Lecture 13: Gaussian Processes
CS480/680 Intro to Machine Learning

2023-2-28

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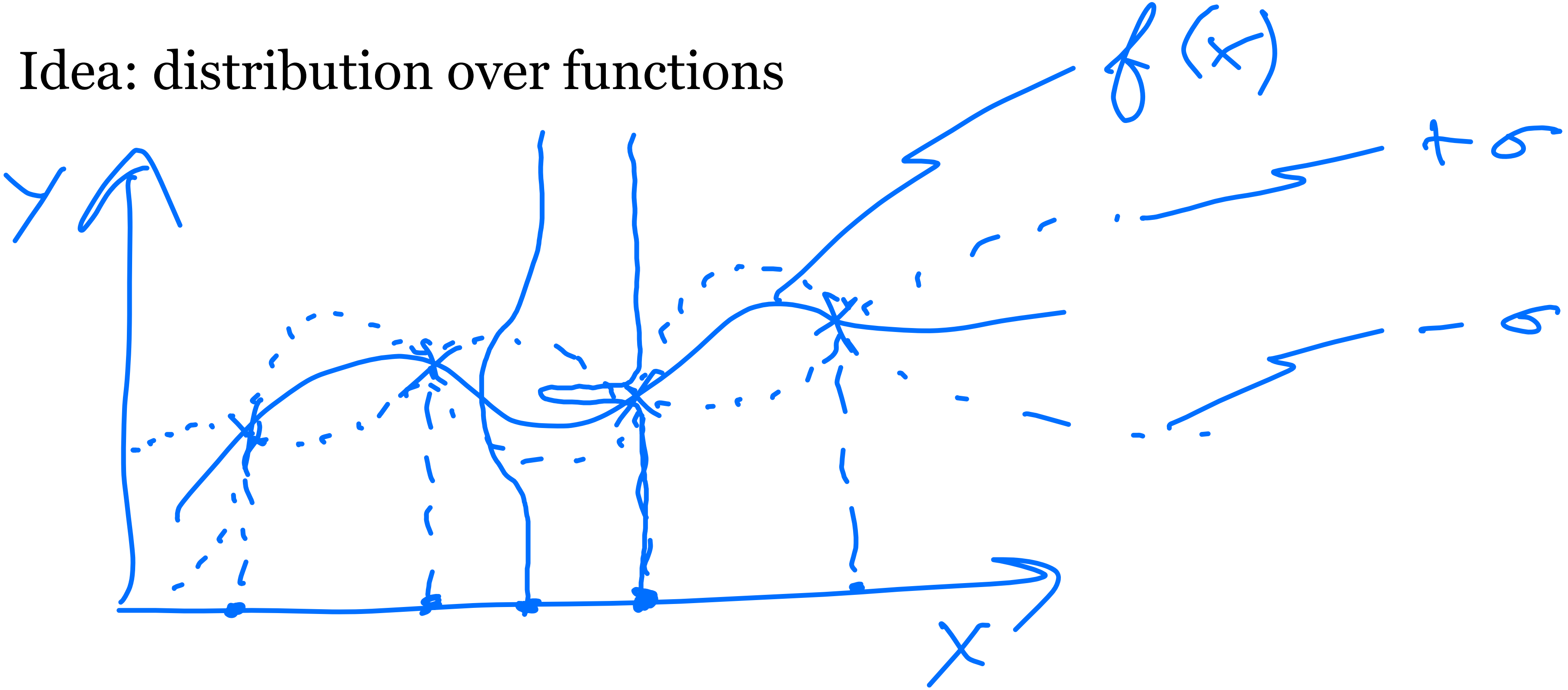
Gaussian Process Regression

- Idea: distribution over functions



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Bayesian Linear Regression

- Setting: $f(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x})$ and $y = f(\boldsymbol{x}) + \epsilon$

  $\boldsymbol{w}$ ↓ unknown; ϵ ↓ $N(0, \sigma^2)$

- Weight space view:
  - Prior: $\Pr(\boldsymbol{w})$
  - Posterior: $\Pr(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) = k \Pr(\boldsymbol{w}) \Pr(\boldsymbol{y}|\boldsymbol{w}, \boldsymbol{X})$

    Gaussian ↑ Gaussian ↑ Gaussian ↑

Bayesian Linear Regression

- Setting: $f(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x})$ and $y = f(\boldsymbol{x}) + \epsilon$

  $\boldsymbol{w}$ ↓ unknown; ϵ ↓ $N(0, \sigma^2)$

- Function space view:
  - Prior: $\Pr(f(\boldsymbol{x}_*)) = \Pr(\boldsymbol{w}^T \phi(\boldsymbol{x}_*))$ ← change of variable ← $\Pr(\boldsymbol{w})$

    $\Pr(f(\boldsymbol{x}_*))$ ↓ Gaussian; $\Pr(\boldsymbol{w})$ ↓ Gaussian
  - Posterior: $\Pr(f(\boldsymbol{x}_*)|\boldsymbol{X}, \boldsymbol{y}) = \Pr(\boldsymbol{w}^T \phi(\boldsymbol{x}_*)|\boldsymbol{X}, \boldsymbol{y})$ ← change of variable ← $\Pr(\boldsymbol{w}^T|\boldsymbol{X}, \boldsymbol{y})$

    $\Pr(f(\boldsymbol{x}_*)|\boldsymbol{X}, \boldsymbol{y})$ ↓ Gaussian; $\Pr(\boldsymbol{w}^T|\boldsymbol{X}, \boldsymbol{y})$ ↓ Gaussian

Gaussian Process

- According to the function view, there is a Gaussian at $f(\boldsymbol{x}_*)$ for every $\boldsymbol{x}_*$. Those Gaussians are correlated through $\boldsymbol{w}$.

- What is the general form of $\Pr(f)$ (i.e., distribution over functions)?

- Answer: **Gaussian Process** (infinite dimensional Gaussian distribution)

Gaussian Process

- Distribution over functions:

$$f(\boldsymbol{x}) \sim GP\big(m(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}')\big)\ \forall \boldsymbol{x}, \boldsymbol{x}'$$

- Where $m(\boldsymbol{x}) = E(f(\boldsymbol{x}))$ is the mean

  and $k(\boldsymbol{x}, \boldsymbol{x}') = E((f(\boldsymbol{x}) - m(\boldsymbol{x}))(f(\boldsymbol{x}') - m(\boldsymbol{x}'))$

  is the kernel covariance function

Mean function $m(\boldsymbol{x})$

- Compute the mean function $m(\boldsymbol{x})$ as follows:

- Let $f(\boldsymbol{x}) = \phi(\boldsymbol{x})^T \boldsymbol{w}$

  with $\boldsymbol{w} \sim N(\boldsymbol{0}, \alpha^{-1}\boldsymbol{I})$

- Then $m(\boldsymbol{x}) = E(f(\boldsymbol{x}))$

$$= E(\boldsymbol{w})^T \phi(\boldsymbol{x})$$

$$= \boldsymbol{0}$$

Kernel covariance function $k(\boldsymbol{x}, \boldsymbol{x}')$

- Compute kernel covariance $k(\boldsymbol{x}, \boldsymbol{x}')$ as follows:

- $k(\boldsymbol{x}, \boldsymbol{x}') = E(f(\boldsymbol{x})f(\boldsymbol{x}'))$

$$= \phi(\boldsymbol{x})^T E\left(\boldsymbol{w}\boldsymbol{w}^T\right)\phi(\boldsymbol{x}')$$

$$= \phi(\boldsymbol{x})^T \frac{I}{\alpha} \phi(\boldsymbol{x}')$$

$$= \frac{\phi(x)^T \phi(x')}{\alpha}$$

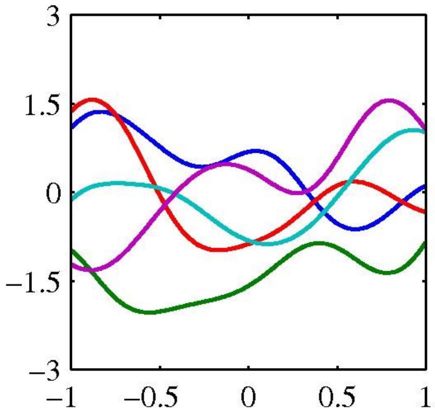
- In some cases we can use domain knowledge to specify k directly.

Examples

- Sampled functions from a Gaussian Process

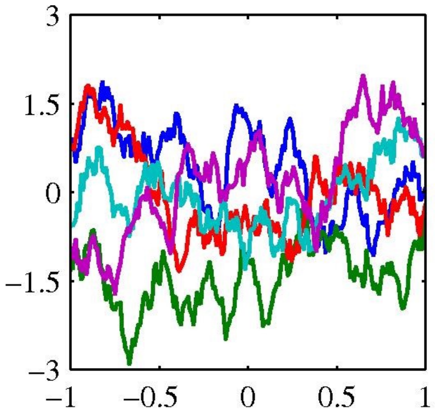
Gaussian kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{||\boldsymbol{x}-\boldsymbol{x}'||^2}{2\sigma^2}}$$



Exponential kernel
(Brownian motion)

$$k(\boldsymbol{x}, \boldsymbol{x}') = e^{-\theta|\boldsymbol{x}-\boldsymbol{x}'|}$$



Gaussian Process Regression

- Gaussian Process Regression corresponds to kernelized Bayesian Linear Regression

- Bayesian Linear Regression:
  - Weight space view
  - Goal: $\Pr(\boldsymbol{w}|\boldsymbol{X},\boldsymbol{y})$ (posterior over $\boldsymbol{w}$)
  - Complexity: cubic in # of basis functions

- Gaussian Process Regression:
  - Function space view
  - Goal: $\Pr(f|\boldsymbol{X},\boldsymbol{y})$ (posterior over f)
  - Complexity: cubic in # of training points

Recap: Bayesian Linear Regression

- Prior: $\Pr(\boldsymbol{w}) = N(\boldsymbol{0}, \boldsymbol{\Sigma})$
- Likelihood: $\Pr(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w}) = N\left(\boldsymbol{w}^T\boldsymbol{\Phi}, \sigma^2\boldsymbol{I}\right)$
- Posterior: $\Pr(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) = N\left(\bar{\boldsymbol{w}}, \boldsymbol{A}^{-1}\right)$
  where $\bar{\boldsymbol{w}} = \sigma^{-2}\boldsymbol{A}^{-1}\boldsymbol{\Phi}\boldsymbol{y}$ and $\boldsymbol{A} = \sigma^{-2}\boldsymbol{\Phi}\boldsymbol{\Phi}^T + \boldsymbol{\Sigma}^{-1}$
- Prediction:
  $\Pr(y_*|\boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}) = N(\sigma^{-2}\phi(\boldsymbol{x}_*)^T\boldsymbol{A}^{-1}\boldsymbol{\Phi}\boldsymbol{y}, \sigma^2 + \phi(\boldsymbol{x}_*)^T\boldsymbol{A}^{-1}\phi(\boldsymbol{x}_*))$
- Complexity: inversion of $\boldsymbol{A}$ is cubic in # of basis functions

Gaussian Process Regression

- Prior: $\Pr(f(\cdot)) = N(m(\cdot), k(\cdot,\cdot))$
- Likelihood: $\Pr(\boldsymbol{y}|\boldsymbol{X}, f) = N(f(\boldsymbol{X}), \sigma^2\boldsymbol{I})$

- Posterior: $\Pr(f(\cdot)|\boldsymbol{X}, \boldsymbol{y}) = N\left(\bar{f}(\cdot), k'(\cdot,\cdot)\right)$

  where $\bar{f}(\cdot) = k(\cdot, \boldsymbol{X})(\boldsymbol{K} + \sigma^2\boldsymbol{I})^{-1}\boldsymbol{y}$ and

  $$k'(\cdot,\cdot) = k(\cdot,\cdot) + \sigma^2\boldsymbol{I} - k(\cdot, \boldsymbol{X})(\boldsymbol{K} + \sigma^2\boldsymbol{I})^{-1}k(\boldsymbol{X},\cdot)$$

- Prediction: $\Pr(y_*|\boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}) = N\left(\bar{f}(\boldsymbol{x}_*), k'(\boldsymbol{x}_*, \boldsymbol{x}_*)\right)$
- Complexity: inversion of $\boldsymbol{K} + \sigma^2\boldsymbol{I}$ is cubic in # of training points

Infinite Neural Networks

- Recall: neural networks with a single hidden layer (that contains sufficiently many hidden units) can approximate any function arbitrarily closely

- Neal 94: The limit of an infinite single hidden layer neural network is a Gaussian Process

Bayesian Neural Networks

- Consider neural network with J hidden units and single identity output unit y_k:

$$y_k = f(\boldsymbol{x}; \boldsymbol{w}) = \sum_{j=1}^{J} w_{kj} h\left(\sum_i w_{ji} x_i + w_{j0}\right) + w_{k0}$$

- Bayesian learning: express prior over the weights
  - Weight space view:

$$\Pr(w_{kj}) \text{ where } E(w_{kj}) = 0, Var(w_{kj}) = \frac{\alpha}{J} \quad \forall kj,$$
$$\Pr(w_{k0}) \text{ where } E(w_{k0}) = 0, Var(w_{k0}) = \sigma^2 \quad \forall k$$

  - Function space view: when $J \to \infty$, by the central limit theorem, an infinite sum of i.i.d. (identically and independently distributed) variables yields a Gaussian

$$\Pr(f(\boldsymbol{x})) = N(f(\boldsymbol{x}) | 0, \alpha E[h(\boldsymbol{x})h(\boldsymbol{x}')] + \sigma^2)$$

Mean Derivation

- Calculation of the mean function:
- $E[f(\boldsymbol{x})] = \sum_{j=1}^{J} E[w_{kj} h(\boldsymbol{x})] + E[w_{k0}]$
  $= \sum_{j=1}^{J} E[w_{kj}] E[h(\boldsymbol{x})] + E[w_{k0}]$
  $= \sum_{j=1}^{J} 0\, E[h(\boldsymbol{x})] + 0$
  $= 0$

Covariance Derivation

- $Cov[f(\boldsymbol{x}), f(\boldsymbol{x}')]$
  $= E[f(\boldsymbol{x})f(\boldsymbol{x}')] - E[f(\boldsymbol{x})]E[f(\boldsymbol{x}')]$
  $= E[f(\boldsymbol{x})f(\boldsymbol{x}')]$
  $= E\left[\left(\sum_j w_{kj}h_j(\boldsymbol{x}) + w_{k0}\right)\left(\sum_j w_{kj}h_j(\boldsymbol{x}') + w_{k0}\right)\right]$
  $= \sum_{j=1}^{J} E\left[w_{kj}h_j(\boldsymbol{x})w_{kj}h_j(\boldsymbol{x}')\right] + E[w_{k0}w_{k0}]$
  $= \sum_{j=1}^{J} E\left[w_{kj}^2\right]E\left[h_j(\boldsymbol{x})h_j(\boldsymbol{x}')\right] + E[w_{k0}^2]$
  $= \sum_{j=1}^{J} Var\left[w_{kj}\right]E[h(\boldsymbol{x})h(\boldsymbol{x}')] + Var(w_{k0})$
  $= \sum_{j=1}^{J} \frac{\alpha}{J} E[h(\boldsymbol{x})h(\boldsymbol{x}')] + \sigma^2$
  $= \alpha E[h(\boldsymbol{x})h(\boldsymbol{x}')] + \sigma^2$

Bayesian Neural Networks

- When # of hidden units $J \to \infty$, then Bayesian neural net is equivalent to a Gaussian Process

$$\Pr\big(f(\cdot)\big) = GP(f(\cdot)|0, \alpha E[h(\cdot)h(\cdot)] + \sigma^2)$$

- Note: this works for
  - Any activation function h
  - Any i.i.d. prior over the weights with mean 0

Case Study: AIBO Gait Optimization

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Gait Optimization

- Problem: find best parameter setting of the gait controller to maximize walking speed
  - Why?: Fast robots have a better chance of winning in robotic soccer

- Solutions:
  - Stochastic hill climbing
  - **Gaussian Processes**
    - Lizotte, Wang, Bowling, Schuurmans (2007) Automatic Gait Optimization with Gaussian Processes, *International Joint Conferences on Artificial Intelligence (IJCAI)*.

Search Problem

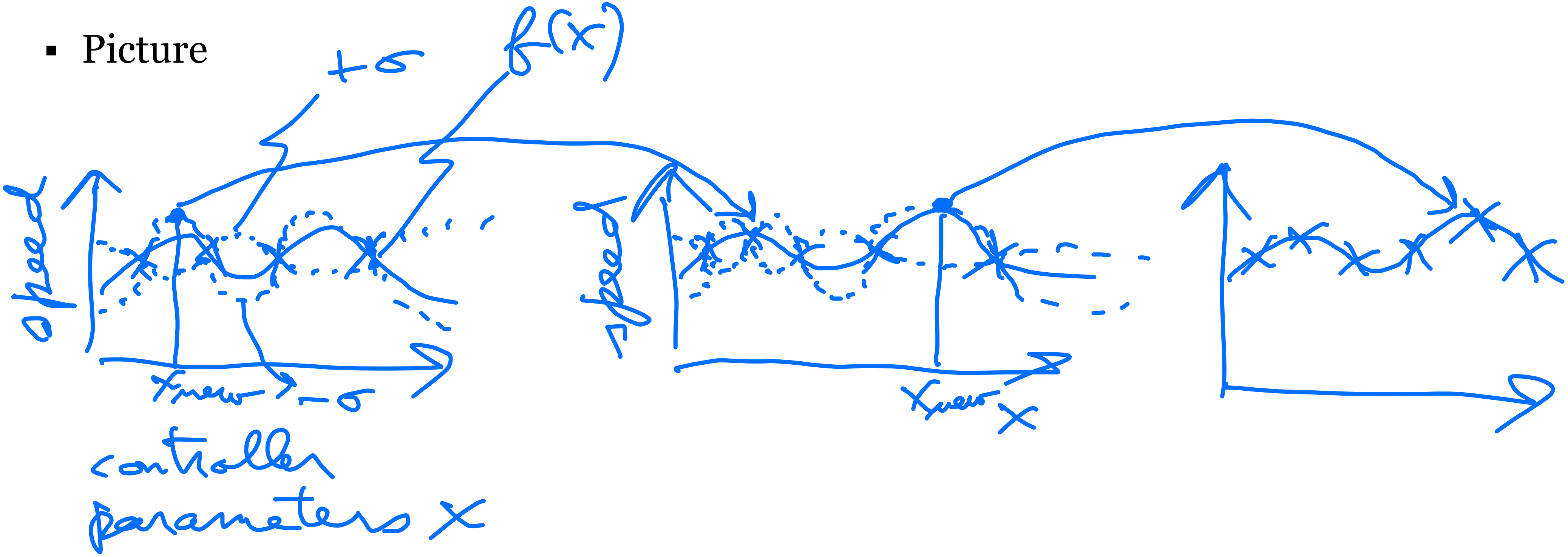
- Let $\boldsymbol{x} \in \Re^{15}$, be a vector of 15 parameters that defines a controller for gait
- Let $f: \boldsymbol{x} \to \Re$ be a mapping from controller parameters to gait speed
- Problem: find parameters $\boldsymbol{x}^*$ that yield highest speed.

$$\boldsymbol{x}^* \leftarrow argmax_{\boldsymbol{x}}\, f(\boldsymbol{x})$$

But f is unknown…

Approach

- Picture



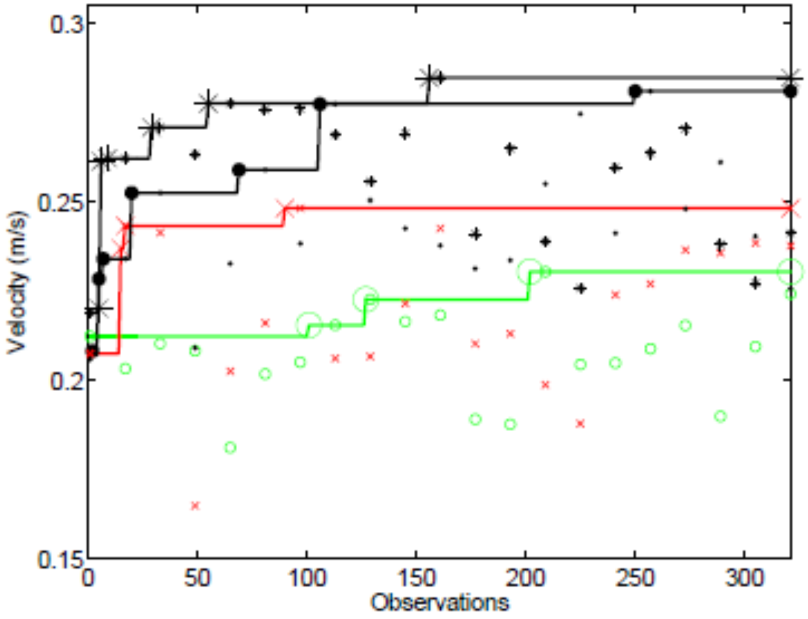
Approach

- Initialize $f(\cdot) \sim GP(m(\cdot), k(\cdot,\cdot))$
- Repeat:
  - Select new $\boldsymbol{x}$:

$$\boldsymbol{x}_{new} \leftarrow argmax_{\boldsymbol{x}} \frac{k(\boldsymbol{x},\boldsymbol{x})}{\max_{\boldsymbol{x}' \in X} f(\boldsymbol{x}') - m(\boldsymbol{x})}$$

  - Evaluate $f(\boldsymbol{x}_{\boldsymbol{new}})$ by observing speed of robot with parameters set to $\boldsymbol{x}_{new}$
  - Update Gaussian process:
    - $\boldsymbol{X} \leftarrow \boldsymbol{X} \cup \{\boldsymbol{x}_{\boldsymbol{new}}\}$ and $\boldsymbol{y} \leftarrow \boldsymbol{y} \cup f(\boldsymbol{x}_{new})$
    - $m(\cdot) \leftarrow k(\cdot, \boldsymbol{X})(\boldsymbol{K} + \sigma^2 \boldsymbol{I})^{-1} \boldsymbol{y}$
    - $k(\cdot,\cdot) \leftarrow k(\cdot,\cdot) + \sigma^2 \boldsymbol{I} - k(\cdot, \boldsymbol{X})(\boldsymbol{K} + \sigma^2 \boldsymbol{I})^{-1} k(\boldsymbol{X},\cdot)$

Results



(•) GP w/MPI 0.281 m/s $\sigma_f^2 = 0.06$

(∗) GP w/MPI 0.285 m/s $\sigma_f^2 = 0.6$

(×) H.Clmb 0.248 m/s

(○) U.Rand 0.230 m/s

Gaussian kernel:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \sigma_f^2 e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}')^T S(\boldsymbol{x}-\boldsymbol{x}')}$$