Sparse Multiscale Gaussian Process Regression

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Outline

Sparse Approximations of GPs and other Kernel Machines
   Coupled Covariance and Function Basis
   De-coupled Covariance and Function Basis

Arbitrary Width Gaussian Covariance and Basis Functions
   Computing the Prior
   Interpretation

Examples
   Gaussian Process Regression
   Support Vector Machine Classification

Summary and Outlook
Basis functions of the form $k(x, \cdot)$

A Brief History of Sparse GP Algorithms

- The posterior mean of the GP takes the form
  \[
  \mu(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x)
  \]

- The simplest sparse approximation enforces
  \[
  \mu_{\text{sparse}}(x) = \sum_{i \in S} \beta_i k(x_i, x), \quad S \subset \{1, 2, \ldots, n\}
  \]

- Alternatively one may sacrifice training time for testing time:
  \[
  \mu_{\text{sparser}}(x) = \sum_{i=1}^{m} \gamma_i k(z_i, x)
  \]
Basis functions NOT of the form $k(\mathbf{x}, \cdot)$

- The next logical step to obtain greater sparsity enforces

$$\mu_{\text{even more sparse}}(\mathbf{x}) = \sum_{i=1}^{m} c_i \mathbf{u}_i(\mathbf{x})$$

where the $\mathbf{u}_i$ belong to some prescribed set of basis functions

- This generalizes the previous approximations which set, e.g.

$$\mathbf{u}_i(\mathbf{x}) = k(\mathbf{z}_i, \mathbf{x})$$

- This was done by Walder et al. [1] using compactly supported basis functions (translated and dilated B$\_3$-splines)

- Gehler and Franz [2] used $\mathbf{u}_i(\mathbf{x}) = (\mathbf{x}^\top \mathbf{x}_i)^p$

- Presently we consider dilated/translated Gaussian basis functions for $\mathbf{u}_i$
Prior probability of arbitrary Gaussian mixtures

Via an infinite limit

- Let $G(k)$ be the zero mean GP with covariance $k$
- Let $u$ be drawn from $G(k)$ and define the random variable
  \[ u_X = (u(x_1), u(x_2), \ldots, u(x_n))^\top \]
- Let $K_{xx} = (k(x_i, x_j))_{ij}$

By the definition of a GP we have

\[
p_{u_X}(\sum_{i=1}^m c_i u_i) = \left| 2\pi K_{xx}^{-1} \right|^{-\frac{1}{2}} \exp \left( -\frac{1}{2} \sum_{i,j=1}^m c_i c_j u_i^\top K_{xx}^{-1} u_j \right).
\]

We take $n \to \infty$ with uniformly distributed $x_i$ so that

- $u_i$ becomes a function $u_i$
- $u_i^\top K_{xx}^{-1} u_j$ becomes

\[
\int \int k^{-1}(x, y) u_i(x) u_j(y) \, dx \, dy.
\]
Computing the Prior

### Probability of arbitrary Gaussian mixtures (2)

But what is $k^{-1}(\cdot, \cdot)$?

- For finite $n$ if we let $u = K_{xx}\alpha$ then $\alpha = K_{xx}^{-1}u$.
- Following this finite analogy, if $u = \int \alpha(\mathbf{x})k(\mathbf{x}, \cdot)\,d\mathbf{x}$, then $k^{-1}$ should satisfy
  \[
  \int u(\mathbf{x})k^{-1}(\mathbf{x}, \cdot)\,d\mathbf{x} = \alpha(\cdot).
  \]

Hence if we define

\[
M_k : \alpha \mapsto M_k\alpha = \int \alpha(\mathbf{x})k(\mathbf{x}, \cdot)\,d\mathbf{x},
\]

then $k^{-1}$ is by definition the Green’s function of $M_k$, as it satisfies

\[
\int (M_k\alpha)(\mathbf{x})k^{-1}(\mathbf{x}, \cdot)\,d\mathbf{x} = \alpha(\cdot).
\]
Prior probability of arbitrary Gaussian mixtures (3)

Now define $g$ to be the normalised Gaussian on $\mathbb{R}^d \times \mathbb{R}^d$,

$$
g(x, y, \sigma) \equiv |2\pi \text{diag}(\sigma)|^{-\frac{1}{2}} \exp \left( -\frac{1}{2} \sum_{i=1}^{d} \frac{([x - y]_i)^2}{[\sigma]_i} \right).
$$

If we choose

- $k(x, y) = cg(x, y, \sigma)$, where $c > 0$, $\sigma > 0 \in \mathbb{R}^d$
- $u_i(x) = g(x, v_i, \sigma_i)$

then everything is Gaussian and we obtain in closed form

$$
\int \int k^{-1}(x, y) u_i(x) u_j(y) \, dx \, dy = \frac{1}{c} g(v_i, v_j, \sigma_i + \sigma_j - \sigma).
$$
Prior probability of arbitrary Gaussian mixtures (4)

Summarising Expressions

\[ p_G(cg(\cdot, \cdot, \sigma)) \left( \sum_{i=1}^{m} c_i g(\cdot, v_i, \sigma_i) \right) \]

\[ \propto \exp \left( -\frac{1}{2} \sum_{i,j=1}^{m} \frac{1}{c_i c_j} g(v_i, v_j, \sigma_i + \sigma_j - \sigma) \right). \]

Let \( \mathcal{H} \) be the RKHS with kernel \( g(\cdot, \cdot, \sigma) \). Then

\[ \langle g(\cdot, v_i, \sigma_i), g(\cdot, v_j, \sigma_j) \rangle_\mathcal{H} = g(v_i, v_j, \sigma_i + \sigma_j - \sigma). \]
Prior probability of arbitrary Gaussian mixtures (5)

Interpretation

- $\sigma_1 = \sigma_2 = \cdots = \sigma_n = \sigma$ recovers the “normal” methods.
- The most likely single Gaussian function $u_1$ has $\sigma_1 = \sigma$.
- As the dimension increases, the probability density in $\sigma_1$ centres around $\sigma$ (so smaller dimensions yield greater gains).
- As noted by Bach and Jordan [3], for all $j = 1, 2, \ldots, d$

$$\lim_{[\sigma_1]_j \to (\frac{1}{2}[\sigma]_j)} p_G(g(\cdot, \cdot, \sigma))(u_1(\cdot)) = 0.$$ 

Kernel machines such as the GP cannot recover “any” function — in fact not even a Gaussian function that is too narrow!
One Dimensional Toy Example

(a) Basis $\sigma_i$'s fixed to $\sigma$.  
(b) Basis $\sigma_i$'s variable.  
(c) Exact g.p.

- Predictive distributions  
  (mean curve with $\pm$ two standard deviations shaded)
- For the sparse algorithms, we plot the crossed circles at the $(v_i, \sigma_i) \in \mathbb{R} \times \mathbb{R}$
- The horizontal lines denote the resulting $\sigma \in \mathbb{R}$ of the covariance function $c_g(\cdot, \cdot, \sigma)$
Real World Examples

(d) pumadyn-32nm error  (e) kin-40K error  (f) kin-40K $\sigma_i$ deviation

- **kin-40k**: 10000 training, 30000 test, 9 attributes, see www.igi.tugraz.at/aschwaig/data.html
- **pumadyn-32nm**: 7168 training, 1024 test, 33 attributes, see www.cs.toronto/delve

On the right we plot $\frac{1}{md} \sum_{i=1}^{m} \sum_{j=1}^{d} (\sigma_i - \sigma_j)^2$
This Can be Applied to any Kernel Machine

- Let $\mathcal{H}$ be the RKHS with kernel $g(\cdot, \cdot, \sigma)$.
- We can always “multi-scale sparsify” the solution to

$$\arg \min_{f \in \mathcal{H}} \| f \|_{\mathcal{H}}^2 + \text{risk}$$

By enforcing the solution to take the form $\sum_{i=1}^{m} c_i g(v_i, \cdot, \sigma_i)$. The objective becomes

$$\arg \min_{c_i \in \mathbb{R}, v_i \in \mathbb{R}^d, \sigma_i \in \mathbb{R}^d} \mathbf{c}^T U_{\Psi} \mathbf{c} + \text{risk}$$

where $U_{\Psi} = (g(v_i, v_j, \sigma_i + \sigma_j - \sigma))_{i,j}$ as before.
A Video of the Optimisation Process
SVM Classifier in Two Dimensions

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Summary and Outlook

- We have seen how to approximate Gaussian kernel machines using a multi-scale Gaussian function basis.
- The result is a generalization of previous sparsification methods, and hence is at least as good as them.
- The method is suitable for obtaining very short test times, desirable in real-time applications, for example.
- The lower the input dimensionality, the more benefit the multi-scale basis can provide.
- A similar analysis could be done for other combinations of basis functions and kernels.
References

Christian Walder, Bernhard Schölkopf, and Olivier Chapelle.
Implicit surfaces with globally regularised and compactly supported basis functions.

Peter Gehler and Matthias Franz.
Implicit wiener series, part ii: Regularised estimation.

Francis R. Bach and Michael I. Jordan.
Kernel independent component analysis.

Edward Snelson and Zoubin Ghahramani.
Sparse gaussian processes using pseudo-inputs.

J. Quiñonero-Candela and C. E. Rasmussen.
A unifying view of sparse approximate gaussian process regression.

C. E. Rasmussen and C. K.I. Williams.
*Gaussian Processes for Machine Learning*.