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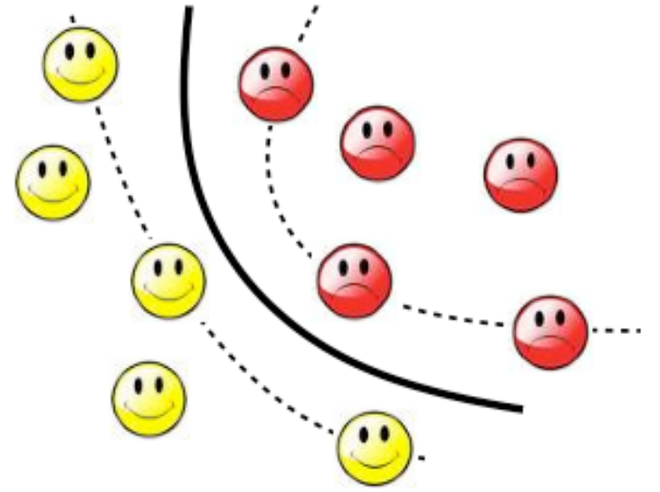

Machine Learning and Data Mining (COMP 5318)

Bayesian Linear Regression And Gaussian Processes

Roman Marchant

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Recap

Linear Regression

Modelling Noisy Observations

Lets assume observations from a deterministic function with added Gaussian noise.

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon \qquad \text{with} \qquad \epsilon \sim \mathcal{N}(0, \beta^{-1})$$

equivalently,

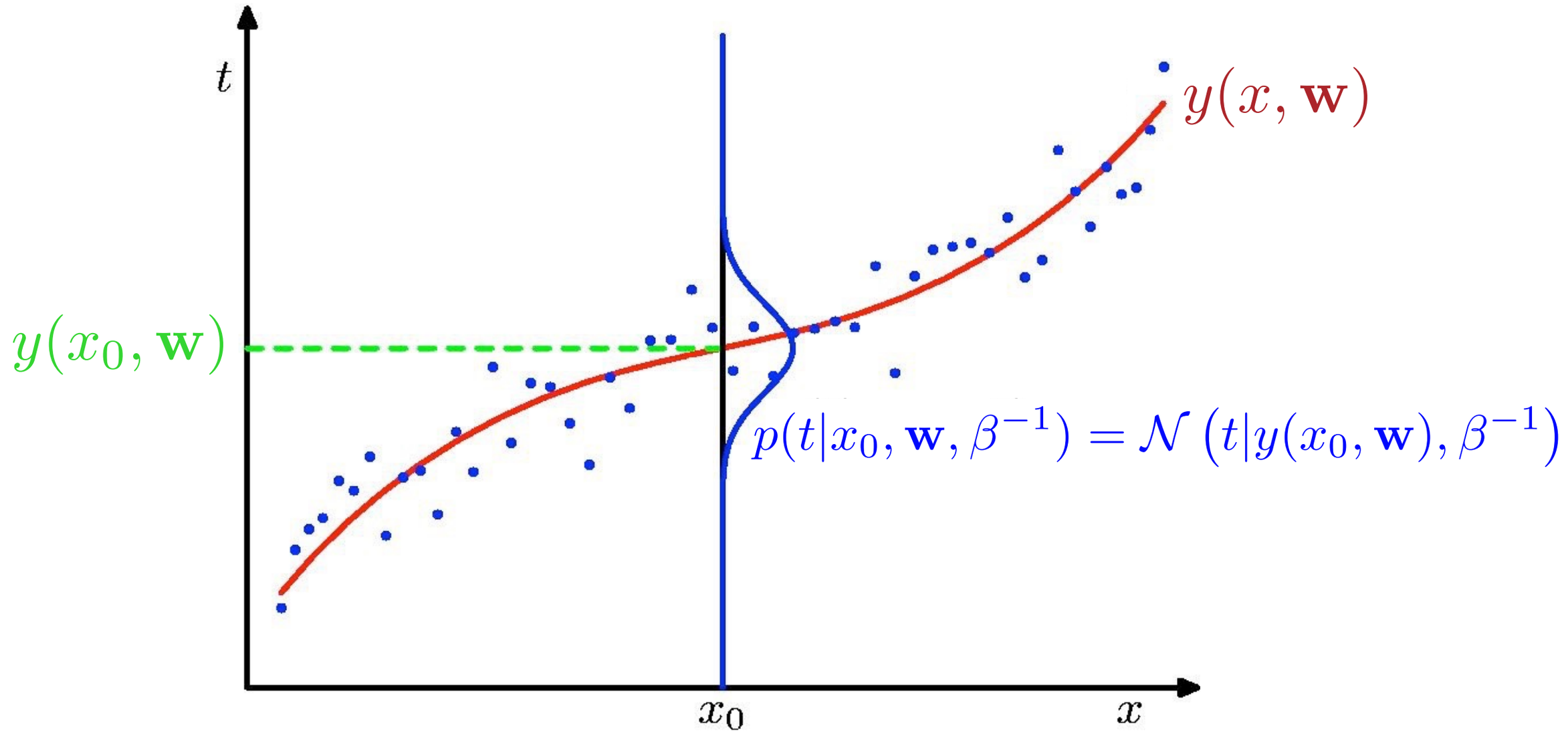
$$p(t|\mathbf{x}, \mathbf{w}, \beta^{-1}) = \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right)$$

Given the training data: $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ $\boldsymbol{\tau} = \{t_1, ..., t_N\}$

The expression of the likelihood of the iid data given the model is:

$$p(\boldsymbol{\tau}|\mathbf{X}, \mathbf{w}, \beta^{-1}) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right)$$

Modelling Noisy Observations



Maximum Likelihood

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$$\mathbf{w}_{\mathrm{ML}} = \underset{\mathbf{w}}{\operatorname{argmax}} \ \ln p(\boldsymbol{\tau}|\mathbf{X}, \mathbf{w}, \beta^{-1})$$

$$\Rightarrow \qquad \left.\frac{\partial \ln p(\boldsymbol{\tau}|\mathbf{w}, \beta^{-1})}{\partial \mathbf{w}}\right|_{\mathbf{w}_{\mathrm{ML}}} = 0$$

$$\sum_{n=1}^{N} \left(t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\right) \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} = 0$$

Solving for $\mathbf{w}_{\mathrm{ML}}$

$$\mathbf{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\tau}$$

where

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}.$$

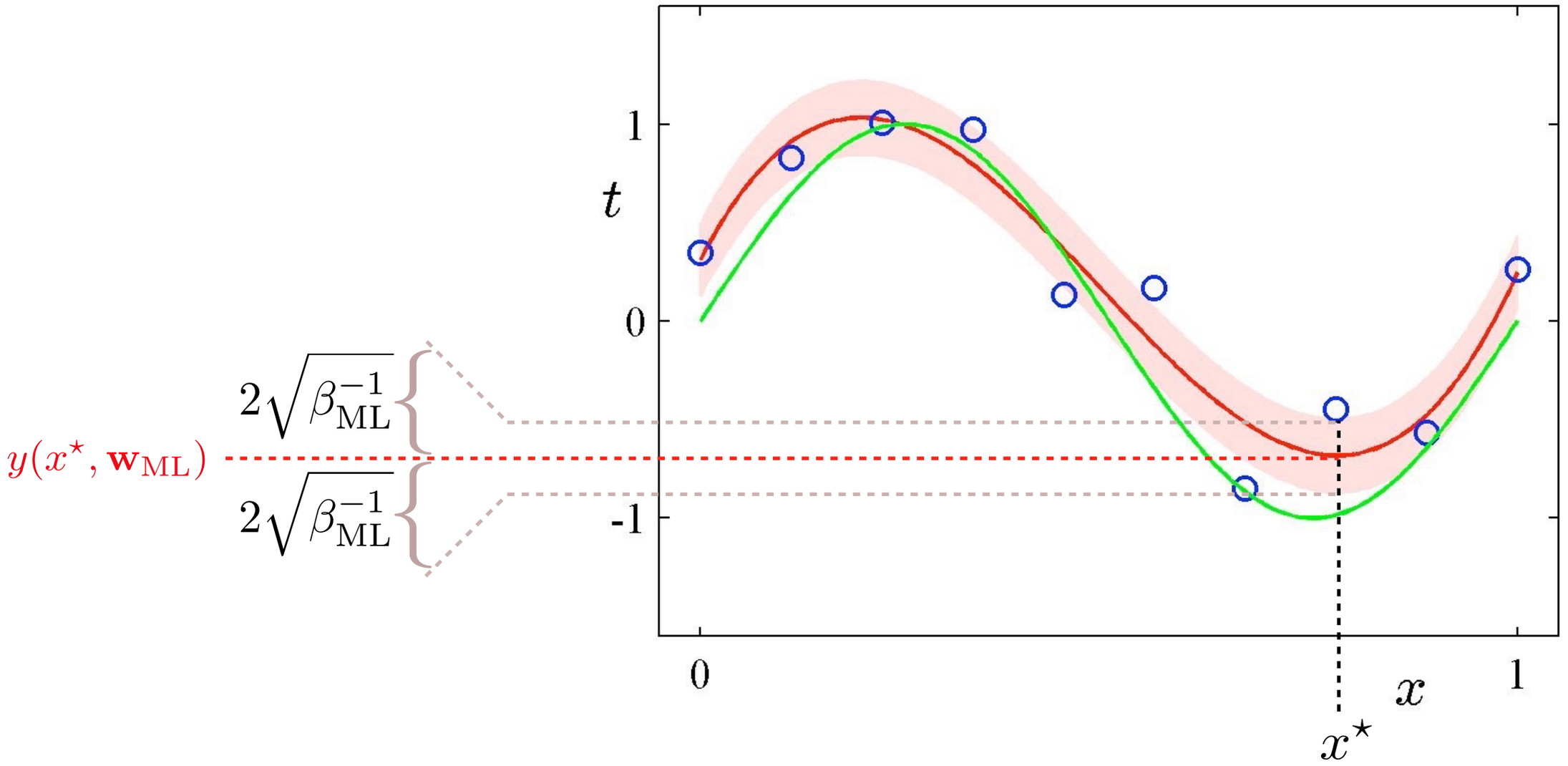
Maximum Likelihood

We can also maximise the log likelihood with respect to the noise precision parameter β .

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\left(t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\right)^2$$

Predictive Distribution

$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1})$$



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Bayesian Linear Regression

C. Bishop, *Pattern Recognition and Machine Learning,* Chapter 3: Linear Models for Regression
Springer New York, 2006

Learning as Optimisation

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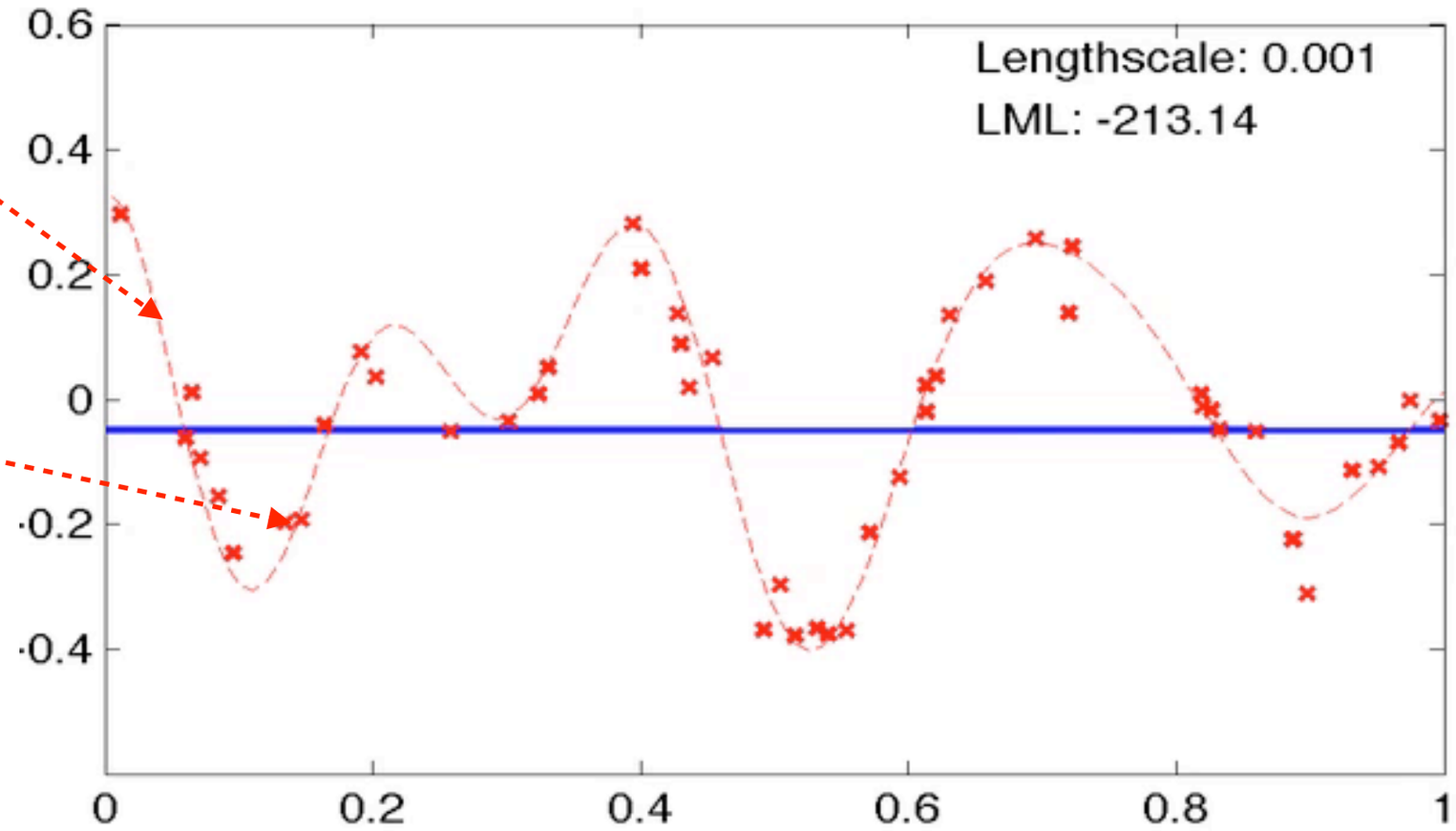
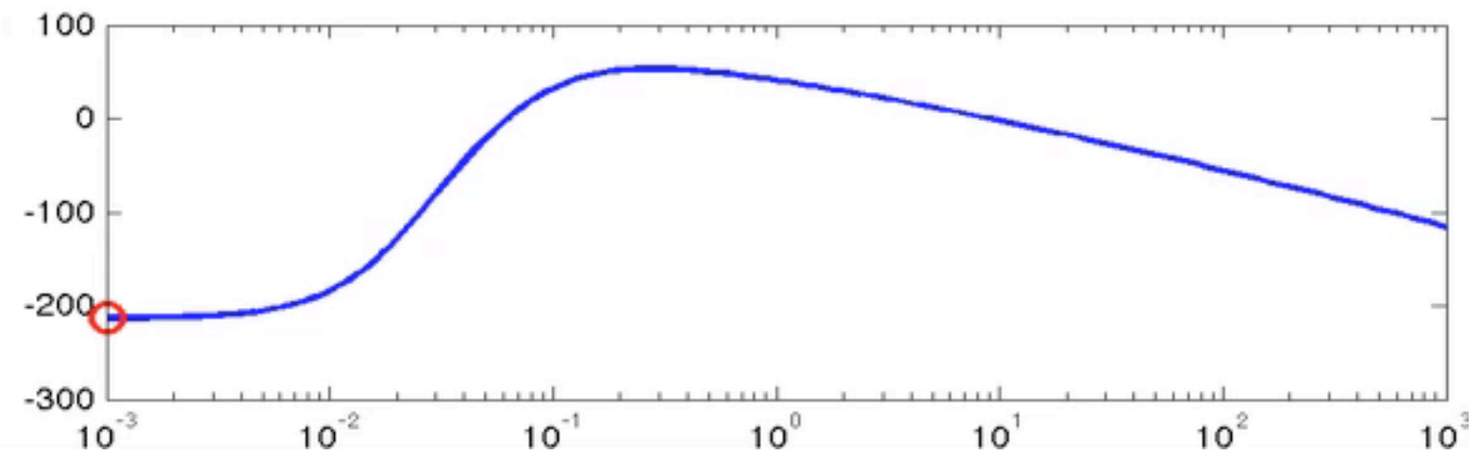
Unknown Function
$f(\mathbf{x})$

Noisy Samples
from f



Log Marginal Likelihood



Deterministic vs Probabilistic Modelling

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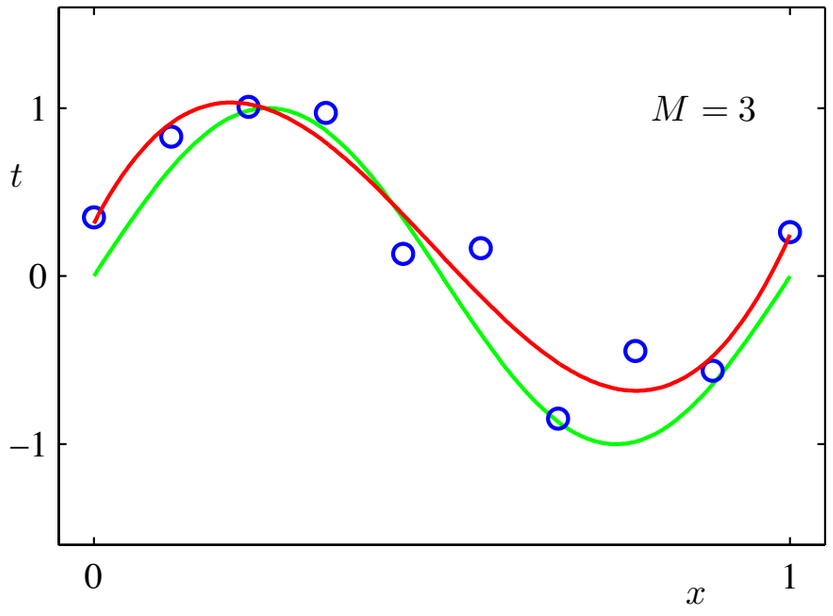
Deterministic

Noisy Data

Ground Truth

Model Fit

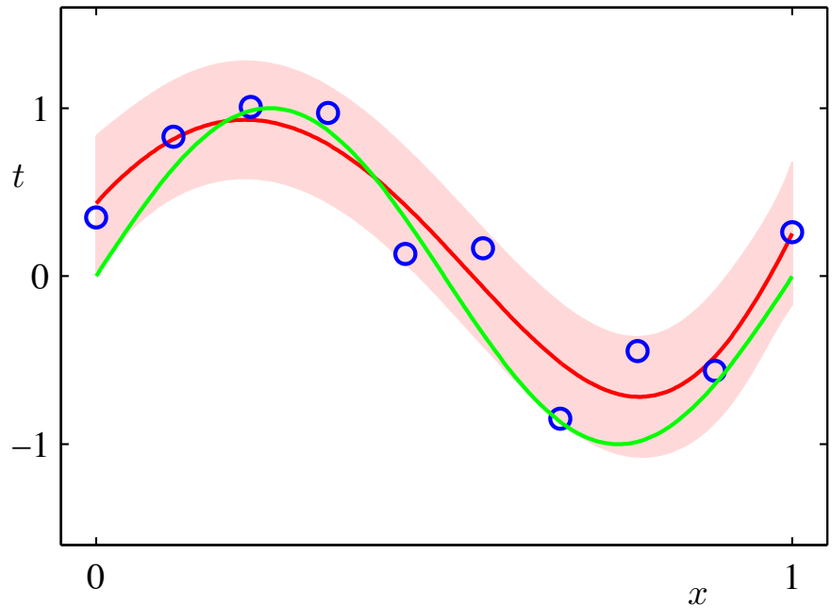


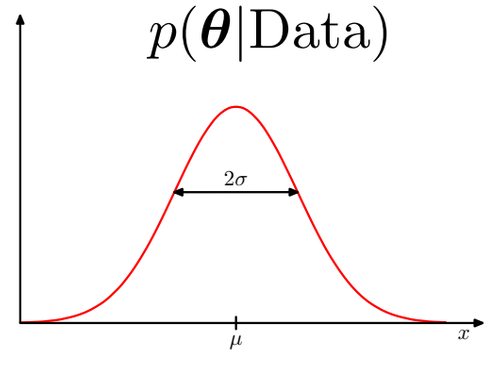
$$y(x, \boldsymbol{\theta}) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$$

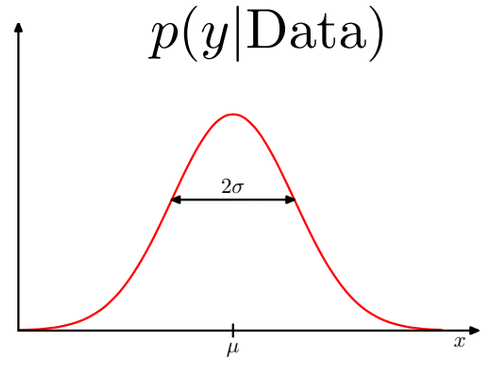
$$\boldsymbol{\theta}^\star = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\ E(\boldsymbol{\theta})$$

Probabilistic

Prediction Uncertainty







Bayes Teorem

Thomas
Bayes
1701–1761

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Likelihood **Prior**

$$\underbrace{p(\boldsymbol{\theta}|\mathcal{D})}_{\textbf{Posterior Distribution (Inference)}} \propto \frac{p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{D})}$$

Normalising Constant

*The data does not speak by itself.

Predictive Distribution

$$p(y|\mathcal{D}) = \int p(y|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathcal{D})\,\mathrm{d}\boldsymbol{\theta}$$

Summing over models.
(integrating over all possible model space)

Bayesian Linear Regression

Apply Bayes theorem to find posterior over parameters:

$$p(\mathbf{w}|\mathbf{X}, \boldsymbol{\tau}, \boldsymbol{\theta}, \beta) \propto p(\boldsymbol{\tau}|\mathbf{X}, \mathbf{w}, \beta)p(\mathbf{w}|\boldsymbol{\theta})$$

Define a conjugate prior (assuming gaussian likelihood):

$$p(\mathbf{w}|\boldsymbol{\theta}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0(\boldsymbol{\theta}), \mathbf{S}_0(\boldsymbol{\theta}))$$

$\boldsymbol{\theta}$ prior parameters (hyper-parameters).

Combining the likelihood and the prior provides the following analytical solution:

$$p(\mathbf{w}|\boldsymbol{\tau}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

where,

$$\mathbf{m}_N = \mathbf{S}_N \left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\tau}\right)$$
$$\mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$$

*Applying theorem from Bishop Section 2.3.3

Bayesian Linear Regression

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Example:

Prior: $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$

Previous Result

$$p(\mathbf{w}|\boldsymbol{\tau}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

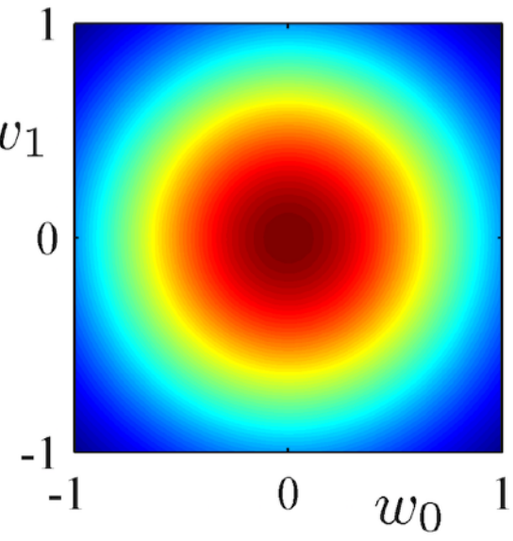
$$\mathbf{m}_N = \mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\tau}\right)$$

$$\mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \beta\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$$

$$\mathbf{m}_0 = 0$$

$$\mathbf{S}_0 = \alpha^{-1}\mathbf{I}$$

2D Zero-mean Isotropic Gaussian



Posterior: $p(\mathbf{w}|\boldsymbol{\tau}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$

$$\mathbf{m}_N = \beta\mathbf{S}_N\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\tau}$$

$$\mathbf{S}_N^{-1} = \alpha\mathbf{I} + \beta\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$$

$$\ln p(\mathbf{w}|\mathbf{t}) = -\frac{\beta}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 - \frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} + \text{const.}$$

Bayesian Linear Regression

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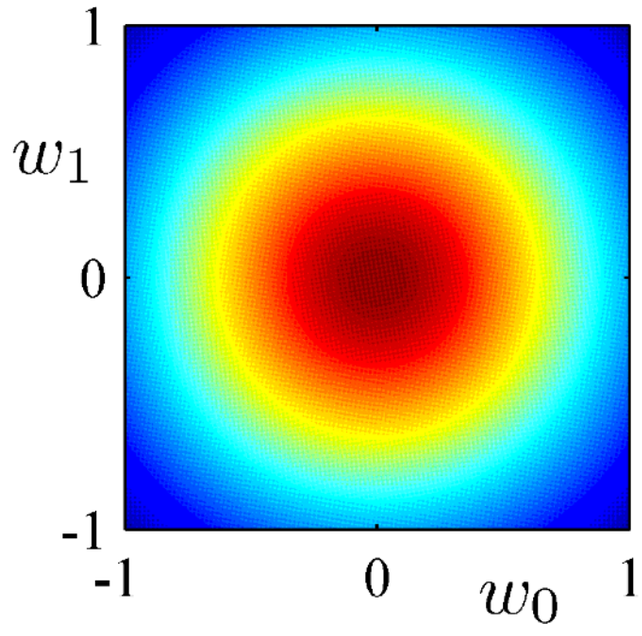
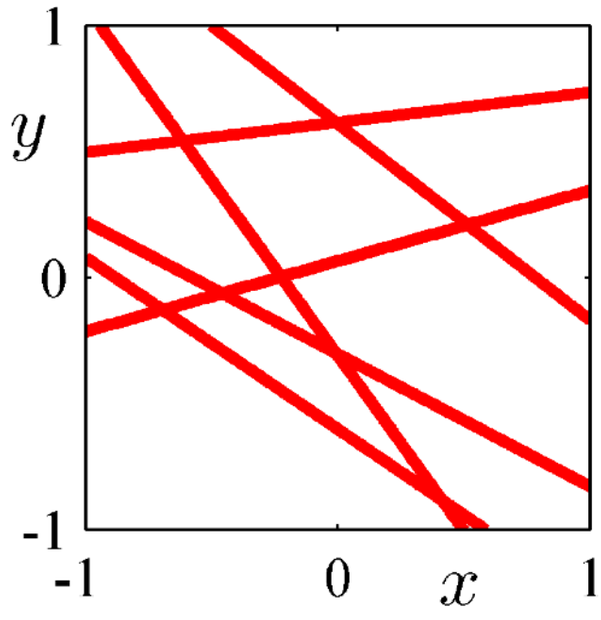
Example:

0 Points Observed

Prior



Data Space



Bayesian Linear Regression

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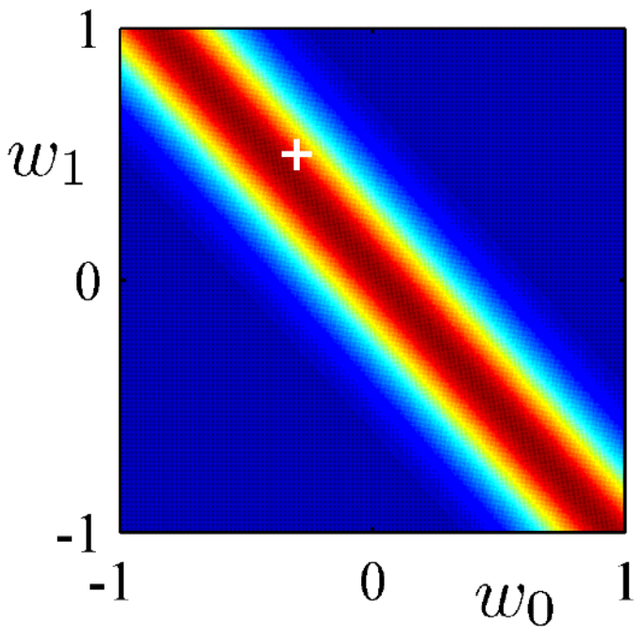
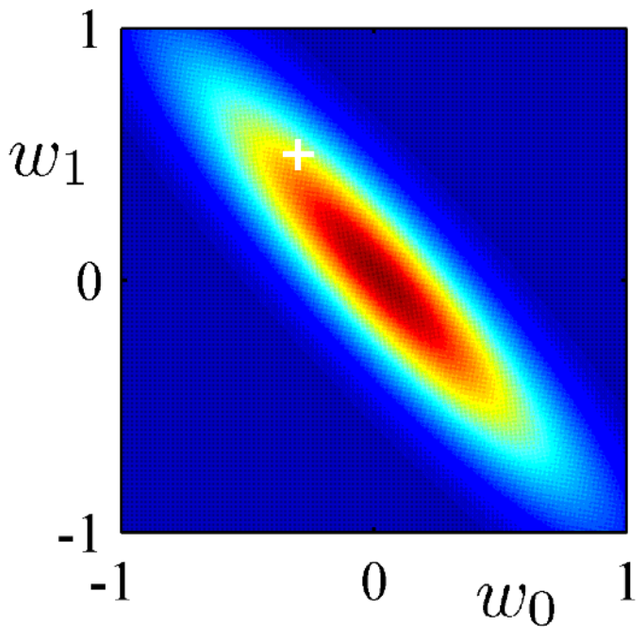
Example:

1 Point Observed

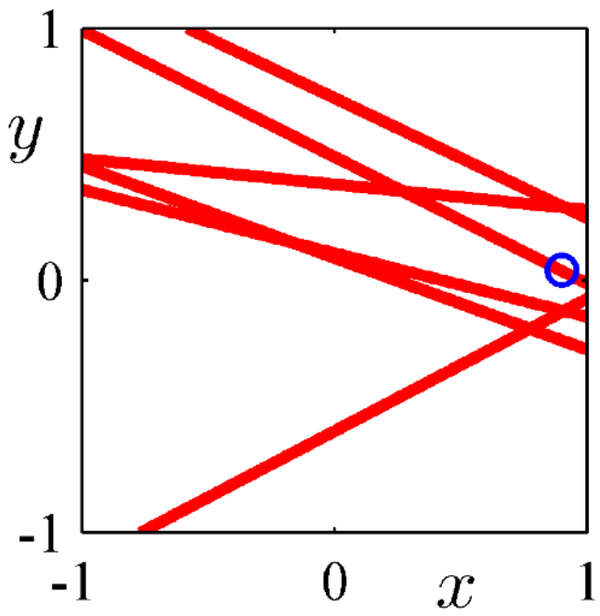
Likelihood



Posterior



Data Space

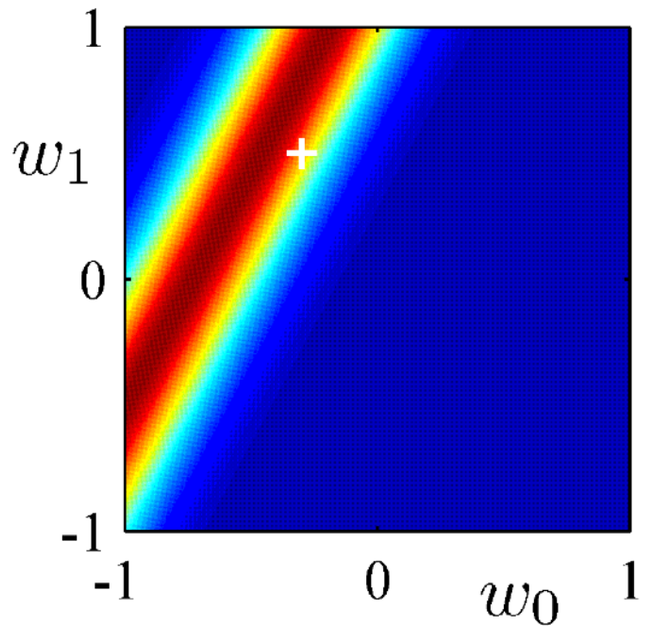


Bayesian Linear Regression

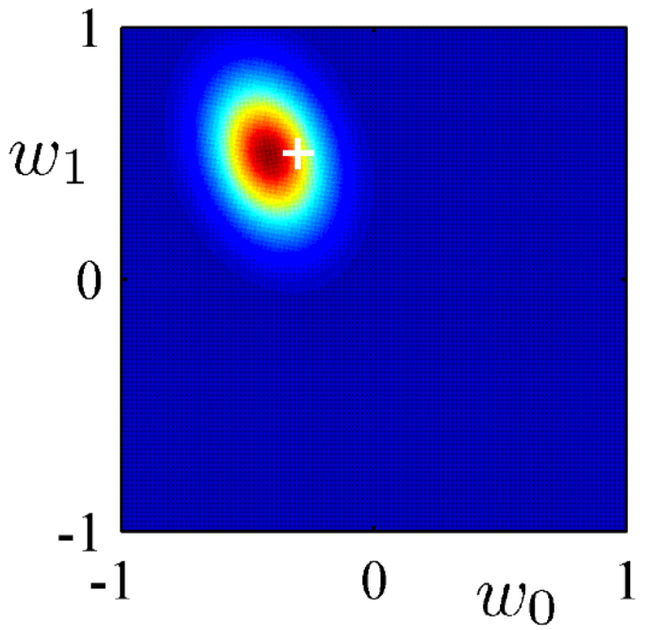
Example:

2 Points Observed

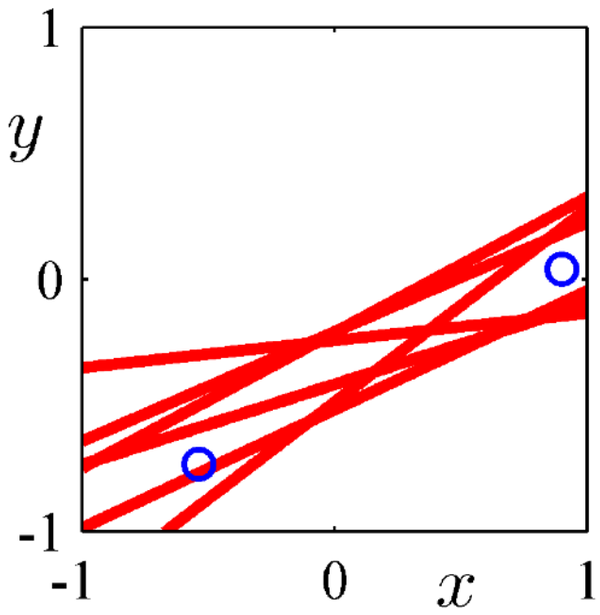
Likelihood



Posterior



Data Space

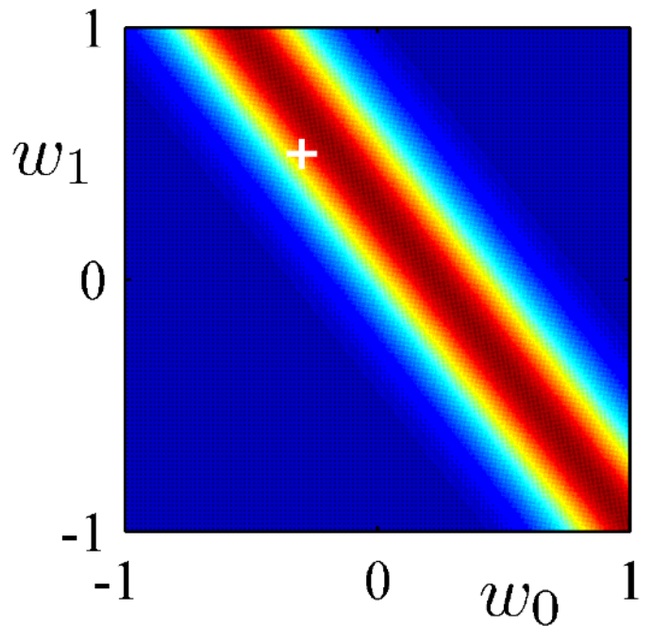


Bayesian Linear Regression

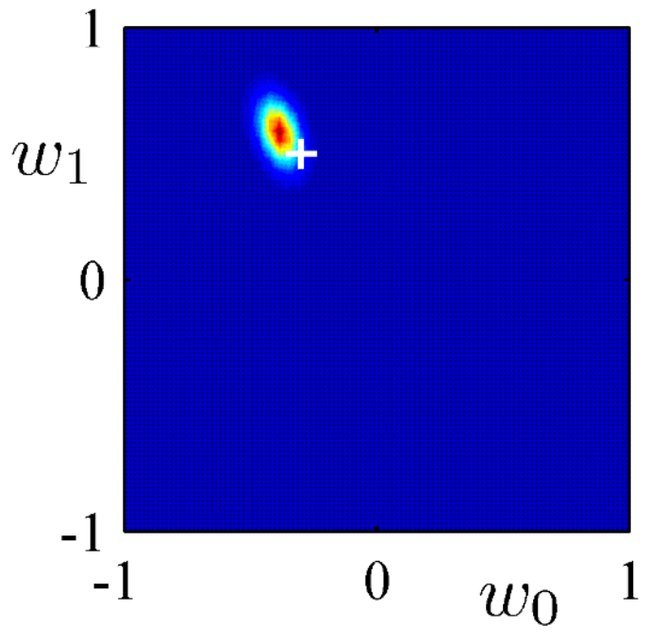
Example:

20 Points Observed

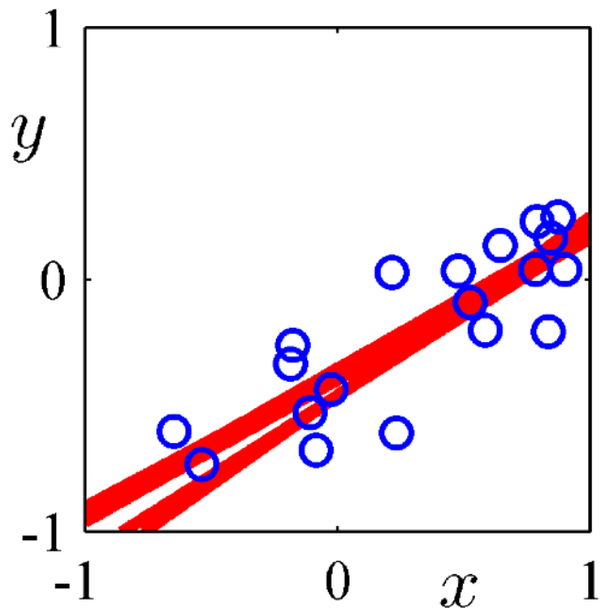
Likelihood



Posterior



Data Space



Predictive Distribution

Predict the value of t for new values of $\mathbf{x}$.

$$p(t|\boldsymbol{\tau}, \alpha, \beta) = \int p(t|\mathbf{w}, \beta) p(\mathbf{w}|\boldsymbol{\tau}, \alpha, \beta) \mathrm{d}\mathbf{w}$$

$$\mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right) \qquad \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{m}_N = \mathbf{S}_N \left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\tau}\right)$$

$$\mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \beta \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}$$

$$p(t|\boldsymbol{\tau}, \alpha, \beta) = \mathcal{N}\left(t|\mathbf{m}_N^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x})\right)$$

Where,

$$\sigma_N^2(\mathbf{x}) = \frac{1}{\beta} + \boldsymbol{\phi}^{\mathrm{T}}(\mathbf{x}) \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})$$

Predictive Distribution

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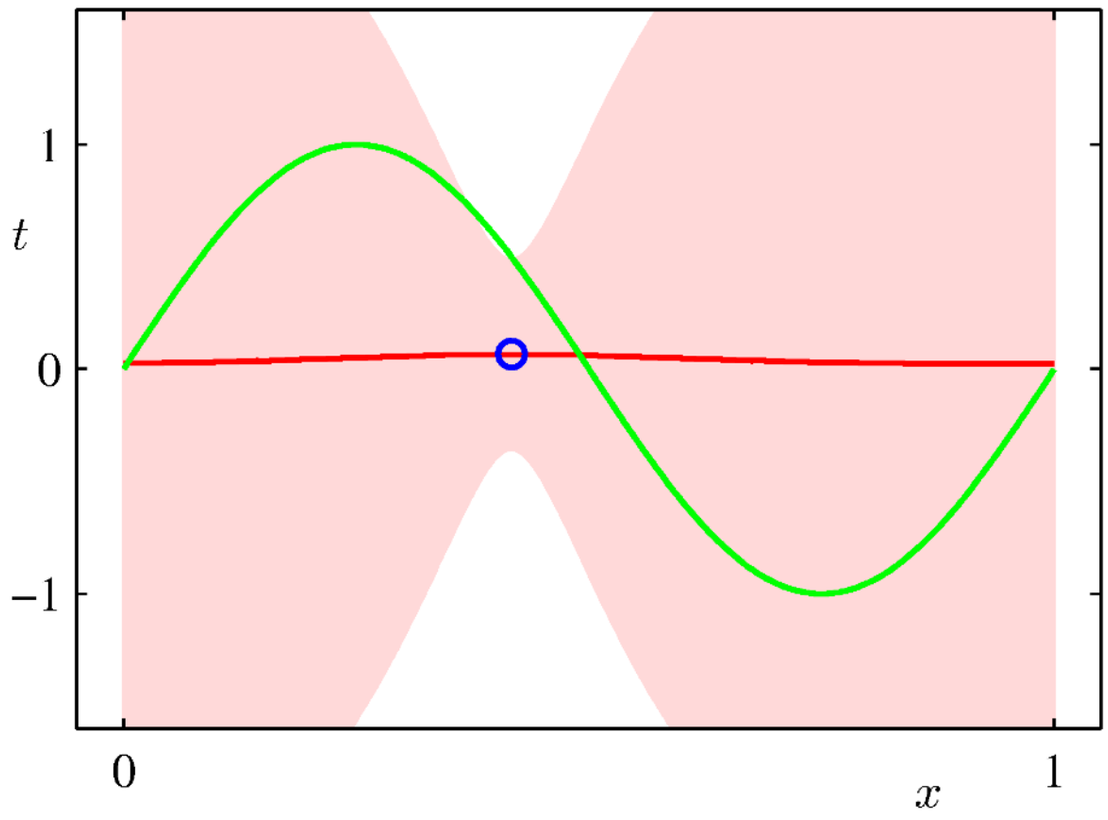
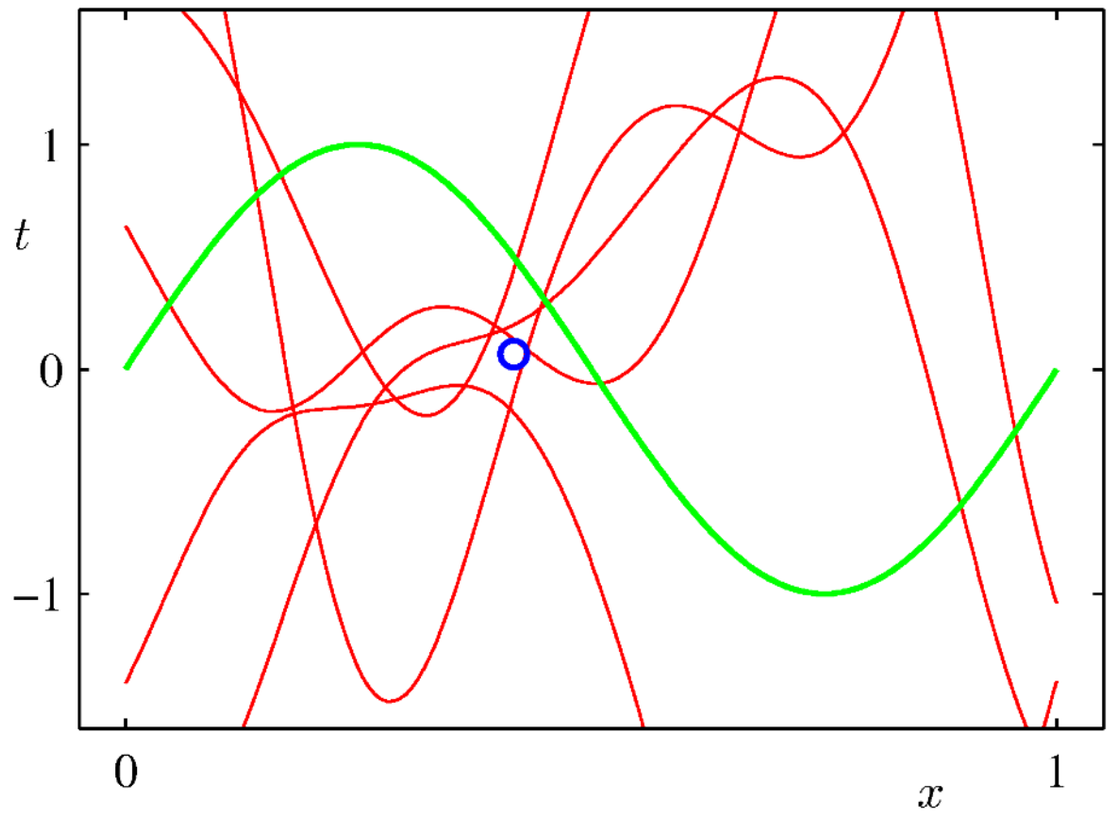
Example: Sinusoidal Data, 9 Gaussian basis functions





Predictive Distribution

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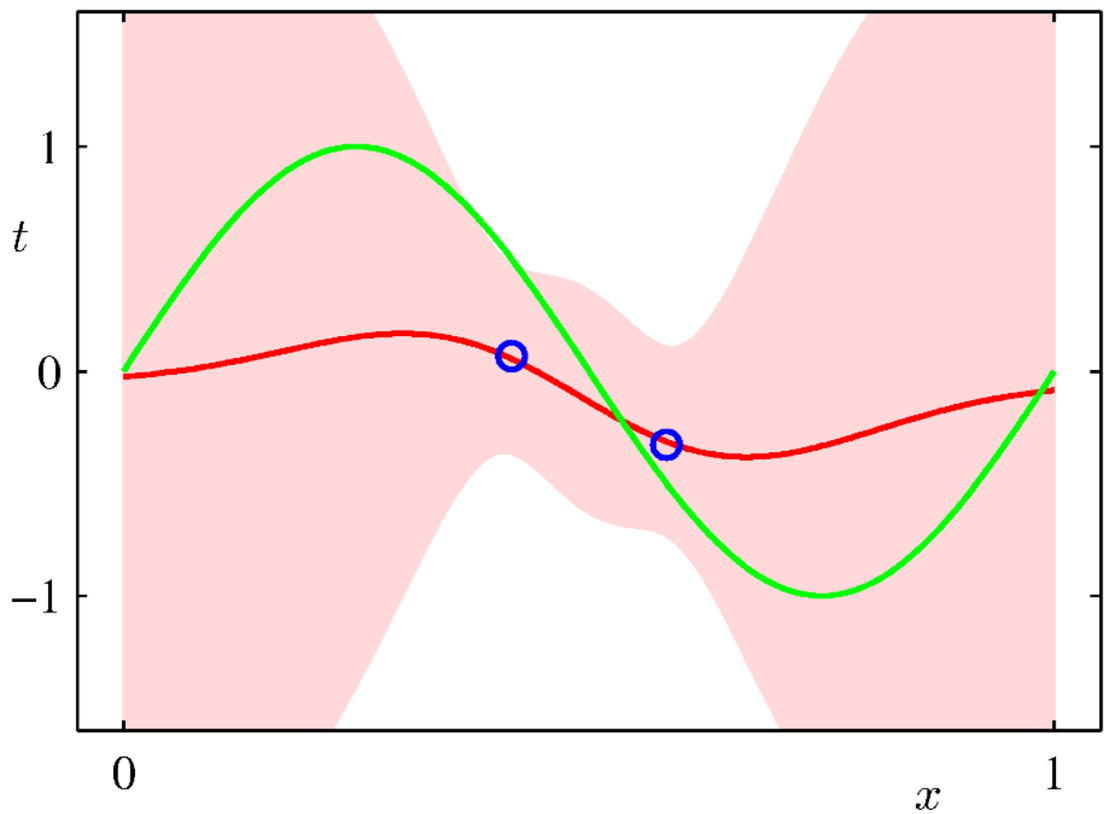
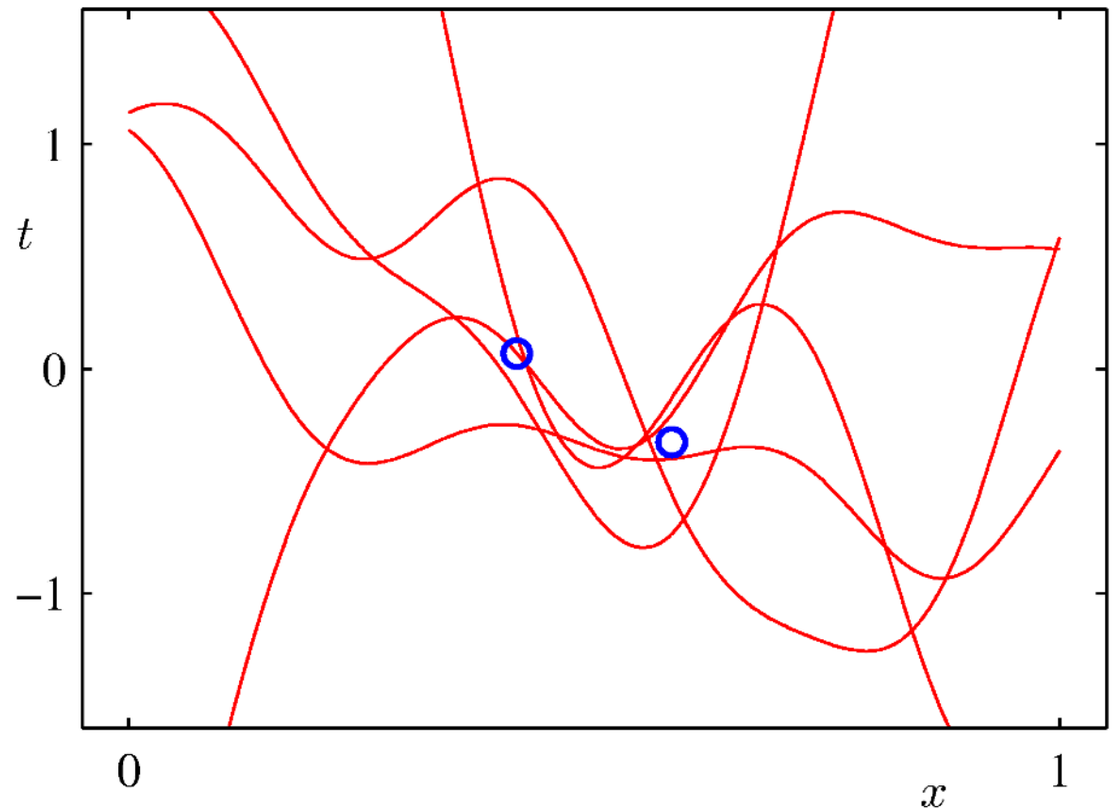
Example: Sinusoidal Data, 9 Gaussian basis functions





Predictive Distribution

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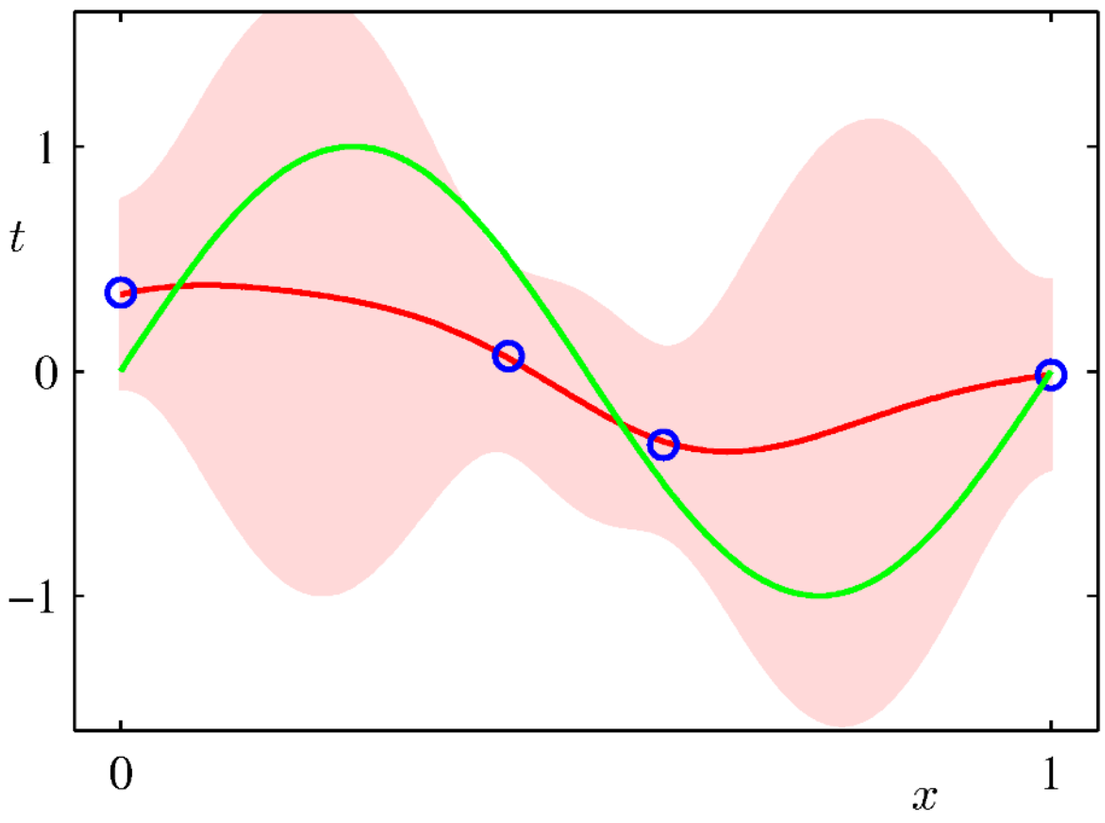
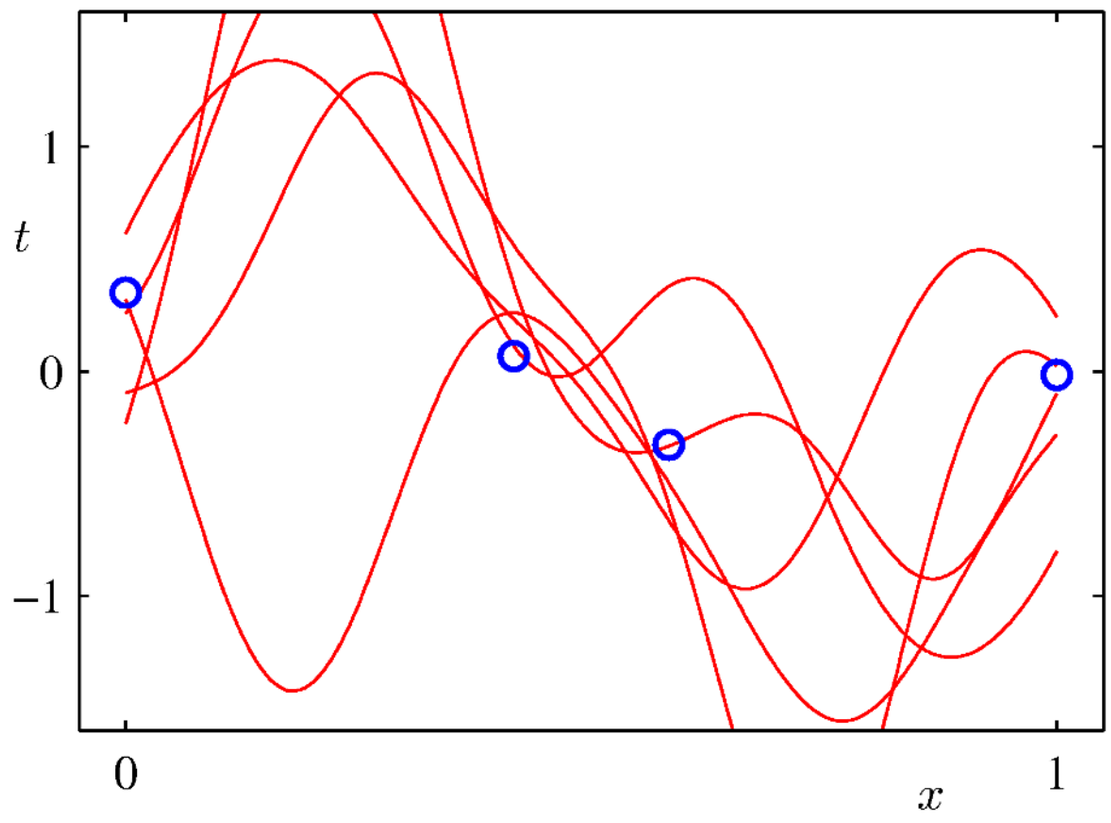
Example: Sinusoidal Data, 9 Gaussian basis functions





Predictive Distribution

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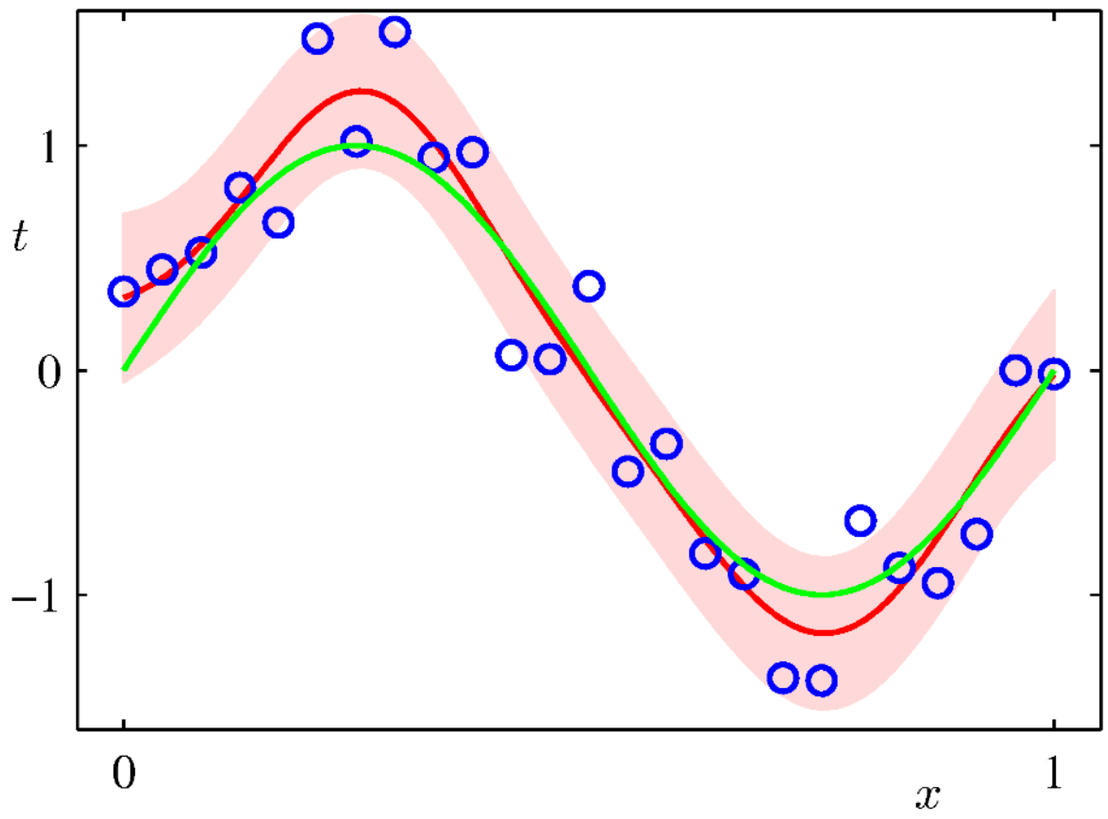
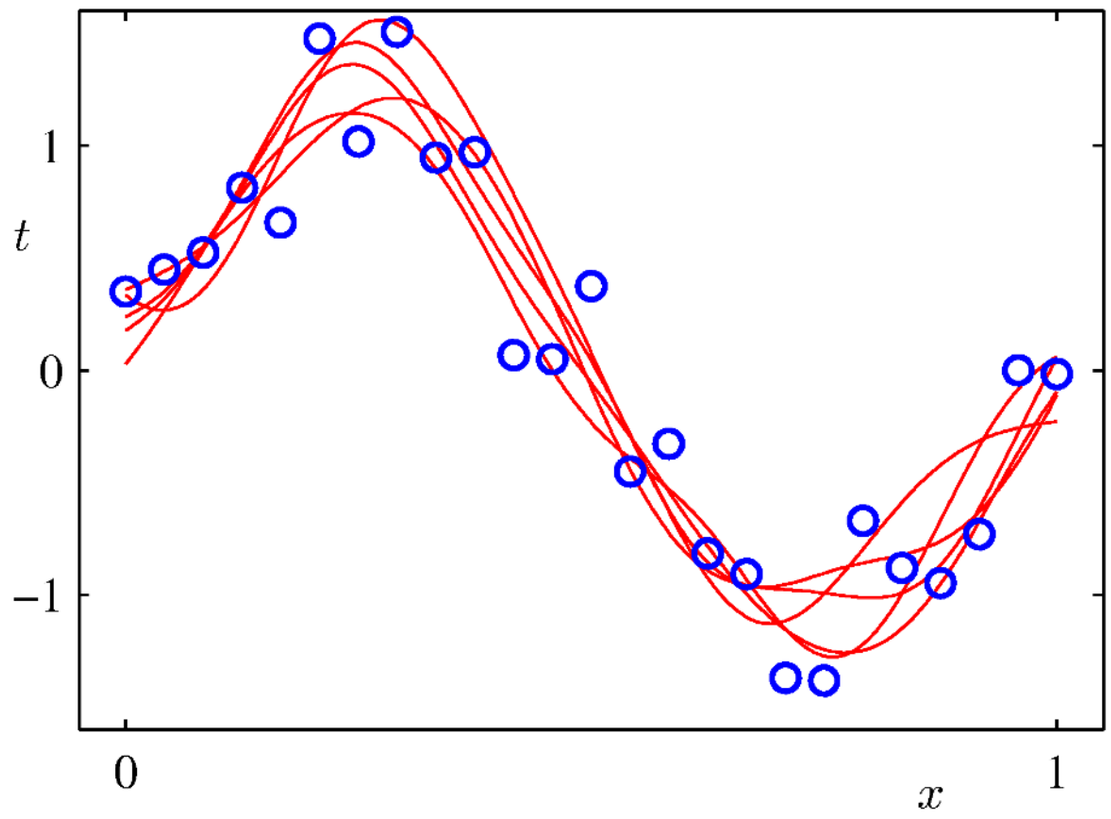
Example: Sinusoidal Data, 9 Gaussian basis functions





Equivalent Kernel

The predictive distribution:

$$p(t|\boldsymbol{\tau}, \alpha, \beta) = \mathcal{N}\left(t|\mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x})\right)$$

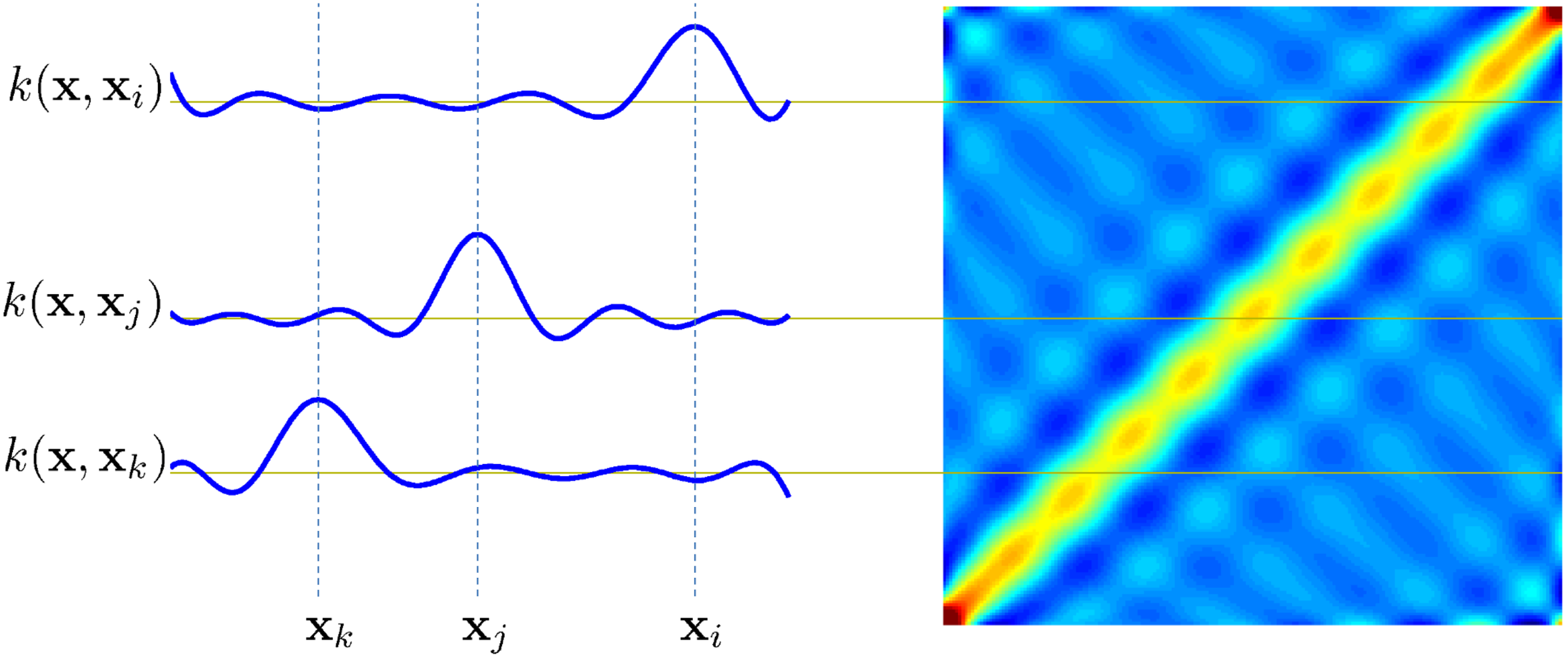
Rewriting the predictive mean:

$$\begin{aligned}\mathbf{m}_N^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}) &= \beta\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{S}_N\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\tau} \\ &= \sum_{n=1}^{N}\beta\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{S}_N\boldsymbol{\phi}(\mathbf{x}_n)t_n \\ &= \sum_{n=1}^{N}k(\mathbf{x}, \mathbf{x}_n)t_n.\end{aligned}$$

Equivalent kernel or *smoother matrix*.

This is a weighted sum of the training data target values.

Equivalent Kernel



Weight of t_n depends on distance between x and x_n; nearby x_n carry more weight.

Equivalent Kernel

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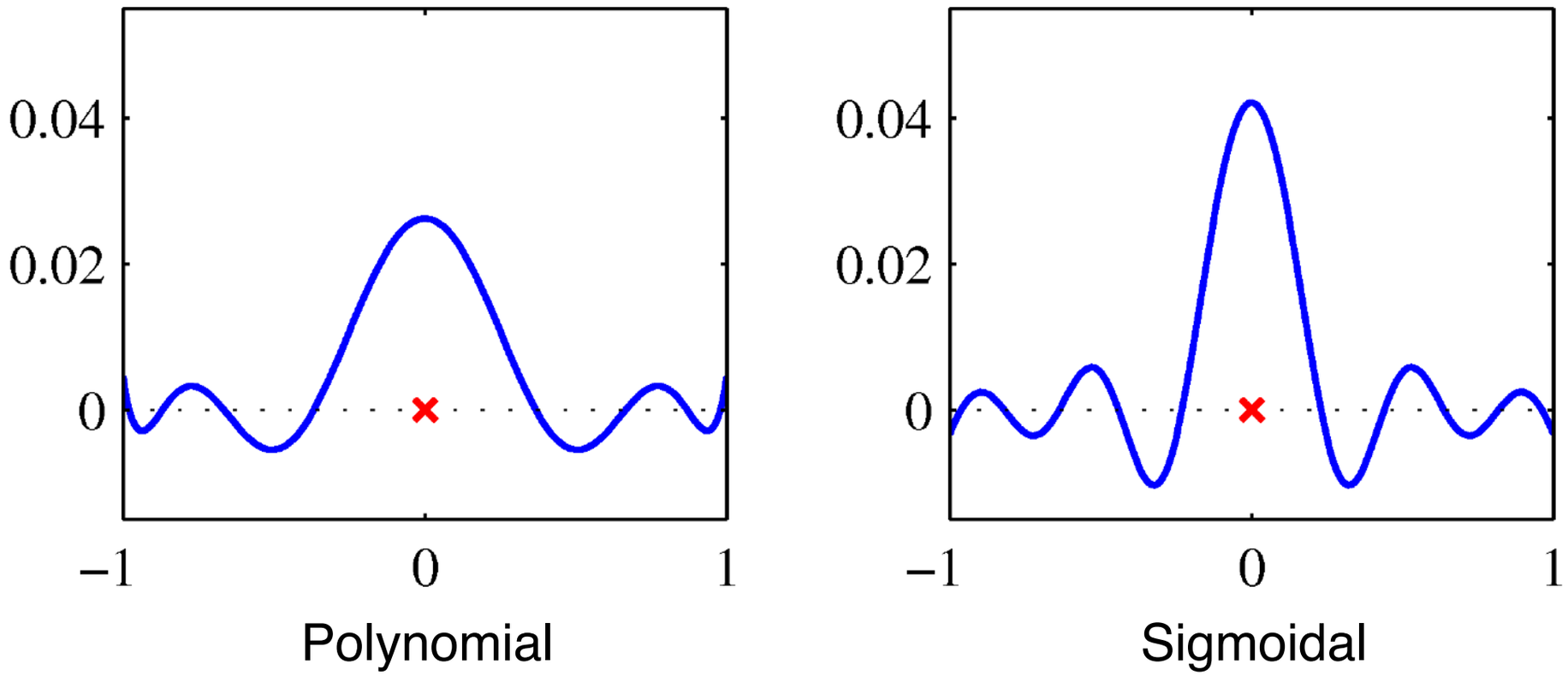
Non-local basis functions have local equivalent



Equivalent Kernel

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The kernel as a covariance function: consider

$$\begin{aligned}\mathrm{cov}[y(\mathbf{x}), y(\mathbf{x}')] &= \mathrm{cov}[\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{w}, \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}')] \\ &= \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{S}_N\boldsymbol{\phi}(\mathbf{x}') = \beta^{-1}k(\mathbf{x}, \mathbf{x}').\end{aligned}$$

We can avoid the use of basis functions and define the kernel function directly, leading to Gaussian Processes.

Gaussian Processes

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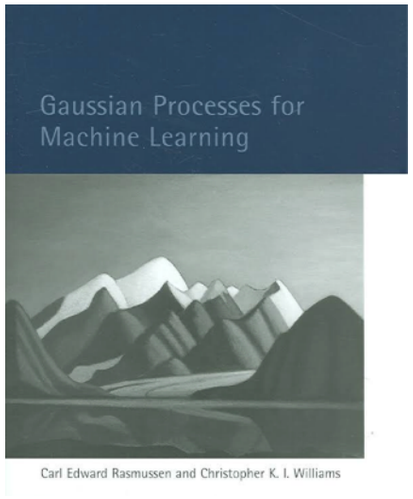
Definition: A Gaussian process is a collection of random variables, any number of which have (consistent) Gaussian distributions.

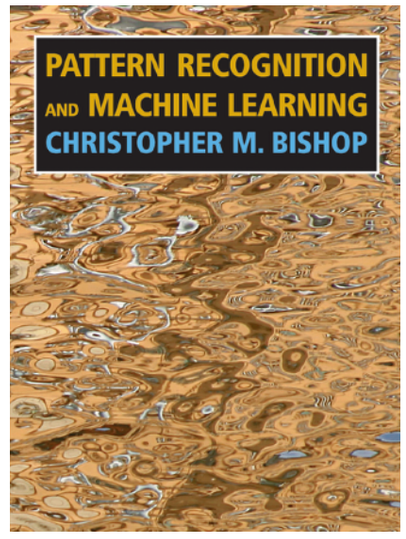
A GP is fully specified by a mean function $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$:

$$f(\mathbf{x}) \sim \mathrm{GP}\left(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')\right)$$

Resources



C. E. Rasmussen and C. Williams, Gaussian processes for machine learning. The MIT Press, Cambridge, Massachuset, 2006.



Chapter 6.4: Kernel Methods
MB Christopher, Pattern Recognition and Machine Learning, Springer-Verlag New York, 2016.

Online resources:
www.gaussianprocess.org

GPy, Stan, gpml, TacoPig

Gaussian Process Regression

Given a set of samples

$$X = [\mathbf{x}_0, \ldots, \mathbf{x}_{N-1}]^T$$
$$\mathbf{y} = [y_0, \ldots, y_{N-1}]^T$$

Choose a covariance function

$$k(\mathbf{x}_i, \mathbf{x}_j \mid \theta)$$

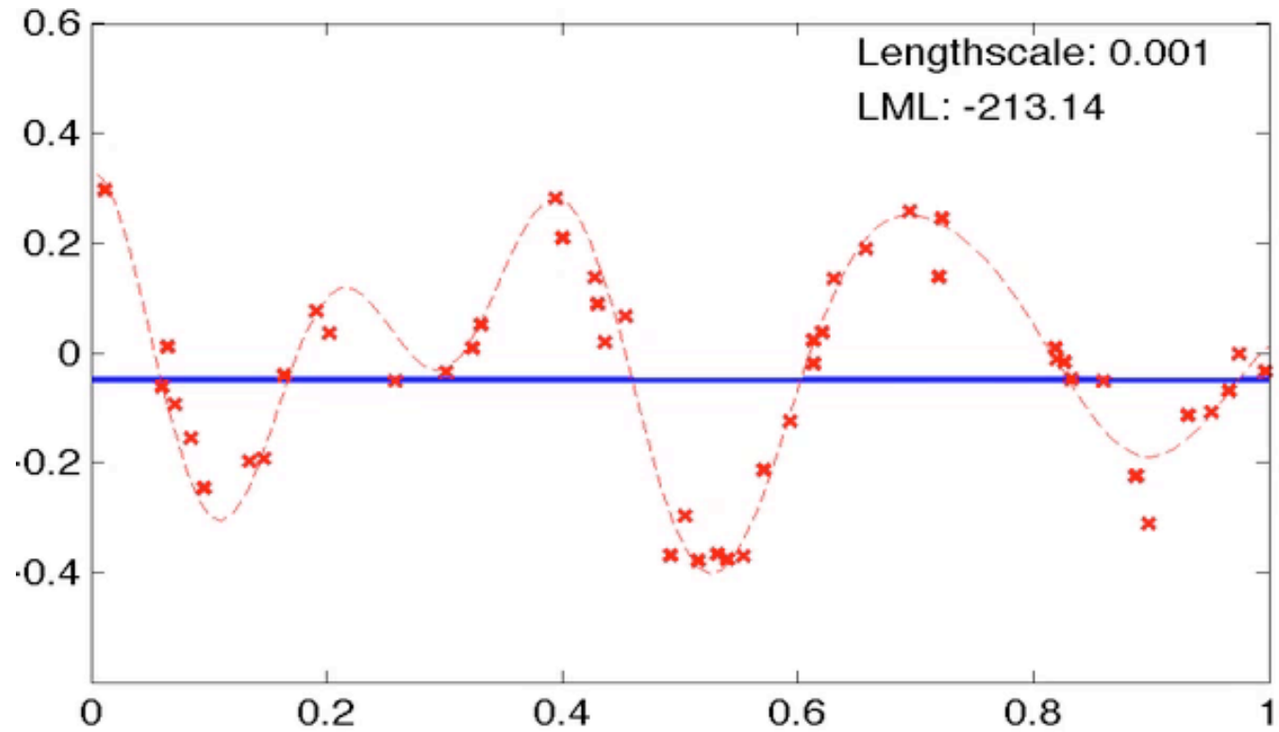
Predict the value of $f(\mathbf{x}_*)$

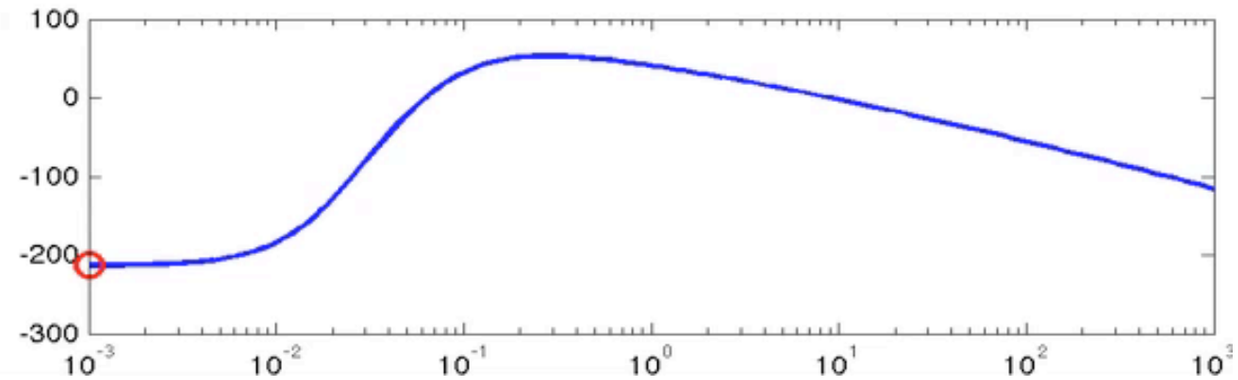
Predictive Posterior Distribution

Mean $\mu(f(\mathbf{x}_*))$

Variance $\sigma(f(\mathbf{x}_*))$

Regression





Log Marginal Likelihood

Gaussian Process Regression

$$y = f(\mathbf{x}) + \epsilon \qquad \text{, with} \qquad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

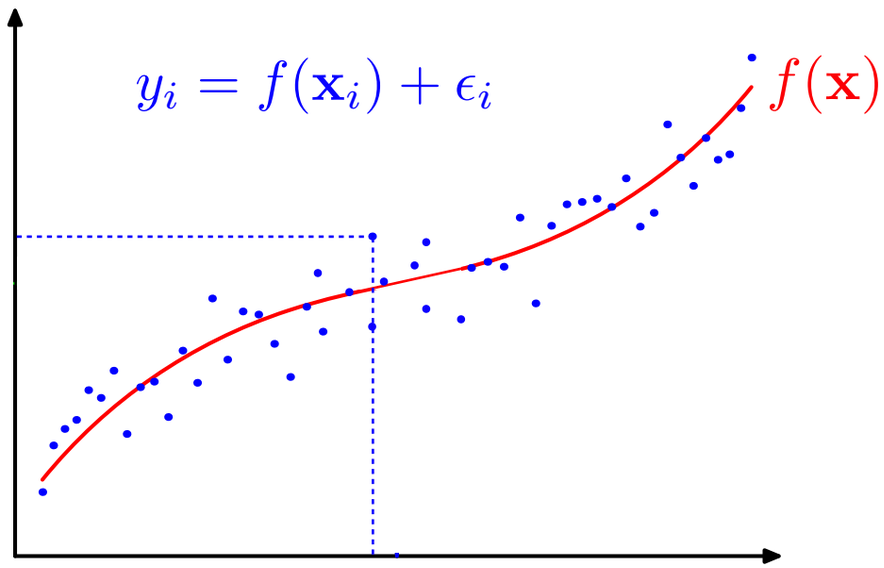
Noisy observations from the function

$$\mathbf{y} = \{y_i\}_{i=1}^N$$

$$X = \{\mathbf{x}_i\}_{i=1}^N$$

Observations Dataset

$$\mathcal{D} = (X, \mathbf{y})$$



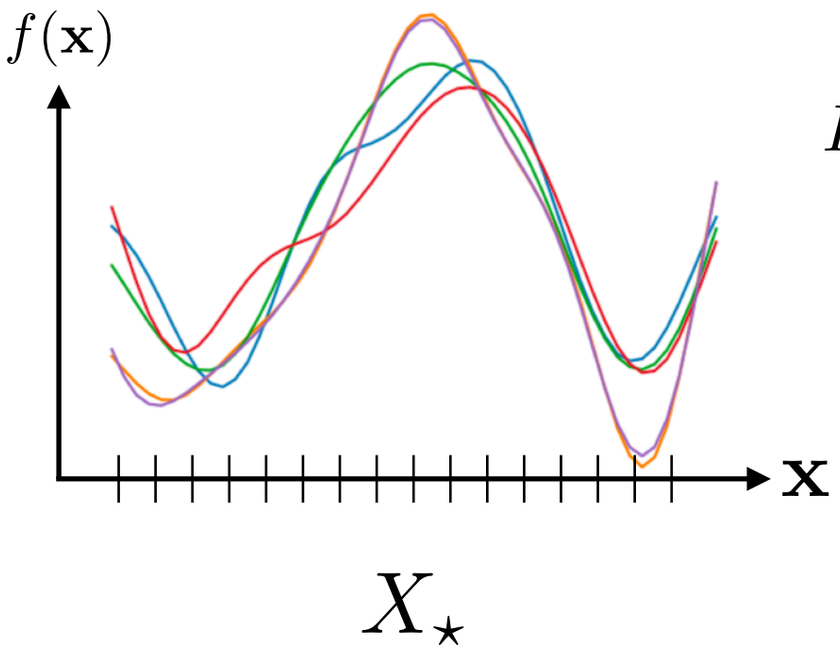
$$f(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}|\boldsymbol{\theta}_m), k(\mathbf{x}, \mathbf{x}'|\boldsymbol{\theta}_c)\right)$$

Samples from a Gaussian Process

$$m(\mathbf{x}) = 0$$

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}(\mathbf{x}-\mathbf{x}')}{2\,\ell^2}\right)$$

$$K(X_\star, X_\star)_{(i,j)} = k(\mathbf{x}_i, \mathbf{x}_j)$$



$$K(X_\star, X_\star) = \begin{bmatrix} k(\mathbf{x}_0,\mathbf{x}_0) & k(\mathbf{x}_0,\mathbf{x}_1) & \cdots & k(\mathbf{x}_0,\mathbf{x}_M) \\ k(\mathbf{x}_1,\mathbf{x}_0) & k(\mathbf{x}_1,\mathbf{x}_1) & & \\ \vdots & & \ddots & \\ k(\mathbf{x}_M,\mathbf{x}_0) & & & k(\mathbf{x}_M,\mathbf{x}_M) \end{bmatrix}$$

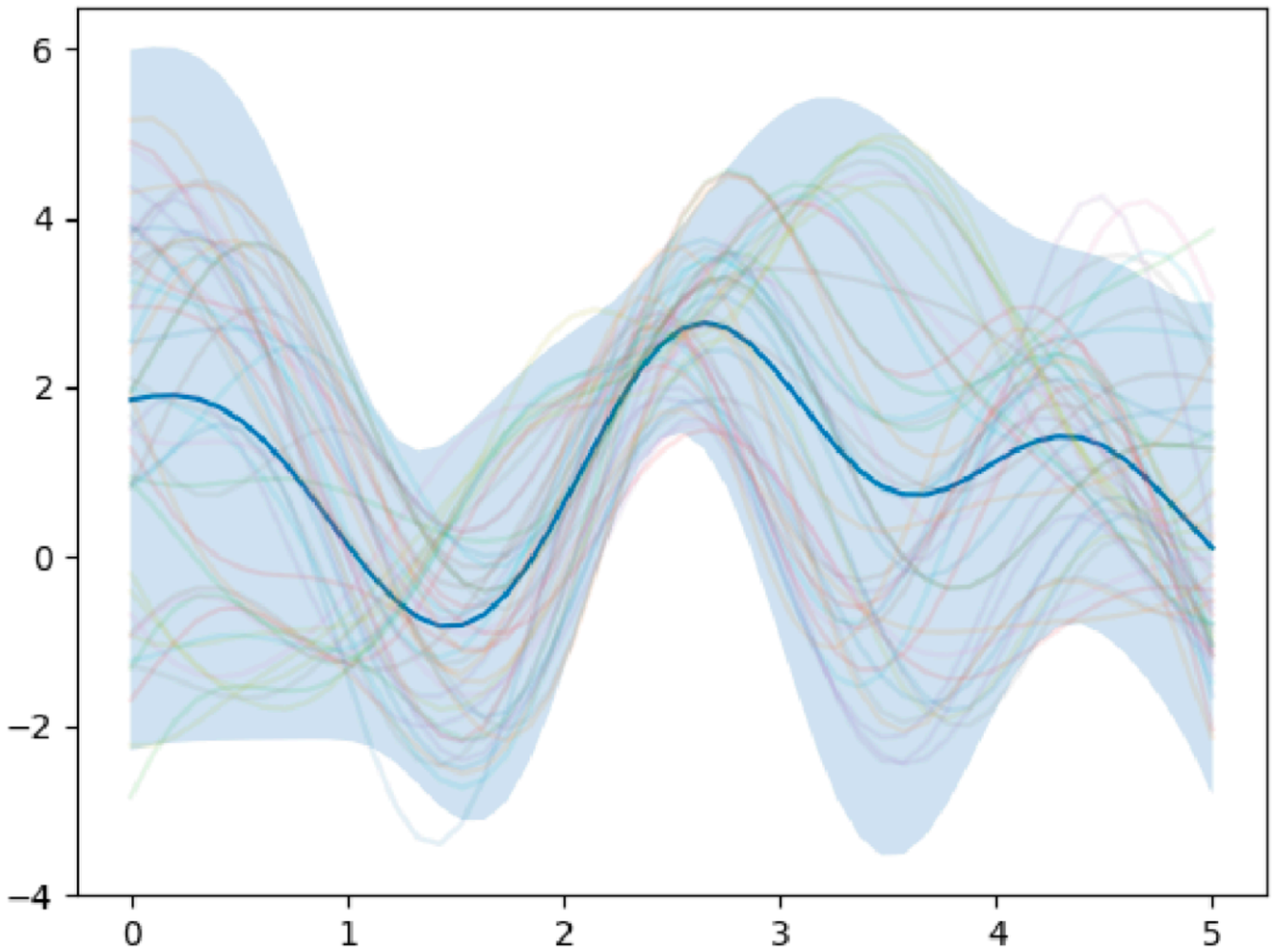
$$\mathbf{f}_\star \sim \mathcal{N}(\mathbf{0}, K(X_\star, X_\star))$$

How to draw samples?

$$K = LL^{\mathrm{T}} \quad \mathbf{u} \sim \mathcal{N}(\mathbf{0}, I) \quad \mathbf{f}_\star = L\mathbf{u}$$

Cholesky decomposition

Stan GP Samples



Covariance Functions

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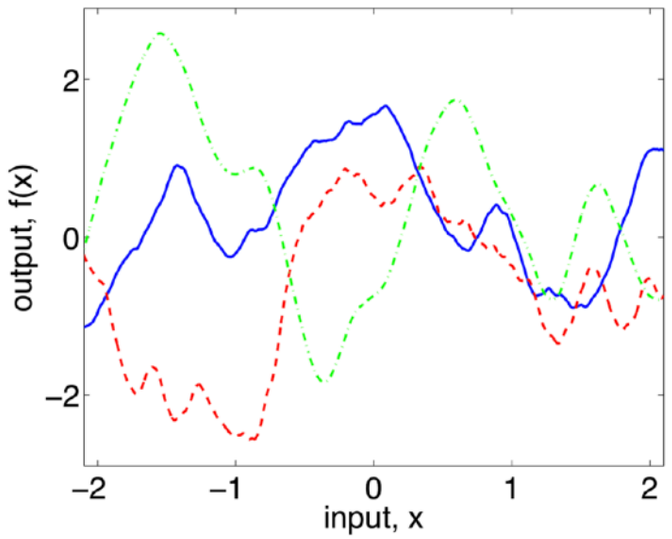
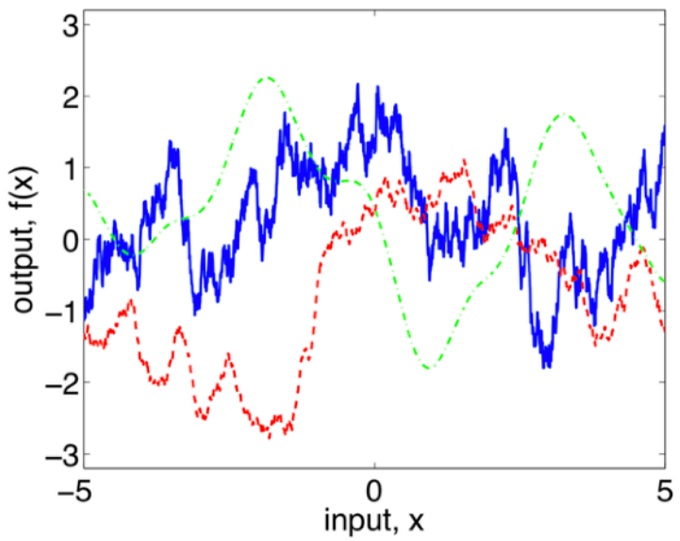
Name	Expression $k(\mathbf{x}', \mathbf{x}'')$	Hyper-Parameters
Linear	$\sigma_f^2(\sigma_0^2 + \mathbf{x}'^T L \mathbf{x}'')$	$\boldsymbol{\theta}_c = \{\sigma_f, \sigma_0, L\}$
Matern 3	$\sigma_f^2 \left(1 + \sqrt{3\mathbf{d}}\right) \exp\left(-\sqrt{3\mathbf{d}}\right)$	$\boldsymbol{\theta}_c = \{\sigma_f, L\}$
Matern 5	$\sigma_f^2 \left(1 + \sqrt{5\mathbf{d}} + \frac{5\mathbf{d}}{3}\right) \exp\left(-\sqrt{5\mathbf{d}}\right)$	$\boldsymbol{\theta}_c = \{\sigma_f, L\}$
Polynomial	$\sigma_f^2(\sigma_0^2 + \mathbf{x}'^T L \mathbf{x}'')^p$	$\boldsymbol{\theta}_c = \{\sigma_f, \sigma_0, L, p\}$
Rational Quadratic	$\sigma_f^2 \left(1 + \frac{\mathbf{d}}{2\alpha}\right)^{-\alpha}$	$\boldsymbol{\theta}_c = \{\sigma_f, L, \alpha\}$
Squared Exponential	$\sigma_f^2 \exp\left(-\frac{\mathbf{d}}{2}\right)$	$\boldsymbol{\theta}_c = \{\sigma_f, L\}$
Periodic Exponential	$\sigma_f^2 \exp\left(-\frac{2\sin^2\left(\pi T \sqrt{\mathbf{d}}\right)}{\rho^2}\right)$	$\boldsymbol{\theta}_c = \{\sigma_f, L, T, \rho\}$

$$\mathbf{d} = (\mathbf{x}' - \mathbf{x}'')^\top L (\mathbf{x}' - \mathbf{x}'') \qquad L_{(i,i)} = \frac{1}{\ell_i^2}$$





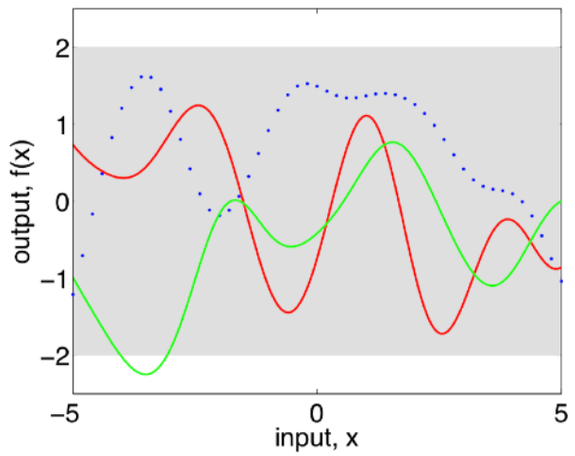
Gaussian Process Regression

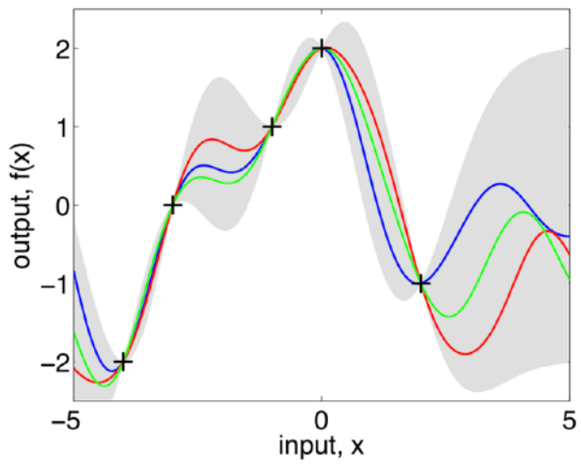
$$y = f(\mathbf{x}) + \epsilon \qquad \text{, with} \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

$$\mathcal{D} = (X, \mathbf{y})$$

Query locations: $X^\star$

$$\mathbf{f}^\star = \{f_i^\star\}_{i=1}^N$$





Predictive distribution over test locations

$$\mathbf{f}^\star | X, \mathbf{y}, X^\star \sim \mathcal{N}(\bar{\mathbf{f}^\star}, \text{cov}(\mathbf{f}^\star))$$

$$\bar{\mathbf{f}^\star} = \mathbb{E}[\mathbf{f}^\star | X, \mathbf{y}, X^\star] = K(X^\star, X)\left[K(X, X) + \sigma_n^2 I\right]^{-1}(\mathbf{y} - M(X))$$

$$\text{cov}(\mathbf{f}^\star) = K(X^\star, X^\star) - K(X^\star, X)\left[K(X, X) + \sigma_n^2 I\right]^{-1} K(X, X^\star) \ ,$$

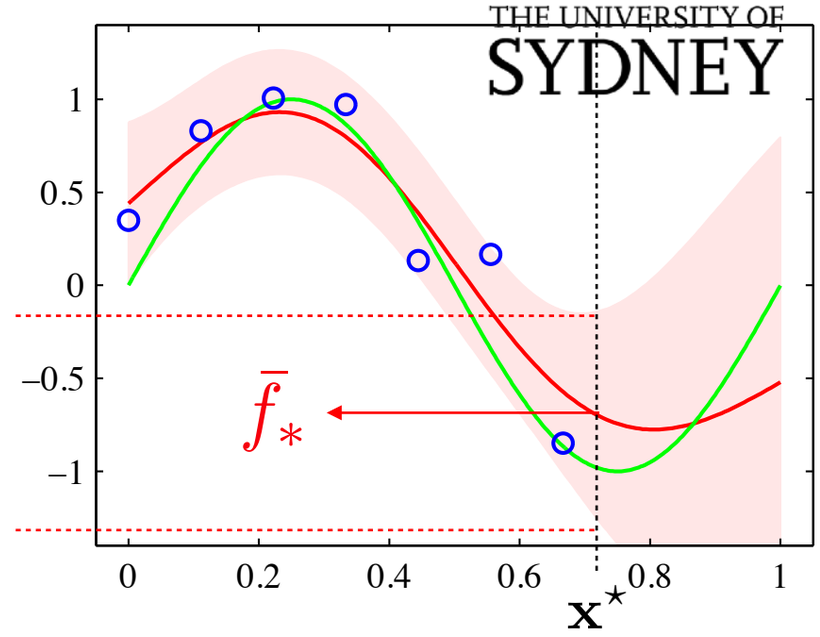
Gaussian Process Regression

One query location: $\mathbf{x}^\star$

$$\bar{f}_* = \mathbf{k}_*^\top (K + \sigma_n^2 I)^{-1} \mathbf{y},$$
$$\mathbb{V}[f_*] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top (K + \sigma_n^2 I)^{-1} \mathbf{k}_*$$

$\bar{f}_* + 2\sqrt{\mathbb{V}[f_*]}$

$\bar{f}_* - 2\sqrt{\mathbb{V}[f_*]}$



input: X (inputs), $\mathbf{y}$ (targets), k (covariance function), σ_n^2 (noise level), $\mathbf{x}_*$ (test input)

$L := \text{cholesky}(K + \sigma_n^2 I)$

$\boldsymbol{\alpha} := L^\top \backslash (L \backslash \mathbf{y})$

$\bar{f}_* := \mathbf{k}_*^\top \boldsymbol{\alpha}$

$\mathbf{v} := L \backslash \mathbf{k}_*$

$\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$

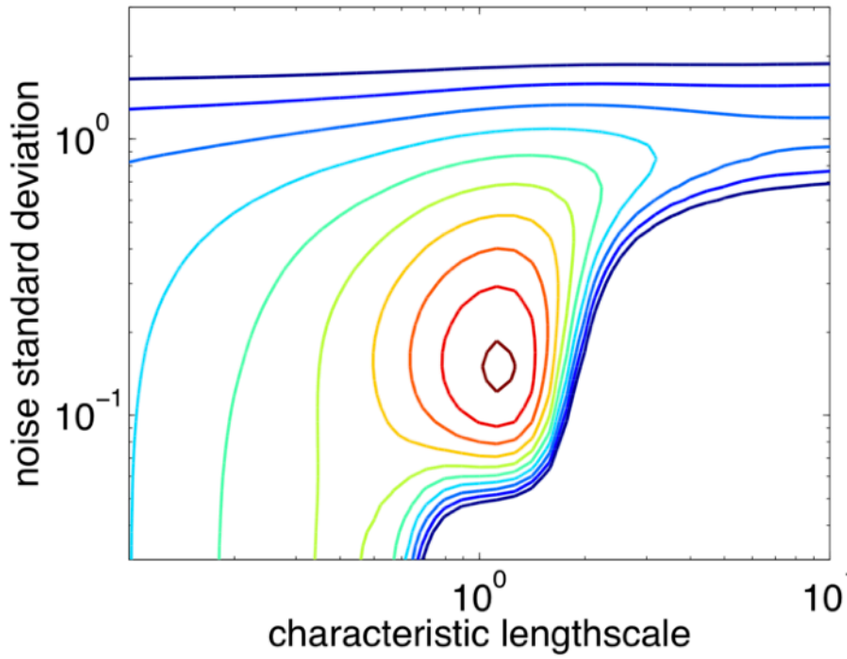
$\log p(\mathbf{y}|X) := -\frac{1}{2}\mathbf{y}^\top \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2} \log 2\pi$

return: $\bar{f}_*$ (mean), $\mathbb{V}[f_*]$ (variance), $\log p(\mathbf{y}|X)$ (log marginal likelihood)

Model Selection - Optimisation

Hyper-parameter Set $\boldsymbol{\theta} = \{\boldsymbol{\theta}_m, \boldsymbol{\theta}_c, \sigma_n\}$

Optimal Hyper-Parameters $\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \ \mathrm{GF}(\mathbf{y}, X, \boldsymbol{\theta})$



Log Marginal Likelihood

$$\mathrm{LML}(\mathbf{y}, X, \boldsymbol{\theta}) = -\frac{1}{2}(\mathbf{y} - M(X))^T K_X^{-1}(\mathbf{y} - M(X)) - \frac{1}{2}\log|K_X| - \frac{n}{2}\log 2\pi$$

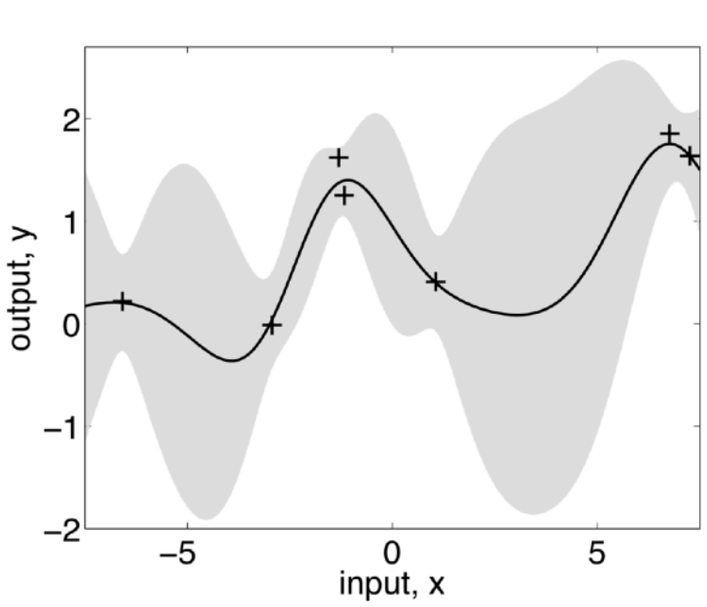
$$K_X = K(X, X) + \sigma_n I \qquad M(X)_{(i)} = m(x_i)$$

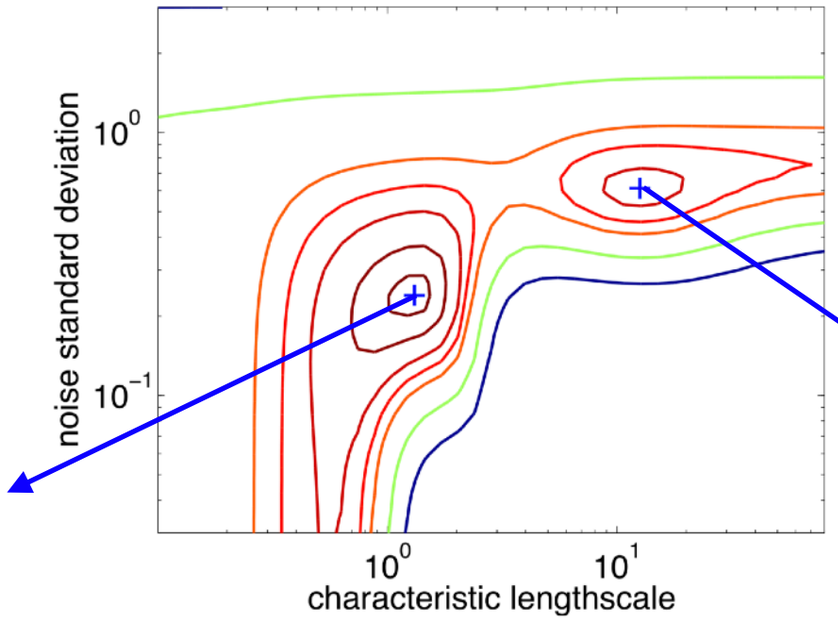
$$\begin{aligned}\frac{\partial}{\partial\theta_j}\log p(\mathbf{y}|X, \boldsymbol{\theta}) &= \frac{1}{2}\mathbf{y}^\top K^{-1}\frac{\partial K}{\partial\theta_j}K^{-1}\mathbf{y} - \frac{1}{2}\,\mathrm{tr}\left(K^{-1}\frac{\partial K}{\partial\theta_j}\right) \\ &= \frac{1}{2}\,\mathrm{tr}\left((\boldsymbol{\alpha}\boldsymbol{\alpha}^\top - K^{-1})\frac{\partial K}{\partial\theta_j}\right) \quad \text{where} \quad \boldsymbol{\alpha} = K^{-1}\mathbf{y}\end{aligned}$$

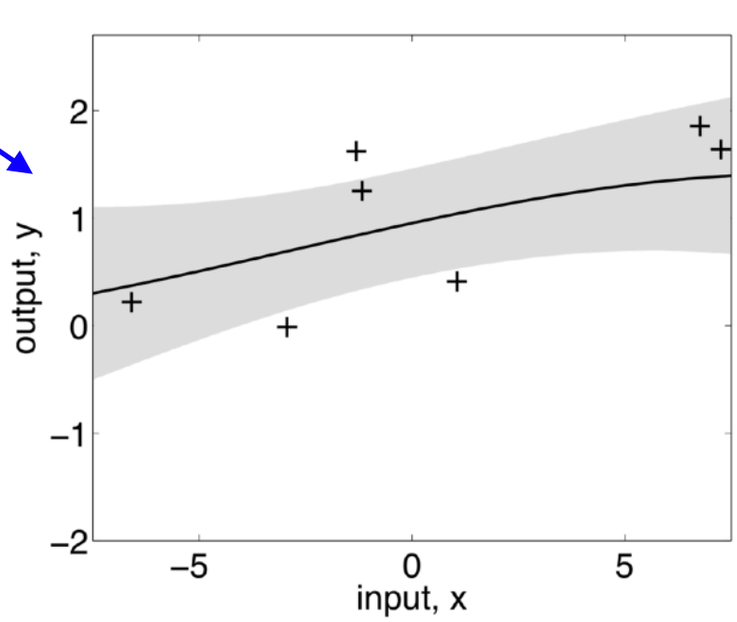
Model Selection (Optimisation)

There is no guarantee that the **marginal likelihood** does not suffer from **multiple local optima**.

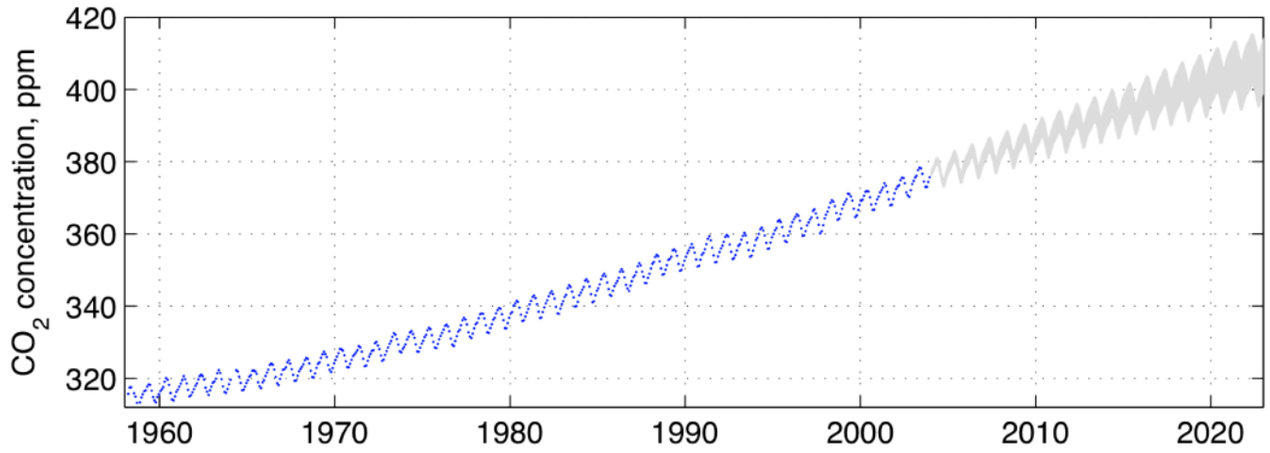
Every local maximum corresponds to a particular interpretation of the data.







Covariance Function Combination

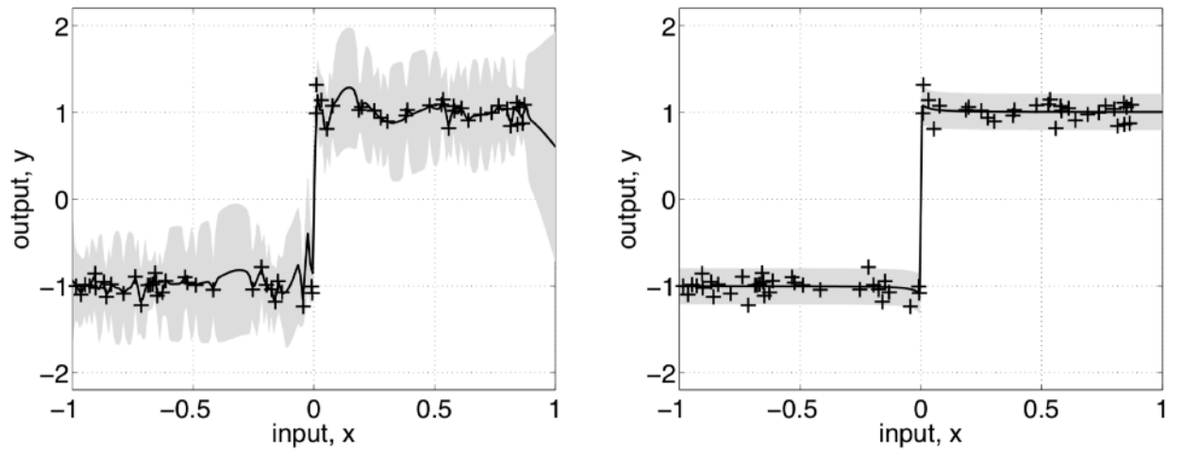


$$k(x, x') = k_1(x, x') + k_2(x, x') + k_3(x, x') + k_4(x, x')$$

$$k_2(x, x') = \theta_3^2 \exp\left(-\frac{(x - x')^2}{2\theta_4^2} - \frac{2\sin^2(\pi(x - x'))}{\theta_5^2}\right)$$

$$k_4(x_p, x_q) = \theta_9^2 \exp\left(-\frac{(x_p - x_q)^2}{2\theta_{10}^2}\right) + \theta_{11}^2 \delta_{pq}$$

Covariance Function Combination



$$k_{\mathrm{NN}}(\mathbf{x}, \mathbf{x}') = \frac{2}{\pi} \sin^{-1}\left(\frac{2\tilde{\mathbf{x}}^\top \Sigma \tilde{\mathbf{x}}'}{\sqrt{(1+2\tilde{\mathbf{x}}^\top \Sigma \tilde{\mathbf{x}})(1+2\tilde{\mathbf{x}}'^\top \Sigma \tilde{\mathbf{x}}')}}\right)$$

Large Datasets

$$\bar{f}_* = \mathbf{k}_*^\top (K + \sigma_n^2 I)^{-1} \mathbf{y},$$
$$\mathbb{V}[f_*] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^\top (K + \sigma_n^2 I)^{-1} \mathbf{k}_*$$

K is a $N \times N$ matrix.

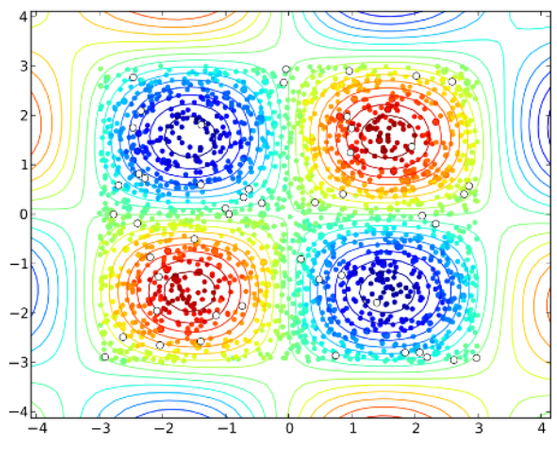
What happens when N is really big?

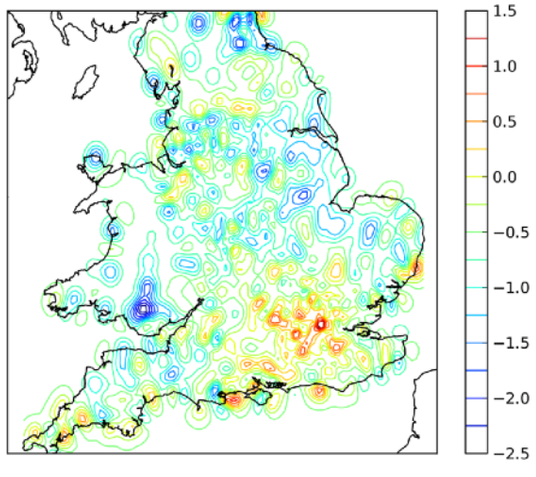
Calculating this inverse $(K + \sigma_n I)^{-1}$ is of order $O(N^3)$

Stochastic Variational Inference.

Current Solutions:

James Hensman, Nicolo Fusi, Neil D. Lawrence, Gaussian Processes for Big Data, arXiv:1309.6835





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Research Example 1

Spatial Temporal Monitoring

Space Time Gaussian Processes

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The domain of the function now contains spatial and temporal components.

$$f\left(\mathbf{s};t\right) \sim \mathcal{GP}\left(m\left(\mathbf{s};t\right), k\left(\left(\mathbf{s};t\right),\left(\mathbf{s};t\right)'\right)\right).$$

Predictive distribution over test locations

$$f((\mathbf{s};t)^*) \sim \mathcal{N}\left(\mu, \sigma^2\right)$$

$$\begin{aligned}\mu((\mathbf{s};t)^*) = &\quad K((\mathbf{s};t)^*, X)K_X^{-1}(\mathbf{y} - m(X)) \,, \\ \sigma^2((\mathbf{s};t)^*) = &\quad K((\mathbf{s};\mathbf{t})^*, (\mathbf{s};t)^*) - K((\mathbf{s};\mathbf{t})^*, X)K_X^{-1}K(X, (\mathbf{s};\mathbf{t})^*) \,.\end{aligned}$$

Spatial Temporal Process
Ozone Concentration

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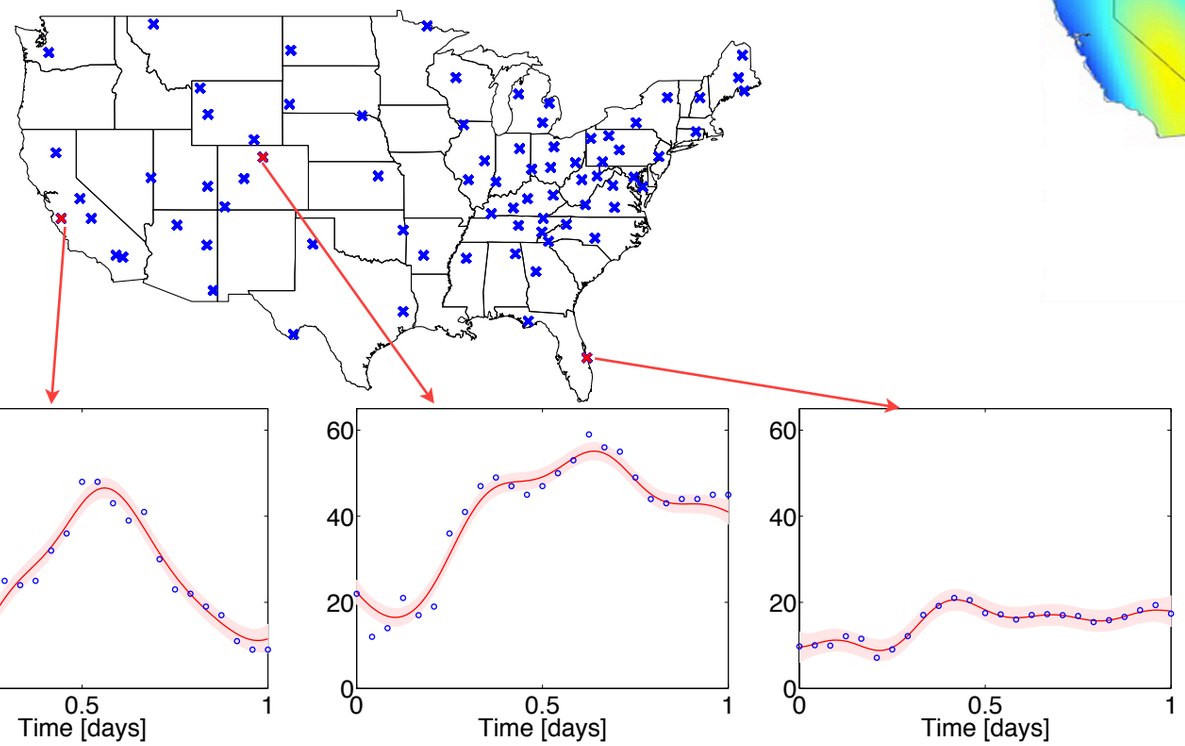
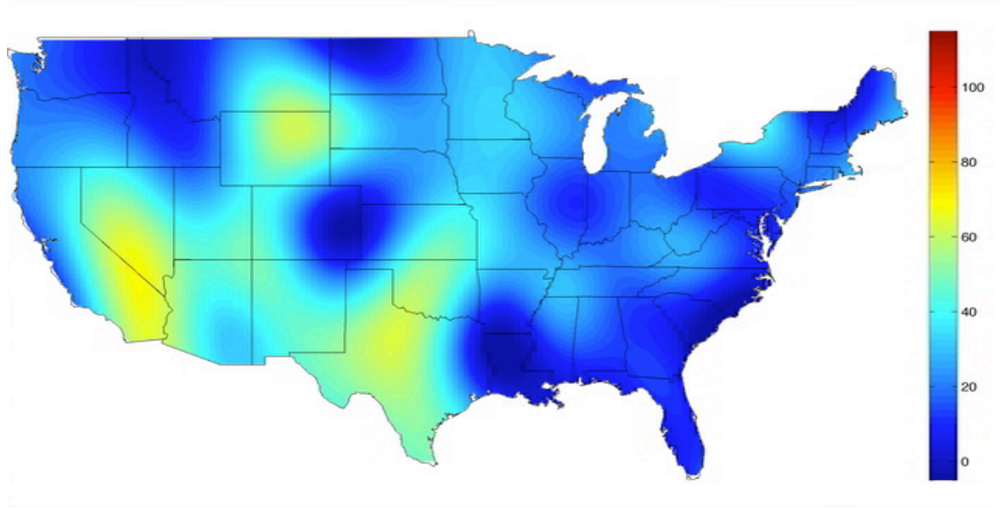




Space Time Covariance Functions

Able to capture spatial and temporal specific behaviour.

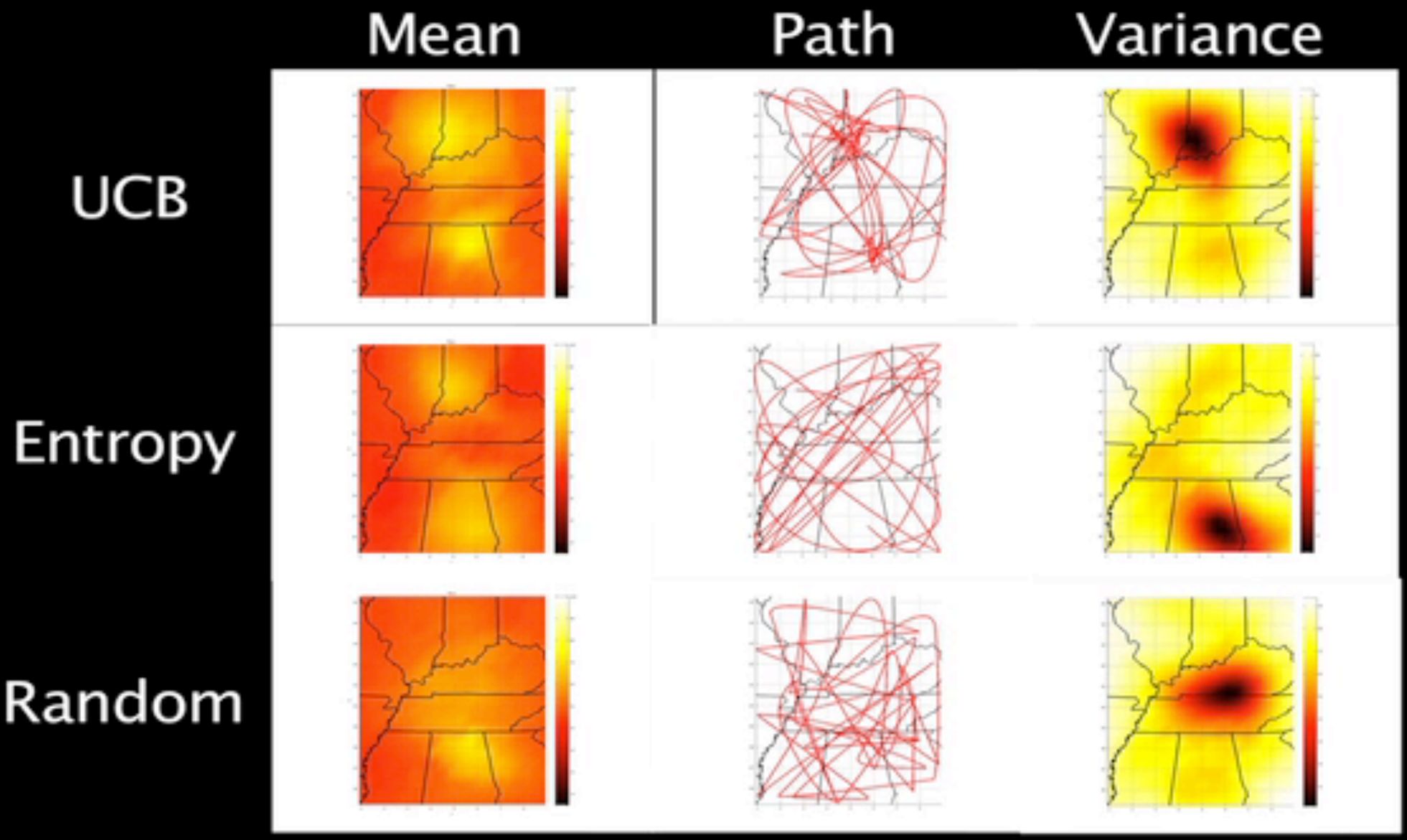
When spatial and temporal patterns are not coupled:

$$k_{sep}\left((\mathbf{s};t),(\mathbf{s};t)'|\boldsymbol{\theta}_c\right) = k_{\text{space}}(\mathbf{s},\mathbf{s}'|\boldsymbol{\theta}_{\text{space}})\, k_{\text{time}}(t,t'|\boldsymbol{\theta}_{\text{time}})$$

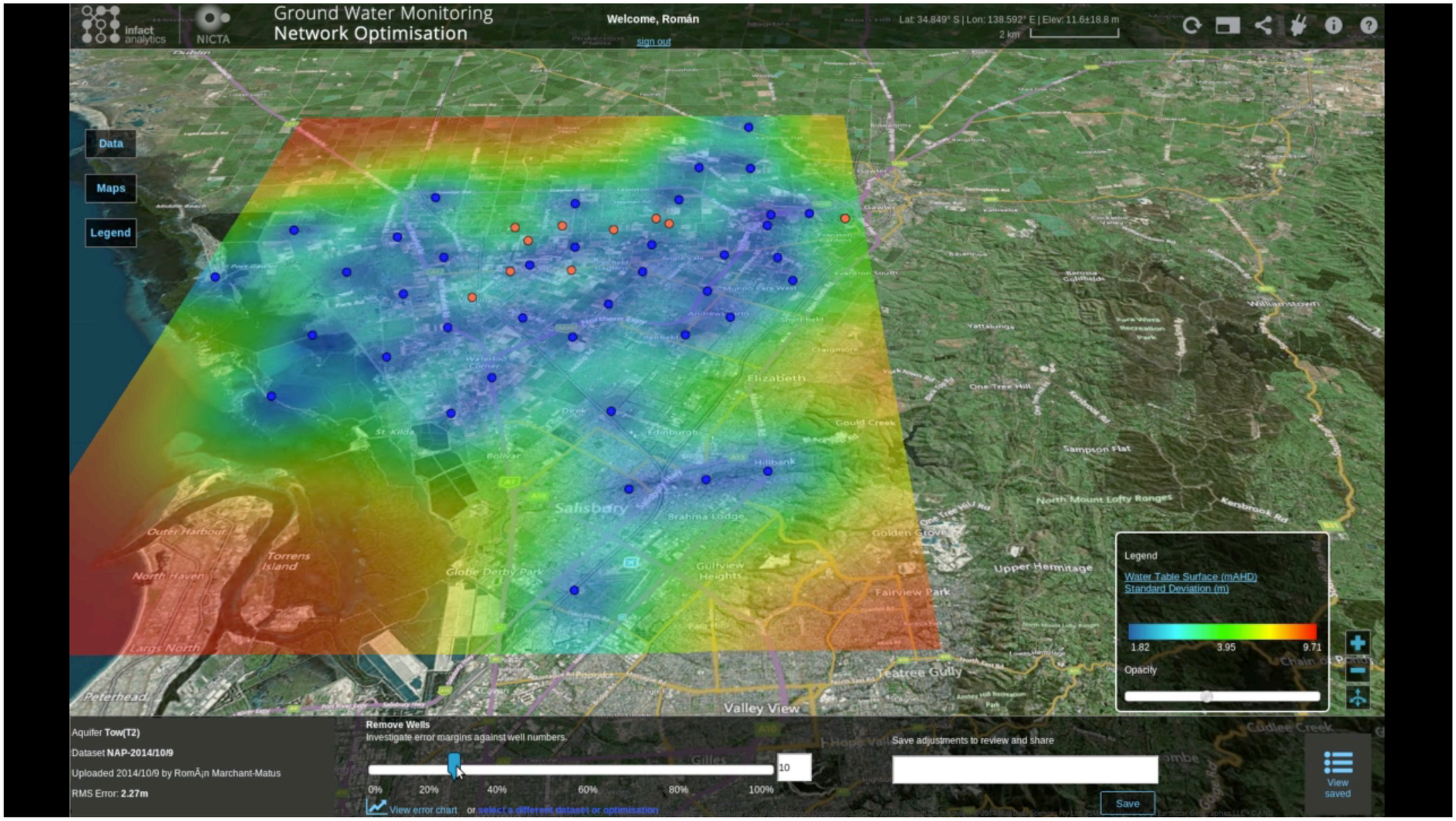
For example: Separable Non-Stationary

$$k(\mathbf{s},\mathbf{s}';t,t' \mid \boldsymbol{\theta}) = \sigma^2 \exp\{-b^2\|\mathbf{s}+\mathbf{s}'\|^2 - a^2(t+t')^2\} + \sigma^2 \exp\{-b^2\|\mathbf{s}-\mathbf{s}'\|^2 - a^2(t-t')^2\} \quad (13)$$

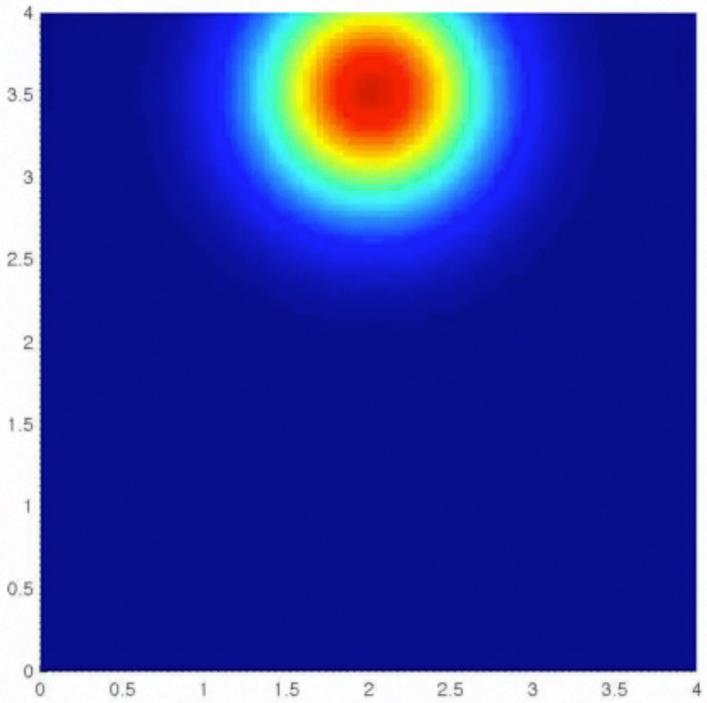
$$-2[\sigma^2\exp\{-b^2\|\mathbf{s}\|^2-a^2(t)^2\}+\sigma^2\exp\{-b^2\|\mathbf{s}'\|^2-a^2(t')^2\}-\sigma^2].$$


Mean
Path
Variance
UCB
Entropy
Random
explores the unknown environment and at the same time identif

Example: Ground Water Monitoring

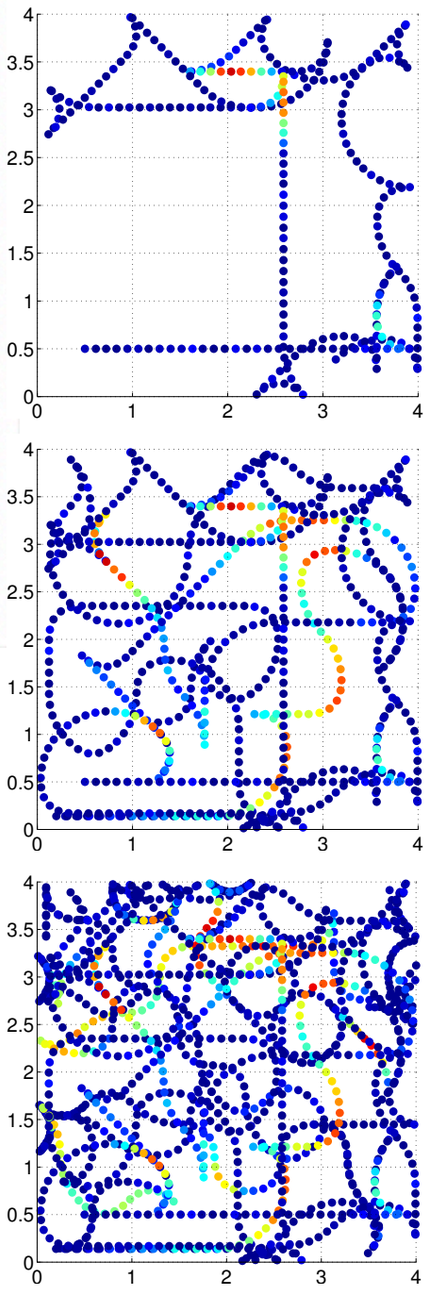


Path Planning

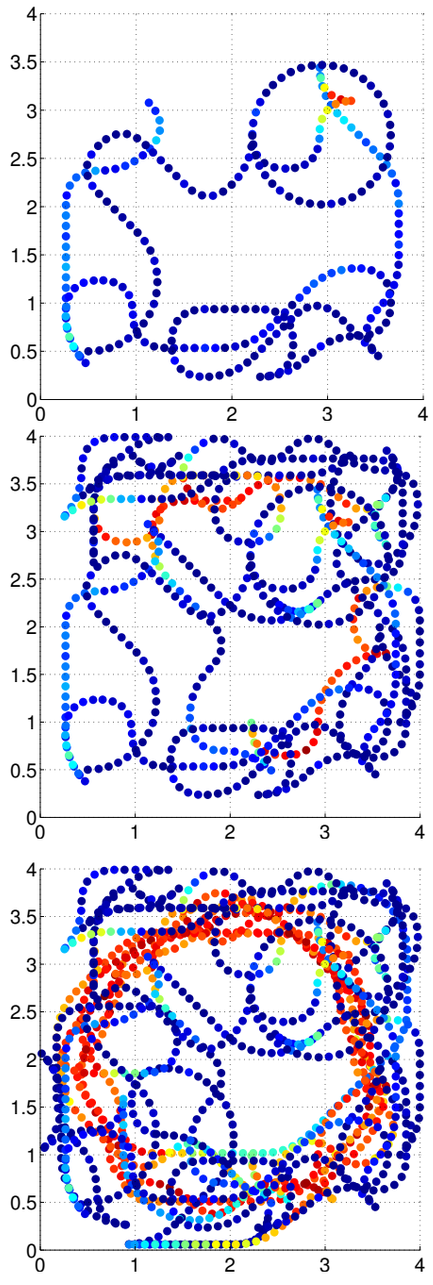


Space Time Function
Ground Truth

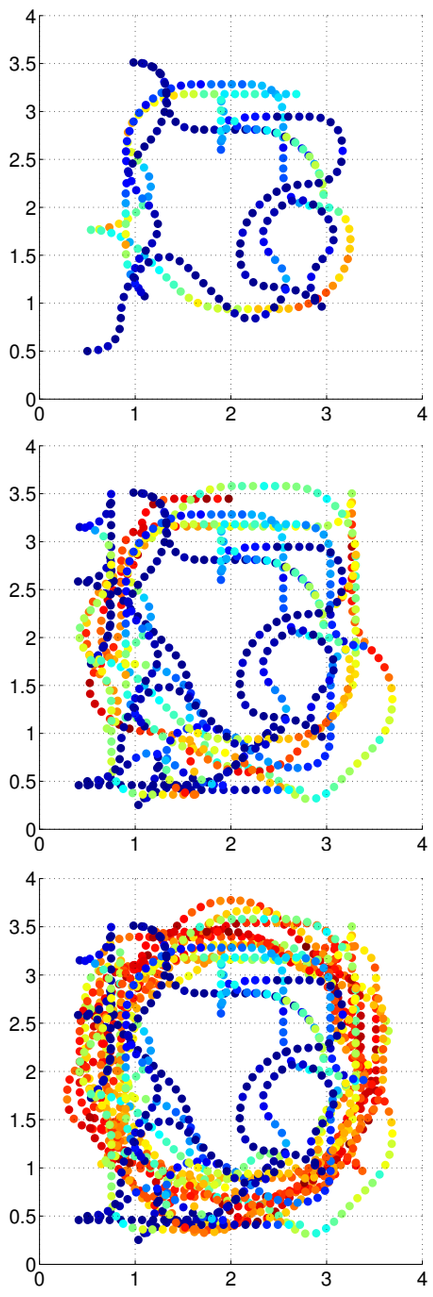
Depth 1



Depth 2



Depth 5



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Research Example 2

Mapping with Gaussian Processes

Simulated Dataset: Probability of Occupancy Versus Location

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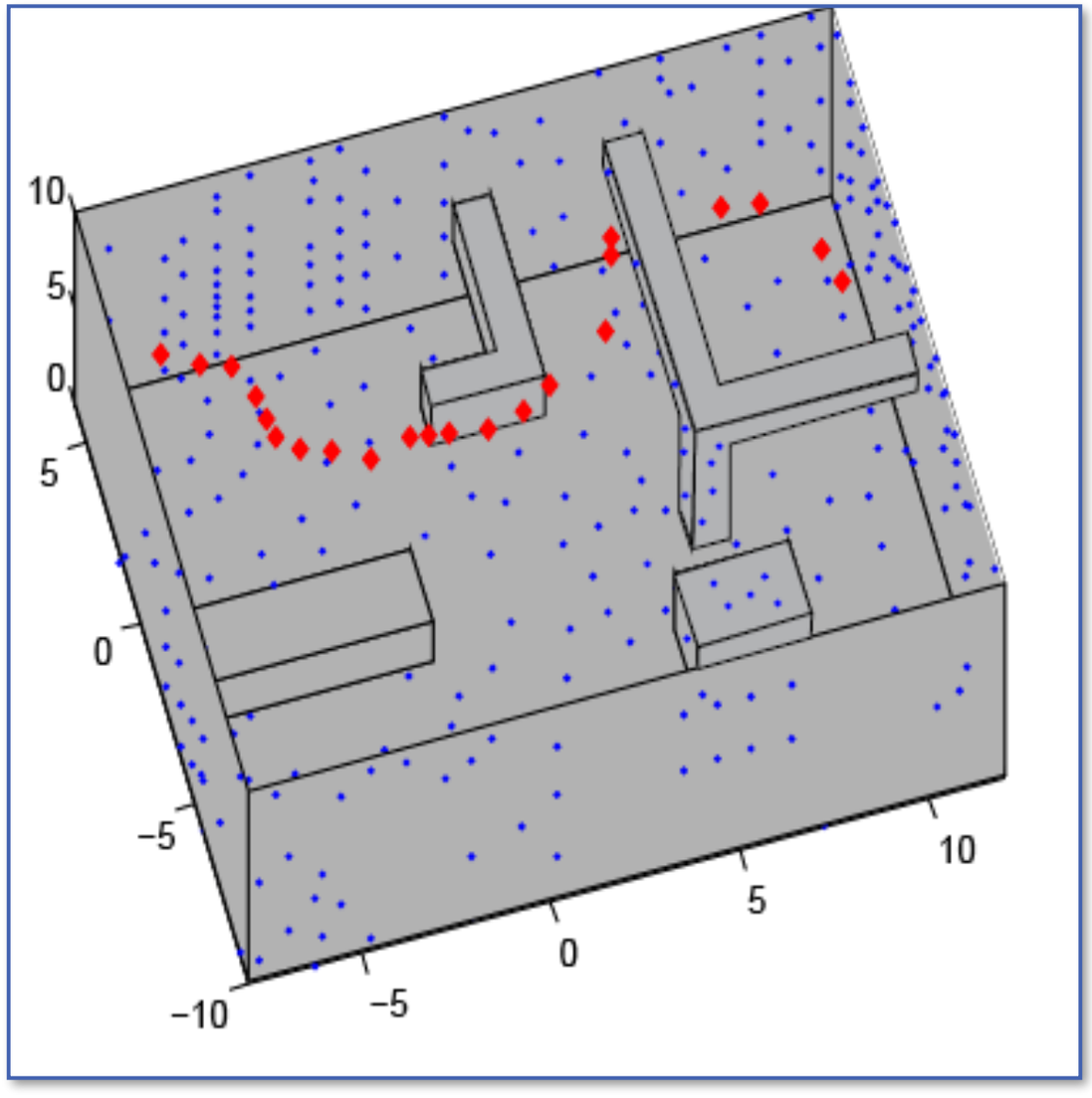

Simulated Dataset: Predicted Occupied Points

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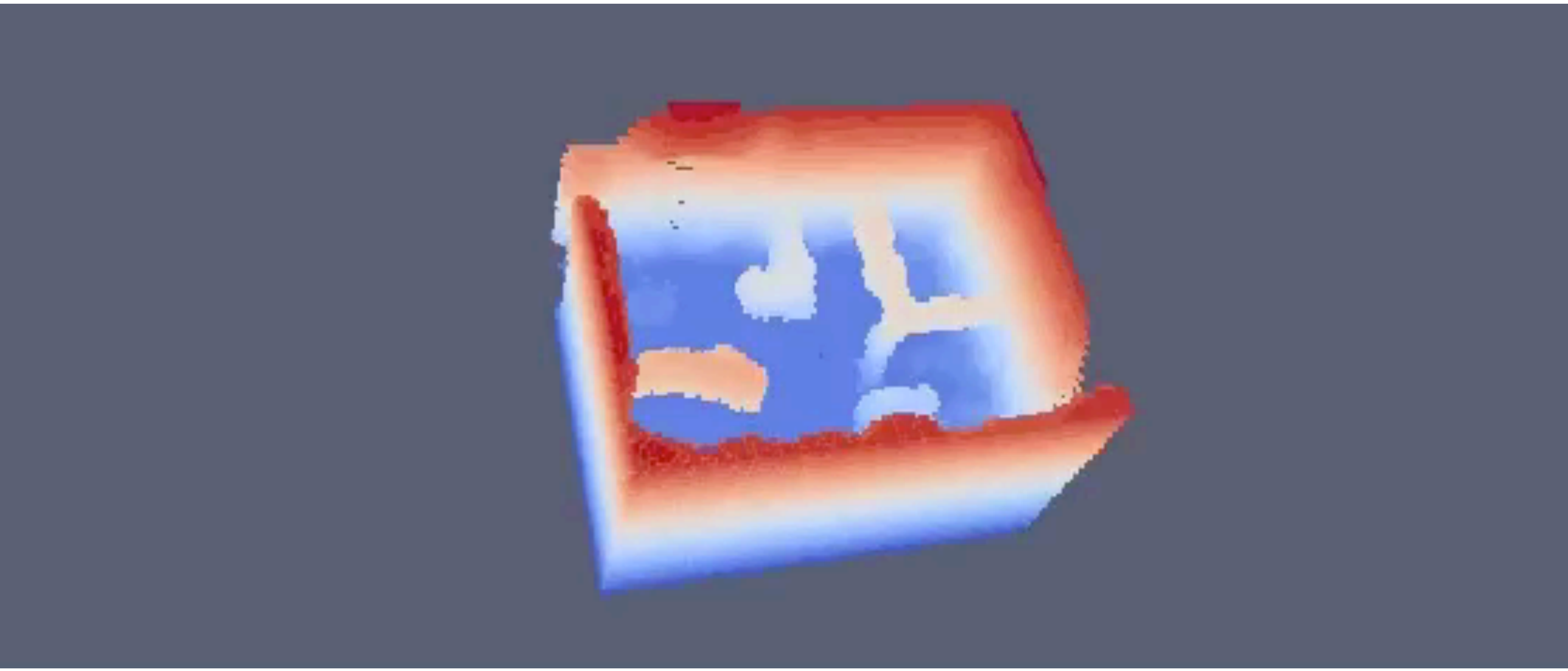

Outdoor Dataset:
Subsampled Reigl Rangefinder Point Cloud

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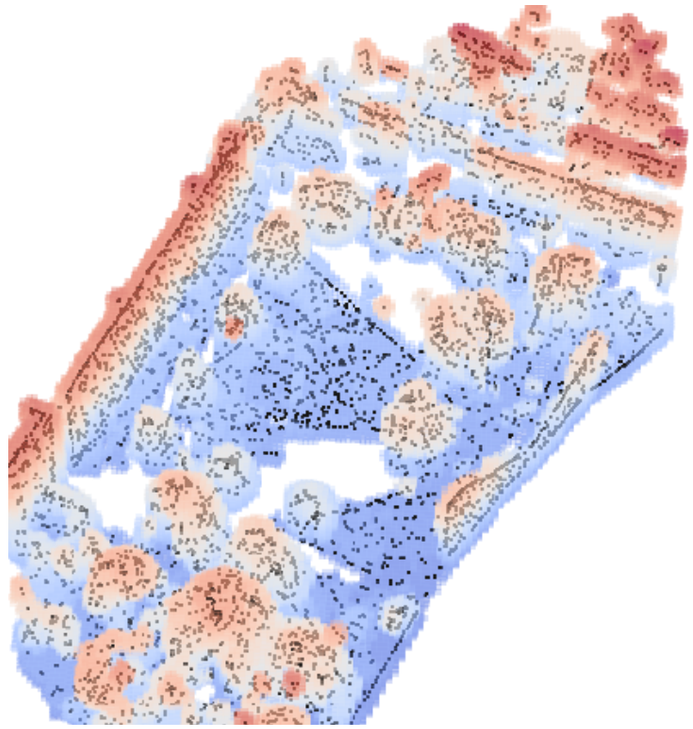

Outdoor Dataset:
Subsampled Rangefinder Point Cloud

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