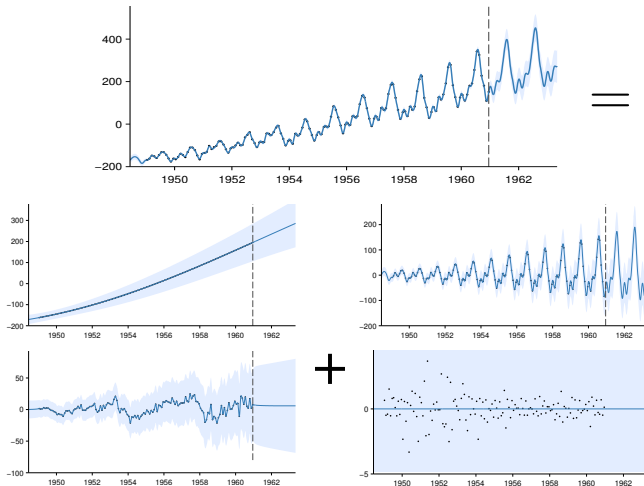
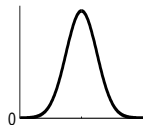


Structure Discovery in Nonparametric Regression through Compositional Kernel Search

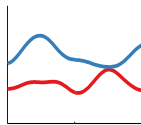


David Duvenaud, James Robert Lloyd, Roger Grosse,
Joshua B. Tenenbaum, Zoubin Ghahramani

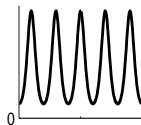
KERNEL CHOICE IS IMPORTANT



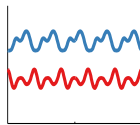
Squared-exp
(SE)



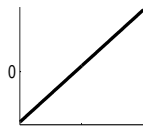
local
variation



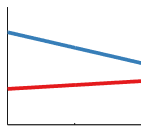
Periodic
(PER)



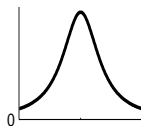
repeating
structure



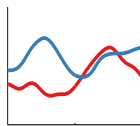
Linear (LIN)



linear
functions

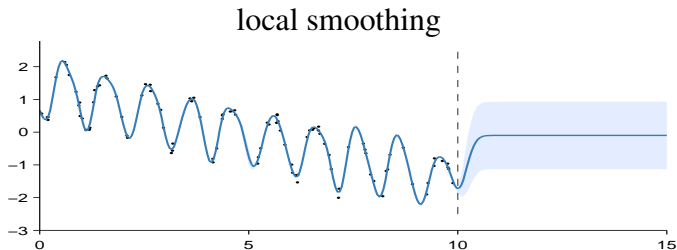


Rational-
quadratic(RQ)

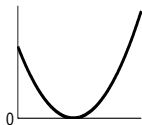


multi-scale
variation

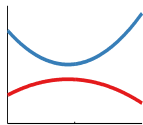
IDENTIFYING STRUCTURE IS CRUCIAL FOR EXTRAPOLATION



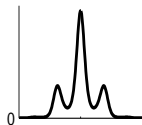
KERNELS CAN BE COMPOSED



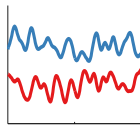
$\text{LIN} \times \text{LIN}$



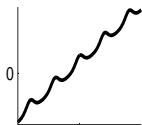
quadratic
functions



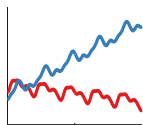
$\text{SE} \times \text{PER}$



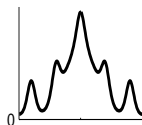
locally
periodic



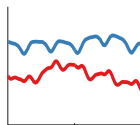
$\text{LIN} + \text{PER}$



periodic
with trend



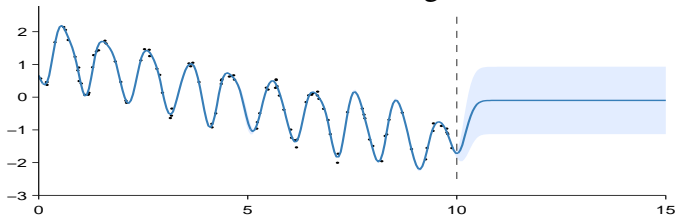
$\text{SE} + \text{PER}$



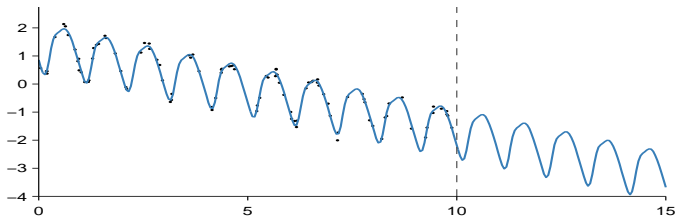
periodic
with noise

IDENTIFYING STRUCTURE IS CRUCIAL FOR EXTRAPOLATION

local smoothing



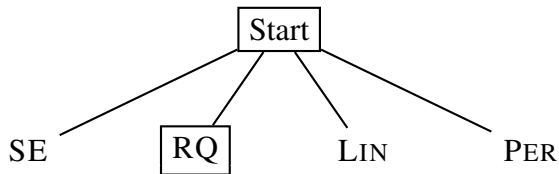
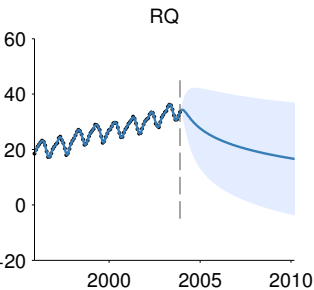
structured model



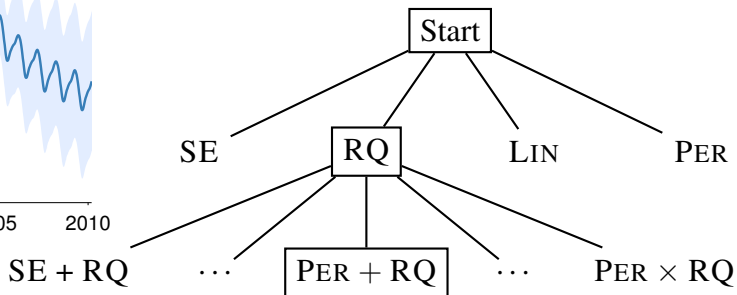
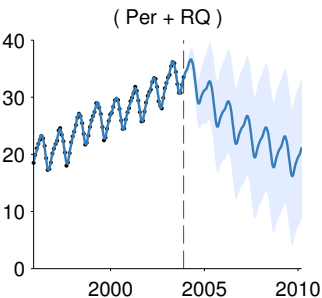
COMPOSITIONAL STRUCTURE SEARCH

- ▶ We define simple grammar over kernels:
 - ▶ $K \rightarrow K + K$
 - ▶ $K \rightarrow K \times K$
 - ▶ $K \rightarrow \text{SE} \mid \text{RQ} \mid \text{LIN} \mid \text{PER}$
- ▶ Can automatically search open-ended space of kernels by applying production rules, then checking model fit (approximate marginal likelihood).

COMPOSITIONAL STRUCTURE SEARCH

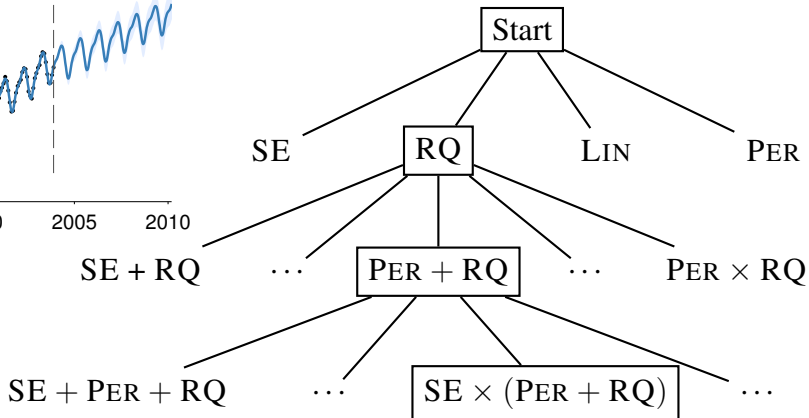
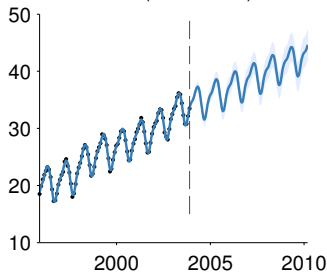


COMPOSITIONAL STRUCTURE SEARCH

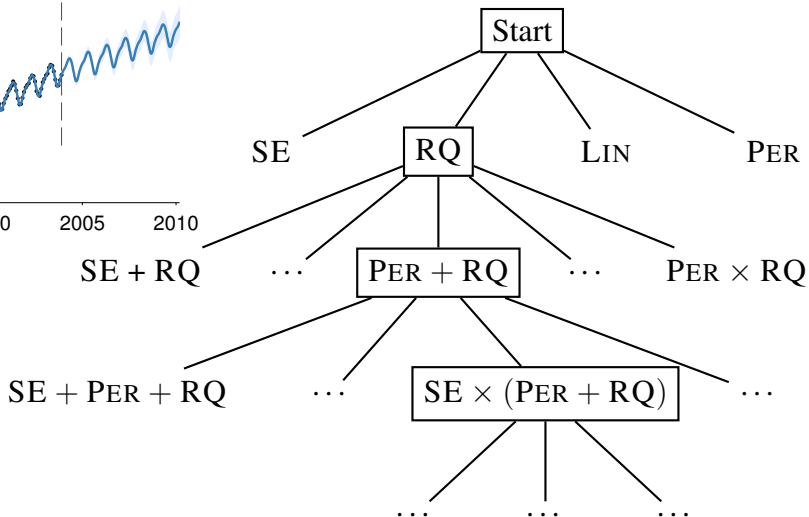
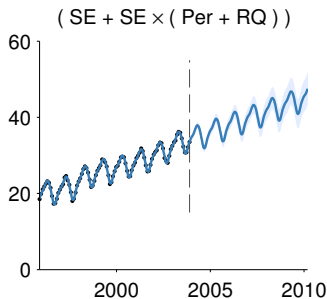


COMPOSITIONAL STRUCTURE SEARCH

$SE \times (Per + RQ)$

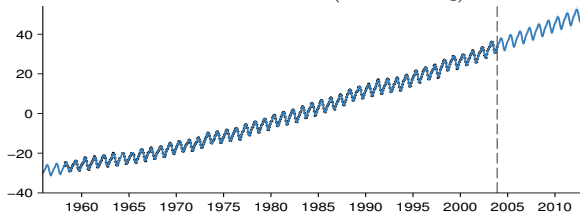


COMPOSITIONAL STRUCTURE SEARCH

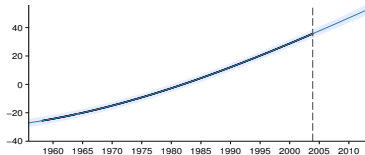


DECOMPOSING THE POSTERIOR

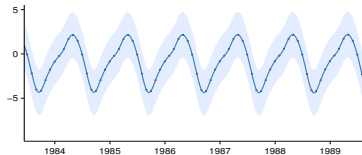
$$\text{LIN} \times \text{SE} + \text{SE} \times (\text{PER} + \text{RQ})$$



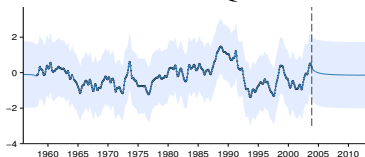
$\text{LIN} \times \text{SE}$



$\text{SE} \times \text{PER}$

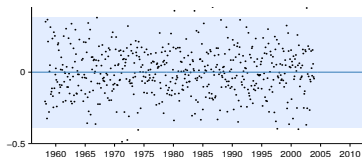


$\text{SE} \times \text{RQ}$



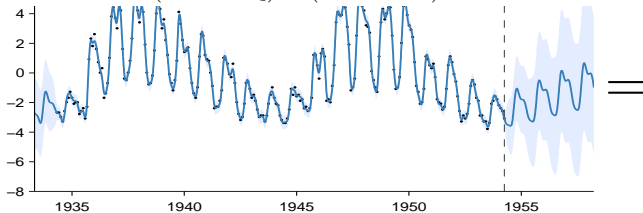
+

Residuals

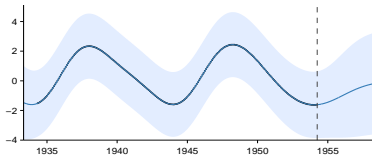


EXAMPLE: RADIO CRITICAL FREQUENCY

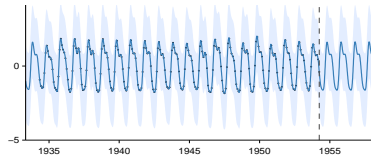
$$(\text{SE} + \text{RQ}) \times (\text{PER} + \text{CS})$$



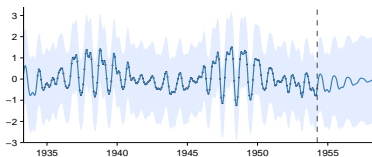
SE



PER \times RQ

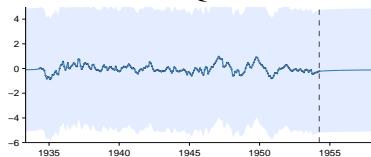


PER \times SE



+

RQ



AUTOMATED MODEL CONSTRUCTION

