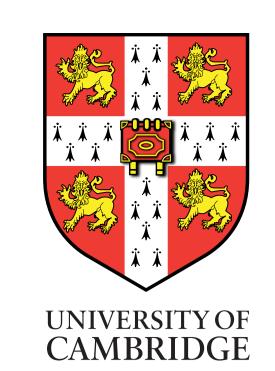


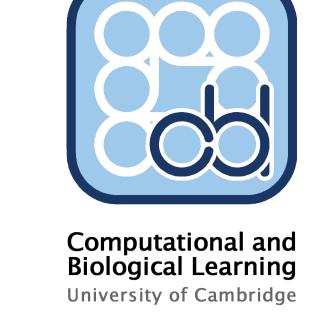
Automating pattern discovery and the statistical process for regression

David Duvenaud¹, **James Robert Lloyd**¹, Roger Grosse²,

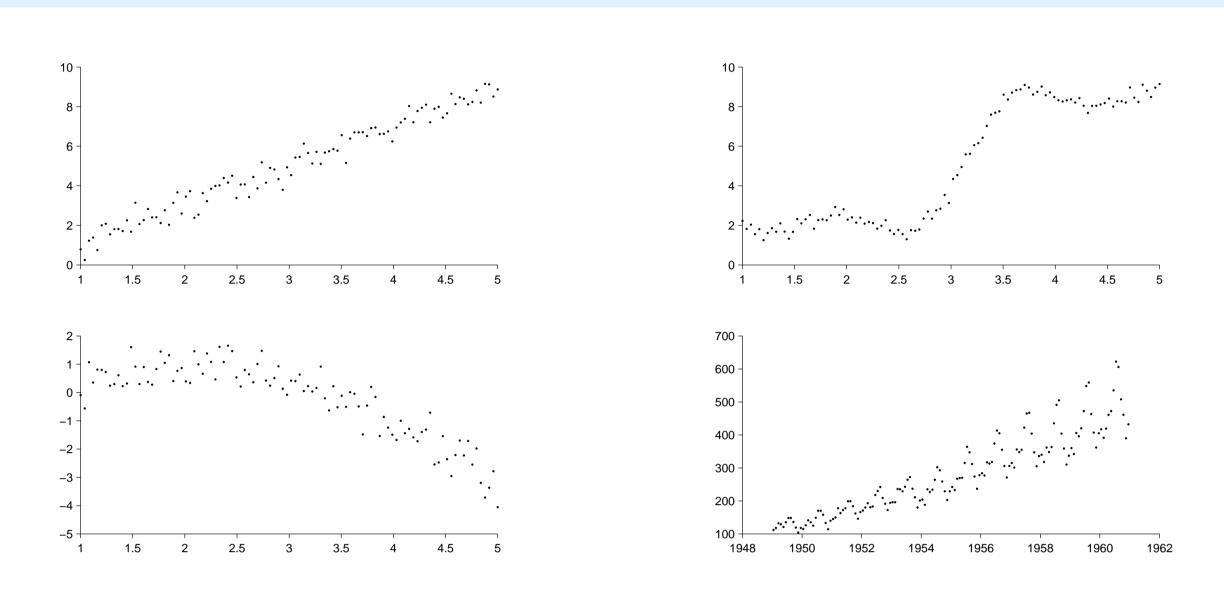
Joshua B. Tenenbaum², Zoubin Ghahramani¹

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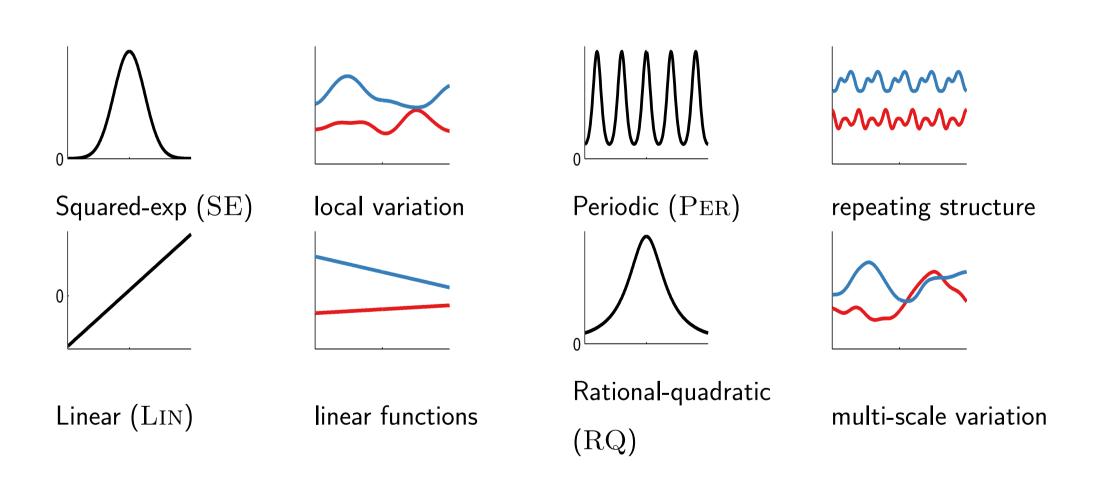
Data often exhibits high level structure



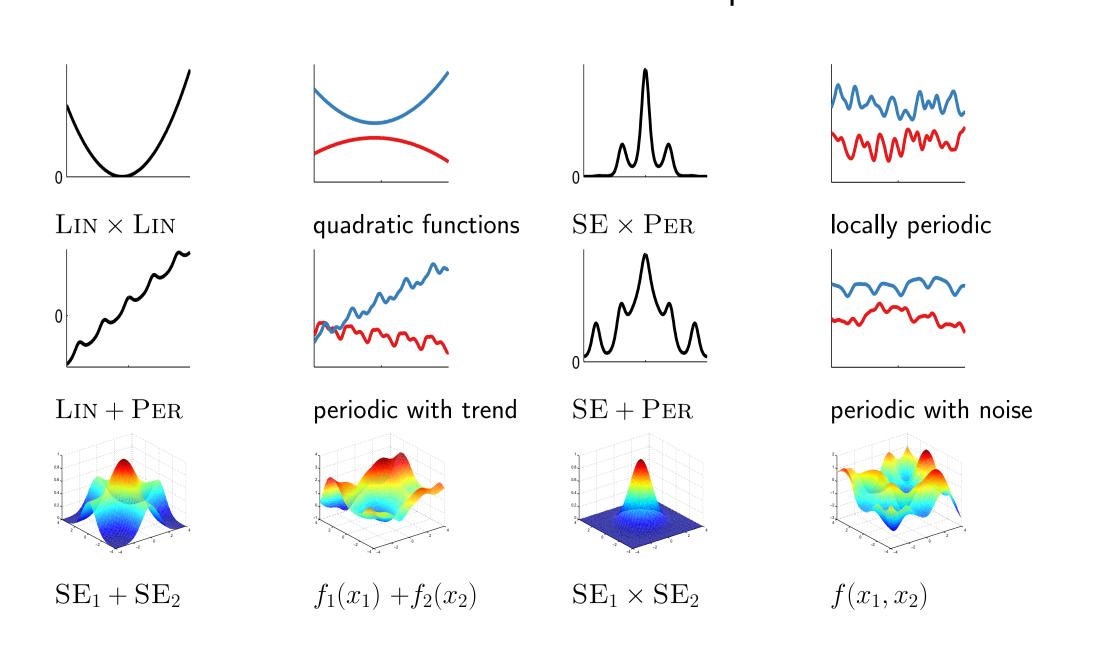
- Traditionally, a researcher / scientist / statistician would select an appropriate model for the type of structures present
- Automatic model selection techniques already exist, typically choosing between a finite or restricted set of models
- Instead, we automate statistical model *construction*, which allows for a very large set of models to be considered

Gaussian process regression can model many structures with an appropriately chosen kernel

- The kernel encodes the inductive bias of the model i.e. the types of functions the model 'believes in'
- Below we depict standard base kernels, and examples of functions the model believes in (samples from the prior)



• Base kernels can be combined to create more complicated structural assumptions



We consider all kernel expressions derived from a generative grammar...

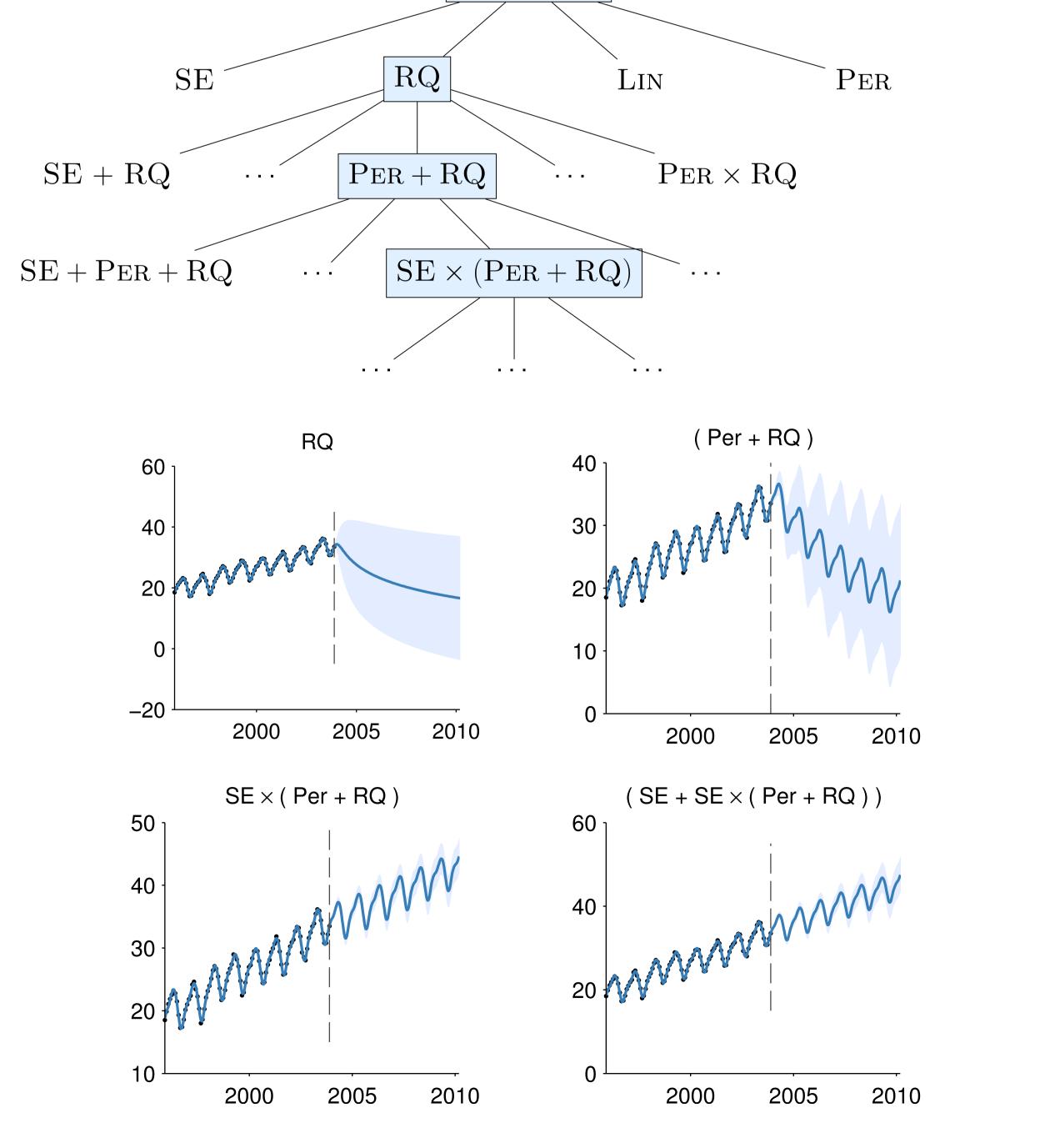
- Constructing appropriate composite kernels has previously been the domain of Gaussian process experts
- ullet We consider all algebraic expressions involving a small number of base kernels and the operations '+' and '×', which includes

Lin
$ Lin \times Lin \times \dots $
PER + PER + .
$\sum_{d=1}^{D} ext{SE}_d$
$igg \overline{\prod_{d=1}^{ ilde{D}}} \mathrm{SE}_d$
Lin + SE
$Lin \times SE$

. . . which we search greedily, producing progressively better statistical models

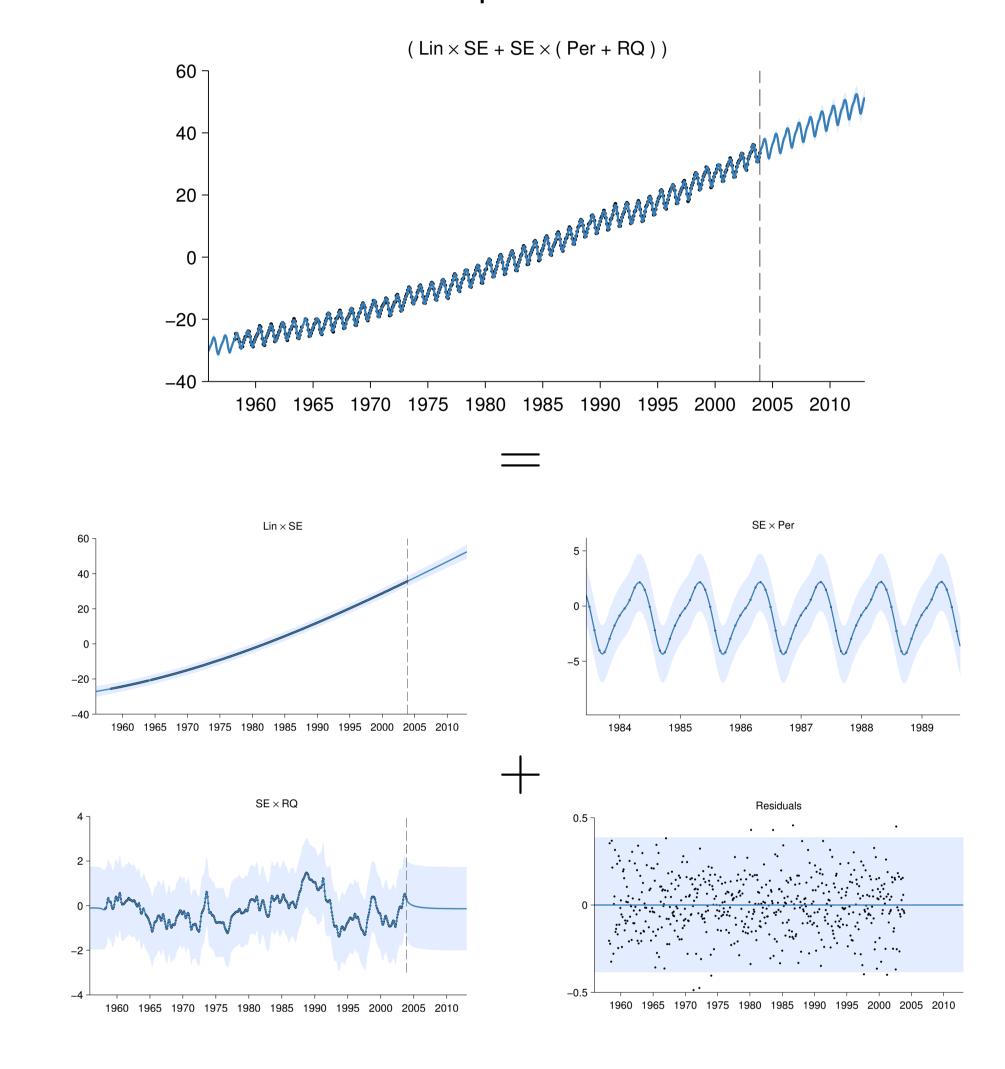
- We try all base kernels, selecting the one with the highest (approximate) marginal likelihood which balances data fit and model complexity
- The search continues by adding an extra term to the current best kernel, stopping when marginal likelihood no longer improves

No structure



Example: Mauna Loa CO₂ concentration

 By automatically inferring an appropriate kernel, we can also automatically decompose functions into additive components



Example: International airline passengers

