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Gaussian Processes with Probabilistic Programming

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Abstract

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1 Introduction

MCMC lends itself to Bayesian interpretations of Gaussian Processes since they can provide a vehicle to express otherwise intractable integrals necessary for a fully Bayesian representation.

2 Gaussian Processes

In the following, we will introduce GP related theory and notations. We will exclusively work on two variable regression problems. Let the data be real-valued scalars $\{x_i, y_i\}_{i=1}^n$ (complete data will be denoted by column vectors \mathbf{x}, \mathbf{y}). GPs present a non-parametric way to express prior knowledge on the space of possible functions f that we assume to have generated the data. f is assumed latent and the GP prior is given by a multivariate Gaussian with mean and covariance $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$, where $m(\mathbf{x})$ is a function of the mean of all functions that map to y_i at x_i and $k(\mathbf{x}, \mathbf{x}')$ is a kernel or covariance function that summarizes the covariance of all functions that map to y_i at x_i . We can absorb the mean function into the covariance function so without loss of generality we can set the mean to zero. The marginal likelihood can be expressed as:

$$p(\mathbf{y}|\mathbf{x}) = \int p(\mathbf{y}|\mathbf{f}, \mathbf{x}) p(\mathbf{f}|\mathbf{x}) d\mathbf{f} \quad (1)$$

where the prior is Gaussian $\mathbf{f}|\mathbf{x} \sim \mathcal{N}(0, k(\mathbf{x}, \mathbf{x}'))$. For a zero mean Gaussian Process this results in a Gaussian posterior $\mathcal{N}(\boldsymbol{\mu}, \Sigma)$ with mean:

$$\boldsymbol{\mu} = \mathbf{K}(\mathbf{x}, \mathbf{x}^*) \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{y} \quad (2)$$

and covariance

$$\Sigma = \mathbf{K}(\mathbf{x}, \mathbf{x}) + \mathbf{K}(\mathbf{x}, \mathbf{x}^*) \mathbf{K}(\mathbf{x}^*, \mathbf{x}^*)^{-1} \mathbf{K}(\mathbf{x}^*, \mathbf{x}). \quad (3)$$

where \mathbf{K} is a covariance function. The covariance function covers general high-level properties of the observed data such as linearity, periodicity and smoothness. The most widely used type of covariance function is the squared exponential covariance function:

$$k(x, x') = \sigma^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right) \quad (4)$$

where σ and ℓ are hyper-parameters. σ is a scaling factor and ℓ is the typical length-scale. Smaller variations can be achieved by exchanging these hyper-parameters. Below, we see how we can express simple GP smoothing with a few

054 lines of Venture code while allowing users to custom design covariance functions.
 055

056 Listing 1: GP Smoothing

```

057 [ASSUME 1 1] ∈ {hyper-parameters}
058 [ASSUME sf 2] ∈ {hyper-parameters}
059
060  $k(x, x') := \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ 
061
062 [ASSUME f VentureFunction(k, σ, ℓ) ]
063 [ASSUME SE make-se (apply-function f 1 sf) ]
064 [ASSUME (make-gp 0 SE) ]
065
066 [SAMPLE GP (array 1 2 3)] % Prior
067
068 [OBSERVE GP D]
069
070 [SAMPLE GP (array 1 2 3)]
071
072 [INFER (MH {hyper-parameters} one 100) ]
073
074 [SAMPLE GP (array 1 2 3)] % Posterior

```

075 The first two lines depict the hyper-parameters. We tag both of them to belong to the set {hyper-
 076 parameters}. Every member of this set belongs to the same inference scope. This scope controls the
 077 application of the inference procedure used. In this paper, we use MH throughout. Each scope is
 078 further subdivided into blocks that allow to do block-proposals. In the following we omit the block
 079 notation for readability, since we always choose the block of a certain scope at random.

080 The ASSUME directives describe the assumptions we make for the GP model, we assume the hyper-
 081 parameters 1 and sf (corresponding to ℓ, σ) to be 1 and 2. The squared exponential covariance
 082 function can be defined outside the Venture code with foreign conventional programming languages,
 083 e.g. Python. In that way, the user can define custom covariance functions without being restricted to
 084 the most common ones. We then integrate the foreign function into Venture as VentureFunction. In
 085 the next line this function is associated with the hyper-parameters. Finally, we assume a Gaussian
 086 Process SP with a zero mean and the previously assumed squared exponential covariance function.

087 In the case where hyper-parameters are unknown they can be found deterministically by optimizing
 088 the marginal likelihood using a gradient based optimizer. Non-deterministic, Bayesian representa-
 089 tions of this case are also known (Neal, 1997). Extending the program described in listing 1 for a
 090 Bayesian treatment of hyper-parameters is simple using the build in stochastic procedure that simu-
 091 lates drawing samples from a gamma distribution:

092

093 Listing 2: Bayesian GP Smoothing

```

094 [ASSUME 1 (gamma 1 3)]
095 [ASSUME sf (gamma 1 2)]
096
097  $k(x, x') := \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ 
098
099 [ASSUME f VentureFunction(k, σ, ℓ) ]
100 [ASSUME SE make-se (apply-function f 1 sf) ]
101 [ASSUME (make-gp 0 SE) ]

```

102

103 Larger variations are achieved by changing the type of the covariance function structure. A different
 104 type could be a linear covariance function:

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107

$$k(x, x') = \sigma^2(x - \ell)(x' - \ell). \quad (5)$$

108 Note that covariance function structures are compositional. We can add covariance functions if we
 109 want to model globally valid structures

$$111 \quad k_3(x, x') = k_1(x, x') + k_2(x, x') \quad (6)$$

112 and we can multiply covariance functions if the data is best explained by local structure

$$114 \quad k_4(x, x') = k_1(x, x') \times k_2(x, x'); \quad (7)$$

115 both, k_3 and k_4 are valid covariance function structures. This leads to an infinite space of possible
 116 structures that could potentially explain the observed data best (e.g. Fig. ??). In the following, we
 117 will refer to covariance functions that are not composite as base covariance functions. Note that this
 118 form of composition can be easily expressed in Venture, for example if one wishes to add a linear
 119 and a periodic kernel:

121 Listing 3: LIN \times PER

```
122 [ASSUME 1 (gamma 1 3)]
123 [ASSUME sf (gamma 1 2)]
124 [ASSUME a (gamma 2 2)]
125
126  $k_{LIN}(x, x') = \sigma_1^2(x - \ell)(x' - \ell)$ 
127
128  $k_{PER}(x, x') := \sigma_2^2 \exp\left(-\frac{2 \sin^2(\pi(x-x')/p)}{\ell^2}\right)$ 
129
130 [ASSUME f_LIN VentureFunction(k_LIN, sigma_1) ]
131 [ASSUME f_PER VentureFunction(k_PER, sigma_2, ell, p) ]
132 [ASSUME LIN (make-LIN (apply-function f_LIN a)) ]
133 [ASSUME PER (make-PER (apply-function f_PER 1 sf)) ]
134 [ASSUME (make-gp 0 (function-times LIN PER)) ]
```

135 Knowledge about the composite nature of covariance functions is not new, however, until recently,
 136 the choice and the composition of covariance functions were done ad-hoc. The Automated Statisti-
 137 cian Project came up with an approximate search over the possible space of kernel structures (Du-
 138 venaud et al., 2013; Lloyd et al., 2014).

140 2.1 A Bayesian interpretation

142 In the following, we will explore a Bayesian representation of GP. The probability of the hyper-
 143 parameters of a GP with assumptions as above and given covariance function structure \mathbf{K} can be
 144 described as:

$$145 \quad P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) = \frac{P(\mathbf{D} | \boldsymbol{\theta}, \mathbf{K})P(\boldsymbol{\theta} | \mathbf{K})}{P(\mathbf{D} | \mathbf{K})}. \quad (8)$$

147 We are interested in the case where covariance structure is not given. Our probabilistic programming
 148 based MCMC framework approximates the following intractable integrals of the expectation for the
 149 prediction:

$$151 \quad \mathbb{E}[y^* | x^*, D, \mathbf{K}_\Omega^s] = \int \int f(x^*, \boldsymbol{\theta}, \mathbf{K}) P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) P(\mathbf{K} | \boldsymbol{\Omega}, s, n) d\boldsymbol{\theta} d\mathbf{K}. \quad (9)$$

153 This is done by sampling from the posterior probability distribution of the hyper-parameters and the
 154 possible kernel:

$$155 \quad y^* \approx \frac{1}{T} \sum_{t=1}^T f(x^* | \boldsymbol{\theta}^{(t)}, \mathbf{K}^{(t)}). \quad (10)$$

158 3 Stochastic Processes

161 In order to provide the sampling of the kernel, we introduce a stochastic process to the SP that
 simulates the grammar for algebraic expressions of kernel algebra. Here, we start with a set of

possible kernels and draw a random subset. For this subset of size n , we sample a set of possible operators that operate on the base kernels.

The marginal probability of a kernel structure which allows us to sample is characterized by the probability of a uniformly chosen subset of the set of n possible covariance functions times the probability of sampling a global or a local structure which is given by a binomial distribution:

$$P(\mathbf{K} \mid \Omega, s, n) = P(\Omega \mid s, n) \times P(s \mid n) \times P(n), \quad (11)$$

with

$$P(\Omega \mid s, n) = \binom{n}{r} p_{+ \times}^k (1 - p_{+ \times})^{n-k} \quad (12)$$

and

$$P(s \mid n) = \frac{n!}{|s|!} \quad (13)$$

where $P(n)$ is a prior on the number of base kernels used. It is possible to also assign a prior for the probability to sample global or local priors, however, we have assigned complete uncertainty to this with the binomial $p = 0.5$.

4 Experiments

Neal suggested the treatment of outliers as a use-case for a Bayesian treatment of Gaussian processes (1997). He evaluates his MCMC setting using the following synthetic data problem. Let f be the underlying function that generates the data:

$$f(x) = 0.3 + 0.4x + 0.5 \sin(2.7x) + \frac{1.1}{(1+x^2)} + \eta \quad \text{with } \eta \sim \mathcal{N}(0, \sigma) \quad (14)$$

We synthetically generate outliers by setting $\sigma = 0.1$ in 95% of the case and to $\sigma = 1$ in the remaining cases. Venture GPs can capture the true underlying function within only 100 MH steps (see Fig. 2). Note that Neal devices an additional noise model and performs large numbe of Hybrid-Monte Carlo and Gibbs steps.

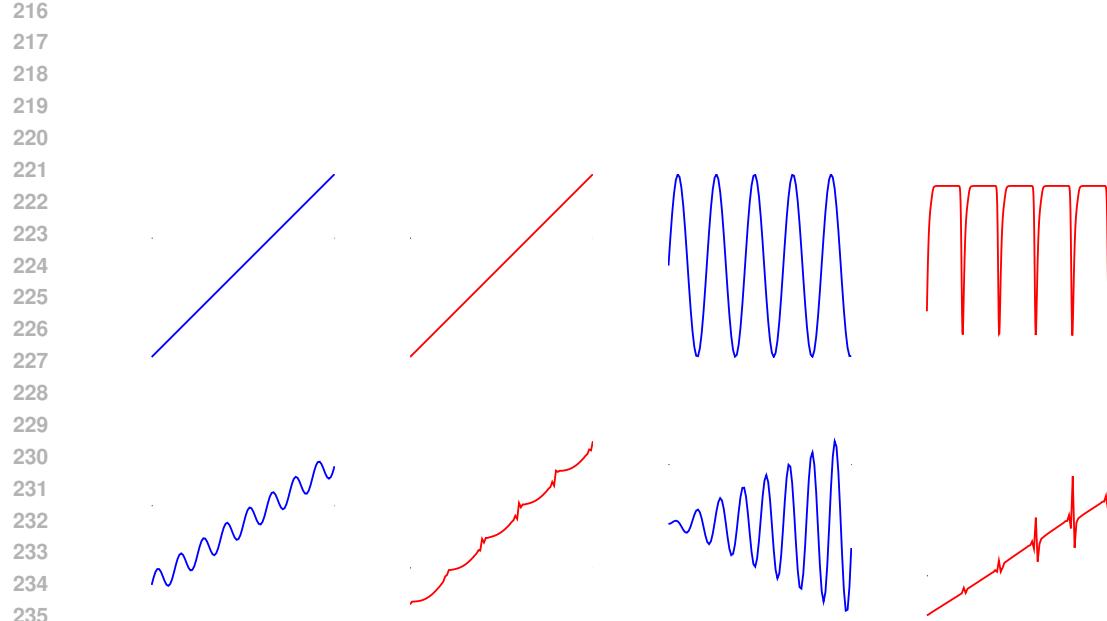
4.1 Structure Learning

Many equivalent covariance structures can be sampled due to covariance function algebra and equivalent representations with different parameterization (Lloyd et al., 2014). Certain covariance functions can differ in terms of the hyper-parameterization but can be absorbed into a single covariance function with a different parameterization. To inspect the posterior of these equivalent structures we convert each kernel expression into a sum of products and subsequently simplify expressions using the following grammar:

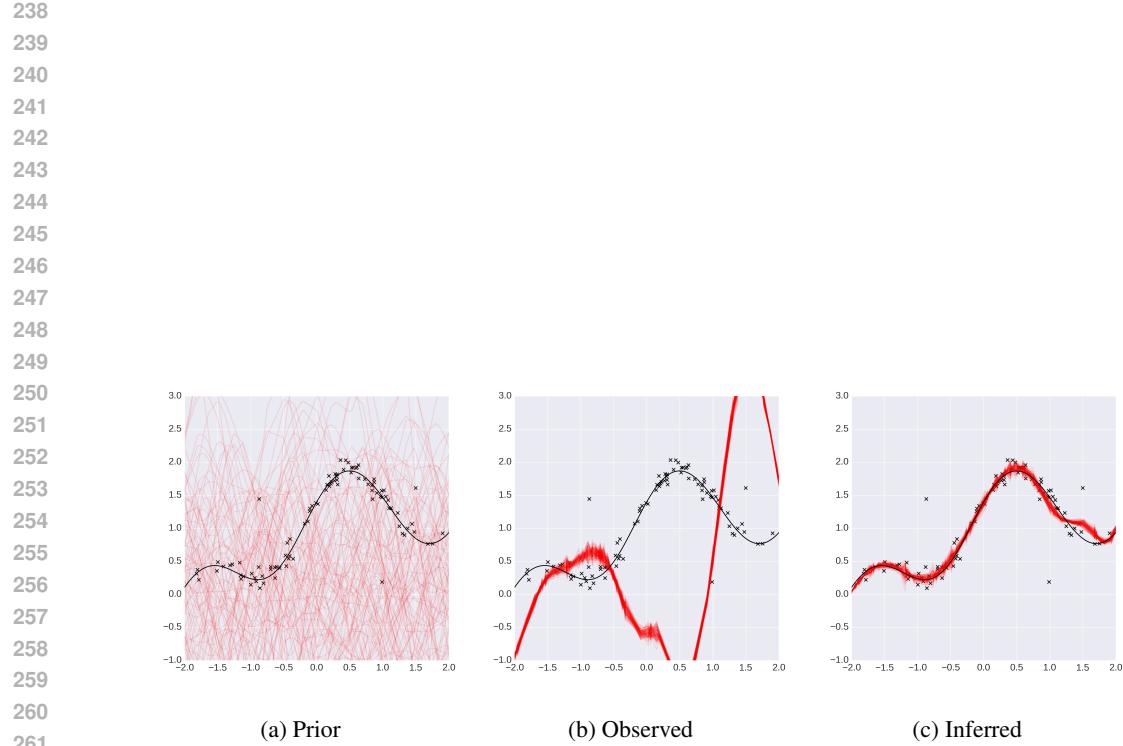
Listing 4: Grammar to simplify expressions

SE × SE	→ SE
{SE, PER, C, WN} × WN	→ WN
LIN + LIN	→ LIN
{SE, PER, C, WN, LIN} × C	→ {SE, PER, C, WN, LIN}

For reproducing results from the Automated Statistician Project in a Bayesian fashion we first define a prior on the hypothesis space. Note that, as in the implementation of the Automated Statistician, we upper-bound the complexity of the space of covariance functions we want to explore. We also put vague priors on hyper-parameters.



236 Figure 1: Composition of covariance functions (blue, left) and samples from the distribution of
237 curves they can produce (red, right).



262 Figure 2: Running a Venture GP on Neal's example for MCMC showing the prior, after having
263 observed the data and after performing inference on the hyper-parameters. Note how the GP is
264 choosing outliers to smooth instead of essential data.

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271 Listing 5: Venture Code for Bayesian GP Structure Learning
272 [ASSUME S (array K1,K2,...,Kn)] // (defined as above)
273 [ASSUME pn (uniform_structure n)]
274 [ASSUME S (array K1,K2,...,Kn)]
275 [ASSUME K* (grammar S pn)]
276 [ASSUME GP (make-gp 0 K*)]

277 [OBSERVE GP D]

278 [INFER (REPEAT 2000 (DO
279   (MH 10 pn one 1)
280   (MH 10 K* one 1)
281   (MH 10 {hyper-parameters} one 10)) ]
282
283

284 We defined the space of covariance structures in a way allowing us to reproduce results for covari-
285 ance function structure learning as in the Automated Statistician. We ran a leave one out cross-
286 validation to gain confidence on the posterior. This resulted in 545 independent runs of the Markov
287 chain that produced a coherent posterior. Our Bayesian interpretation of GP structure and GPs pro-
288 duced a posterior of structures that is in line with previous results on this data set ( Duvenaud et al.,
289 2013; see Fig. 3).
290 We found the final sample of multiple runs to be most informative. This kind of Markov Chain
291 seems to produce samples that are highly auto-correlated.
292

293 4.2 Log-Likelihood
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295 4.3 Residuals
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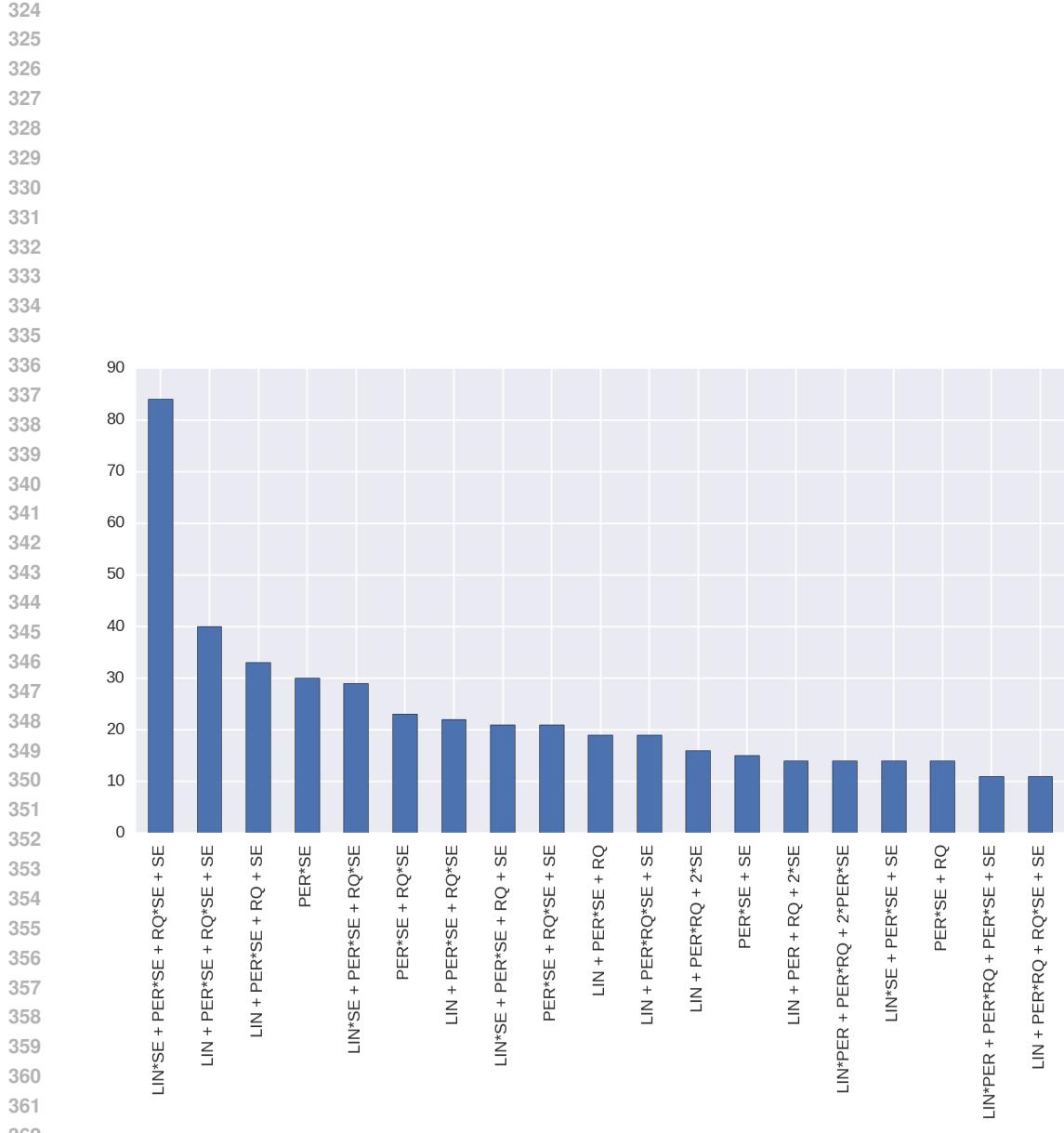
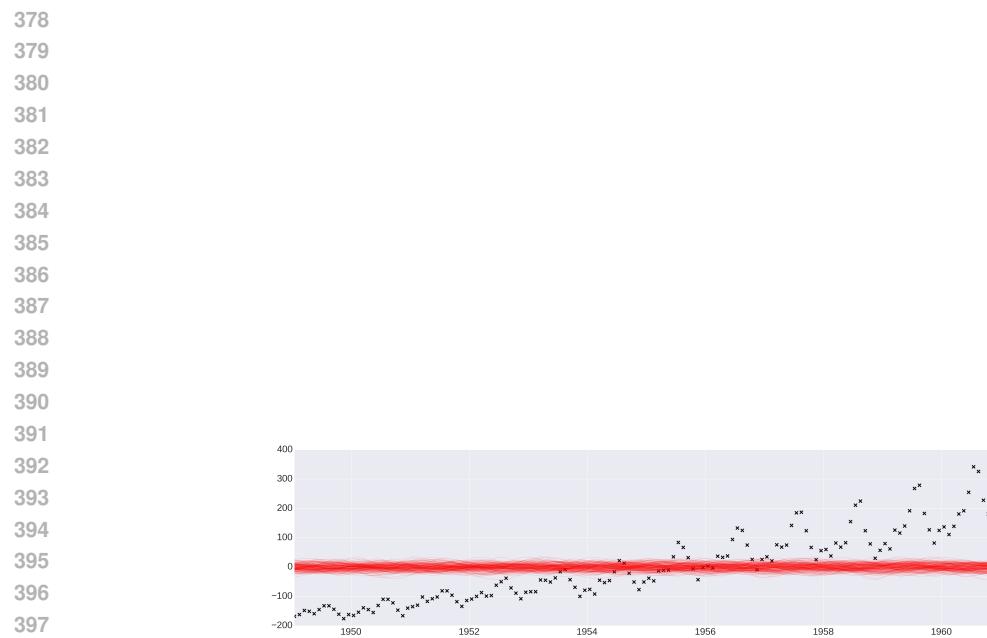


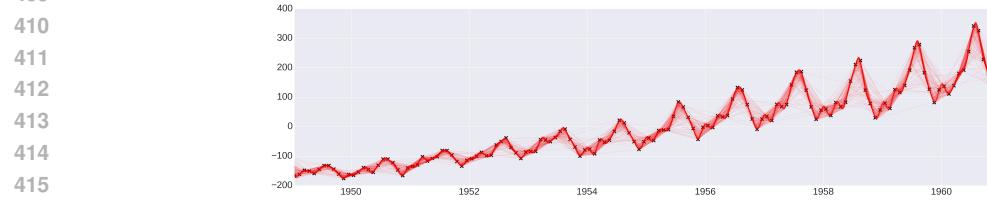
Figure 3: Posterior on structure of the CO₂ data. We have cut the tail of the distribution for space reasons since the number of possible structures is large. We see the final sample of the each of the 545 chains with 2000 nested steps each. Note that Duvenaud et al. (2013) report LIN × SE + PER × SE + RQ × SE.



(a) Prior, before having seen any data.



(b) After having seen any data but before inference



(c) After 1000 MH steps.

Figure 4: Running a Venuter GP with covariance structure PER x SE on the airline data