Probabilistic Programming with Gaussian Process Memoization

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Abstract

Gaussian process memoizer is a probabilistic programming technique that uses Gaussian processes to provides a statistical alternative to memorization. Memoizing a target procedure results in a self-caching wrapper that remembers previously computed values. Gaussian process memoization additionally produces a statistical emulator based on a Gaussian process whose predictions automatically improve whenever a new value of the target procedure becomes available. The work also introduces an efficient implementation, named `gpmem`, that can use kernels given by a broad class of probabilistic programs. The flexibility of `gpmem` is illustrated via three applications: (i) GP regression with hierarchical hyper-parameter learning, (ii) Bayesian structure learning and (iii) a bandit formulation of Bayesian optimization.

GP Memoization: `gpmem`

Gaussian Processes

For any finite set of inputs $\mathbf{x}$, the marginal prior on $f(\mathbf{x})$ is the multivariate Gaussian $f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}))$, where $k(\mathbf{x}, \mathbf{x}') = \mathrm{Cov}_f\left(f(\mathbf{x}), f(\mathbf{x}')\right)$ is the covariance function, a.k.a. kernel. The marginal likelihood can be expressed as:

$$p\left(f(\mathbf{x}) = \mathbf{y} \mid \mathbf{x}\right) = \int p\left(f(\mathbf{x}) = \mathbf{y} \mid f, \mathbf{x}\right)\, p(f|\mathbf{x})\, df$$

where here $p(f|\mathbf{x}) = p(f) \sim \mathcal{GP}(m, k)$ since we assume no dependence of f on $\mathbf{x}$. We can sample a vector of unseen data $\mathbf{y}^* = f(\mathbf{x}^*)$ from the predictive posterior with $\mathbf{y}^* \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\mu} = k(\mathbf{x}, \mathbf{x}^*)\, k(\mathbf{x}^*, \mathbf{x}^*)^{-1}\, \mathbf{y}$ and $\boldsymbol{\Sigma} = k(\mathbf{x}, \mathbf{x}) - k(\mathbf{x}, \mathbf{x}^*) k(\mathbf{x}^*, \mathbf{x}^*)^{-1} k(\mathbf{x}^*, \mathbf{x})$.

Memoization

Memoization is the practice of storing previously computed values of a function so that future calls with the same inputs can be evaluated by lookup rather than re-computation. Gaussian Process memoization:

- is a statistical alternative to standard memoization;
- changes semantics of a probabilistic program; and
- produces a statistical emulator whose predictions improve with memoization.

Bayesian GP

We show how we can use `gpmem` to reproduce Neal's Hierarchical Bayesian GP [2] for data with outliers.

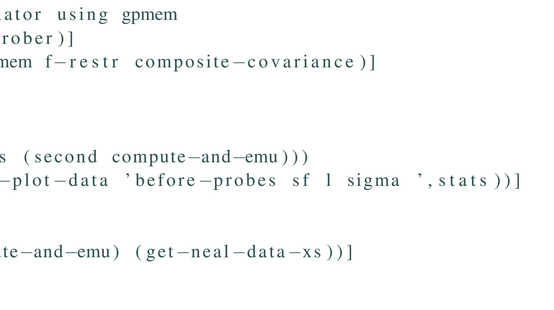
Listing 1: Hierarchical GP Smoothing

```
[INFER (load-plugin (quote symbol<"gppaper-plugin.py">) 'neal)]

;;; SETTING UP THE MODEL
[ASSUME alpha-sf (tag 'hyperhyper 0 (gamma 7 1))]
[ASSUME beta-sf (tag 'hyperhyper 2 (gamma 1 0.5))]
[ASSUME alpha-l (tag 'hyperhyper 1 (gamma 7 1))]
[ASSUME beta-l (tag 'hyperhyper 3 (gamma 1 0.5))]
[ASSUME alpha-s (tag 'hyperhyper 4 (gamma 7 1))]
[ASSUME beta-s (tag 'hyperhyper 5 (gamma 1 0.5))]
;; Parameters of the covariance function
[ASSUME sf (tag 'hyper 0 (log (gamma alpha-sf beta-sf )))]
[ASSUME l (tag 'hyper 1 (log (gamma alpha-l beta-l )))]
[ASSUME sigma (tag 'hyper 2 (uniform-continuous 0 2 ))]
;;  The covariance function
[ASSUME se (make-se sf l)]
[ASSUME wn (make-whitenoise sigma)]
[ASSUME composite-covariance (add-funcs se wn)]


;; Create a prober and emulator using gpmem
[ASSUME f-restr (get-neal-prober)]
[ASSUME compute-and-emu (gpmem f-restr composite-covariance)]

;; Plot data collection
[INFER (do
    (stats <- (extract-stats (second compute-and-emu)))
    (call-back collect-neal-plot-data 'before-probes sf l sigma ',stats))]

;; Probe all data points
[PREDICT (mapv (first compute-and-emu) (get-neal-data-xs))]

;; Plot data collection
[INFER (do
    (stats <- (extract-stats (second compute-and-emu)))
    (call-back collect-neal-plot-data 'after-probes sf l sigma ',stats))]

;; Infer hypers and hyperhypers
[INFER (repeat 100 (do
    (mh 'hyperhyper one 2)
    (mh 'hyper one 1)))]

;; Plot data collection
[INFER (do
    (stats <- (extract-stats (second compute-and-emu)))
    (call-back collect-neal-plot-data 'after-hyperinf sf l sigma ',stats))]

[INFER (call-back dump-neal-plot-data)]
```

Observed data is generated with the following model:

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

where σ is 0.1 with probability 0.95, 1 otherwise.



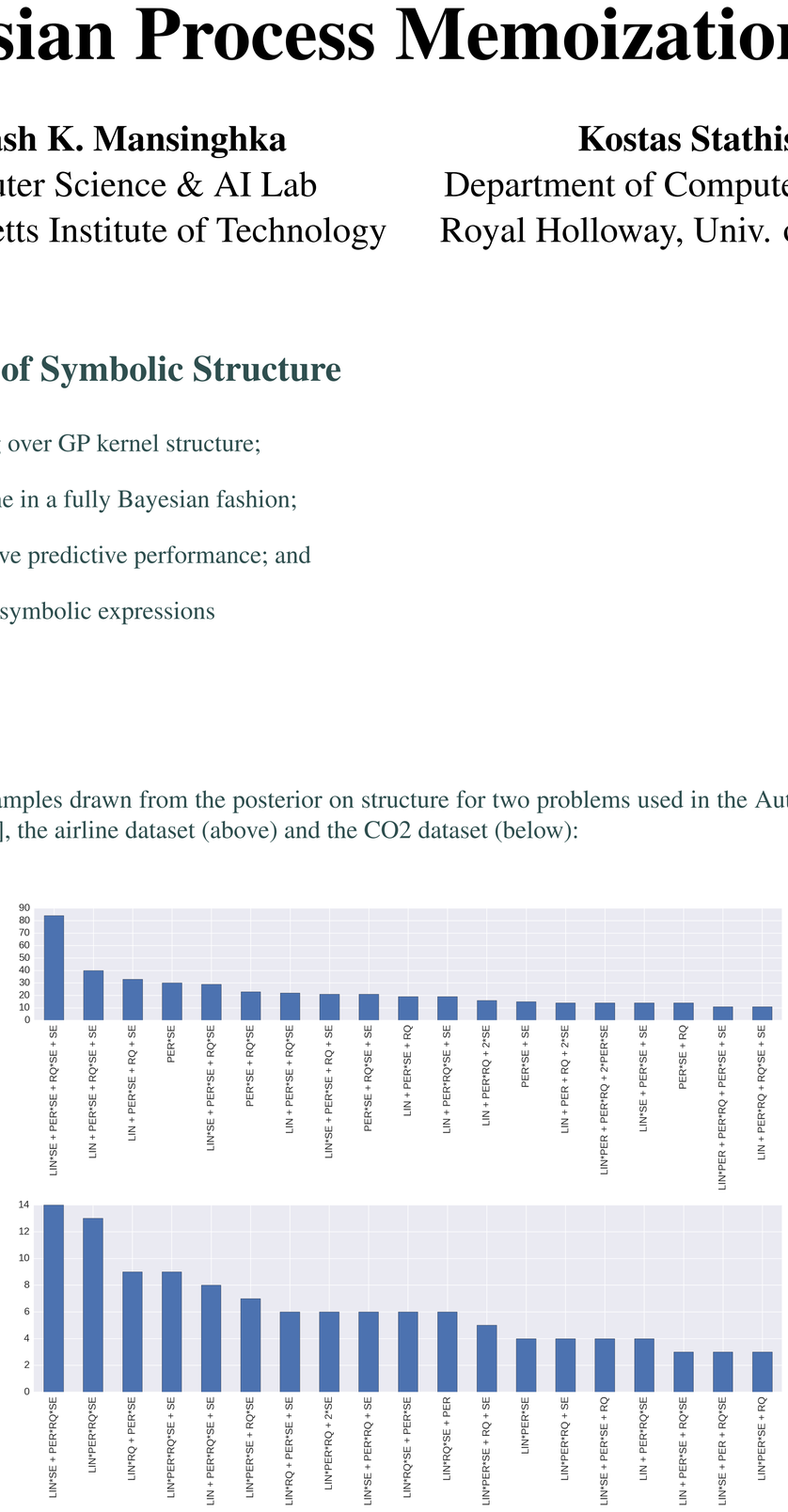
Above, we (left to right) we see predictions before data has been observed, after data has been observed, after we inferred over these observations. On the right, we see a contour plot and marginals of the the ℓ and θ hyper-parameters of the above program after inference (right).

Learning of Symbolic Structure

- reasoning over GP kernel structure;
- never done in a fully Bayesian fashion;
- competitive predictive performance; and
- adequate symbolic expressions

Results

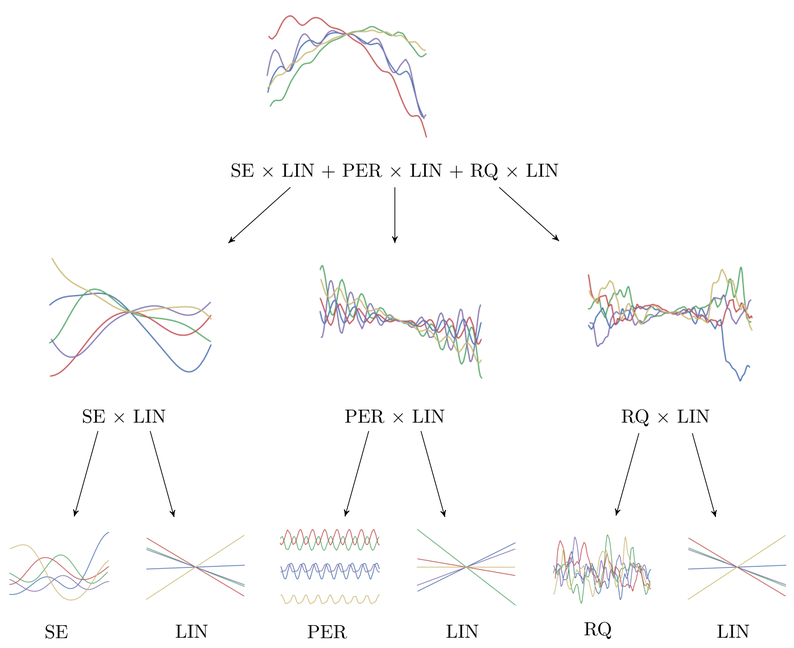
500 and 100 samples drawn from the posterior on structure for two problems used in the Automated Statistician Project [1], the airline dataset (above) and the CO2 dataset (below):



Listing 2: Venture Code for Bayesian GP Structure Learning

```
Place Holder
```

Decomposing a candidate Structure



Bayesian Optimization

Thompson Sampling

In Thompson sampling, the goal is to maximize the total reward received for all actions by placing a prior distribution $P(\theta)$ on the possible "contexts" $\theta \in \Theta$ with reward $r \in \mathbb{R}$.

Repeat:

1. Sample a context $\theta \sim P(\theta)$.
2. Choose an action $a \in \mathcal{A}$ which (approximately) maximizes $V(a|\theta) = \mathbb{E}\left[r|a, \theta\right]$.
3. Let r_{true} be the reward received for action a. Update the believed distribution on θ, i.e., $P(\theta) \leftarrow P_{\text{new}}(\theta)$ where $P_{\text{new}}(\theta) = P\left(\theta \mid a \mapsto r_{\text{true}}\right)$.

Listing 3: Venture Code for Bayesian Optimization

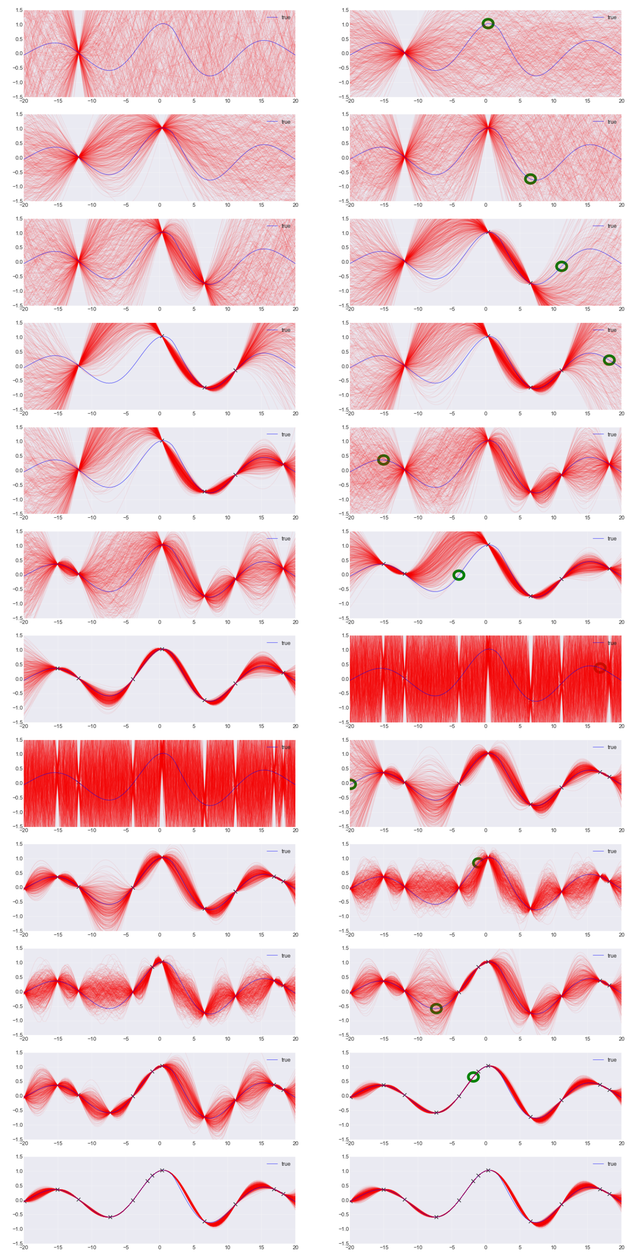
```
[INFER (load-plugin (quote symbol<"gppaper-plugin.py">) 'bayesopt)]

[ASSUME sf1 (tag 'hyper 0 (log (uniform-continuous 0 10)))]
[ASSUME l1 (tag 'hyper 1 (log (uniform-continuous 0 10)))]
[ASSUME se (make-se sf1 l1)]
[ASSUME blackbox-f (get-bayesopt-blackbox)]
[ASSUME compute-and-emu (gpmem blackbox-f se)]

[DEFINE get-uniform-candidate (lambda (prev-xs) (uniform-continuous -20 20))]
[DEFINE mc-argmax
        (lambda (emulator prev-xs)
          ((lambda (candidate-xs)
             (lookup candidate-xs
                     (argmax-of-array (mapv emulator candidate-xs))))
           (mapv (lambda (i) (get-uniform-candidate prev-xs))
                 (linspace 0 19 20))))]
[DEFINE emulator-point-sample
        (lambda (x)
          (run (sample
            (lookup ((second compute-and-emu) (array ,x))
                    0)))))]

[INFER
    (repeat 15 (do pass

      ;; Call f-compute on the next point
      (predict ((first compute-and-emu)
                ,(mc-argmax emulator-point-sample '-)))

      ;; Stats collection
      (stats-before <- (extract-stats (second compute-and-emu)))
      (call-back collect-bayesopt-plot-data sf1 l1 ',stats-before)

      ;; Hyperparameter inference
      (mh 'hyper one 50)

      ;; More stats collection
      (stats-after <- (extract-stats (second compute-and-emu)))
      (call-back collect-bayesopt-plot-data sf1 l1 ',stats-after)))]

[INFER (call-back dump-bayesopt-plot-data)]
```

Bayesian Optimization with `gpmem`

- contexts $\theta = (\mu, K)$ are Gaussian processes over the action space $\mathcal{A} = \mathbb{R}$.
- $K_{\text{prior}} = K_{\text{prior},\sigma,\ell}$ is a procedure, with parameters σ, ℓ, to be used as the prior covariance function: $K_{\text{prior}}(a, a') = \sigma^2 \exp\left(-\frac{(a-a')^2}{2\ell^2}\right)$
- σ and ℓ are (hyper)parameters for K_{prior}
- $\mathbf{a}_{\text{past}} = (a_i)_{i=1}^n$ are the previously probed actions
- $\mathbf{r}_{\text{past}} = (r_i)_{i=1}^n$ are the corresponding rewards

Right: Dynamics of Thompson sampling

- the blue curve is the true function V;
- the red region is a blending of 100 samples of the curve generated (jointly) by a GP-based emulator V_{emu};
- the left and right columns show the state of V_{emu} before and after hyperparameter inference
- in the right column, the next chosen probe point is circled in green;
- each successive probe point a is the (stochastic) maximum of V_{emu}, sampled pointwise and conditioned on the values of the previously probed points; and
- probes tend to happen at points either where the value of V_{emu} is high, or where V_{emu} has high uncertainty.



Conclusions

`gpmem` is a generalization of a number of GP related models and can be applied to:

- Hierarchical Bayesian GP
- Kernel Structure Learning
- Bayesian Optimization

References

[1] D. Duvenaud, J. R. Lloyd, R. Grosse, J. Tenenbaum, and Z. Ghahramani. Structure discovery in nonparametric regression through compositional kernel search. In *Proceedings of the 30th International Conference on Machine Learning (ICML-13)*, pages 1166–1174, 2013.

[2] R. M. Neal. Monte carlo implementation of gaussian process models for bayesian regression and classification. *arXiv preprint physics/9701026*, 1997.