Advanced Introduction to Machine Learning CMU-10715

Gaussian Processes

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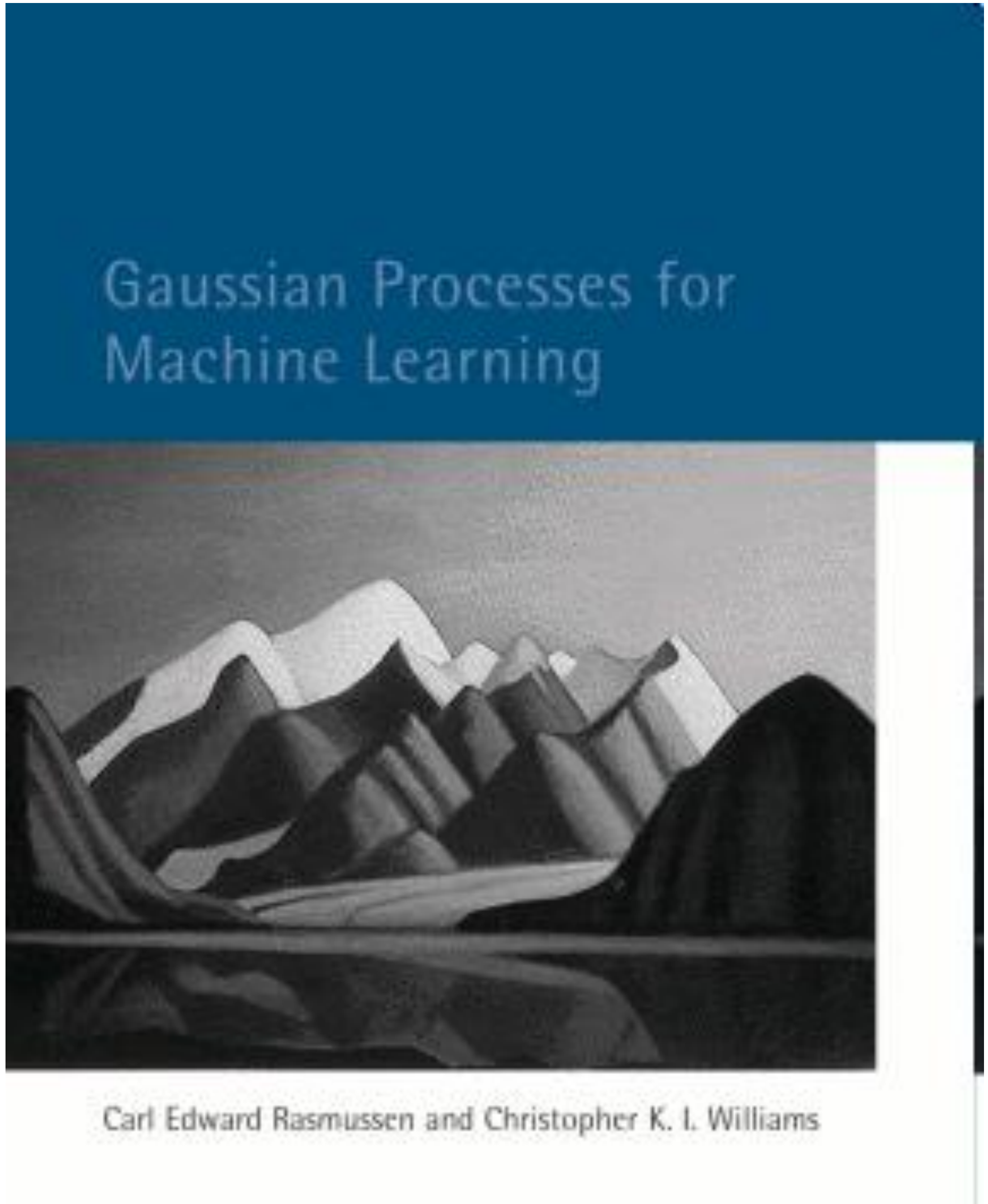
Introduction



http://www.gaussianprocess.org/

Some of these slides in the intro are taken from D. Lizotte, R. Parr, C. Guesterin

Contents

- Introduction
  - Regression
  - Properties of Multivariate Gaussian distributions

- Ridge Regression

- Gaussian Processes

  - Weight space view
    - Bayesian Ridge Regression + Kernel trick

  - Function space view
    - Prior distribution over functions
      + calculation posterior distributions

Regression

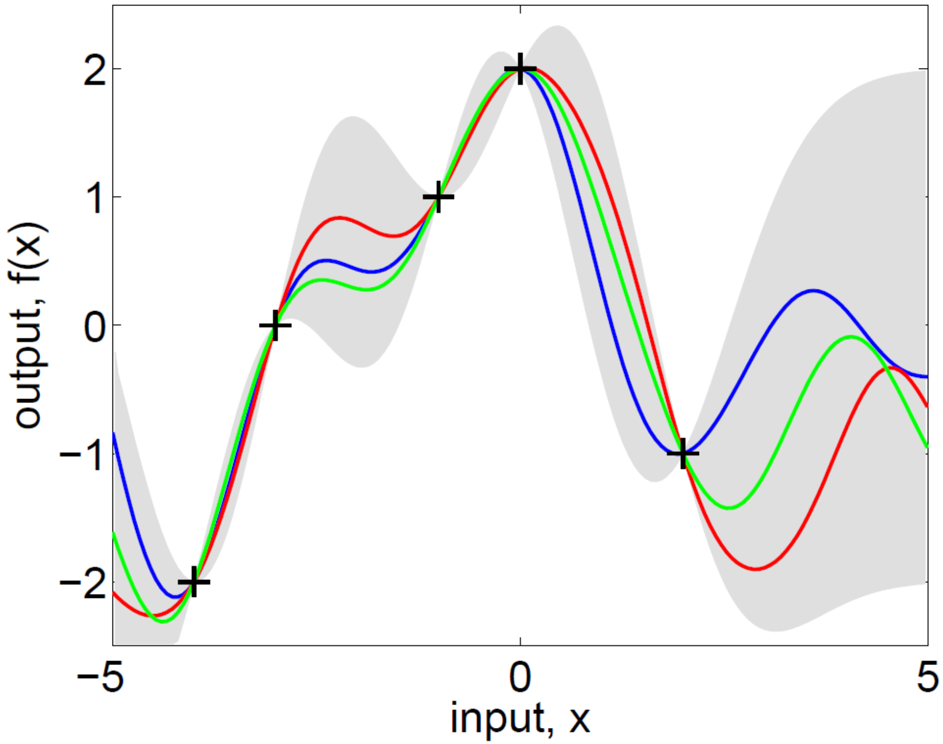
Why GPs for Regression?

Regression methods:

Linear regression, ridge regression, support vector regression, kNN regression, etc…

Motivation 1:

All the above regression method give point estimates. We would like a method that could also provide confidence during the estimation.



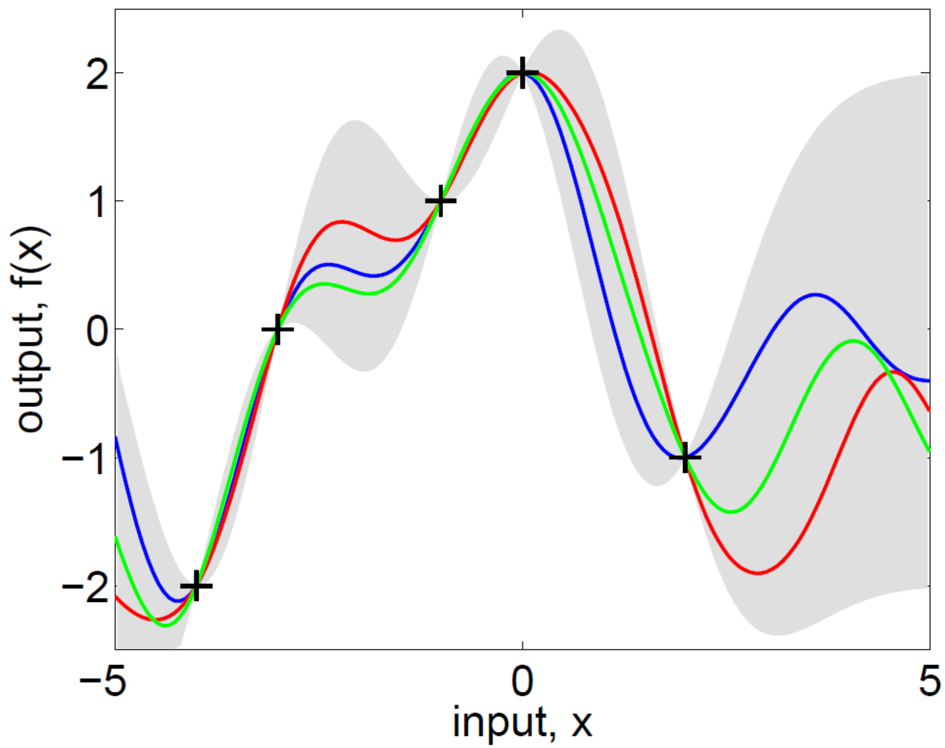
Motivation 2:

Let us kernelize linear ridge regression, and see what we get…

Why GPs for Regression?

GPs can answer the following questions

- Here's where the function will **most likely be.** (expected function)
- Here are some **examples** of what it might look like. (sampling from the posterior distribution)
- Here is a prediction of what you'll see if you evaluate your function at x', **with confidence**

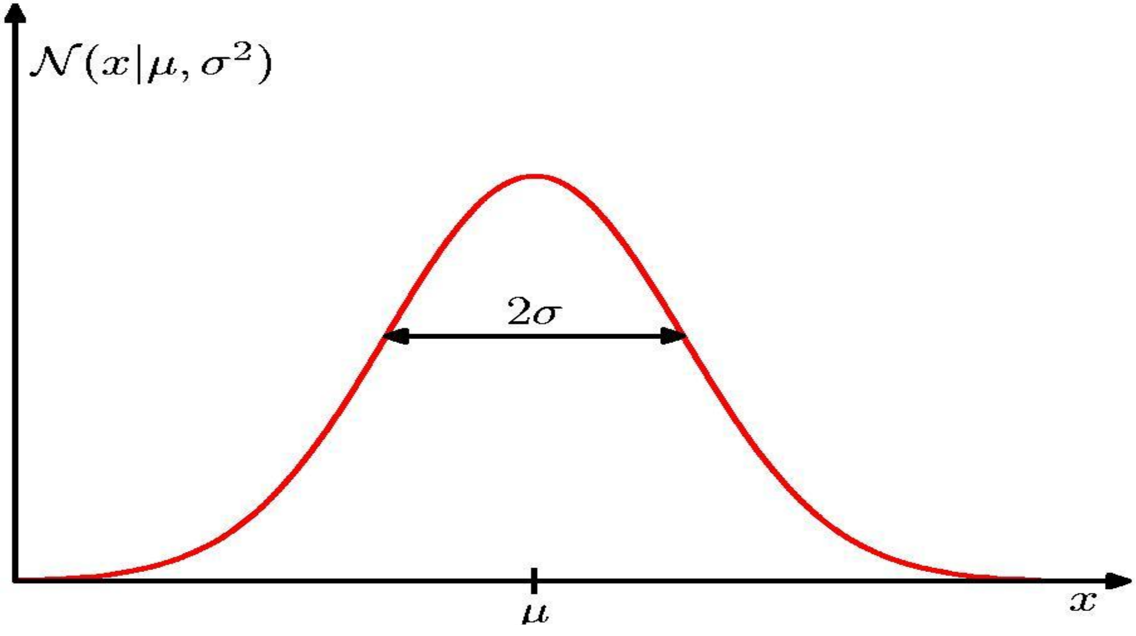


Properties of Multivariate Gaussian Distributions

1D Gaussian Distribution

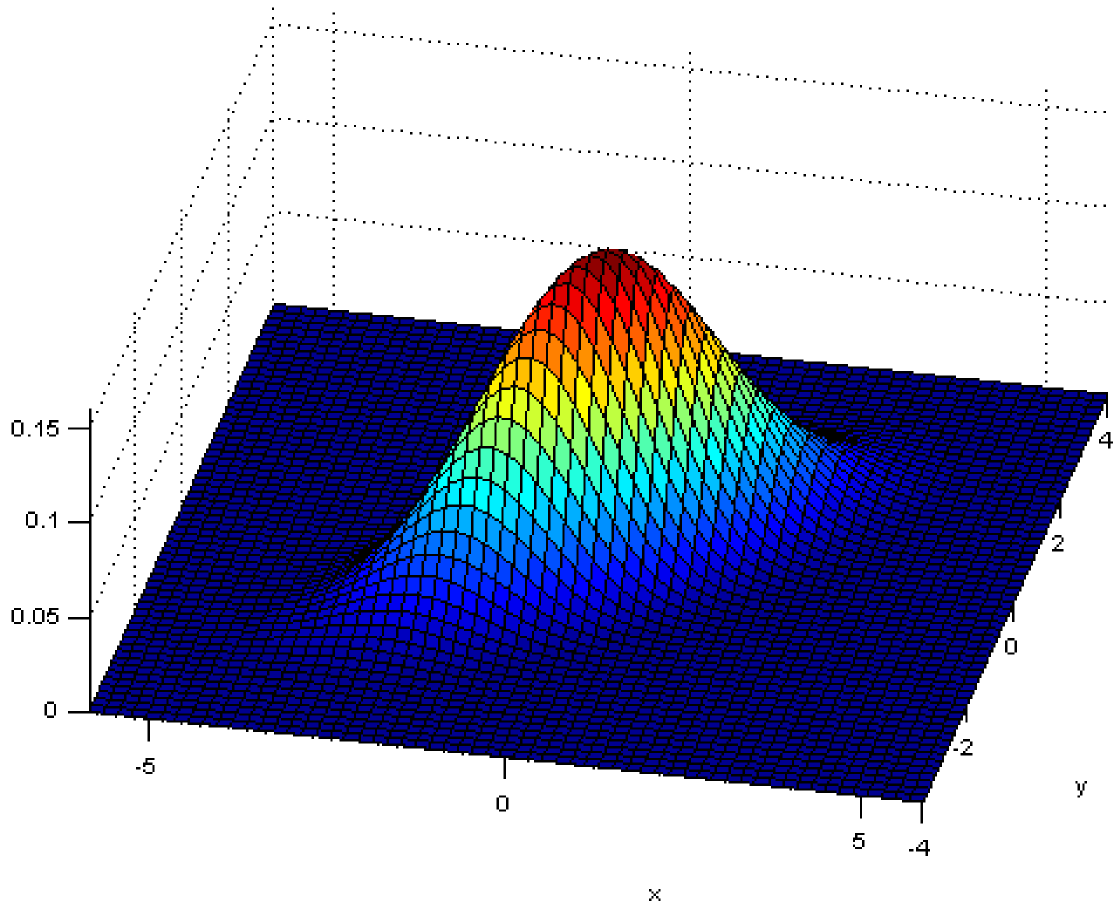
Parameters

- Mean, μ
- Variance, σ^2



$$P(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Multivariate Gaussian



$$p(\mathbf{x} \mid \boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\left\{\frac{-1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu})\right\}$$

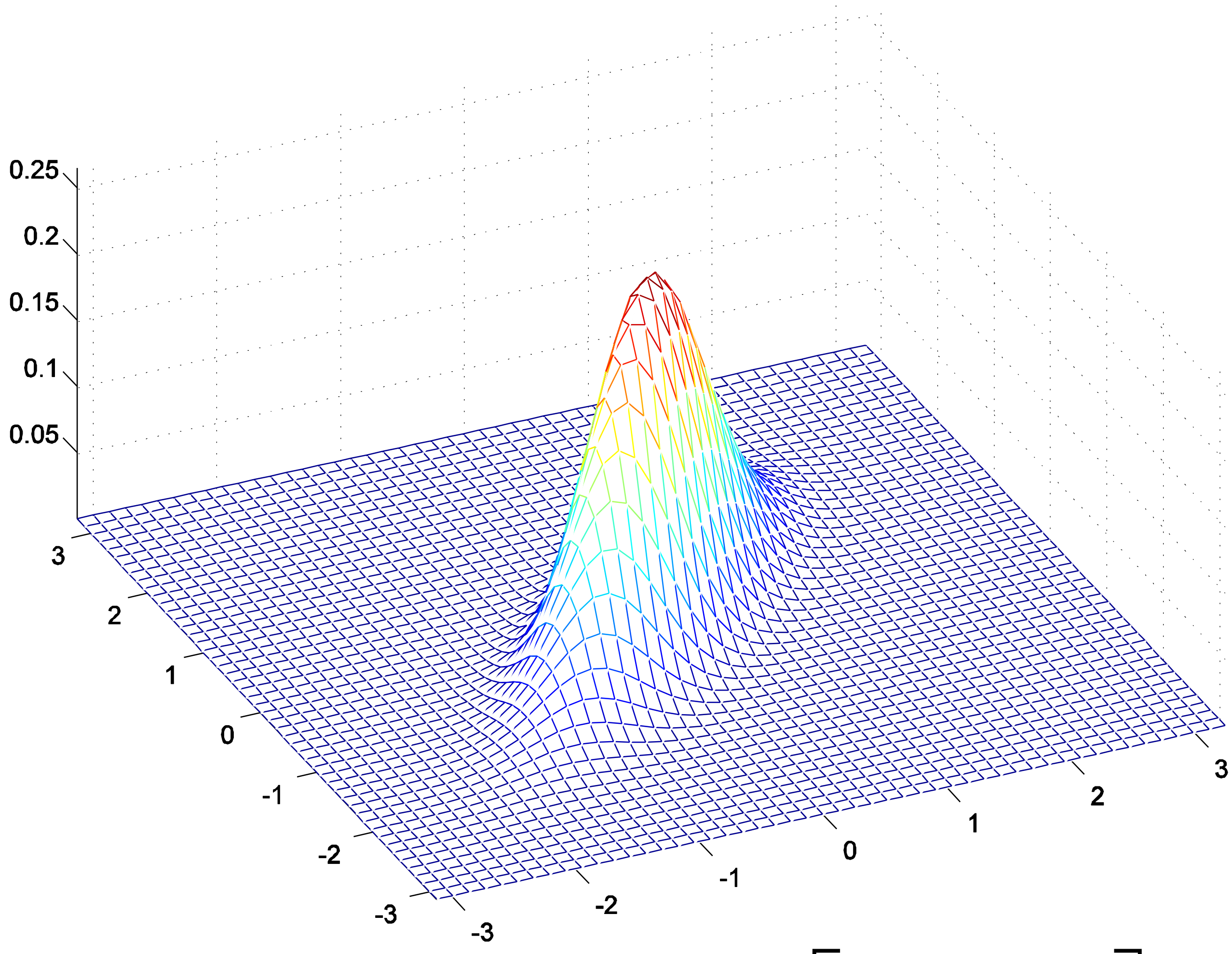
Multivariate Gaussian

- A 2-dimensional Gaussian is defined by
  - a mean vector $\mu = [\ \mu_1, \mu_2\ ]$
  - a covariance matrix: $\Sigma = \begin{bmatrix} \sigma_{1,1}^2 & \sigma_{2,1}^2 \\ \sigma_{1,2}^2 & \sigma_{2,2}^2 \end{bmatrix}$

  where $\sigma_{i,j}^2 = E[\ (x_i - \mu_i)\ (x_j - \mu_j)\ ]$
  is (co)variance

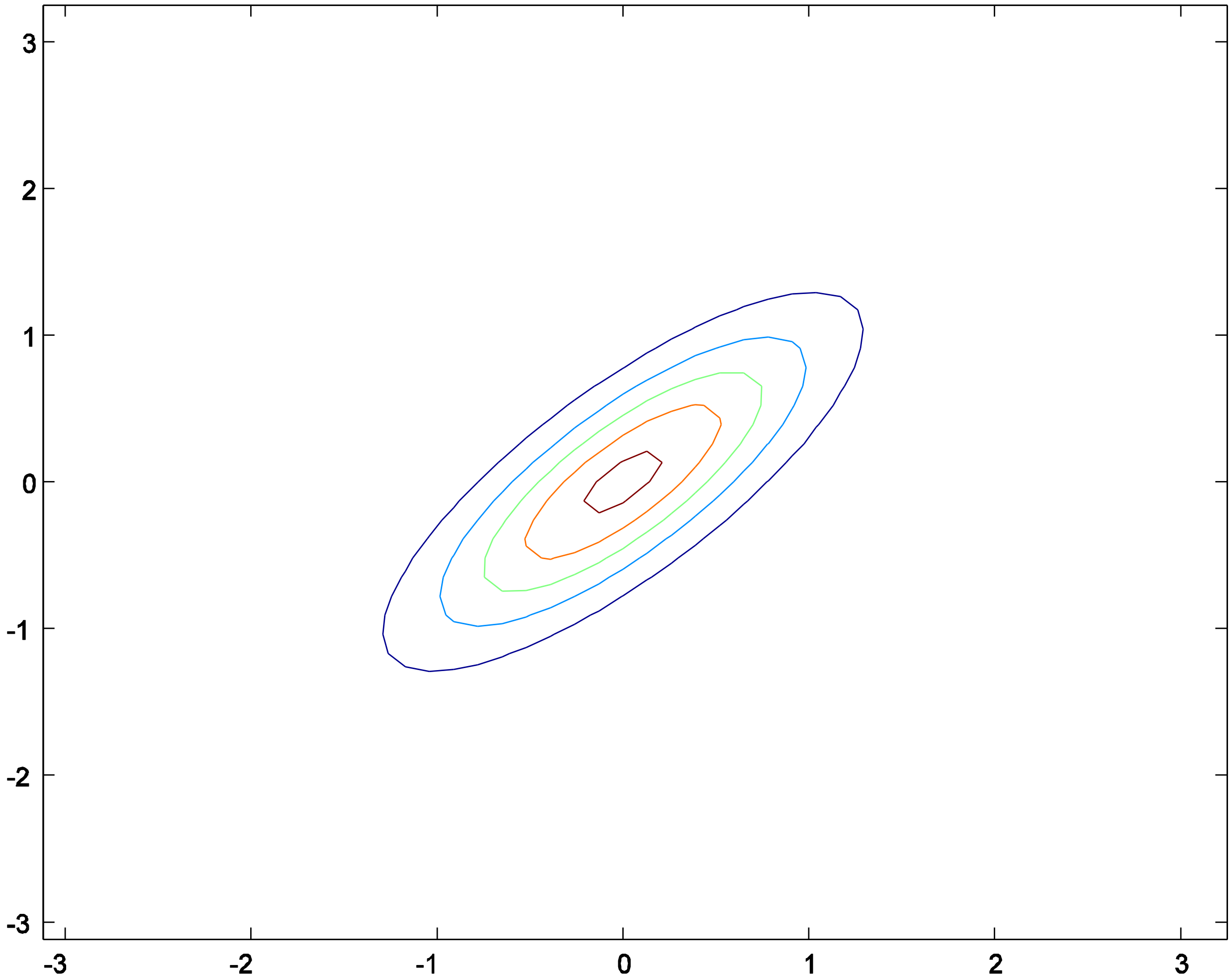
- Note: Σ is symmetric,
  "positive semi-definite": $\forall x$: $x^T \Sigma x \geq 0$

Multivariate Gaussian examples



$\mu = (0,0)$ $\Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$

Multivariate Gaussian examples



$$\mu = (0,0) \qquad \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$

Useful Properties of Gaussians

- Marginal distributions of Gaussians are Gaussian

- Given:

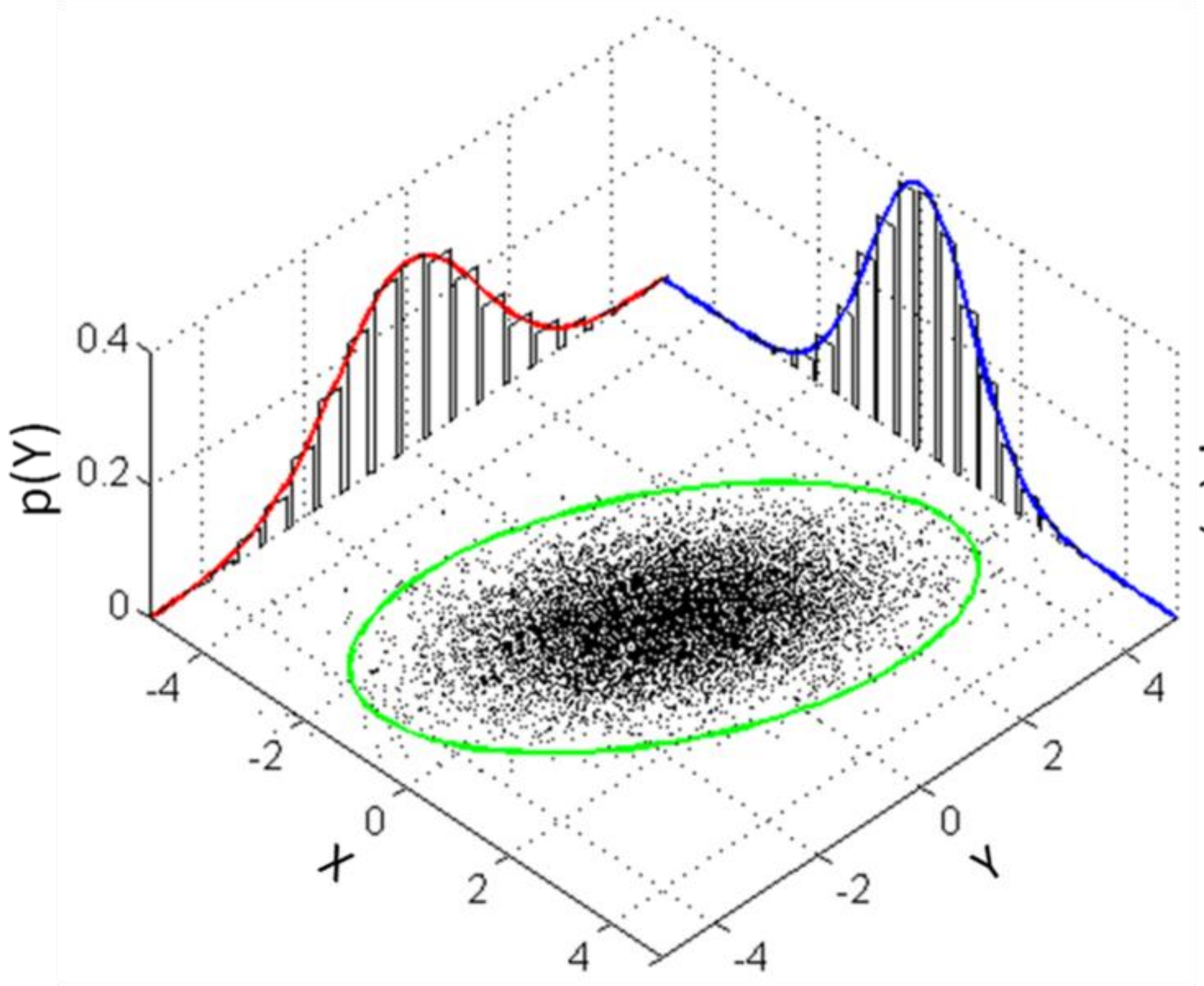
$$x = (x_a, x_b), \mu = (\mu_a, \mu_b)$$

$$\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}$$

- Marginal Distribution:

$$p(X_a) = \mathcal{N}(x_a \mid \mu_a, \Sigma_{aa})$$

Marginal distributions of Gaussians are Gaussian



Block Matrix Inversion

Theorem

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix}$$

$$= \begin{bmatrix} S_D^{-1} & -A^{-1}BS_A^{-1} \\ -D^{-1}CS_D^{-1} & S_A^{-1} \end{bmatrix}$$

Definition: Schur complements

Schur complements of A: $S_A = D - CA^{-1}B$

Schur complements of D: $S_D = A - BD^{-1}C$

Useful Properties of Gaussians

- Conditional distributions of Gaussians are Gaussian
- Notation:

$$\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix} \qquad \Lambda = \Sigma^{-1} = \begin{pmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{pmatrix}$$

- Conditional Distribution:

$$p(X_a|X_b) = \mathcal{N}(x_a \mid \mu_{a|b}, \Lambda_{aa}^{-1})$$

$$\mu_{a|b} = \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(\mathbf{x}_b - \mu_a) = \mu_a - \Sigma_{ab}\Sigma_{bb}^{-1}(\mathbf{x}_b - \mu_a)$$

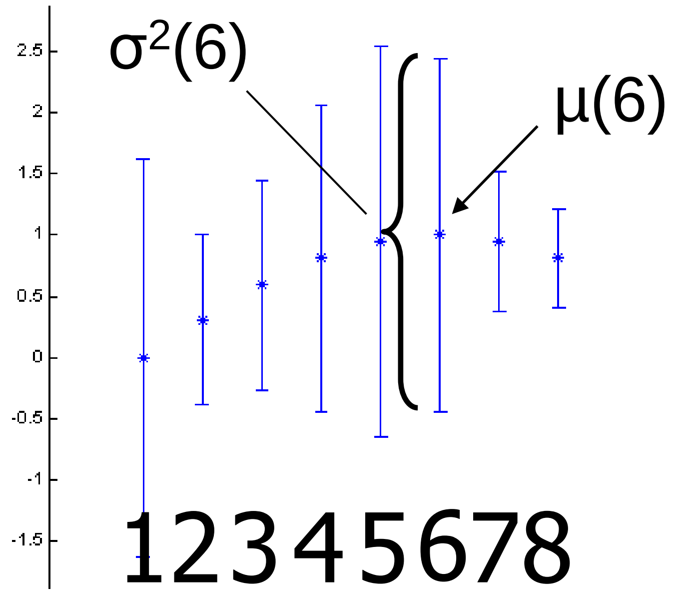
$$\Lambda_{aa}^{-1} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$$

Schur complement of Σ_{bb} in Σ

Higher Dimensions

- **Visualizing > 3 dimensions is… difficult**
- Means and marginals are practical, but then we don't see correlations between those variables
- Marginals are Gaussian, e.g., $f(6) \sim N(\mu(6), \sigma^2(6))$

Visualizing an 8-dimensional Gaussian f:

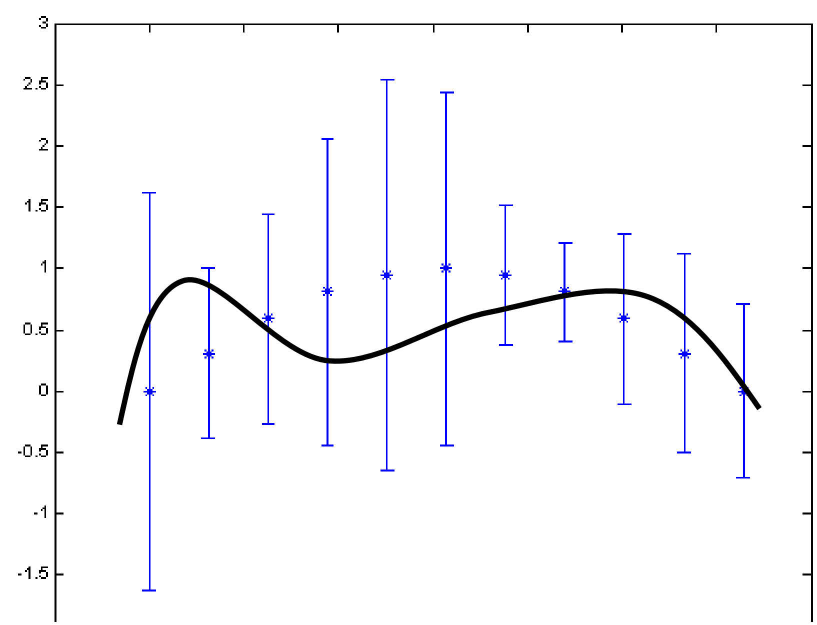


Yet Higher Dimensions

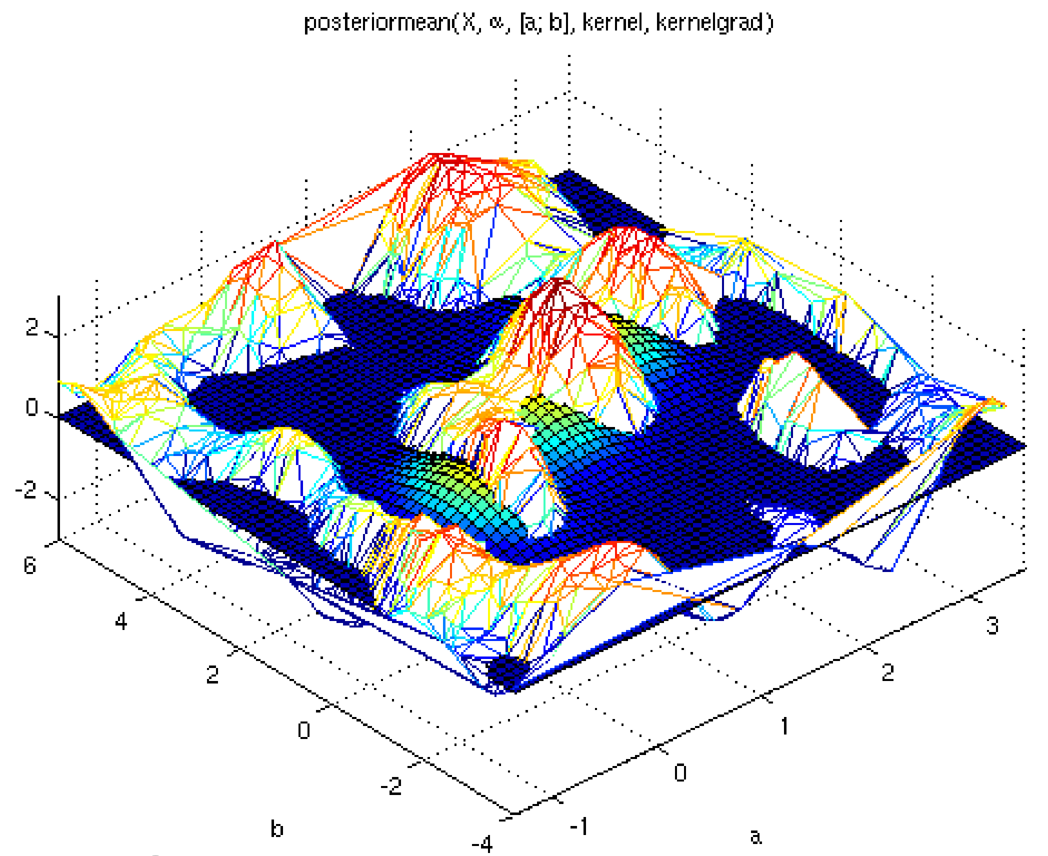
Why stop there?

- We indexed before with $\{1, 2, 3, 4, 5, 6, 7, 8\}$.
- Why noy indexing with $\mathbb{Z}$, or $\mathbb{R}$?
- Need functions $\mu(x), k(x, z)$, $\forall x, z \in \mathbb{R}$
- x and z are indexes over the random variables
- f is now an uncountably

Don't panic: It's just a function



Getting Ridiculous



Why stop there?

- We indexed before with $\mathbb{R}$, why not with $\mathbb{R}^D$?
- Need functions $\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{z})$, $\forall \mathbf{x}, \mathbf{z} \in \mathbb{R}^D$

Gaussian Process

Definition:

- Probability distribution *indexed by* an arbitrary set (integer, real, finite dimensional vector, etc)

- Each element gets a Gaussian distribution over the reals with mean $\mu(x)$

- These distributions are dependent/correlated as defined by $k(x,z)$

- Any finite subset of indices defines a multivariate Gaussian distribution

Gaussian Process

- Distribution over *functions….*

  Yayyy! If our regression model is a GP, then it won't be a point estimate anymore! It can provide regression estimates with confidence

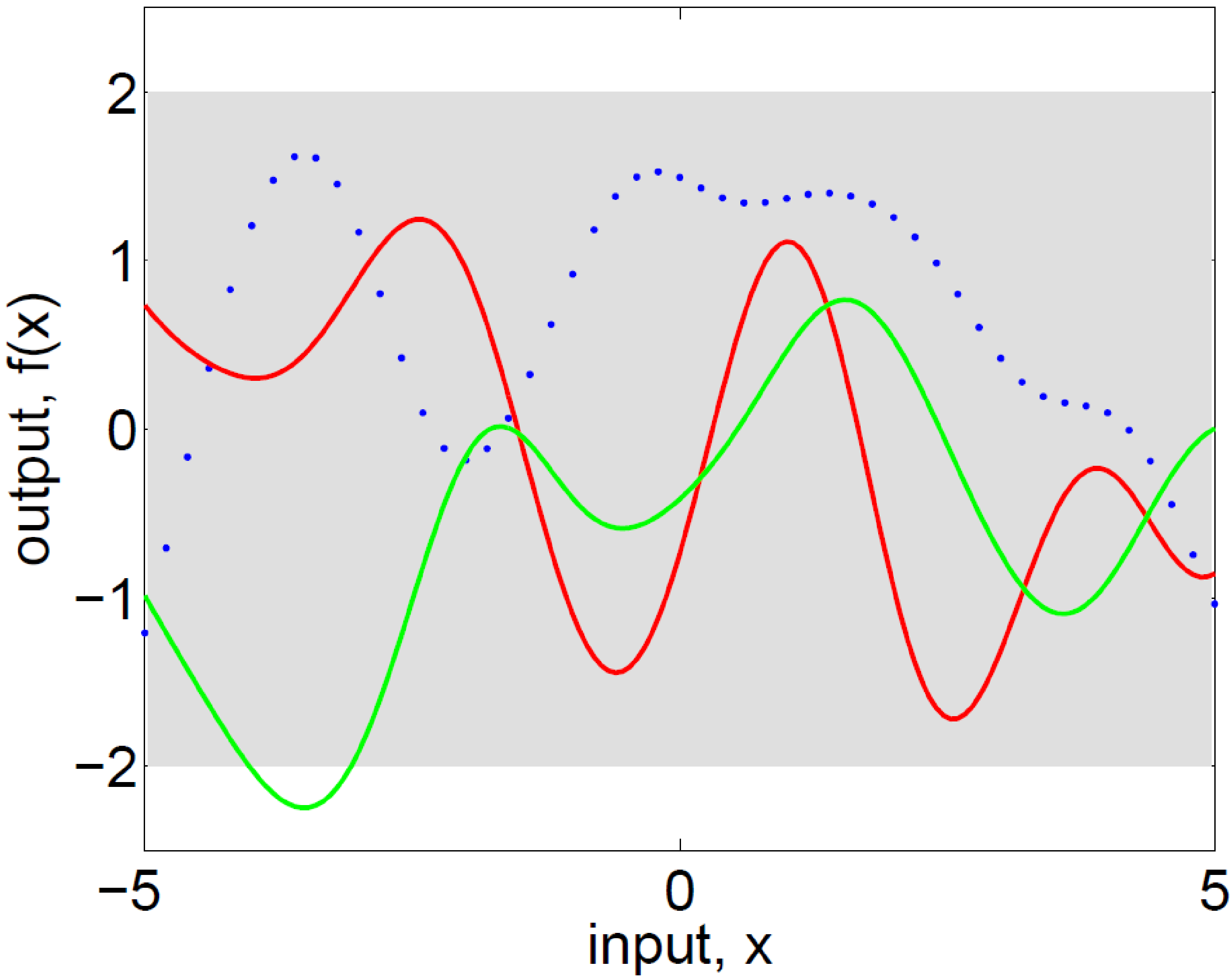
- Domain (index set) of the functions can be pretty much whatever
  - Reals
  - Real vectors
  - Graphs
  - Strings
  - Sets
  - …

Bayesian Updates for GPs

- How can we do regression and learn the GP from data?

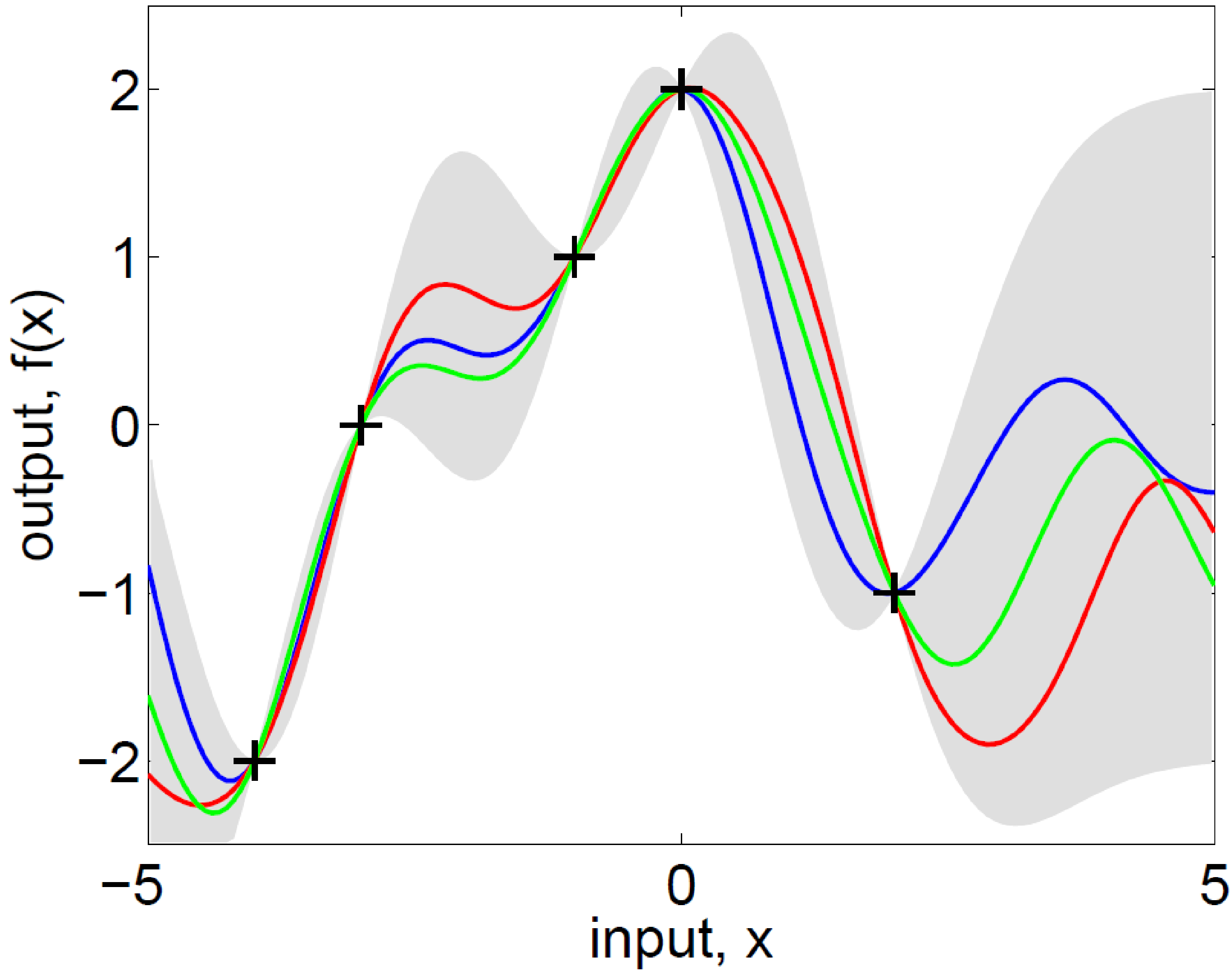
- We will be Bayesians today:
  - Start with GP prior
  - Get some data
  - Compute a posterior

Samples from the prior distribution



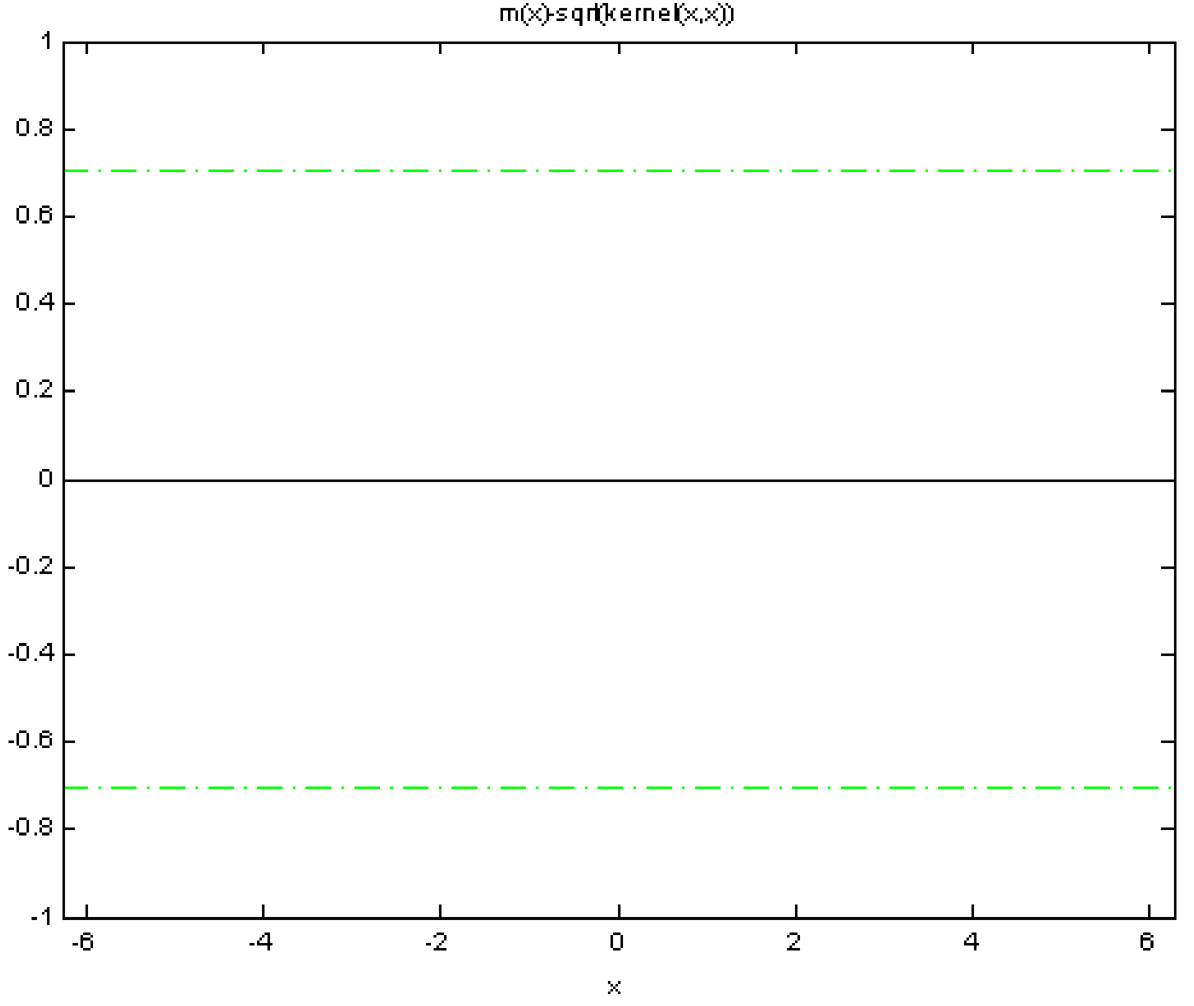
Picture is taken from Rasmussen and Williams

Samples from the posterior distribution

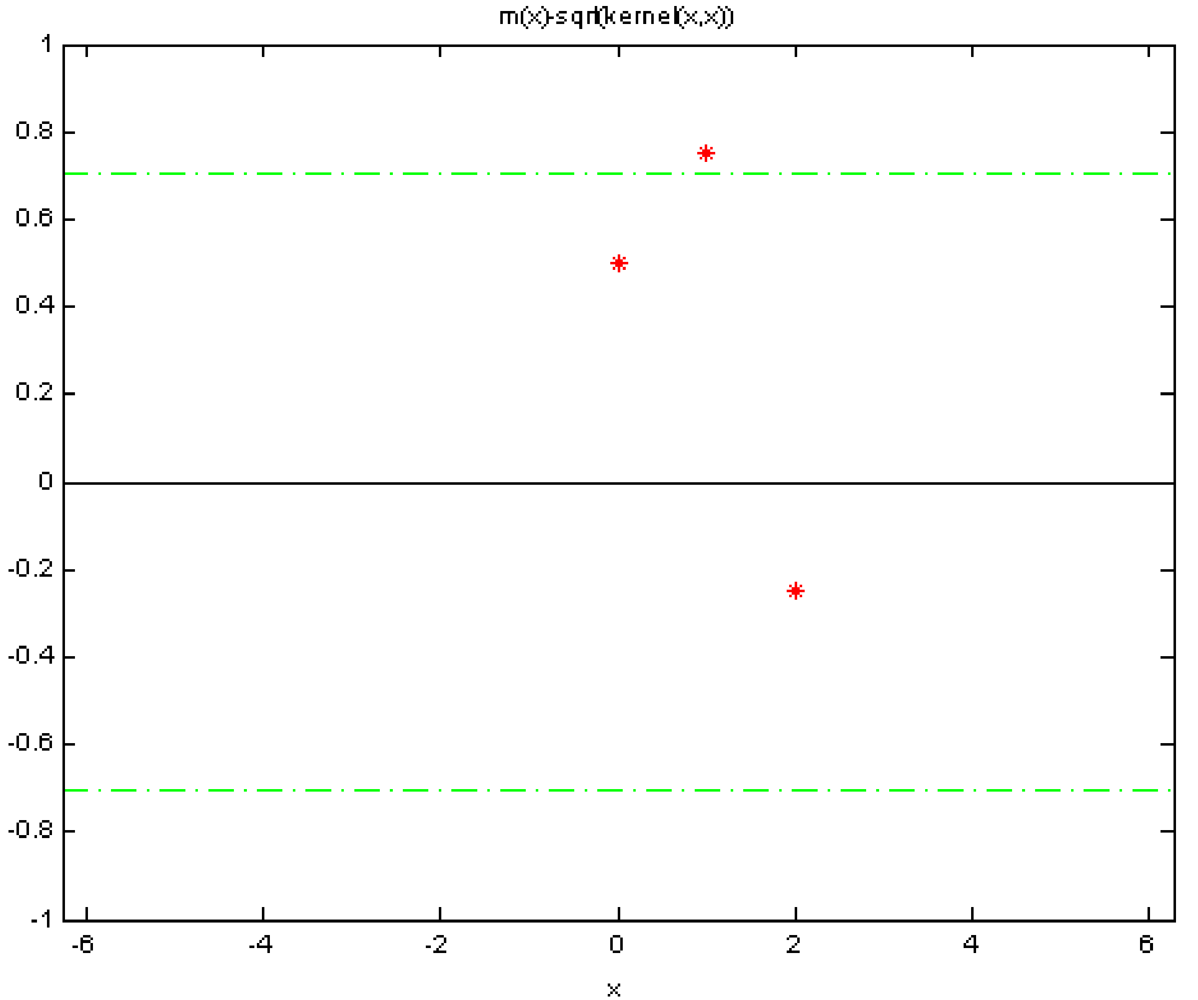


Picture is taken from Rasmussen and Williams

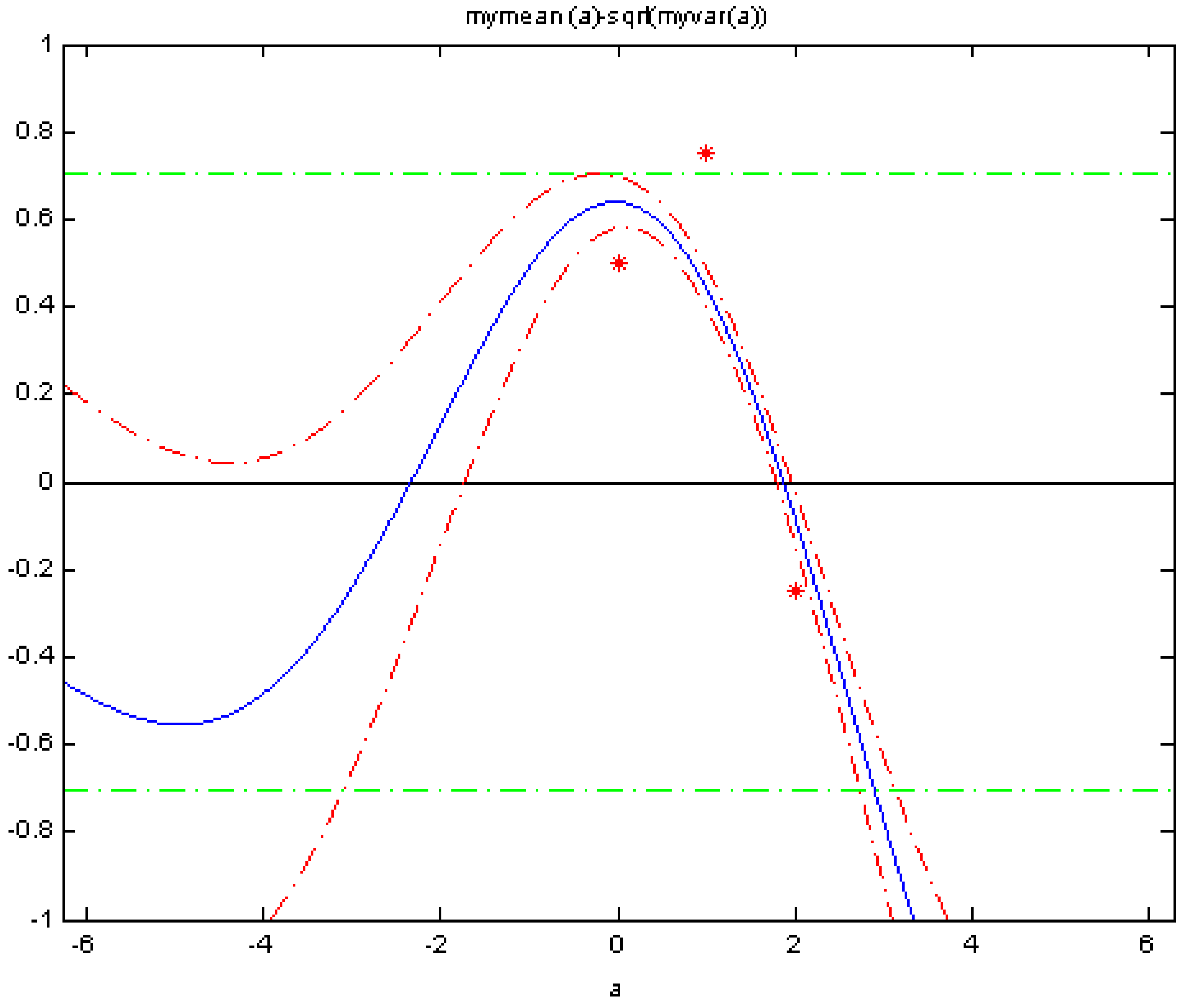
Prior



Data



Posterior



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Ridge Regression

Training set: $D = \{(x_i, y_i) | i = 1, \ldots, n\}$

Linear regression: $f(x) = \langle \mathbf{w}, \phi(x) \rangle$

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathcal{K}} \sum_{i=1}^{m} (y_i - \langle \underbrace{\phi(x_i)}_{\mathbf{x}_i}, \mathbf{w} \rangle)^2$$

Ridge regression:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w} \in \mathcal{K}} \sum_{i=1}^{m} (y_i - \langle \underbrace{\phi(x_i)}_{\mathbf{x}_i}, \mathbf{w} \rangle)^2 + \lambda \|\mathbf{w}\|^2$$

The Gaussian Process is a Bayesian Generalization of the kernelized ridge regression

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Weight Space View

GP = Bayesian ridge regression in feature space
+ Kernel trick to carry out computations

Training set: $D = \{(\mathbf{x}_i, y_i) | i = 1, \ldots, n\}$

$$\left.\begin{array}{l} X = \begin{bmatrix} \mathbf{x}_1 \Big| & \ldots & \Big| \mathbf{x}_n \end{bmatrix} \in \mathbb{R}^{D \times n}, \text{ design matrix} \\[2em] \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^n \end{array}\right\} \textbf{The training data}$$

Bayesian Analysis of Linear Regression with Gaussian noise

$$f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} \in \mathbb{R},\ \mathbf{x}, \mathbf{w} \in \mathbb{R}^D$$

$$y = f(\mathbf{x}) + \epsilon = \mathbf{x}^T\mathbf{w} + \epsilon \in \mathbb{R}$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2) \in \mathbb{R}$$

Let us calculate the likelihood:

$$P(\mathbf{y}|X, \mathbf{w}) = \prod_{i=1}^{n} P(y_i|\mathbf{x}_i^T\mathbf{w})$$

and then put $\mathbf{w} \sim \mathcal{N}_{\mathbf{w}}(0, \Sigma_p)$ prior over parameters $\mathbf{w}$.

Bayesian Analysis of Linear Regression with Gaussian noise

The likelihood:

$$\begin{aligned}
P(\mathbf{y}|X,\mathbf{w}) &= \prod_{i=1}^{n} P(y_i|\mathbf{x}_i^T\mathbf{w}) \\
&= \prod_{i=1}^{n} \mathcal{N}_{y_i}(\mathbf{x}_i^T\mathbf{w},\sigma^2) \\
&= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{-(y_i-\mathbf{x}_i^T\mathbf{w})^2}{2\sigma^2}\right] \\
&= \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left[\frac{-1}{2\sigma^2}\|\mathbf{y}-X^T\mathbf{w}\|^2\right] \\
&= \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w},\sigma^2\mathbf{I}_n)
\end{aligned}$$

Bayesian Analysis of Linear Regression with Gaussian noise

The prior:

$$\mathbf{w} \sim \mathcal{N}_{\mathbf{w}}(0, \Sigma_p)$$

Now, we can calculate the posterior:

$$\begin{aligned}
P(\mathbf{w}|X,\mathbf{y}) &= \frac{P(\mathbf{y}|X,\mathbf{w})P(\mathbf{w})}{P(\mathbf{y}|X)} \\
&= \frac{P(\mathbf{y}|X,\mathbf{w})P(\mathbf{w})}{\int P(\mathbf{y}|X,\mathbf{w})d\mathbf{w}} \\
&= \frac{\mathcal{N}_{\mathbf{y}}(X^T\mathbf{w},\sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0,\Sigma_p)}{\int \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w},\sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0,\Sigma_p)\,d\mathbf{w}} \\
&\sim \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w},\sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0,\Sigma_p)
\end{aligned}$$

Bayesian Analysis of Linear Regression with Gaussian noise

Ridge Regression

$$
\begin{aligned}
P(\mathbf{w}|X,\mathbf{y}) &\sim \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w}, \sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0,\Sigma_p) \\
&\sim \exp\{\frac{-1}{2\sigma^2}(\mathbf{y}-X^T\mathbf{w})^T(\mathbf{y}-X^T\mathbf{w})\}\exp\{\frac{-1}{2}\mathbf{w}^T\Sigma_p^{-1}\mathbf{w}\} \\
&\sim \exp\{\frac{-1}{2}(\mathbf{w}-\bar{\mathbf{w}})^T\underbrace{\left(\frac{1}{\sigma^2}XX^T+\Sigma_p^{-1}\right)}_{A}(\mathbf{w}-\bar{\mathbf{w}})\} \\
&\sim \boxed{\mathcal{N}_{\mathbf{w}}(\bar{\mathbf{w}}, A^{-1})}
\end{aligned}
$$

After "completing the square"

where $\boxed{\bar{\mathbf{w}} \doteq \sigma^{-2}\underbrace{\left(\sigma^{-2}XX^T+\Sigma_p^{-1}\right)^{-1}}_{A^{-1}\in\mathbb{R}^{D\times D}}X\mathbf{y}\in\mathbb{R}^D}$

MAP estimation

$$\boxed{A \doteq \left(\sigma^{-2}XX^T+\Sigma_p^{-1}\right)\in\mathbb{R}^{D\times D}}$$

Bayesian Analysis of Linear Regression with Gaussian noise

We want to use $P(\mathbf{w}|X,\mathbf{y}) = N_{\mathbf{w}}(\bar{\mathbf{w}}, A^{-1})$ posterior for predicting f in a test point $\mathbf{x}_*$.

$$f_* \doteq f(\mathbf{x}_*) \qquad f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} \in \mathbb{R}, \ \mathbf{x}, \mathbf{w} \in \mathbb{R}^D$$

$$y = f(\mathbf{x}) + \epsilon = \mathbf{x}^T\mathbf{w} + \epsilon \in \mathbb{R}$$

$$P(\underbrace{f_*}_{\mathbf{x}_*^T\mathbf{w}} |\mathbf{x}_*, X, \mathbf{y}) = \int \underbrace{P(f_*|\mathbf{x}_*, \mathbf{w})}_{\delta(f_*, \mathbf{x}_*^T\mathbf{w})} \underbrace{P(\mathbf{w}|\mathbf{y}, X)}_{\mathcal{N}_{\mathbf{w}}(\bar{\mathbf{w}}, A^{-1})} \, d\mathbf{w}$$

$$= \mathcal{N}_{f_*}(\mathbf{x}_*^T\bar{\mathbf{w}}, \mathbf{x}_*^T A^{-1}\mathbf{x}_*)$$

This posterior covariance matrix doesn't depend on the observations **y**,

A strange property of Gaussian Processes $\quad \mathbf{y}^T = [y_1, \ldots, y_n]$

Projections of Inputs into Feature Space

The reviewed Bayesian linear regression suffers from

limited expressiveness

$\Downarrow$

To overcome the problem $\Rightarrow$
go to a feature space and do linear regression there

a., **explicit** features $\phi(\mathbf{x}) = [x_1, x_1 x_2^2, x_1 - x_2, \ldots]^T$

b., **implicit** features (kernels) $k(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|^2)$

Explicit Features

$$\phi(\mathbf{x}) = [x_1, x_1 x_2^2, x_1 - x_2, \ldots]^T \in \mathbb{R}^N$$

$$\phi(X) = \left[\phi(\mathbf{x}_1) \middle| \phi(\mathbf{x}_2) \middle| \quad \ldots \quad \middle| \phi(\mathbf{x}_n) \right] \in \mathbb{R}^{N \times n}$$

$$f(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w} \in \mathbb{R}, \qquad \phi(\mathbf{x}), \mathbf{w} \in \mathbb{R}^N$$

$$y = f(\mathbf{x}) + \epsilon = \phi(\mathbf{x})^T \mathbf{w} + \epsilon \in \mathbb{R}$$

Linear regression in the feature space

Explicit Features

The predictive distribution after feature map:

$$P(\underbrace{f_*}_{\phi(\mathbf{x}_*)^T \mathbf{w}} |\mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}\left(\phi(x_*)^T \bar{\mathbf{w}}, \phi(x_*)^T A^{-1} \phi(x_*)\right)$$

where $\bar{\mathbf{w}}$ $\boxed{\doteq \sigma^{-2} \underbrace{\left(\sigma^{-2}\phi(X)\phi(X)^T + \Sigma_p^{-1}\right)^{-1}}_{A^{-1} \in \mathbb{R}^{N \times N}} \underbrace{\phi(X)}_{\in \mathbb{R}^{N \times n}} \underbrace{\mathbf{y}}_{\in \mathbb{R}^{n \times 1}} \in \mathbb{R}^N}$

$$A \doteq \boxed{\left(\sigma^{-2}\phi(X)\phi(X)^T + \Sigma_p^{-1}\right) \in \mathbb{R}^{N \times N}}$$

Explicit Features

Shorthands:

$$\phi_* \doteq \phi(\mathbf{x}_*) \in \mathbb{R}^N \qquad N = \text{dim of feature space}$$

$$\phi \doteq \phi(X) = \left[\phi(\mathbf{x}_1) \middle| \phi(\mathbf{x}_2) \middle| \quad \ldots \quad \middle| \phi(\mathbf{x}_n) \right] \in \mathbb{R}^{N \times n}$$

$$A \doteq \left(\sigma^{-2} \phi \phi^T + \Sigma_p^{-1} \right) \in \mathbb{R}^{N \times N}$$

$$\bar{\mathbf{w}} \doteq \sigma^{-2} \underbrace{\left(\sigma^{-2} \phi \phi^T + \Sigma_p^{-1} \right)^{-1}}_{A^{-1} \in \mathbb{R}^{N \times N}} \phi \mathbf{y} \in \mathbb{R}^N$$

The predictive distribution after feature map:

$$P(\underbrace{f_*}_{\phi_*^T \mathbf{w} \in \mathbb{R}} | \mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*} \left(\phi_*^T \bar{\mathbf{w}}, \phi_*^T A^{-1} \phi_* \right)$$

Explicit Features

The predictive distribution after feature map:

$$P(\underbrace{f_*}_{\phi_*^T \mathbf{w} \in \mathbb{R}} \mid \mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}\left(\phi_*^T \bar{\mathbf{w}}, \phi_*^T A^{-1} \phi_*\right) \qquad (*)$$

$$= \mathcal{N}_{f_*}\left(\overbrace{\sigma^{-2}\phi_*^T \left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1}\phi\mathbf{y}}^{\mathbb{R}}, \phi_*^T \overbrace{\left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1}}^{\mathbb{R}^{N\times N}}\phi_*\right)$$

A problem with (*) is that it needs an NxN matrix inversion...

Let $K \doteq \phi^T \Sigma_p \phi \in \mathbb{R}^{n\times n}$

Theorem:

(*) can be rewritten: $P(f_* | \mathbf{x}_*, X, \mathbf{y}) =$

$$\boxed{\mathcal{N}_{f_*}\left(\underbrace{(\phi_*^T \Sigma_p \phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K + \sigma^2 \mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T \Sigma_p \phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T \Sigma_p \phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K + \sigma^2 \mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{(\phi^T \Sigma_p \phi_*)}_{\mathbb{R}^{n\times 1}}\right)}$$

Proofs

- **Mean expression.** We need:

$$\sigma^{-2}\phi_*^T \underbrace{\left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1}}_{A^{-1}} \phi\mathbf{y} = (\phi_*^T \underbrace{\Sigma_p\phi)(K + \sigma^2\mathbf{I}_n)^{-1}}_{\sigma^{-2}A^{-1}\phi}\mathbf{y}$$

Lemma:

$$\sigma^{-2}\phi(K + \sigma^2\mathbf{I}_n) = \sigma^{-2}\phi(\phi^T\Sigma_p\phi + \sigma^2\mathbf{I}_n) = A\Sigma_p\phi$$

- **Variance expression.** We need:

$$\phi_*^T\left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1}\phi_* = (\phi_*^T\Sigma_p\phi_*) - (\phi_*^T\Sigma_p\phi)(K + \sigma^2\mathbf{I}_n)^{-1}(\phi^T\Sigma_p\phi_*)$$

Matrix inversion Lemma:

$$(\underbrace{U}_{\phi}\underbrace{W}_{\sigma^{-2}}\underbrace{V^T}_{\phi^T} + \underbrace{Z}_{\Sigma_p^{-1}})^{-1} = Z^{-1} - Z^{-1}U(W^{-1} + \underbrace{V^TZ^{-1}U}_{K})^{-1}V^TZ^{-1}$$

From Explicit to Implicit Features

$P(f_*|\mathbf{x}_*, X, \mathbf{y}) =$

$$\boxed{\mathcal{N}_{f_*}\left(\underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T\Sigma_p\phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{(\phi^T\Sigma_p\phi_*}_{\mathbb{R}^{n\times 1}}\right)}$$

We have to work only with $n \times n$ matrices, and not $N \times N$

Reminder: This was the original formulation:

$$P(\underbrace{f_*}_{\phi(\mathbf{x}_*)^T\mathbf{w}}|\mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}\left(\phi(x_*)^T\bar{\mathbf{w}}, \phi(x_*)^T A^{-1}\phi(x_*)\right)$$

where $\bar{\mathbf{w}} \doteq \sigma^{-2}\underbrace{\left(\sigma^{-2}\phi(X)\phi(X)^T + \Sigma_p^{-1}\right)^{-1}}_{A^{-1}\in\mathbb{R}^{N\times N}}\underbrace{\phi(X)}_{\in\mathbb{R}^{N\times n}}\underbrace{\mathbf{y}}_{\in\mathbb{R}^{n\times 1}} \in \mathbb{R}^N$

$$A \doteq \left(\sigma^{-2}\phi(X)\phi(X)^T + \Sigma_p^{-1}\right) \in \mathbb{R}^{N\times N}$$

From Explicit to Implicit Features

$$P(f_*|\mathbf{x}_*, X, \mathbf{y}) =$$

$$\boxed{\mathcal{N}_{f_*}\left(\underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T\Sigma_p\phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{(\phi^T\Sigma_p\phi_*)}_{\mathbb{R}^{n\times 1}}\right)}$$

The feature space always enters in the form of:

$(\phi_*^T\Sigma_p\phi_*)$, $(\phi_*^T\Sigma_p\phi)$, $(\phi^T\Sigma_p\phi)$, ($\in \mathbb{R}^{n\times n}$ matrices)

$$\boxed{\text{Let } k(x,\tilde{x}) \doteq \phi(x)^T\Sigma_p\phi(x)}$$

No need to know the explicit N dimensional features.

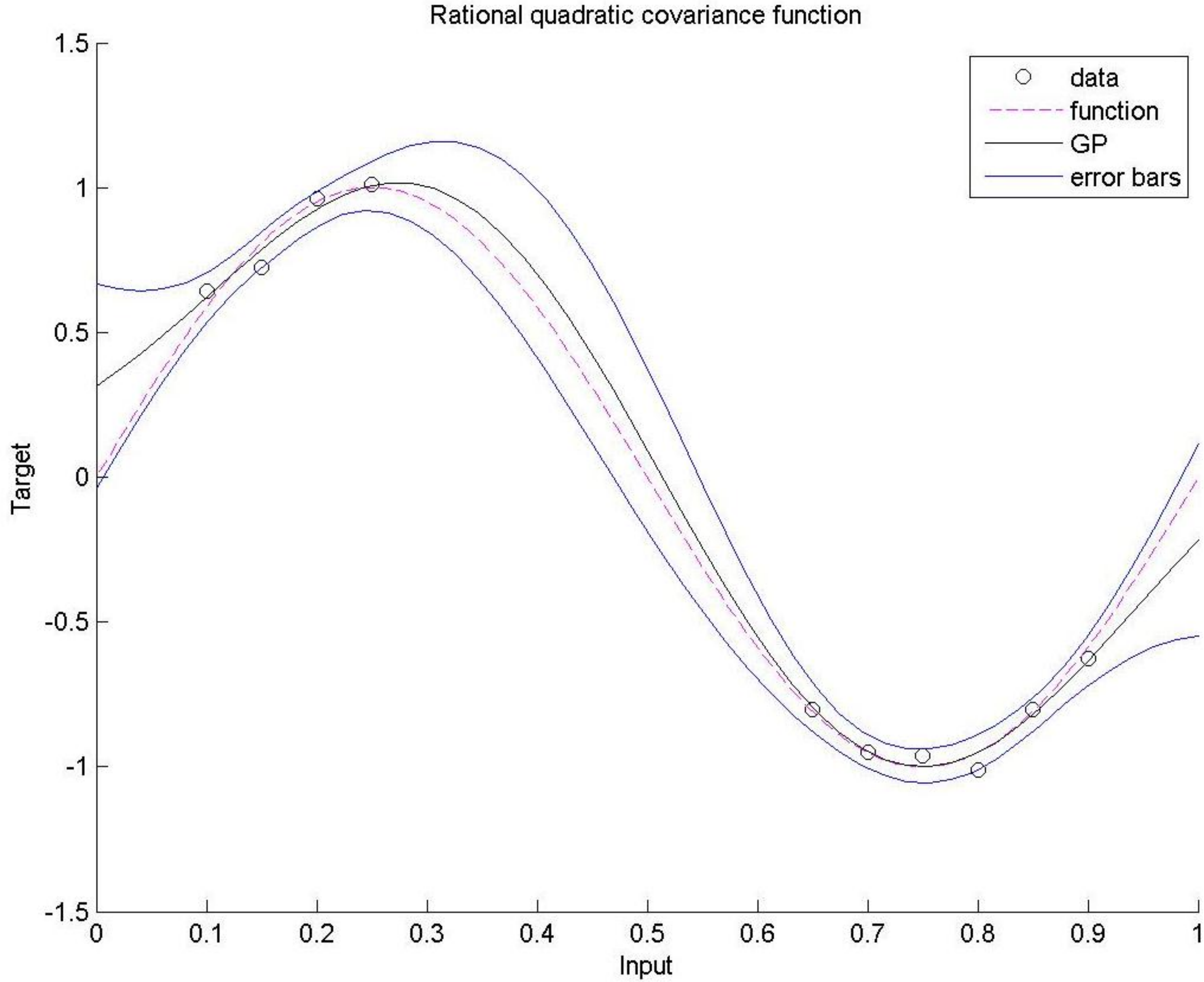
Their inner product is enough.

Lemma:

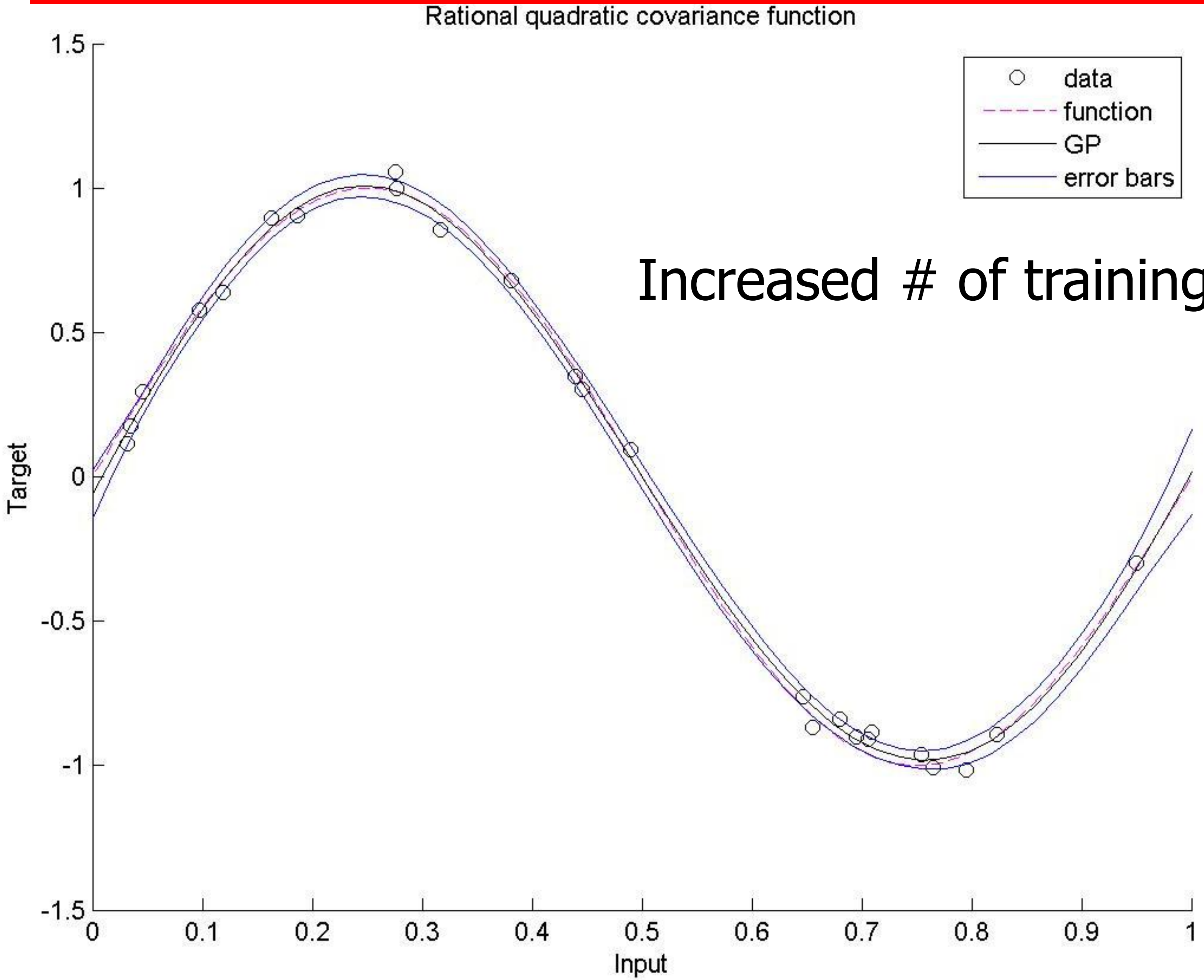
$k(x,\tilde{x})$ is an inner product in the feature space: $\psi(x) \doteq \Sigma_p^{1/2}\phi(x)$

Results

Results using Netlab , Sin function

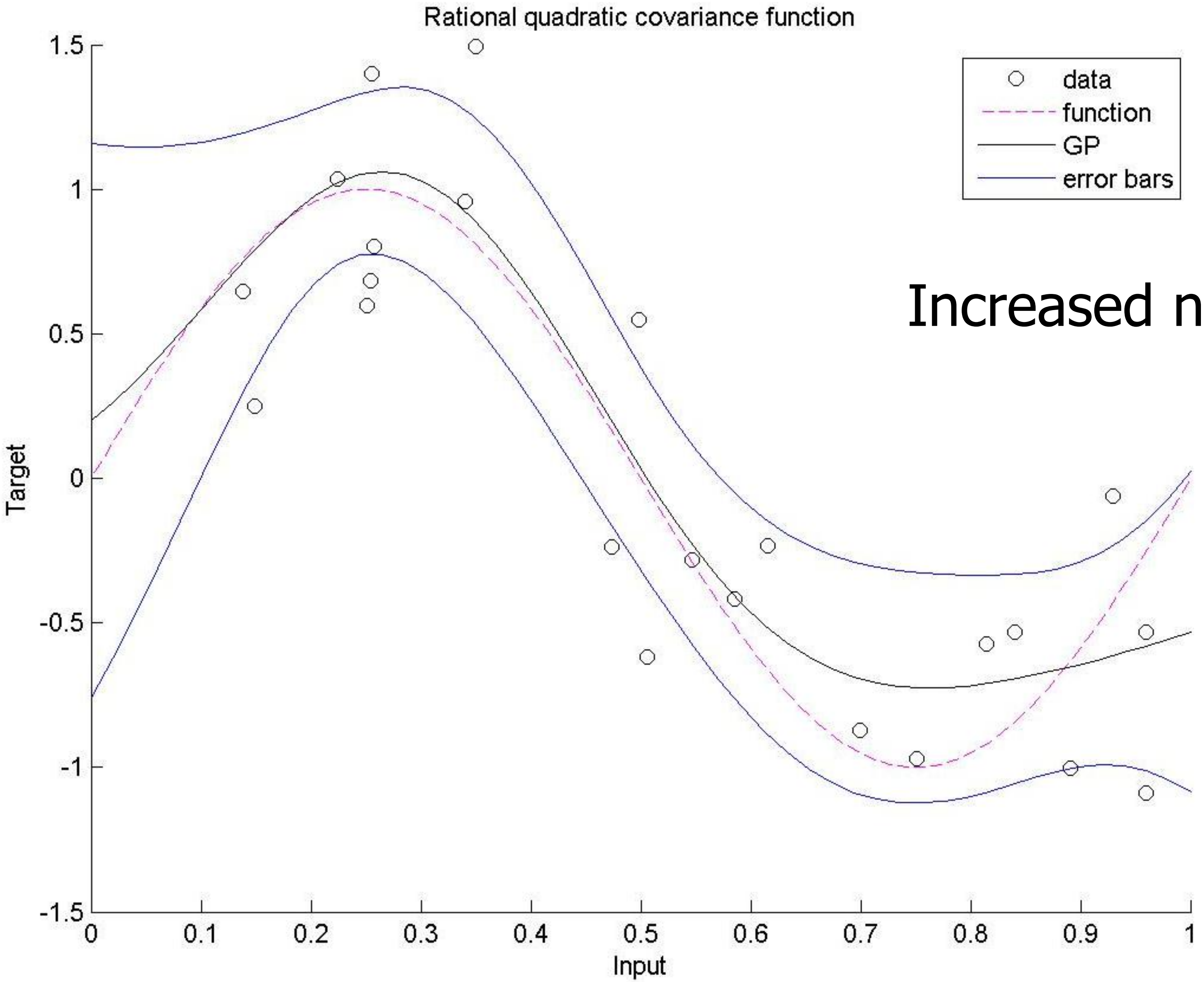


Results using Netlab, Sin function



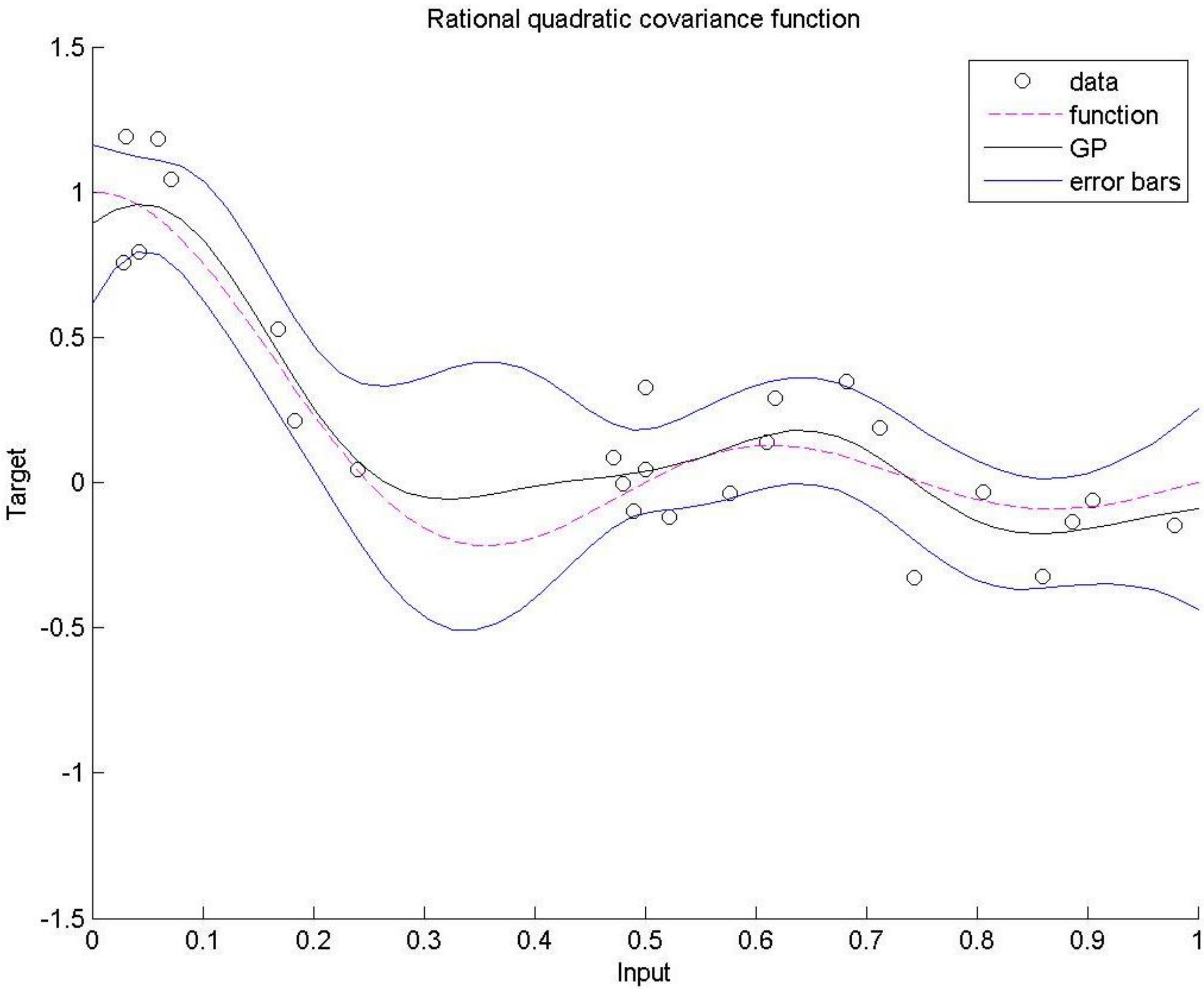
Increased # of training points

Results using Netlab, Sin function



Increased noise

Results using Netlab, Sinc function



Thanks for the Attention! ☺

Extra Material

Contents

- Introduction
- Ridge Regression
- Gaussian Processes
  - Weight space view
    - Bayesian Ridge Regression + Kernel trick
  - Function space view
    - Prior distribution over functions
      + calculation posterior distributions

Function Space View

- An alternative way to get the previous results

- Inference directly in function space

Definition: (Gaussian Processes)

GP is a collection of random variables, s.t. any finite number of them have a joint Gaussian distribution

Function Space View

Notations:

$$f(\mathbf{x}) \sim GP(m(\mathbf{x}), k(\mathbf{x}, \tilde{\mathbf{x}})) \in \mathbb{R},\ \mathbf{x} \in \mathbb{R}^D$$

$$m(\mathbf{x}) = \mathbb{E}[f(x)] \in \mathbb{R},\ \text{(mean function)}$$

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbb{E}[(f(x) - m(\mathbf{x}))(f(\tilde{\mathbf{x}}) - m(\tilde{\mathbf{x}}))^T] \in \mathbb{R}$$

(covariance function)

GP is **completely specified** by its

mean function $m(\mathbf{x})$, and

covariance function $k(\mathbf{x}, \tilde{\mathbf{x}})$

Function Space View

Gaussian Processes:

For each $\mathbf{x} \in \mathbb{R}^D$ we associate a Gaussian variable $f(\mathbf{x})$ such that $\mathbb{R} \ni f(\mathbf{x}) \sim \mathcal{N}_{f(\mathbf{x})}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}))$, and its correalation with other $f(\tilde{\mathbf{x}})$ variables is $k(\mathbf{x}, \tilde{\mathbf{x}})$.

$$\mathbb{R} \ni f(\mathbf{x}) \sim \mathcal{N}_{f(\mathbf{x})}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}))$$

$$\begin{bmatrix} f(\mathbf{x}) \\ f(\tilde{\mathbf{x}}) \end{bmatrix} \sim \mathcal{N}_{\begin{bmatrix} f(\mathbf{x}) \\ f(\tilde{\mathbf{x}}) \end{bmatrix}} \left\{ \begin{bmatrix} m(\mathbf{x}) \\ m(\tilde{\mathbf{x}}) \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}, \mathbf{x}) & k(\tilde{\mathbf{x}}, \mathbf{x}) \\ k(\mathbf{x}, \tilde{\mathbf{x}}) & k(\tilde{\mathbf{x}}, \tilde{\mathbf{x}}) \end{bmatrix} \right\}$$

Function Space View

The Bayesian linear regression is an example of GP

$$f(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w} \in \mathbb{R},\ \phi(\mathbf{x}), \mathbf{w} \in \mathbb{R}^N \quad \mathbf{w} \sim \mathcal{N}_{\mathbf{w}}(0, \Sigma_p)$$

$\Rightarrow [f(\mathbf{x}_1), \ldots, f(\mathbf{x}_k)]$ are jointly Gaussian $\forall \mathbf{x}_1, \ldots, \mathbf{x}_k$
thus f is GP.

$$\mathbb{E}[f(\mathbf{x})] = \phi(\mathbf{x})^T \mathbb{E}[\mathbf{w}] = 0 \Rightarrow m(\mathbf{x}) = 0$$

$$\mathbb{E}[f(x) f(\tilde{\mathbf{x}})^T] = \phi(\mathbf{x})^T \underbrace{\mathbb{E}[\mathbf{w}\mathbf{w}^T]}_{\Sigma_p} \phi(\tilde{\mathbf{x}}) = k(\mathbf{x}, \tilde{\mathbf{x}})$$

Function Space View

Special case

$$\left.\begin{aligned} m(\mathbf{x}) &= 0 \\ k(\mathbf{x}, \tilde{\mathbf{x}}) &= \exp\left(-\tfrac{1}{2}\|\mathbf{x} - \tilde{\mathbf{x}}\|^2\right) \end{aligned}\right\} \Rightarrow f \text{ GP is given}$$

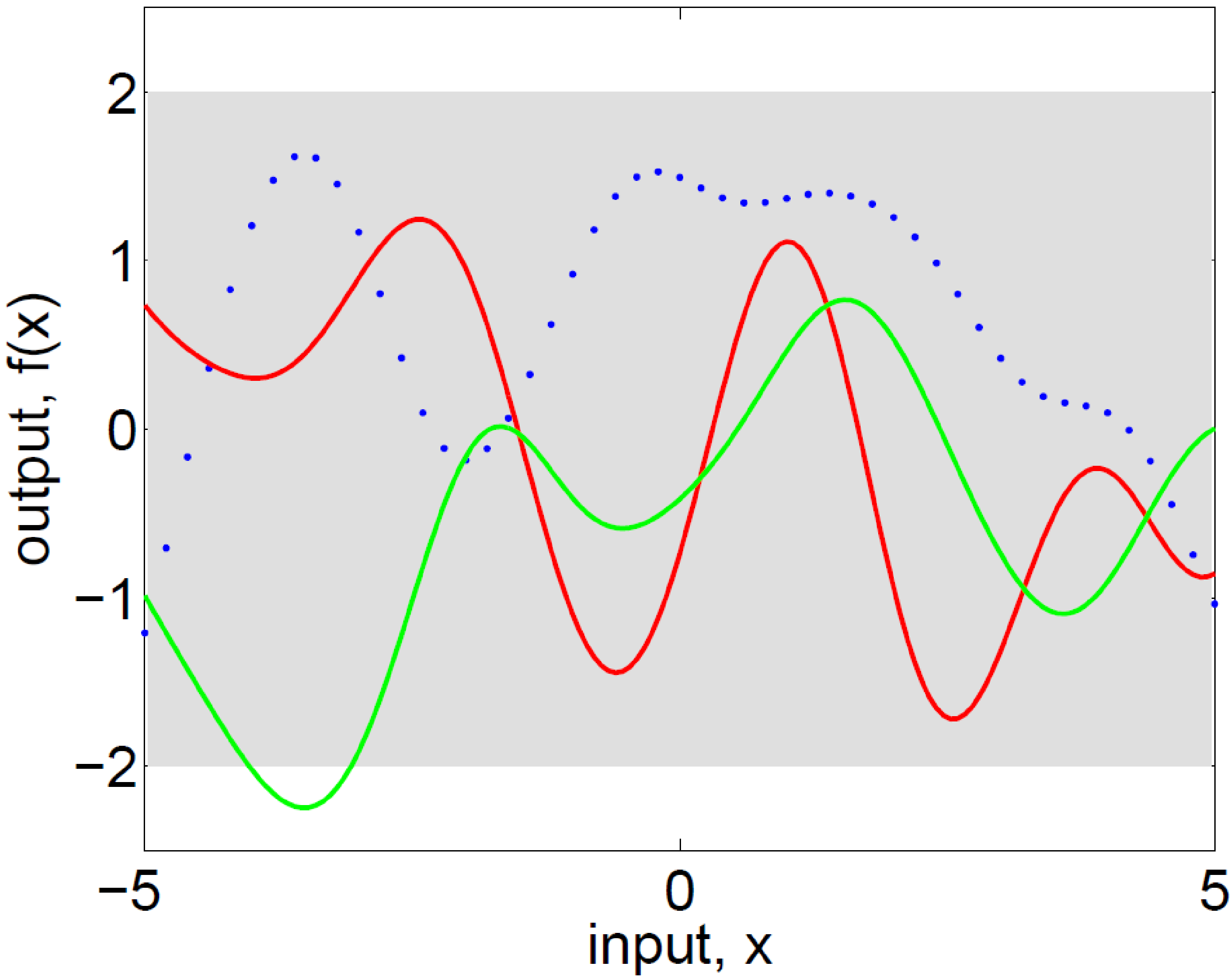
$\Rightarrow$ implies a distribution over functions.

$$\text{Let } X_* = \begin{bmatrix} \mathbf{x}_{*1}^T \\ \vdots \\ \mathbf{x}_{*m}^T \end{bmatrix} \; m \text{ input points}$$

$$\Rightarrow \mathbb{R}^m \ni f_* \sim \mathcal{N}_{f_*}(\underbrace{\mathbf{0}}_{\in \mathbb{R}^m}, \underbrace{k(X_*, X_*)}_{\in \mathbb{R}^{m \times m}})$$

At arbitray $\mathbf{x}_{*1}, \ldots, \mathbf{x}_{*m}$ places, we can generate m points from f (denoted by f_*) and plot them .

Function Space View



Picture is taken from Rasmussen and Williams

Function Space View

Observation

The plotted $f(\mathbf{x}_{*1}), \ldots, f(\mathbf{x}_{*m})$ function looks smooth.

Explanation

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{1}{2}\|\mathbf{x} - \tilde{\mathbf{x}}\|^2\right)$$

Thus if $\|\mathbf{x}_{*i} - \mathbf{x}_{*j}\|$ is small, then $corr(f(\mathbf{x}_{*i}), f(\mathbf{x}_{*j}))$ is high.

Prediction with noise free observations

Training set: $D = \{(\mathbf{x}_i, f_i) | i = 1, \ldots, n\}$

noise free observations

$$X = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} \in \mathbb{R}^{n \times D}, \ m \text{ training inputs}$$

$$X_* = \begin{bmatrix} \mathbf{x}_{*1}^T \\ \vdots \\ \mathbf{x}_{*m}^T \end{bmatrix} \in \mathbb{R}^{m \times D}, \ m \text{ test inputs}$$

$$f = \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix} \in \mathbb{R}^{n}, \ n \text{ training targets}$$

$$f_* = \begin{bmatrix} f_{*1} \\ \vdots \\ f_{*m} \end{bmatrix} \in \mathbb{R}^{m}, \ m \text{ test targets}$$

Prediction with noise free observations

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N}_{\begin{bmatrix} f \\ f_* \end{bmatrix}} \left\{ \begin{bmatrix} \mathbf{0}_n \\ \mathbf{0}_m \end{bmatrix}, \underbrace{\begin{bmatrix} k(X,X) & k(X,X_*) \\ k(X_*,X) & k(X_*,X_*) \end{bmatrix}}_{\in \mathbb{R}^{(m+n)\times(m+n)}} \right\}$$

Goal:

We want to calculate the posterior distribution $f_*|X_*, X, f$

Prediction with noise free observations

Lemma:

$$P(f_*|X_*, X, f) =$$

$$\mathcal{N}_{f_*}\left(k(X_*, X)k(X, X)^{-1}f, k(X_*, X_*) - k(X_*, X)k(X, X)^{-1}k(X, X_*)\right)$$

Proofs: a bit of calculation using the joint (n+m) dim density

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N}_{\begin{bmatrix} f \\ f_* \end{bmatrix}}\left\{\begin{bmatrix} \mathbf{0}_n \\ \mathbf{0}_m \end{bmatrix}, \begin{bmatrix} k(X, X) & k(X, X_*) \\ k(X_*, X) & k(X_*, X_*) \end{bmatrix}\right\}$$

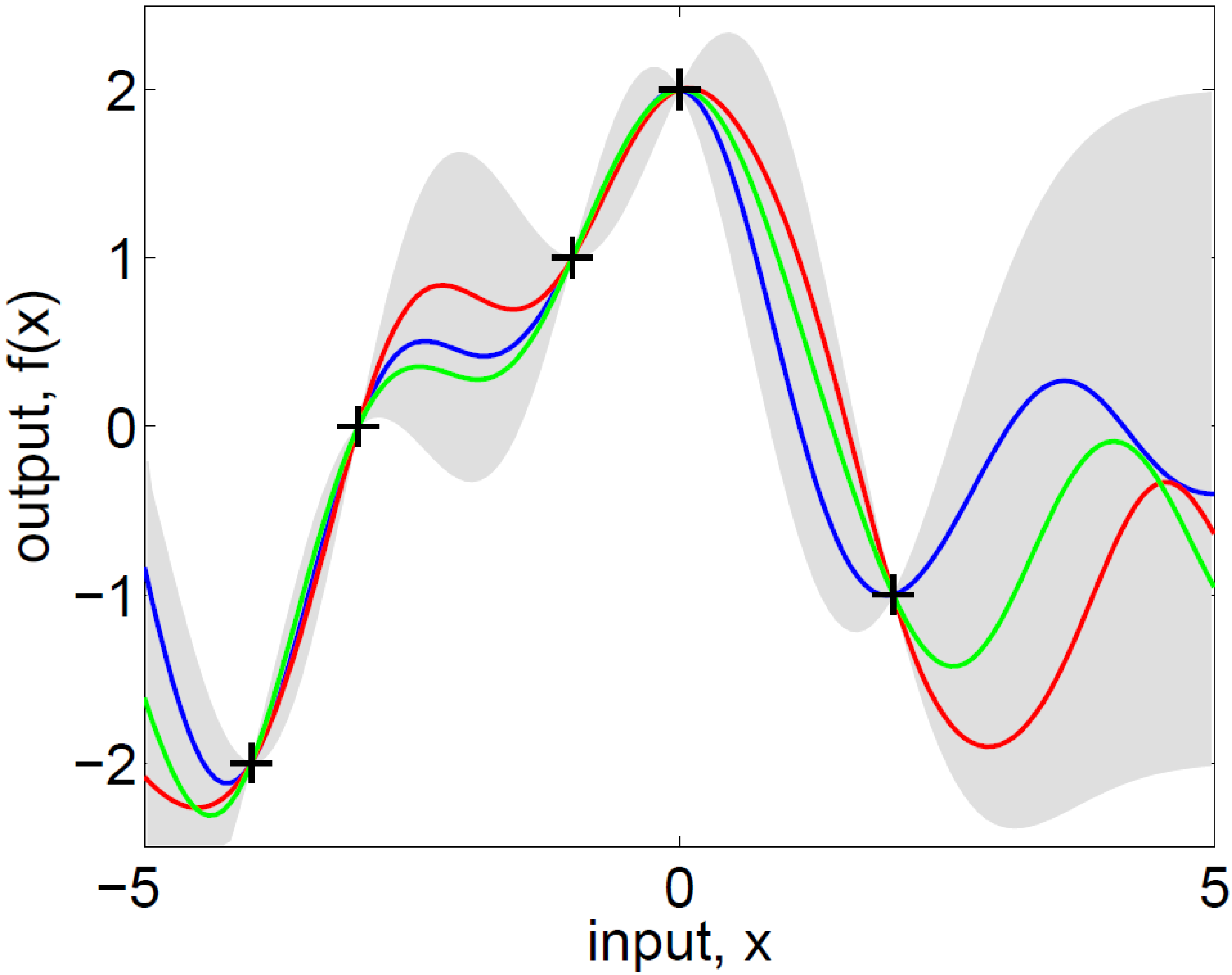
Remarks:

- If $X_* = X \Rightarrow f_* = f$ and the cov is 0. (nosie free observations)
- $P(f_*|X_*, X, f)$ is similar to the previous results:

$$P(f_*|\mathbf{x}_*, X, f) =$$

$$\mathcal{N}_{f_*}\left((\phi_*^T \Sigma_p \phi)(K + \sigma^2 \mathbf{I}_n)^{-1} f, (\phi_*^T \Sigma_p \phi_*) - (\phi_*^T \Sigma_p \phi)(K + \sigma^2 \mathbf{I}_n)^{-1}(\phi^T \Sigma_p \phi_*)\right)$$

Prediction with noise free observations



Picture is taken from Rasmussen and Williams

Prediction using noisy observations

$$y = f(\mathbf{x}) + \epsilon \in \mathbb{R}$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2) \in \mathbb{R}$$

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N}_{\begin{bmatrix} f \\ f_* \end{bmatrix}} \left\{ \begin{bmatrix} \mathbf{0}_n \\ \mathbf{0}_m \end{bmatrix}, \begin{bmatrix} k(X,X) & k(X,X_*) \\ k(X_*,X) & k(X_*,X_*) \end{bmatrix} \right\}$$

$$\Rightarrow cov(y_p, y_q) = k(\mathbf{x}_p, \mathbf{x}_q) + \sigma^2 \delta_{p,q}$$
$$\Rightarrow cov([y_1, \ldots, y_n]) = k(X,X) + \sigma^2 \mathbf{I}_n \in \mathbb{R}^{n \times n}$$

The joint distribution:

$$\Rightarrow \begin{bmatrix} y \\ f_* \end{bmatrix} \sim \mathcal{N}_{\begin{bmatrix} y \\ f_* \end{bmatrix}} \left\{ \begin{bmatrix} \mathbf{0}_n \\ \mathbf{0}_m \end{bmatrix}, \begin{bmatrix} k(X,X) + \sigma^2 \mathbf{I}_n & k(X,X_*) \\ k(X_*,X) & k(X_*,X_*) \end{bmatrix} \right\}$$

Prediction using noisy observations

The posterior for the noisy observations:

$$P(f_*|X, \mathbf{y}, X_*) = \mathcal{N}_{f_*}(\bar{f}_*, cov(f_*))$$

where

$$\bar{f}_* = \mathbb{E}[f_*|X, \mathbf{y}, X_*] = k(X_*, X)[k(X, X) + \sigma^2 I_n]^{-1}\mathbf{y} \in \mathbb{R}^m$$

$$cov(f_*) = k(X_*, X_*) - k(X_*, X)[k(X, X) + \sigma^2 I_n]^{-1} K(X, X_*) \in \mathbb{R}^{m \times m}$$

In the weight space view we had:

$$\bar{f}_* = (\phi_*^T \Sigma_p \phi)(\phi^T \Sigma_p \phi + \sigma^2 \mathbf{I}_n)^{-1}\mathbf{y}$$

$$cov(f_*) = (\phi_*^T \Sigma_p \phi_*) - (\phi_*^T \Sigma_p \phi)(\phi^T \Sigma \phi + \sigma^2 \mathbf{I}_n)^{-1}(\phi^T \Sigma_p \phi_*)$$

If $k(\mathbf{x}, \tilde{\mathbf{x}}) = \phi(x)^T \Sigma_p \phi(\tilde{x})$, then they are the same.

Prediction using noisy observations

Short notations:

$$K = k(X, X) \in \mathbb{R}^{n \times n}$$

$$K_* = k(X, X_*) \in \mathbb{R}^{n \times m}$$

$$k(\mathbf{x}_*) = k_* = k(X, \mathbf{x}_*) = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_*) \\ \vdots \\ k(\mathbf{x}_n, \mathbf{x}_*) \end{bmatrix} \in \mathbb{R}^n$$

$\Rightarrow$ for a single test point $\mathbf{x}_*$:

$$\bar{f}_* = \underbrace{k_*^T}_{\mathbb{R}^{1\times n}} \underbrace{[K + \sigma^2 I_n]^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{\mathbf{y}}_{\mathbb{R}^n} \in \mathbb{R}$$

$$cov(f_*) = \underbrace{k(\mathbf{x}_*, \mathbf{x}_*)}_{\mathbb{R}} - \underbrace{k_*^T}_{\mathbb{R}^{1\times n}} \underbrace{[K + \sigma^2 I_n]^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{k_*}_{\mathbb{R}^n} \in \mathbb{R}$$

Prediction using noisy observations

$$\bar{f}_* = \underbrace{k_*^T}_{\mathbb{R}^{1\times n}} \underbrace{[K + \sigma^2 I_n]^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{\mathbf{y}}_{\mathbb{R}^n} \in \mathbb{R}$$

Two ways to look at it:

- **Linear predictor**

$$\bar{f}_* = \boldsymbol{\beta}^T \mathbf{y} = \beta_1 y_1 + \ldots + \beta_n y_n$$

where $\boldsymbol{\beta}^T = k_*^T [K + \sigma^2 I_n]^{-1} \in \mathbb{R}1 \times n$

- **Manifestation of the Representer Theorem**

$$\bar{f}_* = \boldsymbol{\alpha}^T k_* = \alpha_1 k(\mathbf{x}_1, \mathbf{x}_*) + \ldots + \alpha_n k(\mathbf{x}_n, \mathbf{x}_*)$$

where $\boldsymbol{\alpha} = [K + \sigma^2 I_n]^{-1} \mathbf{y}$

$\bar{f}_*$ is a linear combination of n kernel values.

Prediction using noisy observations

$$\bar{f}_* = \underbrace{k_*^T}_{\mathbb{R}^{1\times n}} \underbrace{[K + \sigma^2 I_n]^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{\mathbf{y}}_{\mathbb{R}^n} \in \mathbb{R}$$

Remarks:

- While the GP in general is quite complex, for the prediction of $\bar{f}_* = f(\mathbf{x}_*)$ we need only the (n+1) dimensional joint Gaussian distibution of $[y_1, \ldots, y_n, f(\mathbf{x}_*)]$

- The posterior covariance of

$$cov(f_*|X, \mathbf{y}, X_*) = k(X_*, X_*) - k(X_*, X)[k(X, X) + \sigma^2 I_n]^{-1} K(X, X_*)$$

does not depend on the observed targets $\mathbf{y}$.
This is a peculiarity of GP.

GP pseudo code

Inputs:

$$X = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} \in \mathbb{R}^{n \times D},\ n \text{ training inputs}$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^{n},\ n \text{ training targets}$$

$k(\cdot,\cdot) : \mathbb{R}^{D \times D} \rightarrow \mathbb{R}$ covariance function (kernel)

$\mathbf{x}_*$ test input

σ^2 noise level on the observations

$$[y(\mathbf{x}) = f(\mathbf{x}) + \epsilon,\ \epsilon \sim \mathcal{N}(0, \sigma^2)]$$

GP pseudo code (continued)

1., $K \in \mathbb{R}^{n\times n}$ Gram matrix. $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$

$$k(\mathbf{x}_*) = k_* = k(X, \mathbf{x}_*) = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_*) \\ \vdots \\ k(\mathbf{x}_n, \mathbf{x}_*) \end{bmatrix} \in \mathbb{R}^n$$

2., $\boldsymbol{\alpha} = (K + \sigma^2 \mathbf{I}_n)^{-1} \mathbf{y}$

3., $\bar{f}_* = k_*^T \boldsymbol{\alpha} \in \mathbb{R}$

4., $cov(f_*) = \underbrace{k(\mathbf{x}_*, \mathbf{x}_*)}_{\mathbb{R}} - \underbrace{k_*^T}_{\mathbb{R}^{1\times n}} \underbrace{[K + \sigma^2 I_n]^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{k_*}_{\mathbb{R}^n} \in \mathbb{R}$

Outputs: $\bar{f}_*$, $cov(f_*)$

Thanks for the Attention! ☺