Iterative Gaussian Process Regression for Potential Energy Surfaces

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Outline

• Motivation:
  • Calculation of potential energy surfaces (PES)

• Gaussian Process Regression (GPR):
  • Background
  • Motivation - can we use GPR to reduce the CPU time needed to calculate a PES?
  • Method; iteration

• Results for PES for fission of $^{240}$Pu:
  • 1D
  • 2D

• Future work
Motivation: potential energy surfaces (PES)

- E.g. fission:
  - Nucleus slowly deforms, from roughly spherical shape to 2 distinct nuclei
  - Nucleus has different potential energy for different deformations
  - PES can yield properties like path taken to fission, lifetime, mass distributions of fission fragments

- Computationally expensive NDFT is used - 5-10 CPU hours per calculation
- 1000s of calculations required

- By how much can we reduce the number of calculations with GPR?

Calculated PES for fission of $^{258}$Fm
Gaussian Process Regression (GPR)

- Regression method from machine learning
- Outputs a model/prediction which is a smooth interpolation of points on a surface
- Predictions at unknown locations on surface are made using all calculated points
- Most useful for expensive computer simulations, with smoothly-varying outputs
- Surface $Y(x)$ is modelled as the sum of a regression model (comprising $k$ regression functions $f_j$) and a random (Gaussian) process $Z$:

$$Y(x) = \sum_{j=1}^{k} \beta_j f_j(x) + Z(x)$$

- Used previously in atmospheric chemistry, locating mineral ores, modelling of oceans and diseases, atomic physics
GPR example in 1D

Increase number of design points:
• Increase accuracy of emulation
• Decrease size of confidence intervals

Design points (red) (with error bars)
GPR prediction (black line)

Unknown function/surface (blue dotted line)
Linear trend line
95% confidence intervals (shaded)

Increase number of design points:
• Increase accuracy of emulation
• Decrease size of confidence intervals
Gaussian Process Regression (GPR) - kernels

- Gaussian correlation model (covariance kernel), for $d$ dimensions:
  \[ V(x', x) = \sigma^2 \prod_{j=1}^{d} \exp \left( -\frac{(x'_j - x_j)^2}{2\theta_j^2} \right) + \tau^2 \delta_0(x' - x) \]

  where $\sigma^2$ is variance of random process $Z$
  - $\theta_j$ are 'characteristic length-scales' $\to$ control spatial correlation lengths
  - $\tau^2$ is 'nugget variance' $\to$ treats numerical instabilities caused by jitters/kinks on surface
  - $\sigma^2, \theta_j$'s, $\tau^2$ optimized to maximise log marginal likelihood
Gaussian Process Regression (GPR) - method

• Use previously calculated surfaces
• Choose a sample of calculated points
• **Normalise the sample**
• Use these ‘design points’ to emulate surface
• Compare emulated surface with original surface (how accurate was the emulation?)

• Iteration:
  • Add new point at location of max $\sigma$ from last iteration
  • Re-emulate
GPR in 1D

Calculated PES for fission of $^{240}$Pu. Plot shows calculated energy (MeV) of nucleus relative to -1840 MeV. Schunck et al. – Phys. Rev. C 90, 054305
• Original slice represented by red points
• Design points in blue
• New points in green

• Blue line gives difference between GPR prediction and original slice

• Occasionally, addition of one new point completely changes the estimation kernel parameters

• When this happens, the prediction changes completely, and the confidence grows suddenly
GPR in 2D

Fission barriers (bottom left) and scission ‘cliff’ (right-hand edge) pose problems
Conclusions and future work

- To successfully perform regression for surface with very different behaviours, need one or both of the following:
  - non-stationary correlation model - $\theta_j$ allowed to vary across surface
  - better pre-processing of data, to make it more normally distributed before regression is performed
- Better iteration method:
  - Bias against selection of new points at edges
  - More cautious selection of new points to avoid sudden changes in GPR output
  - Multiple new points at once
  - We know location of fission barriers/ other tricky areas – take advantage of this knowledge
- Compare fission observables from emulated and ‘normal’ surfaces
- Emulating higher dimensional fission surfaces:
  - Ideally need 5D surface for description of fission
  - GPR should provide a better speedup for higher dimensional surfaces
Thank you!

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• Introduction to Gaussian Process Regression:
Design point selection for GPR

- Latin Hypercube Sampling (LHS) provides better coverage of surface