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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 [OBSERVE GP D]
067
068 [INFER (REPEAT 100 ( DO ( MH hyper-parameters one 10 ) ) ]
```

069 In the case where hyper-parameters are unknown they can be found deterministically by optimizing
 070 the marginal likelihood using a gradient based optimizer. Non-deterministic, Bayesian representations
 071 of this case are also known (Neal, 1997). Extending the program described in listing 1 for a
 072 Bayesian treatment of hyper-parameters is simple using the build in stochastic procedure that simu-
 073 lates drawing samples from a gamma distribution:
 074

075 Listing 2: Bayesian GP Smoothing

```

076 [ASSUME 1 (gamma 1 3)]
077 [ASSUME sf (gamma 1 2)]
078
079  $k(x, x') := \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ 
080
081 [ASSUME f VentureFunction(k, σ, ℓ) ]
082 [ASSUME SE make-se (apply-function f 1 sf) ]
083 [ASSUME (make-gp 0 SE ) ]
084
```

085 Larger variations are achieved by changing the type of the covariance function structure. A different
 086 type could be a linear covariance function:
 087

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

091 Note that covariance function structures are compositional. We can add covariance functions if we
 092 want to model globally valid structures
 093

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

098 and we can multiply covariance functions if the data is best explained by local structure
 099

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

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

108

109

Listing 3: LIN × PER

```

110 [ASSUME 1 (gamma 1 3)]
111 [ASSUME sf (gamma 1 2)]
112 [ASSUME a (gamma 2 2)]
113
114  $k_{LIN}(x, x') = \sigma_1^2(x - \ell)(x' - \ell)$ 
115  $k_{PER}(x, x') := \sigma_2^2 \exp\left(-\frac{2 \sin^2(\pi(x-x')/p)}{\ell^2}\right)$ 
116
117 [ASSUME fLIN VentureFunction( $k_{LIN}, \sigma_1$ ) ]
118 [ASSUME fPER VentureFunction( $k_{PER}, \sigma_2, \ell, p$ ) ]
119 [ASSUME LIN (make-LIN (apply-function fLIN a)) ]
120 [ASSUME PER (make-PER (apply-function fPER 1 sf)) ]
121 [ASSUME (make-gp 0 (function-times LIN PER)) ]
122

```

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

127

128 2.1 A Bayesian interpretation

129

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

$$133 P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) = \frac{P(\mathbf{D} | \boldsymbol{\theta}, \mathbf{K})P(\boldsymbol{\theta} | \mathbf{K})}{P(\mathbf{D} | \mathbf{K})}. \quad (8)$$

134

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

$$138 \mathbb{E}[y^* | x^*, D, \mathbf{K}_\Omega^s] = \iint f(x^*, \boldsymbol{\theta}, \mathbf{K}) P(\boldsymbol{\theta} | \mathbf{D}, \mathbf{K}) P(\mathbf{K} | \Omega, s, n) d\boldsymbol{\theta} d\mathbf{K}. \quad (9)$$

140

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

$$143 y^* \approx \frac{1}{T} \sum_{t=1}^T f(x^* | \boldsymbol{\theta}^{(t)}, \mathbf{K}^{(t)}). \quad (10)$$

145

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3 Stochastic Processes

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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.

151

152

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:

155

156

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

157

with

158

159

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

160

and

161

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

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

4 Experiments

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

$$173 \quad f(x) = 0.3 + 0.4x + 0.5 \sin(2.7x) + \frac{1.1}{(1+x^2)} + \eta \quad \text{with } \eta \sim \mathcal{N}(0, \sigma) \quad (14)$$

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

4.1 Structure Learning

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

189 Listing 4: Grammar to simplify expressions

190 SE × SE	→ SE
191 {SE, PER, C, WN} × WN	→ WN
192 LIN + LIN	→ LIN
193 {SE, PER, C, WN, LIN} × C	→ {SE, PER, C, WN, LIN}

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

200 Listing 5: Venture Code for Bayesian GP Structure Learning

```
201 [ASSUME S (array K1, K2, ..., Kn)] // (defined as above)
202 [ASSUME pn (uniform_structure n)]
203 [ASSUME S (array K1, K2, ..., Kn)]
204 [ASSUME K* (grammar S pn)]
205 [ASSUME GP (make-gp 0 K*)]
206
207 [OBSERVE GP D]
208
209 [INFER (REPEAT 3000 (DO
210   (MH 10 pn one 1)
211   (MH 10 K* one 1)
212   (MH 10 {hyper-parameters} one 10))]
```

213 We defined a set of covariance structures so that we could reproduce results for covariance function
 214 structure learning as in the Automated Statistician. Our results are very similar to what has been
 215 reported by previous work (Duvenaud et al., 2013; see Fig. 3).

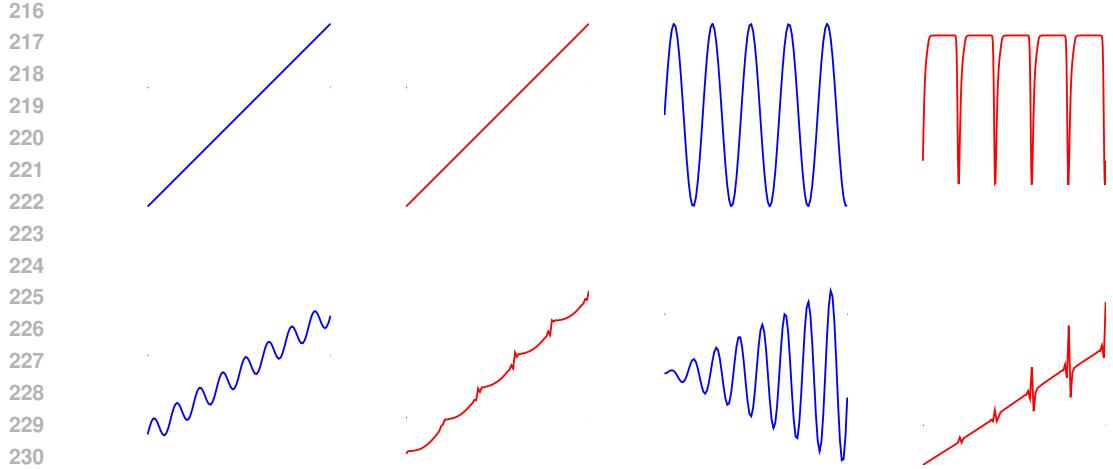


Figure 1: Composition of covariance functions (blue, left) and samples from the distribution of curves they can produce (red, right).

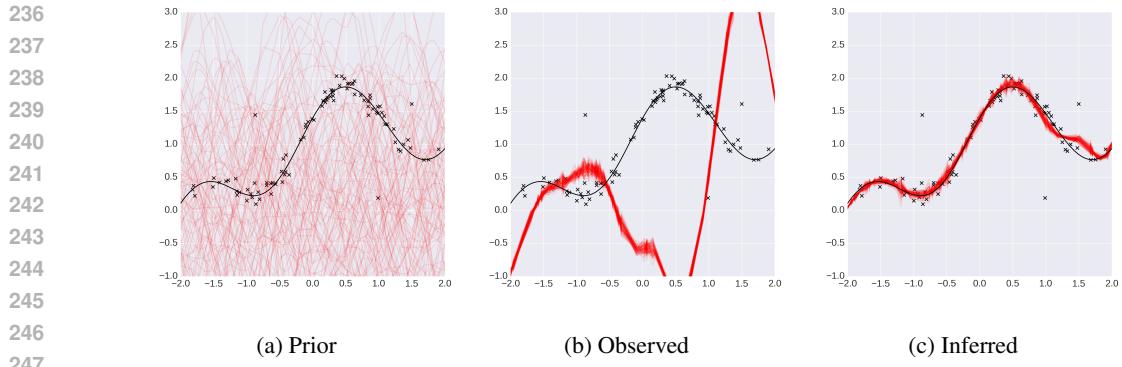


Figure 2: Running a Venture GP on Neal's example for MCMC showing the prior, after having observed the data and after performing inference on the hyper-parameters. Note how the GP is choosing outliers to smooth instead of essential data.

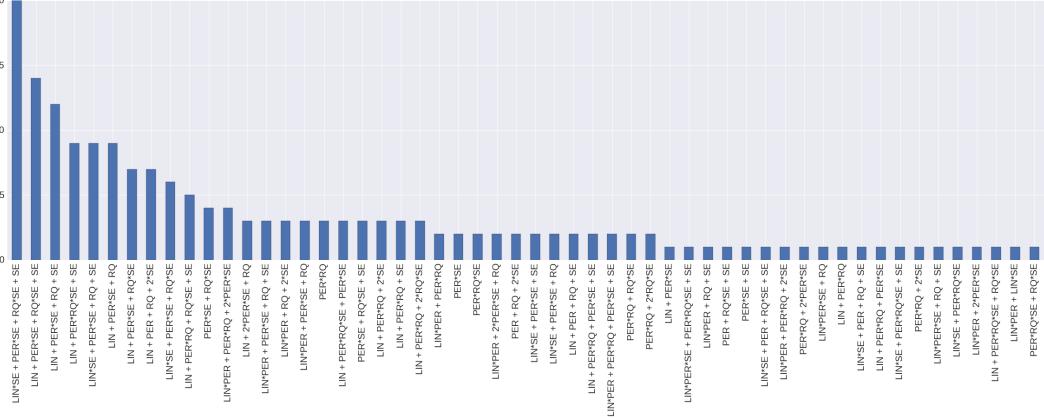
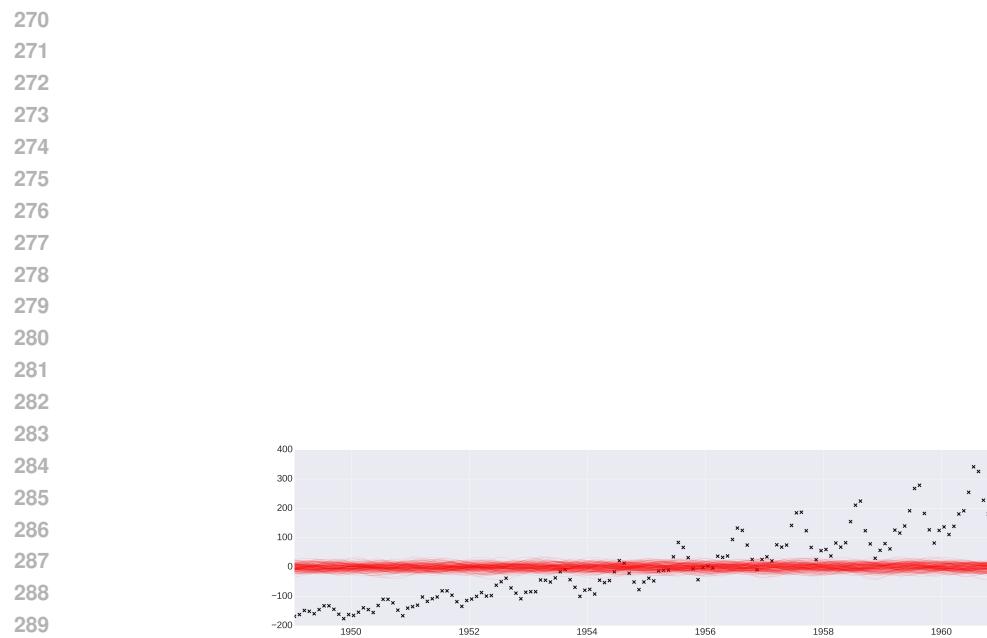
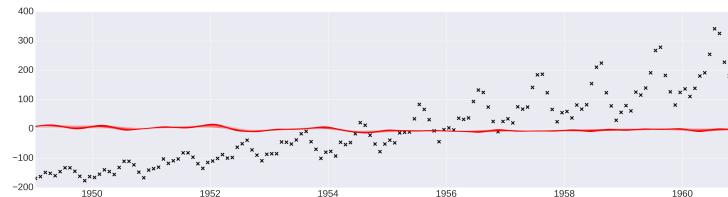


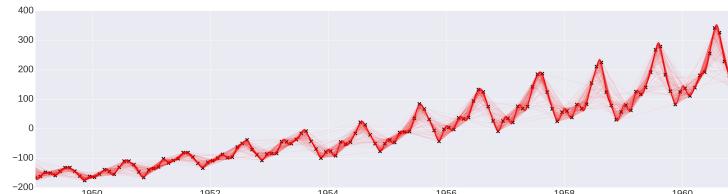
Figure 3: Preliminary results from the cross-validation on the CO2 data. Note that Duvenaud et al. (2013) report $\text{LIN} \times \text{SE} + \text{PER} \times \text{SE} + \text{RQ} \times \text{SE}$. We have run a leave one out cross-validation on this data set. Above we see the preliminary results on 181 validations (of a total of 545×2 runs).



290 (a) Prior, before having seen any data.
291



299 (b) After having seen any data but before inference
300



310 (c) After 1000 MH steps.
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312 Figure 4: Running a Venuter GP with covariance structure PER x SE on the airline data
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- 324 **4.2 Log-Likelihood**
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326 **4.3 Residuals**
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