Structure Discovery in Nonparametric Regression through Compositional Kernel Search

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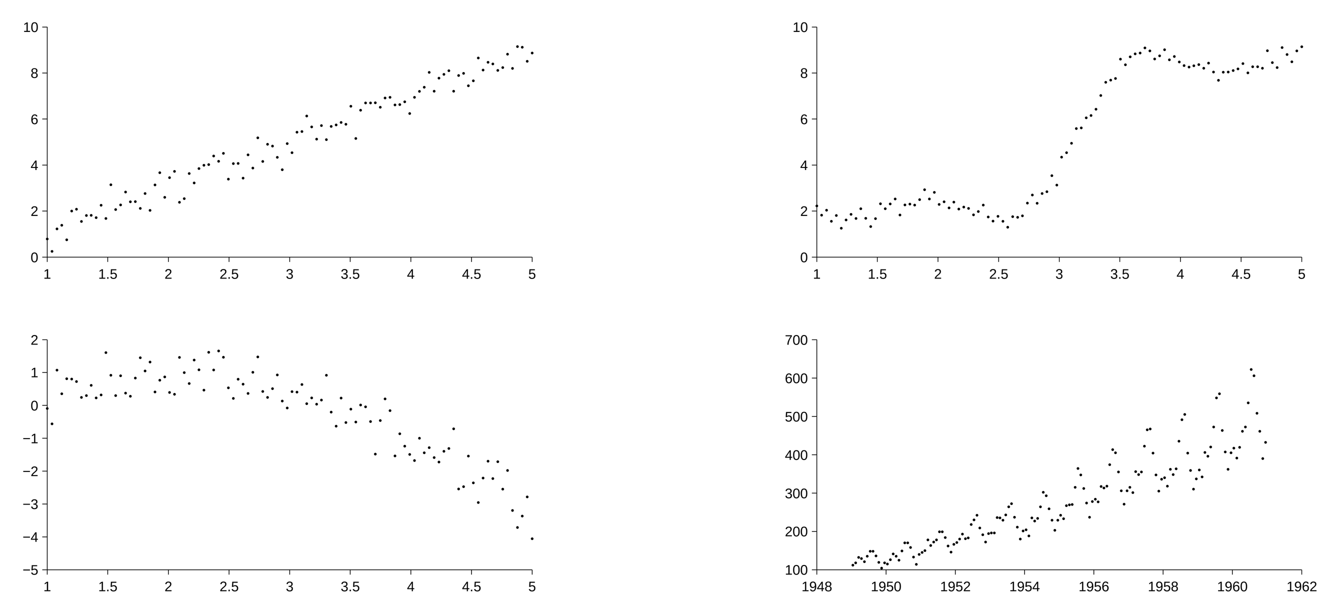
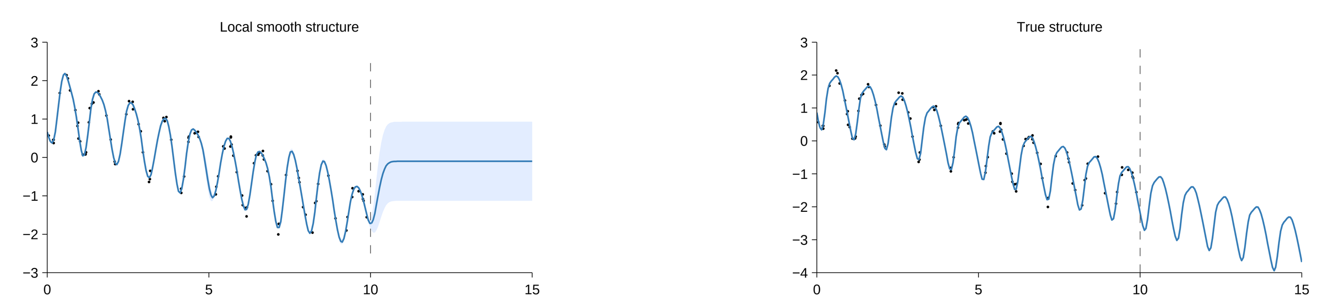
Data often exhibits high level structure or patterns



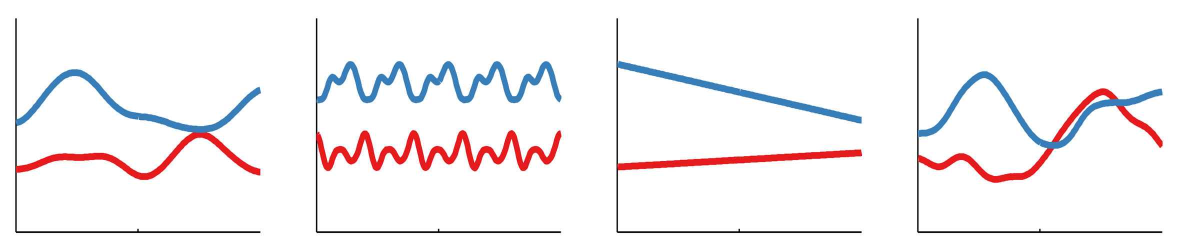
Identifying this structure is crucial for extrapolation



- 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*

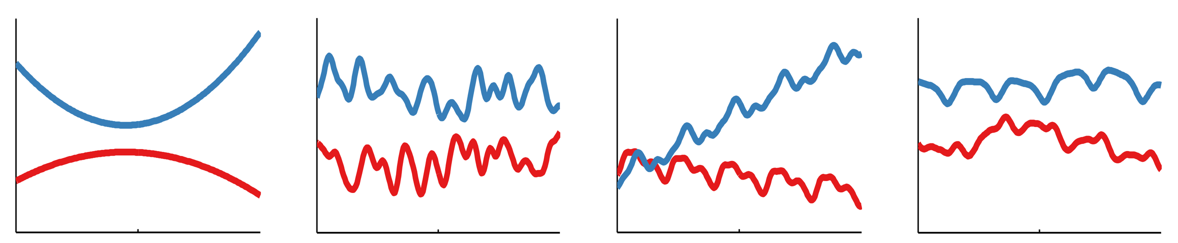
Gaussian process regression can model many structures with an appropriately chosen kernel

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



SE local variation | Per repeating structure | Lin linear functions | RQ multi-scale variation

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



Lin × Lin quadratic functions | SE × Per locally periodic | Lin + Per periodic with trend | SE + Per periodic with noise

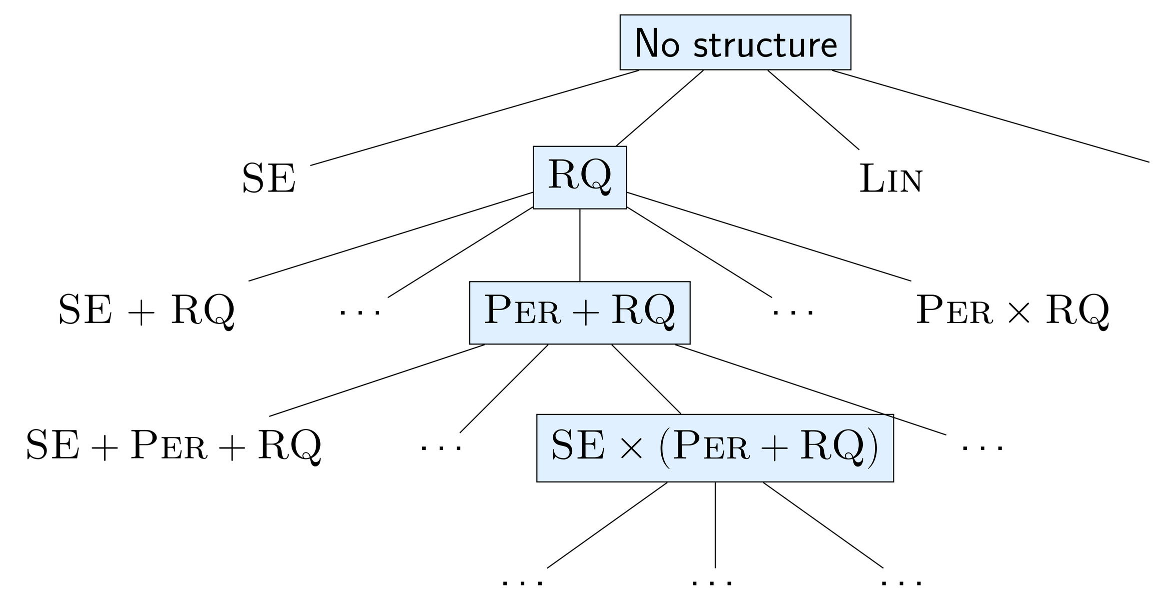
We consider all kernel expressions derived from a generative grammar...

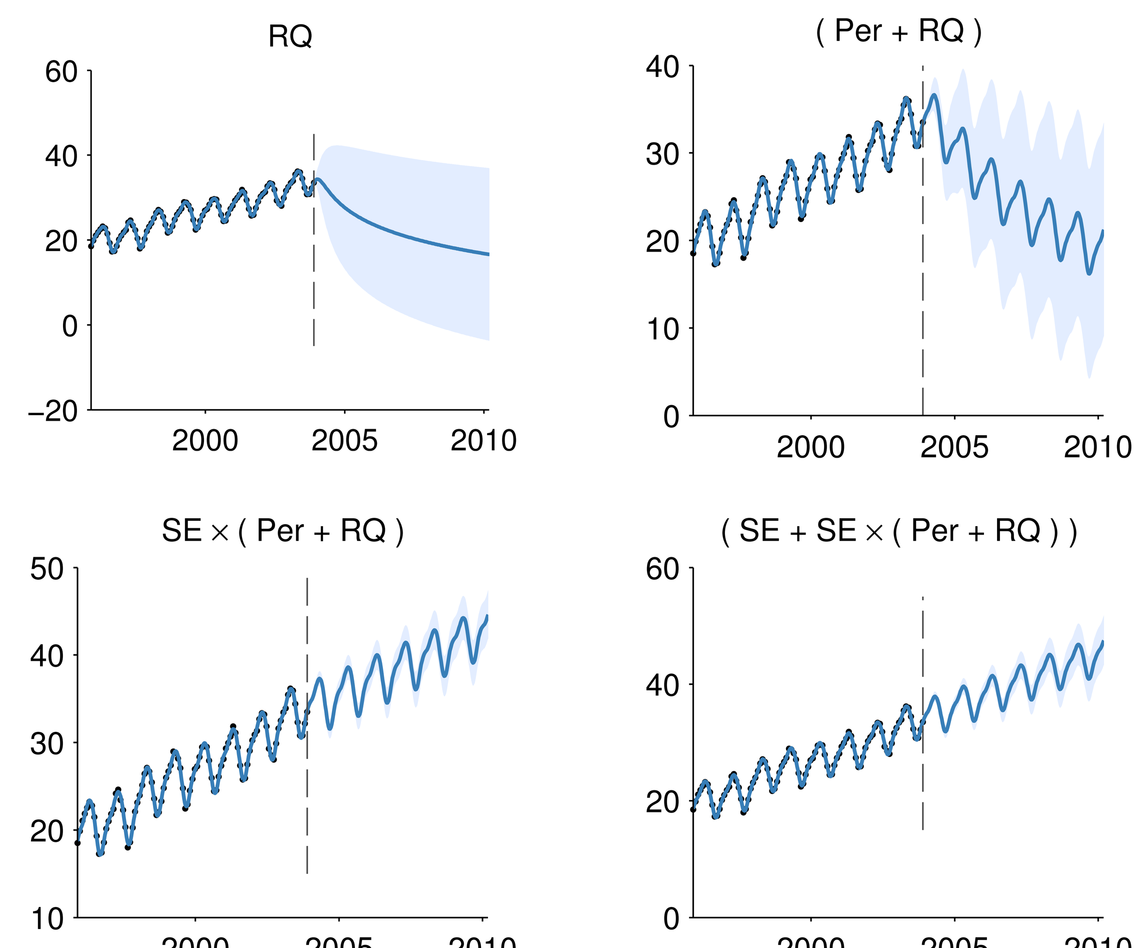
- Constructing appropriate composite kernels has previously been the domain of Gaussian process experts
- We consider all algebraic expressions involving a small number of base kernels and the operations '+' and '×', including e.g.

Bayesian linear regression	Lin
Bayesian polynomial regression	Lin × Lin × ...
Generalized Fourier decomposition	Per + Per + ...
Generalized additive models	$\sum_{d=1}^{D} \mathrm{SE}_d$
Automatic relevance determination	$\prod_{d=1}^{D} \mathrm{SE}_d$
Linear trend with deviations	Lin + SE
Linearly growing amplitude	Lin × SE

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

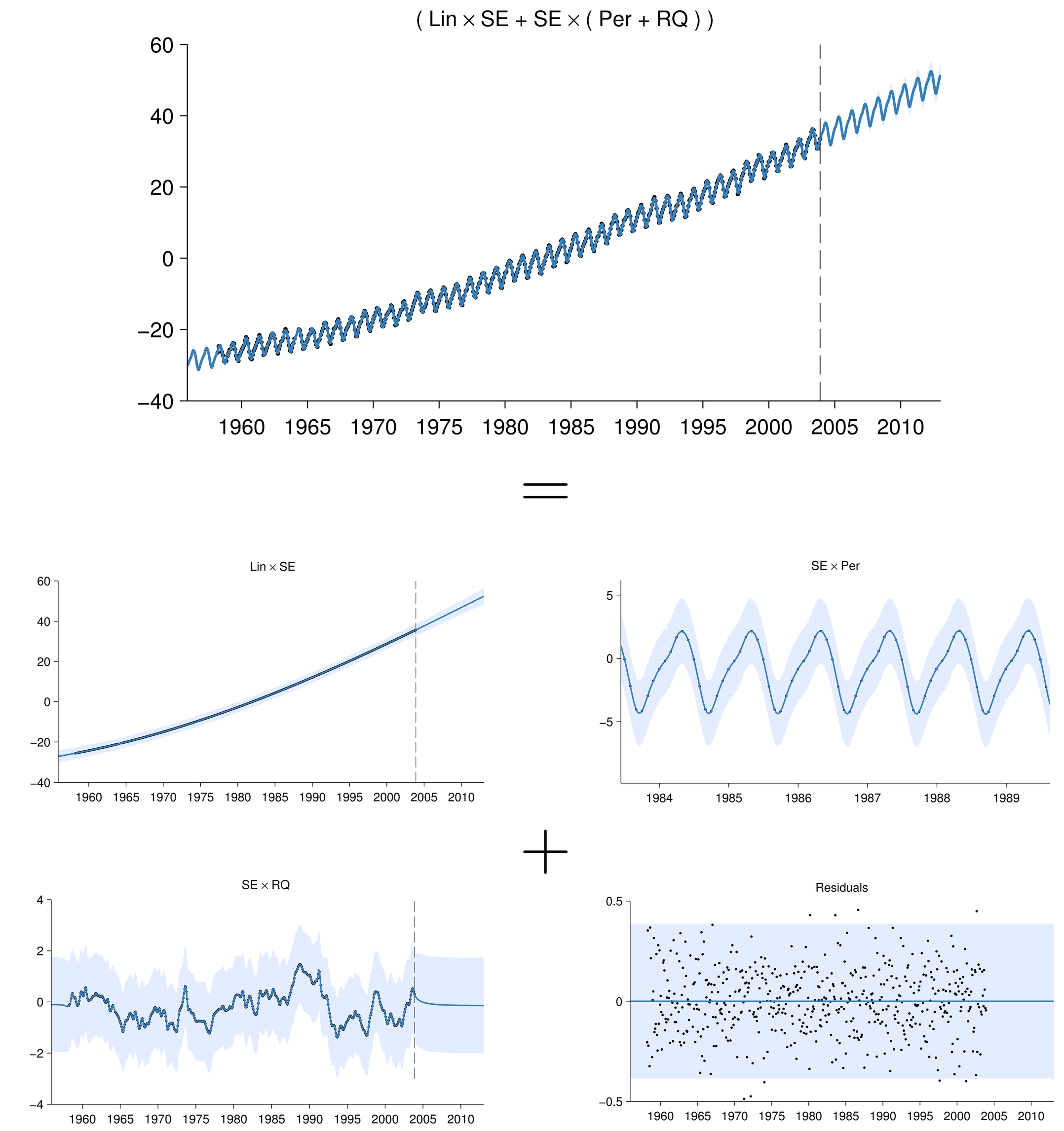
- We try all base kernels, selecting the one with the highest (approximate) marginal likelihood which balances data fit and model complexity
- The search continues by adding an extra term to the current best kernel, stopping when marginal likelihood no longer improves





Example: Mauna Loa CO_2 concentration

- By automatically inferring an appropriate kernel, we can also automatically decompose functions into additive components (additive components of the kernel correspond to independent additive functions)



Example: International airline passengers