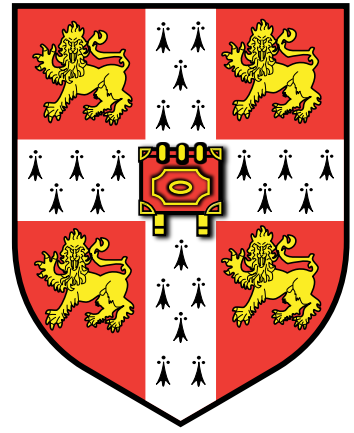
Automated Structure Discovery in Nonparametric Regression through Compositional Grammars



David Duvenaud

Cambridge University
Computational and Biological Learning Lab

April 24, 2013

OUTLINE

- Motivation
- Automated structure discovery in regression
  - Gaussian process regression
  - Structures expressible through kernel composition
  - A massive missing piece
  - grammar & search over models
  - Examples of structures discovered
- Takeaways

CREDIT WHERE CREDIT IS DUE

Talk based on:

- Structure Discovery in Nonparametric Regression through Compositional Kernel Search [ICML 2013]
  David Duvenaud, James Robert Lloyd, Roger Grosse,
  Joshua B. Tenenbaum, Zoubin Ghahramani

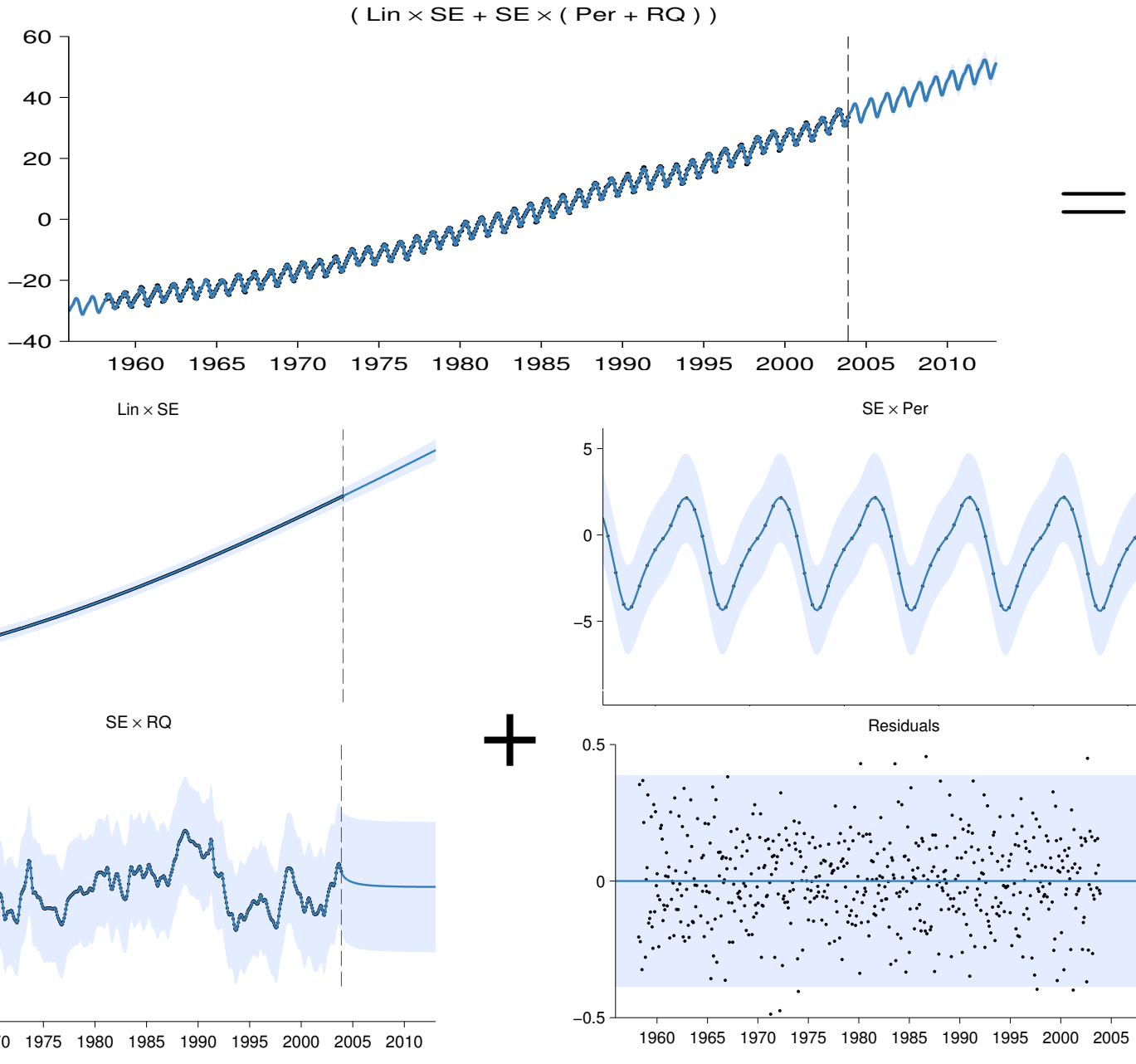
Compositional model building idea from:

- Exploiting compositionality to explore a large space of model structures [UAI 2012]
  Roger B. Grosse, Ruslan Salakhutdinov,
  William T. Freeman, Joshua B. Tenenbaum

Motivation

- Models today built by hand, or chosen from a fixed set.
  - Fixed set sometimes not that rich
    - Just being nonparametric sometimes isn't good enough
    - to learn efficiently, need to have a rich prior that can express most of the structure in your data.
  - Building by hand requires expertise, understanding of the dataset.
  - Follows cycle of: propose model, do inference, check model fit
    - Propose new model
    - Do inference
    - Check model fit
- Andrew Gelman asks: How would an AI do statistics?
- It would need a language for describing arbitrarily complicated models, a way to search over those models, nad a way of checking model fit.

Finding Structure in GP Regression



GAUSSIAN PROCESS REGRESSION

Assume $\mathbf{X}, \mathbf{y}$ is generated by $\mathbf{y} = \mathbf{f}(\mathbf{X}) + \epsilon_\sigma$
A GP prior over $\mathbf{f}$ means that, for any finite set of points $\mathbf{X}$,

$$p(\mathbf{f}(\mathbf{x})) = \mathcal{N}(\mu(\mathbf{X}), K(\mathbf{X}, \mathbf{X}))$$

where

$$K_{ij} = k(\mathbf{X}_i, \mathbf{X}_j)$$

is the *covariance function* or *kernel*. $k(x, x') = \text{cov}\left[f(x), f(x')\right]$

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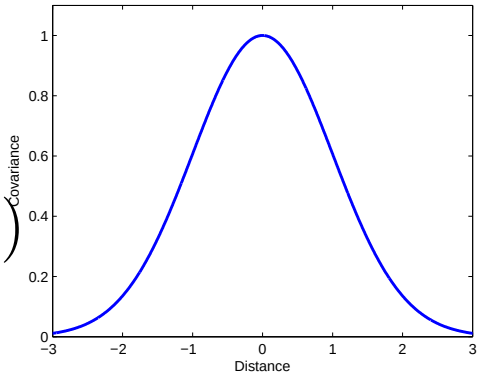
Typically, kernel says that nearby x_1, x_2 will have highly correlated function values $f(x_1), f(x_2)$:

$$k_{\text{SE}}(x, x') = \exp\left(-\frac{1}{2\theta}|x - x'|_2^2\right)$$



SAMPLING FROM A GP

```
function simple_gp_sample

    % Choose a set of x locations.
    N = 100;
    x = linspace( -2, 2, N);

    % Specify the covariance between function
   % values, depending on their location.
    for j = 1:N
        for k = 1:N
            sigma(j,k) = covariance( x(j), x(k) );
        end
    end

   % Specify that the prior mean of f is zero.
   mu = zeros(N, 1);

    % Sample from a multivariate Gaussian.
    f = mvnrnd( mu, sigma );

    plot(x, f);
end

% Squared-exp covariance function.
function k = covariance(x, y)
   k = exp( -0.5*( x - y )^2 );
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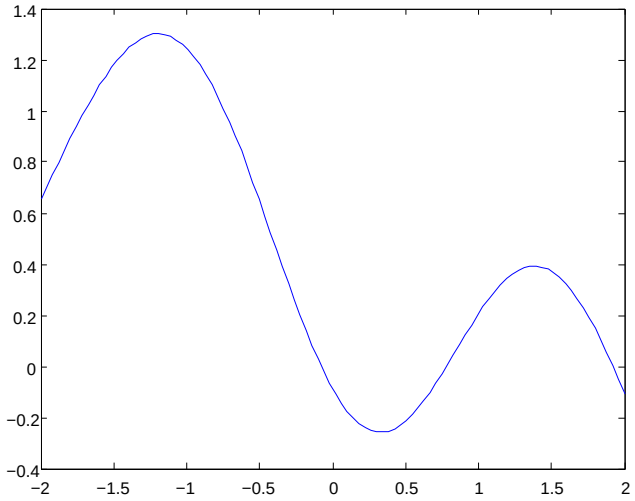

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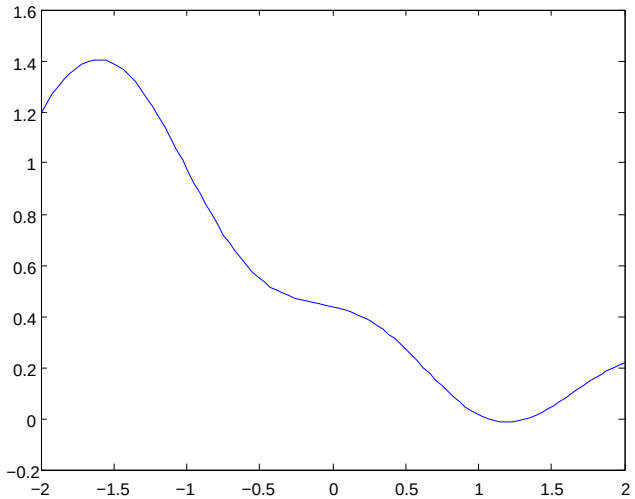

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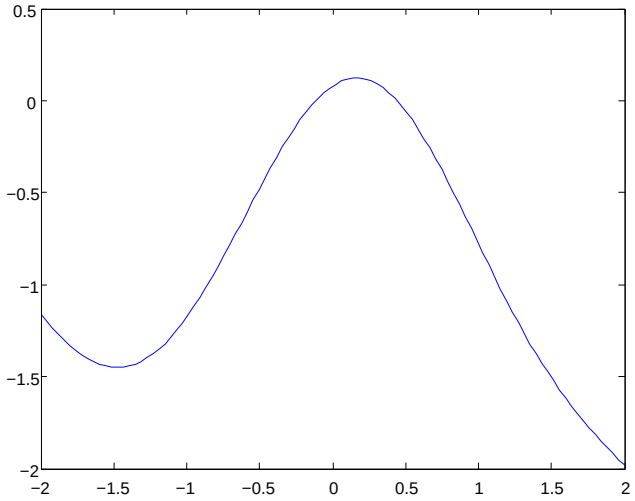

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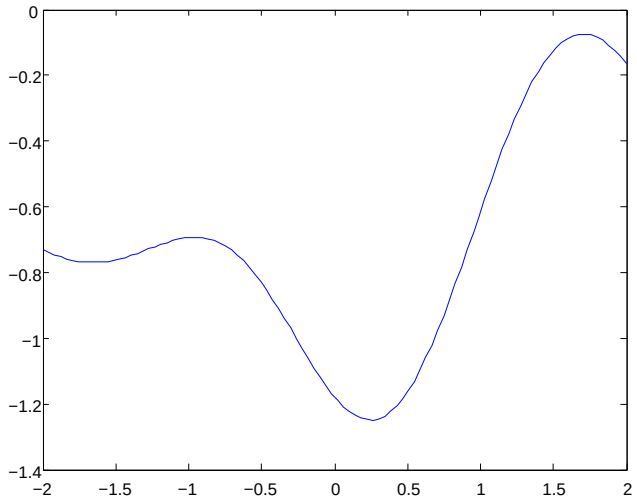

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% Periodic covariance function.
function c = covariance(x, y)
   c = exp( -0.5*( sin(( x - y )*1.5).^2 ));
end
```
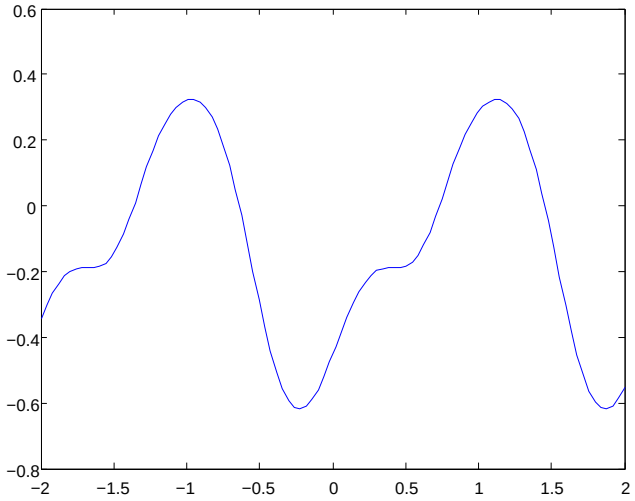
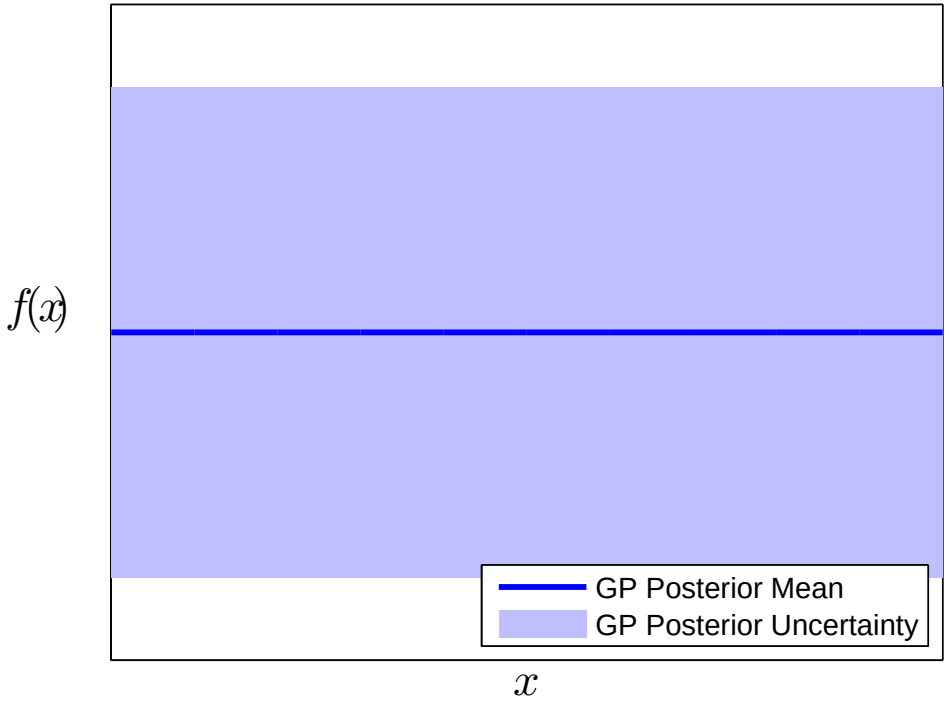



Conditional Posterior

$$f(x^*)|\mathbf{X}, \mathbf{y} \sim \mathcal{N}(k(x^*, \mathbf{X})K^{-1}\mathbf{y}, \\ k(x^*, x^*) - k(x^*, \mathbf{X})K^{-1}k(\mathbf{X}, x^*))$$

With SE kernel:



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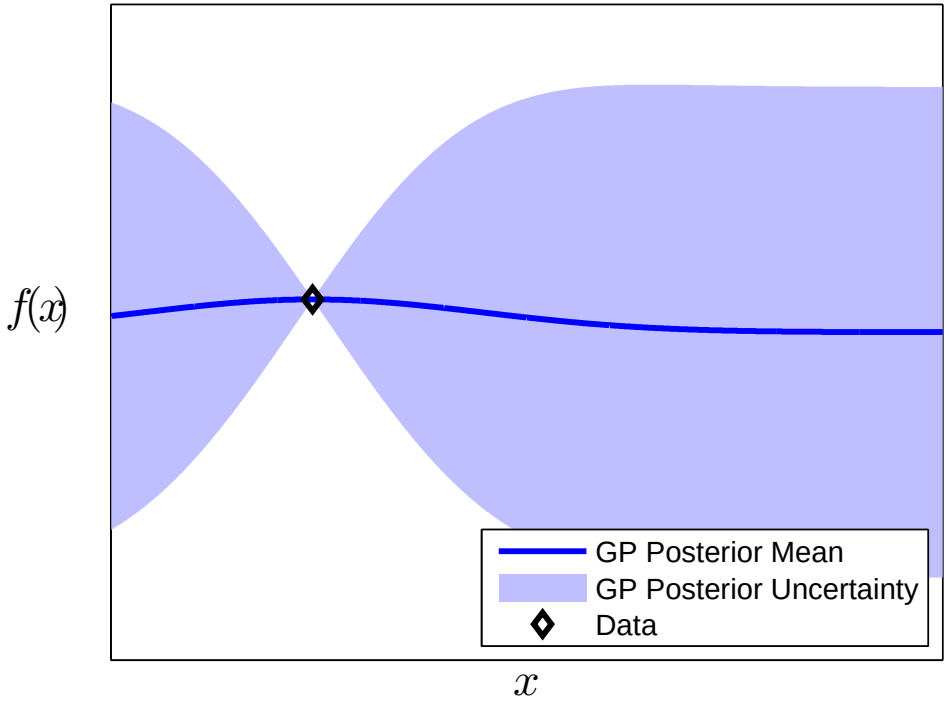

CONDITIONAL POSTERIOR

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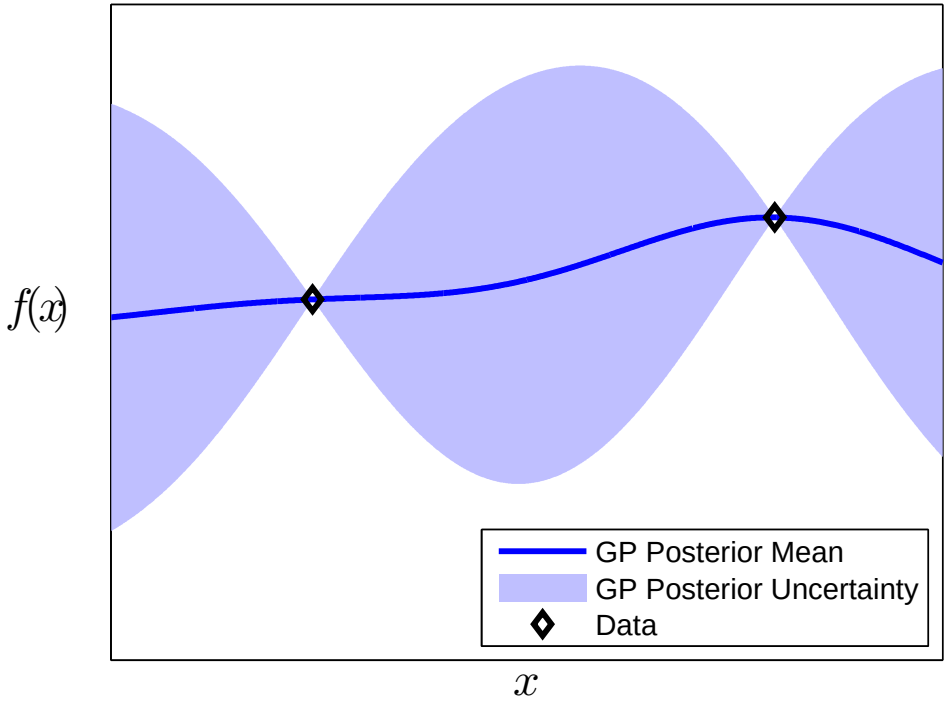

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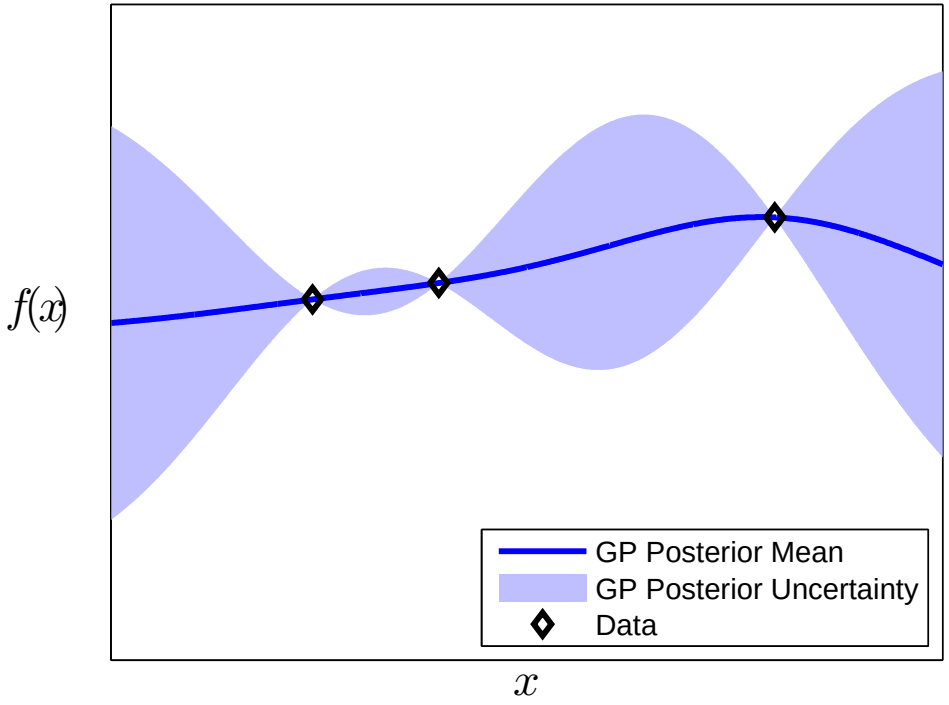

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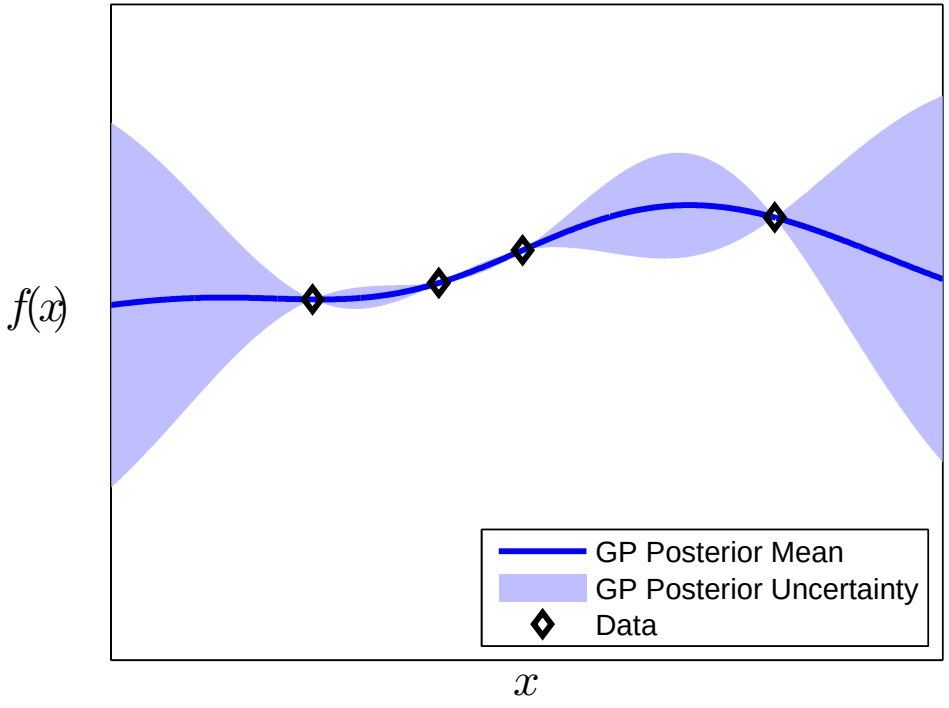
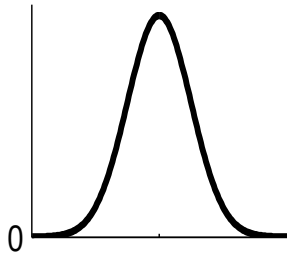
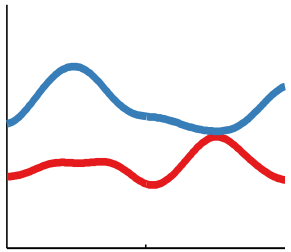


KERNEL CHOICE IS IMPORTANT

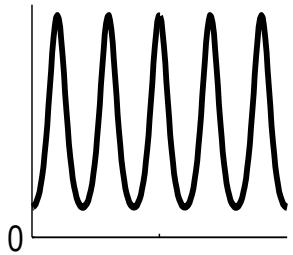
- Kernel determines almost all the properties of the prior.
- Many different kinds, with very different properties:



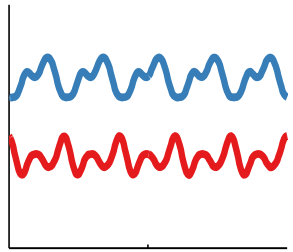
Squared-exp (SE)



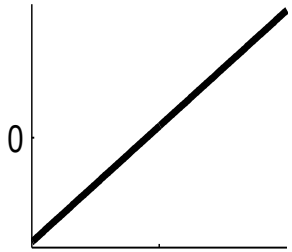
local variation



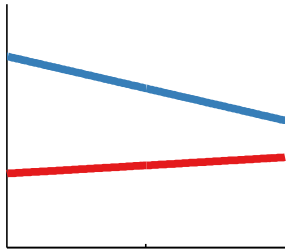
Periodic (PER)



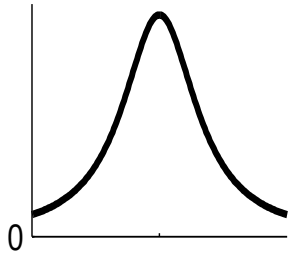
repeating structure



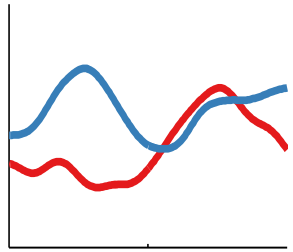
Linear (LIN)



linear functions



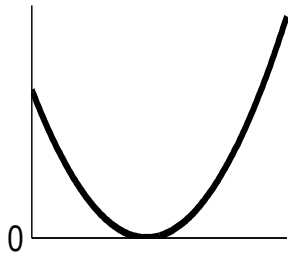
Rational-quadratic(RQ)



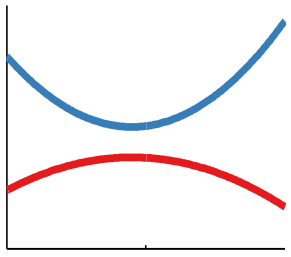
multi-scale variation

KERNELS CAN BE COMPOSED

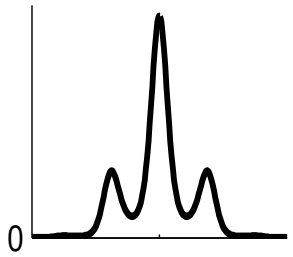
- Two main operations: adding, multiplying



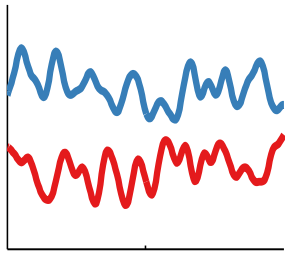
LIN × LIN



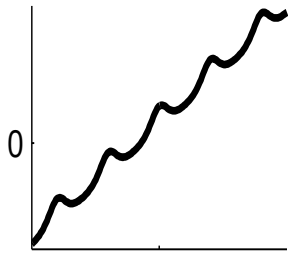
quadratic functions



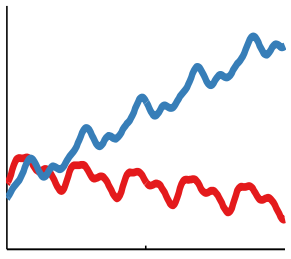
SE × PER



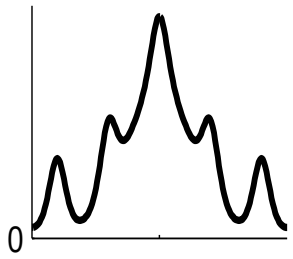
locally periodic



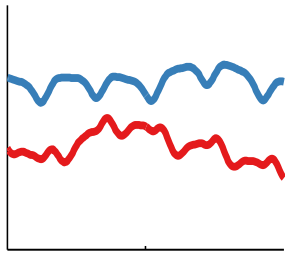
LIN + PER



periodic with trend



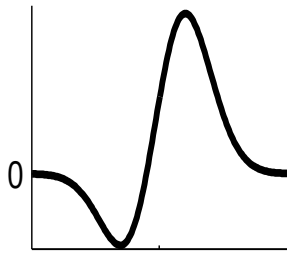
SE + PER



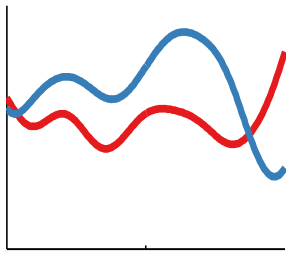
periodic with noise

KERNELS CAN BE COMPOSED

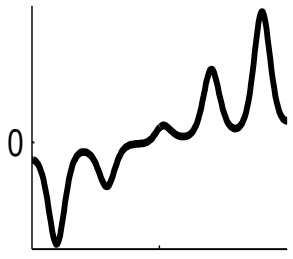
- Can be composed across multiple dimensions



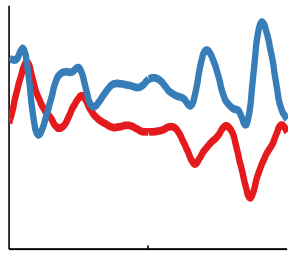
LIN × SE



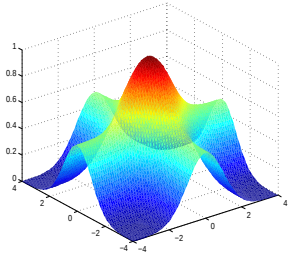
increasing variation



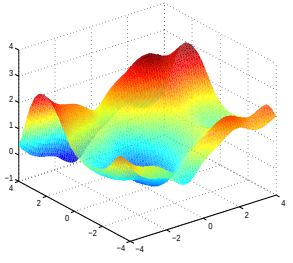
LIN × PER



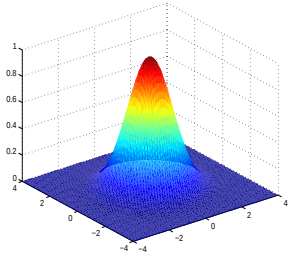
growing amplitude



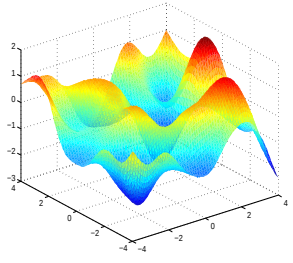
$\mathrm{SE}_1 + \mathrm{SE}_2$



$f_1(x_1) + f_2(x_2)$



$\mathrm{SE}_1 \times \mathrm{SE}_2$



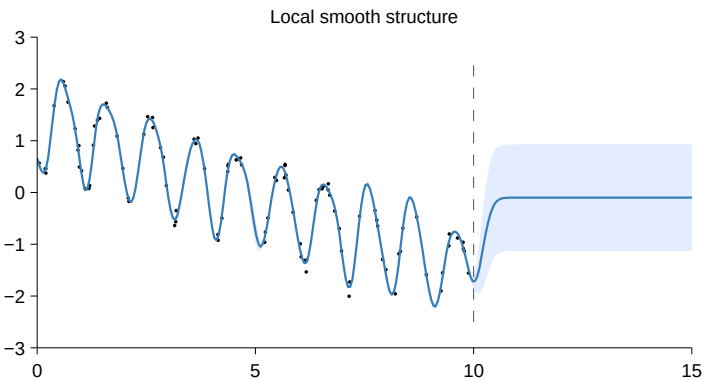
$f(x_1, x_2)$

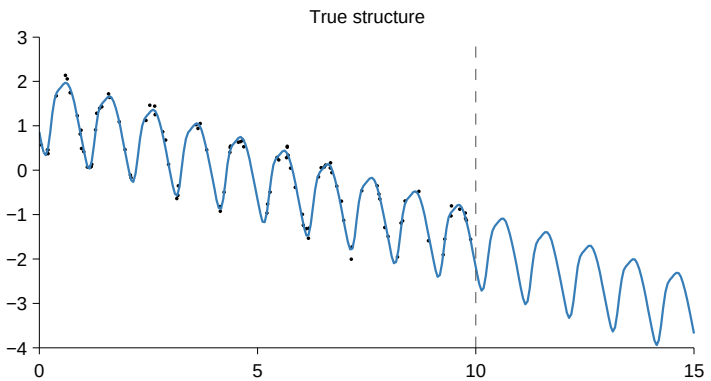
SPECIAL CASES

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

APPROPRIATE KERNELS ARE NECESSARY FOR EXTRAPOLATION

- SE kernel $\rightarrow$ basic smoothing.
- Richer kernels means richer structure can be captured.





KERNELS ARE HARD TO CHOOSE

- Given the diversity of priors available, how to choose one?
- Standard GP software packages include many base kernels and means to combine them, but *no default kernel*
- Software can't choose model for you, you're the expert (?)

KERNELS ARE HARD TO CONSTRUCT

- Carl devotes 4 pages of his book to constructing a custom kernel for CO2 data
- requires specialized knowledge, trial and error, and a dataset small and low-dimensional enough that a human can interpret it.
- In practice, most users can't or won't make custom kernel, and SE kernel became *de facto* standard kernel through inertia.

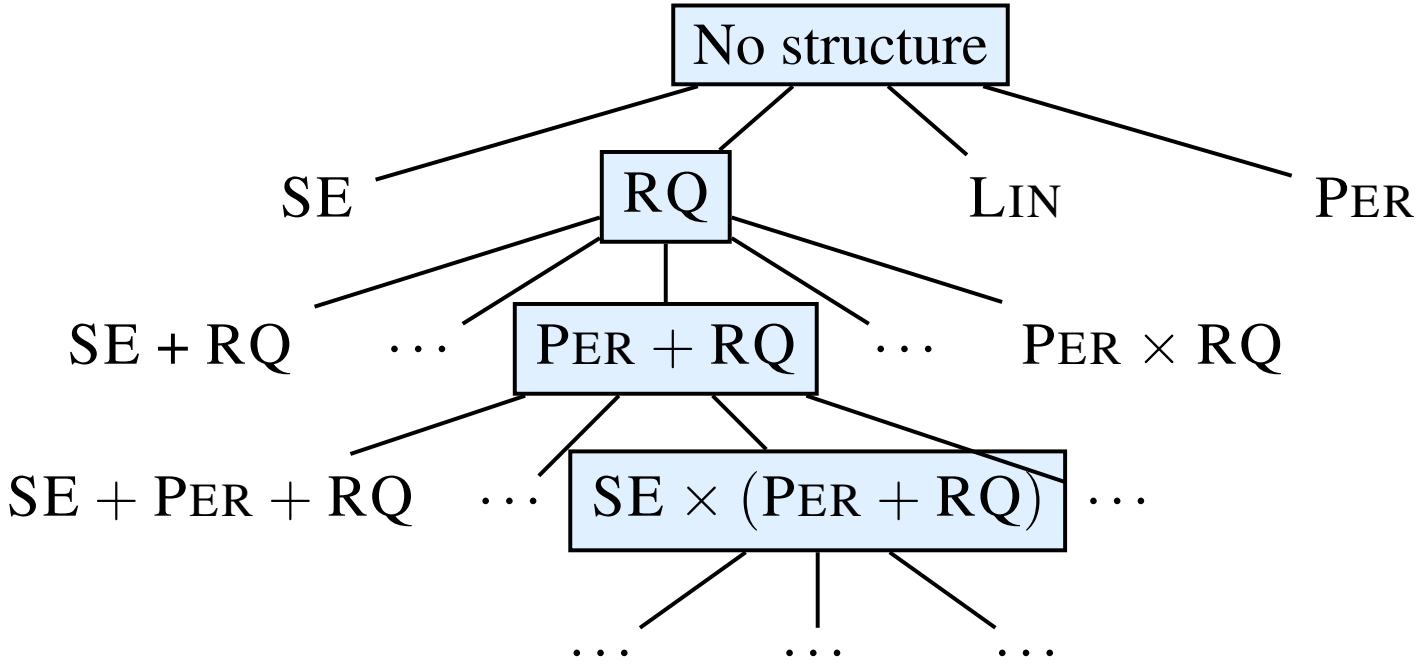
RECAP

- GP Regression is a powerful tool
- Kernel choice allows for rich structure to be captured - different kernels express very different model classes
- Composition generates a rich space of models
- Hard & slow to search by hand
- Can kernel specification be automated?

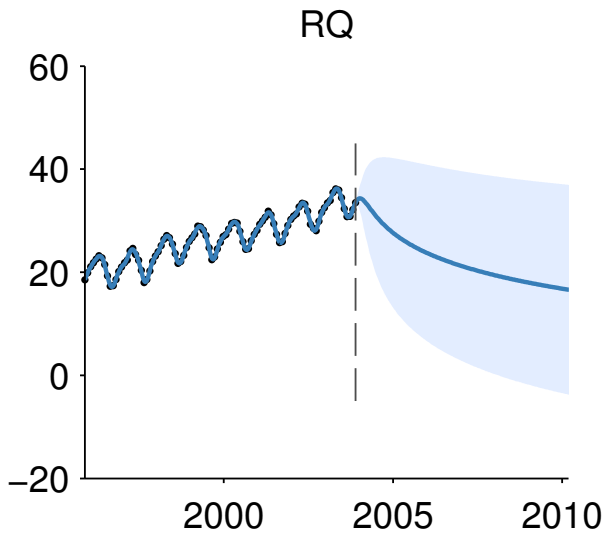
COMPOSITIONAL STRUCTURE SEARCH

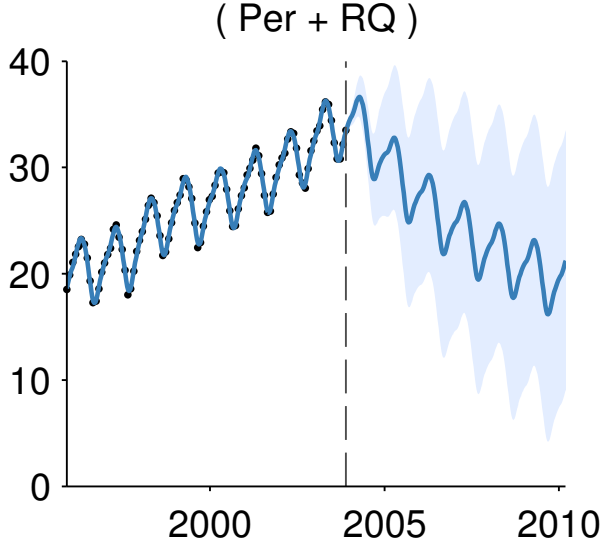
- Define grammar over kernels:
  - $K \to K + K$
  - $K \to K \times K$
  - $K \to \{\text{SE}, \text{RQ}, \text{LIN}, \text{PER}\}$
- Search the space of kernels greedily by applying production rules, checking model fit (approximate marginal likelihood).

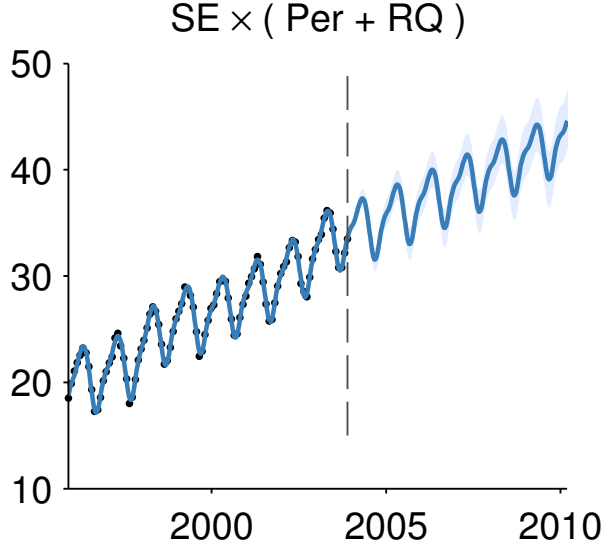
COMPOSITIONAL STRUCTURE SEARCH

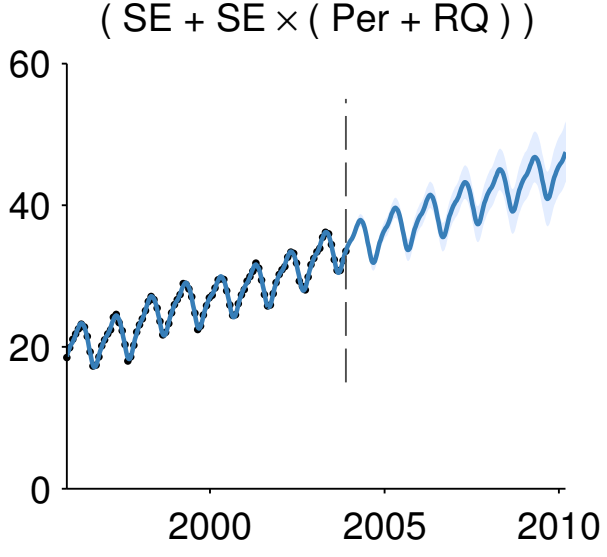


Example Search: Mauna Lua CO_2

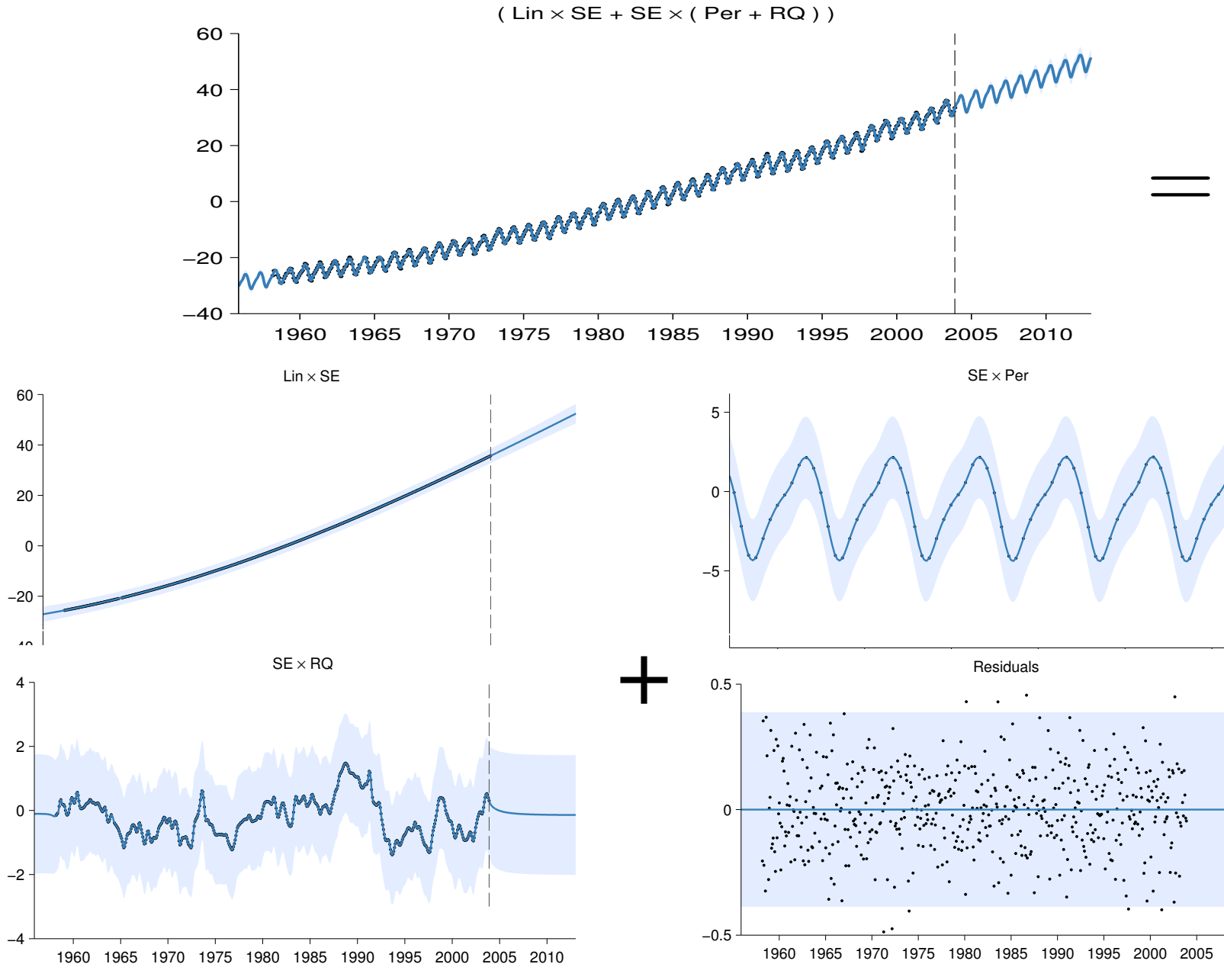








Example Decomposition: Mauna Loa CO_2



COMPOUND KERNELS ARE INTERPRETABLE

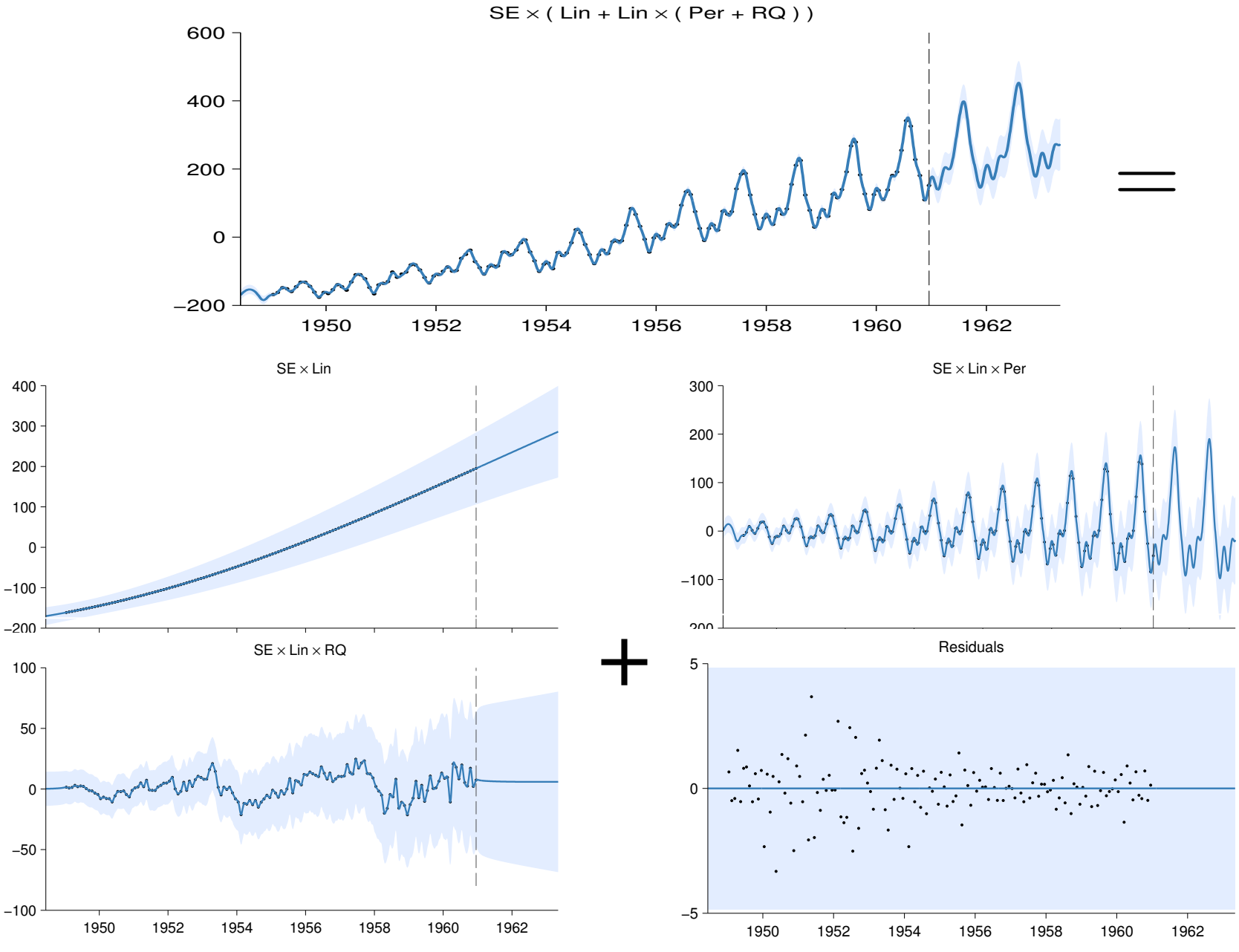
Suppose functions f_1, f_2 are draw from independent GP priors, $f_1 \sim \mathcal{GP}(\mu_1, k_1), f_2 \sim \mathcal{GP}(\mu_2, k_2)$. Then it follows that

$$f := f_1 + f_2 \sim \mathcal{GP}(\mu_1 + \mu_2, k_1 + k_2)$$

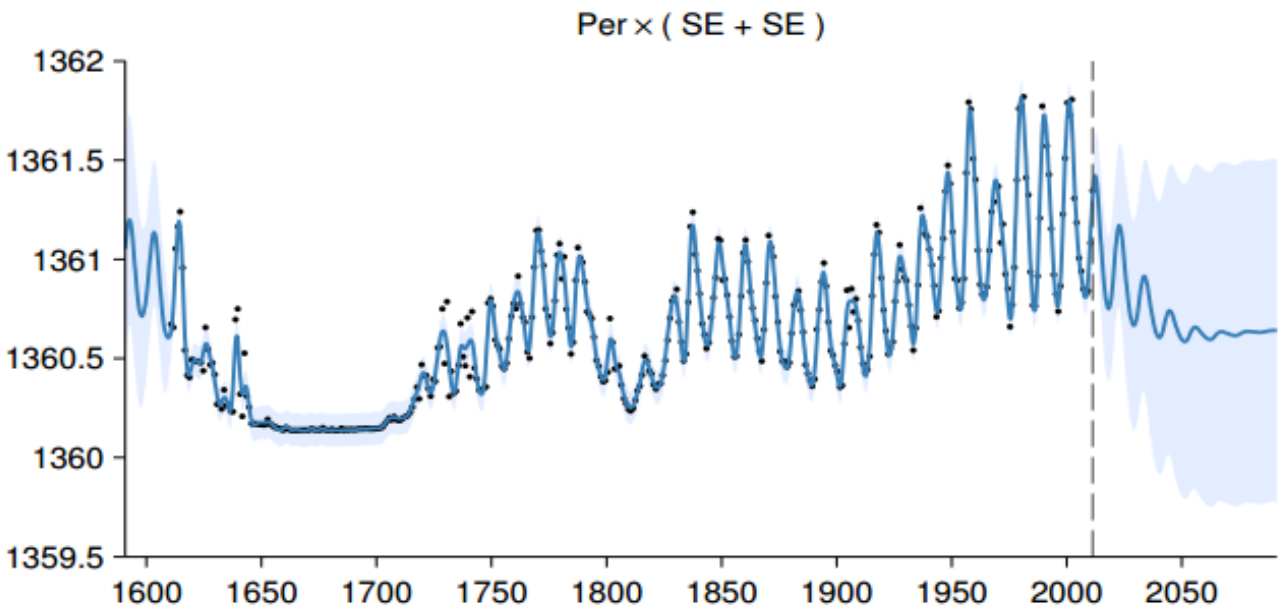
Sum of kernels is equivalent to sum of functions. Distributivity means we can write compound kernels as sums of products of base kernels:

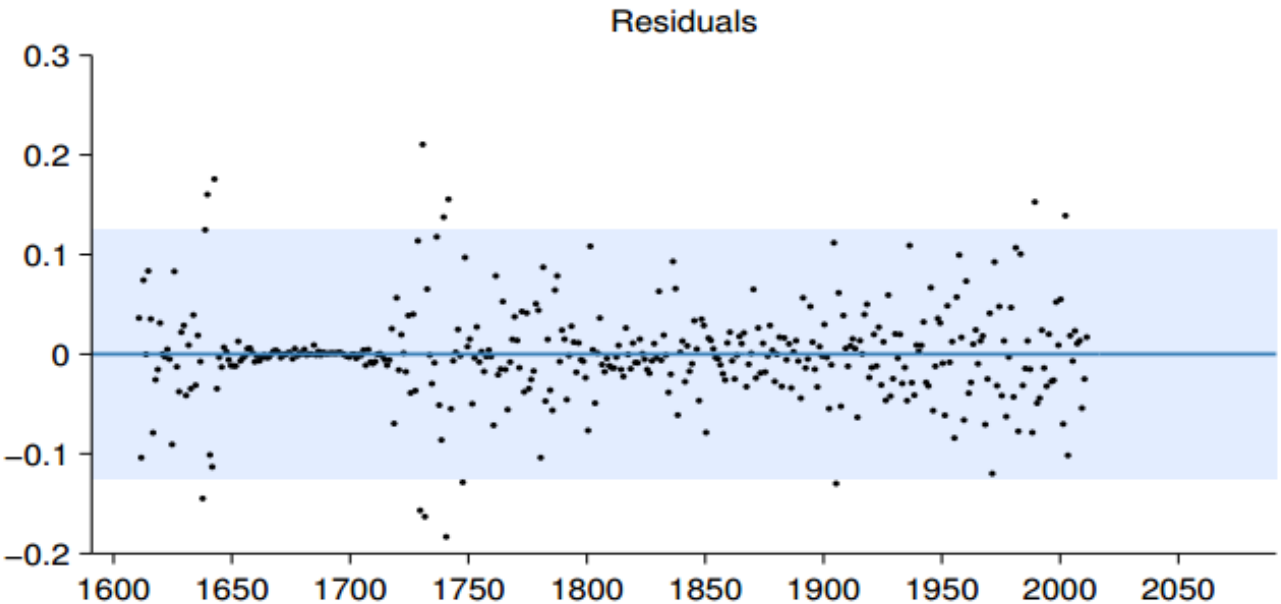
$$\text{SE} \times (\text{RQ} + \text{LIN}) = \text{SE} \times \text{RQ} + \text{SE} \times \text{LIN}.$$

Example Decomposition: Airline



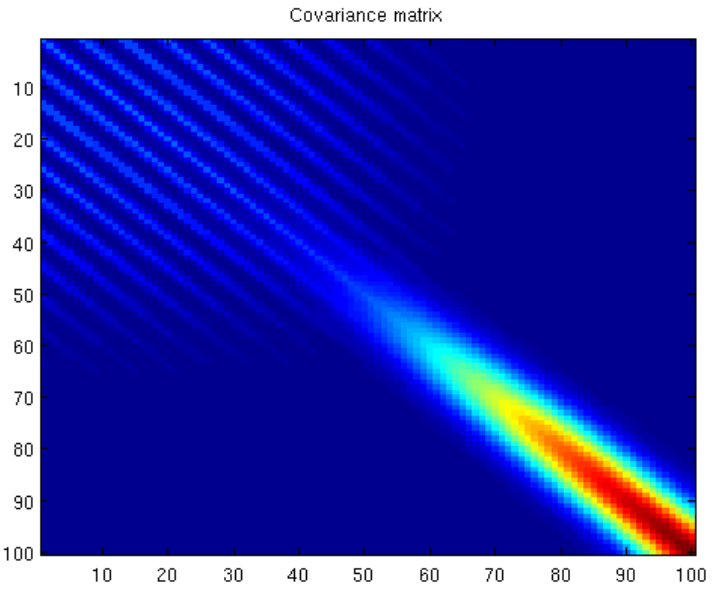
EXAMPLE: SUNSPOTS

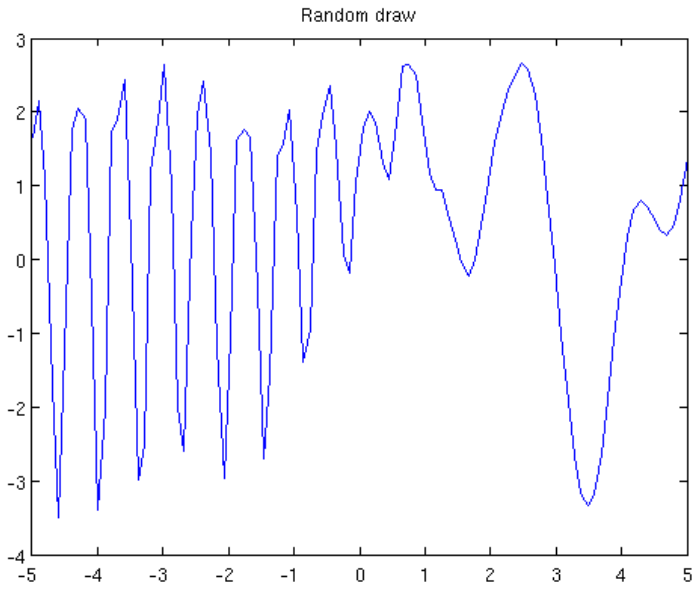




CHANGEPOINT KERNEL

Can express change in covariance:

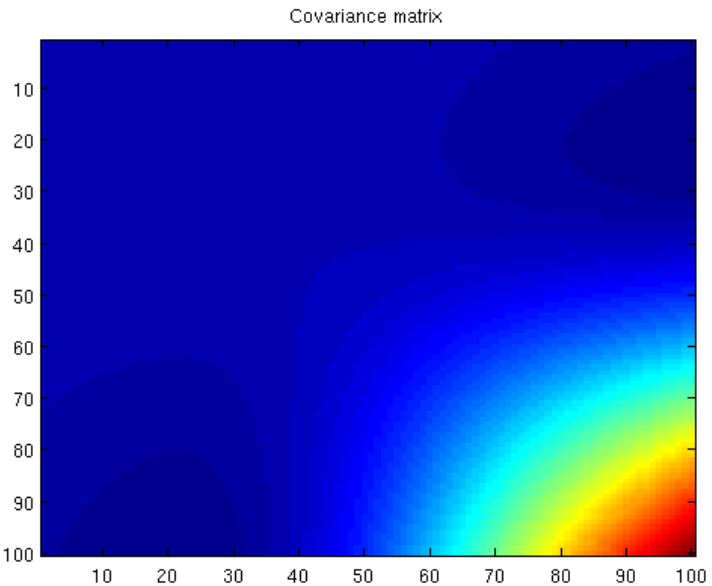


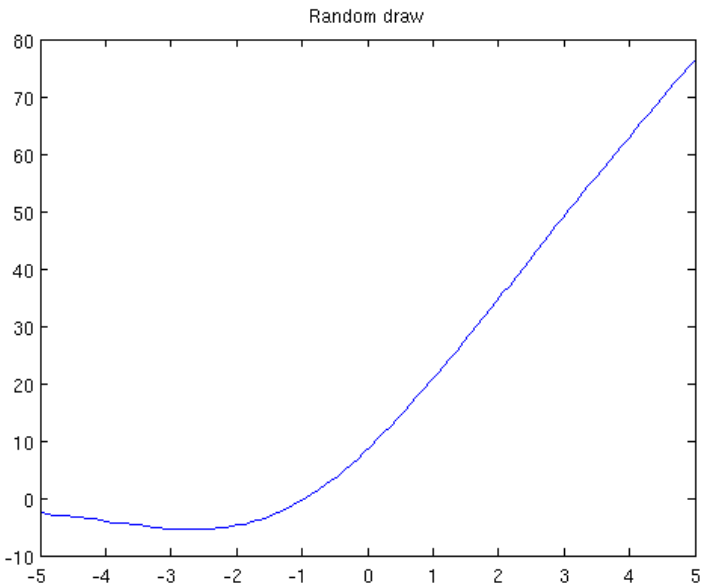


Periodic changing to SE

CHANGEPOINT KERNEL

Can express change in covariance:





SE changing to linear

SUMMARY

- Choosing form of kernel is currently done by hand.
- Compositions of kernels lead to more interesting priors on functions than typically considered.
- A simple grammar specifies all such compositions, and can be searched over automatically.
- Composite kernels lead to interpretable decompositions.

Conclusions

More generally...

- Model-building is currently done mostly by hand.
- Grammars over composite structures are a simple way to specify open-ended model classes.
- Composite structures often imply interpretable decompositions of the data.
- Searching over these model classes is a step towards automating statistical analysis.

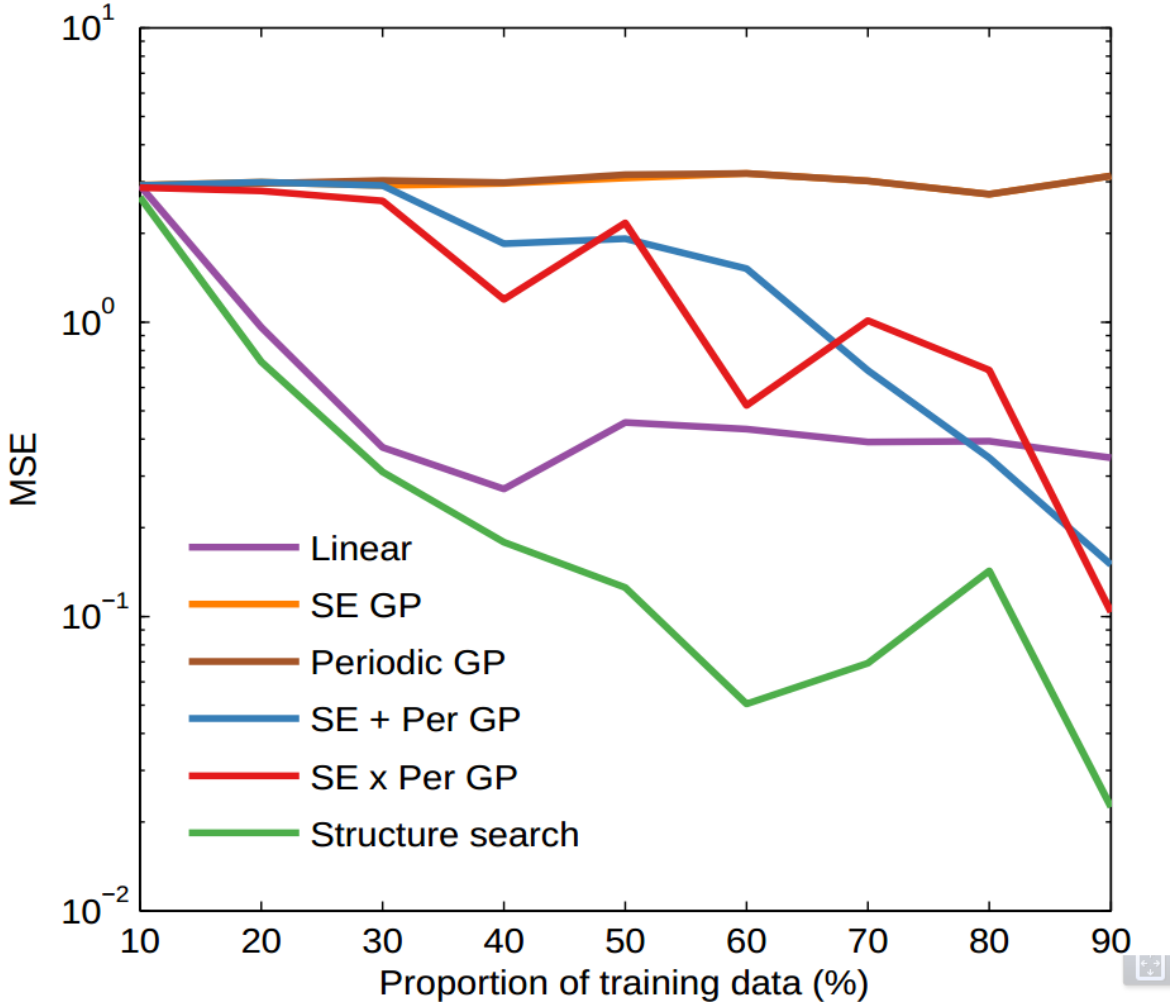
Thanks!

Related Work

(Slide from Roger Grosse)

- Algorithmic information theory, e.g. Solomonoff induction (Solomonoff, 1964)
- Structure learning in other domains
  - Bayesian networks (e.g. Teyssier and Koller, 2005)
  - Markov random fields (e.g. Lee et al., 2006)
- Learning the form of graph embeddings (Kemp and Tenenbaum, 2008)
- Equation discovery
  - BACON knowledge discovery engine (Langley, Simon, and Bradshaw, 1984)
  - exploiting context-free grammar (Todorovski and Dzeroski, 1997)
- Matrix factorization frameworks
  - Exponential family PCA (Collins et al., 2002)
  - Roweis and Ghahramani (1999)
  - Singh and Gordon (2008)

EXTRAPOLATION



Multi-D Interpolation

Method	Mean Squared Error (MSE)				
	bach	concrete	puma	servo	housing
Linear Regression	1.031	0.404	0.641	0.523	0.289
GAM	1.259	0.149	0.598	0.281	0.161
HKL	**0.199**	0.147	0.346	0.199	0.151
GP SE-ARD	**0.045**	0.157	0.317	0.126	**0.092**
GP Additive	**0.045**	**0.089**	**0.316**	**0.110**	0.102
Structure Search	**0.044**	**0.087**	**0.315**	**0.102**	**0.082**