Bayesian Logistic Regression. Laplace Approximation

Evgeny Burnaev

Skoltech, Moscow, Russia

Skoltech
Skolkovo Institute of Science and Technology

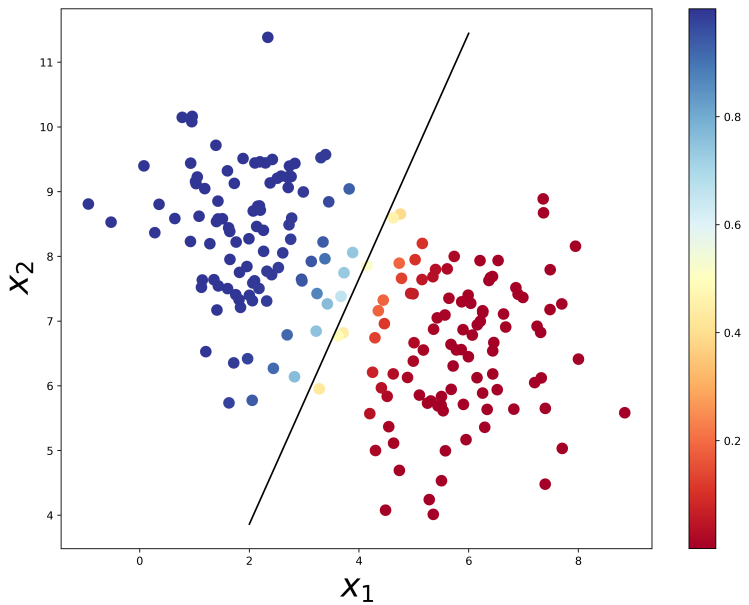
Outline

Logistic Regression

- We consider a two-class classification problem with classes $\mathcal{C}_0$ and $\mathcal{C}_1$.
- A logistic model definies i.i.d. probability to obtain a particular class given vector of inputs $\mathbf{x}$:

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \; p(\mathcal{C}_0|\boldsymbol{\phi}) = 1 - p(\mathcal{C}_1|\boldsymbol{\phi}).$$

  Here $\boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$ is a vector of basis functions
- A data set $\mathcal{D}_m = \{(\boldsymbol{\phi}_i, y_i)\}_{i=1}^m$, where $y_i \in \{0, 1\}$ and $\boldsymbol{\phi}_i = \phi(\mathbf{x}_i)$



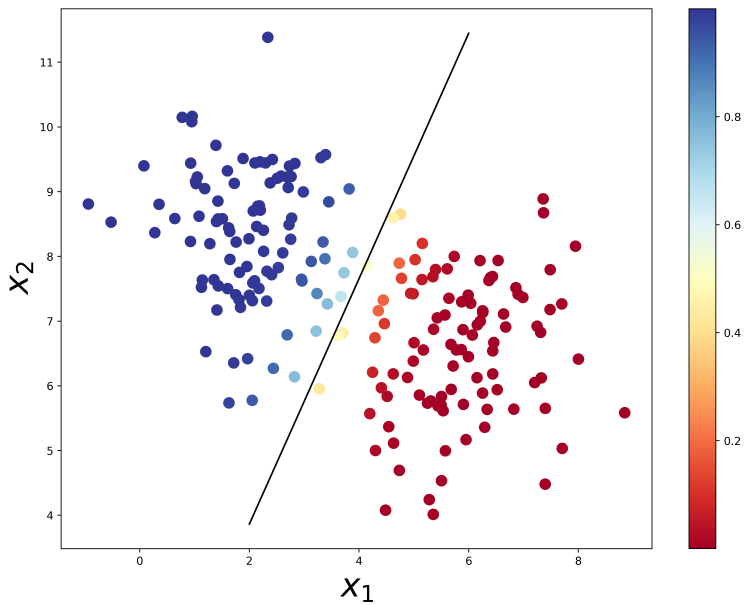
Logistic Regression

- We consider a two-class classification problem with classes $\mathcal{C}_0$ and $\mathcal{C}_1$.
- A logistic model definies i.i.d. probability to obtain a particular class given vector of inputs $\mathbf{x}$:

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \; p(\mathcal{C}_0|\boldsymbol{\phi}) = 1 - p(\mathcal{C}_1|\boldsymbol{\phi}).$$

  Here $\boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$ is a vector of basis functions

- A data set $\mathcal{D}_m = \{(\boldsymbol{\phi}_i, y_i)\}_{i=1}^m$, where $y_i \in \{0, 1\}$ and $\boldsymbol{\phi}_i = \phi(\mathbf{x}_i)$

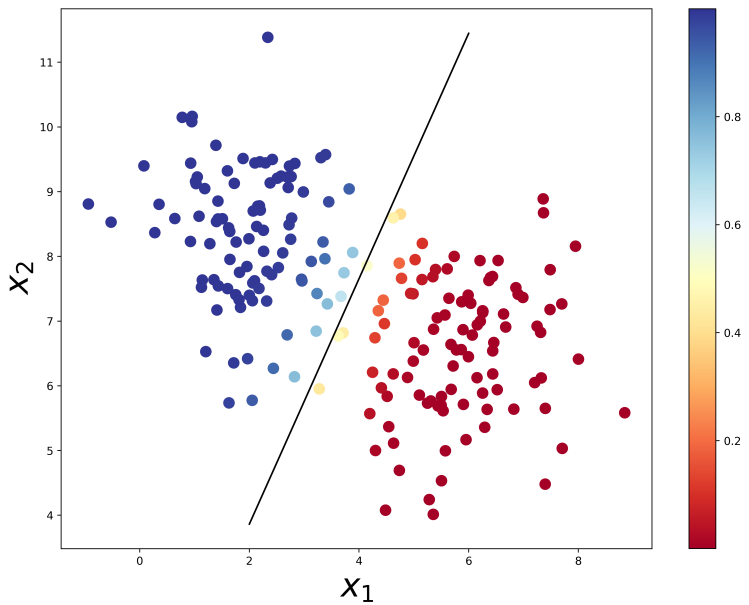


Logistic Regression

- We consider a two-class classification problem with classes $\mathcal{C}_0$ and $\mathcal{C}_1$.
- A logistic model definies i.i.d. probability to obtain a particular class given vector of inputs $\mathbf{x}$:

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \; p(\mathcal{C}_0|\boldsymbol{\phi}) = 1 - p(\mathcal{C}_1|\boldsymbol{\phi}).$$

  Here $\boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$ is a vector of basis functions
- A data set $\mathcal{D}_m = \{(\boldsymbol{\phi}_i, y_i)\}_{i=1}^m$, where $y_i \in \{0, 1\}$ and $\boldsymbol{\phi}_i = \phi(\mathbf{x}_i)$



- We consider a two-class classification problem with classes $\mathcal{C}_0$ and $\mathcal{C}_1$.
- A logistic model definies i.i.d. probability to obtain a particular class given vector of inputs $\mathbf{x}$:

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \; p(\mathcal{C}_0|\boldsymbol{\phi}) = 1 - p(\mathcal{C}_1|\boldsymbol{\phi}).$$

  Here $\boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$ is a vector of basis functions
- A data set $\mathcal{D}_m = \{(\boldsymbol{\phi}_i, y_i)\}_{i=1}^m$, where $y_i \in \{0, 1\}$ and $\boldsymbol{\phi}_i = \phi(\mathbf{x}_i)$
- The likelihood $p(\mathbf{Y}_m|\mathbf{w})$:

- We consider a two-class classification problem with classes $\mathcal{C}_0$ and $\mathcal{C}_1$.
- A logistic model definies i.i.d. probability to obtain a particular class given vector of inputs $\mathbf{x}$:

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \; p(\mathcal{C}_0|\boldsymbol{\phi}) = 1 - p(\mathcal{C}_1|\boldsymbol{\phi}).$$

  Here $\boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$ is a vector of basis functions
- A data set $\mathcal{D}_m = \{(\boldsymbol{\phi}_i, y_i)\}_{i=1}^m$, where $y_i \in \{0, 1\}$ and $\boldsymbol{\phi}_i = \phi(\mathbf{x}_i)$
- The likelihood $p(\mathbf{Y}_m|\mathbf{w})$:

$$p(\mathbf{Y}_m|\mathbf{w}) = \prod_{i=1}^m t_i^{y_i}(1 - t_i)^{1-y_i},$$

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \; t_i = p(\mathcal{C}_1|\boldsymbol{\phi}_i).$$

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- We easily get that

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(t_i - y_i)\boldsymbol{\phi}_i,$$

as

$$\frac{\partial \sigma(a)}{\partial a} = \sigma(a) - \sigma(a)^2.$$

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- We easily get that

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(t_i - y_i)\boldsymbol{\phi}_i,$$

as

$$\frac{\partial \sigma(a)}{\partial a} = \sigma(a) - \sigma(a)^2.$$

Newton-Raphson method

- Newton-Raphson method to minimizes a twice continuously differentiable function $f(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$
- Obtain a quadratic approximation about the current point $\mathbf{x}^{(k)}$

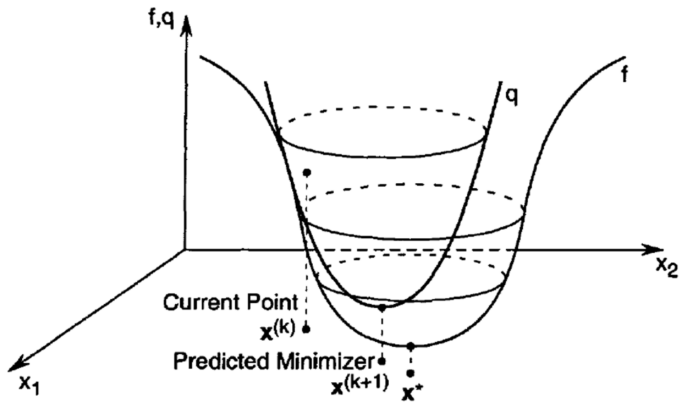
$$f(\mathbf{x}) \approx q(\mathbf{x}) = f(\mathbf{x}^{(k)}) + (\mathbf{x} - \mathbf{x}^{(k)})^\top \mathbf{g}^{(k)} + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(k)})^\top F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}),$$

  where $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$, $F(\mathbf{x}^{(k)}) = \nabla\nabla f(\mathbf{x}^{(k)})$
- Applying first-order necessary condition to q we get

$$\mathbf{0} = \nabla q(\mathbf{x}) = \mathbf{g}^{(k)} + F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)})$$

- If $F(\mathbf{x}^{(k)}) > 0$, then $q(\mathbf{x})$ achieves minimum at

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - F(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}$$



Newton-Raphson method

- Newton-Raphson method to minimizes a twice continuously differentiable function $f(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$
- Obtain a quadratic approximation about the current point $\mathbf{x}^{(k)}$

$$f(\mathbf{x}) \approx q(\mathbf{x}) = f(\mathbf{x}^{(k)}) + (\mathbf{x} - \mathbf{x}^{(k)})^\top \mathbf{g}^{(k)} + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(k)})^\top F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}),$$

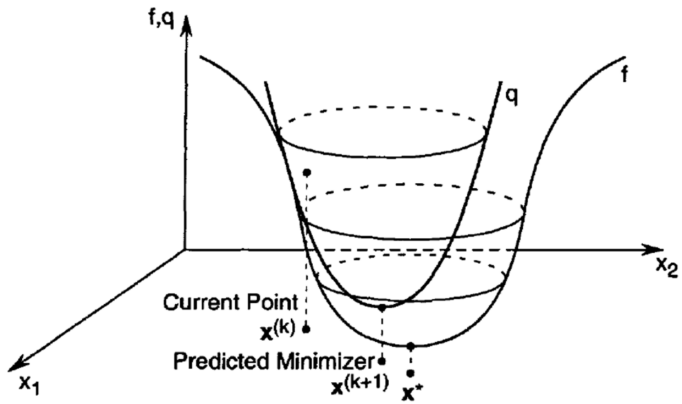
where $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$, $F(\mathbf{x}^{(k)}) = \nabla\nabla f(\mathbf{x}^{(k)})$

- Applying first-order necessary condition to q we get

$$\mathbf{0} = \nabla q(\mathbf{x}) = \mathbf{g}^{(k)} + F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)})$$

- If $F(\mathbf{x}^{(k)}) > 0$, then $q(\mathbf{x})$ achieves minimum at

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - F(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}$$



Newton-Raphson method

- Newton-Raphson method to minimizes a twice continuously differentiable function $f(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$
- Obtain a quadratic approximation about the current point $\mathbf{x}^{(k)}$

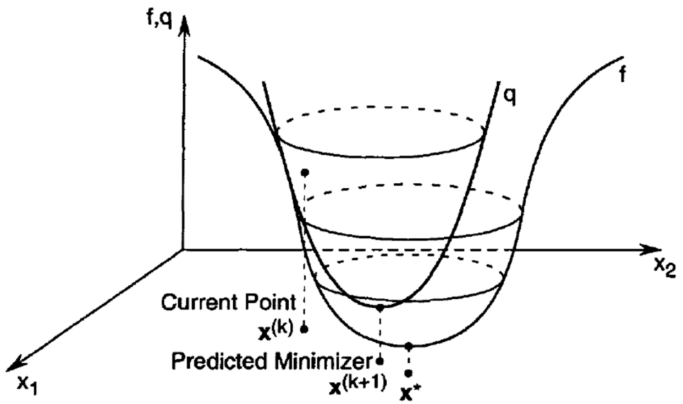
$$f(\mathbf{x}) \approx q(\mathbf{x}) = f(\mathbf{x}^{(k)}) + (\mathbf{x} - \mathbf{x}^{(k)})^\top \mathbf{g}^{(k)} + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(k)})^\top F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}),$$

  where $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$, $F(\mathbf{x}^{(k)}) = \nabla\nabla f(\mathbf{x}^{(k)})$
- Applying first-order necessary condition to q we get

$$\mathbf{0} = \nabla q(\mathbf{x}) = \mathbf{g}^{(k)} + F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)})$$

- If $F(\mathbf{x}^{(k)}) > 0$, then $q(\mathbf{x})$ achieves minimum at

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - F(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}$$



Newton-Raphson method

- Newton-Raphson method to minimizes a twice continuously differentiable function $f(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$
- Obtain a quadratic approximation about the current point $\mathbf{x}^{(k)}$

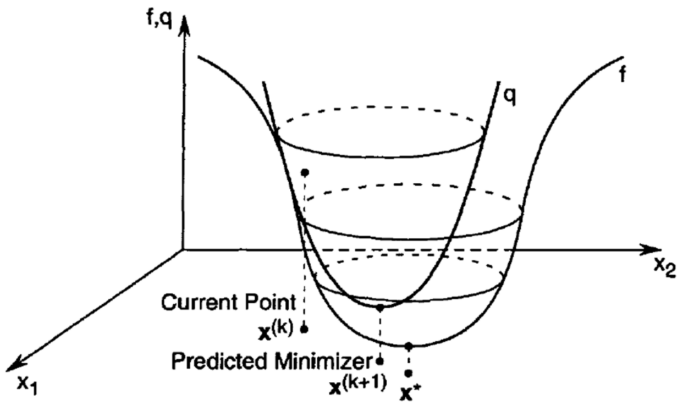
$$f(\mathbf{x}) \approx q(\mathbf{x}) = f(\mathbf{x}^{(k)}) + (\mathbf{x} - \mathbf{x}^{(k)})^\top \mathbf{g}^{(k)} + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(k)})^\top F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}),$$

  where $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$, $F(\mathbf{x}^{(k)}) = \nabla\nabla f(\mathbf{x}^{(k)})$
- Applying first-order necessary condition to q we get

$$\mathbf{0} = \nabla q(\mathbf{x}) = \mathbf{g}^{(k)} + F(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)})$$

- If $F(\mathbf{x}^{(k)}) > 0$, then $q(\mathbf{x})$ achieves minimum at

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - F(\mathbf{x}^{(k)})^{-1}\mathbf{g}^{(k)}$$



Newton-Raphson method

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

- For a Newtown-Raphson method we get

Newton-Raphson method

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

- For a Newtown-Raphson method we get

Newton-Raphson method

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w} \cdot \boldsymbol{\phi}_i^{\top})^2,$$

- For a Newtown-Raphson method we get

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\cdot\boldsymbol{\phi}_i^\top)^2,$$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(\mathbf{w}\cdot\boldsymbol{\phi}_i^\top - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w} - \boldsymbol{\Phi}^\top\mathbf{Y}_m,$$

- For a Newtown-Raphson method we get

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\cdot\boldsymbol{\phi}_i^\top)^2,$$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(\mathbf{w}\cdot\boldsymbol{\phi}_i^\top - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w} - \boldsymbol{\Phi}^\top\mathbf{Y}_m,$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m}\boldsymbol{\phi}_i^\top\cdot\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}.$$

- For a Newtown-Raphson method we get

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\cdot\boldsymbol{\phi}_i^\top)^2,$$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(\mathbf{w}\cdot\boldsymbol{\phi}_i^\top - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w} - \boldsymbol{\Phi}^\top\mathbf{Y}_m,$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m}\boldsymbol{\phi}_i^\top\cdot\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}.$$

- For a Newtown-Raphson method we get

Newton-Raphson method

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\cdot\boldsymbol{\phi}_i^\top)^2,$$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(\mathbf{w}\cdot\boldsymbol{\phi}_i^\top - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w} - \boldsymbol{\Phi}^\top\mathbf{Y}_m,$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m}\boldsymbol{\phi}_i^\top\cdot\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}.$$

- For a Newtown-Raphson method we get

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}\left(\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}\mathbf{Y}_m\right)$$

- Newton-Raphson method

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - \mathbf{H}^{-1}\nabla E(\mathbf{w})$$

- In case of the linear regression with sum-of-squares error and $m \times M$ design matrix $\boldsymbol{\Phi}$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\cdot\boldsymbol{\phi}_i^\top)^2,$$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(\mathbf{w}\cdot\boldsymbol{\phi}_i^\top - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w} - \boldsymbol{\Phi}^\top\mathbf{Y}_m,$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m}\boldsymbol{\phi}_i^\top\cdot\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top\boldsymbol{\Phi}.$$

- For a Newtown-Raphson method we get

$$\begin{aligned}\mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}\left(\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}\mathbf{Y}_m\right)\\ &= (\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top\mathbf{Y}_m.\end{aligned}$$

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- Newton-Raphson method for logistic regression

- Since $0 < t_i < 1$, then $\mathbf{z}^\top \mathbf{H}\mathbf{z} > 0$, i.e. $\mathbf{H}$ is positive definite. Thus the error function is a concave function.

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

  where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.
- Newton-Raphson method for logistic regression

- Since $0 < t_i < 1$, then $\mathbf{z}^\top \mathbf{H}\mathbf{z} > 0$, i.e. $\mathbf{H}$ is positive definite. Thus the error function is a concave function.

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- Newton-Raphson method for logistic regression

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(t_i - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m),$$

- Since $0 < t_i < 1$, then $\mathbf{z}^\top \mathbf{H}\mathbf{z} > 0$, i.e. $\mathbf{H}$ is positive definite. Thus the error function is a concave function.

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- Newton-Raphson method for logistic regression

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(t_i - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m),$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m} t_i(1-t_i)\boldsymbol{\phi}_n^\top \boldsymbol{\phi}_n = \boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}.$$

- Since $0 < t_i < 1$, then $\mathbf{z}^\top \mathbf{H}\mathbf{z} > 0$, i.e. $\mathbf{H}$ is positive definite. Thus the error function is a concave function.

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- Newton-Raphson method for logistic regression

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(t_i - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m),$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m} t_i(1-t_i)\boldsymbol{\phi}_n^\top \boldsymbol{\phi}_n = \boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}.$$

Here $\mathbf{R}$ is a diagonal matrix $m \times m$ with elements $R_{ii} = t_i(1-t_i)$

- Since $0 < t_i < 1$, then $\mathbf{z}^\top\mathbf{H}\mathbf{z} > 0$, i.e. $\mathbf{H}$ is positive definite. Thus the error function is a concave function.

- Cross Entropy error function

$$E(\mathbf{w}) = -\log p(\mathbf{Y}_m|\mathbf{w}) = -\sum_{i=1}^{m}\{y_i \log t_i + (1-y_i)\log(1-t_i)\},$$

where $t_i = \sigma(a_i)$ and $a_i = \mathbf{w} \cdot \boldsymbol{\phi}_i^\top$.

- Newton-Raphson method for logistic regression

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{m}(t_i - y_i)\boldsymbol{\phi}_i = \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m),$$

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{i=1}^{m} t_i(1-t_i)\boldsymbol{\phi}_n^\top \boldsymbol{\phi}_n = \boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}.$$

Here $\mathbf{R}$ is a diagonal matrix $m \times m$ with elements $R_{ii} = t_i(1-t_i)$

- Since $0 < t_i < 1$, then $\mathbf{z}^\top\mathbf{H}\mathbf{z} > 0$, i.e. $\mathbf{H}$ is positive definite. Thus the error function is a concave function.

- We get that

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\mathbb{E}[y_i] = \sigma(a_i) = t_i,$$
$$\text{var}[y_i] = \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.$$

- We get that

$$\mathbf{w}^{(new)} = \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top \mathbf{R} \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\top (\mathbf{t} - \mathbf{Y}_m)$$

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\mathbb{E}[y_i] = \sigma(a_i) = t_i,$$
$$\text{var}[y_i] = \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.$$

- We get that

$$\begin{aligned}\mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m) \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\left\{\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m)\right\}\end{aligned}$$

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\mathbb{E}[y_i] = \sigma(a_i) = t_i,$$
$$\mathrm{var}[y_i] = \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.$$

- We get that

$$\begin{aligned}\mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m) \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\left\{\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\left\{\boldsymbol{\Phi}\mathbf{w}^{(old)} - \mathbf{R}^{-1}(\mathbf{t} - \mathbf{Y}_m)\right\}\end{aligned}$$

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\mathbb{E}[y_i] = \sigma(a_i) = t_i,$$
$$\mathrm{var}[y_i] = \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.$$

- We get that

$$\begin{aligned}\mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m) \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\left\{\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\left\{\boldsymbol{\Phi}\mathbf{w}^{(old)} - \mathbf{R}^{-1}(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\mathbf{z}.\end{aligned}$$

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\mathbb{E}[y_i] = \sigma(a_i) = t_i,$$
$$\mathrm{var}[y_i] = \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.$$

- We get that

$$\begin{aligned}\mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m) \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\left\{\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\left\{\boldsymbol{\Phi}\mathbf{w}^{(old)} - \mathbf{R}^{-1}(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\mathbf{z}.\end{aligned}$$

  Here

$$\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^{(old)} - \mathbf{R}^{-1}(\mathbf{t} - \mathbf{Y}_m).$$

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\mathbb{E}[y_i] = \sigma(a_i) = t_i,$$
$$\mathrm{var}[y_i] = \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.$$

- We get that

$$\begin{aligned}\mathbf{w}^{(new)} &= \mathbf{w}^{(old)} - (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m) \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\left\{\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi}\mathbf{w}^{(old)} - \boldsymbol{\Phi}^\top(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\left\{\boldsymbol{\Phi}\mathbf{w}^{(old)} - \mathbf{R}^{-1}(\mathbf{t} - \mathbf{Y}_m)\right\} \\ &= (\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^\top \mathbf{R}\mathbf{z}.\end{aligned}$$

  Here

$$\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^{(old)} - \mathbf{R}^{-1}(\mathbf{t} - \mathbf{Y}_m).$$

- $\mathbf{R}$ can be interpreted as a covariance matrix, since

$$\begin{aligned}\mathbb{E}[y_i] &= \sigma(a_i) = t_i, \\ \mathrm{var}[y_i] &= \mathbb{E}[y_i^2] - (\mathbb{E}[y_i])^2 = \sigma(a_i) - \sigma^2(a_i) = t_i(1 - t_i) = [\mathbf{R}]_{ii}.\end{aligned}$$

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0, 1)d\theta$$

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0, 1)d\theta$$

$$\text{erf}(a) = \frac{2}{\sqrt{\pi}} \int_{0}^{a} \exp(-\theta^2/2)d\theta$$

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0, 1)d\theta$$

$$\text{erf}(a) = \frac{2}{\sqrt{\pi}} \int_{0}^{a} \exp(-\theta^2/2)d\theta$$

$$f(a) = \Phi(a) = \frac{1}{2}\left\{1 + \frac{1}{\sqrt{2}}\text{erf}(a)\right\}$$

Probit regression

- The general model

$$p(t = 1|a) = f(a),\ a = \mathbf{w} \cdot \boldsymbol{\phi}^\top,$$

  $f(\cdot)$ is an activation function:
  - $t_i = 1$, if $a_i \geq \theta$
  - $t_i = 0$, otherwise
- Usually we consider the noisy threshold model $\theta \sim p(\theta)$, $f(a) = \int_{-\infty}^{a} p(\theta)d\theta$.
- For the logit (logistic) regression $f(a) = \sigma(a)$ and a logistic distribution as $p(\theta)$.
- For the probit regression

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0, 1)d\theta$$

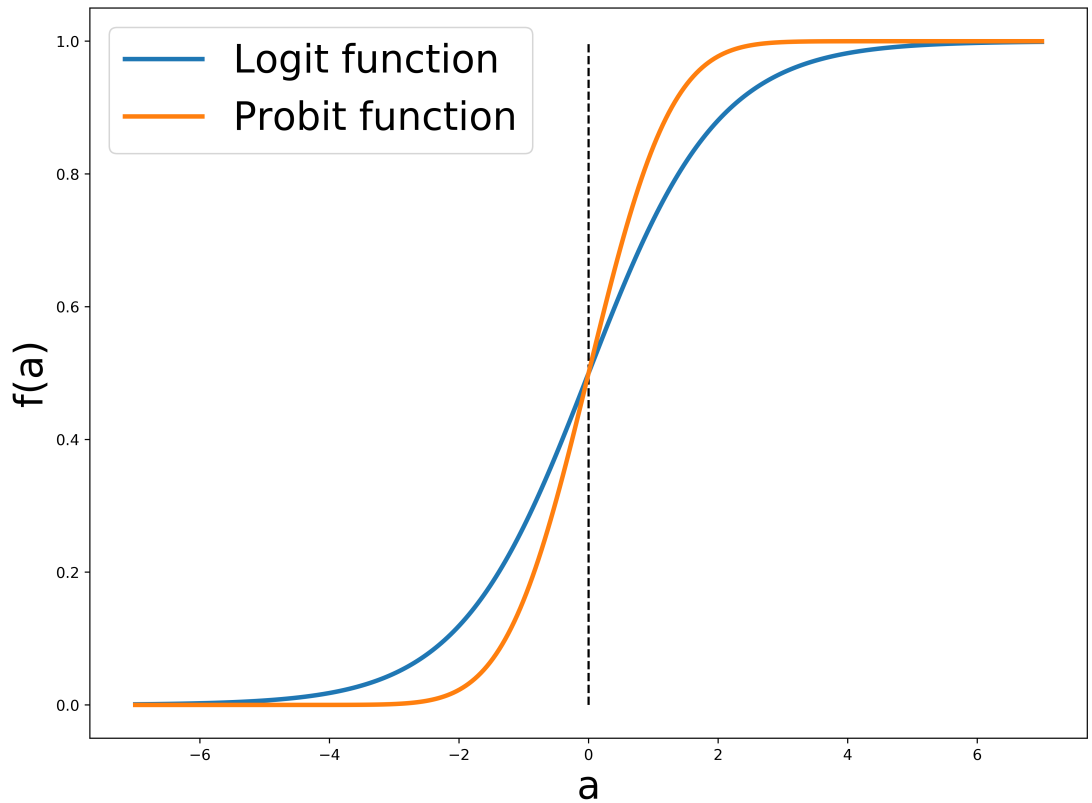
$$\text{erf}(a) = \frac{2}{\sqrt{\pi}} \int_{0}^{a} \exp(-\theta^2/2)d\theta$$

$$f(a) = \Phi(a) = \frac{1}{2}\left\{1 + \frac{1}{\sqrt{2}}\text{erf}(a)\right\}$$

$$p(\mathcal{C}_1|\boldsymbol{\phi}) = t(\boldsymbol{\phi}) = \Phi(\mathbf{w} \cdot \boldsymbol{\phi}^\top)$$

Difference between the logit and the probit regression

- They are not that much different.
- But the probit is a more Bayes-friendly option (more on this later!).



Approximate inference

- We have a distribution $p(z)$.
- This distribution $p(z)$
  - is too complex
  - is known only up to a normalization constant
  - doesn't integrate analytically (almost every Bayesian inference problem).
- We want to find $q(z)$ that is in some sense close to $p(z)$, but is better from our point of view (e.g. the integral is tractable):

$$q(z) \approx p(z).$$

Approximate inference

- We have a distribution $p(z)$.
- This distribution $p(z)$
  - is too complex
  - is known only up to a normalization constant
  - doesn't integrate analytically (almost every Bayesian inference problem).
- We want to find $q(z)$ that is in some sense close to $p(z)$, but is better from our point of view (e.g. the integral is tractable):

$$q(z) \approx p(z).$$

Approximate inference

- We have a distribution $p(z)$.
- This distribution $p(z)$
  - is too complex
  - is known only up to a normalization constant
  - doesn't integrate analytically (almost every Bayesian inference problem).
- We want to find $q(z)$ that is in some sense close to $p(z)$, but is better from our point of view (e.g. the integral is tractable):

$$q(z) \approx p(z).$$

Laplace Approximation: univariate case

- Density with an unknown normalization constant

$$p(z) = \frac{1}{Z} f(z), \;\; Z = \int f(z) dz.$$

- We calculate a mode of the distribution

$$p'(z_0) = 0 \Leftrightarrow \frac{df(z)}{dz}\Big|_{z=z_0} = 0$$

- Using the Taylor approximation we get that

$$\log f(z) \approx \log f(z_0) - \frac{1}{2} A (z - z_0)^2, \;\; A = -\frac{d^2}{dz^2} \log f(z)\Big|_{z=z_0}$$

- Thus we get that

$$f(z) \approx f(z_0) \exp\left\{ -\frac{A}{2} (z - z_0)^2 \right\}$$

Laplace Approximation: univariate case

- Density with an unknown normalization constant

$$p(z) = \frac{1}{Z} f(z), \;\; Z = \int f(z) dz.$$

- We calculate a mode of the distribution

$$p'(z_0) = 0 \Leftrightarrow \frac{df(z)}{dz}\Big|_{z=z_0} = 0$$

- Using the Taylor approximation we get that

$$\log f(z) \approx \log f(z_0) - \frac{1}{2} A (z - z_0)^2, \;\; A = -\frac{d^2}{dz^2} \log f(z)\Big|_{z=z_0}$$

- Thus we get that

$$f(z) \approx f(z_0) \exp\left\{ -\frac{A}{2} (z - z_0)^2 \right\}$$

Laplace Approximation: univariate case

- Density with an unknown normalization constant

$$p(z) = \frac{1}{Z} f(z), \;\; Z = \int f(z) dz.$$

- We calculate a mode of the distribution

$$p'(z_0) = 0 \Leftrightarrow \frac{df(z)}{dz}\Big|_{z=z_0} = 0$$

- Using the Taylor approximation we get that

$$\log f(z) \approx \log f(z_0) - \frac{1}{2} A (z - z_0)^2, \;\; A = -\frac{d^2}{dz^2} \log f(z)\Big|_{z=z_0}$$

- Thus we get that

$$f(z) \approx f(z_0) \exp\left\{ -\frac{A}{2} (z - z_0)^2 \right\}$$

Laplace Approximation: univariate case

- Density with an unknown normalization constant

$$p(z) = \frac{1}{Z} f(z), \;\; Z = \int f(z) dz.$$

- We calculate a mode of the distribution

$$p'(z_0) = 0 \Leftrightarrow \frac{df(z)}{dz}\Big|_{z=z_0} = 0$$

- Using the Taylor approximation we get that

$$\log f(z) \approx \log f(z_0) - \frac{1}{2} A (z - z_0)^2, \;\; A = -\frac{d^2}{dz^2} \log f(z)\Big|_{z=z_0}$$

- Thus we get that

$$f(z) \approx f(z_0) \exp\left\{ -\frac{A}{2} (z - z_0)^2 \right\}$$

- The normalization constant

$$Z = \int f(z)dz \approx f(z_0) \int \exp\left\{-\frac{A}{2}(z - z_0)^2\right\} dz = f(z_0)\left(\frac{2\pi}{A}\right)^{1/2}$$

- Thus we get that

- The normalization constant

$$Z = \int f(z)dz \approx f(z_0) \int \exp\left\{-\frac{A}{2}(z - z_0)^2\right\} dz = f(z_0)\left(\frac{2\pi}{A}\right)^{1/2}$$

- Thus we get that

- The normalization constant

$$Z = \int f(z)dz \approx f(z_0) \int \exp\left\{-\frac{A}{2}(z - z_0)^2\right\} dz = f(z_0)\left(\frac{2\pi}{A}\right)^{1/2}$$

- Thus we get that

$$p(z) = \frac{f(z)}{Z} \approx \frac{f(z_0)\exp\left\{-\frac{A}{2}(z - z_0)^2\right\}}{f(z_0)\left(\frac{2\pi}{A}\right)^{1/2}}$$

- The normalization constant

$$Z = \int f(z)dz \approx f(z_0) \int \exp\left\{-\frac{A}{2}(z - z_0)^2\right\} dz = f(z_0) \left(\frac{2\pi}{A}\right)^{1/2}$$

- Thus we get that

$$p(z) = \frac{f(z)}{Z} \approx \frac{f(z_0) \exp\left\{-\frac{A}{2}(z - z_0)^2\right\}}{f(z_0) \left(\frac{2\pi}{A}\right)^{1/2}}$$
$$= \left(\frac{A}{2\pi}\right)^{1/2} \exp\left\{-\frac{A}{2}(z - z_0)^2\right\}$$

Laplace Approximation is an approximation by Gaussian distribution

- We got the density

$$p(z) \approx q(z) = \left(\frac{A}{2\pi}\right)^{1/2} \exp\left\{-\frac{A}{2}(z - z_0)^2\right\}.$$

- It is the density of Gaussian distribution:

$$q(z) = \mathcal{N}(z|z_0, A^{-1}).$$

Laplace Approximation is an approximation by Gaussian distribution

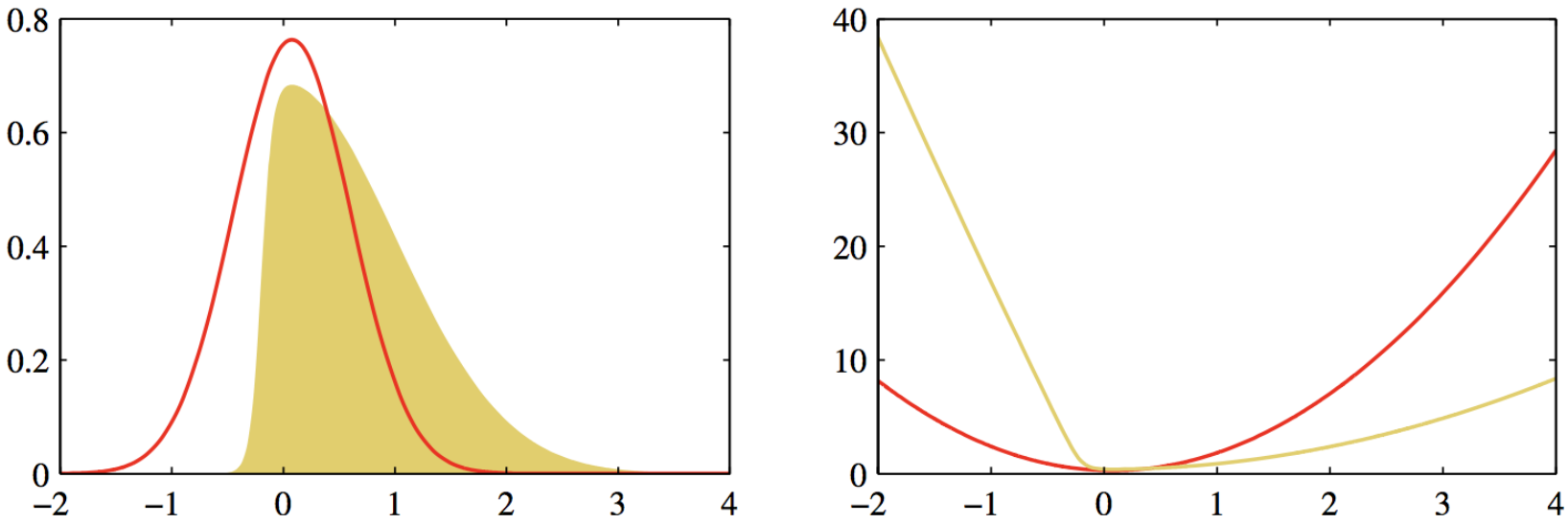
- We got the density

$$p(z) \approx q(z) = \left(\frac{A}{2\pi}\right)^{1/2} \exp\left\{-\frac{A}{2}(z - z_0)^2\right\}.$$

- It is the density of Gaussian distribution:

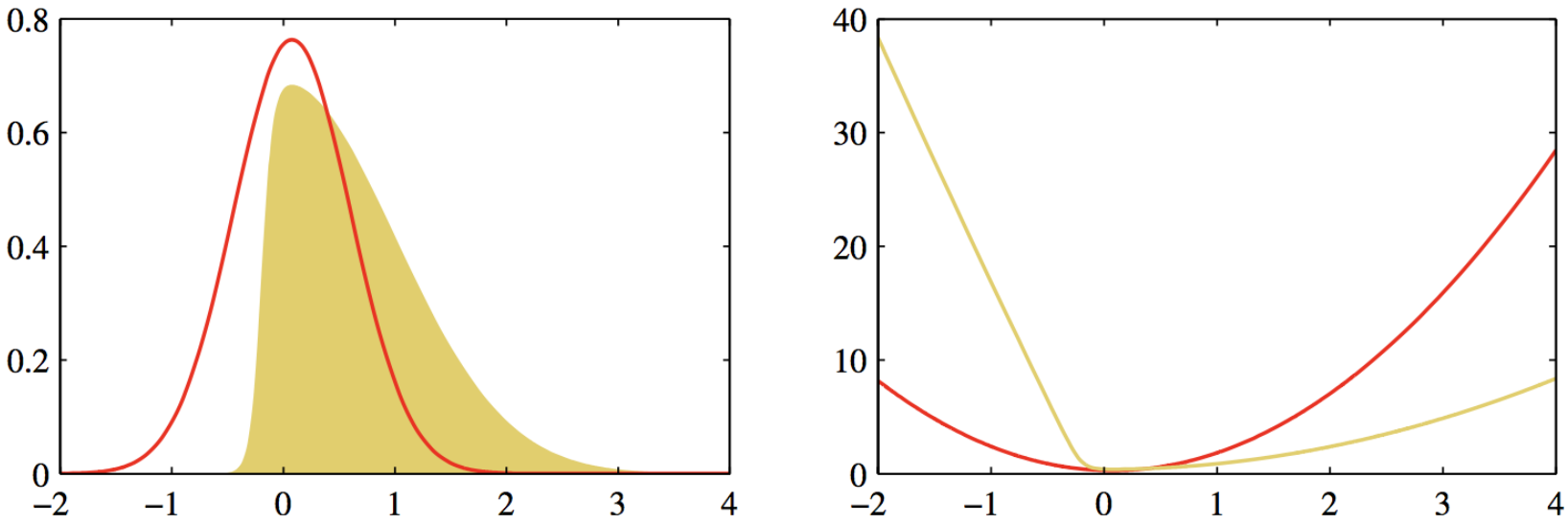
$$q(z) = \mathcal{N}(z|z_0, A^{-1}).$$

Laplace Approximation



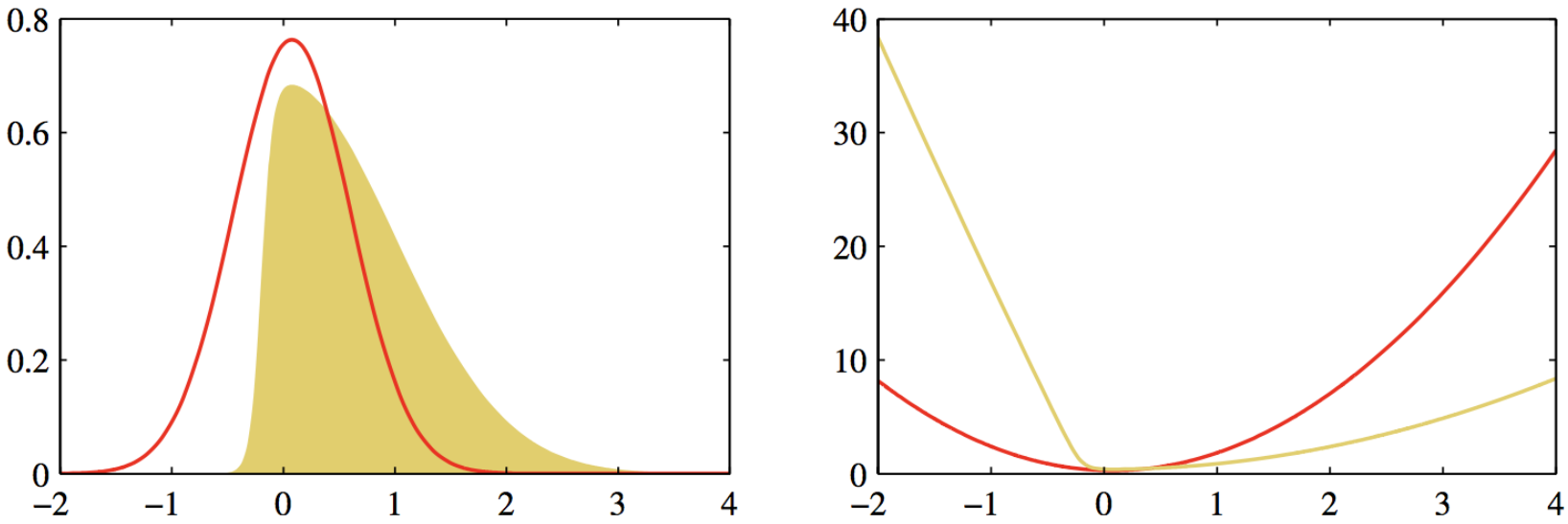
- Laplace approximation for $p(z) \sim \exp(-z^2/2)\sigma(20z + 4)$
- The left plot: the normalized distribution $p(z)$ — in yellow, the Laplace approximation centred on the mode z_0 of $p(z)$ — in red
- The right plot: the negative logarithms of the corresponding curves

Laplace Approximation



- Laplace approximation for $p(z) \sim \exp(-z^2/2)\sigma(20z + 4)$
- The left plot: the normalized distribution $p(z)$ — in yellow, the Laplace approximation centred on the mode z_0 of $p(z)$ — in red
- The right plot: the negative logarithms of the corresponding curves

Laplace Approximation



- Laplace approximation for $p(z) \sim \exp(-z^2/2)\sigma(20z + 4)$
- The left plot: the normalized distribution $p(z)$ — in yellow, the Laplace approximation centred on the mode z_0 of $p(z)$ — in red
- The right plot: the negative logarithms of the corresponding curves

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z}) \Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z}) \Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z}) \Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z}) \Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

$$Z = \int f(\mathbf{z}) d\mathbf{z}$$

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$
$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

$$Z = \int f(\mathbf{z}) d\mathbf{z}$$
$$\approx f(\mathbf{z}_0) \int \exp\{-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)\} d\mathbf{z}$$

Laplace Approximation: multivariate case

- Density with unknown normalization constant

$$p(\mathbf{z}) = f(\mathbf{z})/Z, \;\; Z = \int f(\mathbf{z}) d\mathbf{z}$$

- Taylor expansion

$$\log f(\mathbf{z}) \approx \log f(\mathbf{z}_0) - (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2,$$
$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get

$$f(\mathbf{z}) \approx f(\mathbf{z}_0) \exp\left\{-(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)/2\right\}$$

- Normalization constant

$$\begin{aligned} Z &= \int f(\mathbf{z}) d\mathbf{z} \\ &\approx f(\mathbf{z}_0) \int \exp\{-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)\} d\mathbf{z} \\ &= f(\mathbf{z}_0) \frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}} \end{aligned}$$

Multidimensional Laplace Approximation

- Laplace approximation has the form

$$p(\mathbf{z}) = \frac{f(\mathbf{z})}{Z}$$

- Here

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- It is again a Gaussian distribution

Multidimensional Laplace Approximation

- Laplace approximation has the form

$$p(\mathbf{z}) = \frac{f(\mathbf{z})}{Z}$$
$$\approx \frac{f(\mathbf{z}_0)\exp\left\{-(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)/2\right\}}{f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}}}$$

- Here

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- It is again a Gaussian distribution

Multidimensional Laplace Approximation

- Laplace approximation has the form

$$p(\mathbf{z}) = \frac{f(\mathbf{z})}{Z}$$
$$\approx \frac{f(\mathbf{z}_0)\exp\left\{-(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)/2\right\}}{f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}}}$$
$$= \frac{|\mathbf{A}|^{1/2}}{(2\pi)^{M/2}}\exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\} = \mathcal{N}(\mathbf{z}|\mathbf{z}_0, \mathbf{A}^{-1})$$

- Here

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- It is again a Gaussian distribution

- Laplace approximation has the form

$$p(\mathbf{z}) = \frac{f(\mathbf{z})}{Z}$$
$$\approx \frac{f(\mathbf{z}_0)\exp\left\{-(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)/2\right\}}{f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}}}$$
$$= \frac{|\mathbf{A}|^{1/2}}{(2\pi)^{M/2}}\exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\} = \mathcal{N}(\mathbf{z}|\mathbf{z}_0, \mathbf{A}^{-1})$$

- Here

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),$$

$$\mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- It is again a Gaussian distribution

Bayesian Logistic Regression

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

Bayesian Logistic Regression

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

Bayesian Logistic Regression

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) +$$

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

Bayesian Logistic Regression

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) +$$

$$+ \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const} \to \max_{\mathbf{w}}$$

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

Bayesian Logistic Regression

- Prior over parameters

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

- Probability is

$$t_i = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}_i^\top)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Log-posterior

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) +$$
$$+ \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const} \to \max_{\mathbf{w}}$$

- Maximizing $\log p(\mathbf{w}|\mathbf{Y}_m)$ we estimate $\mathbf{w}_{MAP}$

Bayesian Logistic Regression

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

Bayesian Logistic Regression

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) +$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) + \\ + \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const}$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

Bayesian Logistic Regression

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) + \\ + \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const}$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) + \\ + \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const}$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) + \\ + \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const}$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) + \\ + \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const}$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

$$\mathbf{S}_m^{-1} = -\nabla\nabla \log p(\mathbf{w}|\mathbf{Y}_m) = \mathbf{S}_0^{-1} + \sum_{i=1}^{m} t_i(1 - t_i)\boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_i^\top \Big|_{\mathbf{w}=\mathbf{w}_{MAP}}$$

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

- Bayes formula

$$\mathbf{Y}_m = (y_1, \ldots, y_m)^\top, \;\; p(\mathbf{w}|\mathbf{Y}_m) \sim p(\mathbf{w})p(\mathbf{Y}_m|\mathbf{w})$$

$$\log p(\mathbf{w}|\mathbf{Y}_m) = -\frac{1}{2}(\mathbf{w} - \boldsymbol{\omega}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \boldsymbol{\omega}_0) + \\ + \sum_{i=1}^{m} \{y_i \log t_i + (1 - y_i) \log(1 - t_i)\} + \text{const}$$

- Gaussian approximation to the posterior:
  - first we maximize the posterior to get the MAP
  - second we estimate the Hessian to get covariance matrix

$$\mathbf{S}_m^{-1} = -\nabla\nabla \log p(\mathbf{w}|\mathbf{Y}_m) = \mathbf{S}_0^{-1} + \sum_{i=1}^{m} t_i(1 - t_i)\boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_i^\top \Big|_{\mathbf{w}=\mathbf{w}_{MAP}}$$

- Laplace (Gaussian) approximation to the posterior $p(\mathbf{w}|\mathbf{Y}_m)$ has the form

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{MAP}, \mathbf{S}_m)$$

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function

- We get

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

$$\int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} =$$

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

$$\int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} = \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} \right] \sigma(a) da$$

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

$$\int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} = \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} \right] \sigma(a) da$$
$$= \int \sigma(a) p(a) da$$

Predictive Distribution

- $p(\mathbf{w}|\mathbf{Y}_m)$ is approximated by a Gaussian $q(\mathbf{w})$
- The class probability

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \int p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{w}) p(\mathbf{w}|\mathbf{Y}_m) d\mathbf{w} \approx \int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Let us denote $a = \mathbf{w} \cdot \boldsymbol{\phi}^\top$. We represent

$$\sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) \sigma(a) da$$

  Here $\delta(\cdot)$ is a delta-function
- We get

$$\begin{aligned}\int \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} &= \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w} \right] \sigma(a) da \\ &= \int \sigma(a) p(a) da \\ \text{with} \quad p(a) &= \int \delta(a - \mathbf{w}^\top \boldsymbol{\phi}) q(\mathbf{w}) d\mathbf{w}\end{aligned}$$

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Delta function imposes a linear constraint on $\mathbf{w}$ and so forms a marginal distribution by integrating out all directions orthogonal to ϕ
- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Delta function imposes a linear constraint on $\mathbf{w}$ and so forms a marginal distribution by integrating out all directions orthogonal to $\boldsymbol{\phi}$
- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Delta function imposes a linear constraint on $\mathbf{w}$ and so forms a marginal distribution by integrating out all directions orthogonal to $\boldsymbol{\phi}$
- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Delta function imposes a linear constraint on $\mathbf{w}$ and so forms a marginal distribution by integrating out all directions orthogonal to $\boldsymbol{\phi}$
- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\mu_a = \mathbb{E}[a] = \int p(a) a da = \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) a da \right] q(\mathbf{w}) d\mathbf{w}$$

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- Delta function imposes a linear constraint on $\mathbf{w}$ and so forms a marginal distribution by integrating out all directions orthogonal to $\boldsymbol{\phi}$
- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\mu_a = \mathbb{E}[a] = \int p(a) a da = \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) a da \right] q(\mathbf{w}) d\mathbf{w}$$

$$= \int \mathbf{w} \cdot \boldsymbol{\phi}^\top q(\mathbf{w}) d\mathbf{w} = \left[\int \mathbf{w} q(\mathbf{w}) d\mathbf{w} \right] \cdot \boldsymbol{\phi}^\top = \mathbf{w}_{MAP} \cdot \boldsymbol{\phi}^\top$$

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\sigma_a^2 = \text{var}[a] = \int p(a)(a^2 - (\mathbb{E}[a])^2) da$$

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\begin{aligned}\sigma_a^2 = \text{var}[a] &= \int p(a)(a^2 - (\mathbb{E}[a])^2) da \\ &= \int \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w})(a^2 - (\mathbb{E}[a])^2) da d\mathbf{w}\end{aligned}$$

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\begin{aligned}
\sigma_a^2 = \mathrm{var}[a] &= \int p(a)(a^2 - (\mathbb{E}[a])^2) da \\
&= \int \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) (a^2 - (\mathbb{E}[a])^2) da d\mathbf{w} \\
&= \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) (a^2 - (\mathbb{E}[a])^2) da \right] q(\mathbf{w}) d\mathbf{w}
\end{aligned}$$

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\begin{aligned}
\sigma_a^2 = \mathrm{var}[a] &= \int p(a)(a^2 - (\mathbb{E}[a])^2) da \\
&= \int \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) (a^2 - (\mathbb{E}[a])^2) da d\mathbf{w} \\
&= \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top)(a^2 - (\mathbb{E}[a])^2) da \right] q(\mathbf{w}) d\mathbf{w} \\
&= \int \{(\mathbf{w} \cdot \boldsymbol{\phi}^\top)^2 - (\mathbf{w}_{MAP} \cdot \boldsymbol{\phi}^\top)^2\} q(\mathbf{w}) d\mathbf{w}
\end{aligned}$$

Predictive Distribution

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\begin{aligned}
\sigma_a^2 = \mathrm{var}[a] &= \int p(a)(a^2 - (\mathbb{E}[a])^2) da \\
&= \int \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) (a^2 - (\mathbb{E}[a])^2) da d\mathbf{w} \\
&= \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) (a^2 - (\mathbb{E}[a])^2) da \right] q(\mathbf{w}) d\mathbf{w} \\
&= \int \{ (\mathbf{w} \cdot \boldsymbol{\phi}^\top)^2 - (\mathbf{w}_{MAP} \cdot \boldsymbol{\phi}^\top)^2 \} q(\mathbf{w}) d\mathbf{w} \\
&= \int \boldsymbol{\phi}^\top (\mathbf{w} - \mathbf{w}_{MAP})^\top (\mathbf{w} - \mathbf{w}_{MAP}) \boldsymbol{\phi} q(\mathbf{w}) d\mathbf{w}
\end{aligned}$$

- Recall

$$p(a) = \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) d\mathbf{w}$$

- So $p(a)$ is 1d Gaussian distribution $\mathcal{N}(\mu_a, \sigma_a^2)$ with

$$\begin{aligned}
\sigma_a^2 = \mathrm{var}[a] &= \int p(a)(a^2 - (\mathbb{E}[a])^2) da \\
&= \int \int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top) q(\mathbf{w}) (a^2 - (\mathbb{E}[a])^2) da d\mathbf{w} \\
&= \int \left[\int \delta(a - \mathbf{w} \cdot \boldsymbol{\phi}^\top)(a^2 - (\mathbb{E}[a])^2) da \right] q(\mathbf{w}) d\mathbf{w} \\
&= \int \{(\mathbf{w} \cdot \boldsymbol{\phi}^\top)^2 - (\mathbf{w}_{MAP} \cdot \boldsymbol{\phi}^\top)^2\} q(\mathbf{w}) d\mathbf{w} \\
&= \int \boldsymbol{\phi}^\top (\mathbf{w} - \mathbf{w}_{MAP})^\top (\mathbf{w} - \mathbf{w}_{MAP}) \boldsymbol{\phi} q(\mathbf{w}) d\mathbf{w} \\
&= \boldsymbol{\phi}^\top \left[\int (\mathbf{w} - \mathbf{w}_{MAP})^\top (\mathbf{w} - \mathbf{w}_{MAP}) q(\mathbf{w}) d\mathbf{w} \right] \boldsymbol{\phi} = \boldsymbol{\phi}^\top \mathbf{S}_m \boldsymbol{\phi}
\end{aligned}$$

Predictive Distribution

- Thus we get that

$$p(\mathcal{C}_1|\mathbf{Y}_m) = \int \sigma(a)p(a)da = \int \sigma(a)\mathcal{N}(a|\mu_a, \sigma_a^2)da$$

- We approximate $\sigma(a)$ by $\Phi(\lambda a)$. Here $\lambda^2 = \pi/8$ (same slope at the origin)

$$\sigma(a) \approx \Phi(\lambda a)$$

- We get that

$$\int \Phi(\lambda a)\mathcal{N}(a|\mu, \sigma^2)da = \Phi\left(\frac{\mu}{(\lambda^{-2} + \sigma^2)^{1/2}}\right)$$

- Applying the approximation $\sigma(a) \approx \Phi(\lambda a)$ to both sides we get that

$$\int \sigma(a)\mathcal{N}(a|\mu, \sigma^2)da \approx \sigma(\varkappa(\sigma^2)\mu),\ \varkappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

- Finally

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \sigma(\varkappa(\sigma_a^2)\mu_a)$$

Predictive Distribution

- Thus we get that

$$p(\mathcal{C}_1|\mathbf{Y}_m) = \int \sigma(a)p(a)da = \int \sigma(a)\mathcal{N}(a|\mu_a, \sigma_a^2)da$$

- We approximate $\sigma(a)$ by $\Phi(\lambda a)$. Here $\lambda^2 = \pi/8$ (same slope at the origin)

$$\sigma(a) \approx \Phi(\lambda a)$$

- We get that

$$\int \Phi(\lambda a)\mathcal{N}(a|\mu, \sigma^2)da = \Phi\left(\frac{\mu}{(\lambda^{-2} + \sigma^2)^{1/2}}\right)$$

- Applying the approximation $\sigma(a) \approx \Phi(\lambda a)$ to both sides we get that

$$\int \sigma(a)\mathcal{N}(a|\mu, \sigma^2)da \approx \sigma(\varkappa(\sigma^2)\mu),\ \varkappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

- Finally

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \sigma(\varkappa(\sigma_a^2)\mu_a)$$

- Thus we get that

$$p(\mathcal{C}_1|\mathbf{Y}_m) = \int \sigma(a)p(a)da = \int \sigma(a)\mathcal{N}(a|\mu_a, \sigma_a^2)da$$

- We approximate $\sigma(a)$ by $\Phi(\lambda a)$. Here $\lambda^2 = \pi/8$ (same slope at the origin)

$$\sigma(a) \approx \Phi(\lambda a)$$

- We get that

$$\int \Phi(\lambda a)\mathcal{N}(a|\mu, \sigma^2)da = \Phi\left(\frac{\mu}{(\lambda^{-2} + \sigma^2)^{1/2}}\right)$$

- Applying the approximation $\sigma(a) \approx \Phi(\lambda a)$ to both sides we get that

$$\int \sigma(a)\mathcal{N}(a|\mu, \sigma^2)da \approx \sigma(\varkappa(\sigma^2)\mu),\ \varkappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

- Finally

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \sigma(\varkappa(\sigma_a^2)\mu_a)$$

- Thus we get that

$$p(\mathcal{C}_1|\mathbf{Y}_m) = \int \sigma(a)p(a)da = \int \sigma(a)\mathcal{N}(a|\mu_a, \sigma_a^2)da$$

- We approximate $\sigma(a)$ by $\Phi(\lambda a)$. Here $\lambda^2 = \pi/8$ (same slope at the origin)

$$\sigma(a) \approx \Phi(\lambda a)$$

- We get that

$$\int \Phi(\lambda a)\mathcal{N}(a|\mu, \sigma^2)da = \Phi\left(\frac{\mu}{(\lambda^{-2} + \sigma^2)^{1/2}}\right)$$

- Applying the approximation $\sigma(a) \approx \Phi(\lambda a)$ to both sides we get that

$$\int \sigma(a)\mathcal{N}(a|\mu, \sigma^2)da \approx \sigma(\varkappa(\sigma^2)\mu),\ \varkappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

- Finally

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \sigma(\varkappa(\sigma_a^2)\mu_a)$$

- Thus we get that

$$p(\mathcal{C}_1|\mathbf{Y}_m) = \int \sigma(a)p(a)da = \int \sigma(a)\mathcal{N}(a|\mu_a, \sigma_a^2)da$$

- We approximate $\sigma(a)$ by $\Phi(\lambda a)$. Here $\lambda^2 = \pi/8$ (same slope at the origin)

$$\sigma(a) \approx \Phi(\lambda a)$$

- We get that

$$\int \Phi(\lambda a)\mathcal{N}(a|\mu, \sigma^2)da = \Phi\left(\frac{\mu}{(\lambda^{-2} + \sigma^2)^{1/2}}\right)$$

- Applying the approximation $\sigma(a) \approx \Phi(\lambda a)$ to both sides we get that

$$\int \sigma(a)\mathcal{N}(a|\mu, \sigma^2)da \approx \sigma(\varkappa(\sigma^2)\mu),\ \varkappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

- Finally

$$p(\mathcal{C}_1|\boldsymbol{\phi}, \mathbf{Y}_m) = \sigma(\varkappa(\sigma_a^2)\mu_a)$$

- Class probability

$$t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$$

- Log-posterior for the prior

$$p(\mathbf{w}|\boldsymbol{\alpha}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\alpha}^{-1}), \ \boldsymbol{\alpha} = \mathrm{diag}\{\alpha_1, \ldots, \alpha_M\}$$

has the form

- Class probability

$$t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$$

- Log-posterior for the prior

$$p(\mathbf{w}|\boldsymbol{\alpha}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\alpha}^{-1}), \ \boldsymbol{\alpha} = \mathrm{diag}\{\alpha_1, \ldots, \alpha_M\}$$

  has the form

- Class probability

$$t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$$

- Log-posterior for the prior

$$p(\mathbf{w}|\boldsymbol{\alpha}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\alpha}^{-1}), \ \boldsymbol{\alpha} = \mathrm{diag}\{\alpha_1, \ldots, \alpha_M\}$$

has the form

$$\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = \log\{p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})\} - \log p(\mathbf{Y}_m|\boldsymbol{\alpha})$$

- Class probability

$$t(\boldsymbol{\phi}) = \sigma(\mathbf{w} \cdot \boldsymbol{\phi}^\top), \boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$$

- Log-posterior for the prior

$$p(\mathbf{w}|\boldsymbol{\alpha}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\alpha}^{-1}), \ \boldsymbol{\alpha} = \mathrm{diag}\{\alpha_1, \ldots, \alpha_M\}$$

has the form

$$\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = \log\{p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})\} - \log p(\mathbf{Y}_m|\boldsymbol{\alpha})$$
$$= \sum_{i=1}^{m}\{y_i \log t_i + (1 - y_i)\log(1 - t_i)\} - \mathbf{w}^\top \boldsymbol{\alpha}\mathbf{w}/2 + \mathrm{const}$$

- Due to the Laplace approximation

$$\int f(\mathbf{z})d\mathbf{z} \approx f(\mathbf{z}_0)\int \exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\}d\mathbf{z} = f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}},$$

where

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),\ \mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get that

$$\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = \boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \boldsymbol{\alpha}\mathbf{w},$$
$$\nabla\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = -\left(\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha}\right),$$

where $\mathbf{R}$ is an $m \times m$ diagonal matrix with elements $R_{ii} = t_i(1-t_i)$

- We get that MAP estimate fulfils equality

$$\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \mathbf{A}\mathbf{w} = 0 \Rightarrow$$

- We can use an approximation to get an estimate $\mathbf{w}^*$:

$$\mathbf{w}^* = \mathbf{A}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}).$$

- Due to the Laplace approximation

$$\int f(\mathbf{z})d\mathbf{z} \approx f(\mathbf{z}_0)\int \exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\}d\mathbf{z} = f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}},$$

where

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),\ \mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get that

$$\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = \boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \boldsymbol{\alpha}\mathbf{w},$$
$$\nabla\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = -\left(\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha}\right),$$

where $\mathbf{R}$ is an $m \times m$ diagonal matrix with elements $R_{ii} = t_i(1-t_i)$

- We get that MAP estimate fulfils equality

$$\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \mathbf{A}\mathbf{w} = 0 \Rightarrow$$

- We can use an approximation to get an estimate $\mathbf{w}^*$:

$$\mathbf{w}^* = \mathbf{A}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}).$$

- Due to the Laplace approximation

$$\int f(\mathbf{z})d\mathbf{z} \approx f(\mathbf{z}_0)\int \exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\}d\mathbf{z} = f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}},$$

where

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),\ \mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get that

$$\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = \boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \boldsymbol{\alpha}\mathbf{w},$$
$$\nabla\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = -\left(\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha}\right),$$

where $\mathbf{R}$ is an $m \times m$ diagonal matrix with elements $R_{ii} = t_i(1-t_i)$

- We get that MAP estimate fulfils equality

$$\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \mathbf{A}\mathbf{w} = 0 \Rightarrow$$

- We can use an approximation to get an estimate $\mathbf{w}^*$:

$$\mathbf{w}^* = \mathbf{A}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}).$$

- Due to the Laplace approximation

$$\int f(\mathbf{z})d\mathbf{z} \approx f(\mathbf{z}_0)\int \exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^\top \mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\}d\mathbf{z} = f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}},$$

where

$$\mathbf{z}_0 = \arg\max_{\mathbf{z}} f(\mathbf{z}),\ \mathbf{A} = -\nabla\nabla \log f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

- We get that

$$\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = \boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \boldsymbol{\alpha}\mathbf{w},$$
$$\nabla\nabla \log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha}) = -\left(\boldsymbol{\Phi}^\top \mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha}\right),$$

where $\mathbf{R}$ is an $m \times m$ diagonal matrix with elements $R_{ii} = t_i(1-t_i)$

- We get that MAP estimate fulfils equality

$$\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}) - \mathbf{A}\mathbf{w} = 0 \Rightarrow$$

- We can use an approximation to get an estimate $\mathbf{w}^*$:

$$\mathbf{w}^* = \mathbf{A}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}).$$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that
- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

$$\mathbf{w}^* = \boldsymbol{\alpha}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}),$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

$$\mathbf{w}^* = \boldsymbol{\alpha}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}),\ \mathbf{S}_m = (\boldsymbol{\Phi}^\top\mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha})^{-1}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm

- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

$$\mathbf{w}^* = \boldsymbol{\alpha}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}),\ \mathbf{S}_m = (\boldsymbol{\Phi}^\top\mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha})^{-1}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

$$\mathbf{w}^* = \boldsymbol{\alpha}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}),\ \mathbf{S}_m = (\boldsymbol{\Phi}^\top\mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha})^{-1}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

$$\mathbf{w}^* = \boldsymbol{\alpha}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}),\ \mathbf{S}_m = (\boldsymbol{\Phi}^\top\mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha})^{-1}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm

- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

Iterative update

- The maximum and the hessian of $\log p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})$ coincide with that of $\log p(\mathbf{w}|\mathbf{Y}_m, \boldsymbol{\alpha})$. Therefore, using the Laplace approximation we get that

$$p(\mathbf{Y}_m|\boldsymbol{\alpha}) = \int p(\mathbf{Y}_m|\mathbf{w})p(\mathbf{w}|\boldsymbol{\alpha})d\mathbf{w} \approx p(\mathbf{Y}_m|\mathbf{w}^*)p(\mathbf{w}^*|\boldsymbol{\alpha})(2\pi)^{M/2}|\mathbf{S}_m|^{\frac{1}{2}}$$

$$\mathbf{w}^* = \boldsymbol{\alpha}^{-1}\boldsymbol{\Phi}^\top(\mathbf{Y}_m - \mathbf{t}),\ \mathbf{S}_m = (\boldsymbol{\Phi}^\top\mathbf{R}\boldsymbol{\Phi} + \boldsymbol{\alpha})^{-1}$$

- Setting the derivative of the marginal likelihood to zero we get

$$-\frac{1}{2}(w_i^*)^2 + \frac{1}{2\alpha_i} - \frac{1}{2}[\mathbf{S}_m]_{ii} = 0$$

- For $\gamma_i = 1 - \alpha_i[\mathbf{S}_m]_{ii}$ we get

$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2}$$

- For $\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^* - \mathbf{R}^{-1}(\mathbf{Y}_m - \mathbf{t})$ and $\mathbf{C} = \mathbf{R} + \boldsymbol{\Phi}\mathbf{A}\boldsymbol{\Phi}^\top$ we get

$$\log p(\mathbf{Y}_m|\boldsymbol{\alpha}) = -\frac{1}{2}\left\{m\log(2\pi) + \log|\mathbf{C}| + (\mathbf{z}\mathbf{C}^{-1}\mathbf{z})\right\}.$$

  The same form as in the regression case $\Rightarrow$ we can apply the same analysis of sparsity and obtain the same fast learning algorithm
- We iterate between tuning of $\mathbf{w}$ and $\boldsymbol{\alpha}$

- K-class classification case
- We set $a_k = \mathbf{w}_k \cdot \mathbf{x}^\top$ and probabilities of specific classes to be equal to

$$t_k(\mathbf{x}) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

- The likelihood function is then given by

$$\log p(\mathbf{Y}_m | \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{i=1}^{m} \prod_{k=1}^{K} t_{ik}^{y_{ik}}$$

- All other steps are exactly the same!

Multiclass classification

- K-class classification case
- We set $a_k = \mathbf{w}_k \cdot \mathbf{x}^\top$ and probabilities of specific classes to be equal to

$$t_k(\mathbf{x}) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

- The likelihood function is then given by

$$\log p(\mathbf{Y}_m | \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{i=1}^{m} \prod_{k=1}^{K} t_{ik}^{y_{ik}}$$

- All other steps are exactly the same!

- K-class classification case
- We set $a_k = \mathbf{w}_k \cdot \mathbf{x}^\top$ and probabilities of specific classes to be equal to

$$t_k(\mathbf{x}) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

- The likelihood function is then given by

$$\log p(\mathbf{Y}_m | \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{i=1}^{m} \prod_{k=1}^{K} t_{ik}^{y_{ik}}$$

- All other steps are exactly the same!

Multiclass classification

- K-class classification case
- We set $a_k = \mathbf{w}_k \cdot \mathbf{x}^\top$ and probabilities of specific classes to be equal to

$$t_k(\mathbf{x}) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

- The likelihood function is then given by

$$\log p(\mathbf{Y}_m | \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{i=1}^{m} \prod_{k=1}^{K} t_{ik}^{y_{ik}}$$

- All other steps are exactly the same!

Support Vector Machines and the Relevance Vector Machine

- A state-of-the-art method for classification and regression
- Given data set comprising m input vectors $\mathbf{x}_i$, model has the form

$$f(\mathbf{x}; \mathbf{w}) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- As many kernel functions $K(\cdot, \mathbf{x}_i)$ as examples, i.e. $M = m + 1$ parameters plus kernel width
- Support vector learning: minimize objective function of the form

$$E(\mathbf{w}) = E_D(\mathbf{w}) - \lambda \times (\text{size of margin})$$

  - gives excellent accuracy (particular in classification)
  - as a side-effect, many $\mathbf{w}_i$ get set to zero — the model is sparse
- RVM is simply a Bayesian model utilising the same data dependent kernel basis as the SVM

$$t(\phi) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- A state-of-the-art method for classification and regression
- Given data set comprising m input vectors $\mathbf{x}_i$, model has the form

$$f(\mathbf{x}; \mathbf{w}) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- As many kernel functions $K(\cdot, \mathbf{x}_i)$ as examples, i.e. $M = m + 1$ parameters plus kernel width
- Support vector learning: minimize objective function of the form

$$E(\mathbf{w}) = E_D(\mathbf{w}) - \lambda \times (\text{size of margin})$$

  - gives excellent accuracy (particular in classification)
  - as a side-effect, many $\mathbf{w}_i$ get set to zero — the model is sparse
- RVM is simply a Bayesian model utilising the same data dependent kernel basis as the SVM

$$t(\phi) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- A state-of-the-art method for classification and regression
- Given data set comprising m input vectors $\mathbf{x}_i$, model has the form

$$f(\mathbf{x}; \mathbf{w}) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- As many kernel functions $K(\cdot, \mathbf{x}_i)$ as examples, i.e. $M = m + 1$ parameters plus kernel width
- Support vector learning: minimize objective function of the form

$$E(\mathbf{w}) = E_D(\mathbf{w}) - \lambda \times (\text{size of margin})$$

  - gives excellent accuracy (particular in classification)
  - as a side-effect, many $\mathbf{w}_i$ get set to zero — the model is sparse
- RVM is simply a Bayesian model utilising the same data dependent kernel basis as the SVM

$$t(\phi) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- A state-of-the-art method for classification and regression
- Given data set comprising m input vectors $\mathbf{x}_i$, model has the form

$$f(\mathbf{x}; \mathbf{w}) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- As many kernel functions $K(\cdot, \mathbf{x}_i)$ as examples, i.e. $M = m + 1$ parameters plus kernel width
- Support vector learning: minimize objective function of the form

$$E(\mathbf{w}) = E_D(\mathbf{w}) - \lambda \times (\text{size of margin})$$

  - gives excellent accuracy (particular in classification)
  - as a side-effect, many $\mathbf{w}_i$ get set to zero — the model is sparse
- RVM is simply a Bayesian model utilising the same data dependent kernel basis as the SVM

$$t(\phi) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

- A state-of-the-art method for classification and regression
- Given data set comprising m input vectors $\mathbf{x}_i$, model has the form

$$f(\mathbf{x}; \mathbf{w}) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

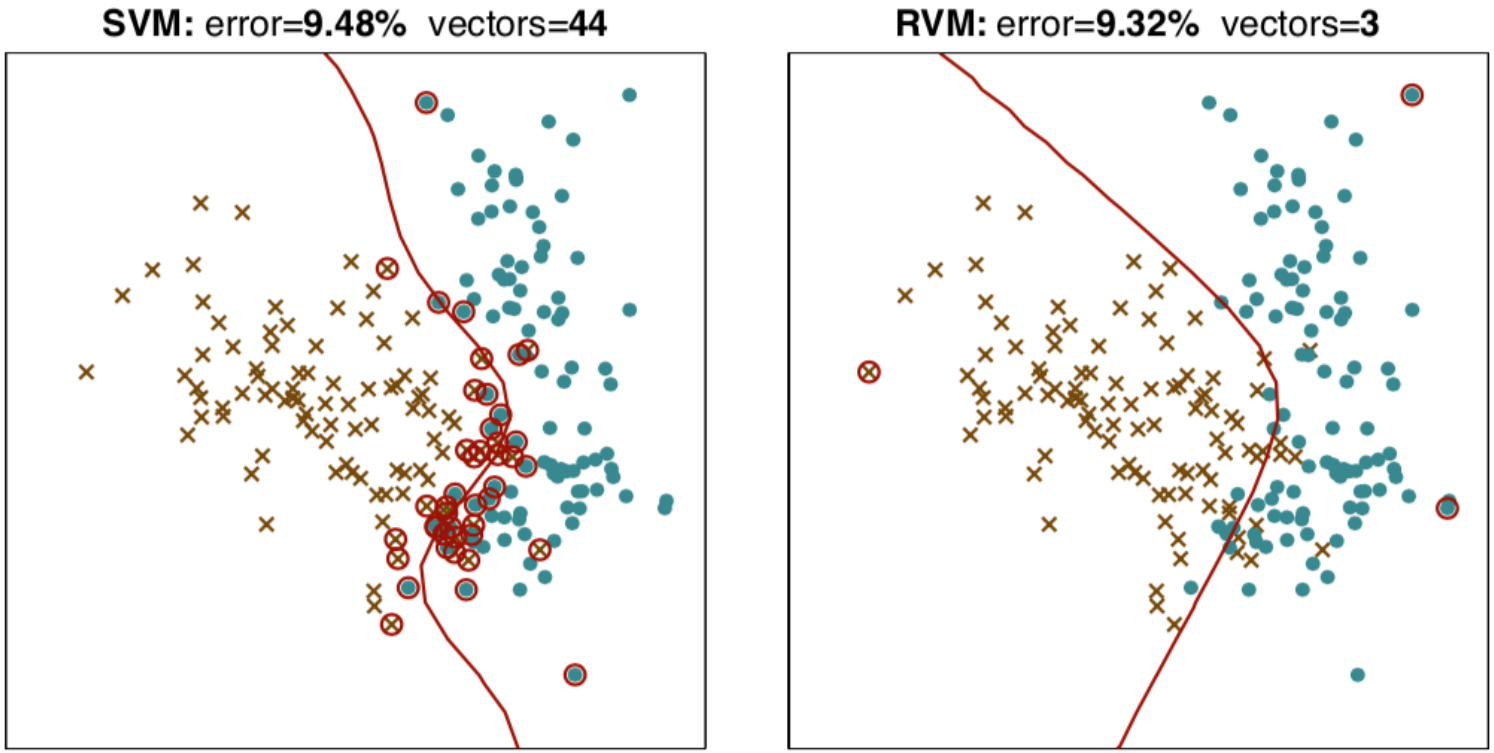
- As many kernel functions $K(\cdot, \mathbf{x}_i)$ as examples, i.e. $M = m + 1$ parameters plus kernel width
- Support vector learning: minimize objective function of the form

$$E(\mathbf{w}) = E_D(\mathbf{w}) - \lambda \times (\text{size of margin})$$

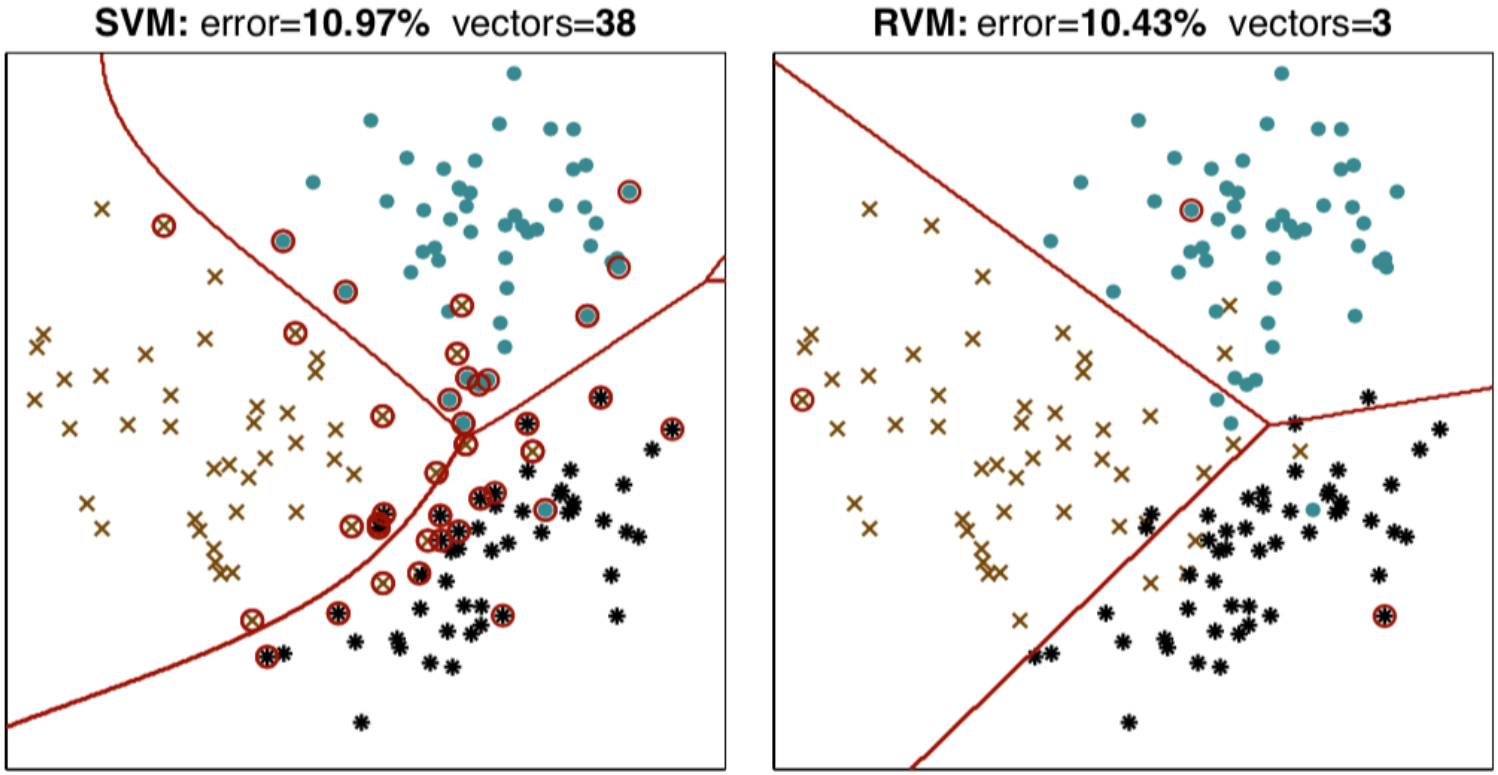
  - gives excellent accuracy (particular in classification)
  - as a side-effect, many $\mathbf{w}_i$ get set to zero — the model is sparse
- RVM is simply a Bayesian model utilising the same data dependent kernel basis as the SVM

$$t(\boldsymbol{\phi}) = \sum_{i=1}^{m} w_i K(\mathbf{x}, \mathbf{x}_i) + w_0$$

RVM Example



RVM Example



Classification Performance Illustration

			errors		vectors	
Data set	***N***	***d***	**SVM**	**RVM**	**SVM**	**RVM**
Pima Diabetes	200	8	20.1%	19.6%	109	4
U.S.P.S.	7291	256	4.4%	5.1%	2540	316
Banana	400	2	10.9%	10.8%	135.2	11.4
Breast Cancer	200	9	26.9%	29.9%	116.7	6.3
Titanic	150	3	22.1%	23.0%	93.7	65.3
Waveform	400	21	10.3%	10.9%	146.4	14.6
German	700	20	22.6%	22.2%	411.2	12.5
Image	1300	18	3.0%	3.9 %	166.6	34.6
Normalised Mean			1.00	**1.08**	1.00	**0.17**

Comparison with the SVM

- General observations:
  - RVM gives better generalization in regression (?)
  - RVM gives better generalization in classification (?)
  - RVM is much sparse (but the SVM is not designed to be sparse)
- There are other advantages of a Bayesian approach:
  - no "nuisance" parameters to set
  - posterior probabilities in classification
  - error bars in regression
  - principled method for more than two classes
  - not limited to Mercer kernels
  - potential to estimate input scale parameters and compare kernels

Comparison with the SVM

- General observations:
  - RVM gives better generalization in regression (?)
  - RVM gives better generalization in classification (?)
  - RVM is much sparse (but the SVM is not designed to be sparse)
- There are other advantages of a Bayesian approach:
  - no "nuisance" parameters to set
  - posterior probabilities in classification
  - error bars in regression
  - principled method for more than two classes
  - not limited to Mercer kernels
  - potential to estimate input scale parameters and compare kernels

Choosing the kernel

- As in the SVM, we must choose the kernel and set any associated parameters
- A Bayesian could compare alternative kernels by computing the fully marginalized probabilities of the data under candidate models, e.g.

$$p(\mathbf{Y}_m|K_1) = \int p(\mathbf{Y}_m|\boldsymbol{\alpha}, K_1)p(\boldsymbol{\alpha}|K_1)d\boldsymbol{\alpha}$$

- We already know this integral isn't analytically tractable
- Approximation via sampling is not feasible for multiple $\boldsymbol{\alpha}$
- Deterministic approximations to this integral have proved inaccurate
- But $p(\mathbf{Y}_m|\boldsymbol{\alpha}_{MAP}, K)$ is a "reasonable" criterion for choosing kernels

Choosing the kernel

- As in the SVM, we must choose the kernel and set any associated parameters
- A Bayesian could compare alternative kernels by computing the fully marginalized probabilities of the data under candidate models, e.g.

$$p(\mathbf{Y}_m|K_1) = \int p(\mathbf{Y}_m|\boldsymbol{\alpha}, K_1)p(\boldsymbol{\alpha}|K_1)d\boldsymbol{\alpha}$$

- We already know this integral isn't analytically tractable
- Approximation via sampling is not feasible for multiple α
- Deterministic approximations to this integral have proved inaccurate
- But $p(\mathbf{Y}_m|\boldsymbol{\alpha}_{MAP}, K)$ is a "reasonable" criterion for choosing kernels

Choosing the kernel

- As in the SVM, we must choose the kernel and set any associated parameters
- A Bayesian could compare alternative kernels by computing the fully marginalized probabilities of the data under candidate models, e.g.

$$p(\mathbf{Y}_m|K_1) = \int p(\mathbf{Y}_m|\boldsymbol{\alpha}, K_1)p(\boldsymbol{\alpha}|K_1)d\boldsymbol{\alpha}$$

- We already know this integral isn't analytically tractable
- Approximation via sampling is not feasible for multiple α
- Deterministic approximations to this integral have proved inaccurate
- But $p(\mathbf{Y}_m|\boldsymbol{\alpha}_{MAP}, K)$ is a "reasonable" criterion for choosing kernels

Choosing the kernel

- As in the SVM, we must choose the kernel and set any associated parameters
- A Bayesian could compare alternative kernels by computing the fully marginalized probabilities of the data under candidate models, e.g.

$$p(\mathbf{Y}_m|K_1) = \int p(\mathbf{Y}_m|\boldsymbol{\alpha}, K_1)p(\boldsymbol{\alpha}|K_1)d\boldsymbol{\alpha}$$

- We already know this integral isn't analytically tractable
- Approximation via sampling is not feasible for multiple $\boldsymbol{\alpha}$
- Deterministic approximations to this integral have proved inaccurate
- But $p(\mathbf{Y}_m|\boldsymbol{\alpha}_{MAP}, K)$ is a "reasonable" criterion for choosing kernels

Choosing the kernel

- As in the SVM, we must choose the kernel and set any associated parameters
- A Bayesian could compare alternative kernels by computing the fully marginalized probabilities of the data under candidate models, e.g.

$$p(\mathbf{Y}_m|K_1) = \int p(\mathbf{Y}_m|\boldsymbol{\alpha}, K_1)p(\boldsymbol{\alpha}|K_1)d\boldsymbol{\alpha}$$

- We already know this integral isn't analytically tractable
- Approximation via sampling is not feasible for multiple $\boldsymbol{\alpha}$
- Deterministic approximations to this integral have proved inaccurate
- But $p(\mathbf{Y}_m|\boldsymbol{\alpha}_{MAP}, K)$ is a "reasonable" criterion for choosing kernels

Choosing the kernel

- As in the SVM, we must choose the kernel and set any associated parameters
- A Bayesian could compare alternative kernels by computing the fully marginalized probabilities of the data under candidate models, e.g.

$$p(\mathbf{Y}_m|K_1) = \int p(\mathbf{Y}_m|\boldsymbol{\alpha}, K_1)p(\boldsymbol{\alpha}|K_1)d\boldsymbol{\alpha}$$

- We already know this integral isn't analytically tractable
- Approximation via sampling is not feasible for multiple $\boldsymbol{\alpha}$
- Deterministic approximations to this integral have proved inaccurate
- But $p(\mathbf{Y}_m|\boldsymbol{\alpha}_{MAP}, K)$ is a "reasonable" criterion for choosing kernels

Choosing the kernel

- E.g. consider choice of η in

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\{-\eta \|\mathbf{x} - \mathbf{x}_i\|^2\}$$

- SVM: cross-validation can be used to set scale parameter η
- RVM: we can optimize the marginal likelihood function w.r.t. η
- Furthermore we can optimize multiple scale parameters η, one for each of the d input dimensions

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\left\{-\sum_{k=1}^{d} \eta_k (\mathbf{x}_k - \mathbf{x}_{ik})^2\right\}$$

- Implementing sparsity of input variables (q.v. Gaussian process models)

Choosing the kernel

- E.g. consider choice of η in

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\{-\eta \|\mathbf{x} - \mathbf{x}_i\|^2\}$$

- SVM: cross-validation can be used to set scale parameter η
- RVM: we can optimize the marginal likelihood function w.r.t. η
- Furthermore we can optimize multiple scale parameters η, one for each of the d input dimensions

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\left\{-\sum_{k=1}^{d} \eta_k (\mathbf{x}_k - \mathbf{x}_{ik})^2\right\}$$

- Implementing sparsity of input variables (q.v. Gaussian process models)

Choosing the kernel

- E.g. consider choice of η in

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\{-\eta \|\mathbf{x} - \mathbf{x}_i\|^2\}$$

- SVM: cross-validation can be used to set scale parameter η
- RVM: we can optimize the marginal likelihood function w.r.t. η
- Furthermore we can optimize multiple scale parameters η, one for each of the d input dimensions

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\left\{-\sum_{k=1}^{d} \eta_k (\mathbf{x}_k - \mathbf{x}_{ik})^2\right\}$$

- Implementing sparsity of input variables (q.v. Gaussian process models)

Choosing the kernel

- E.g. consider choice of η in

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\{-\eta \|\mathbf{x} - \mathbf{x}_i\|^2\}$$

- SVM: cross-validation can be used to set scale parameter η
- RVM: we can optimize the marginal likelihood function w.r.t. η
- Furthermore we can optimize multiple scale parameters η, one for each of the d input dimensions

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\left\{-\sum_{k=1}^{d} \eta_k (\mathbf{x}_k - \mathbf{x}_{ik})^2\right\}$$

- Implementing sparsity of input variables (q.v. Gaussian process models)

Choosing the kernel

- E.g. consider choice of η in

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\{-\eta \|\mathbf{x} - \mathbf{x}_i\|^2\}$$

- SVM: cross-validation can be used to set scale parameter η
- RVM: we can optimize the marginal likelihood function w.r.t. η
- Furthermore we can optimize multiple scale parameters η, one for each of the d input dimensions

$$K(\mathbf{x}, \mathbf{x}_i) = \exp\left\{-\sum_{k=1}^{d} \eta_k (\mathbf{x}_k - \mathbf{x}_{ik})^2\right\}$$

- Implementing sparsity of input variables (q.v. Gaussian process models)

Impact on Regression Benchmarks

- η-RVR: optimization over both $\boldsymbol{\alpha}$ and η

	Test error			# kernels		
Dataset	**SVR**	**RVR**	**η-RVR**	**SVR**	**RVR**	**η-RVR**
Friedman #1	2.92	2.80	0.27	116.6	59.4	11.5
Friedman #2	4140	3505	2593	110.3	6.9	3.9
Friedman #3	0.0202	0.0164	0.0119	106.5	11.5	6.4

- Friedman No. 1: 10-dimensional input space, but functions depends only on variables $1 - 5$. Final η-values shown below

Impact on Regression Benchmarks

- η-RVR: optimization over both $\boldsymbol{\alpha}$ and η

	Test error			# kernels		
Dataset	**SVR**	**RVR**	**η-RVR**	**SVR**	**RVR**	**η-RVR**
Friedman #1	2.92	2.80	0.27	116.6	59.4	11.5
Friedman #2	4140	3505	2593	110.3	6.9	3.9
Friedman #3	0.0202	0.0164	0.0119	106.5	11.5	6.4

- Friedman No. 1: 10-dimensional input space, but functions depends only on variables $1 - 5$. Final η-values shown below