Introduction to Probabilistic Machine Learning

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Bayesian Classification

Overview

1. Bayesian Classification Learning
2. Bayesian Classification Learning via Approximate Message Passing
3. Appendix: Bayesian Classification via Optimization
   - Laplace Approximation
   - Bayesian Linear Logit Regression

Overview

1. **Bayesian Classification Learning**
2. Bayesian Classification Learning via Approximate Message Passing
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Bayesian Classification Learning Setting

- **Given**:
  1. **Training Data**: $D \in (\mathcal{X} \times \{-1, +1\})^n$ of n (labelled) examples from input space $\mathcal{X}$
  2. **Linear Basis Functions**: Basis function mapping $\boldsymbol{\phi}: \mathcal{X} \to \mathbb{R}^M$ and linear function model

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

weight vector — feature vector

  3. **Likelihood of functions**:

$$p(D|f) = p(D|\boldsymbol{w}) = \prod_{i=1}^{n} \int_0^{+\infty} \mathcal{N}\left(t_i; y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(x_i), \beta^2\right) dt_i$$

$$\mathrm{Ber}\left(1; g\left(y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(x_i)\right)\right)$$

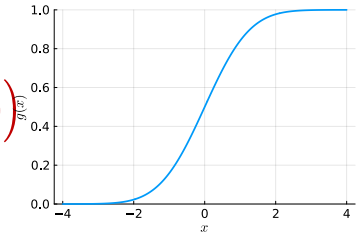
  4. **Prior belief over functions**:

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

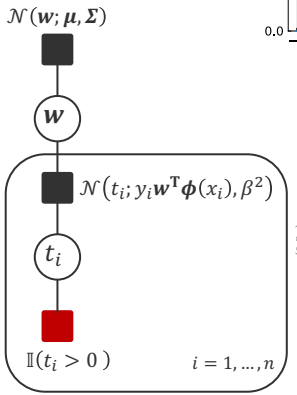
- **Bayesian Inference**:
  - **Posterior belief over functions**:

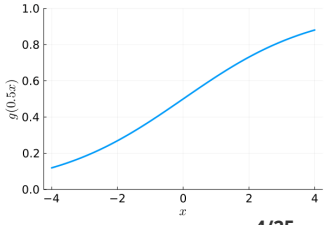
$$p(f|D) = p(\boldsymbol{w}|D) = \frac{\prod_{i=1}^{n} \mathrm{Ber}\left(1; g\left(y_i \boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(x_i)\right)\right) \cdot \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})}{\int_{\mathbb{R}^M} \prod_{i=1}^{n} \mathrm{Ber}\left(1; g\left(y_i \tilde{\boldsymbol{w}}^{\mathrm{T}}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

$$g(t) = \int_0^{\infty} \mathcal{N}(z; t, 1)\, dz$$



$$\lim_{s \to \infty} g(s \cdot t) = \mathbb{I}(t > 0)$$





Bayesian Classification Learning in Pictures

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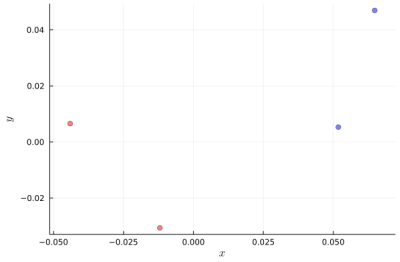
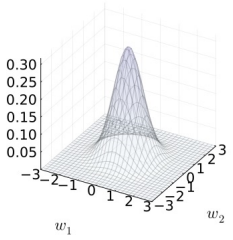
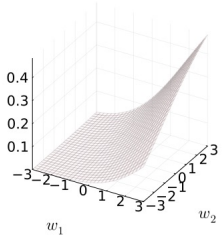
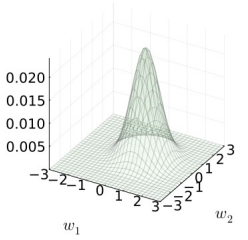
Digital Engineering · Universität Potsdam

$n = 4$

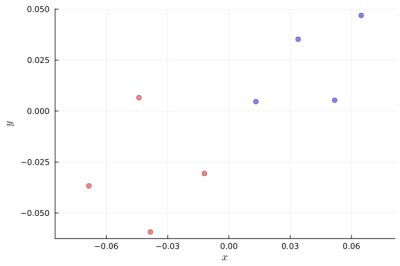


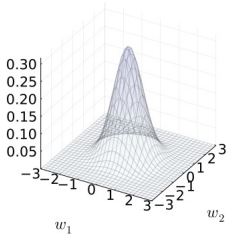


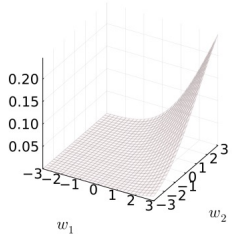


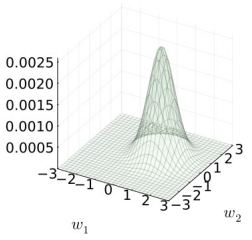


$n = 6$

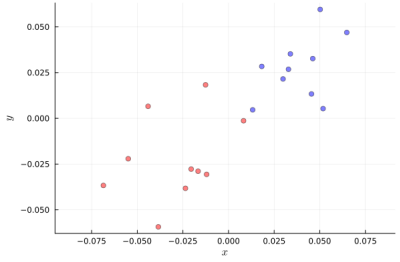


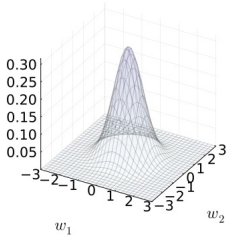


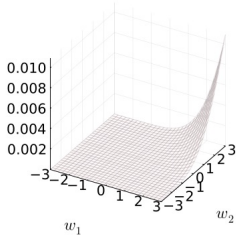


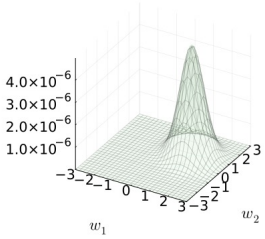


$n = 20$









Overview

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3. Appendix: Bayesian Classification via Optimization
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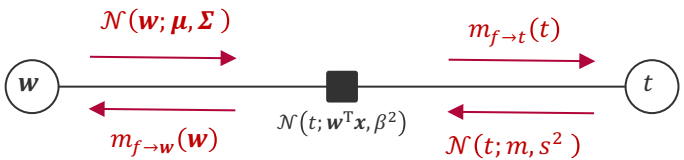
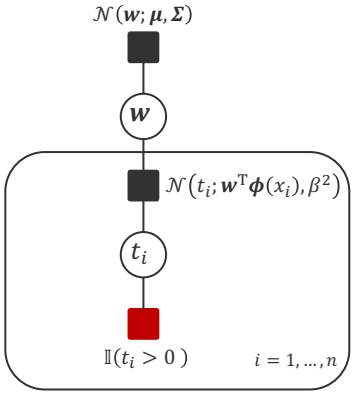
Update Equations for Combined Factors

Gaussian Projection-Noise Factor



$$m_{f\to t}(t) = \mathcal{N}\left(t;\boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{x},\boldsymbol{x}^{\mathrm{T}}\boldsymbol{\Sigma}\boldsymbol{x}+\beta^2\right)$$

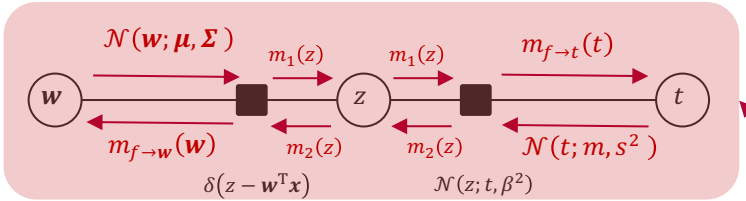
$$m_{f\to \boldsymbol{w}}(\boldsymbol{w}) = \mathcal{G}\left(\boldsymbol{w};\frac{m}{s^2+\beta^2}\boldsymbol{x},\frac{1}{s^2+\beta^2}\boldsymbol{x}\boldsymbol{x}^{\mathrm{T}}\right)$$



$$m_{f\to t}(t) = \int \mathcal{N}\left(t;\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x},\beta^2\right)\cdot\mathcal{N}(\boldsymbol{w};\boldsymbol{\mu},\boldsymbol{\Sigma})\,d\boldsymbol{w} = \int\left[\int \delta\left(z-\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}\right)\cdot\mathcal{N}(\boldsymbol{w};\boldsymbol{\mu},\boldsymbol{\Sigma})\,d\boldsymbol{w}\right]\cdot\mathcal{N}(t;z,\beta^2)\,dz$$

$$m_{f\to \boldsymbol{w}}(\boldsymbol{w}) = \int \mathcal{N}\left(t;\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x},\beta^2\right)\cdot\mathcal{N}(t;m,s^2)\,dt = \int\left[\int \mathcal{N}(t;z,\beta^2)\cdot\mathcal{N}(t;m,s^2)\,dt\right]\cdot\delta\left(z-\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}\right)\,dz$$

$$m_1(z) = \mathcal{N}\left(z;\boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{x},\boldsymbol{x}^{\mathrm{T}}\boldsymbol{\Sigma}\boldsymbol{x}\right)$$
$$m_2(z) = \mathcal{N}\left(z;m,s^2+\beta^2\right)$$



Helper factor tree to derive closed form message equations

Bayesian Linear Classification by Message Passing

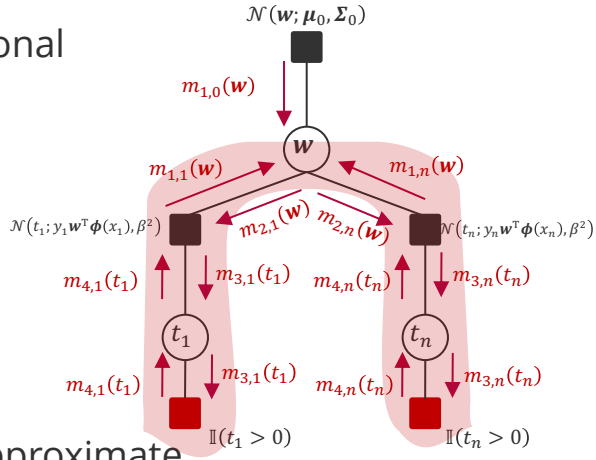
- **Factor Tree**: Each training example is summarized in an M-dimensional message
  - Prior Message $m_{1,0}(\boldsymbol{w}) = \mathcal{G}(\boldsymbol{w}; \boldsymbol{\Sigma}_0^{-1}\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0^{-1}) = p(\boldsymbol{w})$
  - Data Message $m_{1,i}(\boldsymbol{w}) = \mathcal{G}\left(\boldsymbol{w}; a_i y_i \boldsymbol{\phi}(x_i), b_i y_i^2 \boldsymbol{\phi}(x_i)\boldsymbol{\phi}^{\mathrm{T}}(x_i)\right) = p(y_i|\boldsymbol{w})$

$y_i^2 = 1$

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

$$p(\boldsymbol{w}|D) = \mathcal{G}\left(\boldsymbol{w}; \boldsymbol{\Sigma}_0^{-1}\boldsymbol{\mu}_0 + \sum_{i=1}^{n} a_i y_i \boldsymbol{\phi}(x_i), \boldsymbol{\Sigma}_0^{-1} + \sum_{i=1}^{n} b_i \boldsymbol{\phi}(x_i)\boldsymbol{\phi}^{\mathrm{T}}(x_i)\right)$$

- **Iterative Approximations**: Since each data message involves an approximate factor, we need to iterate message passing until convergence!
  - We maintain the (approximate) posterior $p(\boldsymbol{w}|D) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ and the (a_i, b_i)
  1. Compute $m_{2,i}(\boldsymbol{w})$ in scale-location parameters (using Sherman-Morrison formula)
  2. Compute $m_{3,i}(t_i)$ in scale-location parameters by Gaussian projection-noise factor
  3. Compute $m_{4,i}(t_i)$ in natural parameters by matching moments
  4. Update $p(\boldsymbol{w}|D) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ in scale-location parameters (using Sherman-Morrison)



Bayesian Linear Classification: Update of i^{th} Data Message

- **Sherman-Morrison Formula**: For any invertible matrix $\boldsymbol{A}$ it holds that

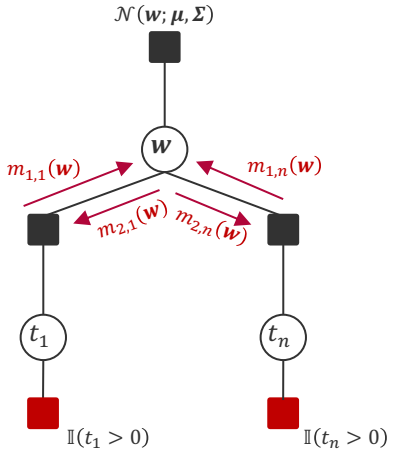
$$\left(\boldsymbol{A} + \boldsymbol{u}\boldsymbol{v}^{\mathrm{T}}\right)^{-1} = \boldsymbol{A}^{-1} - \frac{\boldsymbol{A}^{-1}\boldsymbol{u}\boldsymbol{v}^{\mathrm{T}}\boldsymbol{A}^{-1}}{1 + \boldsymbol{v}^{\mathrm{T}}\boldsymbol{A}^{-1}\boldsymbol{u}}$$

- **Rank-1 Updates** of $\boldsymbol{\Sigma}$ and $\boldsymbol{\mu}$ with addition of $\Delta_i^a \cdot y_i\boldsymbol{\phi}_i$ and $\Delta_i^b \cdot \boldsymbol{\phi}_i\boldsymbol{\phi}_i^{\mathrm{T}}$

$$\boldsymbol{\Sigma}_{\text{new}} = \left(\boldsymbol{\Sigma}^{-1} + \Delta_i^b\boldsymbol{\phi}_i\boldsymbol{\phi}_i^{\mathrm{T}}\right)^{-1} = \boldsymbol{\Sigma} - \frac{\Delta_i^b}{1 + \Delta_i^b \cdot \boldsymbol{\phi}_i^{\mathrm{T}}\boldsymbol{\Sigma}\boldsymbol{\phi}_i} \cdot (\boldsymbol{\Sigma}\boldsymbol{\phi}_i)(\boldsymbol{\Sigma}\boldsymbol{\phi}_i)^{\mathrm{T}}$$

No inverse needed but just matrix multiplications!

$$\boldsymbol{\mu}_{\text{new}} = \left(\boldsymbol{\Sigma}^{-1} + \Delta_i^b\boldsymbol{\phi}_i\boldsymbol{\phi}_i^{\mathrm{T}}\right)^{-1}\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \Delta_i^a y_i\boldsymbol{\phi}_i\right) = \boldsymbol{\mu} + \boldsymbol{\Sigma}\boldsymbol{\phi}_i\left(\frac{\Delta_i^a \cdot y_i - \Delta_i^b \cdot \boldsymbol{\phi}_i^{\mathrm{T}}\boldsymbol{\mu}}{1 + \Delta_i^b \cdot \boldsymbol{\phi}_i^{\mathrm{T}}\boldsymbol{\Sigma}\boldsymbol{\phi}_i}\right)$$



- **Step 1**: Compute mean and covariance of $m_{2,i}(\boldsymbol{w})$ using $\Delta_i^a = -a_i$ and $\Delta_i^b = -b_i$
- **Step 4**: Update $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ of $p(\boldsymbol{w}|D)$ using $\Delta_i^a = a_i^{\text{new}} - a_i$ and $\Delta_i^b = b_i^{\text{new}} - b_i$

Bayesian Linear Classification: Update of i^{th} Data Message

- **Step 2**: $m_{3,i}(t_i) = \mathcal{N}\left(t_i; m_i, s_i^2\right)$ follows from the Gaussian projection-noise factor

$$m_i = \frac{y_i \boldsymbol{\phi}_i^{\mathrm{T}} \boldsymbol{\mu} - a_i \boldsymbol{\phi}_i^{\mathrm{T}} \boldsymbol{\Sigma} \boldsymbol{\phi}_i}{1 - b_i \boldsymbol{\phi}_i^{\mathrm{T}} \boldsymbol{\Sigma} \boldsymbol{\phi}_i} \qquad s_i^2 = \frac{\boldsymbol{\phi}_i^{\mathrm{T}} \boldsymbol{\Sigma} \boldsymbol{\phi}_i}{1 - b_i \cdot \boldsymbol{\phi}_i^{\mathrm{T}} \boldsymbol{\Sigma} \boldsymbol{\phi}_i} + \beta^2$$

- **Step 3**: $m_{4,i}(t_i) = \mathcal{G}(t_i; \tau_i, \rho_i)$ follows from the greater-than factor

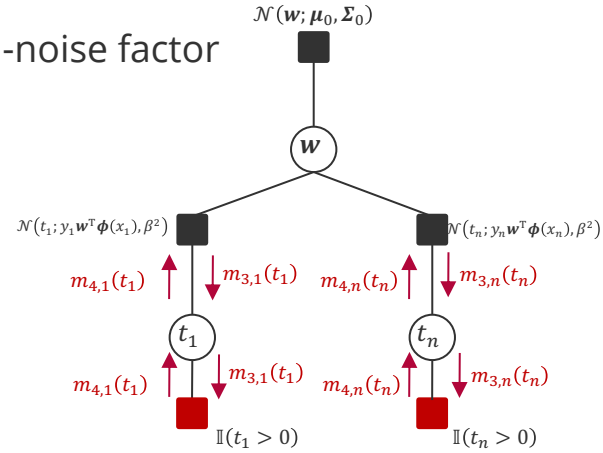
Mean correction of truncated Gaussian

$$\tau_i = \frac{s_i \cdot v\left(\frac{m_i}{s_i}\right) + m_i \cdot w\left(\frac{m_i}{s_i}\right)}{s_i^2 \cdot \left(1 - w\left(\frac{m_i}{s_i}\right)\right)} \qquad \rho_i = \frac{w\left(\frac{m_i}{s_i}\right)}{s_i^2 \cdot \left(1 - w\left(\frac{m_i}{s_i}\right)\right)}$$

Variance correction of truncated Gaussian

- **Final Update**

$$a_i^{\text{new}} = \frac{\tau_i}{1 + \rho_i \cdot \beta^2} \qquad b_i^{\text{new}} = \frac{\rho_i}{1 + \rho_i \cdot \beta^2}$$



Introduction to Probabilistic Machine Learning

Unit 9 – Bayesian Classification

Bayesian Linear Classification: Putting It all Together

Given: n training examples (x_i, y_i) where $y_i \in \{-1, +1\}$ and feature map $\boldsymbol{\phi}: \mathcal{X} \to \mathbb{R}^M$

1. **Initialize** $\boldsymbol{\phi}_i := \boldsymbol{\phi}(x_i)$, $\boldsymbol{\Sigma} = \tau^2 \boldsymbol{I}$, $\boldsymbol{\mu} = \boldsymbol{0}$ and $a_i = b_i = 0$
2. **Repeat until** maximum change componentwisein $\boldsymbol{a}$ and $\boldsymbol{b}$ is small (e.g., $\leq 10^{-6}$)
   For all $i = 1, \ldots, n$
   - Compute $\boldsymbol{z} = \boldsymbol{\Sigma}\boldsymbol{\phi}_i$, $e = \boldsymbol{\phi}_i^{\mathrm{T}}\boldsymbol{z}$, $f = \boldsymbol{\phi}_i^{\mathrm{T}}\boldsymbol{\mu}$, $c = 1 - b_i \cdot e$
   - Compute $m = \frac{y_i \cdot f - a_i \cdot e}{c}$ and $s^2 = \frac{e}{c} + \beta^2$
   - Compute $\tau = \frac{s \cdot V + m \cdot W}{s^2 \cdot (1 - W)}$ and $\rho = \frac{W}{s^2 \cdot (1 - W)}$ for $V = v\left(\frac{m}{s}\right)$ and $W = w\left(\frac{m}{s}\right)$
   - Compute $a_i^{\text{new}} = \frac{\tau}{1 + \rho \cdot \beta^2}$ and $b_i^{\text{new}} = \frac{\rho}{1 + \rho \cdot \beta^2}$
   - Compute $d = 1 + (b_i^{\text{new}} - b_i) \cdot e$
   - Update $\boldsymbol{\Sigma} \leftarrow \boldsymbol{\Sigma} - \frac{b_i^{\text{new}} - b_i}{d} \cdot \boldsymbol{z}\boldsymbol{z}^{\mathrm{T}}$ and $\boldsymbol{\mu} \leftarrow \boldsymbol{\mu} + \frac{y_i \cdot (a_i^{\text{new}} - a_i) - f \cdot (b_i^{\text{new}} - b_i)}{d} \cdot \boldsymbol{z}$
   - Update $a_i \leftarrow a_i^{\text{new}}$ and $a_i \leftarrow a_i^{\text{new}}$

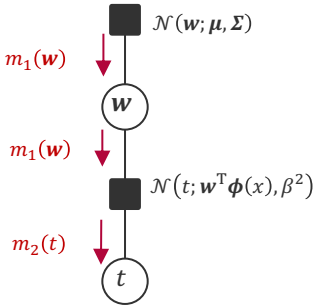
   End For

Majority of algorithm is additions, multiplication, and division of scalars!

Algorithm requires **no** matrix inverses – just matrix products!

Predictions

- **Predicition Tree**: Simple factor chain given posterior $p(\boldsymbol{w}|x, D) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$
  - Posterior Message $m_1(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = p(\boldsymbol{w}|x, D)$
  - Projection-Noise Message $m_2(t) = \mathcal{N}\left(t; \boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{\phi}(x), \boldsymbol{\phi}^{\mathrm{T}}(x)\boldsymbol{\Sigma}\boldsymbol{\phi}(x) + \beta^2\right) = p(t|x, D)$
  - Outcome Probability $\int_0^\infty m_2(t)\, dt = p(y = +1|x, D)$

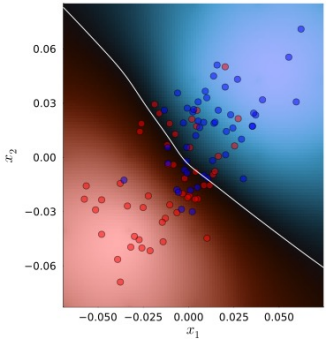
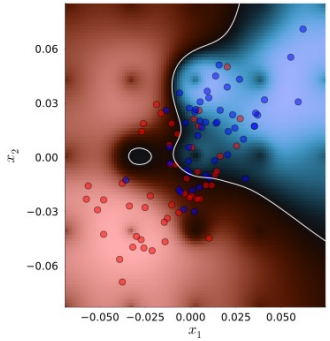
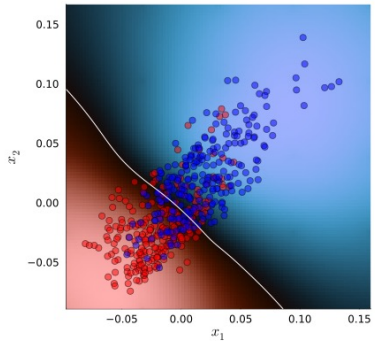
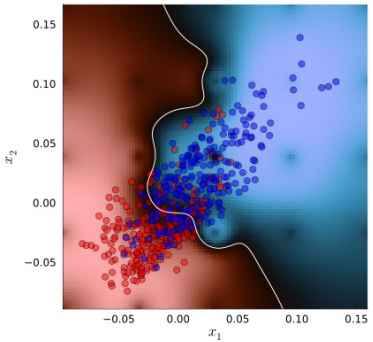


- **Bayesian Linear Probit Regression in Matrix Notation**

$$p(y = +1|x, D) = \int_0^{+\infty} \mathcal{N}\left(y; \boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{\phi}(x), \beta^2 + \boldsymbol{\phi}^{\mathrm{T}}(x)\boldsymbol{\Sigma}\boldsymbol{\phi}(x)\right) dt$$

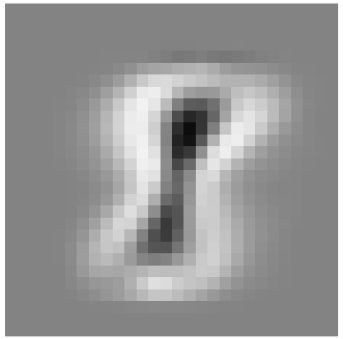
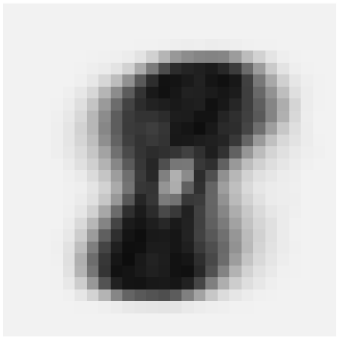
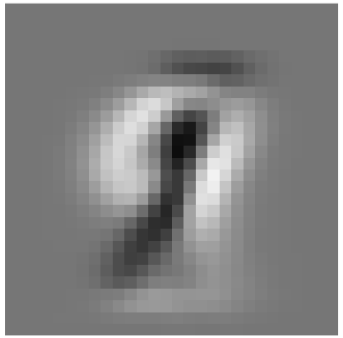
data uncertainty — model uncertainty

Bayesian Linear Classification in Pictures

	$\tau = 1$	$\tau = 10$
$n = 100$		
$n = 500$		

225 features of value of 225 Gaussian density in 2D on a 5×5 grid at 9 resolutions

Bayesian Linear Classification for MNIST

	μ	$\mathrm{diag}(\Sigma)$
"1" vs. "8"		
"1" vs. "9"		

Summary

1. **Bayesian Classification**
   - The likelihood model is no longer conjugate to the prior over the weight vector
   - Approximate inference methods can be used (similar to Bayesian ranking) as the approximation is on a 1D-projection of each feature vector at each training example
   - The message passing algorithm is highly efficient and requires no matrix inversion!
2. **Laplace Approximation**
   - Matches the mode of the true likelihood/posterior to that of a Gaussian
   - Usually easy to compute when we have a posterior that can be differentiated
   - Allows to derive Bayesian linear classification for the logistic likelihood function (though this requires matrix inversion)

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See you next week!