Introduction to Gaussian Processes

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Outline

Prelude: Linear Regression

- Consider data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \subset \mathbb{R}^d \times \mathbb{R}$.
- We want the weight vector $\boldsymbol{w} \in \mathbb{R}^d$ that yields the best linear fit

$$f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x}\,.$$

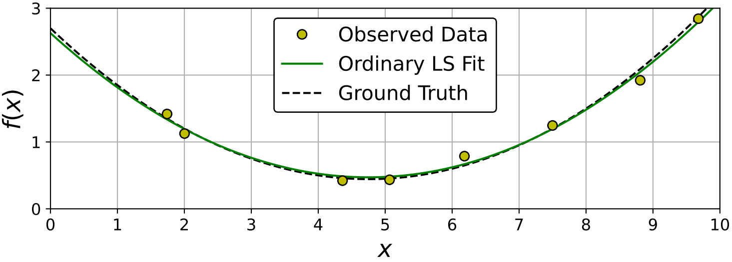
- Let $X \in \mathbb{R}^{n \times d}$ be the design matrix, $\boldsymbol{y} \in \mathbb{R}^n$ the response vector.
- Then $\widehat{\boldsymbol{w}} = X^\dagger \boldsymbol{y} = (X^\top X)^{-1} X^\top \boldsymbol{y}$ minimizes the squared error:

$$X^\dagger \boldsymbol{y} \in \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^d} = \|X\boldsymbol{w} - \boldsymbol{y}\|_2^2\,.$$

Linear Regression with Basis Functions

- Consider data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n} \subset \mathbb{R}^d \times \mathbb{R}$.
- For weight vector $\boldsymbol{w} \in \mathbb{R}^N$ and basis functions $\phi_j : \mathbb{R}^d \to \mathbb{R}$,

$$f(\boldsymbol{x}) = \boldsymbol{w}^\top \phi(\boldsymbol{x}) = \sum_{j=1}^{N} w_j \phi_j(\boldsymbol{x})\,.$$



Bayesian Linear Regression

- The standard linear model for "frequentist" regression is given by

$$\begin{aligned} f(\boldsymbol{x}) &= \boldsymbol{w}^\top \boldsymbol{x}\,, \\ y_i &= f(\boldsymbol{x}_i) + \varepsilon_i\,, \\ \varepsilon_i &\overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma_\varepsilon^2)\,. \end{aligned}$$

- In a Bayesian framework, we have $\boldsymbol{y} \,|\, X, \boldsymbol{w} \sim \mathcal{N}(X\boldsymbol{w}, \sigma_\varepsilon^2\, I)$.
- With prior $\boldsymbol{w} \sim \mathcal{N}(\boldsymbol{0}, \Sigma_p)$, the resulting posterior is

$$\begin{aligned} \boldsymbol{w} \,|\, X, \boldsymbol{y} &\sim \mathcal{N}(\bar{\boldsymbol{w}}, C)\,, \\ C^{-1} &= \sigma_\varepsilon^{-2} X^\top X + \Sigma_p^{-1}\,, \\ \bar{\boldsymbol{w}} &= \sigma_\varepsilon^{-2} C X^\top \boldsymbol{y}\,. \end{aligned}$$

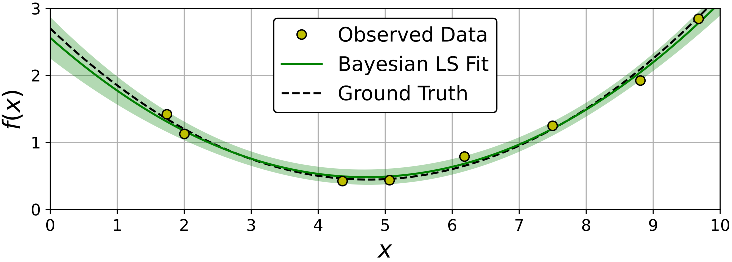
[Rasmussen & Williams, 2006]

Bayesian Linear Regression: Prediction

- We can use the posterior on $\boldsymbol{w}$ to predict new observations.
- For a new input $\boldsymbol{x}_\star \in \mathbb{R}^d$,

$$y_\star \,|\, \boldsymbol{x}_\star, X, \boldsymbol{y} \sim \mathcal{N}(\bar{\boldsymbol{w}}^\top \boldsymbol{x}_\star,\ \boldsymbol{x}_\star^\top C \boldsymbol{x}_\star)\,.$$

[Rasmussen & Williams, 2006]



Gaussian Processes

Definition (Rasmussen and Williams, 2006)

A Gaussian process (GP) is a collection of random variables $\{Y_{\boldsymbol{x}} \mid \boldsymbol{x} \in \mathcal{X}\}$, any finite number of which have a joint Gaussian distribution.

- The index set $\mathcal{X}$ is often an interval $T \subseteq \mathbb{R}$.
- A GP is completely specified by:
  - mean function: $m(\boldsymbol{x}) = \mathbb{E}[Y_{\boldsymbol{x}}]$
  - covariance kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = \mathrm{Cov}[Y_{\boldsymbol{x}}, Y_{\boldsymbol{x}'}]$

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Example (Pavliotis, 2014)

Brownian Motion on $\mathbb{R}$:

$$m(t) = 0 \qquad\qquad k(t, t') = \min(t, t')$$

Ornstein-Uhlenbeck Process:

$$m(t) = x_0 e^{-\alpha t} \qquad\qquad k(t, t') = \frac{1}{\alpha\beta}\left(e^{-\alpha|t-t'|} - e^{-\alpha(t+t')} \right)$$

Function-Space View of GPs

- Any GP defines a distribution over functions $f : \mathcal{X} \to \mathbb{R}$:

$$f(\boldsymbol{x}|\omega) = Y_{\boldsymbol{x}}(\omega)$$

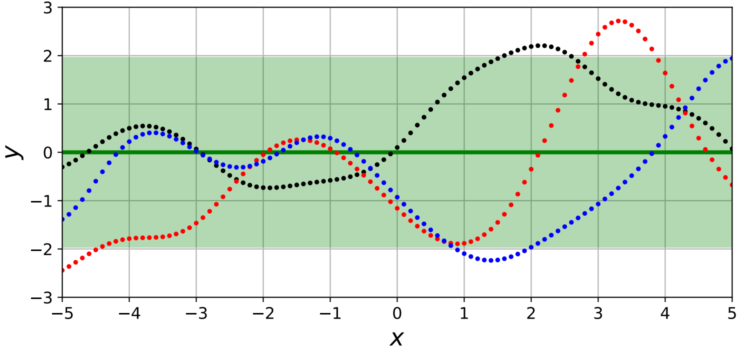
- How do we sample $f \sim \mathcal{GP}\left[m(\cdot), k(\cdot,\cdot)\right]$?
  - Choose $\mathcal{D}_X = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$.
  - Compute $m_i = m(\boldsymbol{x}_i)$, $K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$.
  - Draw $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{m}, K)$ and take $f(\boldsymbol{x}_i) = y_i$.
- Use conditional distributions to sample $y_\star = f(\boldsymbol{x}_\star)$ for $\boldsymbol{x}_\star \notin \mathcal{D}_X$:

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

[Rasmussen & Williams, 2006]

Sampling from a GP

- Prior distribution: $m(x) \equiv 0,\ k(x, x') = \exp\left[-\frac{1}{2}(x - x')^2\right]$
- Can draw (discretized) functions from prior or posterior.
- Plotted points are entries from MVN vectors.



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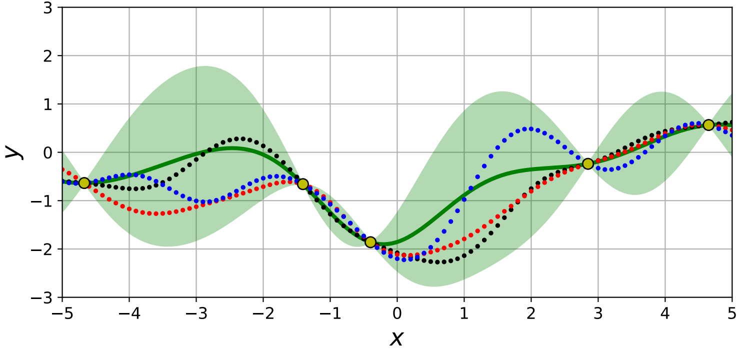


Covariance Functions: Concepts

- A kernel must be symmetric and positive semidefinite.
  - For all $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{X}$, $k(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}', \boldsymbol{x})$.
  - Given measure μ, for all $f \in L^2(\mathcal{X}, \mu)$,

$$\iint_{\mathcal{X} \times \mathcal{X}} k(\boldsymbol{x}, \boldsymbol{x}') f(\boldsymbol{x}) f(\boldsymbol{x}') \, d\mu(\boldsymbol{x}) \, d\mu(\boldsymbol{x}') \geq 0 \,.$$

- We say k is stationary if $k(\boldsymbol{x}, \boldsymbol{x}') = g(\boldsymbol{x} - \boldsymbol{x}')$.
- We say k is isotropic if $k(\boldsymbol{x}, \boldsymbol{x}') = g(\|\boldsymbol{x} - \boldsymbol{x}'\|)$.
- Kernels can be added, multiplied, and scaled:

$$k(\boldsymbol{x}, \boldsymbol{x}') = c_1^2 k_1(\boldsymbol{x}, \boldsymbol{x}') + c_2^2 k_2(\boldsymbol{x}, \boldsymbol{x}') k_3(\boldsymbol{x}, \boldsymbol{x}') \,.$$

[Duvenaud, 2014; Rasmussen & Williams, 2006]

Continuity and Differentiability

Definition (Rasmussen and Williams, 2006)

Let $f \sim \mathcal{GP}\left[m(\cdot), k(\cdot,\cdot)\right]$ be a Gaussian process on $\mathcal{X} \subseteq \mathbb{R}^d$. Then f is continuous in mean square (CMS) at $\boldsymbol{x}_\star \in \mathcal{X}$ if

$$\lim_{\boldsymbol{x} \to \boldsymbol{x}_\star} \mathbb{E}\left[\left|f(\boldsymbol{x}) - f(\boldsymbol{x}_\star)\right|^2\right] = 0\,.$$

We say that f is mean-square differentiable (MSD) at $\boldsymbol{x}_\star$ with partial derivatives $\partial f(\boldsymbol{x}_\star)/\partial x_i$ if, for $i \in \{1, \ldots, d\}$,

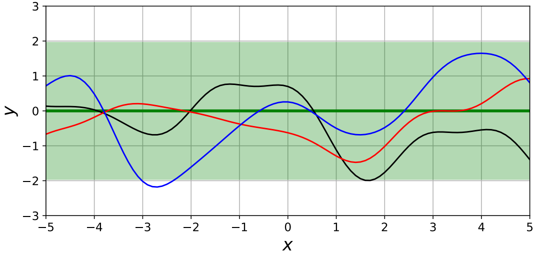
$$\lim_{h \to 0} \mathbb{E}\left[\left(\frac{f(\boldsymbol{x}_\star + h\boldsymbol{e}_i) - f(\boldsymbol{x}_\star)}{h} - \frac{\partial f(\boldsymbol{x}_\star)}{\partial x_i}\right)^2\right] = 0\,.$$

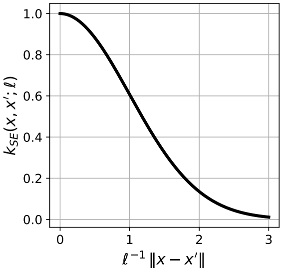
- GP with kernel k is CMS at $\boldsymbol{x}_\star \in \mathcal{X}$ iff k is continuous at $(\boldsymbol{x}_\star, \boldsymbol{x}_\star)$.
- A $2p$-order derivative of $k(\boldsymbol{x}_\star, \boldsymbol{x}_\star)$ ensures f is MSD p times at $\boldsymbol{x}_\star$.

Covariance Kernels: Squared Exponential

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left[-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|^2}{2\ell^2}\right] \qquad \ell > 0$$

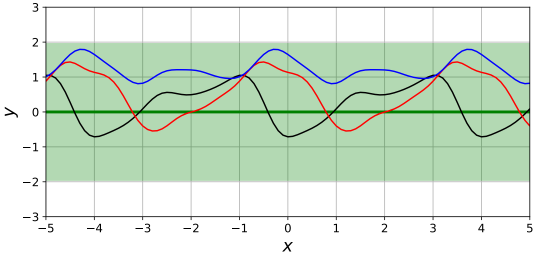
- Infinitely mean-square differentiable
- Often a limiting case of other kernel families

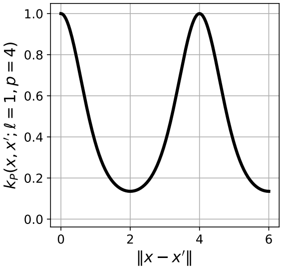




Covariance Kernels: Periodic

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left[-\frac{2\sin^2\left(\pi\|\boldsymbol{x} - \boldsymbol{x}'\|/p\right)}{\ell^2}\right] \qquad \ell, p > 0$$

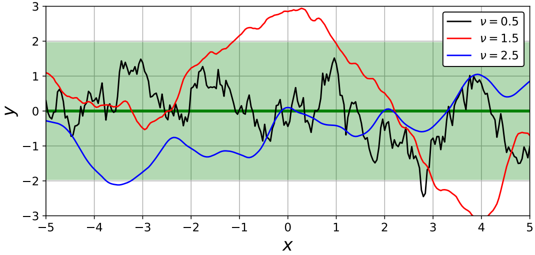


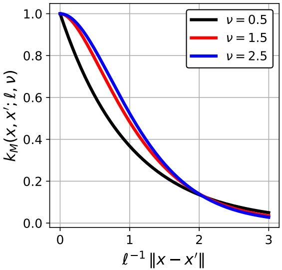


Covariance Kernels: Matérn

$$k(\boldsymbol{x}, \boldsymbol{x}') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{r\sqrt{2\nu}}{\ell} \right)^{\nu} K_{\nu} \left(\frac{r\sqrt{2\nu}}{\ell} \right) \qquad \ell, \nu > 0$$

$K_{\nu}(\cdot)$ is a modified Bessel function





Matérn Kernel Smoothness Parameter

- Mean-square differentiable $\lceil \nu \rceil - 1$ times.
- Reduces to squared exponential as $\nu \to \infty$.
- Simpler forms for $\nu + \frac{1}{2} \in \mathbb{N}$:

$$k_{1/2}(r) = \exp\left[-\frac{r}{\ell}\right] \qquad k_{3/2}(r) = \left(1 + \frac{r\sqrt{3}}{\ell}\right)\exp\left[-\frac{r\sqrt{3}}{\ell}\right]$$

$$k_{5/2}(r) = \left(1 + \frac{r\sqrt{5}}{\ell} + \frac{5r^2}{3\ell^2}\right)\exp\left[-\frac{r\sqrt{5}}{\ell}\right]$$

[Rasmussen & Williams, 2006]

Generalizing Isotropic Kernels

- Most common kernels are defined as $k(\boldsymbol{x}, \boldsymbol{x}') = g(\|\boldsymbol{x} - \boldsymbol{x}'\|)$.
- What if some directions are more important than others?

$$k(\boldsymbol{x}, \boldsymbol{x}') = g\left(\sum_{i=1}^{d} \frac{|x_i - x_i'|}{\ell_i}\right)$$

- For interactions among directions, use a Mahalanobis metric, *e.g.*,

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left[-(\boldsymbol{x} - \boldsymbol{x}')^\top M^{-1}(\boldsymbol{x} - \boldsymbol{x}')\right],$$

with M symmetric, positive definite.

Fitting GPs to Data

- Consider data $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \subset \mathbb{R}^d \times \mathbb{R}$.
- Recall the prediction for $y_\star = f(\boldsymbol{x}_\star)$ at $\boldsymbol{x}_\star \notin \mathcal{D}_X$:

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

- Must account for measurement noise when choosing a model.
- Given $\mathcal{D}$, the GPR model is specified by our choice of kernel.

[Goldberg *et al.*, 1997; Rasmussen & Williams, 2006]

Model Selection

- GP Regression requires:
  - Selecting a kernel function (model).
  - Tuning hyperparameters $\boldsymbol{\theta} \in \mathbb{R}^p$.
- The log-marginal likelihood is

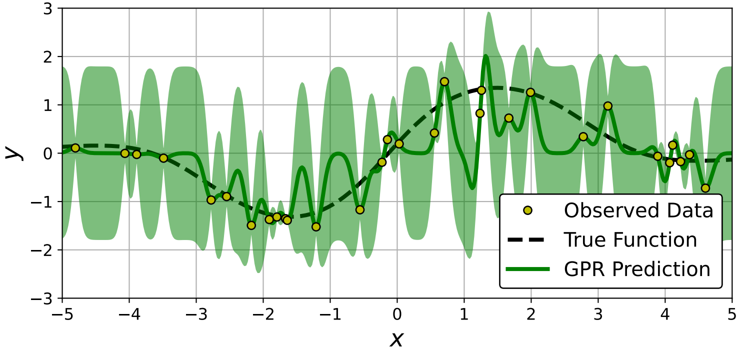
$$\log p(\boldsymbol{y} \mid X, \boldsymbol{\theta}) = -\frac{1}{2}\, \boldsymbol{y}^\top K_{\boldsymbol{\theta}}^{-1} \boldsymbol{y} - \frac{1}{2} \log |K_{\boldsymbol{\theta}}| - \frac{n}{2} \log(2\pi)\,,$$
$$K_{\boldsymbol{\theta}} = K(X, X; \boldsymbol{\theta}) + N(\boldsymbol{\theta})\,,$$

  where $N(\boldsymbol{\theta})$ models noise in outputs, $y_i = f(\boldsymbol{x}_i) + \varepsilon_i$.
- Cross-validation is also possible.
  - Block matrix inversion speeds up prediction.
  - Loss minimization requires expensive derivatives.

[Rasmussen & Williams, 2006]

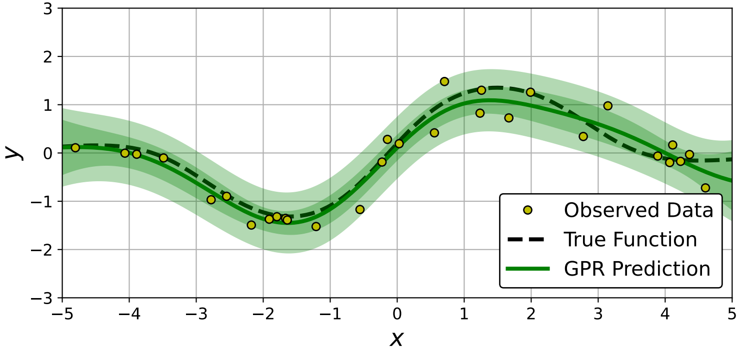
Model Selection: An Illustration

- Observed outputs are corrupted by iid $\mathcal{N}(0, 0.3^2)$ noise.
- Assuming outputs are noiseless: length scale $\ell = 0.0972$



Model Selection: An Illustration

- Observed outputs are corrupted by iid $\mathcal{N}(0, 0.3^2)$ noise.
- Including noise-level hyperparmater: length scale $\ell = 1.42$



Dealing with Noisy Outputs

- Often, we can only observe $y_i = f(\boldsymbol{x}_i) + \varepsilon_i$.
- Standard approach: assume independent $\varepsilon_i \sim \mathcal{N}(0, \sigma_\varepsilon^2)$
- Predictive distribution is given by

$$
\begin{aligned}
\mathbb{E}\left[\boldsymbol{y}_\star | X_\star, X, \boldsymbol{y}\right] &= K(X_\star, X) K_{\boldsymbol{y}}^{-1} \boldsymbol{y} \\
\mathrm{Cov}\left[\boldsymbol{y}_\star | X_\star, X, \boldsymbol{y}\right] &= K_\star - K(X_\star, X) K_{\boldsymbol{y}}^{-1} K(X, X_\star) \\
K_{\boldsymbol{y}} &= K(X, X) + \sigma_\varepsilon^2 I \\
K_\star &= K(X_\star, X_\star) + \sigma_\varepsilon^2 I
\end{aligned}
$$

Uncertainty vs. Variability

- Often wrongly used as synonyms.
  - Uncertainty: Lack of knowledge of a deterministic quantity
  - Variability: Differences in nominally interchangeable objects
- Distinct, but intertwined, concepts.
  - Uncertainty is quantified in probabilistic terms.
  - Variability is expressed in the language of statistics.
- Two main classes of uncertainty:
  - Aleatoric: difference in outcomes from repeated experiments
  - Epistemic: imprecise results from incomplete information

[Begg *et al.*, 2014; Der Kiureghian & Ditlevsen, 2009]

An Important Distinction

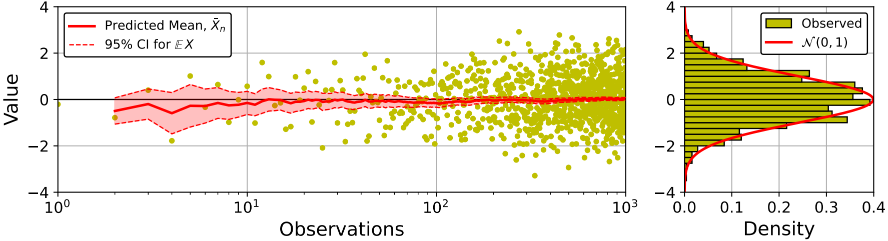
Consider independent variables $X_i \overset{\text{iid}}{\sim} \mathcal{N}(0,1)$.

<u>Estimate the Mean</u>

$$\mathbb{V}\left[\bar{X}_n\right] = \mathbb{V}\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] = \frac{1}{n} \to 0$$

<u>Predict the Next Value</u>

$$\mathbb{V}\left[X_{n+1}\right] = 1 \;\; \forall\, n \in \mathbb{N}$$



Uncertainty Quantification in GPR

- Predictive variance as a measure of confidence in model prediction
- For noiseless observations, no distinction: $\mathbb{V}[y] = \mathbb{V}[f(\boldsymbol{x})]$
- When noise is independent of input $\boldsymbol{x}$,

$$\mathbb{V}[y] = \mathbb{V}[f(\boldsymbol{x}) + \varepsilon] = \mathbb{V}[f(\boldsymbol{x})] + \sigma_\varepsilon^2$$

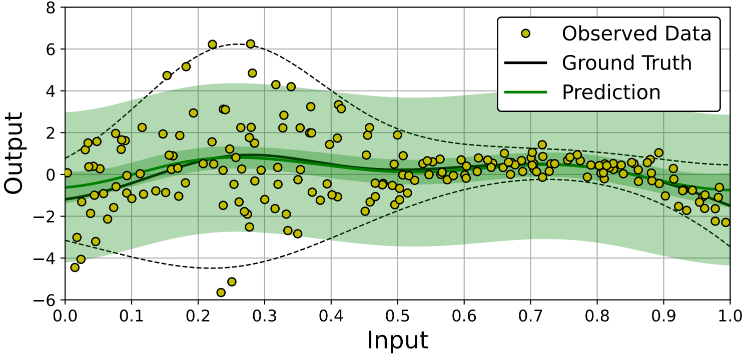
- We can quantify uncertainty "for the mean" or "for outputs."

What if the Noise Level Varies?

- Single hyperparameter σ_ε^2 implies homoscedasticity.
- Estimate $v_i \approx \sigma_\varepsilon^2(\boldsymbol{x}_i)$ and use $K_{\boldsymbol{y}} = K(X, X) + \text{diag}(\boldsymbol{v})$.
- For complete results, also need $v_\star \approx \sigma_\varepsilon^2(\boldsymbol{x}_\star)$ at test points.

GPR with Heteroscedastic Noise

- Use a secondary GPR to model the varying noise level.
- Incorporate noise estimates into likelihood of primary model.



[Kersting *et al.*, 2007; Zhang *et al.*, 2020]

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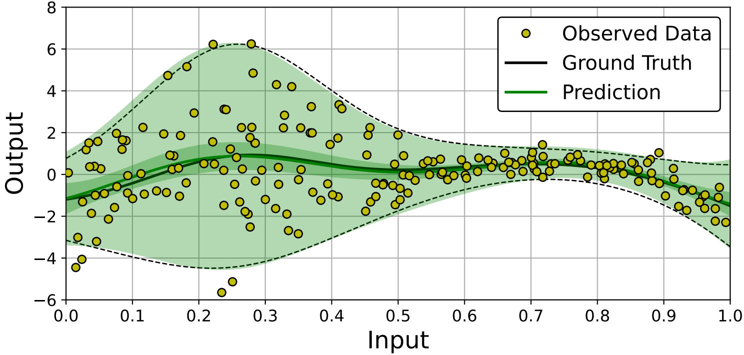


[Kersting *et al.*, 2007; Zhang *et al.*, 2020]

GPR with Qualitative Inputs

- Model a system as $f : \mathbb{R}^d \times S \to \mathbb{R}$ with $S = \{1, 2, \dots, n_s\}$.
- 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.

[Santner *et al.*, 2018]

Modeling Cross-Correlation

- Describe correlation between response surfaces $f(\cdot, s)$.
- Must have $C_{s,s} = 1$ and $|C_{s,s'}| \leq 1$ for all $s, s' \in S$.
- Options include:
  - Exchangable model:

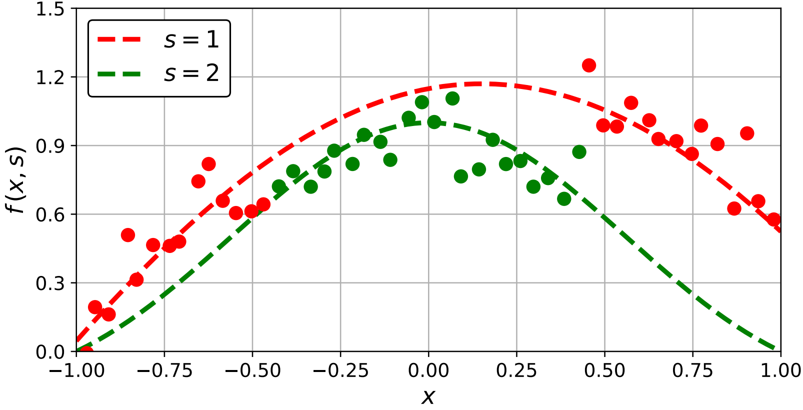
$$C_{s,s'} = \begin{cases} 1 & : s = s' \\ \rho & : s \neq s' \end{cases}$$

  - Toeplitz model for ordinal categories: $C_{s,s'} = e^{-\gamma|s-s'|}$
  - Specify all $\frac{1}{2}n_s(n_s - 1)$ superdiagonal entries.

[Qian *et al.*, 2008; Santner *et al.*, 2018]

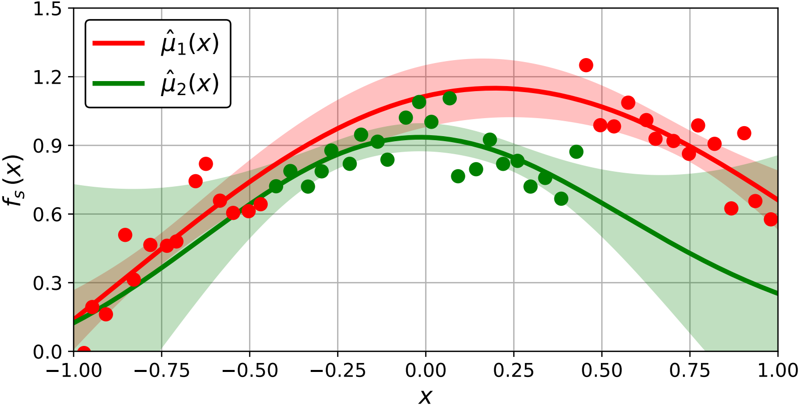
Mixed-Input Example: Data

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



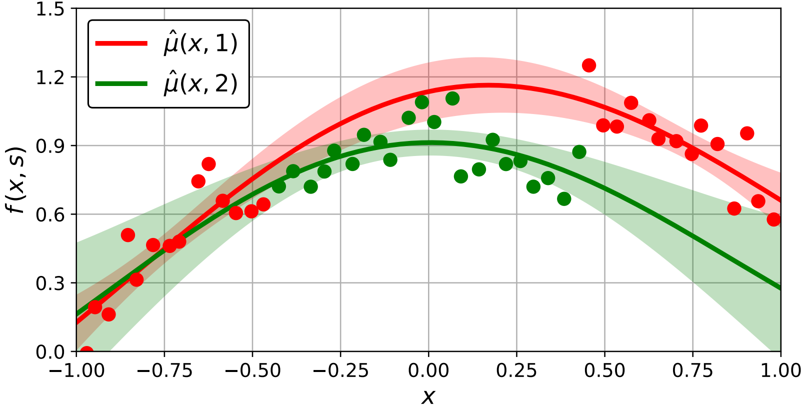
Mixed-Input Example: Disjoint Fits

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



Mixed-Input Example: Combined Fit

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

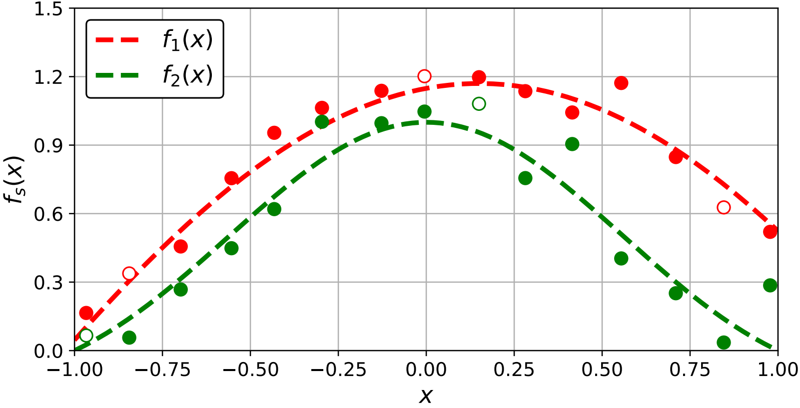


Multiple Regression

- 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.



[Santner *et al.*, 2018]

Bayesian Optimization

- 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.

[Frazier, 2018]

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

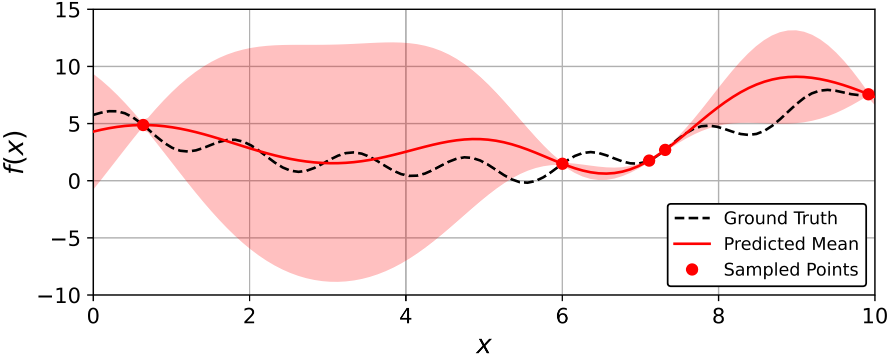
  Update sample $\mathcal{D}_i \leftarrow \mathcal{D}_{i-1} \cup \{(\boldsymbol{x}_i, y_i)\}$;

end

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

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

An Illustrated Example



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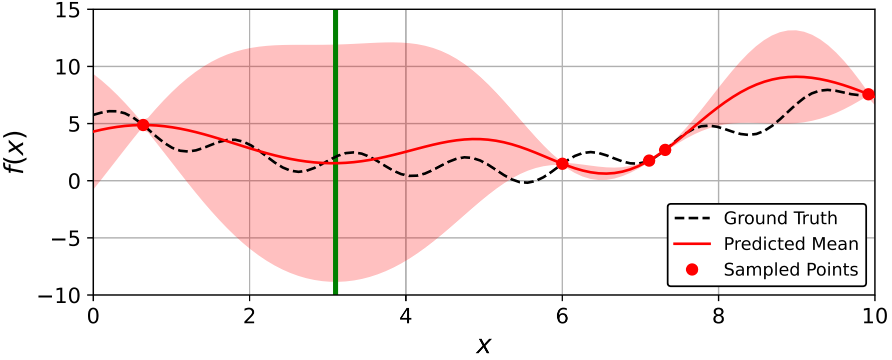

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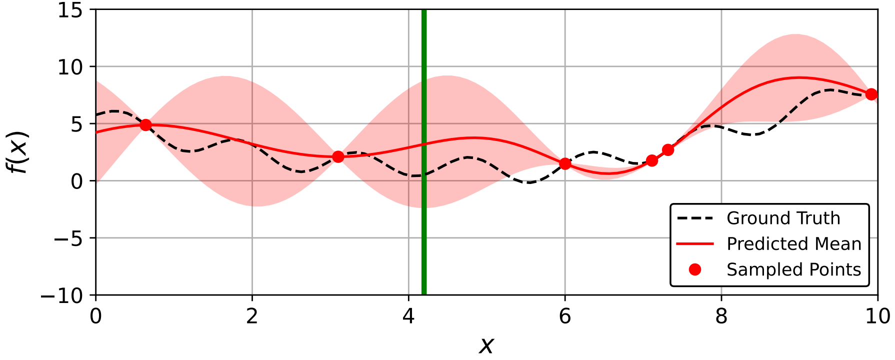
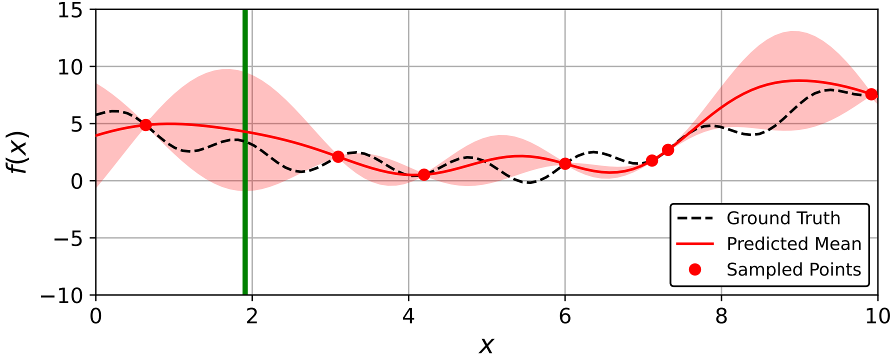


An Illustrated Example



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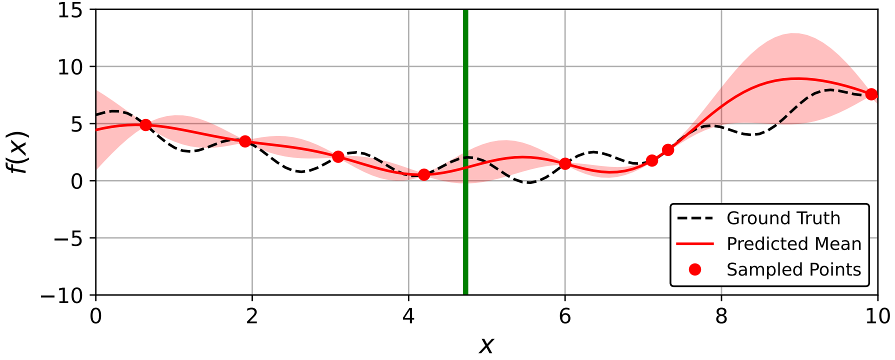

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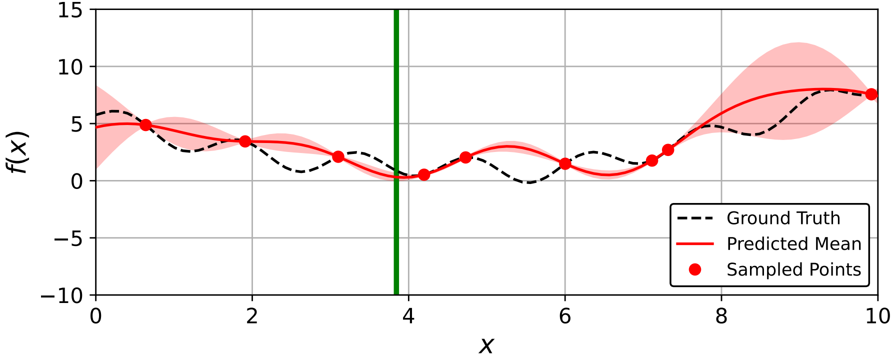

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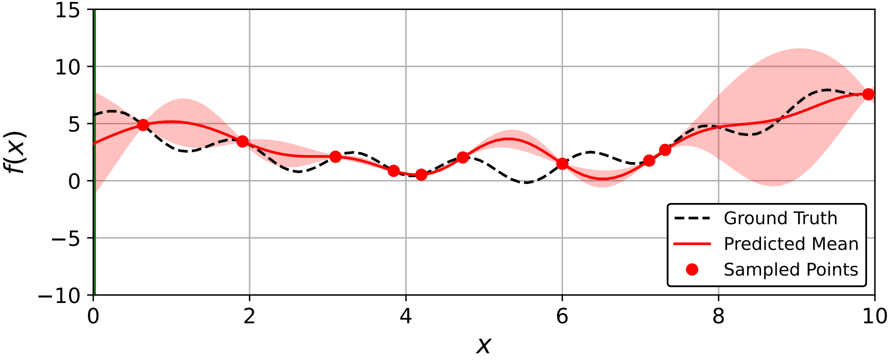

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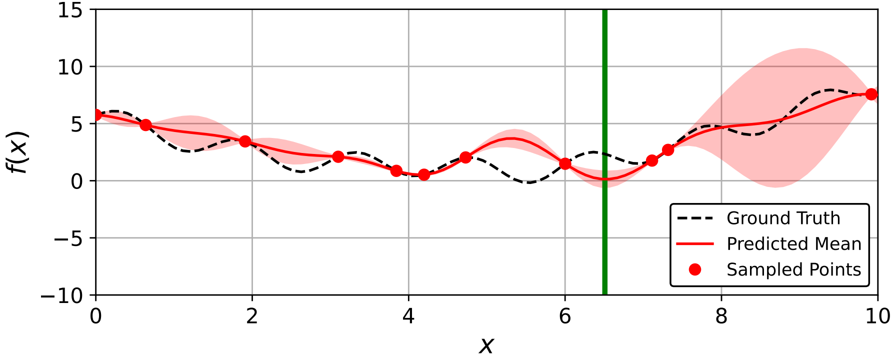

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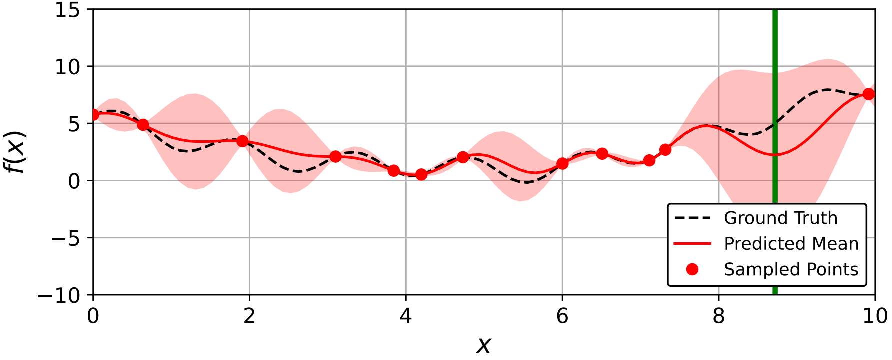

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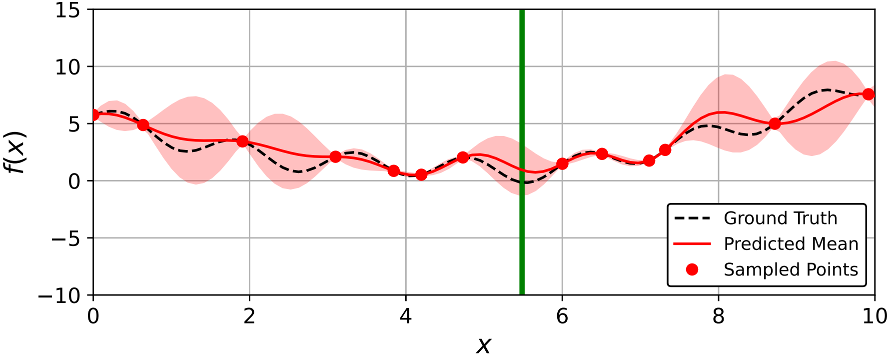

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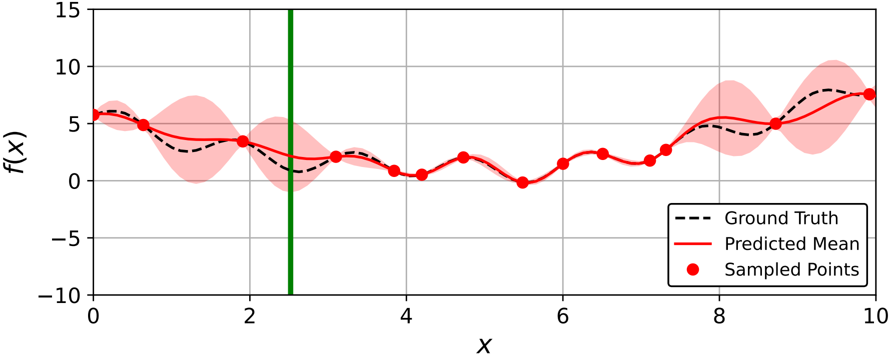

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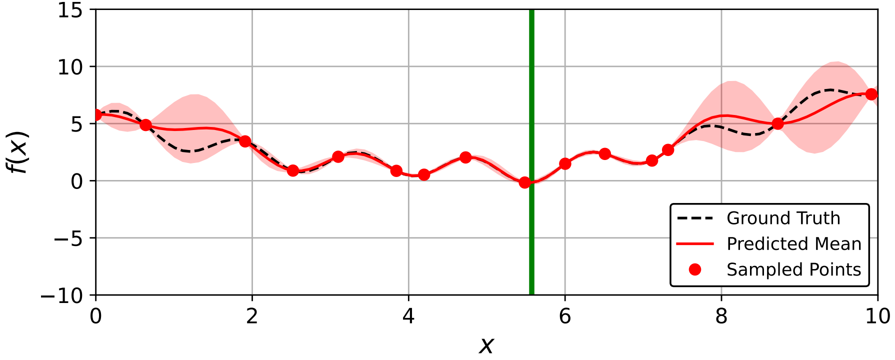

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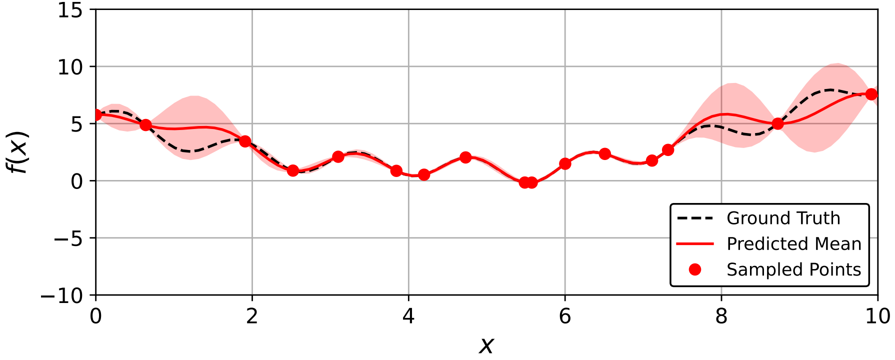


Selecting the Next Sample Point

- 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.

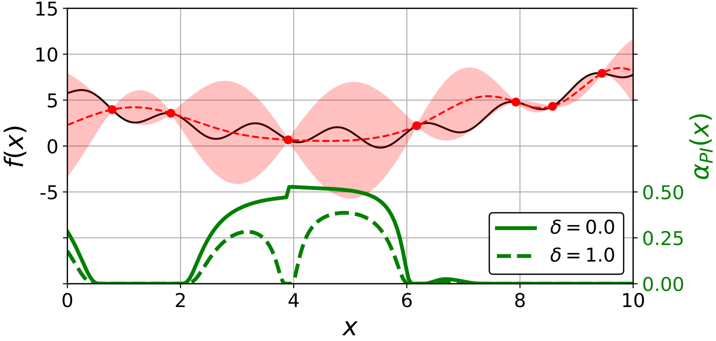
[Shahriari *et al.*, 2015]

Acquisition Function: Probability of Improvement

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

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

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

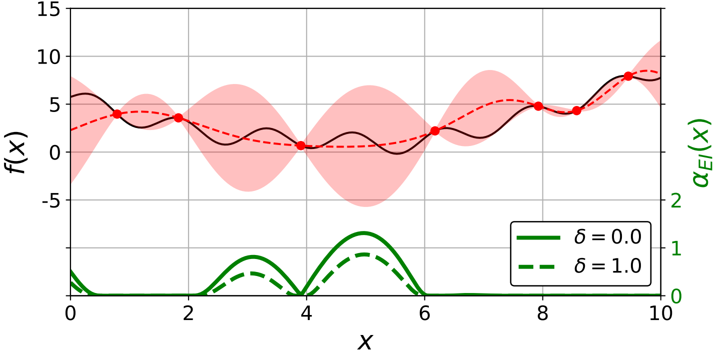


Acquisition Function: Expected Improvement

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

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

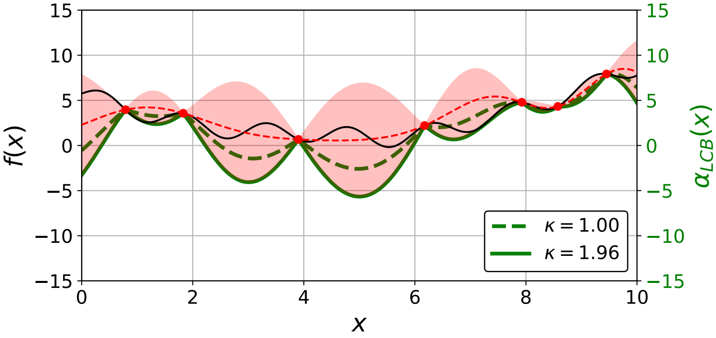
- Less prone than PI to become stuck in a local minimum.



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.

[Duvenaud, 2014; Shahriari *et al.*, 2015]

Pre-processing Data

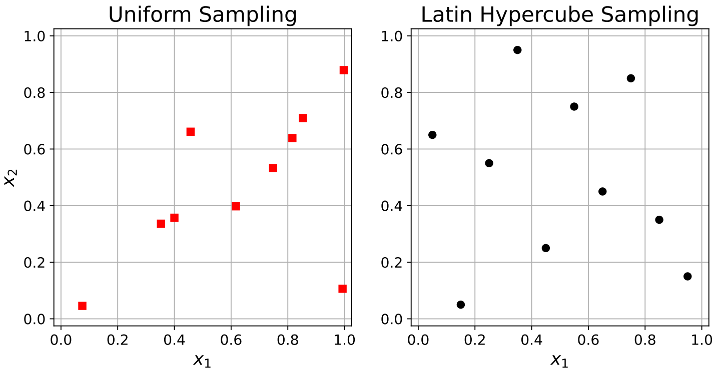
- Transforming sample data can facilitate GPR performance.
  - Normalize observations:

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

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

Generating a Useful Initial Sample

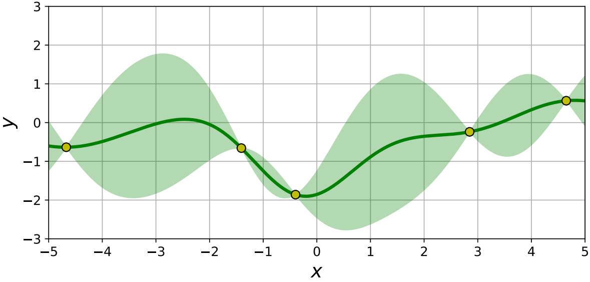
- Samples drawn uniformly may not fill the domain.
- Latin hypercube sampling offers better samples for regression.



[Santner *et al.*, 2018]

Final Thoughts

- GPs offer a rich environment for mathematical modeling.
- Regression is possible without explicit functional forms.
- Bayesian framework provides a natural measure of uncertainty.
- Expensive optimization problems benefit from efficient sampling.



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