

How to build an automatic statistician



James Robert Lloyd¹, David Duvenaud¹, Roger Grosse²,



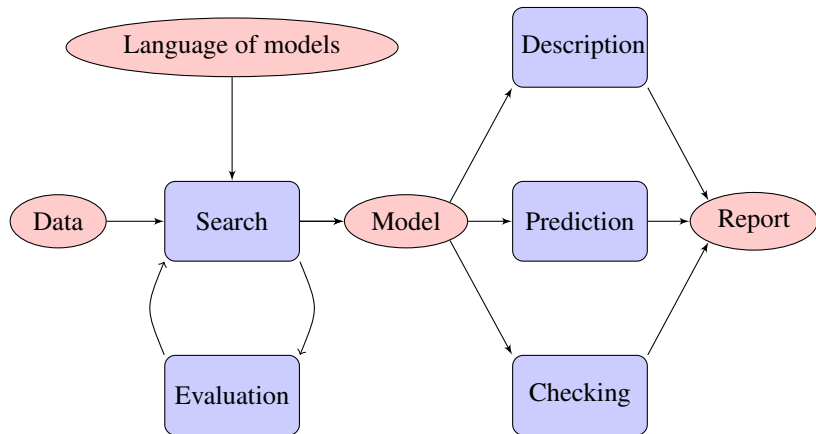
Joshua Tenenbaum², Zoubin Ghahramani¹

1: Department of Engineering, University of Cambridge, UK

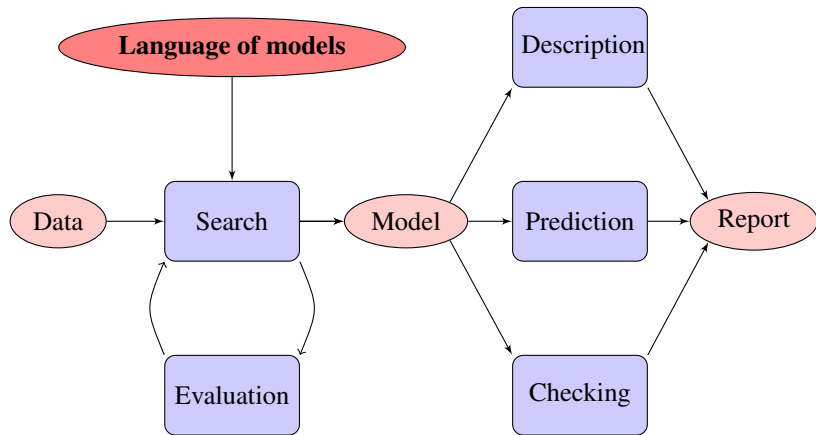
2: Massachusetts Institute of Technology, USA

August 8, 2014

A SYSTEM FOR AUTOMATIC DATA ANALYSIS

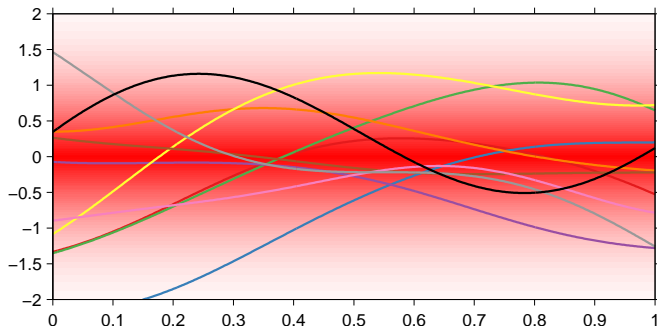


DEFINING A LANGUAGE OF MODELS



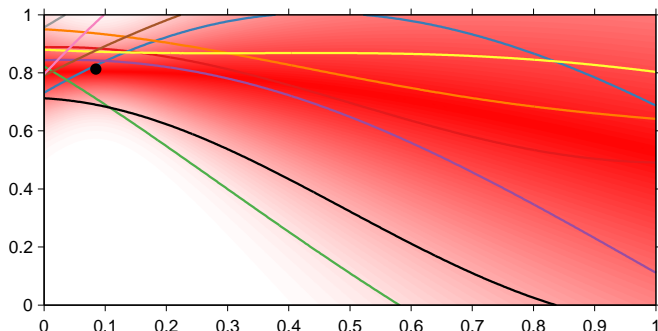
GAUSSIAN PROCESS REGRESSION

We can use Gaussian processes to place priors on functions and perform a Bayesian regression analysis



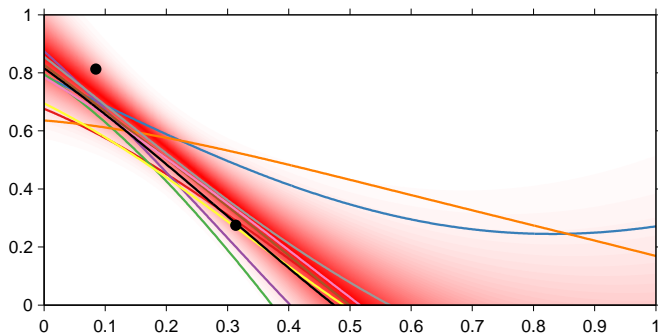
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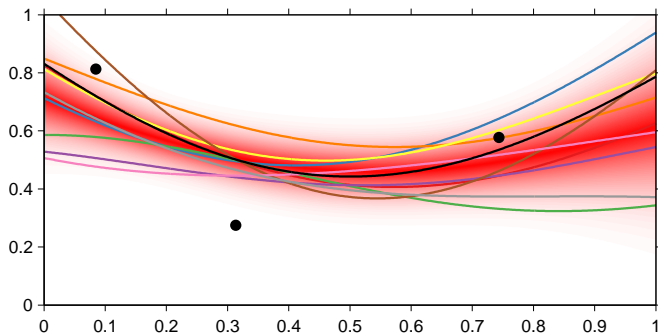
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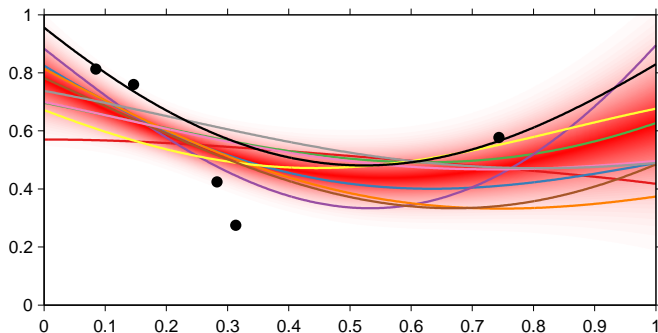
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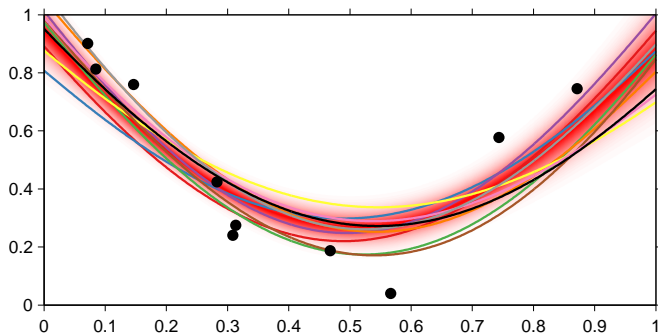
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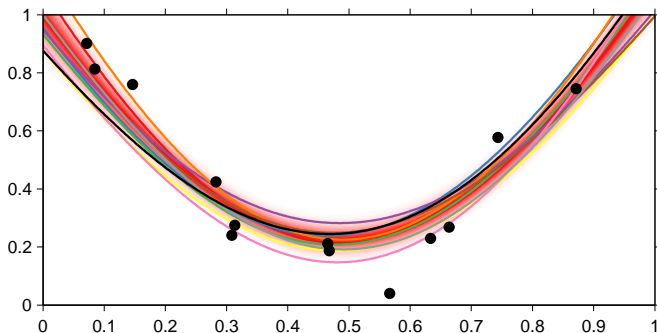
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THE ATOMS OF OUR LANGUAGE

Five base kernels



Squared
exp. (SE)



Periodic
(PER)



Linear
(LIN)



Constant
(C)



White
noise (WN)

Encoding for the following types of functions



Smooth
functions



Periodic
functions



Linear
functions



Constant
functions

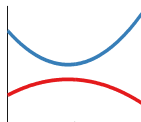


Gaussian
noise

THE COMPOSITION RULES OF OUR LANGUAGE

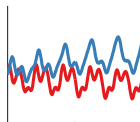
- ▶ Two main operations: addition, multiplication

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



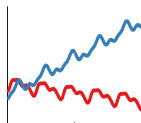
quadratic
functions

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



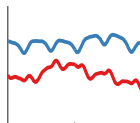
locally
periodic

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



periodic plus
linear trend

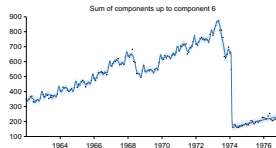
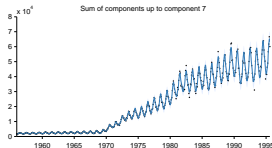
$\text{SE} + \text{PER}$



periodic plus
smooth trend

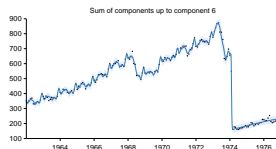
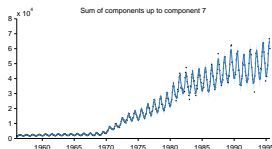
MODELING CHANGEPOINTS

Time series data often exhibit changepoints:



MODELING CHANGEPOINTS

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We can model this by assuming $f_1(x) \sim \text{GP}(0, k_1)$ and $f_2(x) \sim \text{GP}(0, k_2)$ and then defining

$$f(x) = (1 - \sigma(x))f_1(x) + \sigma(x)f_2(x)$$

where σ is a sigmoid function between 0 and 1.

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Then $f \sim \text{GP}(0, k)$, where

$$k(x, x') = (1 - \sigma(x))k_1(x, x')(1 - \sigma(x')) + \sigma(x)k_2(x, x')\sigma(x')$$

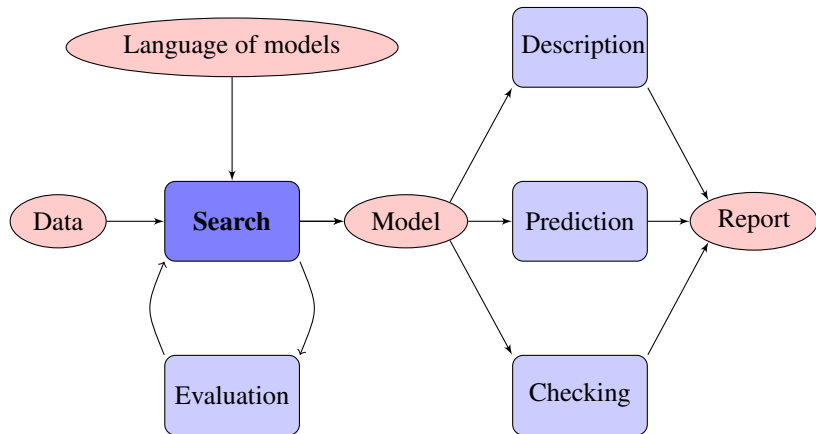
We define the changepoint operator $k = \text{CP}(k_1, k_2)$.

AN EXPRESSIVE LANGUAGE OF MODELS

Regression model	Kernel
GP smoothing	$SE + WN$
Linear regression	$C + LIN + WN$
Multiple kernel learning	$\sum SE + WN$
Trend, cyclical, irregular	$\sum SE + \sum PER + WN$
Fourier decomposition	$C + \sum \cos + WN$
Sparse spectrum GPs	$\sum \cos + WN$
Spectral mixture	$\sum SE \times \cos + WN$
Changepoints	e.g. $CP(SE, SE) + WN$
Heteroscedasticity	e.g. $SE + LIN \times WN$

Note: \cos is a special case of our version of PER

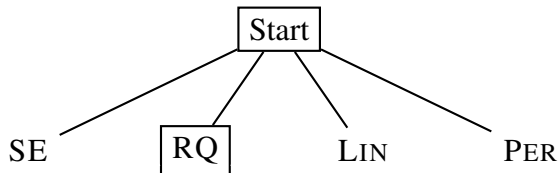
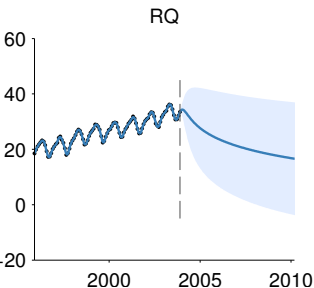
DISCOVERING A GOOD MODEL VIA SEARCH



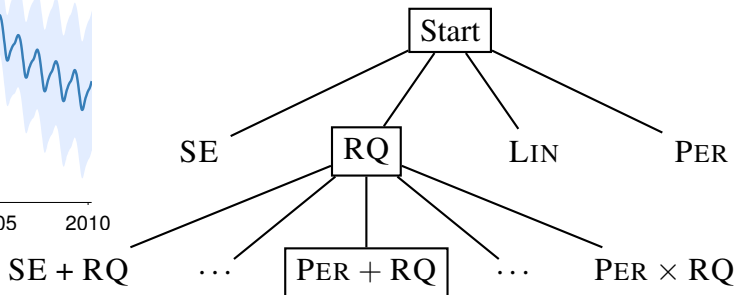
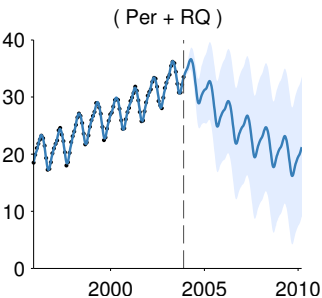
DISCOVERING A GOOD MODEL VIA SEARCH

- ▶ Language defined as the arbitrary composition of five base kernels (WN, C, LIN, SE, PER) via three operators ($+$, \times , CP).
- ▶ The space spanned by this language is open-ended and can have a high branching factor requiring a judicious search
- ▶ We propose a greedy search for its simplicity and similarity to human model-building

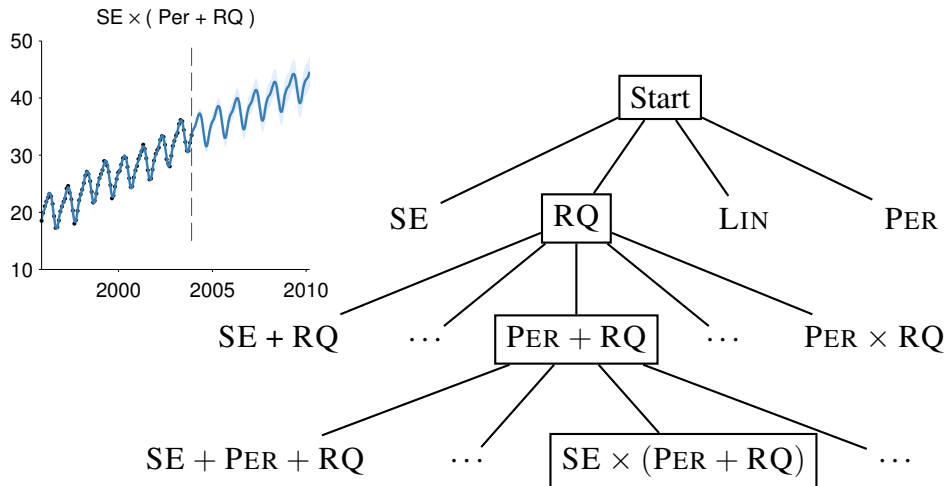
EXAMPLE: MAUNA LOA KEELING CURVE



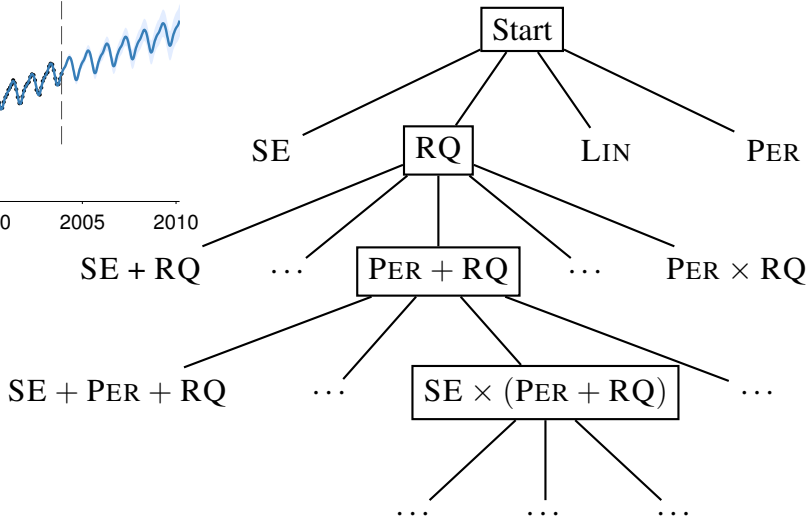
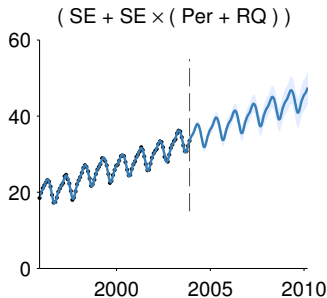
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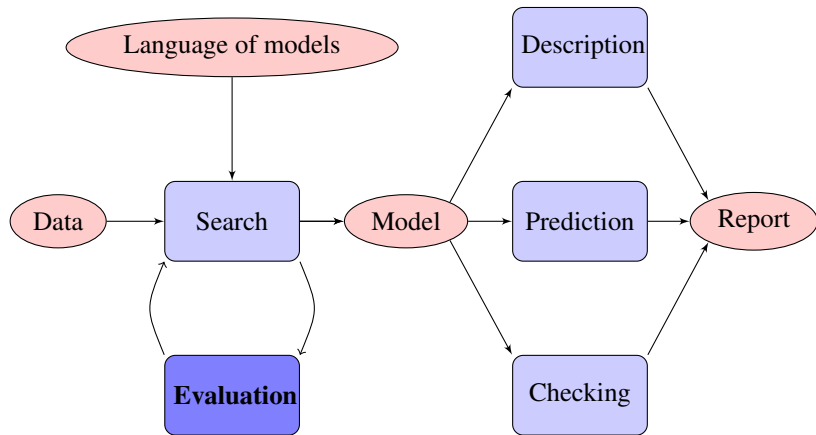
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MODEL EVALUATION



BAYESIAN MODEL SELECTION

Suppose we have a collection of models $\{M_i\}$ and some data D

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Bayes rule tells us

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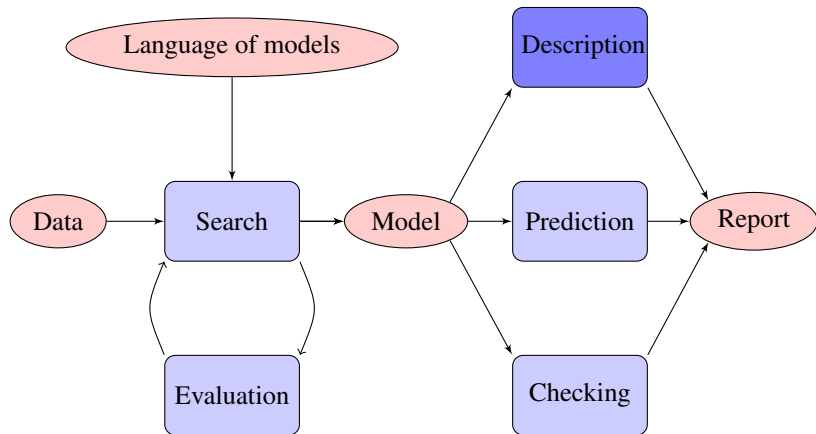
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i.e. The most likely model has the highest **marginal likelihood**

AUTOMATIC TRANSLATION OF MODELS

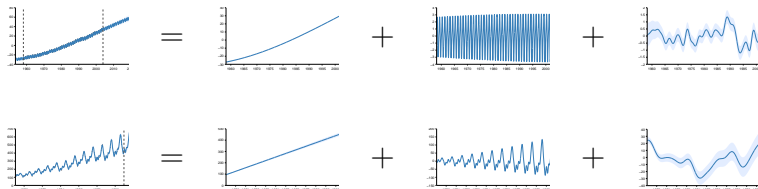


SUMS OF KERNELS ARE SUMS OF FUNCTIONS

If $f_1 \sim \text{GP}(0, k_1)$ and independently $f_2 \sim \text{GP}(0, k_2)$ then

$$f_1 + f_2 \sim \text{GP}(0, k_1 + k_2)$$

e.g.

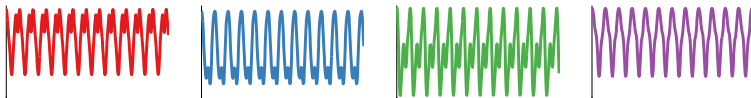


We can therefore describe each component separately

PRODUCTS OF KERNELS

$\underbrace{\text{PER}}$
periodic function

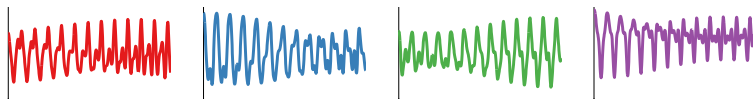
On their own, each kernel is described by a standard noun phrase



PRODUCTS OF KERNELS - SE

$$\underbrace{\text{SE}}_{\text{approximately}} \times \underbrace{\text{PER}}_{\text{periodic function}}$$

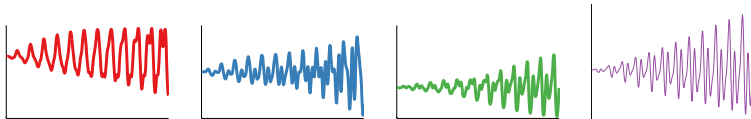
Multiplication by SE removes long range correlations from a model since $\text{SE}(x, x')$ decreases monotonically to 0 as $|x - x'|$ increases.



PRODUCTS OF KERNELS - LIN

$\underbrace{\text{SE}}_{\text{approximately}} \times \underbrace{\text{PER}}_{\text{periodic function}} \times \underbrace{\text{LIN}}_{\text{with linearly growing amplitude}}$

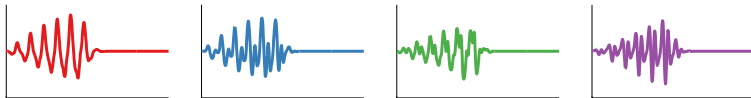
Multiplication by LIN is equivalent to multiplying the function being modeled by a linear function. If $f(x) \sim \text{GP}(0, k)$, then $xf(x) \sim \text{GP}(0, k \times \text{LIN})$. This causes the standard deviation of the model to vary linearly without affecting the correlation.



PRODUCTS OF KERNELS - CHANGEPOINTS

$\underbrace{\text{SE}}_{\text{approximately}} \times \underbrace{\text{PER}}_{\text{periodic function}} \times \underbrace{\text{LIN}}_{\text{with linearly growing amplitude}} \times \underbrace{\sigma}_{\text{until 1700}}$

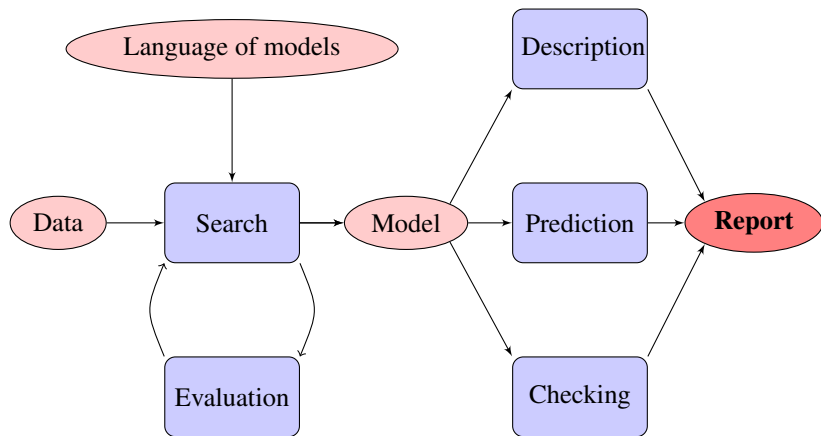
Multiplication by σ is equivalent to multiplying the function being modeled by a sigmoid.



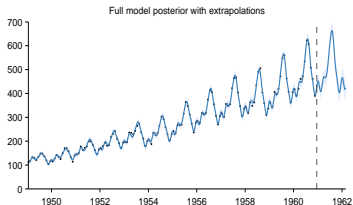
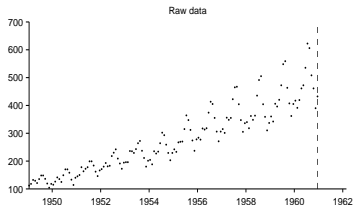
NOUN PHRASE AND POSTMODIFIER FORMS

Kernel	Noun phrase	Postmodifier phrase
WN	uncorrelated noise	n/a
C	constant	n/a
SE	smooth function	whose shape changes smoothly
PER	periodic function	modulated by a periodic function
LIN	linear function	with linearly varying amplitude
$\prod_k \text{LIN}^{(k)}$	polynomial	with polynomially varying amplitude
$\prod_k \sigma^{(k)}$	n/a	which applies until / from [changepoint]

AUTOMATICALLY GENERATED REPORTS



EXAMPLE: AIRLINE PASSENGER VOLUME

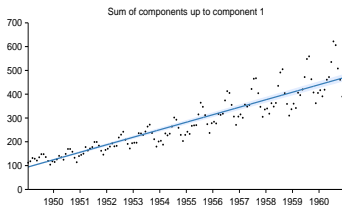
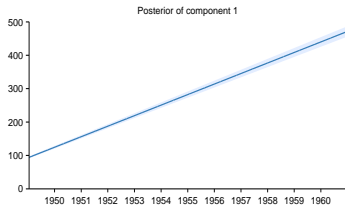


Four additive components have been identified in the data

- ▶ A linearly increasing function.
- ▶ An approximately periodic function with a period of 1.0 years and with linearly increasing amplitude.
- ▶ A smooth function.
- ▶ Uncorrelated noise with linearly increasing standard deviation.

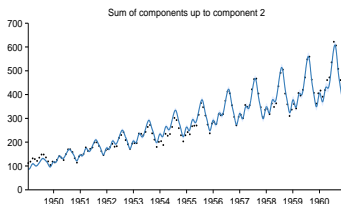
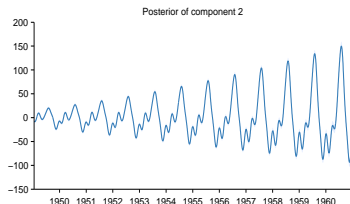
EXAMPLE: AIRLINE PASSENGER VOLUME

This component is linearly increasing.



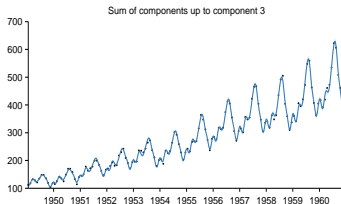
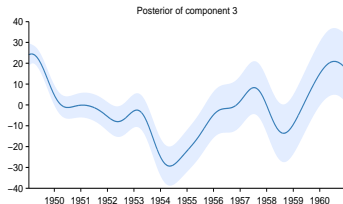
EXAMPLE: AIRLINE PASSENGER VOLUME

This component is approximately periodic with a period of 1.0 years and varying amplitude. Across periods the shape of this function varies very smoothly. The amplitude of the function increases linearly. The shape of this function within each period has a typical lengthscale of 6.0 weeks.



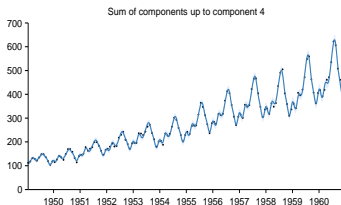
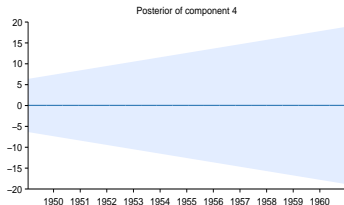
EXAMPLE: AIRLINE PASSENGER VOLUME

This component is a smooth function with a typical lengthscale of 8.1 months.



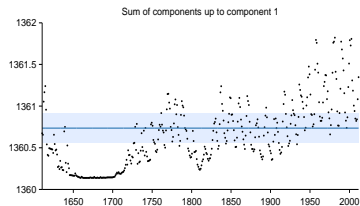
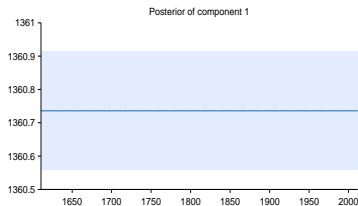
EXAMPLE: AIRLINE PASSENGER VOLUME

This component models uncorrelated noise. The standard deviation of the noise increases linearly.



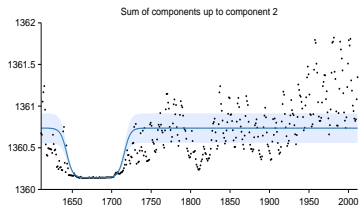
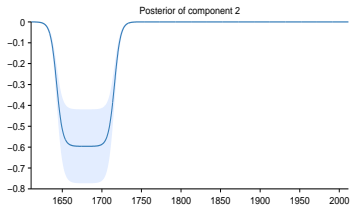
EXAMPLE: SOLAR IRRADIANCE

This component is constant.



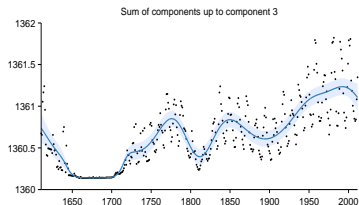
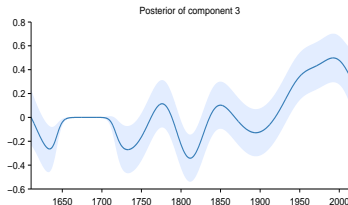
EXAMPLE: SOLAR IRRADIANCE

This component is constant. This component applies from 1643 until 1716.



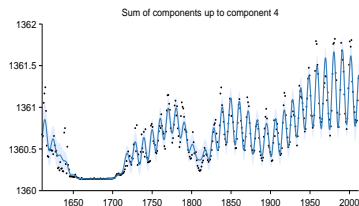
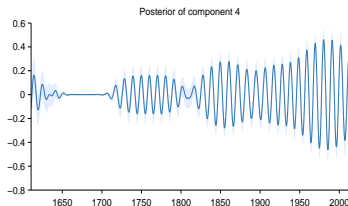
EXAMPLE: SOLAR IRRADIANCE

This component is a smooth function with a typical lengthscale of 23.1 years. This component applies until 1643 and from 1716 onwards.



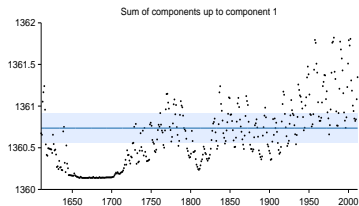
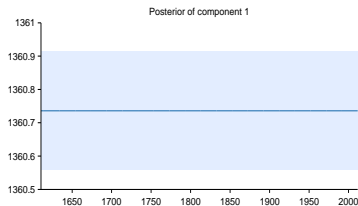
EXAMPLE: SOLAR IRRADIANCE

This component is approximately periodic with a period of 10.8 years. Across periods the shape of this function varies smoothly with a typical lengthscale of 36.9 years. The shape of this function within each period is very smooth and resembles a sinusoid. This component applies until 1643 and from 1716 onwards.



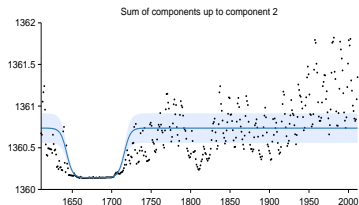
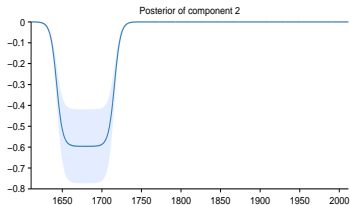
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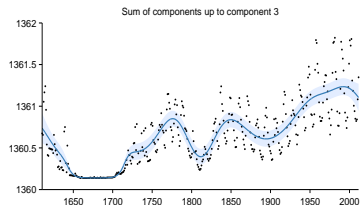
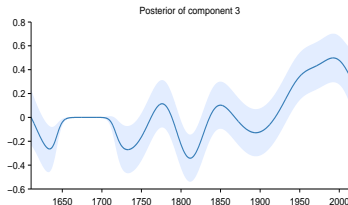
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