Projected Sequential Gaussian Processes and Design for Random Ouput Emulation

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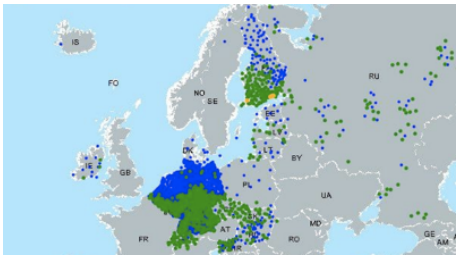
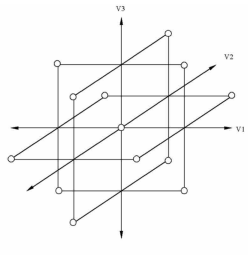
MUCM team meeting, Soton, July 2009

[1] http://wiki.aston.ac.uk/DanCornford/

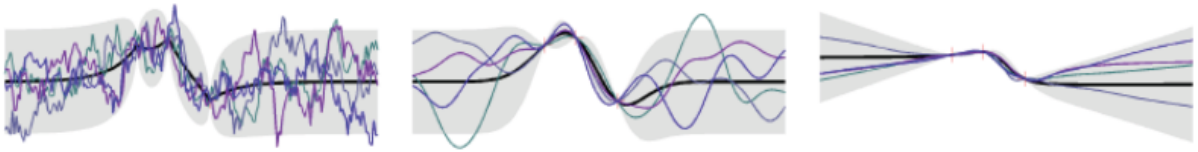
Overview





- Will cover two main areas:
  - How to emulate when we need large numbers of simulator runs?
  - How to select our experimental design when we are emulating random output simulators?
- I will provide a context / motivation for these works first.
- Note: Remi has been working on the INTAMAP project!

Gaussian Processes for Interpolation



- We all use Gaussian processes for emulation.
- A Gaussian process is specified by a mean function $\mu(x)$, and a covariance function, $c(x, x')$.
- Using Gaussian processes with large simulator design sets (of n design points) raises issues:
  - computational issues - likelihood / Bayesian inference scales as $O(n^3)$ - sampling painful, complex simulators impossible?;
  - inferential issues - full Bayesian treatments produce non-Gaussian process posteriors;
- Remi will show a projected, sequential Gaussian processes implementation in C++ to address computational issues.
- Does not address the inferential issues, since it is a maximum-likelihood / MAP method.

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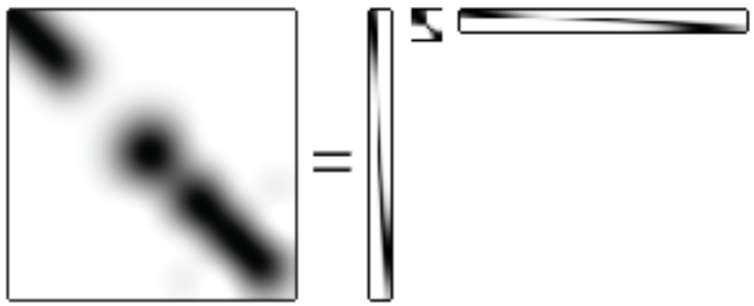
Solutions for large n



- Several options are available for dealing with large training sets:
  - Subset the data into smaller regions of interest – border effects;
  - Select nearest n_{max} outputs for local prediction – discontinuities, parameter inference?;
  - Spectral methods – usually require inputs on a regular grid;
  - Sparse matrices – generally require the scale of variation to be short with respect to the overall domain being studied (might work well if the mean function is doing all the work);
  - Low-rank / projected approximations – difficult to determine the low-rank matrix apriori.
- Here we adopt the low rank (projected) approximation, but determine this sequentially.

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Projected Sequential Gaussian Process

- The basic algorithm is quite simple. The Gaussian process posterior is parametrised using α_i and $C(i,j)$ as:

$$\mu_{posterior}(x) = \mu_{prior}(x) + \sum_{i}^{m} \alpha_i c(x, x_i), \text{ and,}$$

$$c_{posterior}(x, x') = c_{prior}(x, x') + \sum_{i,j=1}^{m} c(x, x_i) C(i,j) c(x_j, x')$$

- If m, the size of the active set, is the same as the data set size n, then this is an exact parametrisation.
- Main benefit is a sequential approach to updating the posterior:
  - as each design point is added it is possible (but not necessary) to increase the size of the active set, depending on how much information would be lost;
  - using the expectation propagation method we can recycle the design points.
- Remi will explain and show more ...

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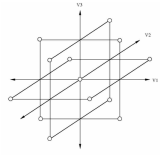
Experimental design for random output simulators



- Alexis has been working on emulation of random output (stochastic) simulators:
  - Initial work has focussed on modelling the output as a heteroscedastic Gaussian process;
  - This has a separate GP for the mean output and (at an input point) variance of the output.
  - Optimal designs for such settings are not known, since the random (heteroscedastic) output means it might well be efficient to run the simulator a number of times at each design point.
  - Here we consider designs which are informative about model parameters and also designs that are informative for model predictions.
- Alexis will focus on the question of designs for parameter estimation in heteroscedastic GPs.

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Final remarks

The projected, sequential Gaussian process is ongoing work

The implementation does not address:

- mean functions (we will be working on that),
- full Bayesian approaches,
- optimisations for compact covariances,
- Remi will show where we are now.

Optimal design for random output emulation is ongoing work

- working with Noha and LSE to link to ASCM,
- early results promising, but still need full results,
- Alexis will show where we are now.

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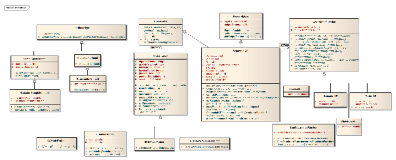
Software implementation



- Implementing the psgp library was important to us – we want to extend and reuse it.
- Implementation details can make a big difference to performance.
- Built in C++ on top of the IT++ libraries for matrix / vector operations and Blas for linear algebra - will produce Matlab and R interfaces.
- Class design based on:
  - `CovarianceFunction` *interface* (abstract class, strictly) for the Gaussian process;
  - `LikelihoodType` for the output characteristics (Gaussian in MUCM);
  - The `sequentialGP` implements two *interfaces*, `ForwardModel` and `Optimisable`.
- This will be released on GoogleCode soon.

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