Applications of Gaussian Processes

EN.540.782: Statistical Uncertainty Quantification

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Outline

Review: Gaussian Processes

Definition

A Gaussian Process (GP) is a collection of random variables $\{X_\alpha \mid \alpha \in \mathcal{X}\}$ any finite number of which have a joint Gaussian distribution.

- A GP is completely specified by:
  - mean function: $m(\boldsymbol{x}) = \mathbb{E}[f(\boldsymbol{x})]$
  - covariance kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = \mathrm{Cov}[f(\boldsymbol{x}), f(\boldsymbol{x}')]$
- Use conditional distributions to predict values at new inputs:
  - Observations: inputs $X \in \mathbb{R}^{n \times d}$, outputs $\boldsymbol{y} \in \mathbb{R}^n$.
  - For new inputs $X_\star \in \mathbb{R}^{n_\star \times d}$,

$$\mathbb{E}[\boldsymbol{y}_\star | X_\star, X, \boldsymbol{y}] = K(X_\star, X) K(X, X)^{-1} \boldsymbol{y}$$
$$\mathrm{Cov}[\boldsymbol{y}_\star | X_\star, X, \boldsymbol{y}] = K(X_\star, X_\star) - K(X_\star, X) K(X, X)^{-1} K(X, X_\star)$$

Problem Setting

- Objective $f : \mathcal{X} \to \mathbb{R}$ on domain $\mathcal{X} \subseteq \mathbb{R}^d$.
- We seek a global minimizer

$$\boldsymbol{x}^\star \in \operatorname*{argmin}_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x}) \,.$$

- Bayesian optimization (BO) is most appropriate when:
  - Evaluating f is expensive (and possibly noisy).
  - We have no derivative information.

Basic BO Algorithm

Algorithm 1: Bayesian Optimization

Data: objective function $f : \mathcal{X} \to \mathbb{R}$; initial sample $\mathcal{D}_n = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$

for $i \in \{n+1, \ldots, N\}$ **do**

  Fit a GPR model to data $\mathcal{D}_{i-1}$;

  Choose a new point $\boldsymbol{x}_i \in \mathcal{X}$;

  Evaluate $y_i \leftarrow f(\boldsymbol{x}_i)$;

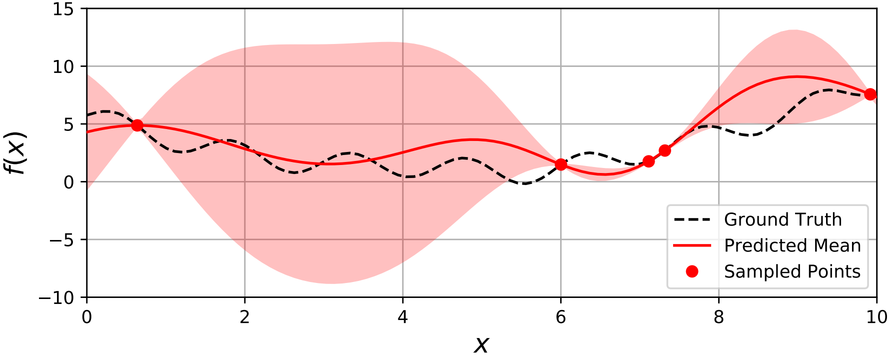
  Update sample $\mathcal{D}_i \leftarrow \mathcal{D}_{i-1} \cup \{(\boldsymbol{x}_i, y_i)\}$;

end

$j \leftarrow \operatorname*{argmin}_{1 \leq i \leq N} y_i$;

Result: approximate global minimizer $\boldsymbol{x}_j$

An Illustrated Example



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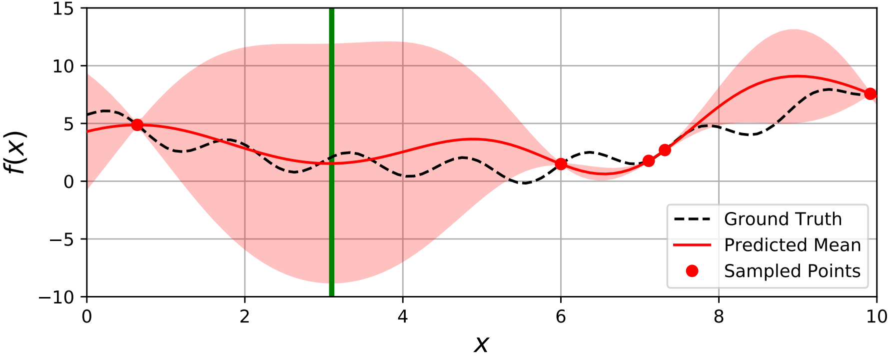

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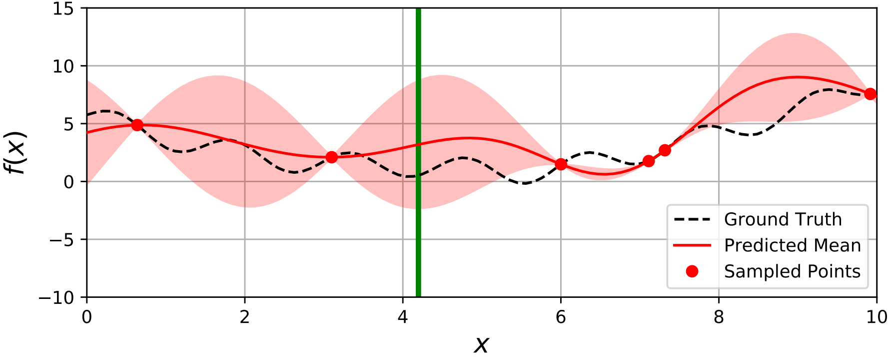

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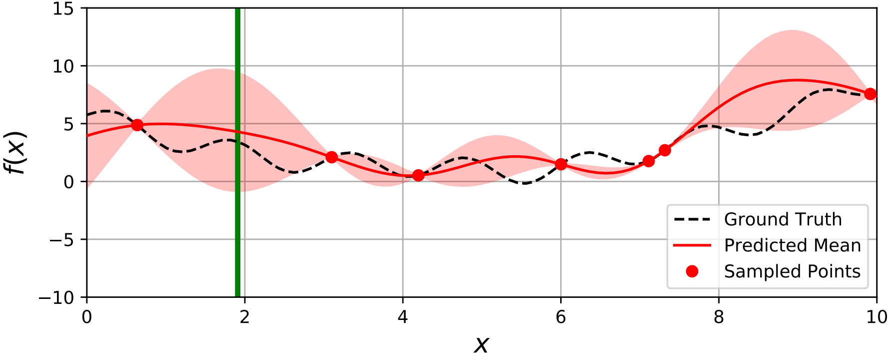

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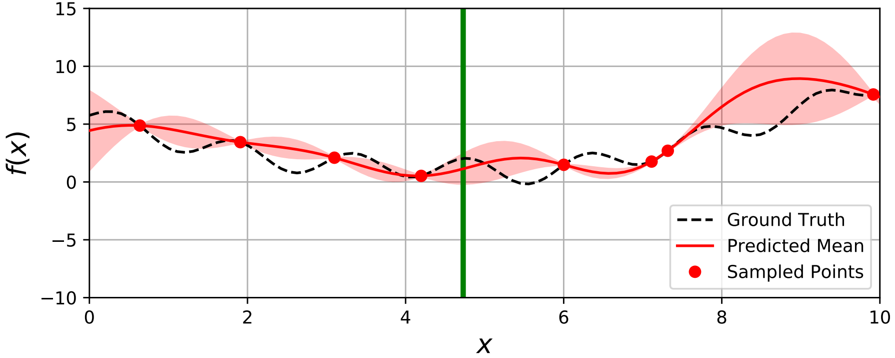

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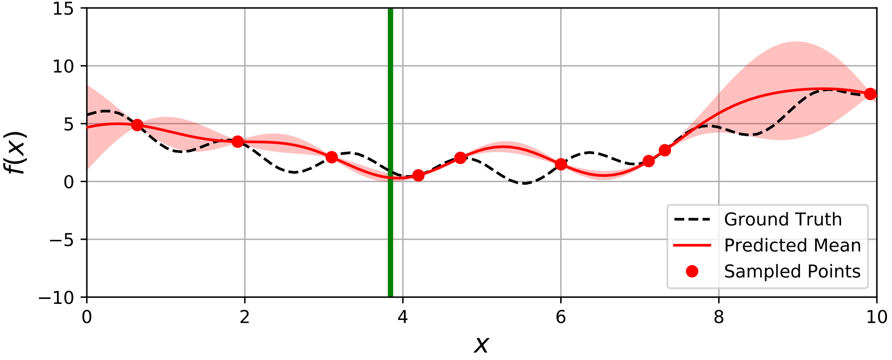

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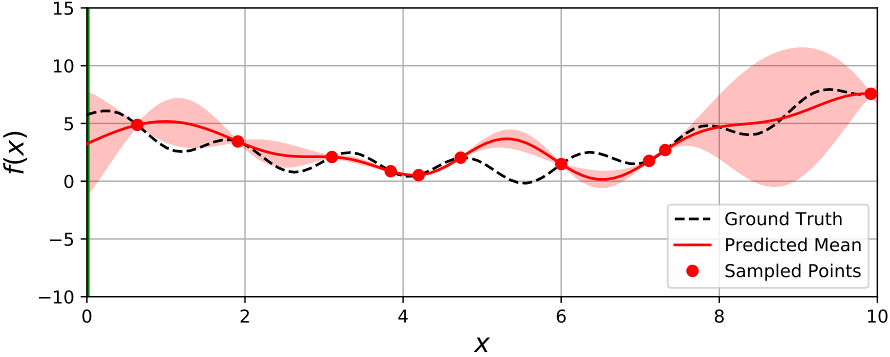

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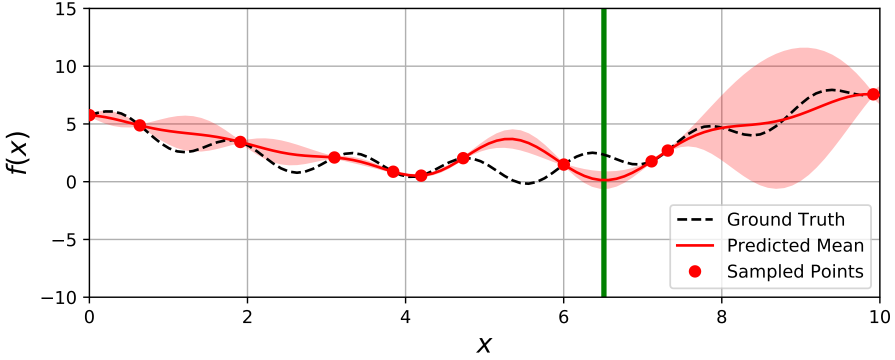

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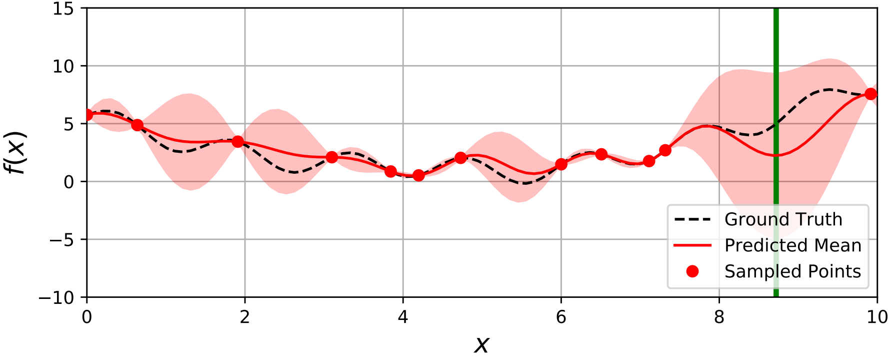

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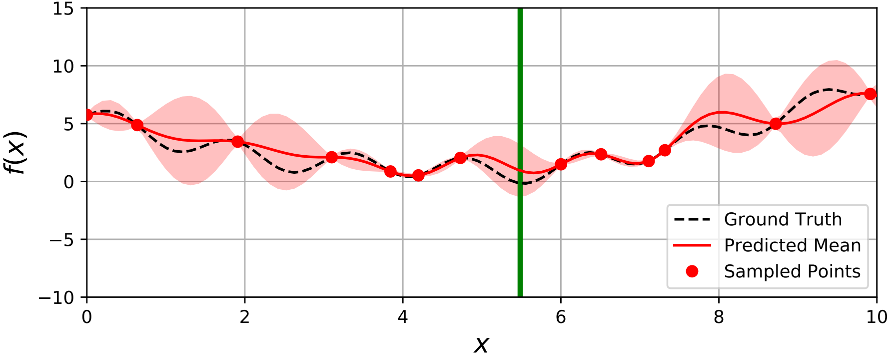

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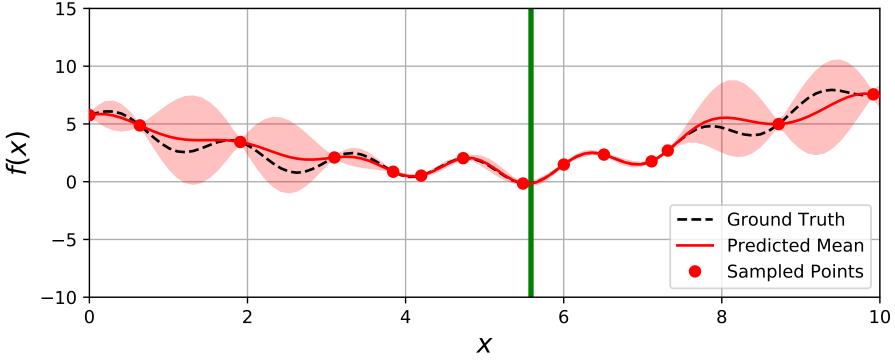

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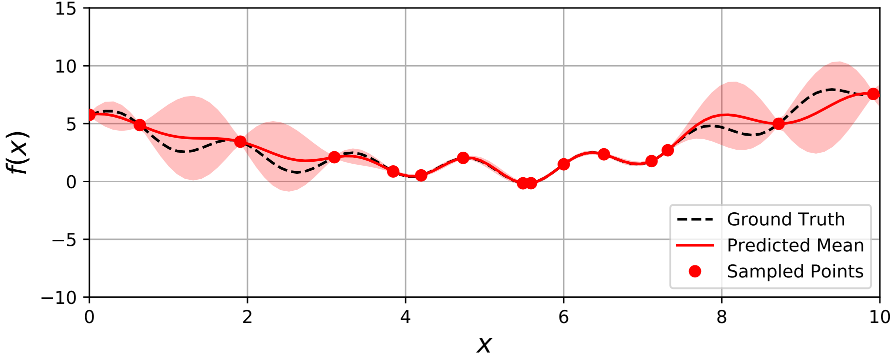


Selecting the Next Sample Point

- Use current knowledge to inform our choice.
- Exploration vs. Exploitation
- An acquisition function measures utility of sampling at $\boldsymbol{x} \in \mathcal{X}$:

$$\boldsymbol{x}_{i+1} = \operatorname*{argmax}_{\boldsymbol{x} \in \mathcal{X}} \alpha(\boldsymbol{x}; \mathcal{D}_i)$$

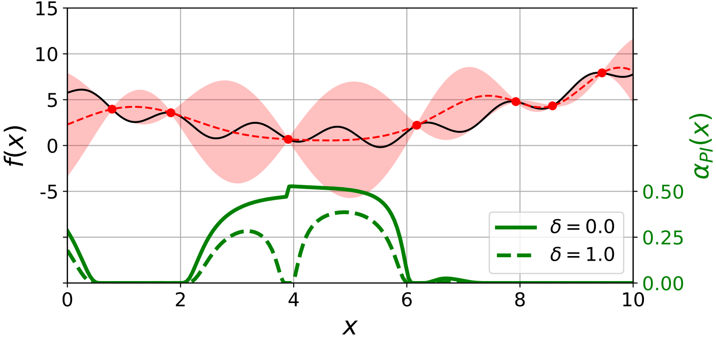
- How is this better? Optimizing α does not require evaluating f.

Acquisition Function: Probability of Improvement

- Which inputs are likely to improve the current best observation?
- Gaussian distribution provides an analytical expression:

$$\alpha_{PI}(\boldsymbol{x}; \mathcal{D}) = \mathbb{P}\left[f(\boldsymbol{x}) < \tau \mid \mathcal{D}\right] = \Phi\left(\frac{\tau - \mu(\boldsymbol{x})}{\sigma(\boldsymbol{x})}\right)$$

- Threshold τ usually written as $\tau = y_{\min} - \delta$ for $\delta \geq 0$.

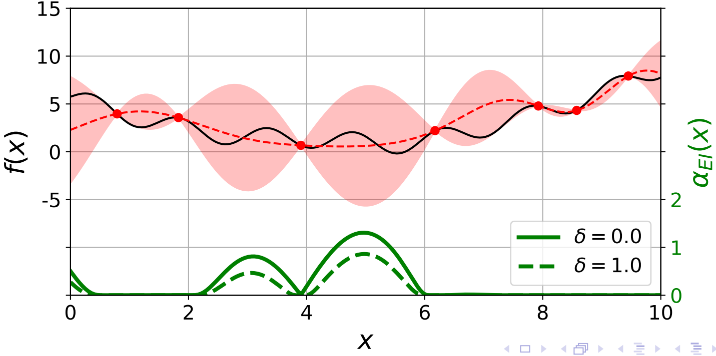


Acquisition Function: Expected Improvement

- Not all improvements are equally helpful.
- Expected improvement compared to threshold τ is

$$\alpha_{EI}(\boldsymbol{x};\mathcal{D}) = \mathbb{E}\left[\max(0,\, \tau - \mathcal{N}\left[\mu(\boldsymbol{x}), \sigma^2(\boldsymbol{x})\right])\right]$$
$$= (\tau - \mu(\boldsymbol{x}))\,\Phi\left(\frac{\tau - \mu(\boldsymbol{x})}{\sigma(\boldsymbol{x})}\right) + \sigma(\boldsymbol{x})\,\phi\left(\frac{\tau - \mu(\boldsymbol{x})}{\sigma(\boldsymbol{x})}\right).$$

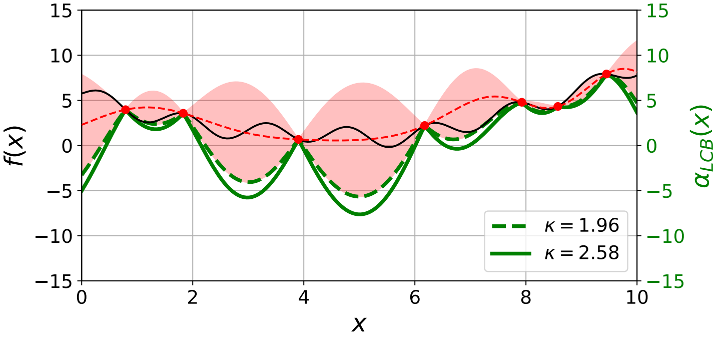
- Less prone than PI to become stuck in a local minimum.



Acquisition Function: Lower Confidence Bound

- Which inputs have superior best-case outputs?
- Usually expressed as a loss to be minimized:

$$\alpha_{LCB}(\boldsymbol{x}; \mathcal{D}) = \mu(\boldsymbol{x}) - \kappa\sigma(\boldsymbol{x})\,.$$



Computational Cost

- Inverting $K(X, X) \in \mathbb{R}^{n \times n}$ requires $O(n^3)$ operations.
- Cholesky decomposition must be updated each iteration.
- Approximation techniques exchange accuracy for speed.
- Using a sparse kernel for the GPR may help.

Pre-processing Data

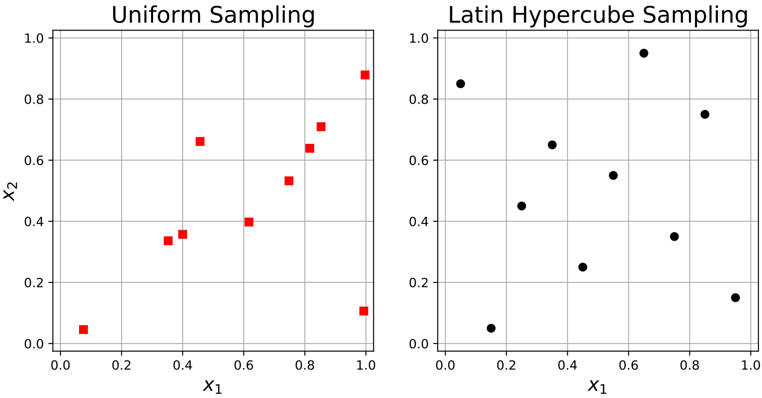
- Transforming sample data can facilitate GPR performance.
  - Normalize observations:

$$\tilde{\boldsymbol{x}}_i = \frac{\boldsymbol{x}_i - \bar{\boldsymbol{x}}}{s_x} \qquad \tilde{y}_i = \frac{y_i - \bar{y}}{s_y}$$

  - If outputs are necessarily positive: $\tilde{y}_i = \log(y_i)$.
  - Dimensionality reduction: focus on important directions.
- Apply knowledge of problem when deciding how to process data.
- Must reverse transformations to recover interpretable quantities.

Generating a Useful Initial Sample

- Samples drawn uniformly may not fill the domain.
- Latin hypercube sampling offers better samples for regression.



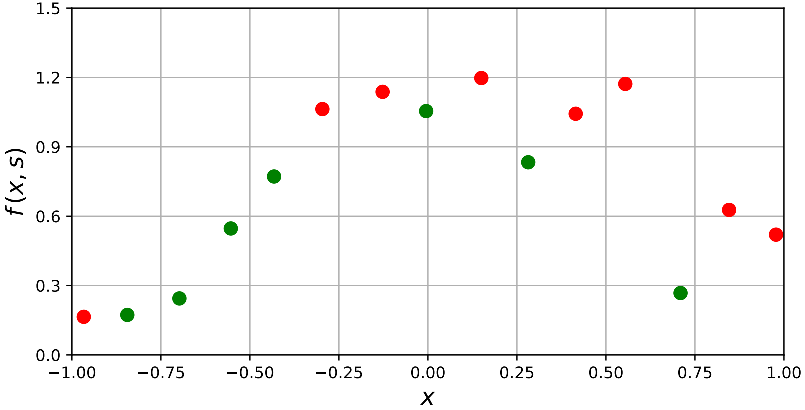
GPR with Qualitative Inputs

- Model a system as $f : \mathbb{R}^d \times S \to \mathbb{R}$ with $S = \{1, \ldots, n_s\}$.
- Can we do better than n_s separate fits?
- If the n_s surfaces are correlated, we can use expanded kernel

$$k\left((\boldsymbol{x}, s), (\boldsymbol{x}', s')\right) = C_{s,s'}\tilde{k}(\boldsymbol{x}, \boldsymbol{x}')\,,$$

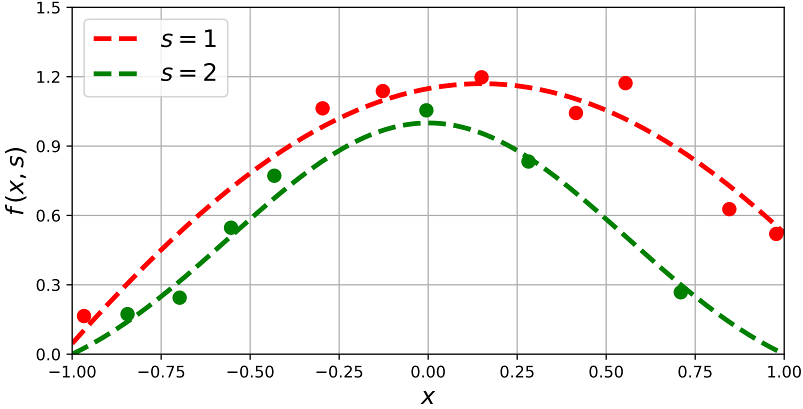
where $C \in \mathbb{R}^{n_s \times n_s}$ is a cross-correlation matrix.

A Mixed-Model Example



A Mixed-Model Example

$$f : [-1, 1] \times \{1, 2\} : (x, s) \mapsto \begin{cases} 1.9\cos(x - 0.15) - 0.73 & : s = 1 \\ (1 - x^2)e^{-x^2} & : s = 2 \end{cases}$$



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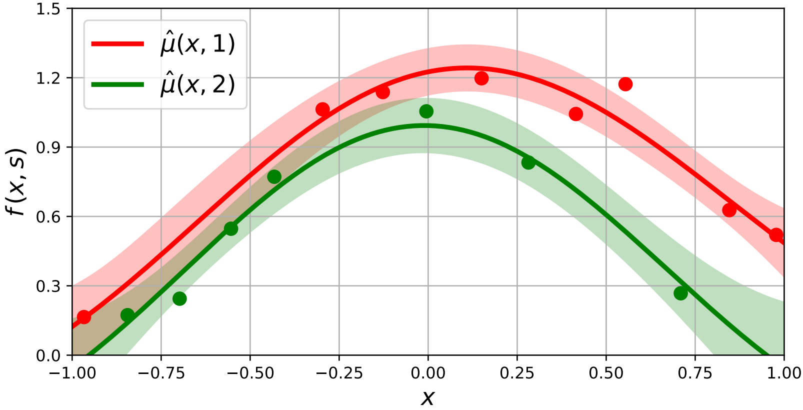
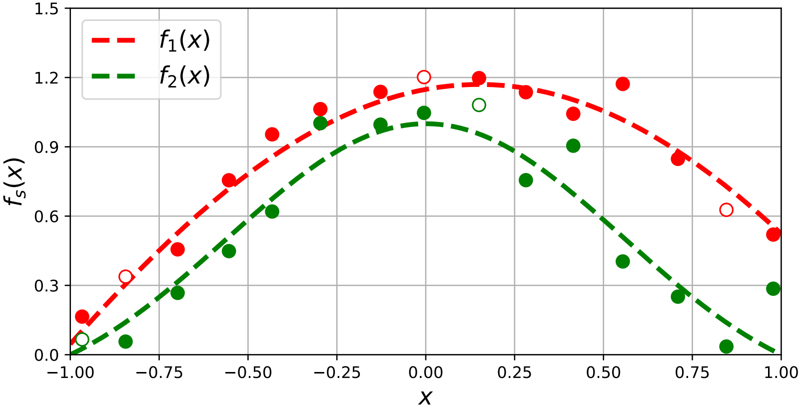


Multiple Regression

- The qualitative input scheme also works for multiple outputs:

$$\boldsymbol{y} = \mathbf{f}(\boldsymbol{x}) \in \mathbb{R}^{d'} \quad \longleftrightarrow \quad y_s = f(\boldsymbol{x}, s)$$

- Such an approach can accommodate missing output data.



References

- Frazier, P.I. "A Tutorial on Bayesian Optimization," *arXiv Preprint*, 22 pp. (2018). arXiv:1807.02811
- Luong, P.; Gupta, S.; Nguyen, D.; Rana, S.; Venkatesh, S. "Bayesian Optimization with Discrete Variables," in *AI 2019: Advances in Artificial Intelligence*, 473–84 (2019).
- Močkus, J. "On Bayesian Methods for Seeking the Extremum," in *Optimization Techniques: IFIP Technical Conference*, 400–04 (1975).
- Rasmussen, C.E.; Williams, C.K.I. *Gaussian Processes for Machine Learning*, MIT Press: Cambridge, MA (2006).
- Santner, T.J.; Williams, B.J.; Notz, W.I. *The Design and Analysis of Computer Experiments*," 2nd ed., Springer: New York, NY (2018).
- Shahriari, B.; Swersky, K.; Wang, Z.; Adams, R.P.; de Freitas, N. "Taking the Human Out of the Loop: A Review of Bayesian Optimization," *Proc. IEEE*, 104(1), 148–75 (2015).