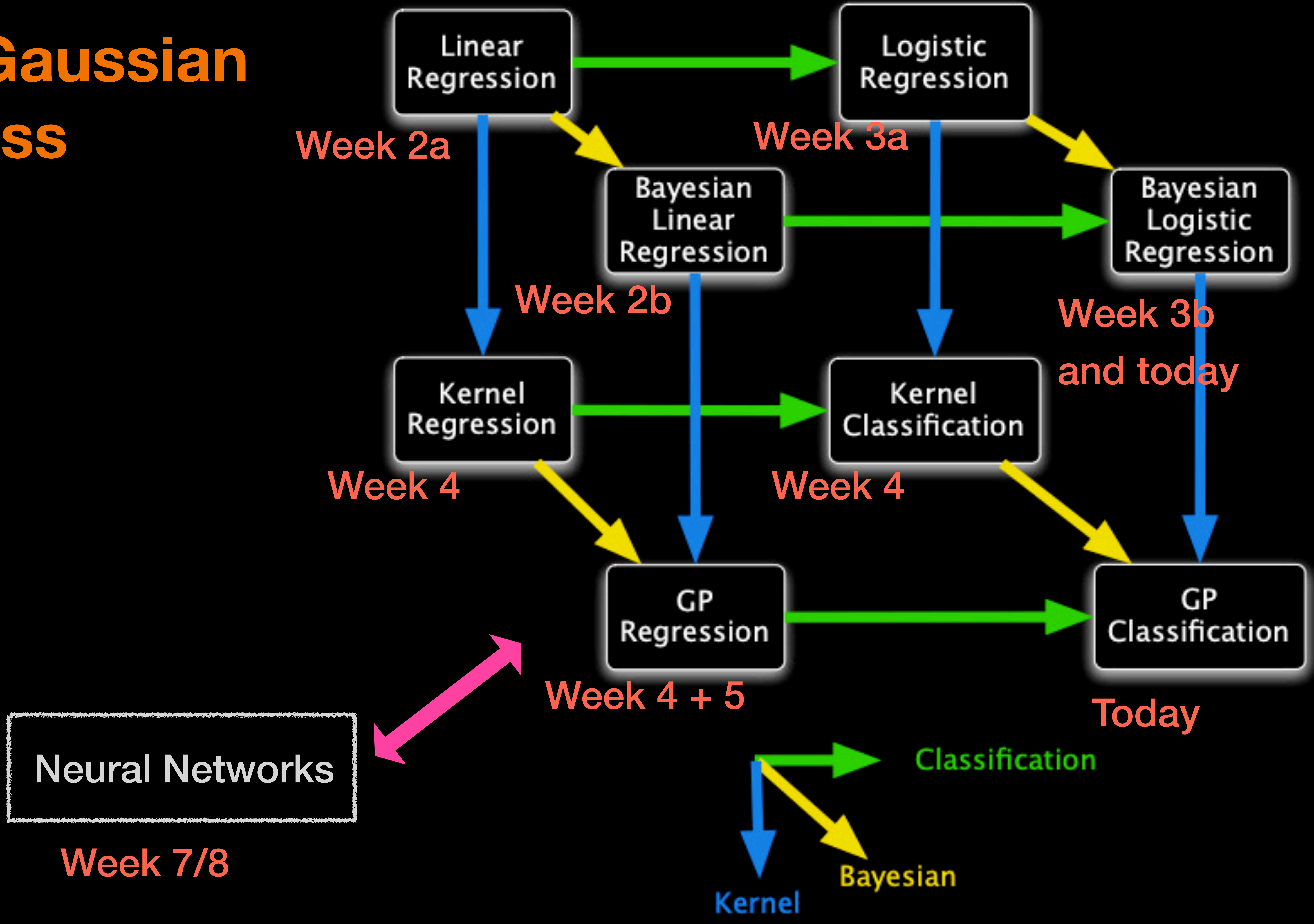
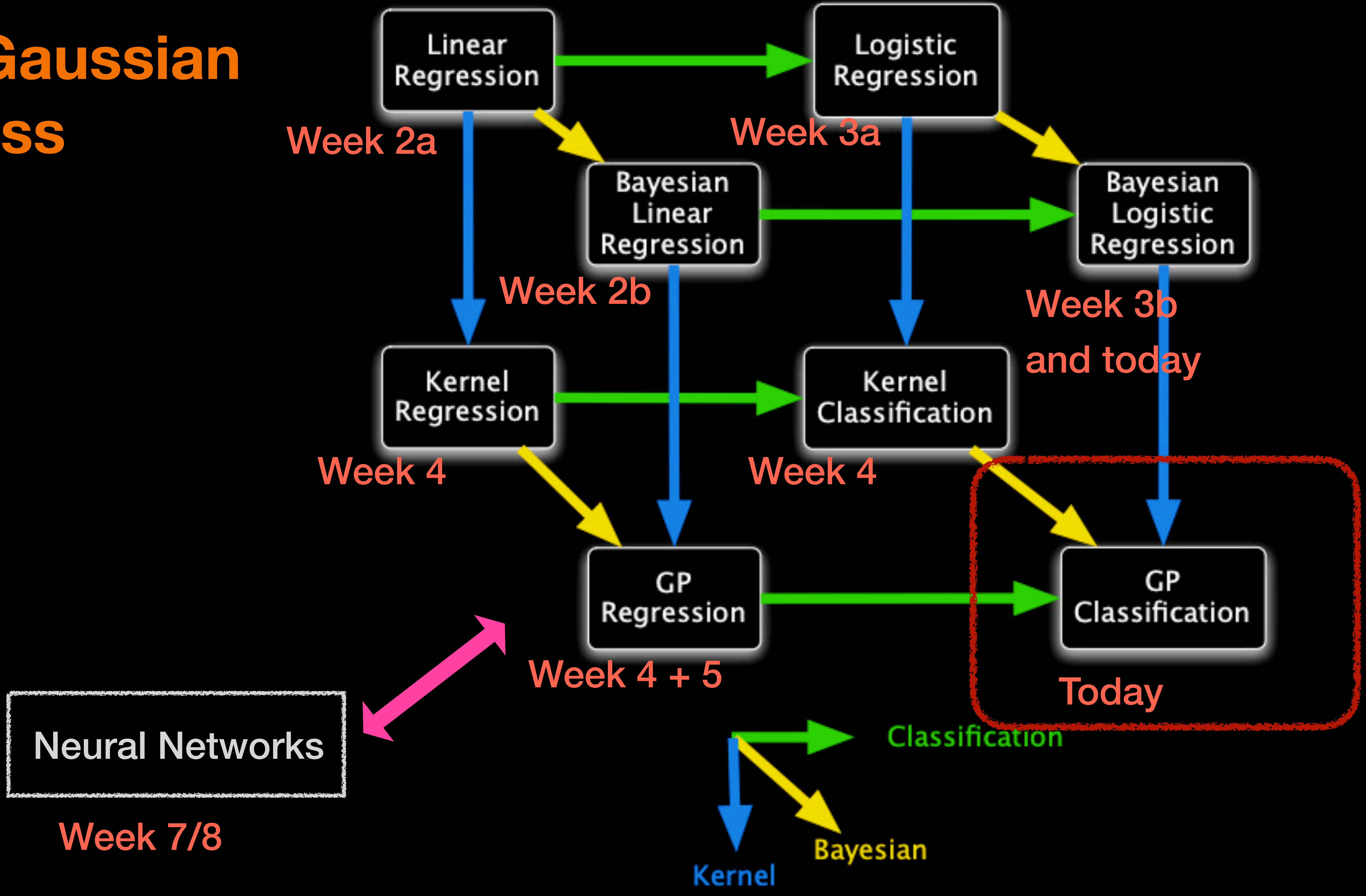
Laplace’s method and GP classification (cont’d)

Week 6a - Statistical ML / Thang Bui / ANU / 2025 S1 - Thanks to Yuan-Sen Ting for many slides

Why Gaussian Process



Why Gaussian Process



Laplace Approximation in Higher Dimensions

Stationary point - local maximum :

$$\nabla f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0} = 0$$

Hessian matrix :

$$\underbrace{\mathbf{A}}_{\mathbb{R}^{m\times m},\ m \text{ number of dimensions}} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

Bishop eq 4.132

Multivariate Gaussian - provided that A is positive definite, i.e. $\mathbf{z}_0$ is a local maximum

$$q(\mathbf{z}) = (2\pi)^{-M/2}|\mathbf{A}|^{-1/2}\exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^{\mathrm{T}}\mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\} = \mathcal{N}(\mathbf{z}\,|\,\mathbf{z}_0, \mathbf{A}^{-1})$$

Bishop eq 4.134, GP Book eq 3.11

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta \mid \theta_{\mathbf{MAP}}, \mathbf{S})$$

Bishop eq 4.144

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} g_n^{y_n} \{1 - g_n\}^{1-y_n}$$

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta \,|\, \mathbf{y}, \mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta \,|\, \theta_{\mathbf{MAP}}, \mathbf{S})$$

Bishop eq 4.144

$$\mathbf{S}^{-1} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z_0}}$$

Bishop eq 4.132

$$p(\theta \,|\, \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} g_n^{y_n} \{1 - g_n\}^{1-y_n}$$

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta \mid \theta_{\mathbf{MAP}}, \mathbf{S})$$

Bishop eq 4.144

$$\mathbf{S}^{-1} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z}_0}$$

Bishop eq 4.132

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0) \cdot \prod_{n=1}^{N} g_n^{y_n} \{1 - g_n\}^{1-y_n}$$

$$-\ln p(\theta \mid \mathbf{y}, \mathbf{X}) = \frac{1}{2}(\theta - \mathbf{m}_0)^T \mathbf{S}_0^{-1}(\theta - \mathbf{m}_0) - \sum_{n=1}^{N} [y_n \ln g_n + (1 - y_n)\ln(1 - g_n)] + \text{const}$$

Bishop eq 4.142

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta \mid \theta_{\mathbf{MAP}}, \mathbf{S})$$

Bishop eq 4.144

$$\mathbf{S}^{-1} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z_0}}$$

Bishop eq 4.132

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} g_n^{y_n} \{1 - g_n\}^{1-y_n}$$

Function of w, $y_n = \sigma\left(\mathbf{w^T}\phi(\mathbf{x_n})\right)$

$$-\ln p(\theta \mid \mathbf{y}, \mathbf{X}) = \frac{1}{2}(\theta - \mathbf{m_0})^T \mathbf{S_0}^{-1}(\theta - \mathbf{m_0}) - \sum_{n=1}^{N} [y_n \ln \overbrace{g_n} + (1 - y_n)\ln(1 - \overbrace{g_n})] + \text{const}$$

Bishop eq 4.142

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta \,|\, \mathbf{y}, \mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta \,|\, \theta_{\mathbf{MAP}}, \mathbf{S})$$

Bishop eq 4.144

$$\mathbf{S}^{-1} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z_0}}$$

Bishop eq 4.132

$$p(\theta \,|\, \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} g_n^{y_n} \{1 - g_n\}^{1-y_n}$$

Function of w, $y_n = \sigma\left(\mathbf{w^T}\phi(\mathbf{x_n})\right)$

$$-\ln p(\theta \,|\, \mathbf{y}, \mathbf{X}) = \frac{1}{2}(\theta - \mathbf{m_0})^T \mathbf{S_0}^{-1}(\theta - \mathbf{m_0}) - \sum_{n=1}^{N} [y_n \ln \overbrace{g_n} + (1 - y_n)\ln(1 - \overbrace{g_n})] + \text{const}$$

Bishop eq 4.142

$$\mathbf{S^{-1}} = -\nabla_\theta \nabla_\theta \log \mathbf{p}(\theta \,|\, \mathbf{t}, \mathbf{X}) =$$

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta\,|\,\mathbf{y},\mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta\,|\,\theta_{\mathbf{MAP}}, \mathbf{S})$$

$$\mathbf{S}^{-1} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z_0}}$$

Bishop eq 4.144

Bishop eq 4.132

$$p(\theta\,|\,\mathbf{y},\mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} g_n^{y_n}\{1-g_n\}^{1-y_n}$$

Function of w, $y_n = \sigma\left(\mathbf{w^T}\phi(\mathbf{x_n})\right)$

$$-\ln p(\theta\,|\,\mathbf{y},\mathbf{X}) = \frac{1}{2}(\theta-\mathbf{m_0})^T\mathbf{S_0}^{-1}(\theta-\mathbf{m_0}) - \sum_{n=1}^{N}[y_n \ln \overbrace{g_n} + (1-y_n)\ln(1-\overbrace{g_n})] + \text{const}$$

Bishop eq 4.142

$$\mathbf{S^{-1}} = -\nabla_\theta\nabla_\theta \log \mathbf{p}(\theta\,|\,\mathbf{t},\mathbf{X}) = \mathbf{S_0^{-1}}$$

Laplace Approximation for Bayesian Logistic Regression

$$p(\theta\,|\,\mathbf{y},\mathbf{X}) \simeq \mathbf{q}(\theta) = \mathcal{N}(\theta\,|\,\theta_{\mathbf{MAP}},\mathbf{S})$$

Bishop eq 4.144

$$\mathbf{S}^{-1} = -\nabla\nabla \ln f(\mathbf{z})\Big|_{\mathbf{z}=\mathbf{z_0}}$$

Bishop eq 4.132

$$p(\theta\,|\,\mathbf{y},\mathbf{X}) \propto \mathcal{N}(\mathbf{m_0},\mathbf{S_0}) \cdot \prod_{n=1}^{N} g_n^{y_n}\{1-g_n\}^{1-y_n}$$

Function of w, $y_n = \sigma\left(\mathbf{w^T}\phi(\mathbf{x_n})\right)$

$$-\ln p(\theta\,|\,\mathbf{y},\mathbf{X}) = \frac{1}{2}(\theta-\mathbf{m_0})^T\mathbf{S_0}^{-1}(\theta-\mathbf{m_0}) - \sum_{n=1}^{N}[y_n \ln \overbrace{g_n} + (1-y_n)\ln(1-\overbrace{g_n})] + \text{const}$$

Bishop eq 4.142

$$\downarrow \nabla_\theta$$

$$\sum_{n=1}^{N}(g_n - y_n)\boldsymbol{\phi_n}$$

$$\downarrow \nabla_\theta$$

$$\mathbf{S^{-1}} = -\nabla_\theta\nabla_\theta \log \mathbf{p}(\theta\,|\,\mathbf{t},\mathbf{X}) = \mathbf{S_0^{-1}} + \sum_{n=1}^{N} g_n(1-g_n)\boldsymbol{\phi}_n\boldsymbol{\phi}_n^T$$

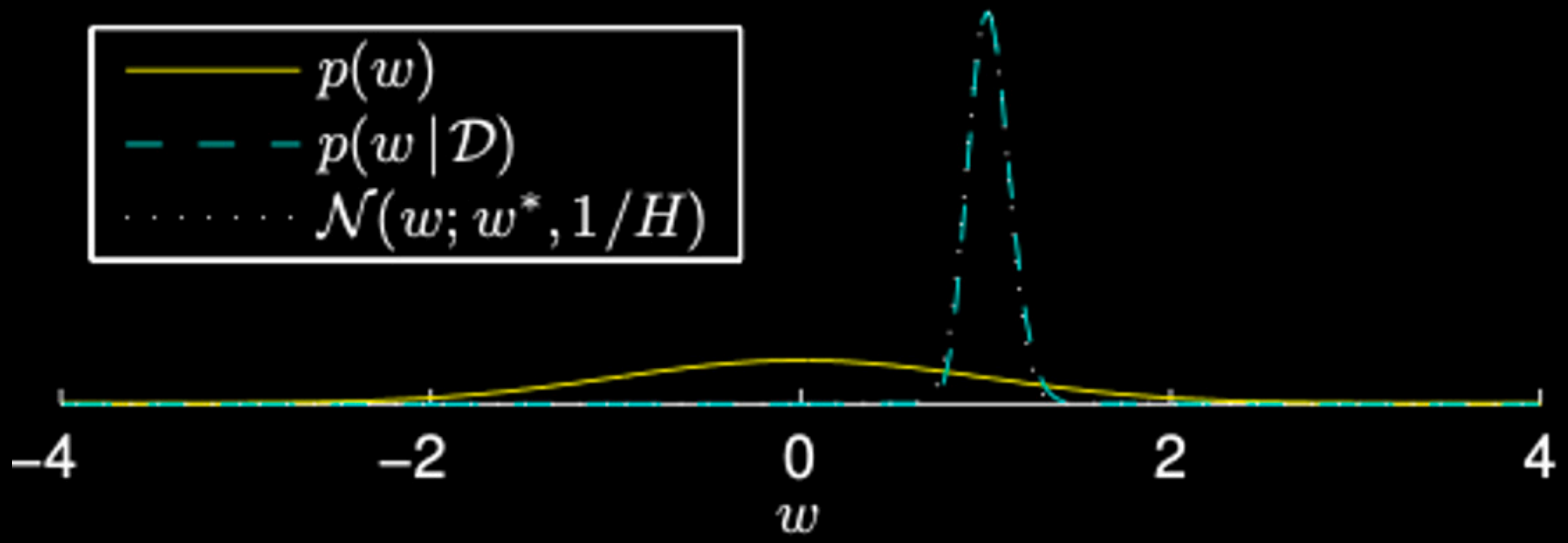
Bishop eq 4.143

Why Laplacian Approximation Works Well

Recall

$$p(\theta \,|\, \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} \sigma(\theta^T \boldsymbol{\phi}(\mathbf{x_n}))^{y_n} \left\{1 - \sigma(\theta^T \boldsymbol{\phi}(\mathbf{x_n})\right\}^{1-y_n}$$

$N = 500$



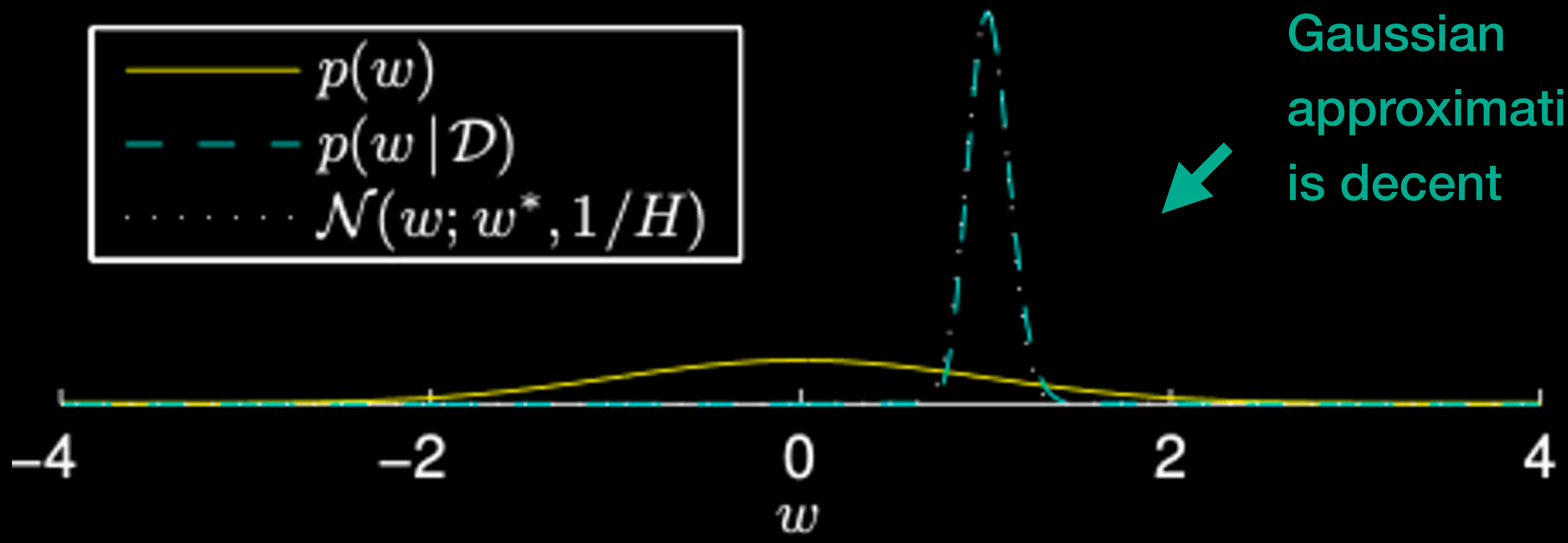
Example courtesy of Edinburgh MLPR course
https://www.inf.ed.ac.uk/teaching/courses/mlpr/2016/notes/w8a_bayes_logistic_regression_laplace.pdf

Why Laplacian Approximation Works Well

Recall

$$p(\theta \mid \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} \sigma(\theta^T \boldsymbol{\phi}(\mathbf{x_n}))^{y_n} \left\{1 - \sigma(\theta^T \boldsymbol{\phi}(\mathbf{x_n}))\right\}^{1-y_n}$$

$N = 500$



Gaussian approximation is decent

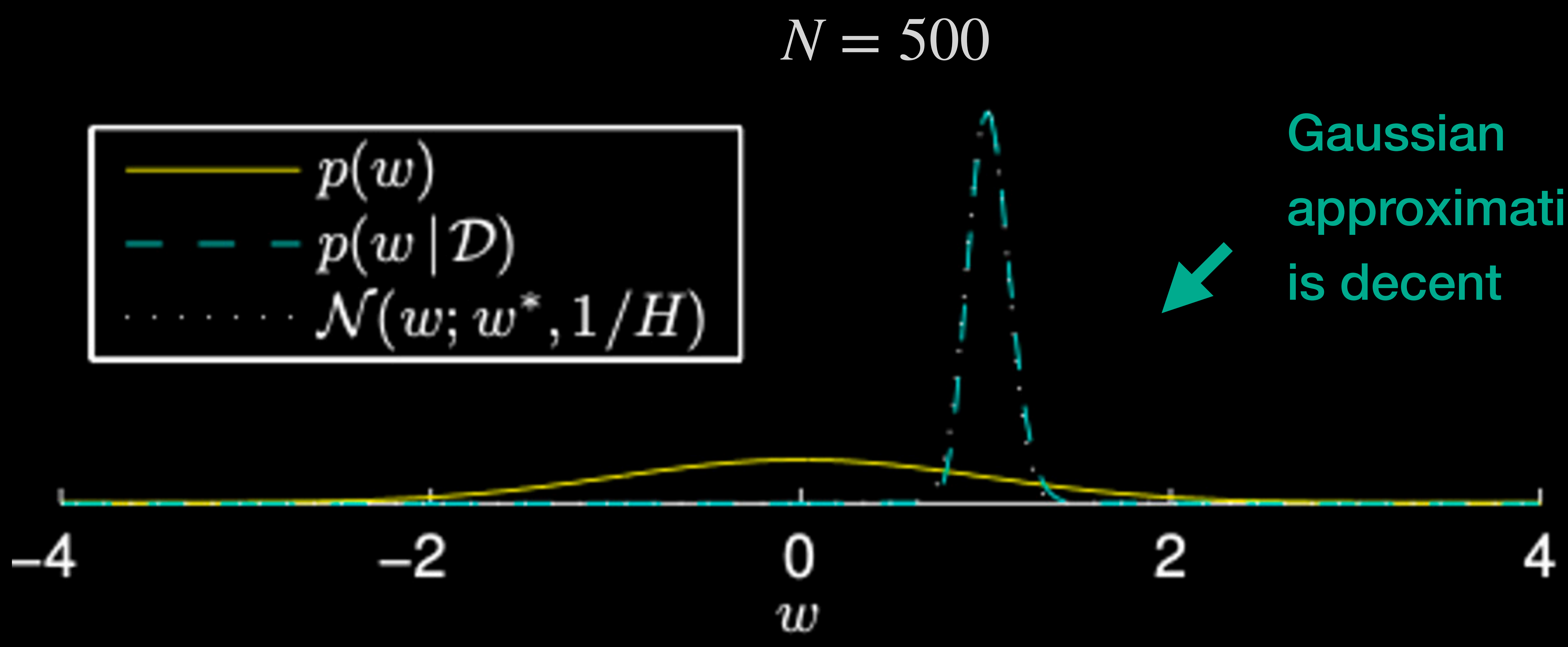
Example courtesy of Edinburgh MLPR course
https://www.inf.ed.ac.uk/teaching/courses/mlpr/2016/notes/w8a_bayes_logistic_regression_laplace.pdf

Why Laplacian Approximation Works Well

Recall

$$p(\theta \,|\, \mathbf{y}, \mathbf{X}) \propto \mathcal{N}(\mathbf{m_0}, \mathbf{S_0}) \cdot \prod_{n=1}^{N} \sigma(\theta^T \boldsymbol{\phi}(\mathbf{x_n}))^{y_n} \left\{1 - \sigma(\theta^T \boldsymbol{\phi}(\mathbf{x_n}))\right\}^{1-y_n}$$

This function is concave and have a unique maximum (exercise)



Gaussian approximation is decent

Example courtesy of Edinburgh MLPR course
https://www.inf.ed.ac.uk/teaching/courses/mlpr/2016/notes/w8a_bayes_logistic_regression_laplace.pdf

Predictive Distribution for Bayesian Logistic Regression

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \mid \mathbf{x}^*, \theta)}_{\text{Sigmoid}} \, \underbrace{\mathbf{p}(\theta \mid \mathbf{y}, \mathbf{X})}_{\approx \mathcal{N}(\theta; \theta_{\mathbf{MAP}}, \mathbf{S})} \, \mathrm{d}\theta$$

Predictive Distribution for Bayesian Logistic Regression

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \mid \mathbf{x}^*, \theta)}_{\text{Sigmoid}} \, \underbrace{\mathbf{p}(\theta \mid \mathbf{y}, \mathbf{X})}_{\approx \mathcal{N}(\theta;\, \theta_{\mathbf{MAP}}, \mathbf{S})} \, \mathrm{d}\theta$$

Still analytically intractable

Probit Function

Recall that, the Sigmoid “logistic” function is used in logistic regression because it falls out naturally from the idea of log odd and can be regarded as generalised linear regression

Probit Function

Recall that, the Sigmoid “logistic” function is used in logistic regression because it falls out naturally from the idea of log odd and can be regarded as generalised linear regression

Probit function (closely related to the erf function)

$$\Phi(x) \equiv \int_{-\infty}^{x} \mathcal{N}(x \mid 0,1)\,\mathrm{d}x$$

Bishop eq 4.114

Probit Function

Recall that, the Sigmoid "logistic" function is used in logistic regression because it falls out naturally from the idea of log odd and can be regarded as generalised linear regression

Probit function (closely related to the erf function)

$$\Phi(x) \equiv \int_{-\infty}^{x} \mathcal{N}(x \,|\, 0,1)\, \mathrm{d}x$$

Bishop eq 4.114

is a close analog, and yet makes the previous integral possible

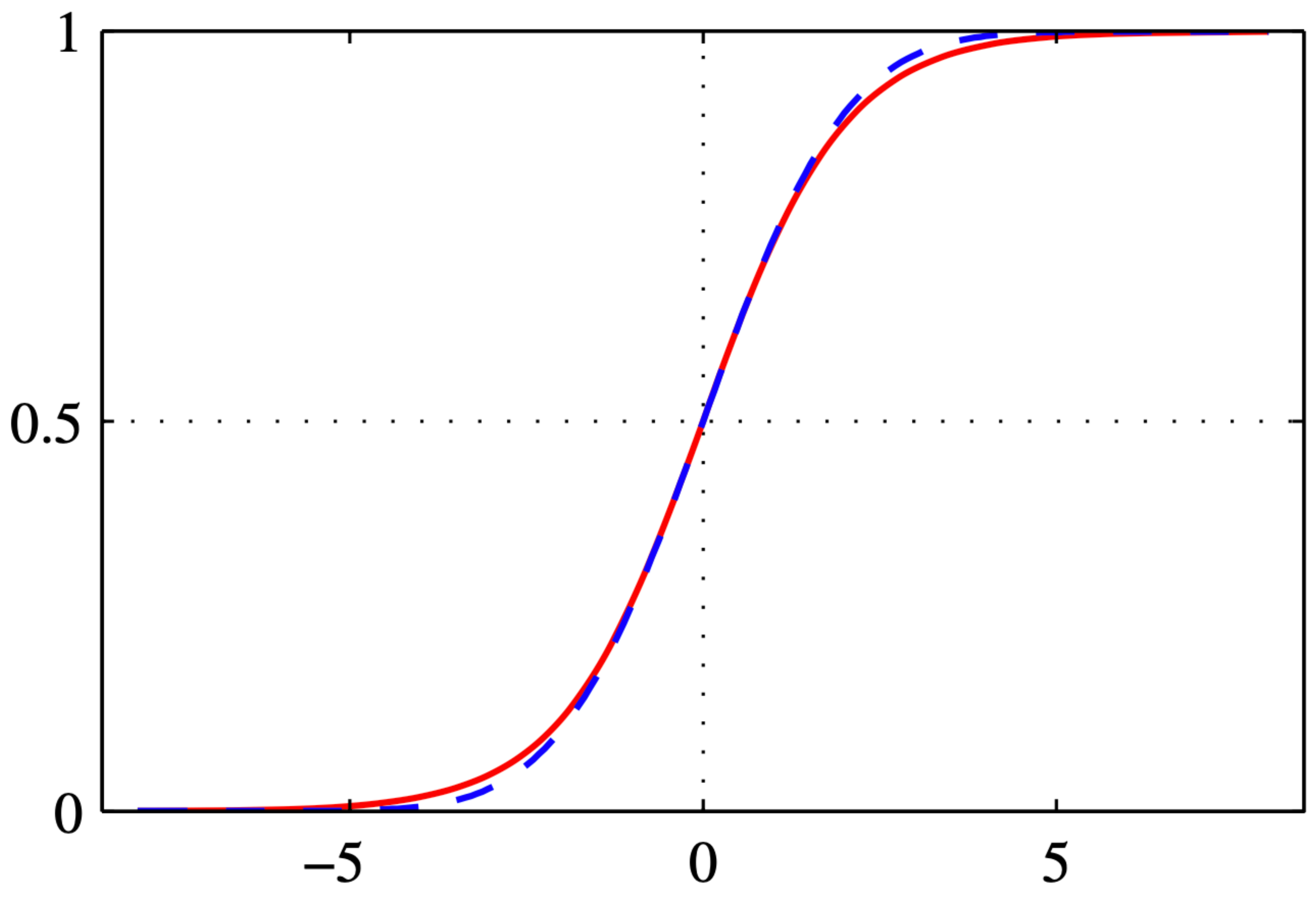
$$\int \Phi(\lambda a)\, \mathcal{N}(a \,|\, \mu, \sigma^2)\, \mathrm{d}a = \Phi\left(\frac{\mu}{\sqrt{\lambda^{-2} + \sigma^2}}\right)$$

Bishop eq 4.152

Approximating Sigmoid Function with Probit Function

$$\sigma(a) \simeq \Phi(\lambda a), \quad \text{with} \quad \lambda^2 = \pi/8$$

Figure 4.9 Plot of the logistic sigmoid function $\sigma(a)$ defined by (4.59), shown in red, together with the scaled probit function $\Phi(\lambda a)$, for $\lambda^2 = \pi/8$, shown in dashed blue, where $\Phi(a)$ is defined by (4.114). The scaling factor $\pi/8$ is chosen so that the derivatives of the two curves are equal for $a = 0$.



Approximating Sigmoid Function with Probit Function

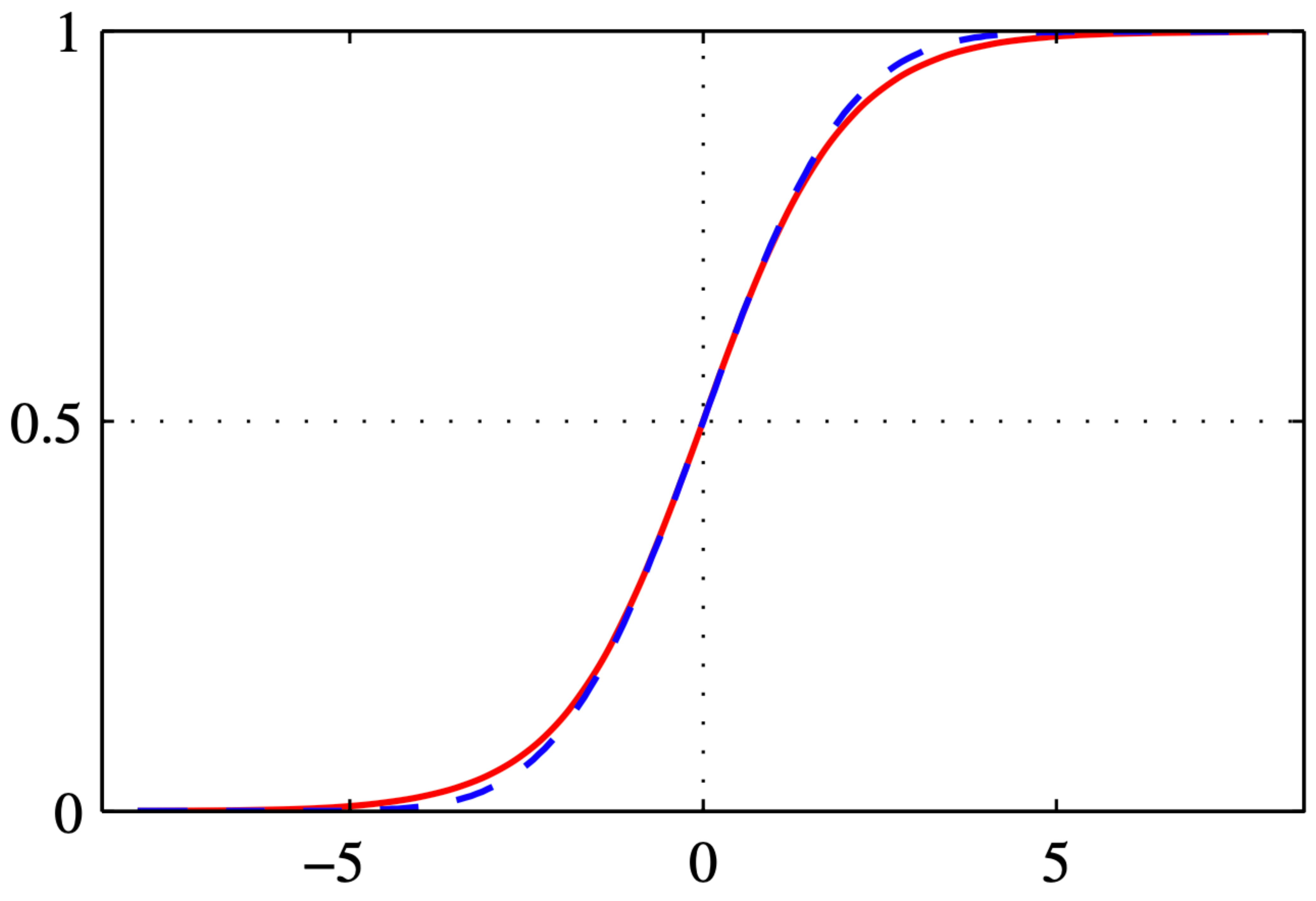
$\sigma(a) \simeq \Phi(\lambda a)$, with $\lambda^2 = \pi/8$

$$\int \sigma(a)\mathcal{N}(a \mid \mu, \sigma^2)\mathrm{d}a \simeq \sigma(\kappa(\sigma^2)\,\mu)$$

$$\kappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

Bishop eq 4.153

Figure 4.9 Plot of the logistic sigmoid function $\sigma(a)$ defined by (4.59), shown in red, together with the scaled probit function $\Phi(\lambda a)$, for $\lambda^2 = \pi/8$, shown in dashed blue, where $\Phi(a)$ is defined by (4.114). The scaling factor $\pi/8$ is chosen so that the derivatives of the two curves are equal for $a = 0$.



Predictive distribution for Bayesian Logistic Regression

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \mid \mathbf{x}^*, \theta)}_{\sigma\left(\theta^T \phi(\mathbf{x}^*)\right)} \underbrace{\mathbf{p}(\theta \mid \mathbf{y}, \mathbf{X})}_{\approx q(\theta) = \mathcal{N}(\theta \mid \theta_{\mathbf{MAP}}, \mathbf{S})} \, \mathrm{d}\theta$$

Let

$$a = \theta^T \phi(\mathbf{x}^*)$$

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \sigma(a) \, p(a) \, \mathrm{d}a$$

Predictive distribution for Bayesian Logistic Regression

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \mid \mathbf{x}^*, \theta)}_{\sigma\left(\theta^T \phi(\mathbf{x}^*)\right)} \underbrace{\mathbf{p}(\theta \mid \mathbf{y}, \mathbf{X})}_{\approx q(\theta) = \mathcal{N}(\theta \mid \theta_{\mathbf{MAP}}, \mathbf{S})} \, \mathrm{d}\theta$$

Let

$$a = \theta^T \phi(\mathbf{x}^*)$$

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \sigma(a) \underbrace{p(a)}_{\substack{\text{Also Gaussian} \\ \mathcal{N}(a \mid \mu_a, \sigma_a^2)}} \mathrm{d}a$$

Predictive distribution for Bayesian Logistic Regression

$$p(y^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \,|\, \mathbf{x}^*, \theta)}_{\sigma\left(\theta^T \phi(\mathbf{x}^*)\right)} \underbrace{\mathbf{p}(\theta \,|\, \mathbf{y}, \mathbf{X})}_{\approx q(\theta) = \mathcal{N}(\theta \,|\, \theta_{\mathbf{MAP}}, \mathbf{S})} \, \mathrm{d}\theta$$

Let

$$a = \theta^T \phi(\mathbf{x}^*)$$

$$p(y^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \sigma(a) \underbrace{p(a)}_{\text{Also Gaussian } \mathcal{N}(a \,|\, \mu_a, \sigma_a^2)} \, \mathrm{d}a$$

$$\mu_a = \theta_{\mathrm{MAP}}^T \phi(\mathbf{x}^*)$$

$$\sigma_a^2 = \phi^T(\mathbf{x}^*) \, \mathbf{S} \, \phi(\mathbf{x}^*)$$

Bishop eq 4.147, 4.151

Predictive distribution for Bayesian Logistic Regression

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \mid \mathbf{x}^*, \theta)}_{\sigma\left(\theta^T \phi(\mathbf{x}^*)\right)} \underbrace{\mathbf{p}(\theta \mid \mathbf{y}, \mathbf{X})}_{\approx q(\theta) = \mathcal{N}(\theta \mid \theta_{\mathbf{MAP}}, \mathbf{S})} \, \mathrm{d}\theta$$

Let

$$a = \theta^T \phi(\mathbf{x}^*)$$

$$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \sigma(a) \underbrace{p(a)}_{\substack{\text{Also Gaussian} \\ \mathcal{N}(a \mid \mu_a, \sigma_a^2)}} \mathrm{d}a$$

$$\mu_a = \theta_{\mathrm{MAP}}^T \phi(\mathbf{x}^*)$$

$$\sigma_a^2 = \phi^T(\mathbf{x}^*) \, \mathbf{S} \, \phi(\mathbf{x}^*)$$

Bishop eq 4.147, 4.151

$$\simeq \sigma\left(\left(1 + \frac{\pi \sigma_a^2}{8}\right)^{-1/2} \mu_a\right)$$

Bishop eq 4.153

Gaussian Process for Classification

Recall in Gaussian Process Regression

$$p(\mathbf{f} \mid \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})$$

Gaussian Process for Classification

Recall in Gaussian Process Regression

$$p(\mathbf{f} \mid \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})$$

we have $y_n \in \{0,1\}$ in classification. We use the same approach as in logistic classification

Gaussian Process for Classification

Recall in Gaussian Process Regression

$$p(\mathbf{f} \mid \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})$$

we have $y_n \in \{0,1\}$ in classification. We use the same approach as in logistic classification

Key idea — using GP as a intermediate step

Gaussian Process for Classification

Recall in Gaussian Process Regression

$$p(\mathbf{f} \,|\, \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})$$

we have $y_n \in \{0,1\}$ in classification. We use the same approach as in logistic classification

Key idea — using GP as a intermediate step

Recall in logistic regression

$$g(\mathbf{x}) = \sigma\left(\theta^{\mathbf{T}} \phi(\mathbf{x})\right)$$

Gaussian Process for Classification

Recall in Gaussian Process Regression

$$p(\mathbf{f} \,|\, \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})$$

we have $y_n \in \{0,1\}$ in classification. We use the same approach as in logistic classification

Key idea — using GP as a intermediate step

And the "squash" it with a sigmoid function

$$g(\mathbf{x}) = \sigma\big(f(\mathbf{x})\big)$$

$$p(y_n \,|\, f, \mathbf{x}_n) = \sigma\left(f(\mathbf{x_n})\right)^{y_n} \left(1 - \sigma(f(\mathbf{x_n}))\right)^{1-y_n}$$

Recall in logistic regression

$$g(\mathbf{x}) = \sigma\big(\theta^{\mathbf{T}} \phi(\mathbf{x})\big)$$

Bishop eq 6.73

Gaussian Process for Classification

Recall in Gaussian Process Regression

$$p(\mathbf{f} \,|\, \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})$$

we have $y_n \in \{0,1\}$ in classification. We use the same approach as in logistic classification

Key idea — using GP as a intermediate step

And the "squash" it with a sigmoid function

$$g(\mathbf{x}) = \sigma\big(f(\mathbf{x})\big)$$

$$p(y_n \,|\, f, \mathbf{x}_n) = \sigma\left(\boxed{f(\mathbf{x_n})}\right)^{y_n} \left(1 - \sigma(f(\mathbf{x_n}))\right)^{1-y_n}$$

Bishop eq 6.73

Recall in logistic regression

$$g(\mathbf{x}) = \sigma\left(\boxed{\theta^{\mathbf{T}} \phi(\mathbf{x})}\right)$$

Substituting the linear model with Gaussian Process

Gaussian Process for Classification

Input Variable

$$[\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_n]$$

Gaussian Process for Classification

Input Variable

$$[\mathbf{x_1}, \mathbf{x_2}, \ldots \mathbf{x_n}]$$

Gaussian Process

Intermediate Variable

$$\mathbf{f} = [f_1, f_2, \ldots f_n]$$

Gaussian Process for Classification

Input Variable

$$[\mathbf{x_1}, \mathbf{x_2}, \ldots \mathbf{x_n}]$$

Gaussian Process

Response Function, e.g. Sigmoid

Intermediate Variable

$$\mathbf{f} = [f_1, f_2, \ldots f_n]$$

Target Variable

$$\mathbf{y} = [y_1, y_2, \ldots y_n]$$

Gaussian Process for the Intermediate Variable

Bishop eq 6.74

$$p(\mathbf{f} \mid \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \underbrace{\mathbf{K}}_{\text{Kernel (X, X)}})$$

Bishop eq 6.75

$$\mathbf{K}_{nm} = k(\mathbf{x}_n, \mathbf{x}_m \mid \underbrace{\boldsymbol{\theta}}_{\text{Kernel hyperparameters}})$$

Gaussian Process for the Intermediate Variable

Bishop eq 6.74

$$p(\mathbf{f} \mid \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \underbrace{\mathbf{K}}_{\text{Kernel (X, X)}})$$

Bishop eq 6.75

$$\mathbf{K}_{nm} = k(\mathbf{x}_n, \mathbf{x}_m \mid \underbrace{\boldsymbol{\theta}}_{\text{Kernel hyperparameters}})$$

Recall from Gaussian Process Regression that

$$\boxed{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y})} = \mathcal{N}(f^* \mid m(\mathbf{x}^*), \sigma^2(\mathbf{x}^*))$$

Gaussian Process for the Intermediate Variable

Bishop eq 6.74

$$p(\mathbf{f} \,|\, \mathbf{X}) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \underbrace{\mathbf{K}}_{\text{Kernel (X, X)}})$$

Bishop eq 6.75

$$\mathbf{K}_{nm} = k(\mathbf{x}_n, \mathbf{x}_m \,|\, \underbrace{\boldsymbol{\theta}}_{\text{Kernel hyperparameters}})$$

Recall from Gaussian Process Regression that

$$\boxed{p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y})} = \mathcal{N}(f^* \,|\, m(\mathbf{x}^*), \sigma^2(\mathbf{x}^*))$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\,(k(\mathbf{X}, \mathbf{X})^{-1} + \sigma^2 \mathrm{I}_N)^{-1}\,\mathbf{y}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\,(k(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathrm{I})^{-1}\,k(\mathbf{X}, \mathbf{x}^*)$$

Bishop eq 6.78

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \mid \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \mid \mathbf{X}) + \text{const}\,.$$

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \mid \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \mid \mathbf{X}) + \text{const}\,.$$

$$\mathbf{y}^T \mathbf{f} - \sum_{n=1}^{N} \ln(1 + e^{f_n})$$

Bishop eq 6.79

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f}\,|\,\mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y}\,|\,\mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f}\,|\,\mathbf{X}) + \text{const}\,.$$

$$\mathbf{y}^T\mathbf{f} - \sum_{n=1}^{N} \ln(1 + e^{f_n})$$

Bishop eq 6.79

$$-\frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f} - \frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln|\,\mathbf{K}\,|$$

Bishop eq 6.80, GP Book eq 3.12

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \,|\, \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \,|\, \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \,|\, \mathbf{X}) + \text{const}\,.$$

$$\mathbf{y}^T\mathbf{f} - \sum_{n=1}^{N} \ln(1 + e^{f_n})$$

Bishop eq 6.79

$$-\frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f} - \frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln|\mathbf{K}|$$

Bishop eq 6.80, GP Book eq 3.12

$$\nabla_{\mathbf{f}} \ln p(\mathbf{f} \,|\, \mathbf{X}, \mathbf{y}) = \mathbf{y} - \sigma(\mathbf{f}) - \mathbf{K}^{-1}\mathbf{f} = 0$$

Bishop eq 6.81, GP Book eq 3.13, 3.15

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f}\,|\,\mathbf{X},\mathbf{y}) = \ln p(\mathbf{y}\,|\,\mathbf{f},\mathbf{X}) + \ln p(\mathbf{f}\,|\,\mathbf{X}) + \text{const}\,.$$

$$\mathbf{y}^T\mathbf{f} - \sum_{n=1}^{N} \ln(1+e^{f_n})$$

Bishop eq 6.79

$$-\frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f} - \frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln|\mathbf{K}|$$

Bishop eq 6.80, GP Book eq 3.12

$$\nabla_{\mathbf{f}} \ln p(\mathbf{f}\,|\,\mathbf{X},\mathbf{y}) = \mathbf{y} - \sigma(\mathbf{f}) - \mathbf{K}^{-1}\mathbf{f} = 0$$

Bishop eq 6.81, GP Book eq 3.13, 3.15

$$\Rightarrow \quad \boxed{\mathbf{f}_{\text{MAP}} = \mathbf{K}(\mathbf{y} - \sigma(\mathbf{f}_{\text{MAP}}))}$$

Bishop eq 6.84, GP Book eq 3.17

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f}\,|\,\mathbf{X},\mathbf{y}) = \ln p(\mathbf{y}\,|\,\mathbf{f},\mathbf{X}) + \ln p(\mathbf{f}\,|\,\mathbf{X}) + \text{const}\,.$$

$$\mathbf{y}^T\mathbf{f} - \sum_{n=1}^{N} \ln(1+e^{f_n})$$

Bishop eq 6.79

$$-\frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f} - \frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln|\mathbf{K}|$$

Bishop eq 6.80, GP Book eq 3.12

$$\nabla_{\mathbf{f}} \ln p(\mathbf{f}\,|\,\mathbf{X},\mathbf{y}) = \mathbf{y} - \sigma(\mathbf{f}) - \mathbf{K}^{-1}\mathbf{f} = 0$$

Bishop eq 6.81, GP Book eq 3.13, 3.15

$$\boxed{\mathbf{f}_{\mathrm{MAP}} = \mathbf{K}(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))}$$

Bishop eq 6.84, GP Book eq 3.17

Implicit function of $\mathbf{f}_{\mathrm{MAP}}$, e.g. solve with Newton's method

See GP Book eq 3.18-3.19, Algorithm 3.1

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \mid \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \mid \mathbf{X}) + \text{const}\,.$$

$$\Rightarrow \quad \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \mathbf{y} - \sigma(\mathbf{f}) - \mathbf{K}^{-1}\mathbf{f} = 0$$

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \mid \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \mid \mathbf{X}) + \text{const}\,.$$

$$\Rightarrow \quad \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \mathbf{y} - \boxed{\sigma(\mathbf{f})} - \boxed{\mathbf{K}^{-1}\mathbf{f}} = 0$$

$$\Rightarrow \quad -\nabla_{\mathbf{f}} \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) \Big|_{\mathbf{f}_{\mathrm{MAP}}} = \boxed{\operatorname{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma\left(\mathbf{f}_{\mathrm{MAP}})\right)\right\}} + \boxed{\mathbf{K}^{-1}} \equiv \mathbf{H}$$

Bishop eq 6.82, GP Book eq 3.14, 3.15

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \mid \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \mid \mathbf{X}) + \text{const}\,.$$

$$\Rightarrow \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \mathbf{y} - \boxed{\sigma(\mathbf{f})} - \boxed{\mathbf{K}^{-1}\mathbf{f}} = 0$$

Factorizes into a diagonal matrix because the sample is i.i.d

$$\Rightarrow -\nabla_{\mathbf{f}} \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) \Big|_{\mathbf{f}_{\text{MAP}}} = \boxed{\text{diag}\left\{\sigma(\mathbf{f}_{\text{MAP}})(1 - \sigma\left(\mathbf{f}_{\text{MAP}}\right))\right\}} + \boxed{\mathbf{K}^{-1}} \equiv \mathbf{H}$$

Bishop eq 6.82, GP Book eq 3.14, 3.15

Laplace Approximation for Gaussian Process Classification

$$\ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \ln p(\mathbf{y} \mid \mathbf{f}, \mathbf{X}) + \ln p(\mathbf{f} \mid \mathbf{X}) + \text{const}\,.$$

$$\Rightarrow \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \mathbf{y} - \sigma(\mathbf{f}) - \mathbf{K}^{-1}\mathbf{f} = 0$$

Factorizes into a diagonal matrix because the sample is i.i.d

$$\Rightarrow -\nabla_{\mathbf{f}} \nabla_{\mathbf{f}} \ln p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) \Big|_{\mathbf{f}_{\mathrm{MAP}}} = \operatorname{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + \mathbf{K}^{-1} \equiv \mathbf{H}$$

Bishop eq 6.82, GP Book eq 3.14, 3.15

Laplace Approximation $\quad q(\mathbf{f}) \simeq p(\mathbf{f} \mid \mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{f}; \mathbf{f}_{\mathrm{MAP}}, \mathbf{H}^{-1})$

Bishop eq 6.86

One More Layer Up …

$$p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{f})\, p(\mathbf{f} \,|\, \mathbf{X}, \mathbf{y})\, \mathrm{d}\mathbf{f}$$

One More Layer Up …

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})\, \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})}\, \mathrm{d}\mathbf{f}$$

$$\mathbf{f}_{\mathrm{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))$$

$$\mathbf{H} = \mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

One More Layer Up ...

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))} \, \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})} \, \mathrm{d}\mathbf{f}$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, \mathbf{f}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\mathrm{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))$$

$$\mathbf{H} = \mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

One More Layer Up …

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})} \, \mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, \mathbf{f}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\mathrm{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))$$

$$\mathbf{H} = \mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

One More Layer Up …

$$p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \,|\, \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})} \,\mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, \mathbf{f}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\mathrm{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))$$

$$\mathbf{H} = \mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

Bishop eq 2.115

One More Layer Up …

$$p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \,|\, \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})} \, \mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, \mathbf{f}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\mathrm{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))$$

$$\mathbf{H} = \mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \,|\, \boldsymbol{\mu}, \mathbf{H}^{-1})$$

$$p(y \,|\, \mathbf{x}) = \mathcal{N}(\mathbf{y} \,|\, \mathbf{A}\mathbf{x} + b, \sigma^2)$$

Bishop eq 2.115

One More Layer Up ...

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*; m(\mathbf{x}^*), \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f}; \mathbf{f}_{\text{MAP}}, \mathbf{H}^{-1})} \, \mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, \mathbf{f}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\text{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\text{MAP}}))$$

$$\mathbf{H} = \operatorname{diag}\left\{\sigma(\mathbf{f}_{\text{MAP}})(1 - \sigma(\mathbf{f}_{\text{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \mathbf{H}^{-1})$$

$$p(y \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\mathbf{x} + b, \sigma^2)$$

$$\Rightarrow \quad p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \sigma^2 + \mathbf{A}\mathbf{H}^{-1}\mathbf{A}^T)$$

Bishop eq 2.115

One More Layer Up …

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))}\, \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})}\, \mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1} \boxed{\mathbf{f}}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\mathrm{MAP}} = \boxed{k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))}$$

$$\mathbf{H} = \mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boxed{\boldsymbol{\mu}}, \mathbf{H}^{-1})$$

$$p(y \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid \boxed{\mathbf{A}\mathbf{x}} + b, \sigma^2)$$

$$\Rightarrow\; p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \boxed{\mathbf{A}\boldsymbol{\mu} + \mathbf{b}}, \sigma^2 + \mathbf{A}\mathbf{H}^{-1}\mathbf{A}^T)$$

Bishop eq 2.115

One More Layer Up …

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})} \,\mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1} \mathbf{f}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)$$

$$\mathbf{f}_{\mathrm{MAP}} = k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))$$

$$\mathbf{H} = \mathrm{diag}\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\} + k(\mathbf{X}, \mathbf{X})^{-1}$$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \mathbf{H}^{-1})$$

$$p(y \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\mathbf{x} + b, \sigma^2)$$

$$\Rightarrow \quad p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \sigma^2 + \mathbf{A}\mathbf{H}^{-1}\mathbf{A}^T)$$

Bishop eq 2.115

$\Rightarrow$

$$c = k(\mathbf{x}^*, \mathbf{X})\big(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}})\big)$$

Bishop eq 6.87,
GP Book eq. 3.21

One More Layer Up …

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*;\, m(\mathbf{x}^*),\, \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f};\, \mathbf{f}_{\mathrm{MAP}},\, \mathbf{H}^{-1})} \,\mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1} \boxed{\mathbf{f}}$$

$$\sigma^2(\mathbf{x}^*) = \boxed{k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)}$$

$$\mathbf{f}_{\mathrm{MAP}} = \boxed{k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}}))}$$

$$\mathbf{H} = \boxed{\mathrm{diag}\left\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\right\} + k(\mathbf{X}, \mathbf{X})^{-1}}$$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boxed{\boldsymbol{\mu}}, \boxed{\mathbf{H}^{-1}})$$

$$p(y \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid \boxed{\mathbf{A}\mathbf{x}} + b, \boxed{\sigma^2})$$

$$\Rightarrow \quad p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \boxed{\mathbf{A}\boldsymbol{\mu} + \mathbf{b}}, \boxed{\sigma^2} + \mathbf{A}\boxed{\mathbf{H}^{-1}}\mathbf{A}^T)$$

Bishop eq 2.115

$$\Rightarrow \quad c = k(\mathbf{x}^*, \mathbf{X})\big(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}})\big)$$

Bishop eq 6.87,
GP Book eq. 3.21

One More Layer Up …

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{f})}_{\mathcal{N}(f^*; m(\mathbf{x}^*), \sigma^2(\mathbf{x}^*))} \underbrace{p(\mathbf{f} \mid \mathbf{X}, \mathbf{y})}_{\mathcal{N}(\mathbf{f}; \mathbf{f}_{\text{MAP}}, \mathbf{H}^{-1})} \, \mathrm{d}\mathbf{f} \qquad = \mathcal{N}(\mathbf{f}^*; c, d^2)$$

$$m(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1} \boxed{\mathbf{f}}$$

$$\sigma^2(\mathbf{x}^*) = \boxed{k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\, k(\mathbf{X}, \mathbf{X})^{-1}\, k(\mathbf{X}, \mathbf{x}^*)}$$

$$\mathbf{f}_{\text{MAP}} = \boxed{k(\mathbf{X}, \mathbf{X})(\mathbf{y} - \sigma(\mathbf{f}_{\text{MAP}}))}$$

$$\mathbf{H} = \boxed{\operatorname{diag}\{\sigma(\mathbf{f}_{\text{MAP}})(1 - \sigma(\mathbf{f}_{\text{MAP}}))\} + k(\mathbf{X}, \mathbf{X})^{-1}}$$

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \mathbf{H}^{-1})$$

$$p(y \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\mathbf{x} + b, \sigma^2)$$

$$\Rightarrow p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \sigma^2 + \mathbf{A}\mathbf{H}^{-1}\mathbf{A}^T)$$

Bishop eq 2.115

$$\Rightarrow$$

$$c = k(\mathbf{x}^*, \mathbf{X})\big(\mathbf{y} - \sigma(\mathbf{f}_{\text{MAP}})\big)$$

Bishop eq 6.87, GP Book eq. 3.21

$$d^2 = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X}) \left(\operatorname{diag}\{\sigma(\mathbf{f}_{\text{MAP}})(1 - \sigma(\mathbf{f}_{\text{MAP}}))\}^{-1} + k(\mathbf{X}, \mathbf{X}) \right)^{-1} k(\mathbf{X}, \mathbf{x}^*)$$

Bishop eq 6.88, GP Book eq 3.22

Predictive Distribution for Gaussian Process Classification

Finally, $p(y^* = 1 \,|\, x^*, \mathbf{X}, \mathbf{y}) = \int p(y^* = 1 \,|\, f^*, \mathbf{x}^*)\, p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y})\, \mathrm{d}f^*$

GP Book eq 3.10

Predictive Distribution for Gaussian Process Classification

Finally, $p(y^* = 1 \,|\, x^*, \mathbf{X}, \mathbf{y}) = \displaystyle\int p(y^* = 1 \,|\, f^*, \mathbf{x}^*)\, \underbrace{p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y})}_{\mathcal{N}(f^*;\, c,\, d^2)}\, \mathrm{d}f^*$

GP Book eq 3.10

Predictive Distribution for Gaussian Process Classification

Finally, $p(y^* = 1 \mid x^*, \mathbf{X}, \mathbf{y}) = \int p(y^* = 1 \mid f^*, \mathbf{x}^*)\, p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y})\, \mathrm{d}f^*$

GP Book eq 3.10

$$\underbrace{p(y^* = 1 \mid f^*, \mathbf{x}^*)}_{\sigma(f^*)} \qquad \underbrace{p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y})}_{\mathcal{N}(f^*; c, d^2)}$$

Predictive Distribution for Gaussian Process Classification

Finally, $p(y^* = 1 \,|\, x^*, \mathbf{X}, \mathbf{y}) = \int p(y^* = 1 \,|\, f^*, \mathbf{x}^*)\, p(f^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y})\, \mathrm{d}f^*$

GP Book eq 3.10

$\sigma(f^*)$ $\quad\quad$ $\mathcal{N}(f^*; c, d^2)$

Recall with Probit approximation

$$\int \sigma(a)\mathcal{N}(a \,|\, \mu, \sigma^2)\mathrm{d}a \simeq \sigma(\kappa(\sigma^2)\,\mu)$$

$$\kappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

Bishop eq 4.153

Predictive Distribution for Gaussian Process Classification

Finally, $p(y^* = 1 \mid x^*, \mathbf{X}, \mathbf{y}) = \int p(y^* = 1 \mid f^*, \mathbf{x}^*)\, p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y})\, \mathrm{d}f^*$

GP Book eq 3.10

$\sigma(f^*)$ $\quad\quad$ $\mathcal{N}(f^*; c, d^2)$

$$p(y^* = 1 \mid x^*, \mathbf{X}, \mathbf{y}) = \sigma\Big((1 + \pi d^2/8)^{-1/2}\, c\Big)$$

$$c = k(\mathbf{x}^*, \mathbf{X})\big(\mathbf{y} - \sigma(\mathbf{f}_{\mathrm{MAP}})\big)$$

Bishop eq 6.87,
GP Book eq 3.21

$$d^2 = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})\Big(\mathrm{diag}\big\{\sigma(\mathbf{f}_{\mathrm{MAP}})(1 - \sigma(\mathbf{f}_{\mathrm{MAP}}))\big\}^{-1} + k(\mathbf{X}, \mathbf{X})\Big)^{-1} k(\mathbf{X}, \mathbf{x}^*)$$

Bishop eq 6.88,
GP Book eq 3.22

Recall with Probit approximation

$$\int \sigma(a)\mathcal{N}(a \mid \mu, \sigma^2)\mathrm{d}a \simeq \sigma(\kappa(\sigma^2)\, \mu)$$

$$\kappa(\sigma^2) = (1 + \pi\sigma^2/8)^{-1/2}$$

Bishop eq 4.153

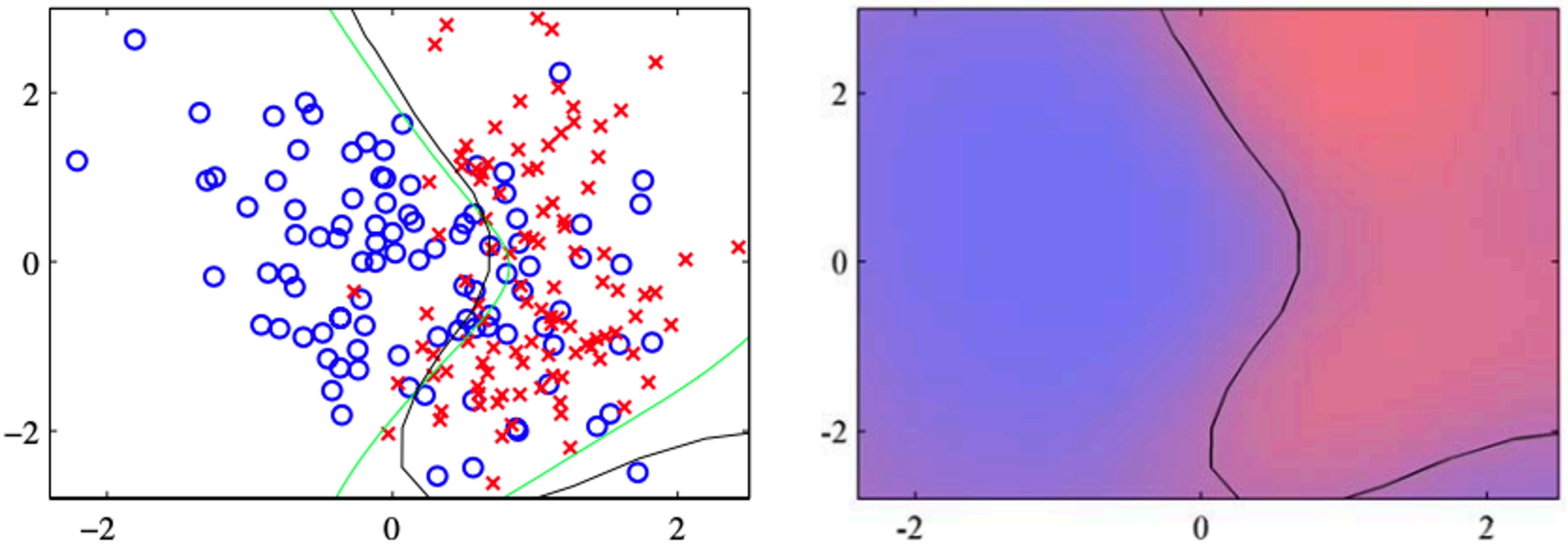


Figure 6.12 Illustration of the use of a Gaussian process for classification, showing the data on the left together with the optimal decision boundary from the true distribution in green, and the decision boundary from the Gaussian process classifier in black. On the right is the predicted posterior probability for the blue and red classes together with the Gaussian process decision boundary.

Recap: Learning Hyperparameters in GP Regression

$$\underbrace{p(\mathbf{y} \mid \mathbf{X}, \overbrace{\theta}^{\text{Kernel hyperparameter}})}_{\text{the marginal likelihood}} = \mathcal{N}(\mathbf{y}; \mathbf{0}, \underbrace{\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathrm{I}}_{\hat{\mathbf{K}}})$$

$$\ln p(\mathbf{y} \mid \mathbf{X}, \theta) = -\sum_{\mathbf{i}} \ln \mathbf{L}_{\mathbf{ii}} - \frac{\mathbf{1}}{\mathbf{2}} \mathbf{y}^{\mathrm{T}} \alpha - \frac{\mathbf{N}}{\mathbf{2}} \ln(\mathbf{2}\pi)$$

$L =$ Cholesky $\hat{\mathbf{K}}$

$\boldsymbol{\alpha} = \mathbf{L}^{\mathbf{T}} \setminus (\mathbf{L} \setminus \mathbf{y})$

Recap: Learning Hyperparameters in GP Regression

$$\underbrace{p(\mathbf{y} \mid \mathbf{X}, \overbrace{\theta}^{\text{Kernel hyperparameter}})}_{\text{the marginal likelihood}} = \mathcal{N}(\mathbf{y}; \mathbf{0}, \underbrace{\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathrm{I}}_{\hat{\mathbf{K}}})$$

$$\ln p(\mathbf{y} \mid \mathbf{X}, \theta) = -\frac{1}{2} \ln |\hat{\mathbf{K}}| - \frac{1}{2} \mathbf{y}^{\mathrm{T}} \hat{\mathbf{K}}^{-1} \mathbf{y} - \frac{\mathrm{N}}{2} \ln(2\pi)$$

(Bishop eq 6.69)

$$\ln p(\mathbf{y} \mid \mathbf{X}, \theta) = -\sum_{\mathrm{i}} \ln \mathbf{L}_{\mathrm{ii}} - \frac{1}{2} \mathbf{y}^{\mathrm{T}} \alpha - \frac{\mathrm{N}}{2} \ln(2\pi)$$

$L =$ Cholesky $\hat{\mathbf{K}}$

$\boldsymbol{\alpha} = \mathbf{L}^{\mathrm{T}} \setminus (\mathbf{L} \setminus \mathbf{y})$

Recap: Learning Hyperparameters in GP Regression

$$\underbrace{p(\mathbf{y} \mid \mathbf{X}, \overbrace{\theta}^{\text{Kernel hyperparameter}})}_{\text{the marginal likelihood}} = \mathcal{N}(\mathbf{y}; \mathbf{0}, \underbrace{\mathbf{K}(\mathbf{X}, \mathbf{X})}_{\hat{\mathbf{K}}} + \sigma^2 \mathrm{I})$$

$$\ln p(\mathbf{y} \mid \mathbf{X}, \theta) = -\frac{1}{2} \ln |\hat{\mathbf{K}}| - \frac{1}{2} \mathbf{y}^{\mathrm{T}} \hat{\mathbf{K}}^{-1} \mathbf{y} - \frac{\mathbf{N}}{2} \ln(2\pi)$$

(Bishop eq 6.69)

Learning through gradient descent

$$\frac{\partial}{\partial x} \ln |\mathbf{A}| = \mathrm{Tr}\left(\mathbf{A}^{-1} \frac{\partial \mathbf{A}}{\partial \mathrm{x}}\right)$$

$$\frac{\partial}{\partial x}(\mathbf{A}^{-1}) = -\mathbf{A}^{-1} \frac{\partial \mathbf{A}}{\partial \mathbf{x}} \mathbf{A}^{-1}$$

(Bishop eq C.21, C.22)

$$\ln p(\mathbf{y} \mid \mathbf{X}, \theta) = -\sum_{\mathbf{i}} \ln \mathbf{L}_{\mathbf{ii}} - \frac{1}{2} \mathbf{y}^{\mathrm{T}} \alpha - \frac{\mathbf{N}}{2} \ln(2\pi)$$

$L =$ Cholesky $\hat{\mathbf{K}}$

$\boldsymbol{\alpha} = \mathbf{L}^{\mathrm{T}} \backslash (\mathbf{L} \backslash \mathbf{y})$

Recap: Learning Hyperparameters in GP Regression

$$\underbrace{p(\mathbf{y}\,|\,\mathbf{X},}_{\text{the marginal likelihood}}\overbrace{\theta}^{\text{Kernel hyperparameter}}) = \mathcal{N}(\mathbf{y}; \mathbf{0}, \underbrace{\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma^2 \mathrm{I}}_{\hat{\mathbf{K}}})$$

$$\ln p(\mathbf{y}\,|\,\mathbf{X}, \theta) = -\frac{1}{2}\ln|\hat{\mathbf{K}}| - \frac{1}{2}\mathbf{y}^{\mathrm{T}}\hat{\mathbf{K}}^{-1}\mathbf{y} - \frac{\mathrm{N}}{2}\ln(2\pi)$$

(Bishop eq 6.69)

$$\frac{\partial}{\partial x}\ln|\mathbf{A}| = \mathrm{Tr}\left(\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial \mathrm{x}}\right)$$

$$\frac{\partial}{\partial x}(\mathbf{A}^{-1}) = -\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{A}^{-1}$$

(Bishop eq C.21, C.22)

Learning through gradient descent

$$\frac{\partial}{\partial \theta_i}\ln p(\mathbf{y}\,|\,\mathbf{X}, \theta) = -\frac{1}{2}\mathrm{Tr}\left(\hat{\mathbf{K}}^{-1}\frac{\partial \hat{\mathbf{K}}}{\partial \theta_{\mathrm{i}}}\right) + \frac{1}{2}\mathbf{y}^{\mathrm{T}}\hat{\mathbf{K}}^{-1}\frac{\partial \hat{\mathbf{K}}}{\partial \theta_{\mathrm{i}}}\hat{\mathbf{K}}^{-1}\mathbf{y}$$

(Bishop eq 6.70)

$$\ln p(\mathbf{y}\,|\,\mathbf{X}, \theta) = -\sum_{\mathrm{i}}\ln \mathbf{L}_{\mathrm{ii}} - \frac{1}{2}\mathbf{y}^{\mathrm{T}}\alpha - \frac{\mathrm{N}}{2}\ln(2\pi)$$

$L =$ Cholesky $\hat{\mathbf{K}}$

$\boldsymbol{\alpha} = \mathbf{L}^{\mathrm{T}} \backslash (\mathbf{L} \backslash \mathbf{y})$

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = \int p(\mathbf{y}\,|\,\mathbf{f},\mathbf{X},\theta)\,p(\mathbf{f}\,|\,\mathbf{X},\theta)\,\mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f}\,|\,\mathbf{X},\theta) = \mathcal{N}(\mathbf{f};\mathbf{0},\mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y} \,|\, \mathbf{X}, \theta) = \int p(\mathbf{y} \,|\, \mathbf{f}, \mathbf{X}, \theta) \underbrace{p(\mathbf{f} \,|\, \mathbf{X}, \theta)}_{\propto\, p(\mathbf{f} \,|\, \mathbf{y}, \mathbf{X}, \theta) \;\simeq\; \mathcal{N}(\mathbf{a} \,|\, \mathbf{a}_{\mathrm{MAP}}, \mathbf{H}^{-1})} \,\mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f} \,|\, \mathbf{X}, \theta) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y} \,|\, \mathbf{X}, \theta) = \int p(\mathbf{y} \,|\, \underbrace{\mathbf{f}, \mathbf{X}, \theta)\, p(\mathbf{f} \,|\, \mathbf{X}}_{\propto\, p(\mathbf{f} \,|\, \mathbf{y}, \mathbf{X}, \theta) \;\simeq\; \mathcal{N}(\mathbf{a} \,|\, \mathbf{a}_{\mathrm{MAP}}, \mathbf{H}^{-1})}, \theta)\, \mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f} \,|\, \mathbf{X}, \theta) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

For a scaled Gaussian, the "normalising" constant

Bishop eq 4.135, 4.137, GP Book eq 3.31

$$p(\mathbf{y} \,|\, \mathbf{X}, \theta) = \qquad \int \exp\left(-\frac{1}{2}(\mathbf{f} - \mathbf{f}_{\mathrm{MAP}})^T \mathbf{H}\, (\mathbf{f} - \mathbf{f}_{\mathrm{MAP}})\right) \mathrm{d}\mathbf{f}$$

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = \int p(\mathbf{y}\,|\,\underbrace{\mathbf{f},\mathbf{X},\theta)\,p(\mathbf{f}\,|}_{\propto\, p(\mathbf{f}\,|\,\mathbf{y},\mathbf{X},\theta)\ \simeq\ \mathcal{N}(\mathbf{a}\,|\,\mathbf{a}_{\mathrm{MAP}},\,\mathbf{H}^{-1})}\mathbf{X},\theta)\,\mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f}\,|\,\mathbf{X},\theta) = \mathcal{N}(\mathbf{f};\mathbf{0},\mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

For a scaled Gaussian, the "normalising" constant

Bishop eq 4.135, 4.137, GP Book eq 3.31

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = p(\mathbf{y}\,|\,\mathbf{f}_{\mathrm{MAP}},\mathbf{X},\theta)\,p(\mathbf{f}_{\mathrm{MAP}}\,|\,\mathbf{X},\theta)\int \exp\left(-\frac{1}{2}(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})^{T}\,\mathbf{H}\,(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})\right)\,\mathrm{d}\mathbf{f}$$

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = \int \underbrace{p(\mathbf{y}\,|\,\mathbf{f},\mathbf{X},\theta)\,p(\mathbf{f}\,|\,\mathbf{X},\theta)}_{\propto\, p(\mathbf{f}\,|\,\mathbf{y},\mathbf{X},\theta)\ \simeq\ \mathcal{N}(\mathbf{a}\,|\,\mathbf{a}_{\mathrm{MAP}},\mathbf{H}^{-1})}\,\mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f}\,|\,\mathbf{X},\theta) = \mathcal{N}(\mathbf{f};\mathbf{0},\mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

For a scaled Gaussian, the "normalising" constant

Bishop eq 4.135, 4.137, GP Book eq 3.31

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = p(\mathbf{y}\,|\,\mathbf{f}_{\mathrm{MAP}},\mathbf{X},\theta)\,p(\mathbf{f}_{\mathrm{MAP}}\,|\,\mathbf{X},\theta)\int \exp\left(-\frac{1}{2}(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})^T\,\mathbf{H}\,(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})\right)\mathrm{d}\mathbf{f}$$

Bishop eq 6.90

$$\ln p(\mathbf{y}\,|\,\mathbf{X},\theta) = \ln p(\mathbf{y}\,|\,\mathbf{f}_{\mathrm{MAP}},\mathbf{X},\theta) + \ln p(\mathbf{f}_{\mathrm{MAP}}\,|\,\mathbf{X},\theta)\ -\frac{1}{2}\ln|\mathbf{H}| + \frac{N}{2}\ln 2\pi$$

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y} \,|\, \mathbf{X}, \theta) = \int \underbrace{p(\mathbf{y} \,|\, \mathbf{f}, \mathbf{X}, \theta)\, p(\mathbf{f} \,|\, \mathbf{X}, \theta)}_{\propto\, p(\mathbf{f} \,|\, \mathbf{y}, \mathbf{X}, \theta) \;\simeq\; \mathcal{N}(\mathbf{a} \,|\, \mathbf{a}_{\mathrm{MAP}}, \mathbf{H}^{-1})}\, \mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f} \,|\, \mathbf{X}, \theta) = \mathcal{N}(\mathbf{f}; \mathbf{0}, \mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

For a scaled Gaussian, the “normalising” constant

Bishop eq 4.135, 4.137, GP Book eq 3.31

$$p(\mathbf{y} \,|\, \mathbf{X}, \theta) = p(\mathbf{y} \,|\, \mathbf{f}_{\mathrm{MAP}}, \mathbf{X}, \theta)\, p(\mathbf{f}_{\mathrm{MAP}} \,|\, \mathbf{X}, \theta) \int \exp\left(-\frac{1}{2} (\mathbf{f} - \mathbf{f}_{\mathrm{MAP}})^T \mathbf{H} (\mathbf{f} - \mathbf{f}_{\mathrm{MAP}}) \right) \mathrm{d}\mathbf{f}$$

Bishop eq 6.90

$$\ln p(\mathbf{y} \,|\, \mathbf{X}, \theta) = \underbrace{\boxed{\ln p(\mathbf{y} \,|\, \mathbf{f}_{\mathrm{MAP}}, \mathbf{X}, \theta)}}_{\text{Goodness of fit at the optimal parameter}} + \ln p(\mathbf{f}_{\mathrm{MAP}} \,|\, \mathbf{X}, \theta) - \frac{1}{2} \ln |\mathbf{H}| + \frac{N}{2} \ln 2\pi$$

Marginal Likelihood for GP Classification and BIC

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = \int \underbrace{p(\mathbf{y}\,|\,\mathbf{f},\mathbf{X},\theta)\,p(\mathbf{f}\,|\,\mathbf{X},\theta)}_{\propto\, p(\mathbf{f}\,|\,\mathbf{y},\mathbf{X},\theta) \;\simeq\; \mathcal{N}(\mathbf{a}\,|\,\mathbf{a}_{\mathrm{MAP}},\mathbf{H}^{-1})}\,\mathrm{d}\mathbf{f}$$

$$\boxed{p(\mathbf{f}\,|\,\mathbf{X},\theta) = \mathcal{N}(\mathbf{f};\mathbf{0},\mathbf{K})}$$

Bishop eq 6.89, GP Book eq 3.30

For a scaled Gaussian, the "normalising" constant

Bishop eq 4.135, 4.137, GP Book eq 3.31

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) = p(\mathbf{y}\,|\,\mathbf{f}_{\mathrm{MAP}},\mathbf{X},\theta)\,p(\mathbf{f}_{\mathrm{MAP}}\,|\,\mathbf{X},\theta)\int \exp\left(-\frac{1}{2}(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})^T\,\mathbf{H}\,(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})\right)\,\mathrm{d}\mathbf{f}$$

Bishop eq 6.90

$$\ln p(\mathbf{y}\,|\,\mathbf{X},\theta) = \boxed{\ln p(\mathbf{y}\,|\,\mathbf{f}_{\mathrm{MAP}},\mathbf{X},\theta)} + \ln p(\mathbf{f}_{\mathrm{MAP}}\,|\,\mathbf{X},\theta)\,\boxed{-\frac{1}{2}\ln|\mathbf{H}| + \frac{N}{2}\ln 2\pi}$$

Goodness of fit at the optimal parameter

Complexity / degree of freedom "penalty"

What we have learned

Bishop's textbook: chapter 4.4-4.5, 6.4.5-6.4.6
GP book: http://gaussianprocess.org/gpml/chapters/
chapter 3.1-3.4

Bishop's textbook: chapter 4.4-4.5, 6.4.5-6.4.6
GP book: http://gaussianprocess.org/gpml/chapters/
chapter 3.1-3.4

What we have learned

- Bayesian Logistic Regression

  - the challenge to computing a non-Gaussian predictive distribution

What we have learned

Bishop's textbook: chapter 4.4-4.5, 6.4.5-6.4.6
GP book: http://gaussianprocess.org/gpml/chapters/
chapter 3.1-3.4

- Bayesian Logistic Regression

  - the challenge to computing a non-Gaussian predictive distribution

- Laplace Approximation for Bayesian Logistic Regression

What we have learned

Bishop's textbook: chapter 4.4-4.5, 6.4.5-6.4.6
GP book: http://gaussianprocess.org/gpml/chapters/
chapter 3.1-3.4

- Bayesian Logistic Regression

  - the challenge to computing a non-Gaussian predictive distribution

- Laplace Approximation for Bayesian Logistic Regression

- Gaussian Process Classification

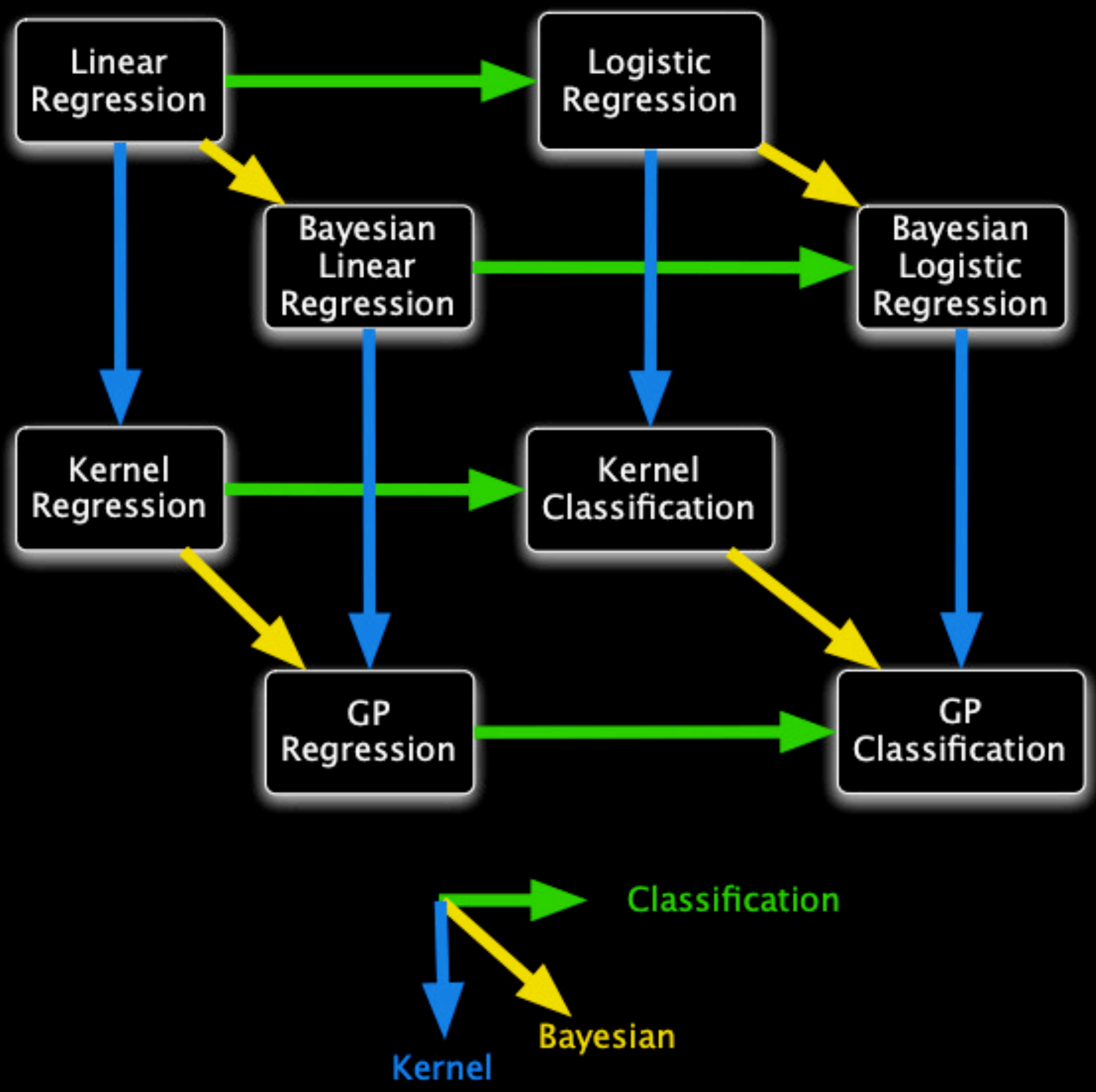
What we have learned

Bishop’s textbook: chapter 4.4-4.5, 6.4.5-6.4.6
GP book: http://gaussianprocess.org/gpml/chapters/
chapter 3.1-3.4

- Bayesian Logistic Regression

  - the challenge to computing a non-Gaussian predictive distribution

- Laplace Approximation for Bayesian Logistic Regression
- Gaussian Process Classification
- Laplace Approximation for Gaussian Process Classification



Tomorrow: recap and unsupervised learning