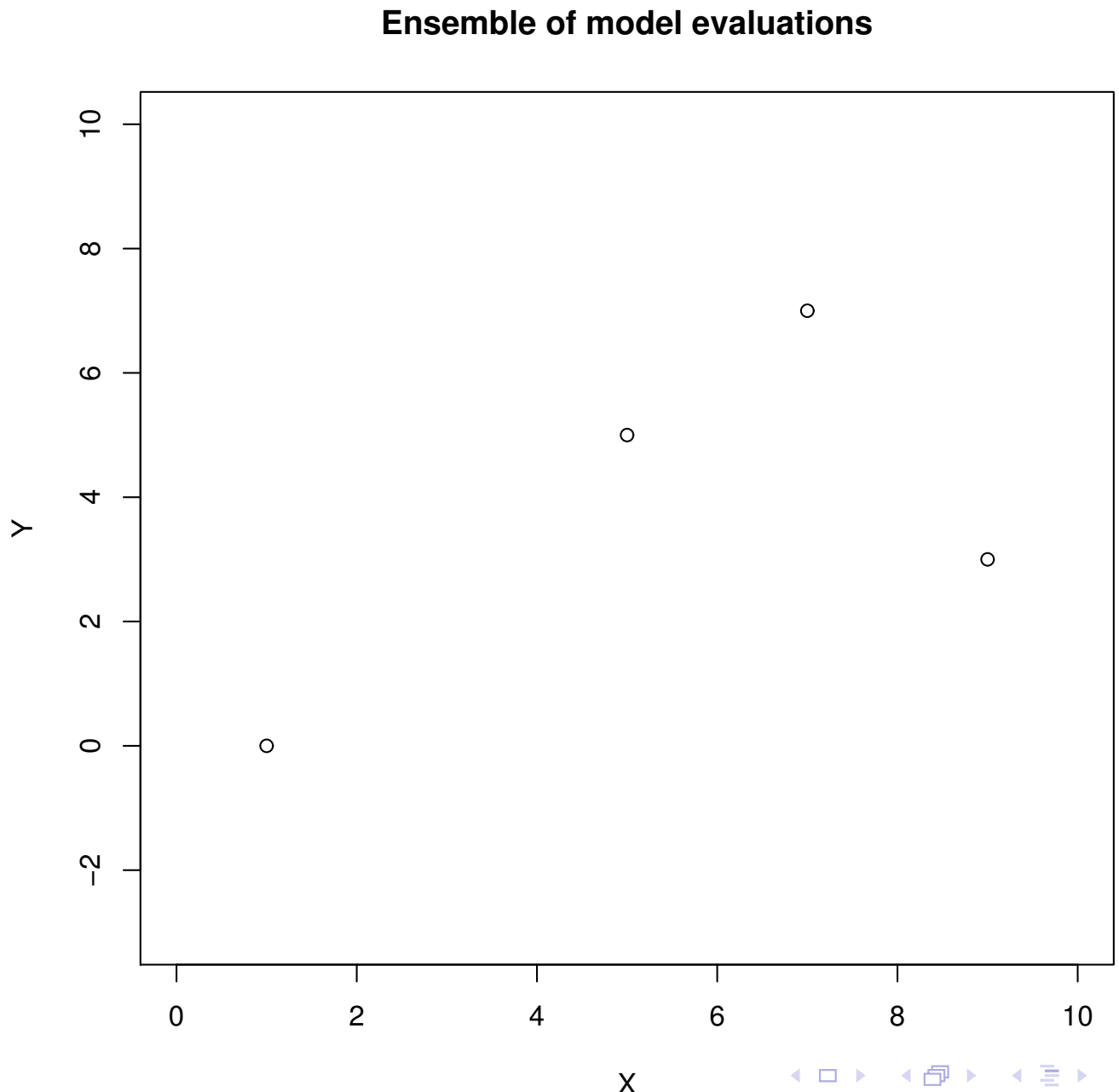

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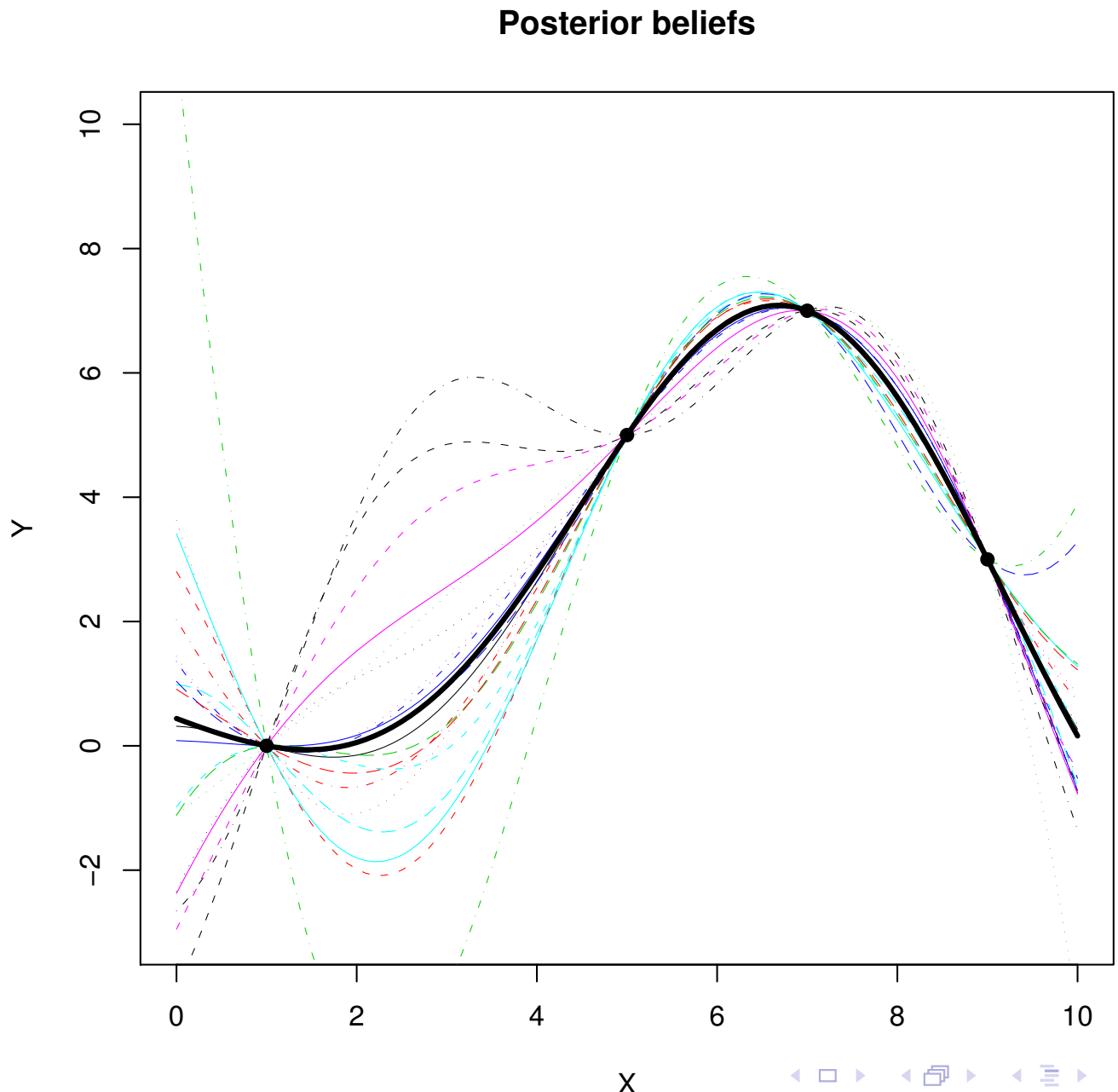

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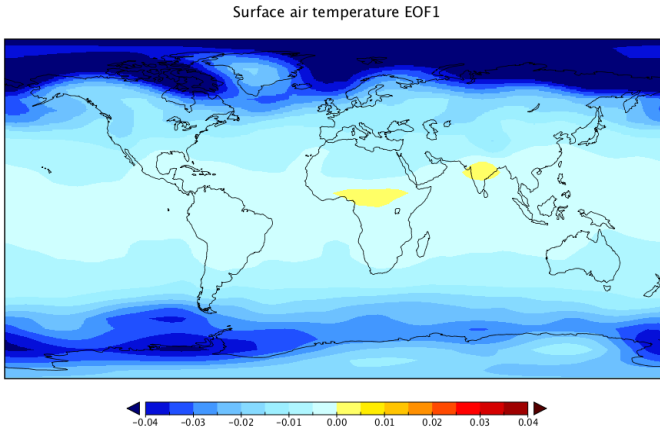
  - Allows us to build in known trends and exploit power of linear regression
- covariance function $c(\cdot, \cdot)$ - cf Nicolas' talk
  - Stationary? Smooth?
  - Length-scale?
  - Nb - we don't want a nugget term

Example 1: Easier regression

PLASIM-ENTS: Holden, Edwards, Garthwaite, W 2015



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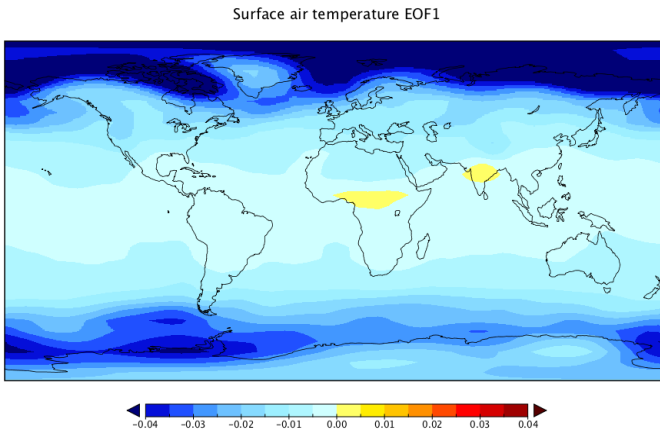

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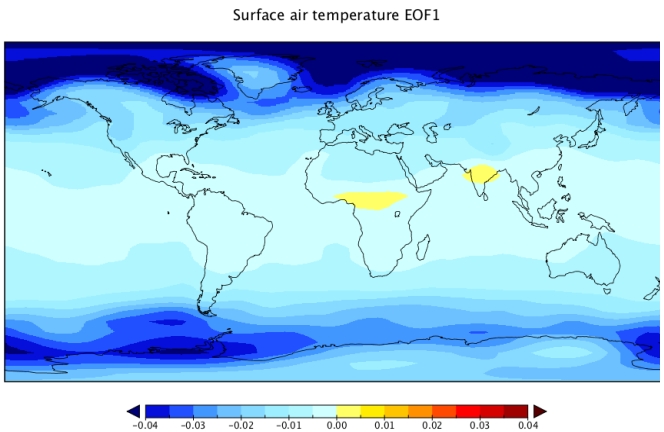

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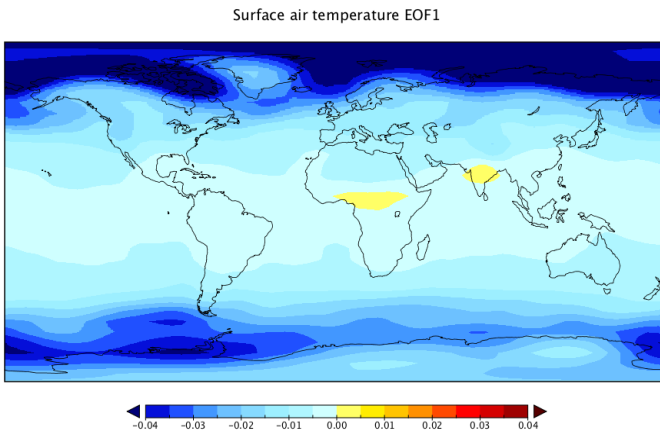

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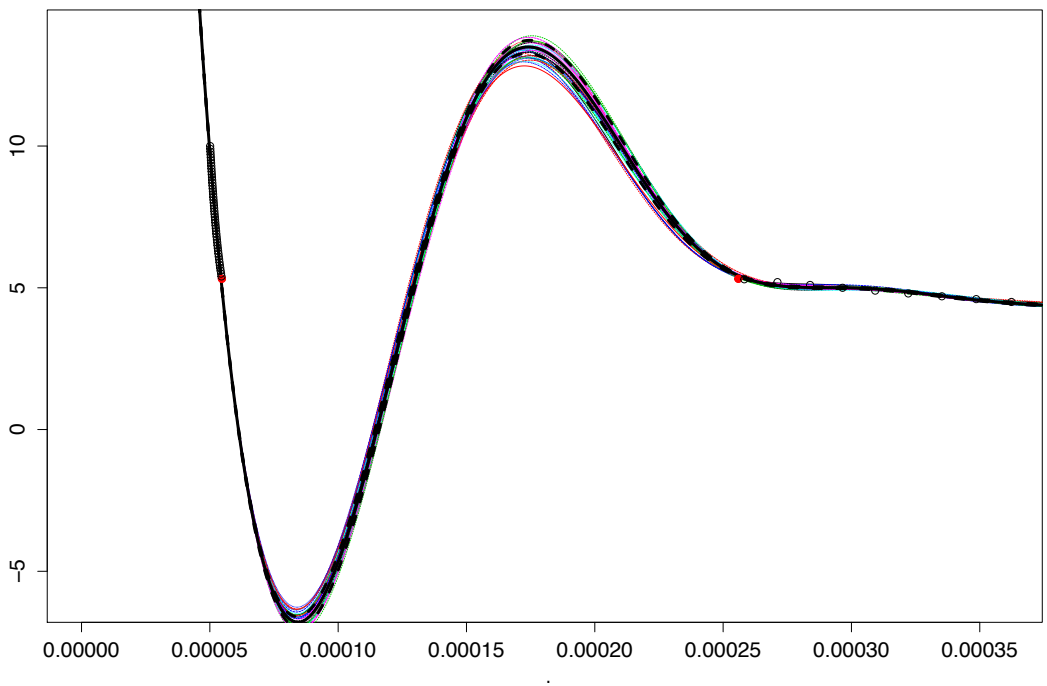
- A GP gave us 82% accuracy (straight out of the box) with no need for transformations.

Example 2: Estimating gas laws for CCS

Cresswell, Wheatley, W., Graham 2016

$PV = nRT$ is an idealised law that holds in the limit.

- it doesn't apply when the gas is near its critical point
- gasses are most easily transported in the super-critical region.
- Impurities in the CO_2 (SO_2 etc) change the fluid behaviour.
- We only have a few measurements of fluid behaviour for impure CO2.



$$\int_{v_l}^{v_g} P(v)dv = P_s(v_g - v_l)$$

$$\text{and } \frac{\partial P}{\partial v}| = \frac{\partial P^2}{\partial v^2}| = 0$$

at $P = P_c, T = T_c$. By incorporating this information we were able to make more accurate predictions.

Example 3: Symmetry

Suppose we are modelling a function that is invariant under the single permutation σ, where $\sigma^2 = e$, e.g.,

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If k is an isotropic kernel (we only actually require isotropy for each pair of vertices that swap in σ), then $k(x, x') = k(\sigma x, \sigma x')$ and $k(x, \sigma x') = k(\sigma x, x')$ as swaps only occur in pairs ($\sigma^2 = e$). So we can use

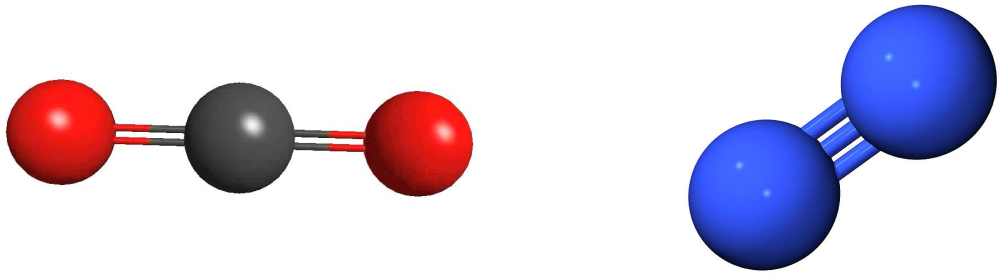
$$k_f(x, x') = k(x, x') + k(\sigma x, x')$$

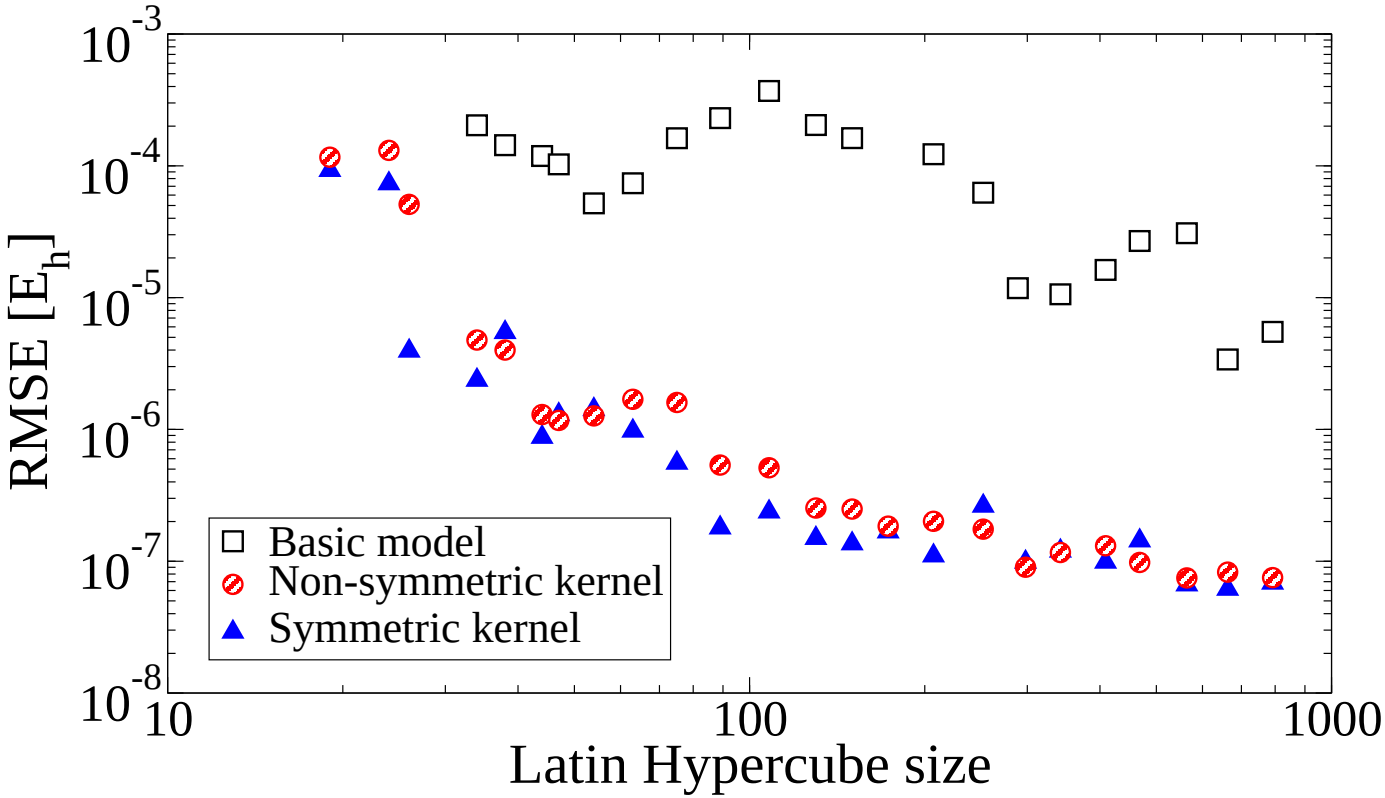
saving half the computation.

Example 3: Modelling intermolecular potentials: Ne-CO2

Uteva, Graham, W, Wheatley 2017

1294 cm-1



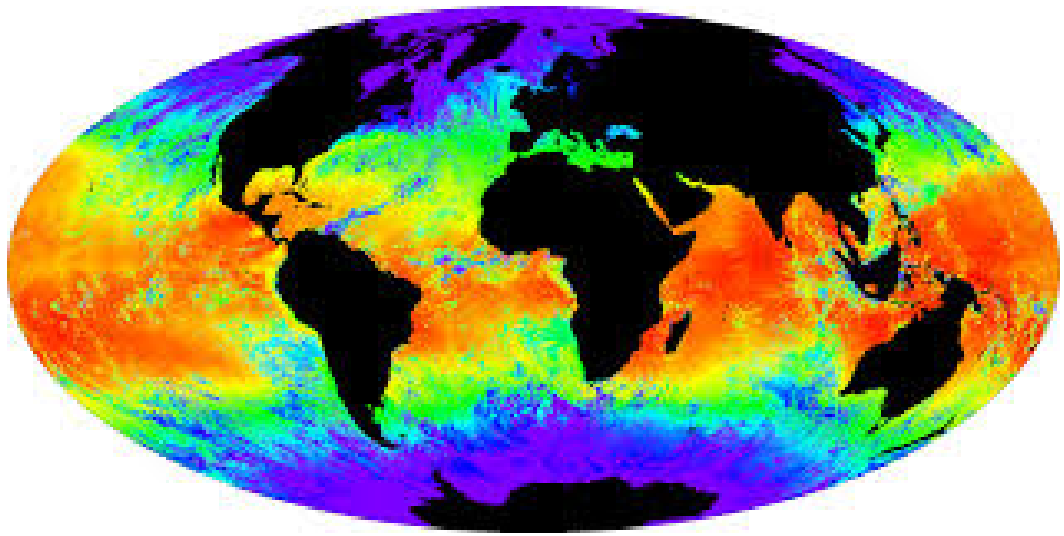


SPDE-INLA: Beyond GPs

Lindgren, Rue, Lindström 2011

The GP viewpoint is somewhat limited in that it relies upon us specifying a positive definite covariance function.

How can we build boutique covariance functions? E.g. emulating SST



The SPDE-INLA approach of Lindgren, Rue, Lindström shows how any Gauss Markov random field (somewhat like a GP) can be written as the solution to a SPDE, which we can solve on a finite mesh.

This gives us more modelling power, but at the cost of much more complex mathematics/algorithms.

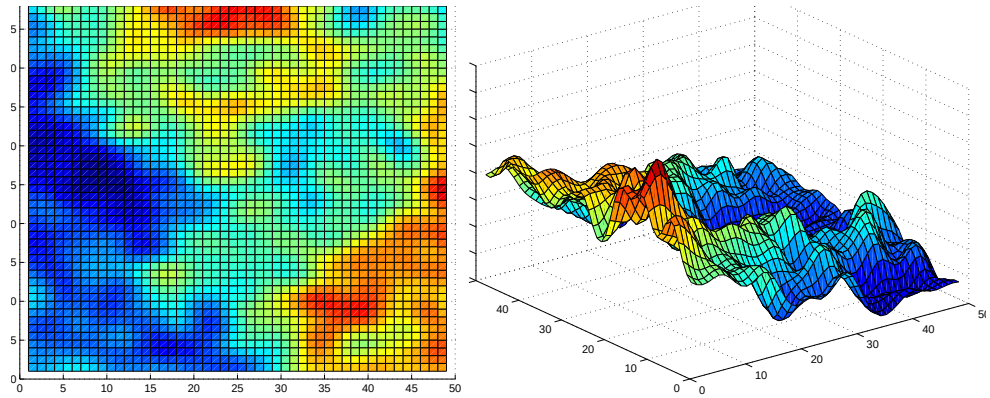
High dimensional problems

Carbon capture and storage

Knowledge of the physical problem is encoded in a simulator f

Inputs:

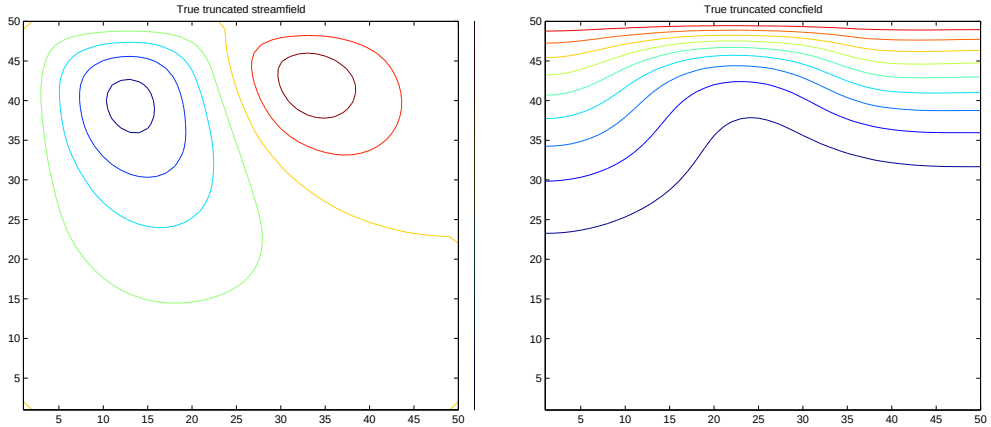
Permeability field, K
(2d field)



$\downarrow f(K)$

Outputs:

Stream func. (2d field),
concentration (2d field),
surface flux (1d scalar),
$\vdots$



Surface Flux= 6.43, ...

Uncertainty quantification (UQ) for CCS

The simulator maps from permeability field K to outputs such as the surface flux $\mathcal{S}$. Let $f(K)$ denote this mapping

$$f : K \rightarrow \mathcal{S}$$

For most problems the permeability K is unknown.

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If we assume a distribution for $K \sim \pi(K)$, we can quantify our uncertainty about $\mathcal{S} = f(K)$.

- e.g., by finding the cumulative distribution function (CDF) of $\mathcal{S}$:

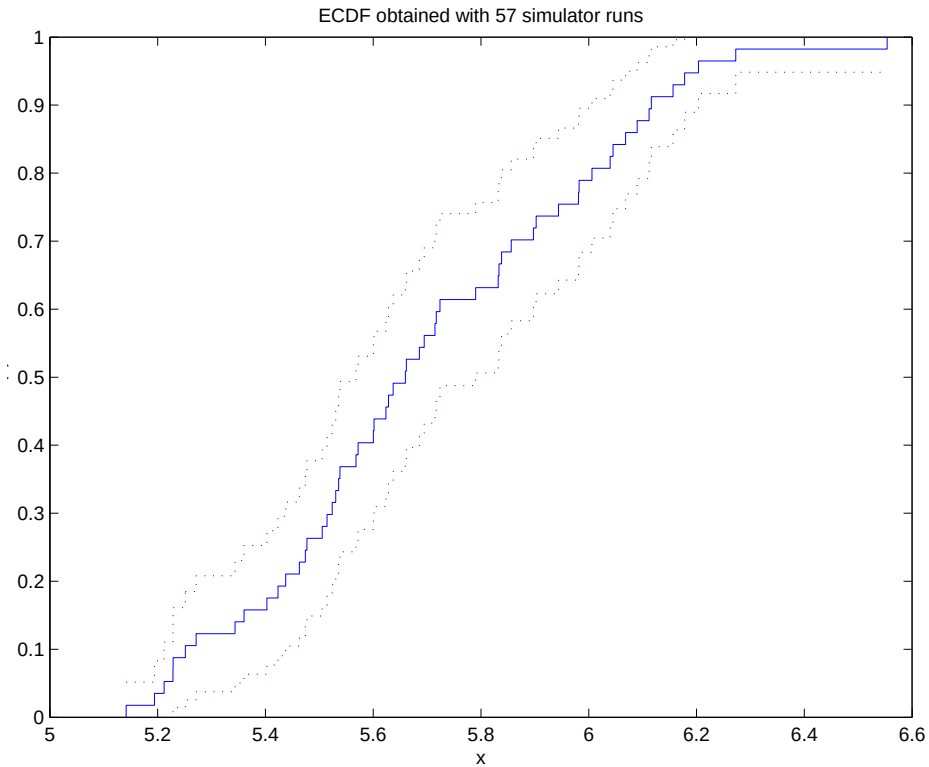
$$F(s) = \mathbb{P}(f(K) \leq s)$$

UQ for complex computer models

Gold standard approach: Monte Carlo simulation

- Draw $K_1, \ldots, K_N \sim \pi(K)$, and evaluate the simulator at each giving fluxes
  $s_1 = f(K_1), \ldots, s_N = f(K_N)$
- Estimate the empirical CDF

$$\widehat{F}(s) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}_{s_i \leq s}$$



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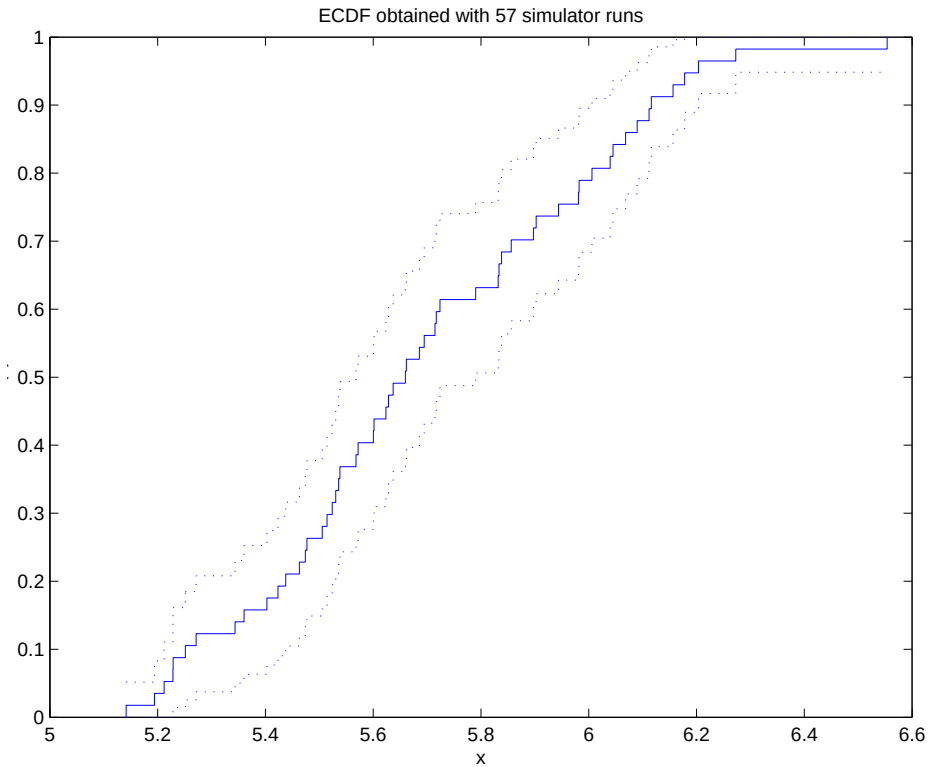

Note that $N = 10^3$ is not large if we want quantiles in the tail of the distribution

However the cost of the simulator means we are limited to $\sim$100 evaluations.

Multivariate Emulation

Wilkinson 2010

How can we deal with multivariate ouput?

- Build independent or separable multivariate emulators,
- Linear model of coregionalization?

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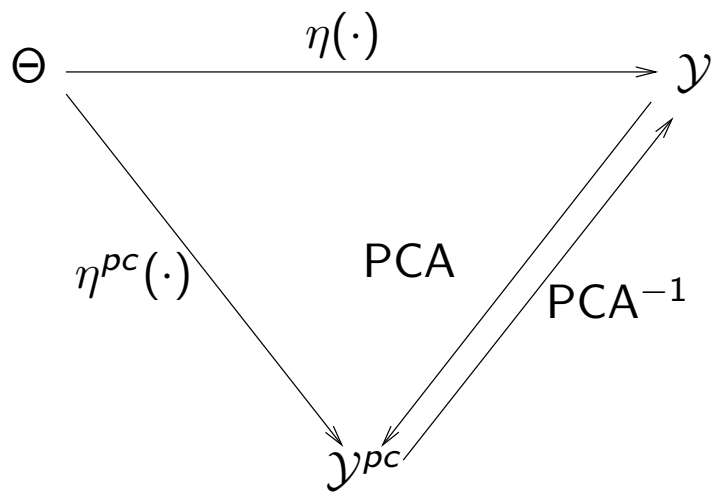
Instead, if the outputs are highly correlated we can reduce the dimension of the data by projecting the data into some lower dimensional space $\mathcal{Y}^{pc}$, i.e., assume

$$y = Wy^{pc} + e$$

where $dim(y) >> dim(y^{pc})$

Emulate from Θ to the reduced dimensional output space $\mathcal{Y}^{pc}$



Principal Component Emulation (EOF)

1. Find the singular value decomposition of Y.

$$Y = U\Gamma V^*.$$

Γ contains the singular values (sqrt of the eigenvalues), and V the principal components (eigenvectors of $Y^\top Y$).

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Why use PCA here?

- The n directions are chosen to maximize the variance captured
- The approximation is the best possible rank n approximation in terms of minimizing the reconstruction error (Frobenius/2-norm)

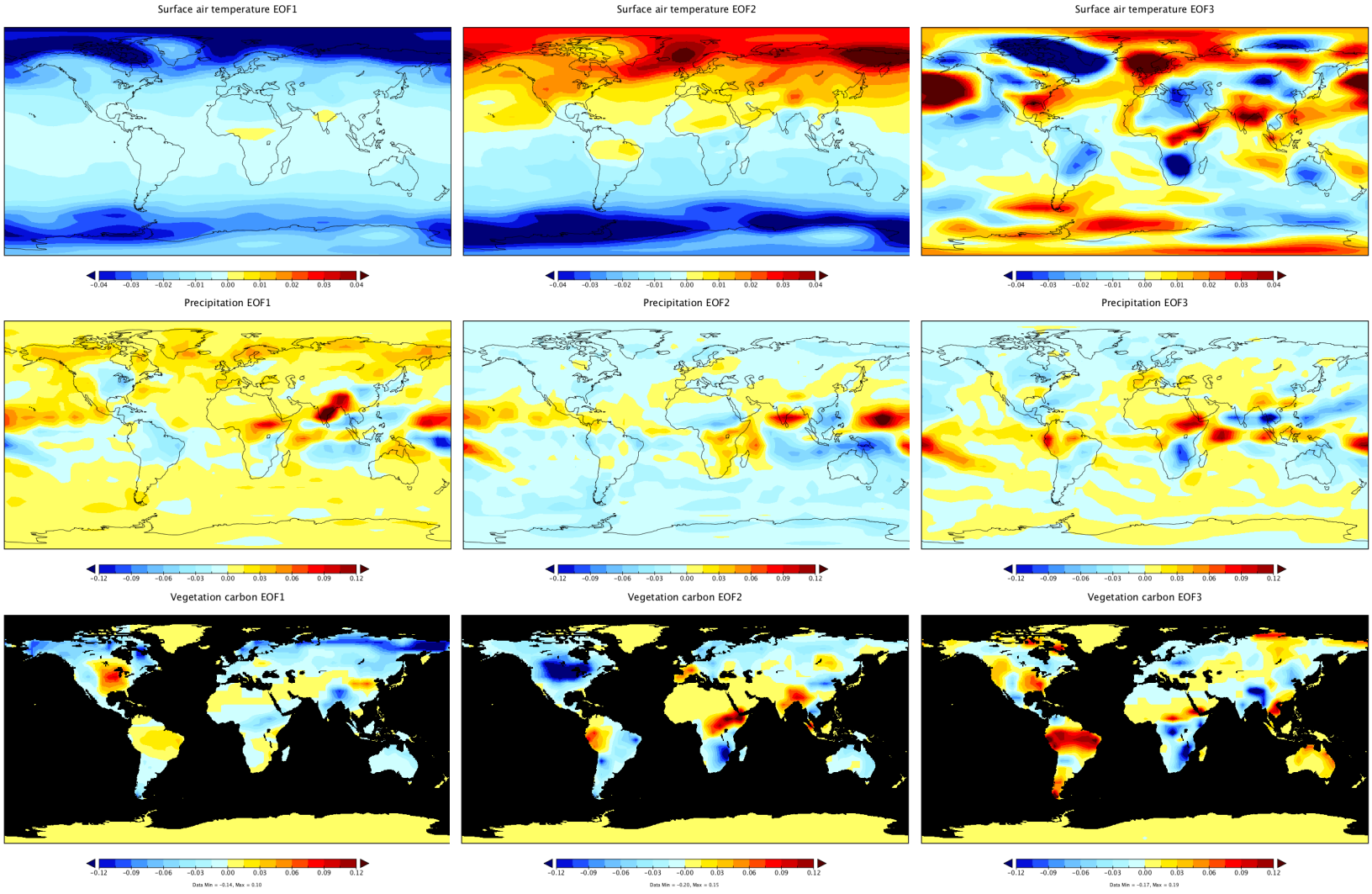
PLASIM-ENTS

Holden, Edwards, Garthwaite, Wilkinson 2015

- Planet Simulator coupled to the terrestrial carbon model ENTS
- Inputs are eccentricity, obliquity, precession describing Earth's orbit around the sun.
- Model climate (annual average surface temperature and rainfall) and vegetation (annual average vegetation carbon density) spatial fields (on a 64×32) grid.

We used an ensemble of 50 simulations

Principal components



PCA emulation

We then emulate the reduced dimension model

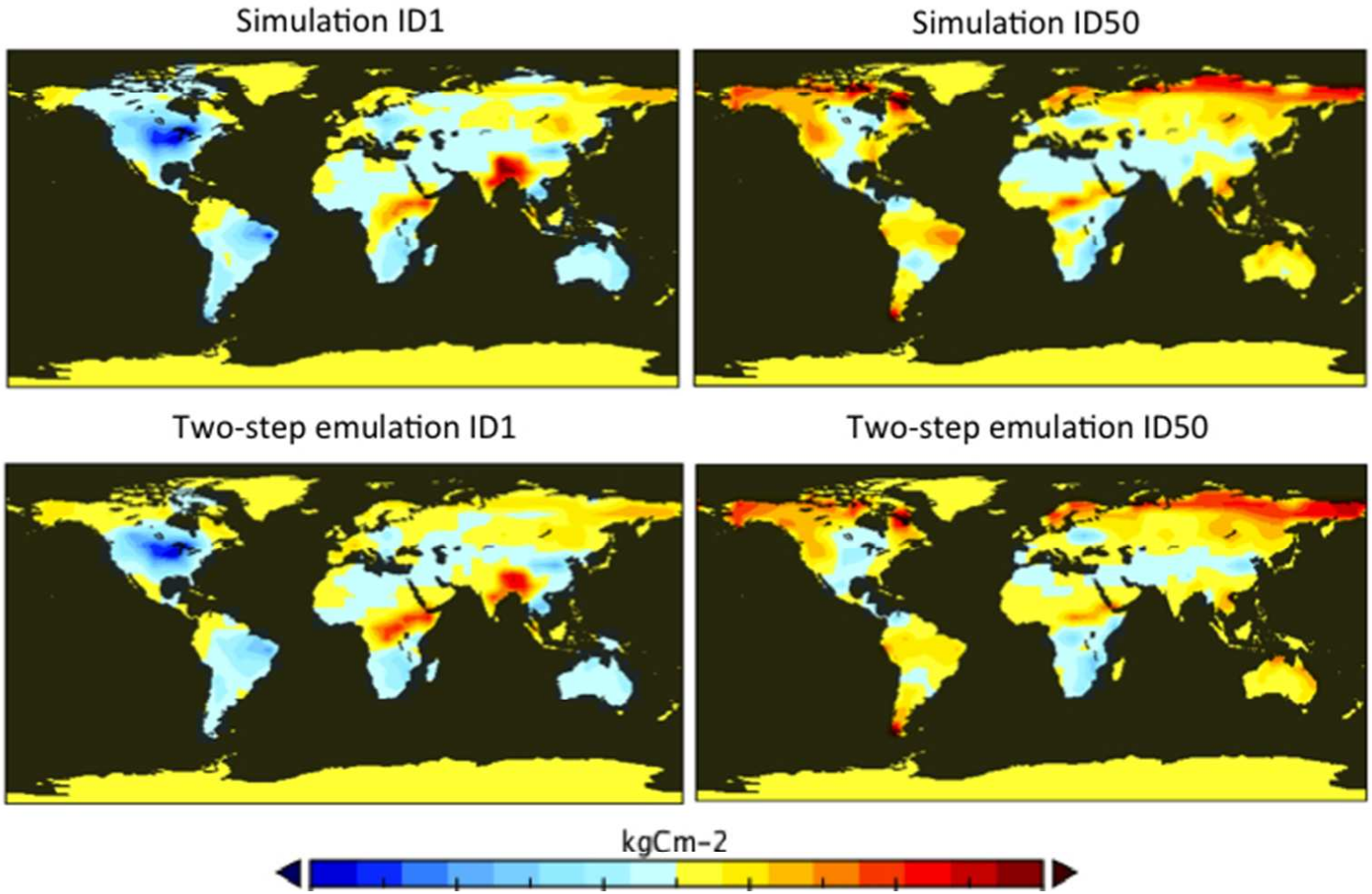
$$\eta_{pc}(\cdot) = (\eta_{pc}^1(\cdot), \ldots, \eta_{pc}^{n^*}(\cdot)).$$

- Each component η_{pc}^i will be uncorrelated (in the ensemble) but not necessarily independent. We use independent Gaussian processes for each component.
- The output can be reconstructed (accounting for reconstruction error) by modelling the discarded components as Gaussian noise with variance equal to the corresponding eigenvalue:

$$\eta(\theta) = V_1 \eta_{pc}(\theta) + V_2 \text{diag}(\Lambda)$$

where $\Lambda_i \sim N(0, \Gamma_{ii})$ ($\Gamma_{ii} = i^{th}$ eigenvalue).

Leave-one-out cross validation of the emulator



We can then use the PC-emulator to do sensitivity analysis.

Comments

- This approach (PCA emulation) requires that the outputs are highly correlated.
- We are assuming that the output $\mathcal{D}_{\text{sim}}$ is really a linear combination of a smaller number of variables,

$$\eta(\theta) = \mathbf{v}_1 \eta_{pc}^1(\theta) + \ldots + \mathbf{v}_{n^*} \eta_{pc}^{n^*}(\theta)$$

  which may be a reasonable assumption in many situations, eg, temporal spatial fields.
- Although PCA is a linear method (we could use kernel-PCA instead), the method can be used on highly non-linear models as we are still using non-linear Gaussian processes to map from Θ to $\mathcal{Y}^{pc}$ – the linear assumption applies only to the dimension reduction (and can be generalised).
- The method accounts for the reconstruction error from reducing the dimension of the data.

Emulating simulators with high dimensional input

Crevilln-Garca, W., Shah, Power, 2016

For the CCS simulator, the input is a permeability field which only needs to be known at a finite but large number of locations,

- e.g. if we use a 100×100 grid in the solver, K contains 10^4 entries
- Impossible to directly model $f : \mathbb{R}^{10,000} \to \mathbb{R}$

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We can use the same idea to reduce the dimension of the inputs. However, because we know the distribution of K, it is more efficient to use the Karhunen-Loève (KL) expansion of K (rather than learn it empirically as in PCA)

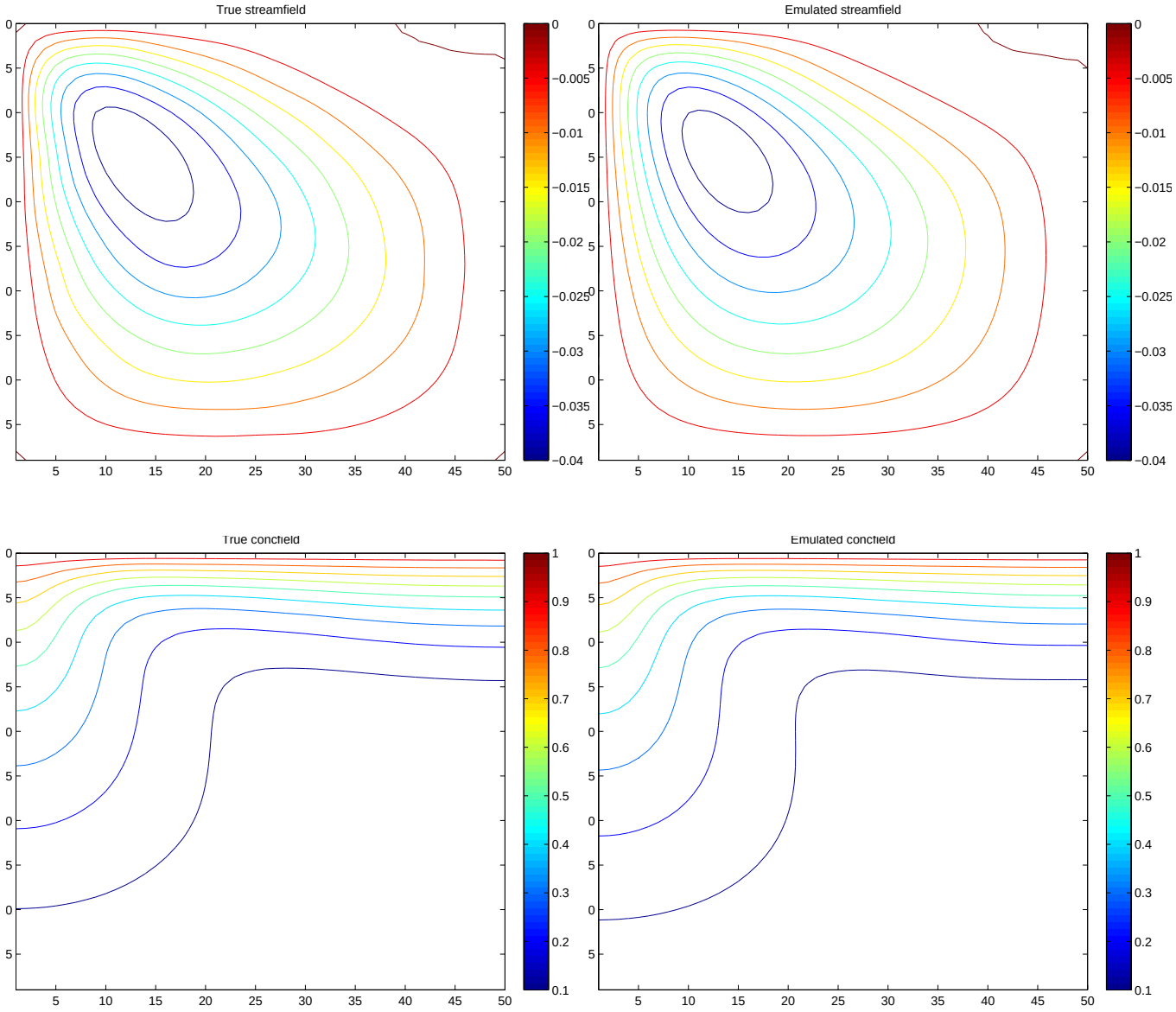
- $K = \exp(Z)$ where $Z \sim GP(m, C)$
- Z can be represented as

$$Z(\cdot) = \sum_{i=1}^{\infty} \lambda_i \xi_i \phi_i(\cdot)$$

where λ_i and ϕ_i are the eigenvalues and eigenfunctions of the covariance function of Z and $\xi_i \sim N(0, 1)$.

Emulating the stream function and concentration fields

Left=true, right = emulated, 118 training runs, held out test set.



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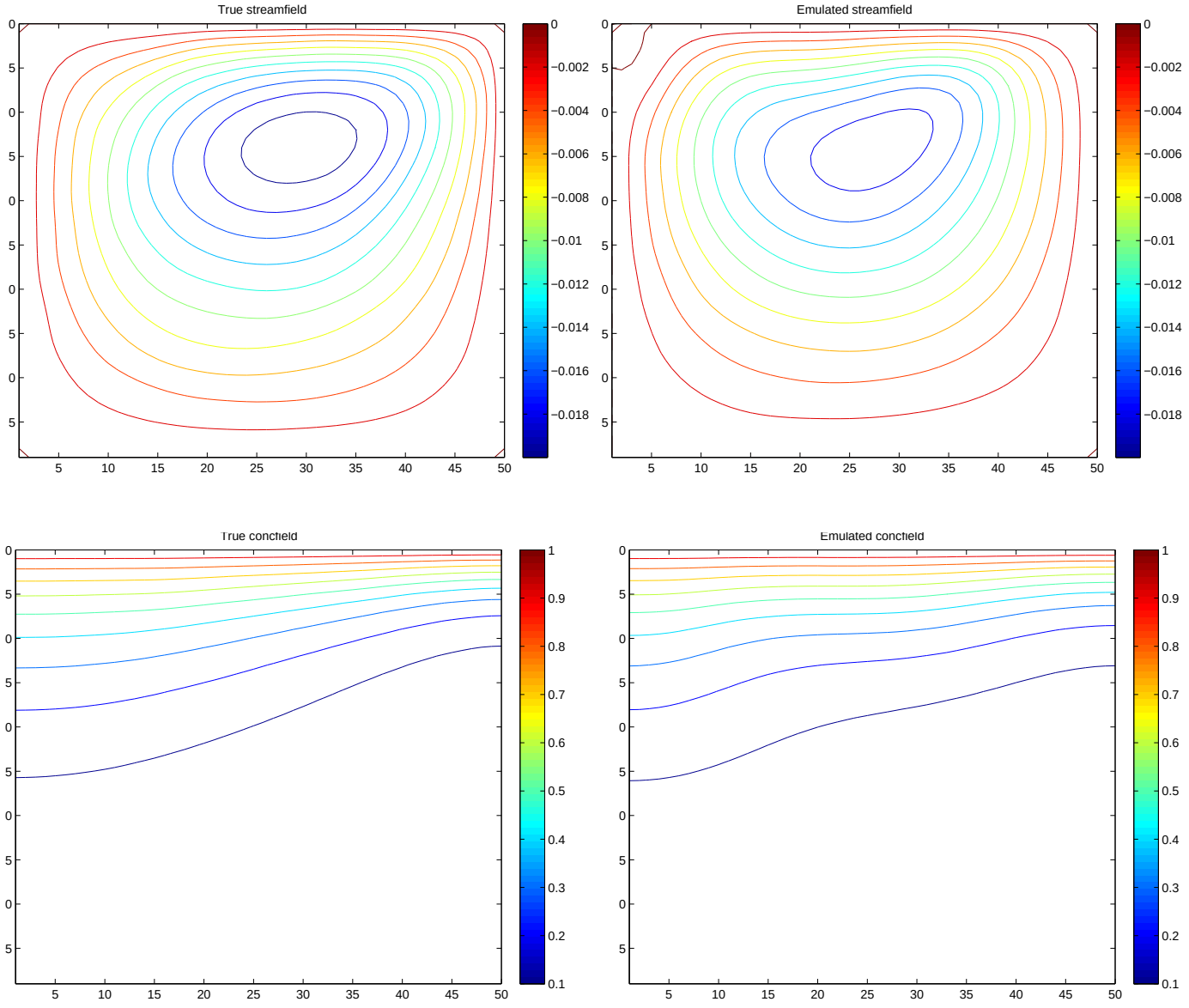

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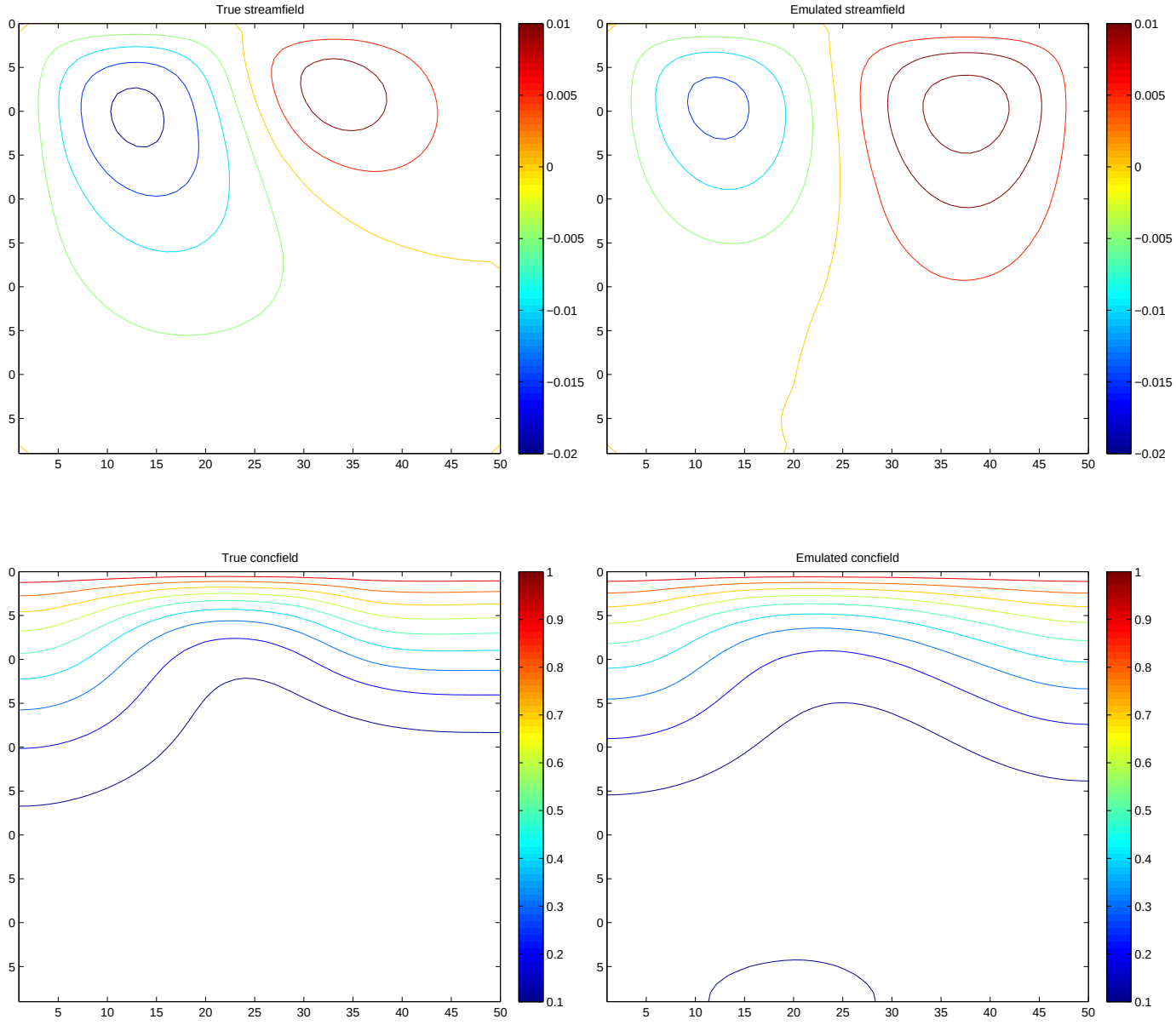
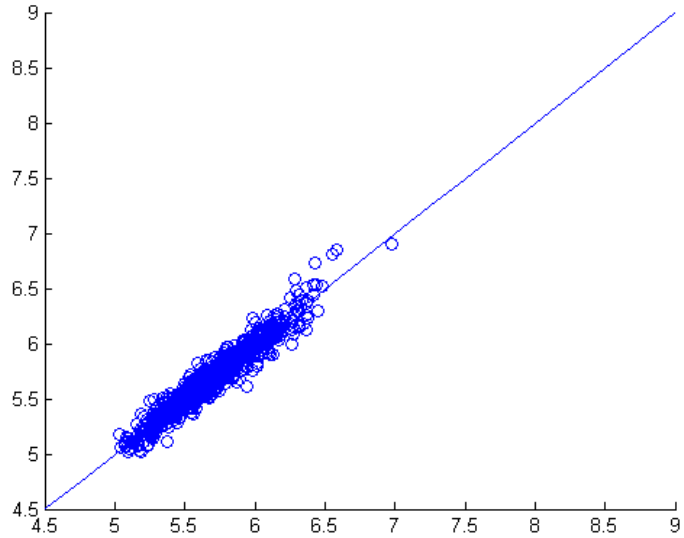
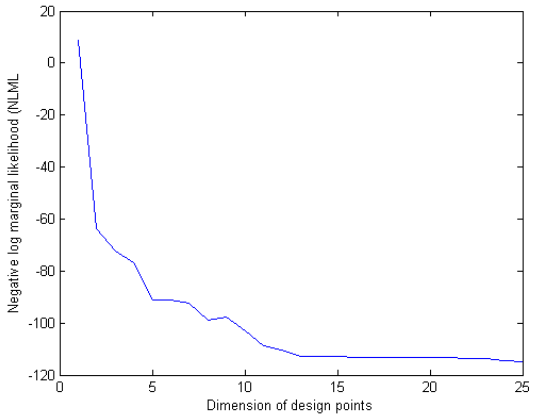


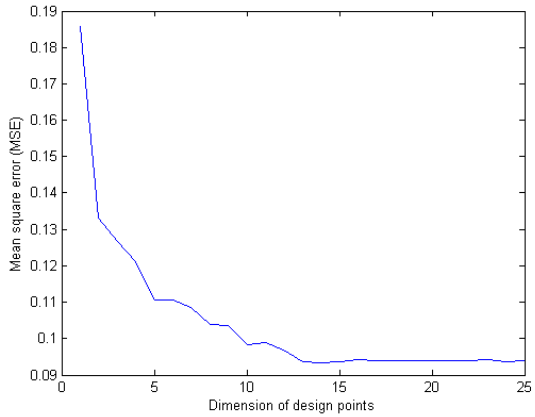
Predictive performance vs n = no. of KL components

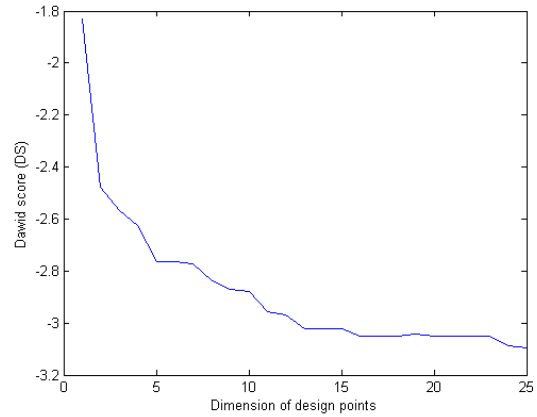
We can assess the accuracy of the emulator by examining the prediction error on a held-out test set. Plotting predicted vs true value indicates the accuracy the GP emulator.



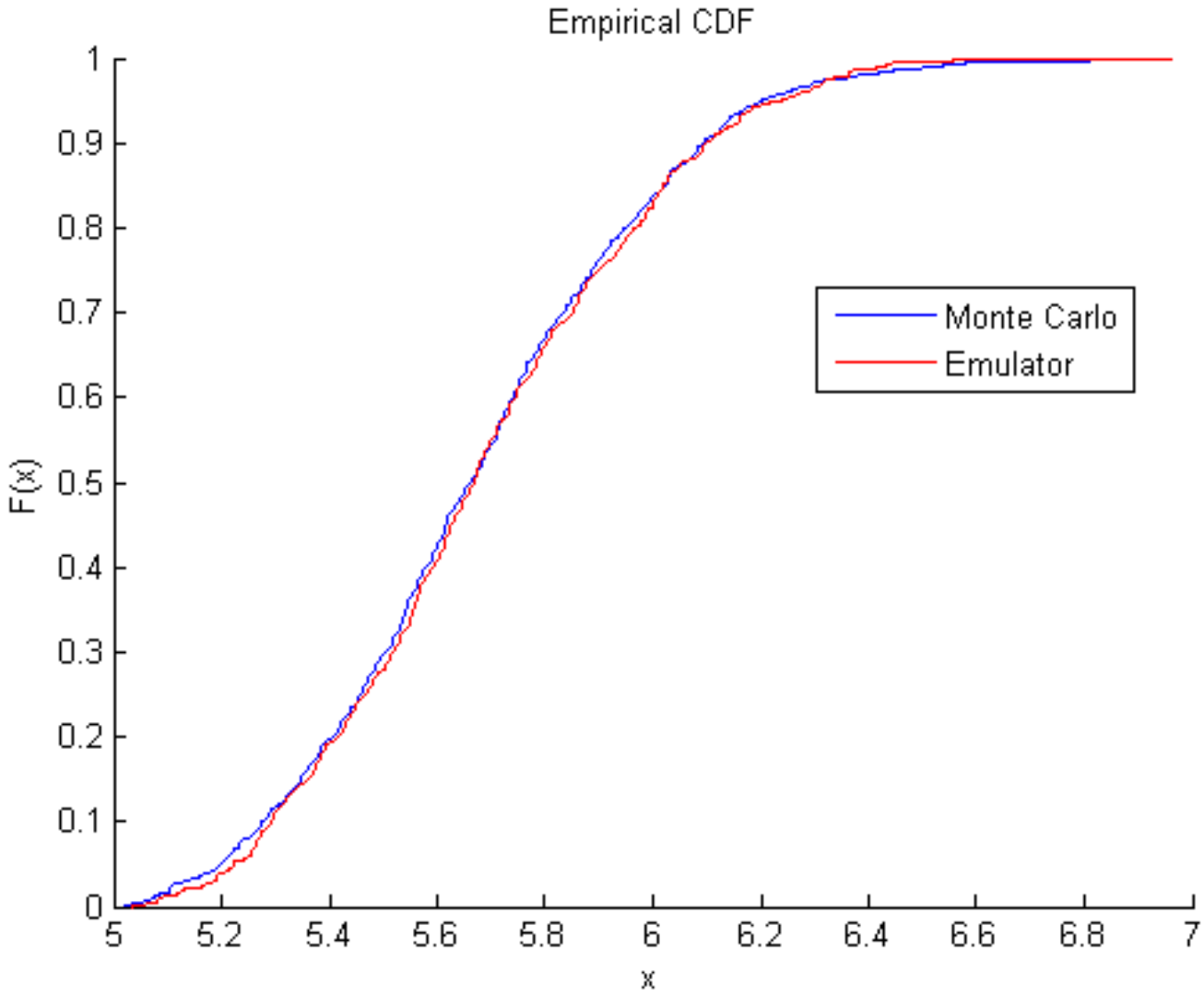
We can also choose the number of KL components to retain using numerical scores







CCS simulator results - 20 simulator training runs



Blue line = CDF from using 10^3 Monte Carlo samples from the simulator
Red line = CDF obtained using emulator (trained with 20 simulator runs, rational quadratic covariance function)

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$$d = f(x) \quad y = g(x)$$

where d are the observations, x the unknown (high dimensional) field, and y the quantity you want to predict.

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  - Less dimension reduction leads to less information loss, but the regression becomes harder.
- Using global sensitivity analysis to select the most influential inputs is a way of doing dimension reduction focused on the important information for regression. However, it is limited to projections onto the original coordinate axes.

Model discrepancy

An appealing idea

Kennedy and O'Hagan 2001

Lets acknowledge that most models are imperfect.

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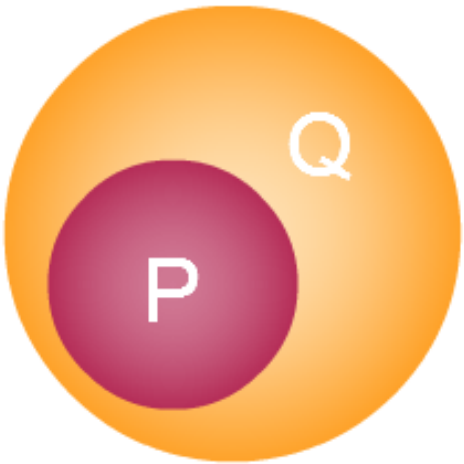
Kennedy and O'Hagan 2001

Lets acknowledge that most models are imperfect.
Can we expand the class of models by adding a GP to our simulator?



If $f(x)$ is our simulator, d the observation, then perhaps we can correct f by modelling

$$y = f(x) + \delta(x) \quad \text{where} \quad \delta \sim GP$$

An appealing, but flawed, idea

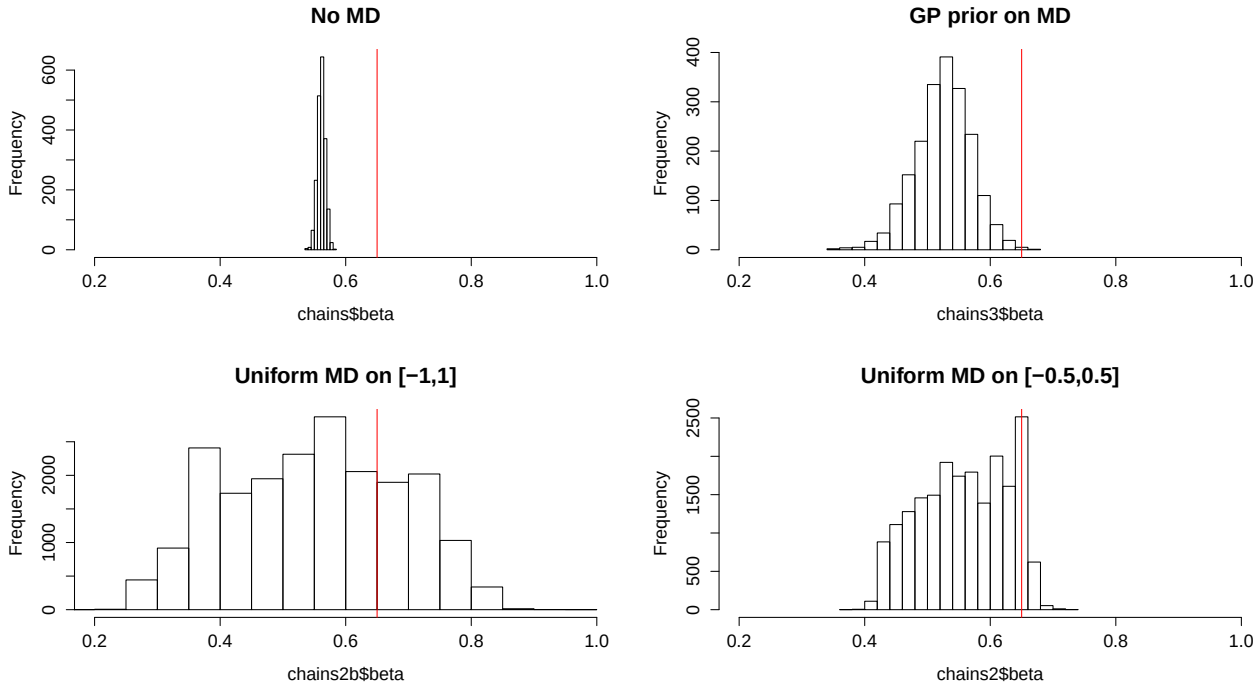
Kennedy and O'Hagan 2001, Brynjarsdottir and O'Hagan 2014

Simulator

$$f(x) = x\theta$$

Reality

$$g(x) = \frac{\theta x}{1 + \frac{x}{a}} \quad \theta = 0.65, a = 20$$



Bolting on a GP can correct your predictions, but won't necessarily fix your inference.

Conclusions

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- Popularity stems from
  - Naturalness of the framework
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Thank you for listening!