

Introduction to Probabilistic Machine Learning

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Bayesian Regression

Overview

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

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

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

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

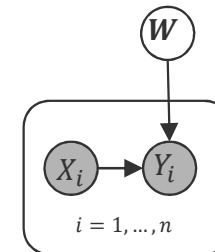
4. **Prior belief over functions:**

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

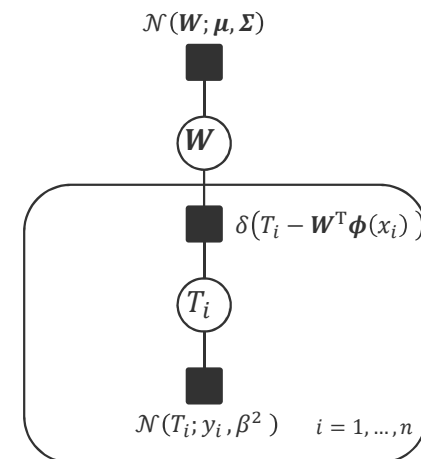
- ## ■ Bayesian Inference: Posterior belief over functions

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

Bayesian Network



Factor Graph



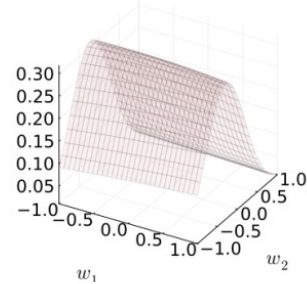
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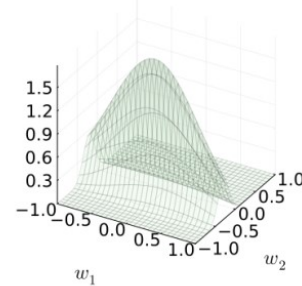
Bayesian Inference in Pictures

$n = 2$

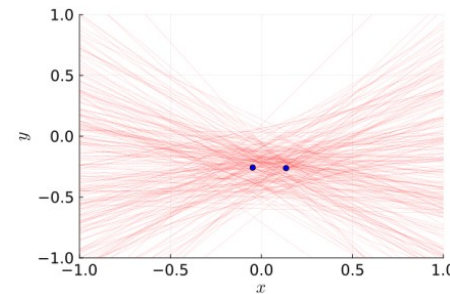
Likelihood



Posterior



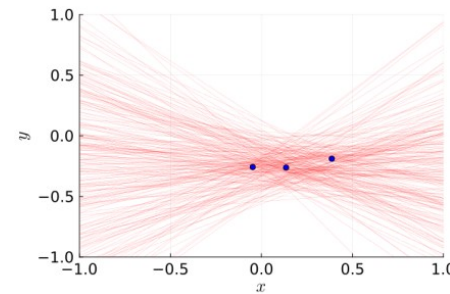
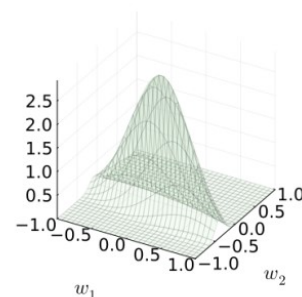
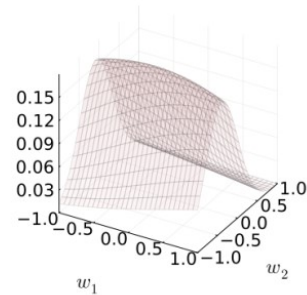
Input Space



$$f(x; \mathbf{w}) = w_1 x + w_2$$

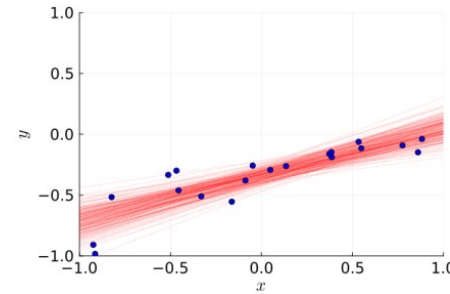
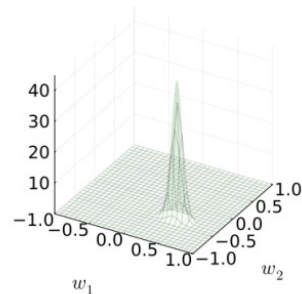
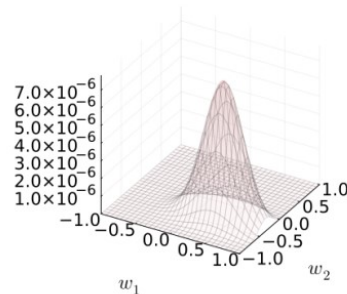
$$p(y|x; \mathbf{w}) = \mathcal{N}(y; f(x), 0.2^2)$$

$n = 3$



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

$m=20$



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Multivariate Normal Distribution

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

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

where Σ must be a positive definite $M \times M$ matrix and $\mu \in \mathbb{R}^M$.

- **Properties:**

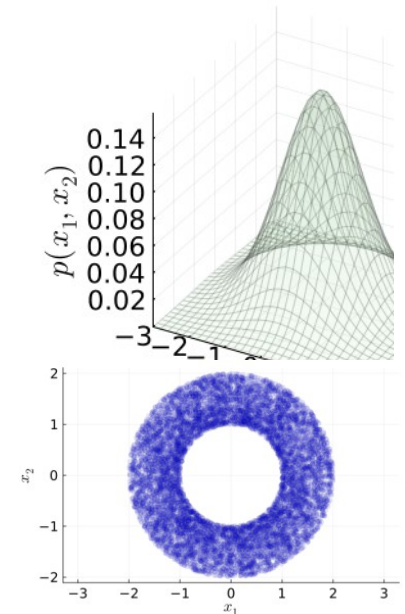
$$E[X] = \mu$$

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

- **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

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

- 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

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

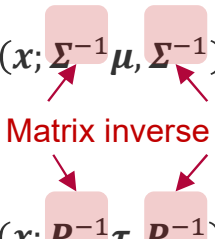
□ Natural Parameters

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

■ Conversions

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{G}(\mathbf{x}; \boxed{\boldsymbol{\Sigma}^{-1}} \boldsymbol{\mu}, \boxed{\boldsymbol{\Sigma}^{-1}})$$

Matrix inverse

$$\mathcal{G}(\mathbf{x}; \boldsymbol{\tau}, \mathbf{P}) = \mathcal{N}(\mathbf{x}; \boxed{\mathbf{P}^{-1}} \boldsymbol{\tau}, \boxed{\mathbf{P}^{-1}})$$


Multivariate Normal Distributions: Products & Divisions

- **Theorem (Multiplication).** Given two multi-dimensional Gaussian distributions $\mathcal{G}(x; \tau_1, P_1)$ and $\mathcal{G}(x; \tau_2, P_2)$ we have

$$\mathcal{G}(x; \tau_1, P_1) \cdot \mathcal{G}(x; \tau_2, P_2) = \mathcal{G}(x; \tau_1 + \tau_2, P_1 + P_2) \cdot \mathcal{N}(\mu_1; \mu_2, \Sigma_1 + \Sigma_2)$$

Additive updates!

Gaussian density

- **Theorem (Division).** Given two multi-dimensional Gaussian distributions $\mathcal{G}(x; \tau_1, P_1)$ and $\mathcal{G}(x; \tau_2, P_2)$ where $P_1 - P_2$ is positive definite we have

$$\frac{\mathcal{G}(x; \tau_1, P_1)}{\mathcal{G}(x; \tau_2, P_2)} = \frac{\mathcal{G}(x; \tau_1 - \tau_2, P_1 - P_2)}{\mathcal{N}(\mu_1; \mu_2, \Sigma_2 - \Sigma_1)} \cdot \frac{|\Sigma_2|}{|\Sigma_2 - \Sigma_1|}$$

Subtractive updates!

Correction factor

Gaussian density

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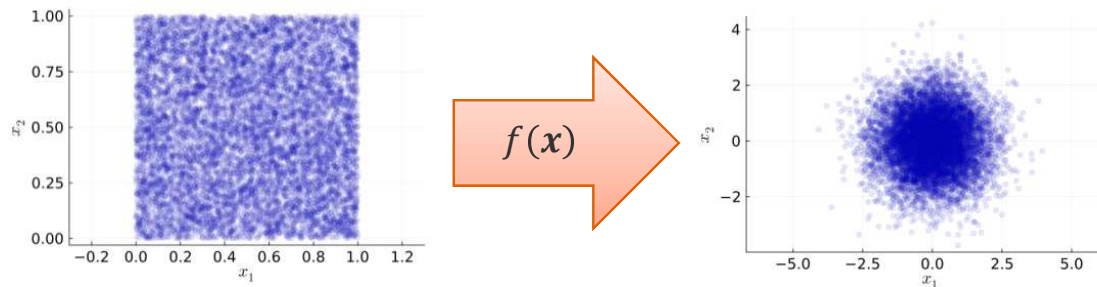
- Natural extension of the one-dimensional multiplication and division rules!

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 $f(\mathbf{X}) \sim N(\cdot; \mathbf{0}, \mathbf{I})$ 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 $\mathbf{X} \sim \mathcal{N}(\cdot; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ then for $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$
$$\mathbf{Y} \sim \mathcal{N}(\cdot; \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$
 - For sampling a multivariate distribution, we require either the SVD or Cholesky decomposition of the covariance matrix, $\boldsymbol{\Sigma} = \mathbf{L}\mathbf{L}^T$
 - Can be easily proven from the properties of expectation and covariance



George Box
(1919 – 2013)



Mervin Mueller
(1928 – 2018)

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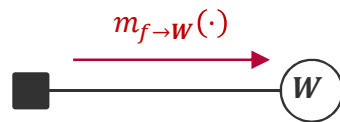
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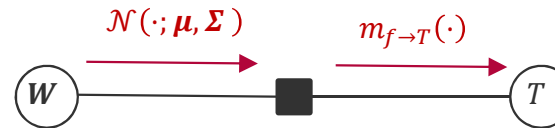
Multivariate Message Update Equations

Gaussian Factor $\mathcal{N}(W; \mu, \Sigma)$

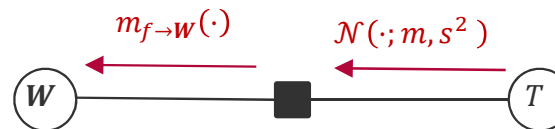


$$m_{f \rightarrow W}(w) = \mathcal{N}(w; \mu, \Sigma)$$

Gaussian Projection Factor $\delta(T - W^T x)$

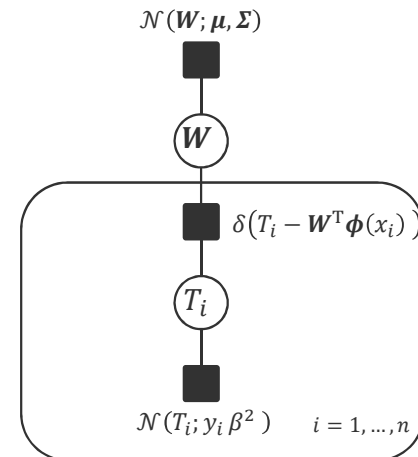


$$m_{f \rightarrow T}(t) = \int \delta(t - w^T x) \cdot \mathcal{N}(w; \mu, \Sigma) dw = \mathcal{N}(t; \mu^T x, x^T \Sigma x)$$



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

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

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

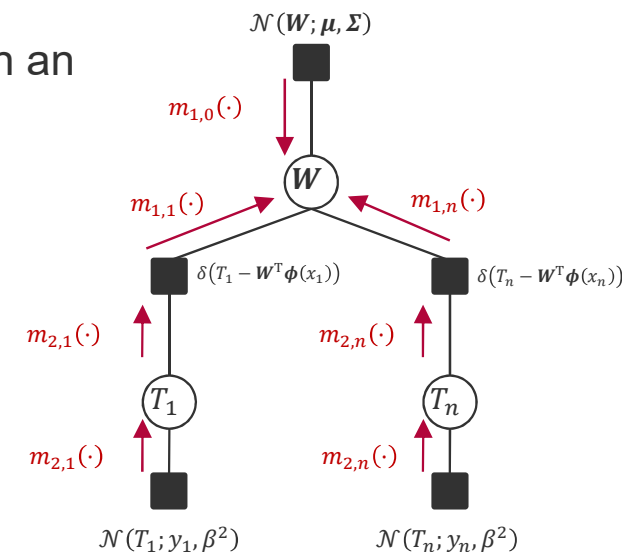
- **Feature Matrix:** All feature vectors are stacked on top of each other in a *feature matrix*

feature vector

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

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

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



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Bayesian Linear Regression: Training & Prediction

- **Posterior:** In terms of the feature matrix, it can be written as

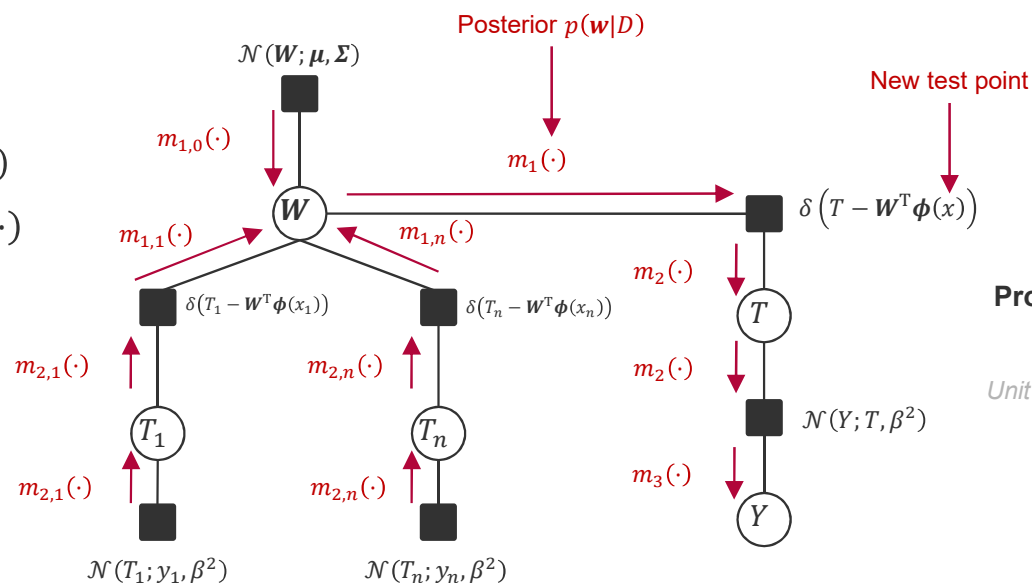
$$p(\mathbf{w}|D) = \mathcal{G}(\mathbf{w}; \Sigma^{-1}\boldsymbol{\mu} + \beta^{-2}\boldsymbol{\Phi}^T\mathbf{y}, \Sigma^{-1} + \beta^{-2}\boldsymbol{\Phi}^T\boldsymbol{\Phi})$$

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

$\mathbf{S}(\Sigma^{-1}\boldsymbol{\mu} + \beta^{-2}\boldsymbol{\Phi}^T\mathbf{y}) \quad (\Sigma^{-1} + \beta^{-2}\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}$

- **Data model for prediction:**

- Prediction at new test point x is $m_3(y)$
- Posterior $p(\mathbf{w}|D)$ is the message $m_1(\cdot)$ to the Gaussian projection factor at the test point x
- To avoid recomputing this message for every test point x we simply store the message $m_1(\mathbf{w}) = p(\mathbf{w}|D)$ as the “model”



Predictions

- **Prediction Tree:** Simple factor chain given posterior $p(\mathbf{w}|D) = \mathcal{N}(\mathbf{w}; \mathbf{m}, \mathbf{S})$

- Posterior Message $m_1(\mathbf{w}) = \mathcal{N}(\mathbf{w}; \mathbf{m}, \mathbf{S}) = p(\mathbf{w}|D)$
- Projection Message $m_2(t) = \mathcal{N}(t; \mathbf{m}^T \boldsymbol{\phi}(x), \boldsymbol{\phi}^T(x) \cdot \mathbf{S} \cdot \boldsymbol{\phi}(x)) = p(t|x, D)$
- Prediction Message $m_3(y) = \mathcal{N}(y; \mathbf{m}^T \boldsymbol{\phi}(x), \beta^2 + \boldsymbol{\phi}^T(x) \cdot \mathbf{S} \cdot \boldsymbol{\phi}(x)) = p(y|x, D)$

- **Bayesian Linear Regression in Matrix Notation**

Training

$$\mathbf{S} = (\boldsymbol{\Sigma}^{-1} + \beta^{-2} \boldsymbol{\Phi}^T \boldsymbol{\Phi})^{-1}$$

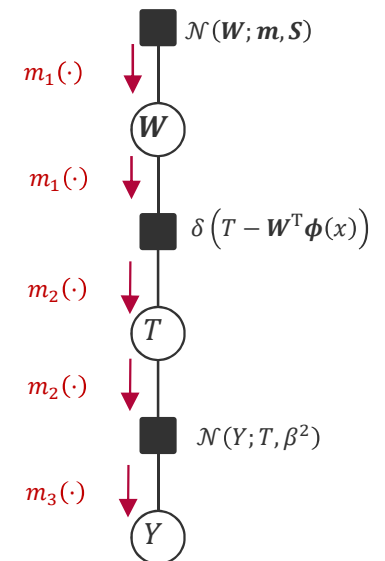
$$\mathbf{m} = \mathbf{S} \cdot (\boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} + \beta^{-2} \boldsymbol{\Phi}^T \mathbf{y})$$

Prediction

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

data uncertainty

model uncertainty



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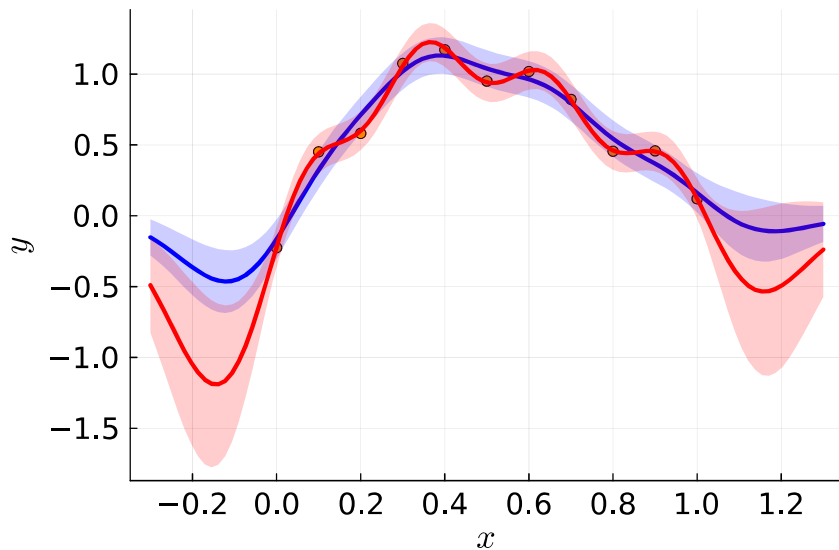
Bayesian Linear Regression: Example

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

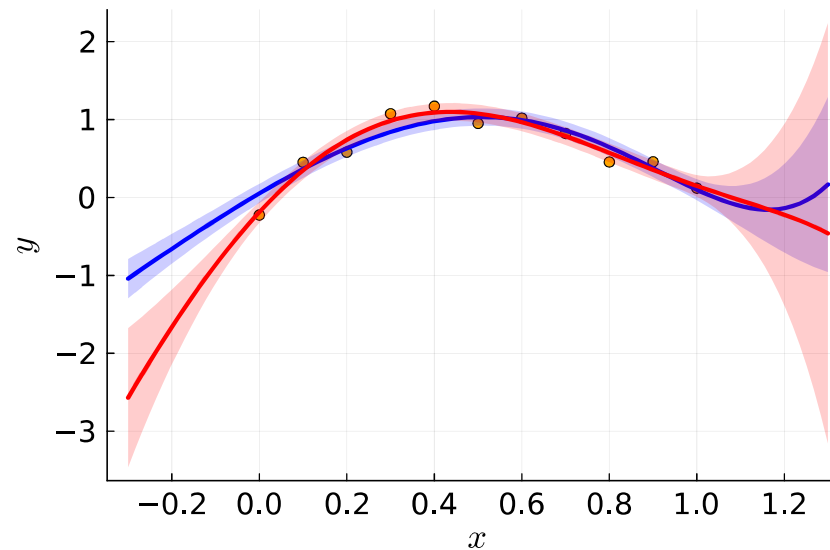
$$\lambda = 10$$

$$\lambda = 1$$

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



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



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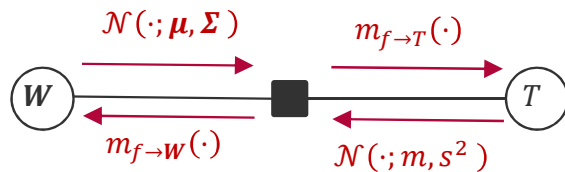
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Gaussian Projection Factor Revisited

Identical factors
but different
assumptions
on $p(W)$

Gaussian Projection Factor $\delta(T - W^T x)$

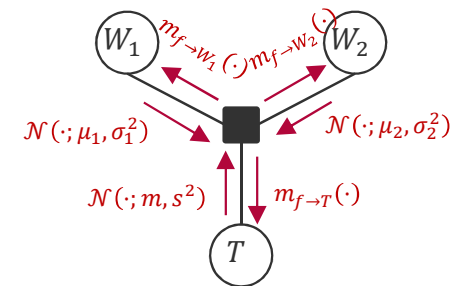


$$m_{f \rightarrow T}(t) = \int \delta(t - w^T x) \cdot \mathcal{N}(w; \mu, \Sigma) dw = \mathcal{N}(t; \mu^T x, x^T \Sigma x)$$

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

Inverting the sum of these matrices is $\mathcal{O}(M^3)$

Weighted Sum Factor $\delta(T - W^T x)$



$$m_{f \rightarrow T}(t) = \mathcal{N}(t; x_1 \mu_1 + x_2 \mu_2, x_1^2 \sigma_1^2 + x_2^2 \sigma_2^2)$$

$$m_{f \rightarrow W_2}(w_2) = \mathcal{N}\left(w_2; \frac{m - x_1 \mu_1}{x_2}, \frac{s^2 + x_1^2 \sigma_1^2}{x_2^2}\right)$$

$$m_{f \rightarrow W_1}(w_1) = \mathcal{N}\left(w_1; \frac{m - x_2 \mu_2}{x_1}, \frac{s^2 + x_2^2 \sigma_2^2}{x_1^2}\right)$$

Computing the 1D-messages is $\mathcal{O}(M)$!

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 $\phi_i(x)$

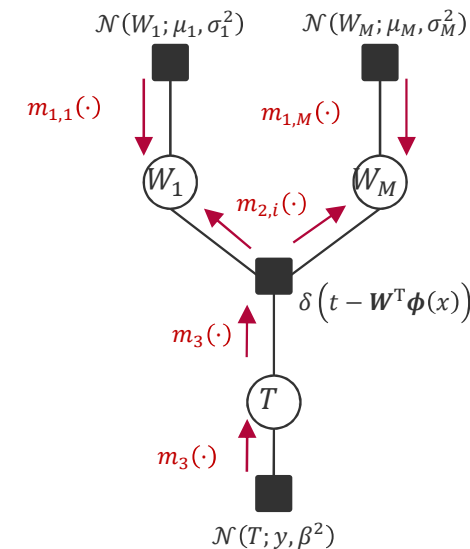
$$\sigma_i^2 \leftarrow \sigma_i^2 \cdot \left[1 - \frac{\phi_i^2(x) \sigma_i^2}{\beta^2 + \sum_{j=1}^M \phi_j^2(x) \sigma_j^2} \right]$$

multiplicative update

largest for parameter with largest uncertainty so far

- In practice, each training example is only processed once.

- Complexity reduces from $\mathcal{O}(n \cdot M^2 + M^3)$ to $\mathcal{O}(n \cdot M)$

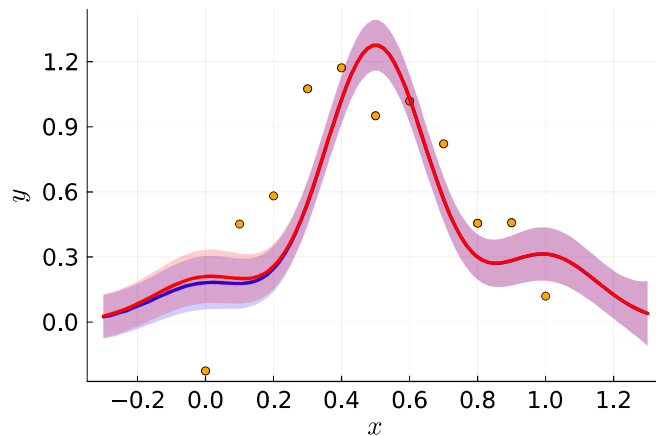


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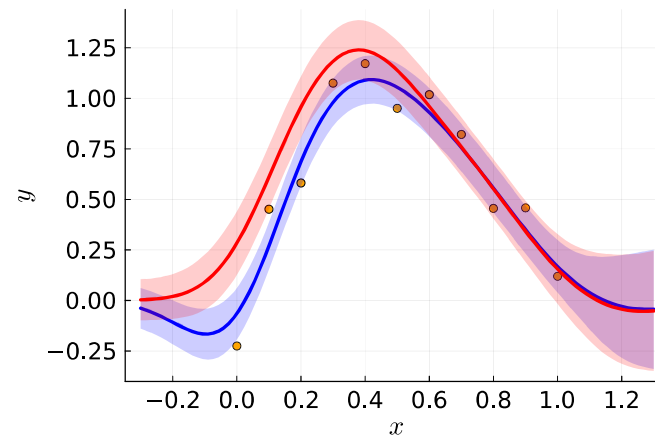
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Speeding up Bayesian Linear Regression

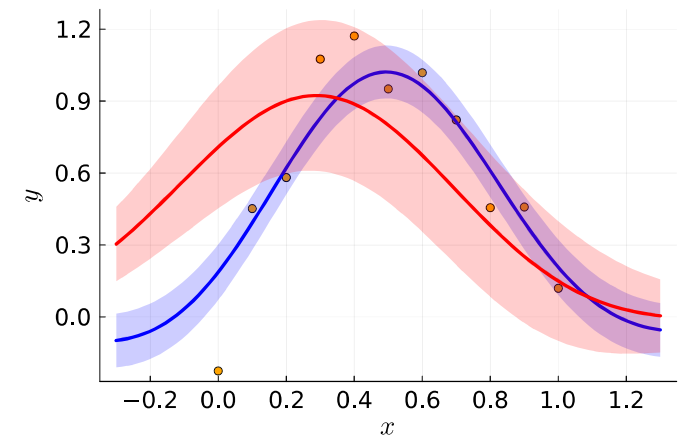
Nearly orthogonal features



Weakly correlated features



Strongly correlated features



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Summary

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)
- 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 in closed form
- Variance of Bayesian regression 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!