

Introduction to Probabilistic Machine Learning

Bayesian Regression

Ralf Herbrich

Overview

1. Bayesian Linear Regression
2. Bayesian Linear Regression via Message Passing
 - Normal Distribution Revisited
 - Posterior and Predictive Distribution
3. Fast Bayesian Linear Regression
4. Bayesian Linear Regression via Linear Algebra

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Unit 7 – Bayesian Regression

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Bayesian Inference of Linear Basis Function Models

■ Given:

1. **Training Data:** $D \in (\mathcal{X} \times \mathbb{R})^n$ of n (labelled) examples (x_i, y_i)
2. **Linear Basis Functions:** Basis function mapping $\phi: \mathcal{X} \rightarrow \mathbb{R}^M$ and linear function model

$$f(x; \mathbf{w}) := \mathbf{w}^T \phi(x)$$

↖ ↘
weight vector feature vector
3. **Likelihood of functions:**

$$p(D|f) = p(D|\mathbf{w}) = \prod_{i=1}^n \mathcal{N}(y_i; \mathbf{w}^T \phi(x_i), \beta^2)$$

4. **Prior belief over functions:**

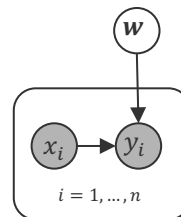
$$p(f) = p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

■ Bayesian Inference:

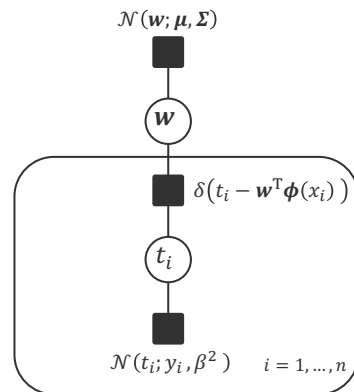
- **Posterior belief over functions:**

$$p(f|D) = p(\mathbf{w}|D) = \frac{\prod_{i=1}^n \mathcal{N}(y_i; \mathbf{w}^T \phi(x_i), \beta^2) \cdot \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\int_{\mathbb{R}^M} \prod_{i=1}^n \mathcal{N}(y_i; \tilde{\mathbf{w}}^T \phi(x_i), \beta^2) \cdot \mathcal{N}(\tilde{\mathbf{w}}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\tilde{\mathbf{w}}}$$

Bayesian Network



Factor Graph



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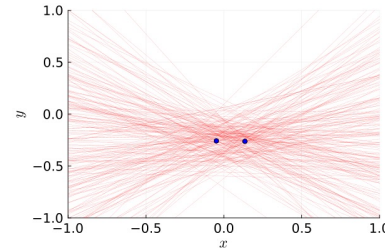
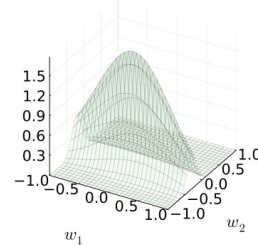
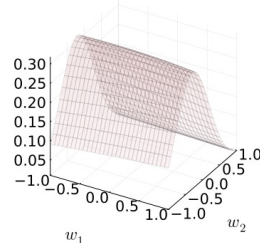
Bayesian Inference in Pictures

Likelihood

Posterior

Input Space

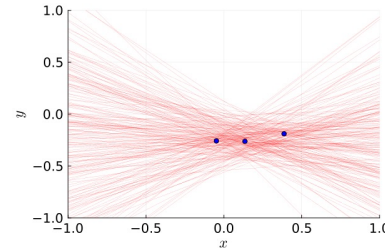
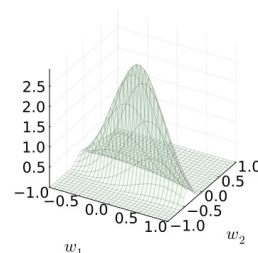
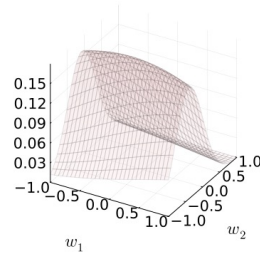
$n = 2$



$$f(x) = w_1x + w_2$$

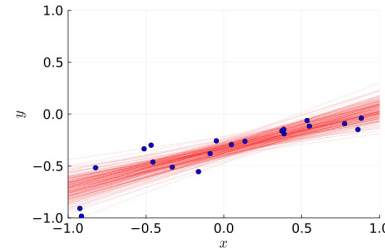
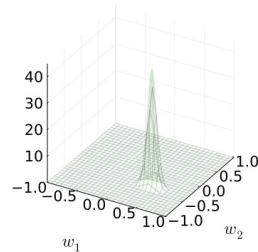
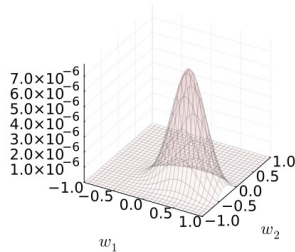
$$P(y|x) = \mathcal{N}(y; f(x), 0.2^2)$$

$n = 3$



$$P(w_j) = \mathcal{N}(w_j; 0, 0.5)$$

$m=20$



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Multivariate Normal Distribution

- **Multivariate Normal Distribution.** A continuous random variable $\mathbf{X} \in \mathbb{R}^M$ is said to have a multivariate normal distribution if the density is given by

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

where $\boldsymbol{\Sigma}$ must be a positive definite $M \times M$ matrix.

- **Properties:**

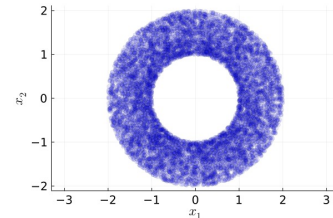
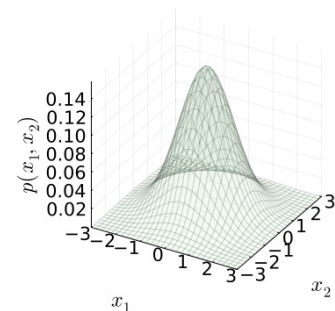
$$E[\mathbf{X}] = \boldsymbol{\mu}$$

$$\text{cov}[\mathbf{X}] = \boldsymbol{\Sigma}$$

- **Covariance.** For any two random variables X_1 and X_2 the covariance expresses the extent to which X_1 and X_2 vary together **linearly** and is given by

$$\text{cov}[X_1, X_2] = E_{X_1 X_2}[(X_1 - E[X_1]) \cdot (X_2 - E[X_2])] = E_{X_1 X_2}[X_1 X_2] - E[X_1] \cdot E[X_2]$$

- Generalization of the variance to two random variables: $\text{var}[X] = \text{cov}[X, X]$
- **Theorem.** If two random variables X_1 and X_2 are independent, then $\text{cov}[X_1, X_2] = 0$. The converse is not true!



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Multivariate Normal Distribution: Representations

■ Two Parameterizations (for different purposes):

□ Scale-Location Parameters

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{M}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \cdot \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

□ Natural Parameters

$$\mathcal{G}(\mathbf{x}; \boldsymbol{\tau}, \mathbf{P}) = (2\pi)^{-\frac{M}{2}} |\mathbf{P}|^{\frac{1}{2}} \cdot \exp\left(-\frac{1}{2}\boldsymbol{\tau}^T \mathbf{P}^{-1} \boldsymbol{\tau}\right) \cdot \exp\left(\boldsymbol{\tau}^T \mathbf{x} - \frac{1}{2}\mathbf{x}^T \mathbf{P} \mathbf{x}\right)$$

■ Conversions

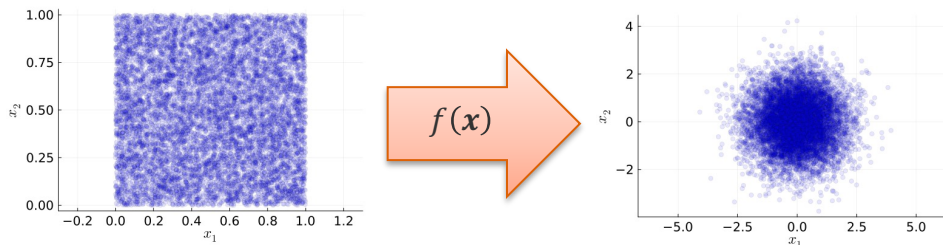
$$\begin{array}{c} \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{G}(\mathbf{x}; \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}, \boldsymbol{\Sigma}^{-1}) \\ \quad \quad \quad \swarrow \quad \quad \searrow \\ \quad \quad \text{Matrix inverse} \\ \quad \quad \swarrow \quad \quad \searrow \\ \mathcal{G}(\mathbf{x}; \boldsymbol{\tau}, \mathbf{P}) = \mathcal{N}(\mathbf{x}; \mathbf{P}^{-1} \boldsymbol{\tau}, \mathbf{P}^{-1}) \end{array}$$

Sampling Multivariate Normal Distribution

- **Assumption:** We have access to a random number generator $x \sim \text{Unif}([0,1])$
- **Box-Mueller:** If $x_1 \sim \text{Unif}([0,1])$ and $x_2 \sim \text{Unif}([0,1])$ then $f(x) \sim N(\cdot; \mathbf{0}, \mathbf{I})$ for

$$f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} \sqrt{-2 \ln(x_1)} \cdot \cos(2\pi x_2) \\ \sqrt{-2 \ln(x_1)} \cdot \sin(2\pi x_2) \end{bmatrix}$$

□ In pictures:



- **Sampling a multivariate Gaussian.** If $x \sim \mathcal{N}(x; \mu, \Sigma)$ then for $y = Ax + b$

$$y \sim \mathcal{N}(y; A\mu + b, A\Sigma A^T)$$

- For sampling a multivariate distribution, we require either the SVD or Cholesky decomposition of the covariance matrix, $\Sigma = LL^T$ (see exercises)
- Can be easily proven from the properties of expectation and covariance



George Box
(1919 – 2013)



Mervin Mueller
(1928 – 2018)

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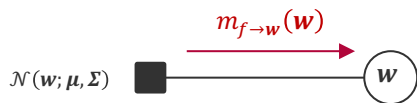
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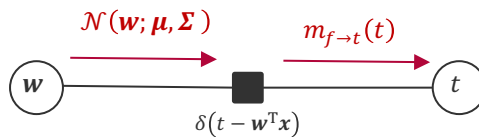
Multivariate Message Update Equations

Gaussian Factor

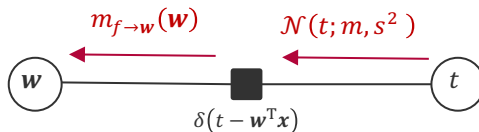


$$m_{f \rightarrow \mathbf{w}}(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Gaussian Projection Factor

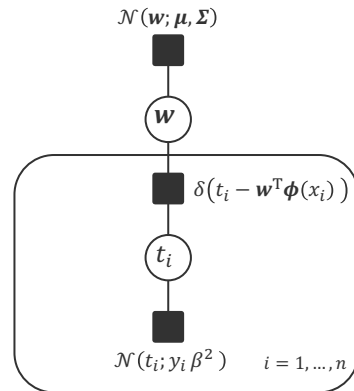


$$m_{f \rightarrow \mathbf{t}}(\mathbf{t}) = \int \delta(\mathbf{t} - \mathbf{w}^T \mathbf{x}) \cdot \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) d\mathbf{w} = \mathcal{N}(\mathbf{t}; \boldsymbol{\mu}^T \mathbf{x}, \mathbf{x}^T \boldsymbol{\Sigma} \mathbf{x})$$



$$m_{f \rightarrow \mathbf{w}}(\mathbf{w}) = \int \delta(\mathbf{t} - \mathbf{w}^T \mathbf{x}) \cdot \mathcal{N}(\mathbf{t}; m, s^2) d\mathbf{t} = \mathcal{G}\left(\mathbf{w}; \frac{m}{s^2} \mathbf{x}, \frac{1}{s^2} \mathbf{x} \mathbf{x}^T\right)$$

Factor Graph



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Bayesian Linear Regression by Message Passing

- **Message:** Simple factor tree where each training example is summarized in an M -dimensional message

- Prior Message $m_{1,0}(\mathbf{w}) = \mathcal{G}(\mathbf{w}; \Sigma^{-1}\boldsymbol{\mu}, \Sigma^{-1}) = p(\mathbf{w})$
- Target Message $m_{2,i}(t_i) = \mathcal{N}(t_i; y_i, \beta^2) = p(y_i|t_i)$
- Data Message $m_{1,i}(\mathbf{w}) = \mathcal{G}(\mathbf{w}; \beta^{-2}y_i\boldsymbol{\phi}(x_i), \beta^{-2}\boldsymbol{\phi}(x_i)\boldsymbol{\phi}^T(x_i)) = p(y_i|\mathbf{w})$

- **Posterior:** Multiplying prior and data messages we have

$$p(\mathbf{w}|D) = \mathcal{G}\left(\mathbf{w}; \Sigma^{-1}\boldsymbol{\mu} + \beta^{-2} \sum_{i=1}^n y_i \boldsymbol{\phi}(x_i), \Sigma^{-1} + \beta^{-2} \sum_{i=1}^n \boldsymbol{\phi}(x_i)\boldsymbol{\phi}^T(x_i)\right)$$

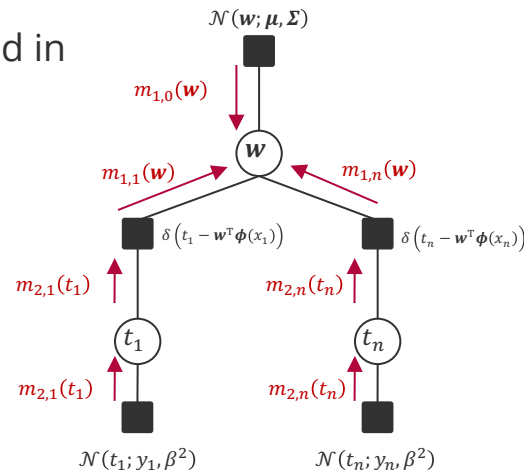
- **Feature Matrix:** All feature vectors are stacked on top of each other in a *feature matrix*

feature vector

$$\Phi = \begin{bmatrix} \phi_1(x_1) & \cdots & \phi_M(x_1) \\ \vdots & \ddots & \vdots \\ \phi_1(x_n) & \cdots & \phi_M(x_n) \end{bmatrix} = \begin{bmatrix} \boldsymbol{\phi}^T(x_1) \\ \vdots \\ \boldsymbol{\phi}^T(x_n) \end{bmatrix}$$

$$\Phi^T \mathbf{y} = [\boldsymbol{\phi}(x_1) \quad \cdots \quad \boldsymbol{\phi}(x_n)] \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^n y_i \boldsymbol{\phi}(x_i)$$

$$\Phi^T \Phi = [\boldsymbol{\phi}(x_1) \quad \cdots \quad \boldsymbol{\phi}(x_n)] \begin{bmatrix} \boldsymbol{\phi}^T(x_1) \\ \vdots \\ \boldsymbol{\phi}^T(x_n) \end{bmatrix} = \sum_{i=1}^n \boldsymbol{\phi}(x_i)\boldsymbol{\phi}^T(x_i)$$



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Predictions

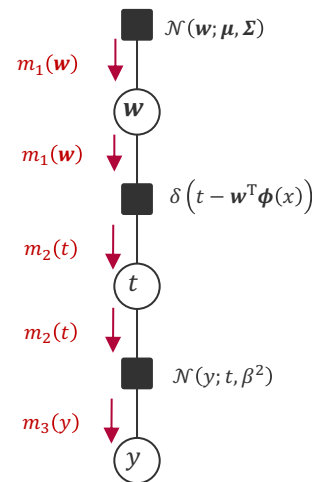
- **Prediction Tree:** Simple factor chain given posterior $p(\mathbf{w}|x, D) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$
 - Posterior Message $m_1(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = p(\mathbf{w}|x, D)$
 - Projection Message $m_2(t) = \mathcal{N}(t; \boldsymbol{\mu}^T \boldsymbol{\phi}(x), \boldsymbol{\phi}^T(x) \boldsymbol{\Sigma} \boldsymbol{\phi}(x)) = p(t|x, D)$
 - Prediction Message $m_3(y) = \mathcal{N}(y; \boldsymbol{\mu}^T \boldsymbol{\phi}(x), \beta^2 + \boldsymbol{\phi}^T(x) \boldsymbol{\Sigma} \boldsymbol{\phi}(x)) = p(y|x, D)$
- **Bayesian Linear Regression in Matrix Notation**

$$p(\mathbf{w}|D) = \mathcal{N}\left(\mathbf{w}; \underbrace{\mathbf{S}_D(\boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} + \beta^{-2} \boldsymbol{\Phi}^T \mathbf{y})}_{\mathbf{m}}, \mathbf{S}_D\right), \quad \mathbf{S}_D = (\boldsymbol{\Sigma}^{-1} + \beta^{-2} \boldsymbol{\Phi}^T \boldsymbol{\Phi})^{-1}$$

$$p(y|x, D) = \mathcal{N}(y; \mathbf{m}^T \boldsymbol{\phi}(x), \beta^2 + \boldsymbol{\phi}^T(x) \mathbf{S}_D \boldsymbol{\phi}(x))$$

data uncertainty

model uncertainty



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Bayesian Linear Regression: Example

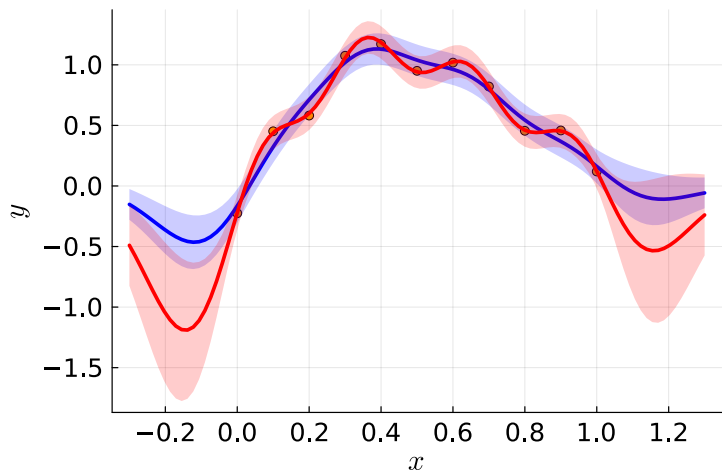
$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \lambda^2 I)$$

$$\lambda = 10$$

$$\lambda = 1$$

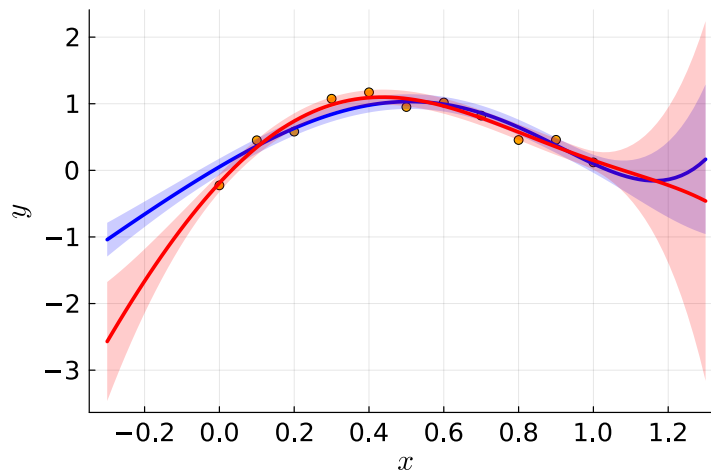
Gaussian Basis

$$\phi_j(x) = \mathcal{N}(x; j, 0.15^2)$$



Polynomial Basis

$$\phi_j(x) = x^j$$



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Fast Bayesian Linear Regression

- **Speeding up Bayesian Linear Regression:** Factorize the prior **and** posterior over the weight vector and then use message passing

- Since x is fixed, we used $\phi := \phi(x)$
- Message $m_{1,i}(w_i) = \mathcal{N}(w_i; \mu_i, \sigma_i^2)$
- Message $m_3(t) = \mathcal{N}(t; y, \beta^2)$
- Message $m_{2,i}(w_i) = \mathcal{N}(w_i; \phi_i^{-1} \cdot (y - \mu^T \phi + \mu_i \phi_i), \phi_i^{-2} \cdot (\beta^2 + \sum_{j=1}^M \phi_j^2 \sigma_j^2 - \phi_i^2 \sigma_i^2))$

- One can show that the product of $m_{1,i}(w_i)$ and $m_{2,i}(w_i)$ gives

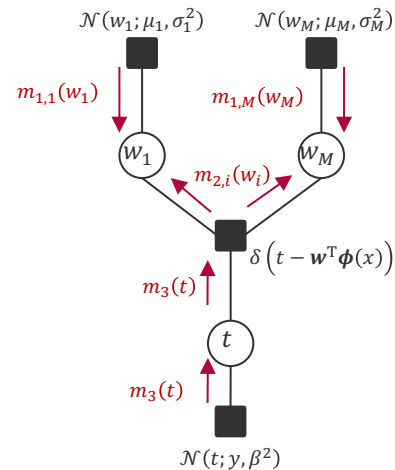
$$\mu_i \leftarrow \mu_i + \frac{y - \mu^T \phi(x)}{\phi_i(x)} \cdot \left[\frac{\phi_i^2(x) \sigma_i^2}{\beta^2 + \sum_{j=1}^M \phi_j^2(x) \sigma_j^2} \right]$$

target mismatch is measured
in units of $\phi_i(x)$

$$\sigma_i^2 \leftarrow \sigma_i^2 \cdot \left[1 - \frac{\phi_i^2(x) \sigma_i^2}{\beta^2 + \sum_{j=1}^M \phi_j^2(x) \sigma_j^2} \right]$$

multiplicative update

largest for parameter with
largest uncertainty so far

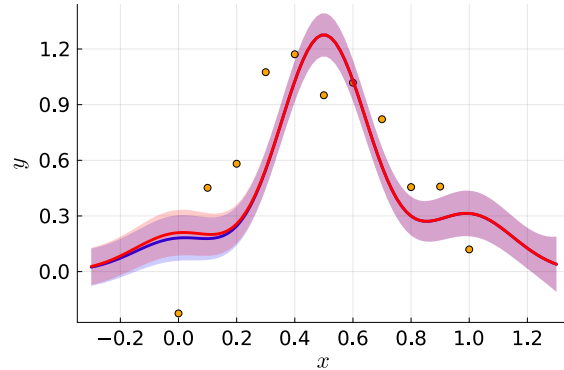


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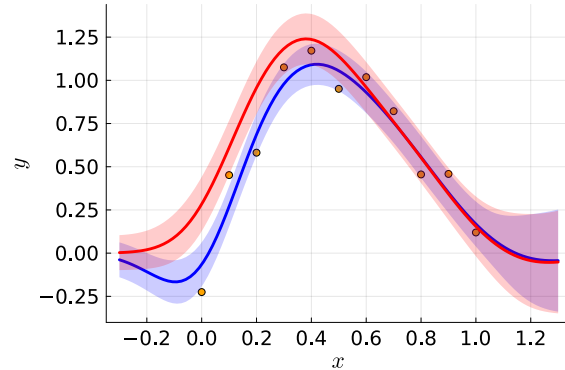
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Speeding up Bayesian Linear Regression

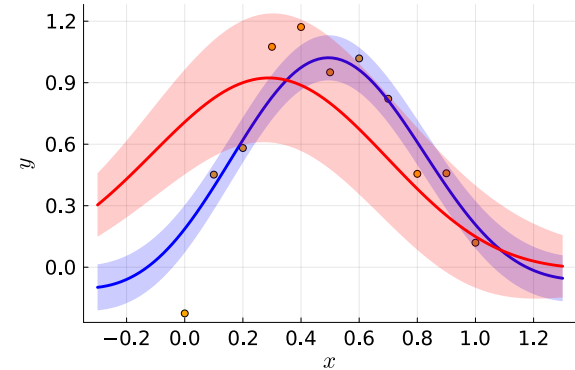
Nearly orthogonal features



Weakly correlated features



Strongly correlated features



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Bayes' Theorem for Normal Distributions

- **Conjugate Gaussians.** Given a normally distributed variable

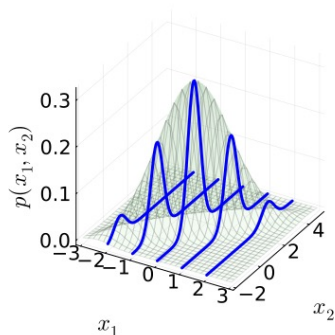
$$\mathbf{x} \sim \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

and a conditional distribution for \mathbf{y} given \mathbf{x} such that $\mathbf{y}|\mathbf{x} \sim \mathcal{N}(\mathbf{y}; \mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{S})$ we have the following for the marginal $p(\mathbf{y})$ and the "inverse" conditional $p(\mathbf{x}|\mathbf{y})$

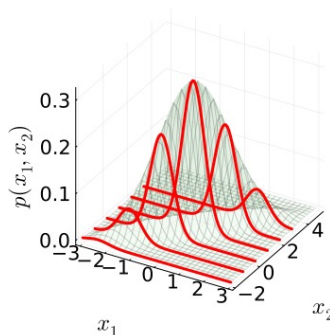
$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}; \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{S} + \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

$$p(\mathbf{x}|\mathbf{y}) = \mathcal{G}(\mathbf{x}; \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \mathbf{A}^T\mathbf{S}^{-1}(\mathbf{y} - \mathbf{b}), \boldsymbol{\Sigma}^{-1} + \mathbf{A}^T\mathbf{S}^{-1}\mathbf{A}),$$

$$p(x_1) = \mathcal{N}(x_1; 0, 1)$$



$$p(x_2|x_1) = \mathcal{N}\left(x_2; x_1 + 1, \frac{1}{2}\right)$$



$$p(x_1|x_2) = \mathcal{N}\left(x_1; \frac{2}{3}(x_2 - 1), \frac{1}{3}\right)$$

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Conjugate Gaussians: Derivation

■ Main Ideas:

1. **Representation:** Represent the Gaussian distribution via natural parameters and introduce a log-normalization constant to capture the marginal
2. **Multiplication:** Derive the update of the multiplication of two Gaussians over x
3. **Linear Mapping:** Derive a relation between Gaussian in x and in $y = Ax$

■ 1D Warm-Up

- **Theorem (Multiplication).** *Given two non-normalized one-dimensional Gaussian distributions $\mathcal{G}(x; \tau_1, \rho_1)$ and $\mathcal{G}(x; \tau_2, \rho_2)$ we have*

$$\mathcal{G}(x; \tau_1, \rho_1) \cdot \mathcal{G}(x; \tau_2, \rho_2) = \mathcal{G}(x; \tau_1 + \tau_2, \rho_1 + \rho_2) \cdot \mathcal{N}(\mu_1; \mu_2, \sigma_1^2 + \sigma_2^2)$$

- **Theorem (Linearity).** *Given a non-normalized one-dimensional Gaussian distribution $\mathcal{N}(y; aw + b, \beta^2)$ we have*

$$\mathcal{N}(y; aw + b, \beta^2) = \mathcal{N}(w; a^{-1}(y - b), a^{-2}\beta^2) \cdot \frac{1}{a}$$

- These two theorems combined allow to both efficiently and robustly compute the posterior parameters and derive the conjugate Gaussian equations

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Bayesian Linear Regression

- **Bayesian Linear Regression:** For the linear basis function model $f(x; \mathbf{w}) := \mathbf{w}^T \boldsymbol{\phi}(x)$ with likelihood $p(D|\mathbf{w}) = \mathcal{N}(\mathbf{y}; \boldsymbol{\Phi} \mathbf{w}, \beta^2 \mathbf{I})$ and prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$p(\mathbf{w}|D) = \mathcal{N}\left(\mathbf{w}; \mathbf{S}\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \frac{1}{\beta^2}\boldsymbol{\Phi}^T\mathbf{y}\right), \mathbf{S}\right), \quad \mathbf{S}^{-1} = \boldsymbol{\Sigma}^{-1} + \frac{1}{\beta^2}\boldsymbol{\Phi}^T\boldsymbol{\Phi}$$

- **Special Case:** $\boldsymbol{\mu} = \mathbf{0}$ and $\boldsymbol{\Sigma} = \tau^2 \mathbf{I}$

- For the posterior **mean** we have (Why?):

$$\boldsymbol{\mu}_{\text{posterior}} = \left(\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \frac{\beta^2}{\tau^2}\mathbf{I}\right)^{-1} \boldsymbol{\Phi}^T\mathbf{y} = \mathbf{w}_{\text{MAP}}$$

- If the mean of the full Bayesian inference and the maximum-a-posteriori are the same, what's the difference?! The **variance** of the predictive distribution!

$$p(y|x, D) = \int p(y|x, \mathbf{w}) \cdot p(\mathbf{w}|D) d\mathbf{w} = \int \mathcal{N}(y; \mathbf{w}^T \boldsymbol{\phi}(x), \beta^2) \cdot p(\mathbf{w}|D) d\mathbf{w}$$

$$p(y|x, D) = \mathcal{N}\left(y; \left(\mathbf{S}\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \frac{1}{\beta^2}\boldsymbol{\Phi}^T\mathbf{y}\right)\right)^T \boldsymbol{\phi}(x), \beta^2 + \boldsymbol{\phi}^T(x) \mathbf{S} \boldsymbol{\phi}(x)\right)$$

Properties of Gaussians

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$p(\mathbf{v}|\mathbf{w}) = \mathcal{N}(\mathbf{v}; \mathbf{A}\mathbf{w}, \boldsymbol{\Xi})$$

$$p(\mathbf{v}) = \mathcal{N}(\mathbf{v}; \mathbf{A}\boldsymbol{\mu}, \boldsymbol{\Xi} + \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

$$p(\mathbf{w}|\mathbf{v}) = \mathcal{N}(\mathbf{w}; \mathbf{m}, \mathbf{S})$$

$$\mathbf{m} = \mathbf{S}\left(\mathbf{A}^T\boldsymbol{\Xi}^{-1}\mathbf{v} + \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}\right)$$

$$\mathbf{S}^{-1} = \boldsymbol{\Sigma}^{-1} + \mathbf{A}^T\boldsymbol{\Xi}^{-1}\mathbf{A}$$

Introduction to Probabilistic Machine Learning

Unit 7 – Bayesian Regression

1. Bayesian Linear Regression

- Averaging over all functions weighting them by their posterior probability gives both a smoother mean and confidence intervals for each prediction (predictive distribution)
- Marginals and conditionals for multivariate Normals are linearly transformed Normals!
- Message passing on the Bayesian Regression factor graph involves no loops and is exact
- For linear basis function models with Normal noise, the posterior can be computed closed form
- Mean of Bayesian regression equals MAP solution but variance accounts for model uncertainty

2. Fast Bayesian Linear Regression

- The Bayesian linear regression algorithm is of cubic complexity in the features and quadratic in the training set size
- By factorizing *both* the prior and posterior distribution over the weight vector, we get a completely linear-complexity algorithm!

See you next week!