Structure Discovery in Nonparametric Regression through Compositional Kernel Search

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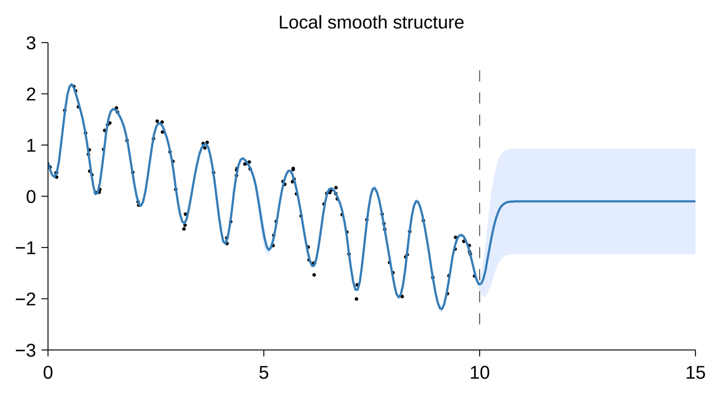
Identifying structure is crucial for extrapolation

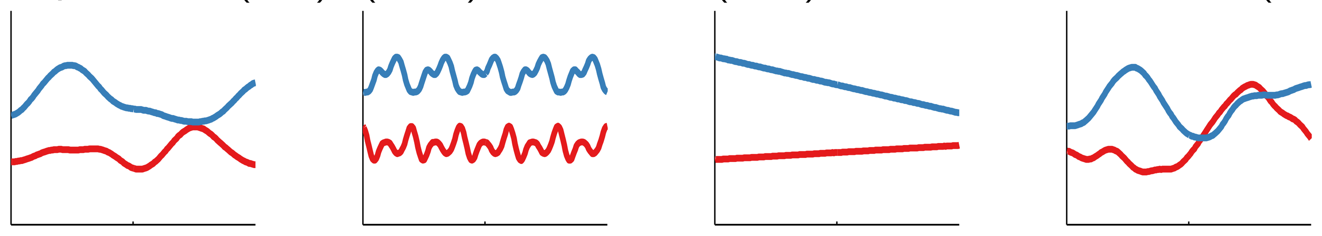


- Traditionally, a statistician proposes an appropriate model for the type of structures present
- Automatic model selection techniques already exist, typically choosing between a finite or restricted set of models
- Instead, we automate statistical model *construction*

Gaussian processes model structure through kernels

- The kernel specifies which structures are likely under the GP prior, which in turn determines the generalization properties of the model.
- Below we list standard base kernels, and draws from the corresponding GP priors:

Squared Exponential (SE) | Periodic (PER) | Linear (LIN) | Rational Quadratic (RQ)

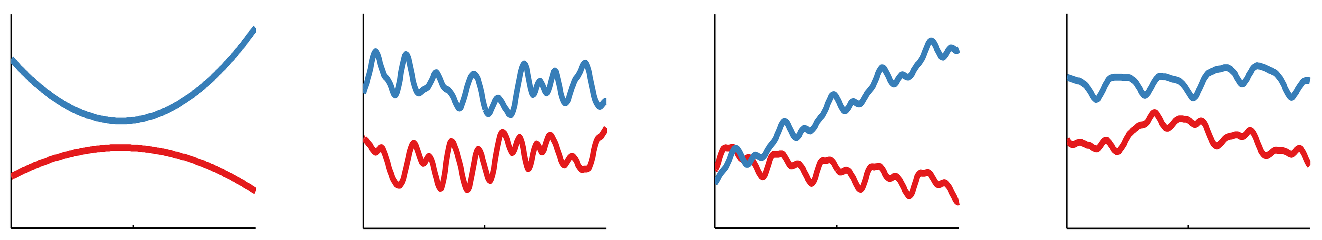


local variation | repeating structure | linear functions | multiscale variation

Kernels can be Composed

- Constructing appropriate composite kernels has previously been done by experts

LIN × LIN | SE × PER | LIN + PER | SE + PER



quadratic functions | locally periodic | periodic with trend | periodic with noise

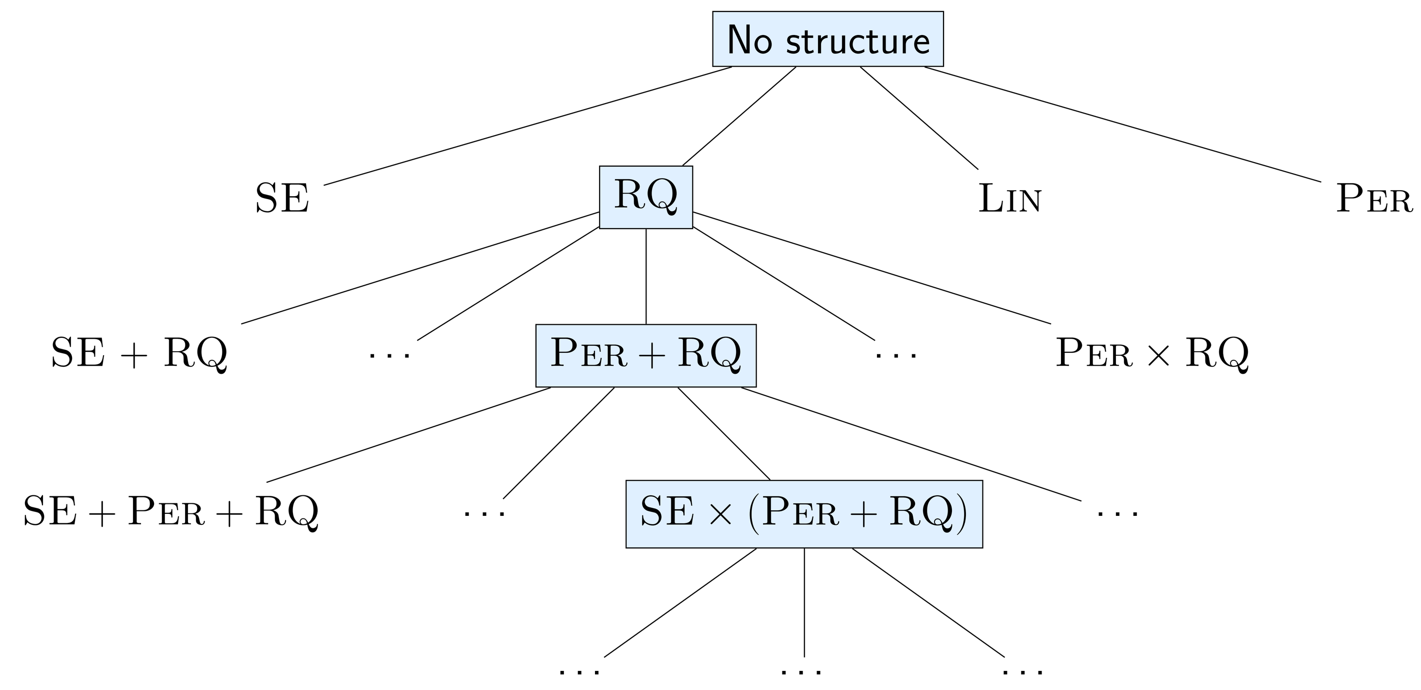
. . . defining an open-ended set of structures

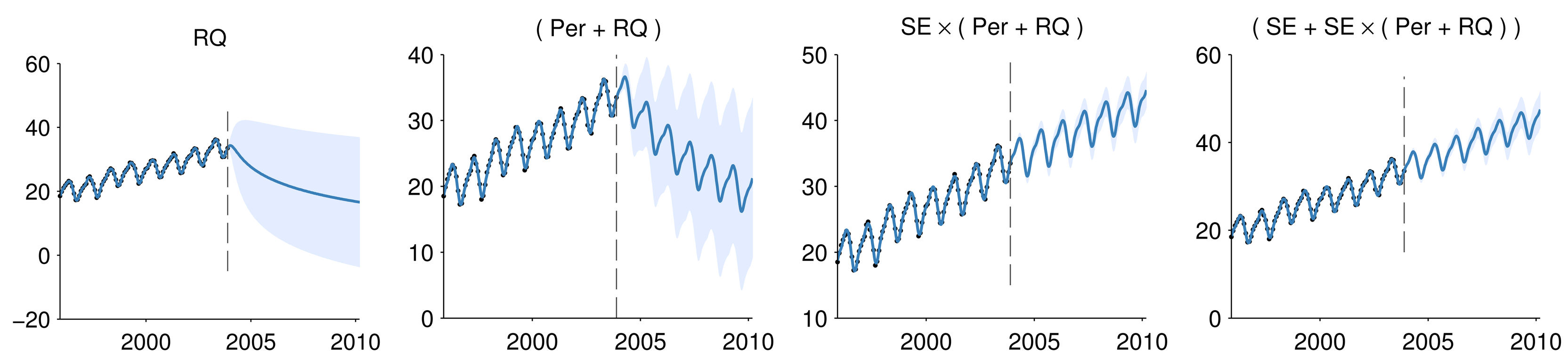
- We consider all algebraic expressions involving a small number of base kernels and the operations '+' and '×', including e.g.

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 local deviations	LIN + SE
Linearly growing amplitude	LIN × SE

. . . by a greedy search

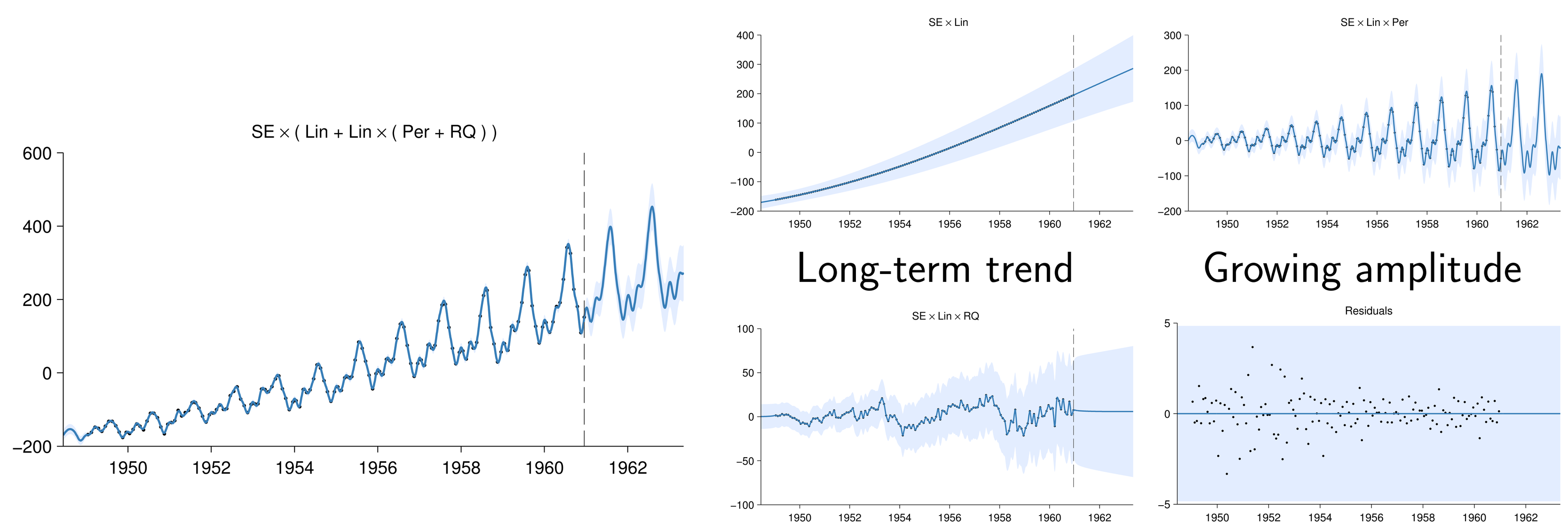
- We try all base kernels, selecting the one with the highest (approximate) marginal likelihood which balances data fit and model complexity
- The search continues by adding an extra term to the current best kernel, stopping when marginal likelihood no longer improves





Compound Kernels are Interpretable

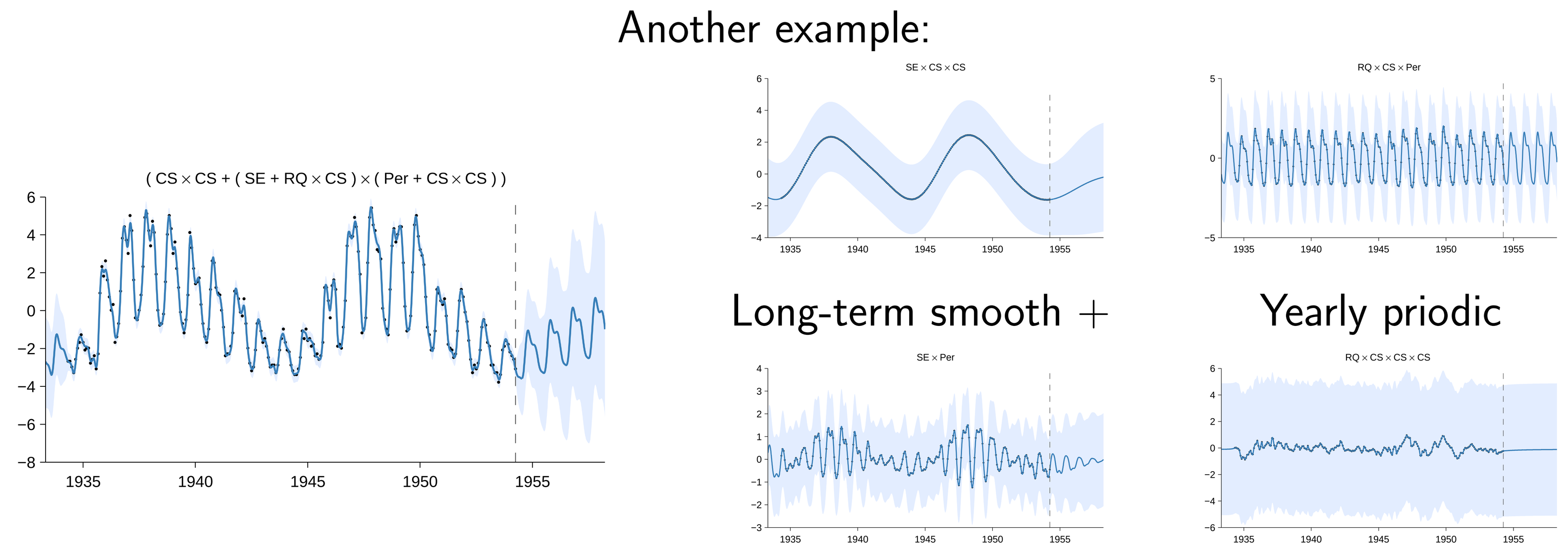
- Compound kernels decompose functions into additive components



Long-term trend | Growing amplitude

Short-term deviatinos | noise

Another example:



Long-term smooth + | Yearly priodic

Long-term amlpitude + | Short-term noise