LaTeX command declarations here.

In [1]:
```
from __future__ import division

# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
import matplotlib as mpl;
from mpl_toolkits.mplot3d import Axes3D
if "bmh" in plt.style.available: plt.style.use("bmh");

# matplotlib objects
from matplotlib import mlab;
from matplotlib import gridspec;

# scientific
import numpy as np;
import scipy as scp;
import scipy.stats;

# scikit-learn
import sklearn;
from sklearn.kernel_ridge import KernelRidge;

# python
import random;

# warnings
import warnings
warnings.filterwarnings("ignore")
```

In [2]:
```
# rise config
from notebook.services.config import ConfigManager
cm = ConfigManager()
cm.update('livereveal', {
              'theme': 'simple',
              'start_slideshow_at': 'selected',
              'transition':'fade',
              'scroll': False
});
```

EECS 545: Machine Learning

Lecture 11: Bayesian Linear Regression & Gaussian Processes

- Instructor: **Jacob Abernethy**
- Date: February 17, 2015

Lecture Exposition Credit: Ben & Valli

References

This lecture draws upon the following resources:

- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://www.springer.com/us/book/9780387310732). 2006.
- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[CS229]** Ng, Andrew. CS 229: Machine Learning (http://cs229.stanford.edu/). Autumn 2015.
  - Gaussian Processes (http://cs229.stanford.edu/section/cs229-gaussian_processes.pdf)
  - More on Gaussians (http://cs229.stanford.edu/section/more_on_gaussians.pdf)

Outline

- Review Multivariate Gaussians
  - Partitioned Marginals and Conditionals
  - Bayes' Theorem for Gaussians
- Bayesian Linear Regression
- Gaussian Process Regression
  - Gaussian Processes

More on Multivariate Gaussians

> Taken from **[PRML]** §2.3, **[MLAPP]** §4.3, 4.4, and **[CS229]**

Review: Multivariate Gaussians

Recall the **Multivariate Normal / Gaussian** distribution with

- mean $\mu \in \mathbb{R}^D$
- covariance matrix $\Sigma \in \mathbb{R}^{D \times D}$

$$\mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right]$$

Partitioned Gaussian Distributions

Partition $x \sim \mathcal{N}(\mu, \Sigma)$ as $x = [x_a, x_b]^T$, and

- Mean and covariance

$$\mu = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}$$

- Precision Matrix

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

Partitioned Marginals

Exercise: Marginals are obtained by taking a subset of rows and columns:

$$\begin{aligned} P(x_a) &= \int P(x_a, x_b)\, dx_b \\ &= \mathcal{N}(x_a | \mu_a, \Sigma_{aa}) \end{aligned}$$

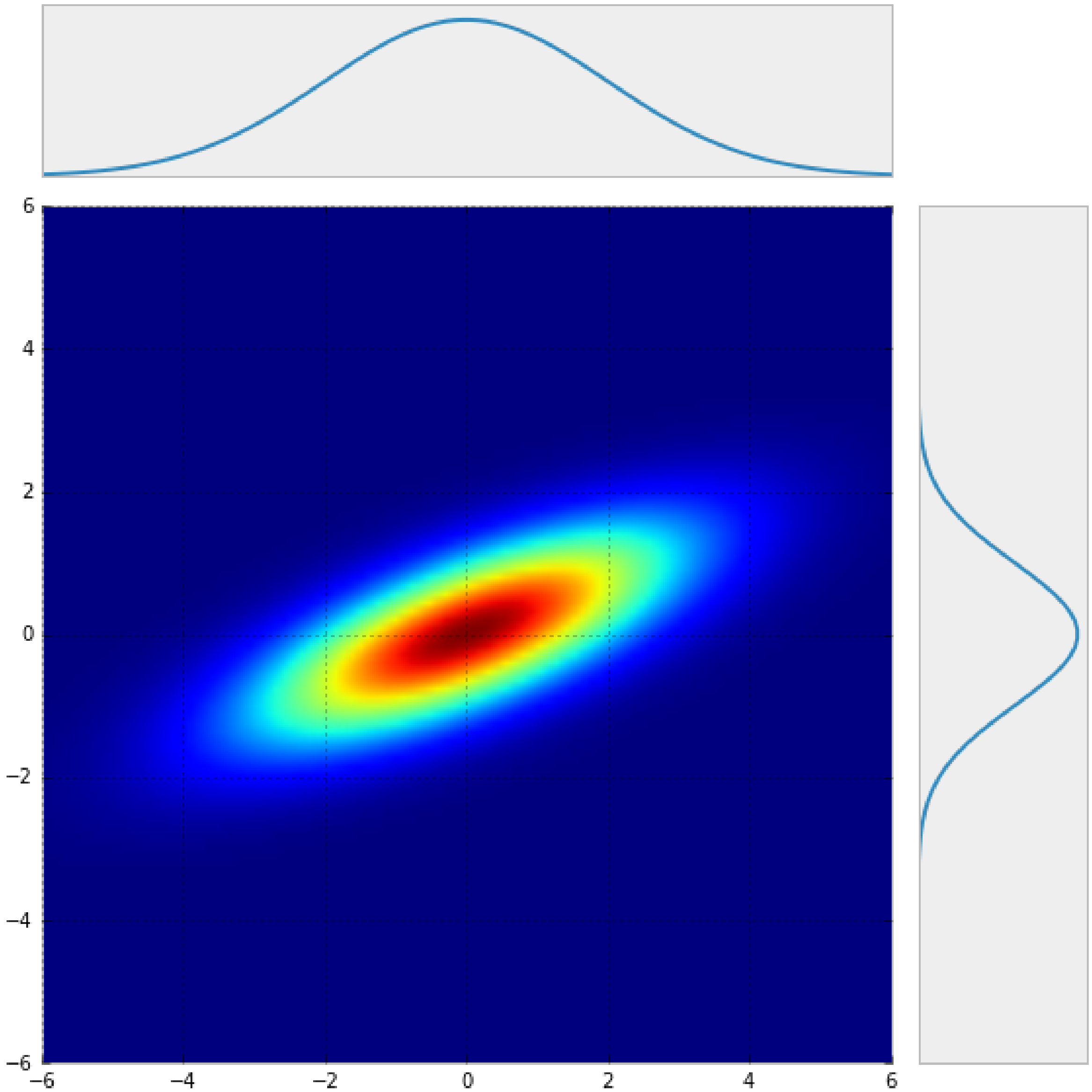
> Marginals are Gaussian!

Partitioned Marginals: Example Code

In [8]:
```
def plot_mvn(sigmax, sigmay, mux, muy, corr):
    # dimensions
    radius = 3 * max(sigmax, sigmay);
    # create grid
    x = np.linspace(mux-radius, mux+radius, 100);
    y = np.linspace(muy-radius, muy+radius, 100);
    X, Y = np.meshgrid(x, y);

    # data limits
    xlim = (x.min(), x.max());
    ylim = (y.min(), y.max());

    # bivariate and univariate normals
    sigmaxy = corr * np.sqrt(sigmax * sigmay);
    Z = mlab.bivariate_normal(X, Y, sigmax, sigmay, mux, muy, sigma
xy);
    zx = np.sum(Z, axis=0); #mlab.normpdf(x, mux, sigmax);
    zy = np.sum(Z, axis=1); #mlab.normpdf(y, muy, sigmay);

    # figure
    fig = plt.figure(figsize=(8,8));

    # subplots
    gs = gridspec.GridSpec(2, 2, width_ratios=[5,1], height_ratios=
[1,5]);
    ax_xy = fig.add_subplot(gs[1,0]);
    ax_x  = fig.add_subplot(gs[0,0], sharex=ax_xy);
    ax_y  = fig.add_subplot(gs[1,1], sharey=ax_xy);

    # plot
    ax_xy.imshow(Z, origin='lower', extent=xlim+ylim, aspect='aut
o');
    ax_x.plot(x, zx);
    ax_y.plot(zy, y);

    # hide labels
    ax_x.xaxis.set_visible(False);
    ax_x.yaxis.set_visible(False);
    ax_y.xaxis.set_visible(False);
    ax_y.yaxis.set_visible(False);

    # layout & title
    plt.tight_layout();
```

Partitioned Marginals: Bivariate Example

In [9]:
```
# sigmax, sigmay, mux, muy, corr
plot_mvn(2, 1, 0, 0, 1);
```



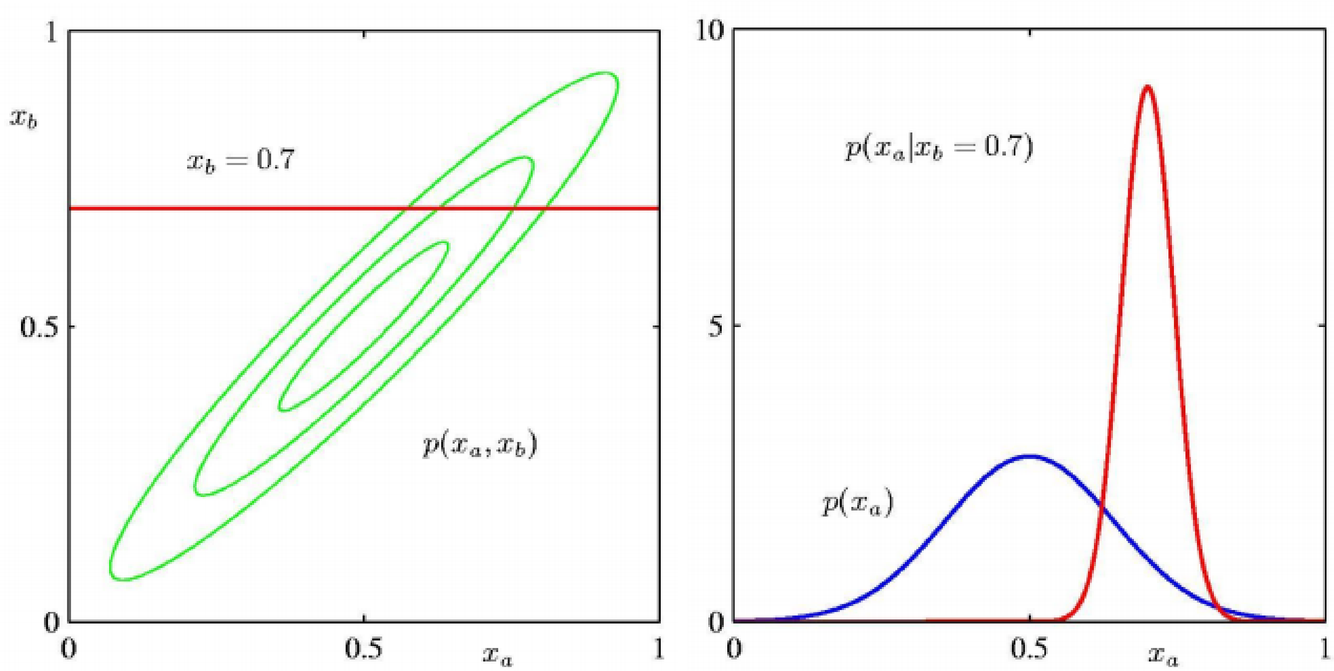
Partitioned Conditionals

Exercise: Conditionals are given by

$$
\begin{aligned}
P(x_a|x_b) &= \mathcal{N}(x_a|\mu_{a|b}, \Sigma_{a|b}) \\
\Sigma_{a|b} &= \Lambda_{aa}^{-1} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \\
\mu_{a|b} &= \Sigma_{a|b}\left[\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b - \mu_b)\right] \\
&= \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b - \mu_b) \\
&= \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b)
\end{aligned}
$$

Partitioned Conditionals

> Obtained by "slicing" the joint pdf



Linear Gaussian Systems: Model

Suppose $x \in \mathbb{R}^{D_x}$ and $y \in \mathbb{R}^{D_y}$, and

$$x \sim \mathcal{N}(\mu_x, \Sigma_x)$$
$$y|x \sim \mathcal{N}(Ax + b, \Sigma_y)$$

for fixed $A \in \mathbb{R}^{D_y \times D_x}$ and $b \in \mathbb{R}^{D_y}$.

Linear Gaussian Systems: Bayes' Theorem

Exercise: Show that

$$\boxed{P(y) = \mathcal{N}(y|A\mu_x + b, \Sigma_y + A\Sigma_x A^T)}$$

Linear Gaussian Systems: Bayes' Theorem

Exercise: Show that

$$\boxed{P(x|y) = \mathcal{N}(x|\mu_{x|y}, \Sigma_{x|y})}$$

where

$$\begin{aligned}
\Sigma_{x|y}^{-1} &= \Sigma_x^{-1} + A^T \Sigma_y^{-1} A \\
\mu_{x|y} &= \Sigma_{x|y} \left[A^T \Sigma_y^{-1} (y-b) + \Sigma_x^{-1} \mu_x \right]
\end{aligned}$$

Bayesian Linear Regression

> Taken from **[PRML]** §3.3, **[MLAPP]** §7.6, and **[CS229]**

Review: Regression

Data: Given data $\mathcal{D} = \{(x_k, t_k)\}_{k=1}^N$

- Observations $x = \{x_1, \dots, x_N\}$
- Target values $t = \{t_1, \dots, t_N\}$

Predict: Learn a function $y(x) = t$, e.g.

- Linear Regression, $y(x) = w^T \phi(x)$
- Kernel Regression, Locally Weighted Regression, etc.

Review: Linear Regression

In linear regression, we had a **likelihood** and **prior**

$$\begin{aligned}
w &\sim \mathcal{N}(w_0, S_0) \\
t|x, w, \beta &\sim \mathcal{N}(w^T \phi(x_n), \beta^{-1})
\end{aligned}$$

- Alternatively, $y = w^T x + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \beta^{-1})$
- Ridge regression corresponds to $w_0 = 0$ and $S_0 = \tau^2 I$.

Review: Linear Regression

Regularized linear regression gave a **MAP Estimate**:

$$w_{MAP} = (\lambda I + \Phi^T \Phi)^{-1} \Phi^T t$$

- where λ is a function of S_0 and β
- this is a *point estimate* of the full posterior $P(w|\mathcal{D})$

Review: Bayesian Updating

Bayesian Linear Regression will compute the full posterior. Recall that

$$\text{posterior} \propto \text{likelihood} \cdot \text{prior}$$

> weight the *data likelihood* by your *prior beliefs*

Bayesian Linear Regression

Instead, **Bayesian Linear Regression** computes the full posterior over the weights,

$$\begin{aligned} P(w|x,t) &\propto P(t|x,w)P(w) \\ &= \mathcal{N}(t \mid w^T \phi(x), \beta^{-1}) \mathcal{N}(w \mid w_0, S_0) \\ &= \mathcal{N}(w \mid m_N, S_N) \end{aligned}$$

where

- $m_N = S_N(S_0^{-1} w_0 + \beta \Phi^T t)$
- $S_N^{-1} = S_0^{-1} + \beta \Phi^T \Phi$

We got this simply by apply the calcuations on Linear Gaussian Systems (see prev. slides)!

BLR: Simplifying the Prior

Assume $w_0 = 0$ and $S_0 = \alpha^{-1} I$ (zero-mean isotropic Gaussian):

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

Exercise: By Bayes' Rule for Gaussians, the corresponding posterior is:

$$P(w|x, t) = \mathcal{N}(w|m_N, S_N)$$

where

- $m_N = \beta S_N \Phi^T t$
- $S_N^{-1} = \alpha I + \beta \Phi^T \Phi$

BLR: Using the Posterior

We have just shown the posterior is:

$$P(w|x, t) = \mathcal{N}(w|m_N, S_N)$$

where $m_N = \beta S_N \Phi^T t$ and $S_N^{-1} = \alpha I + \beta \Phi^T \Phi$

- Note the **posterior mean** is $m_N = w_{MAP}$ from regularized linear regression!
- Now we also have the **posterior variance** S_N! This tells us how *confident* we are in our prediction w_{MAP}.

Break time!

Sequential Bayesian Learning

Note: The posterior and prior are both Gaussians.

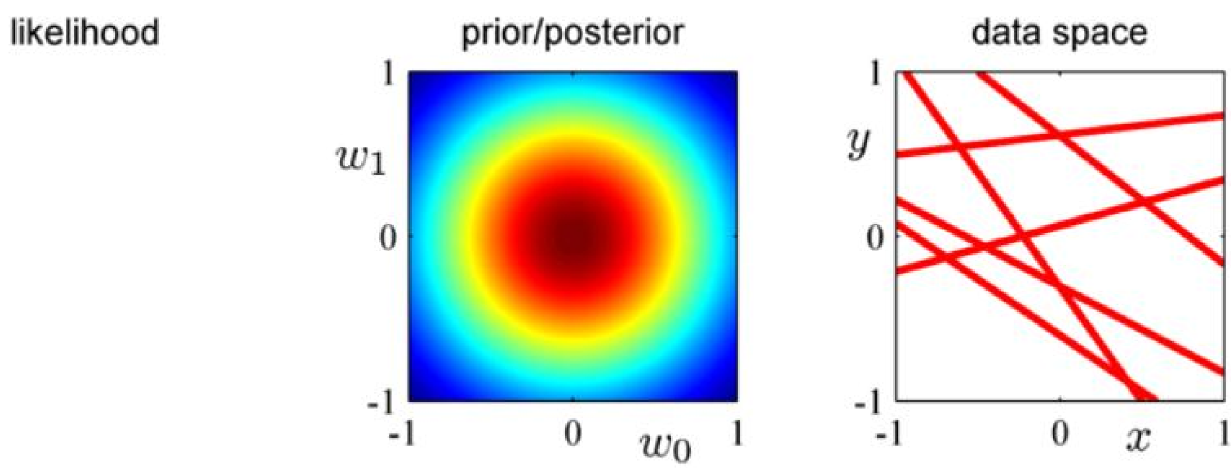
- If our data is *streaming*, we can use the posterior for one observation as a prior for the next set of observations.
- Starting from a fixed prior, sequentially update our beliefs as new data arrives.

This is **Bayesian Updating**.

Sequential Bayesian Learning

Simple model: $y(x, w) = w_0 + w_1 x$

$$\text{posterior} \propto \text{likelihood} \cdot \text{prior}$$



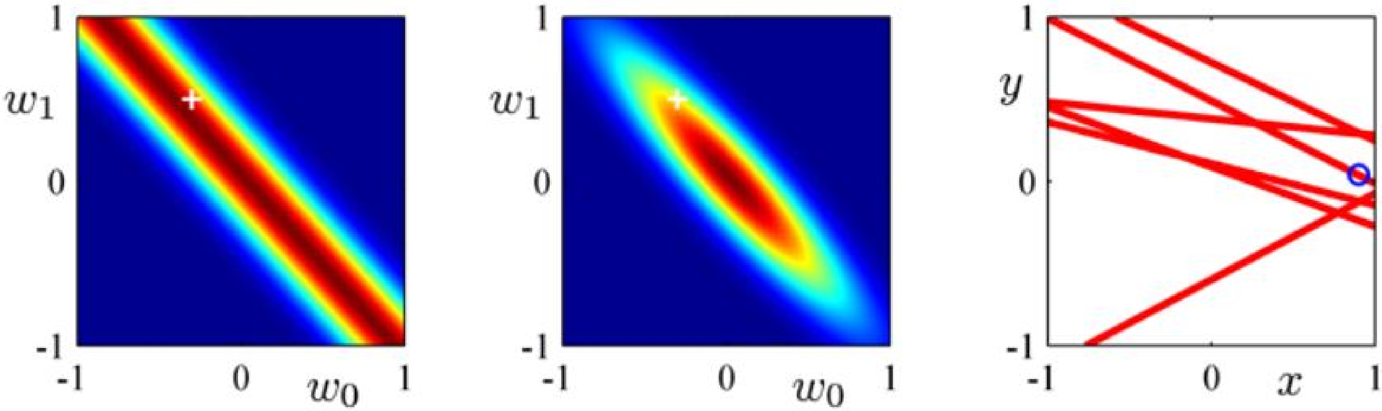
(A) (B) $p(\mathbf{w}|\mathbf{x}, t)$ (C) samples of $\mathbf{w}|\mathbf{x}, t$

Sequential Bayesian Learning

Simple model: $y(x, w) = w_0 + w_1 x$

$$\text{posterior} \propto \text{likelihood} \cdot \text{prior}$$

We can sample lines (*hypotheses*) from the posterior:



(A) $p(t|\mathbf{x}, \mathbf{w})$ (B) $p(\mathbf{w}|\mathbf{x}, t)$ (C) samples of $\mathbf{w}|\mathbf{x}, t$

Sequential Bayesian Learning

Simple model: $y(x, w) = w_0 + w_1 x$

$$\text{posterior} \propto \text{likelihood} \cdot \text{prior}$$

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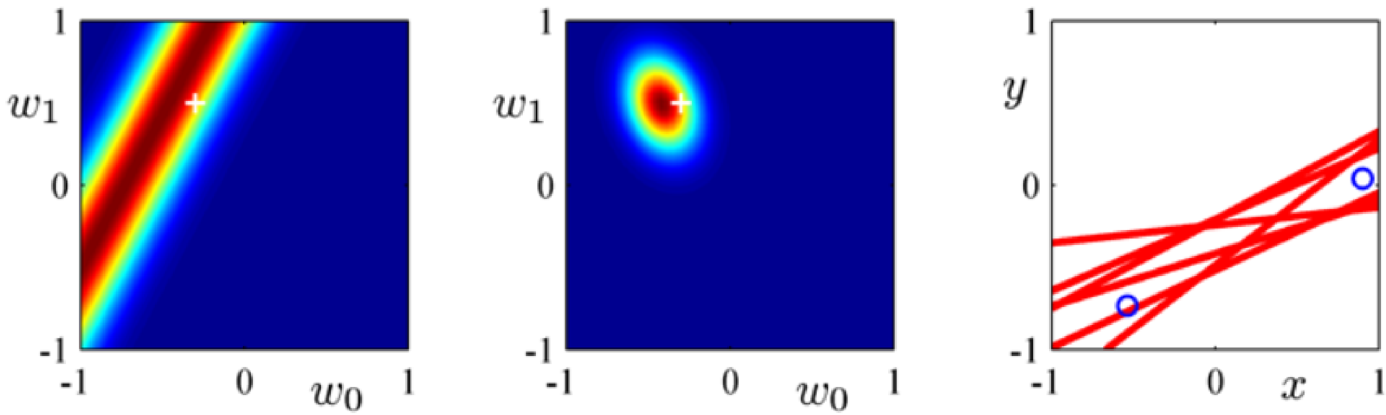

(A) $p(t|\mathbf{x}, \mathbf{w})$ (B) $p(\mathbf{w}|\mathbf{x}, t)$ (C) samples of $\mathbf{w}|\mathbf{x}, t$

Sequential Bayesian Learning

Simple model: $y(x, w) = w_0 + w_1 x$

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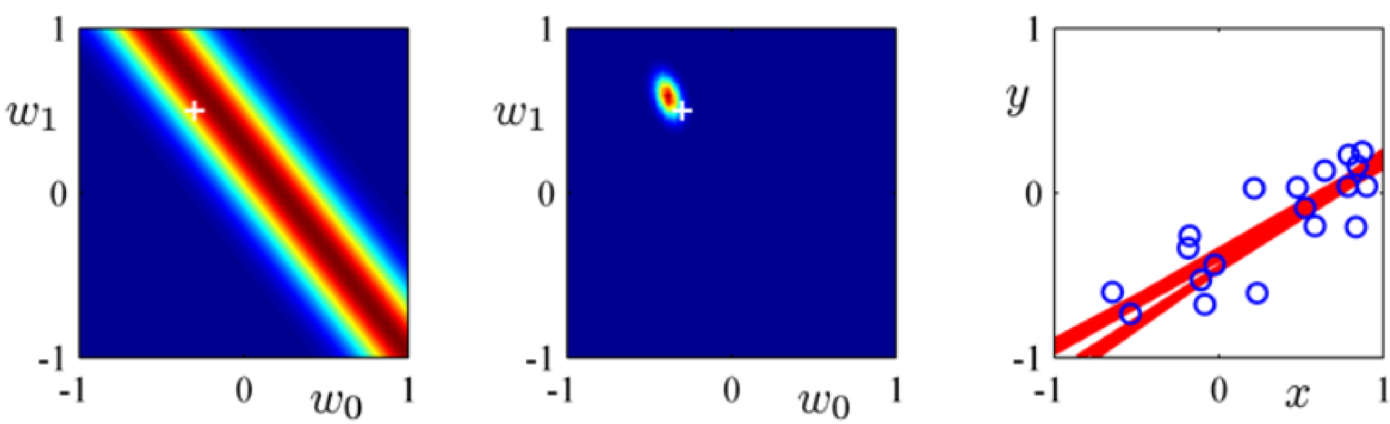


(A) $p(t|\mathbf{x}, \mathbf{w})$ (B) $p(\mathbf{w}|\mathbf{x}, t)$ (C) samples of $\mathbf{w}|\mathbf{x}, t$

Predictive Distribution

Our real goal is to predict t given new x using the **predictive distribution**,

$$\begin{aligned} P(t|x, \mathcal{D}) &= \int_w P(t|x, w, \mathcal{D}) P(w|\mathcal{D})\, dw \\ &= \int_w \mathcal{N}(t|w^T \phi(x), \beta^{-1}) \mathcal{N}(0, \alpha^{-1} I) \end{aligned}$$

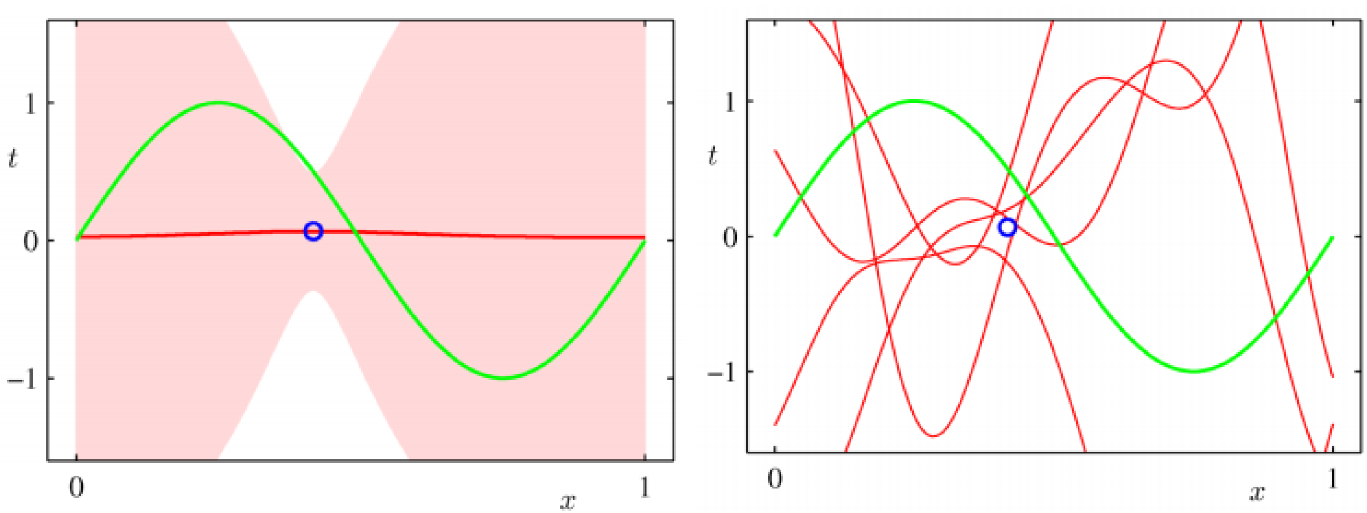
Exercise: Show that $P(t|x, \mathcal{D}) = \mathcal{N}(t|m_N^T \phi(x), \sigma_N^2(x))$, where

- $\sigma_N^2(x) = \frac{1}{\beta} + \phi(x)^T S_n \phi(x)$

Intuitively, this corresponds to noise in data + uncertainty in w.

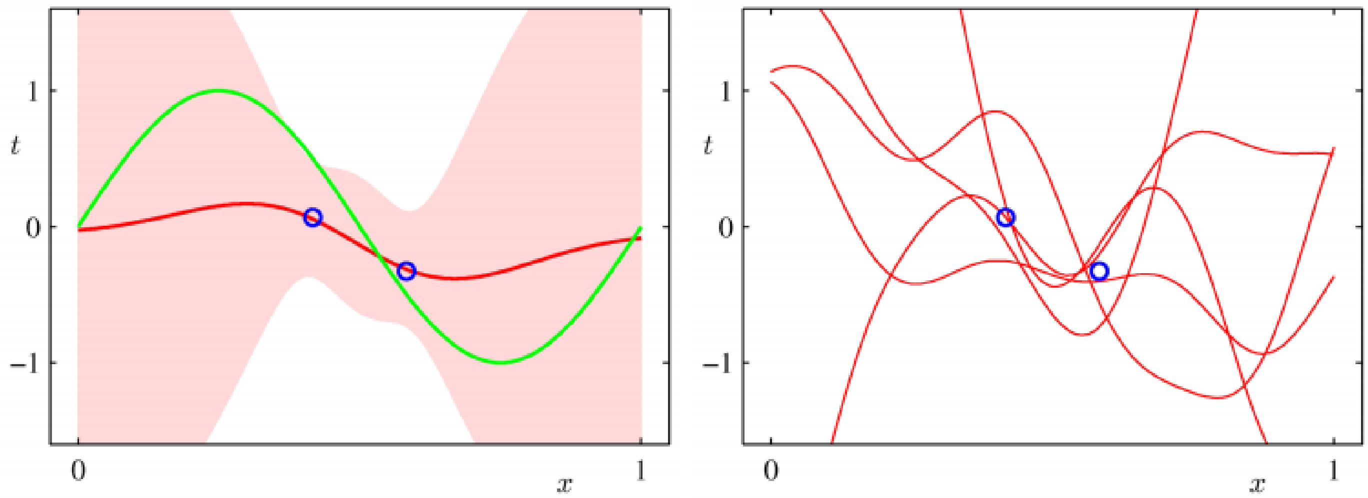
Predictive Distribution: Samples

Using 9 Gaussian basis functions $\phi_j(x) = exp\left\{-\frac{(x-\mu_j)}{2s^2}\right\}$



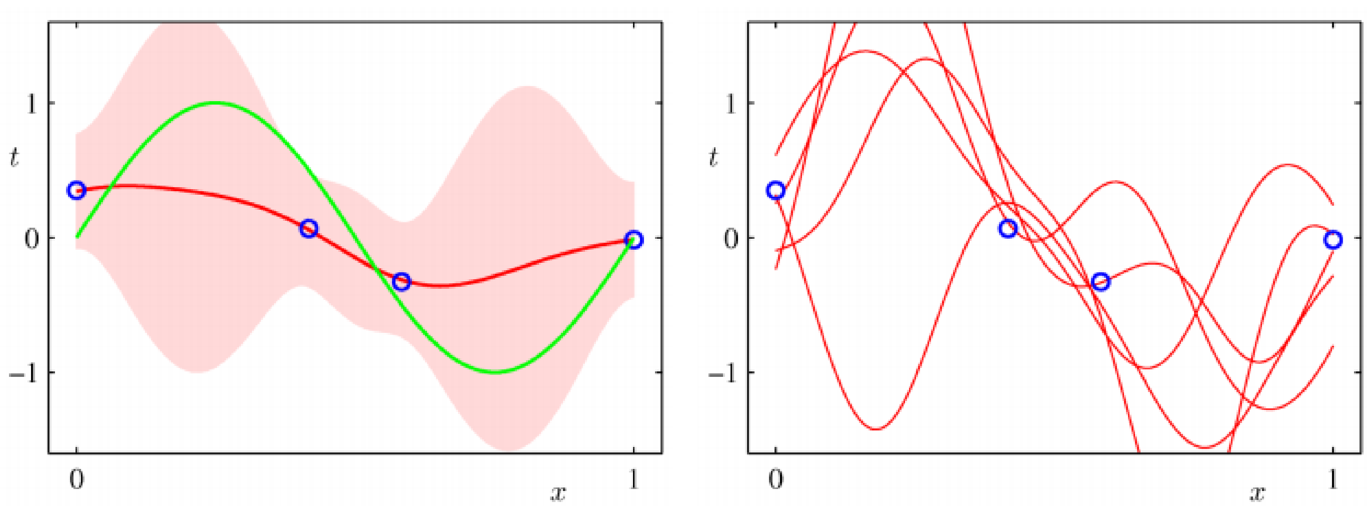
$N = 1$ observed point

Predictive Distribution: Samples



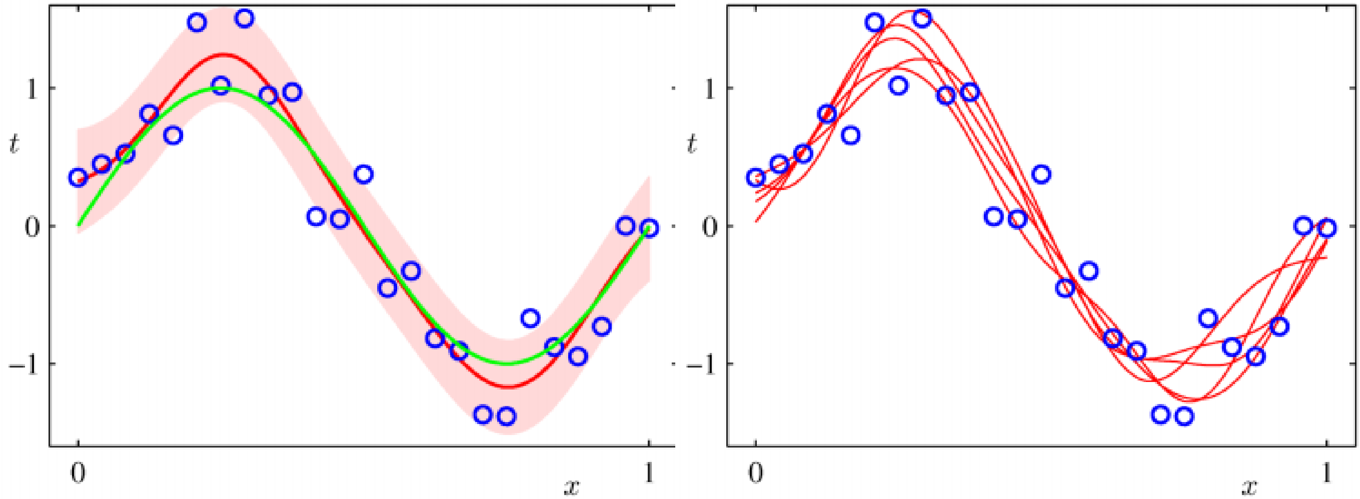
$N = 2$ observed points

Predictive Distribution: Samples



$N = 4$ observed points

Predictive Distribution: Samples



$N = 25$ observed points

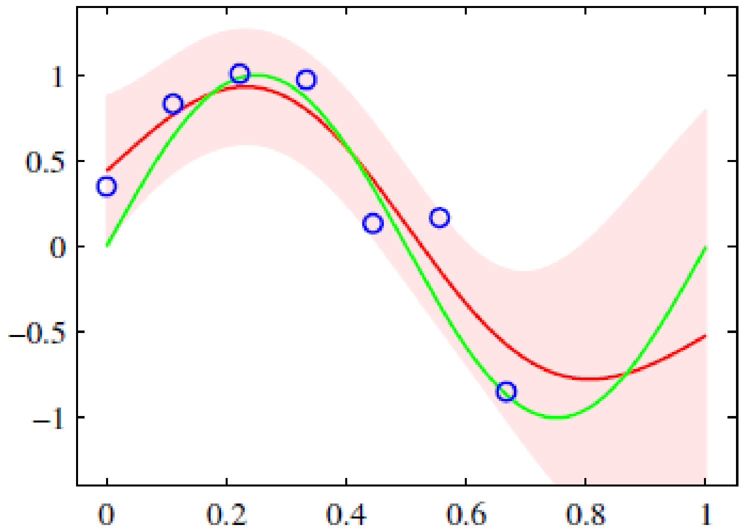
Gaussian Processes

> Taken from **[CS229]** and **[MLAPP]**

Gaussian Processes

Motivation: Here are some data points. What function did they come from?

- GPs are a nice way of expressing “priors on functions”
- Applications: Regression and Classification



Gaussian Processes: Motivation

Multivariate Gaussians are useful for modeling *finite* collections of real-valued variables.

- Nice analytical properties
- Distribution over **random vectors**
- Easily model *correlations* between variables

Gaussian Processes extend Multivariate Gaussians to *infinite-sized* collections of real-valued variables.

- Distribution over **random functions**

How can we parameterize probability distributions over functions?

Distributions over Functions: Finite Domain

Consider the following simple example:

- Let $\mathcal{X} = \{x_1, \ldots, x_m\}$ be any finite set.
- Let $\mathcal{H}$ be the set of all functions $h : \mathcal{X} \mapsto \mathbb{R}$.

For example, one function $h_0 \in \mathcal{H}$ is

$$h_0(x_1) = 5 \quad h_0(x_2) = 2.3 \quad \cdots \quad h_0(x_{m-1}) = -\pi \quad h_0(x_m) = 8$$

Any function $h \in \mathcal{H}$ can be represented as a vector:

$$\overrightarrow{h_0} = [5, 2.3, \ldots, \pi, 8]$$

Distributions over Functions: Finite Domain

To specify a distribution over $\mathcal{H}$, exploit the one-one mapping to $\mathbb{R}^m$

- Assume a distribution over vectors, $\vec{h} \sim \mathcal{N}(\vec{\mu}, \sigma^2 I)$.

This **induces** a distribution over $\mathcal{H}$ given by likelihoods at each "*sample point*":

$$P(h) = P(\vec{h}) = \prod_{k=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2\sigma^2}(f(x_k) - \mu_k)^2\right]$$

Distributions over Functions: Infinite Domain

A **stochastic process** is a collection of random variables, $f = \{f(x)\}_{x \in \mathcal{X}}$ with index set $\mathcal{X}$, e.g.

- Dirichlet Processes, Poisson Processes, etc.

A **Gaussian Process** is a stochastic process such that any finite subcollection of random variables has a multivariate Gaussian distribution

Gaussian Processes: Definition

We say $f(\cdot) \sim \mathcal{GP}(m, k)$ is drawn from a Gaussian process with

- mean function $m(\cdot) : \mathcal{X} \mapsto \mathbb{R}$
- covariance or kernel function $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$

provided that for any finite set $\{x_1, \ldots, x_m\} \subset \mathcal{X}$, the associated random variables have distribution

$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_m) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} m(x_1) \\ \vdots \\ m(x_m) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & \cdots & k(x_1, x_m) \\ \vdots & \ddots & \vdots \\ k(x_m, x_1) & \cdots & k(x_m, x_m) \end{bmatrix} \right)$$

Gaussian Processes: Interpretation

Intuitively, $f \sim \mathcal{GP}(m, k)$ is an

- extremely high-dimensional vector
- drawn from an extremely high-dimensional Gaussian

Each dimension corresponds to an element $x \in \mathcal{X}$,

- the corresponding component of the vector represents $f(x)$

Gaussian Processes: Mean and Covariance

The **mean function** $m(\cdot) : \mathcal{X} \mapsto \mathbb{R}$ can be any function.

- For most applications, set $m \equiv 0$.

The **covariance function** $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ must be a valid kernel.

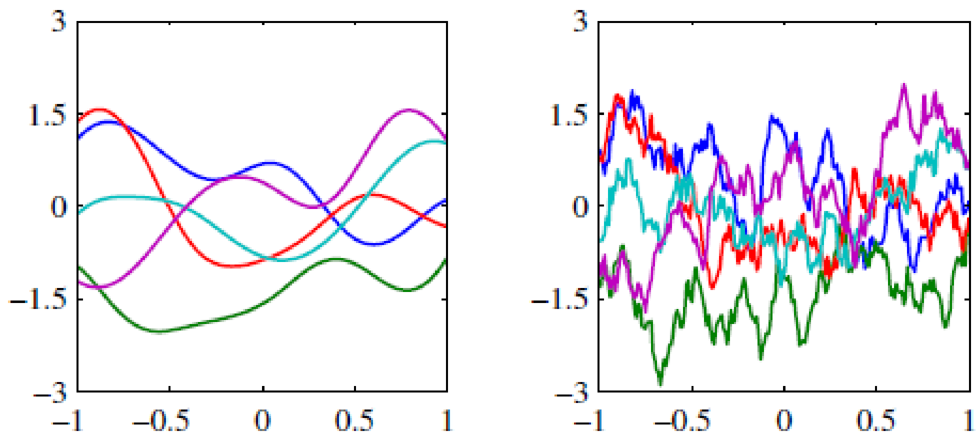
- $f(x)$ and $f(x')$ will have high covariance if x and x' are "nearby"
- Therefore, kernel controls **smoothness**

Gaussian Processes: Example

When $m \equiv 0$, the choice of kernel defines the prior.

- (Left) Gaussian Kernel $k(x, x') = exp(-\theta \|x - x'\|_2^2)$
- (Right) Exponential Kernel $k(x, x') = exp(-\theta \|x - x'\|_1)$

Samples from a Gaussian Process:



Linear Regression Revisited

Model: Assume $y \approx w^T \phi(x)$ is a combination of M fixed basis functions.

$$w \sim \mathcal{N}(w_0, S_0)$$
$$y|x, w, \beta \sim \mathcal{N}(w^T \phi(x_n), \beta^{-1})$$

Given training points $x_1, \ldots, x_N$, what is the joint distribution $P(\vec{y})$ of $y(x_1), \ldots, y(x_N)$?

$$\vec{y} = \Phi w = \begin{bmatrix} y(x_1) & \cdots & y(x_N) \end{bmatrix}^T$$

Linear Regression Revisited

Note $\vec{y} = \Phi w$ is a linear combination of Gaussians w, so is itself Gaussian!

$$\mathrm{E}[\vec{y}] = \Phi E[w] = 0$$
$$\mathrm{Cov}[\vec{y}] = \mathrm{E}[yy^T] = \Phi \mathrm{E}[ww^T]\Phi^T = \frac{1}{\alpha}\Phi\Phi^T = K$$

where $K = [k(x_i, x_j)]_{i,j} \in \mathbb{R}^{N \times N}$ is the **Gram Matrix** over the training data with kernel

$$k(x_i, x_j) = \frac{1}{\alpha}\phi(x_i)^T \phi(x_j)$$

Bayesian Linear Regression

So, Bayesian Kernel Linear Regression is a Gaussian Process!

- Kernel $k(\cdot, \cdot)$ is dot product in feature space.

$$
\begin{aligned}
y &= f(x) + \epsilon \\
f &\sim \mathcal{GP}(0, k(\cdot, \cdot)) \\
\epsilon &\sim \mathcal{N}(0, \sigma^2)
\end{aligned}
$$

> Features in BLR $\Longleftrightarrow$ Kernel functions for GPs

Gaussian Process Regression

In general, $k(\cdot, \cdot)$ can be any valid kernel,

$$
\begin{aligned}
y &= f(x) + \epsilon \\
f &\sim \mathcal{GP}(0, k(\cdot, \cdot)) \\
\epsilon &\sim \mathcal{N}(0, \sigma^2)
\end{aligned}
$$

> See the book for more details.