# Laplace’s method and GP classification

Week 5b - Statistical ML / Thang Bui / ANU / 2025 S1 - Thanks to Yuan-Sen Ting for many slides

# Plan for today and next Wed

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

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- Bayesian Logistic Regression

  - the challenge to computing a non-Gaussian predictive distribution

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- Laplace Approximation for Bayesian Logistic Regression
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- Bayesian Logistic Regression

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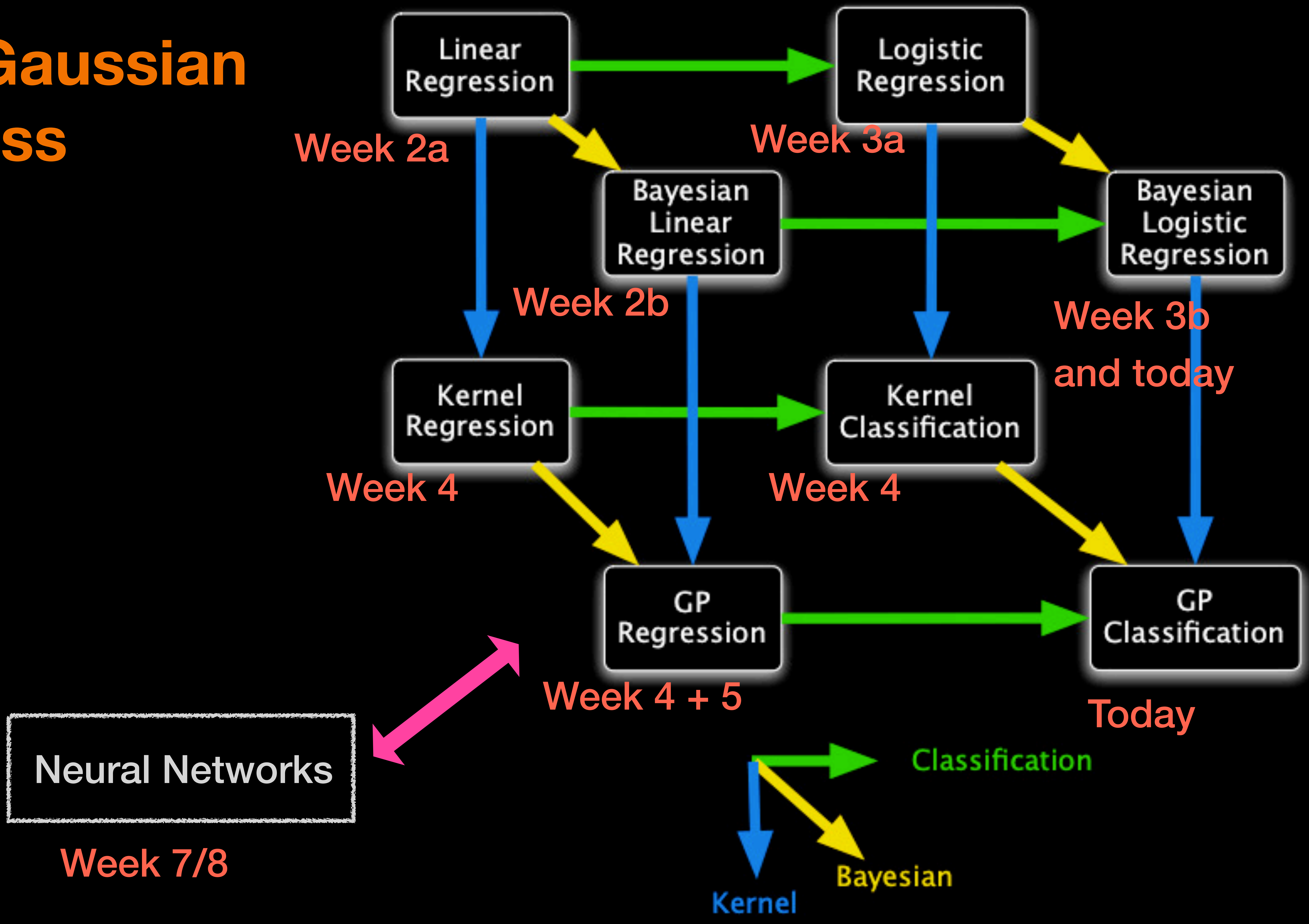
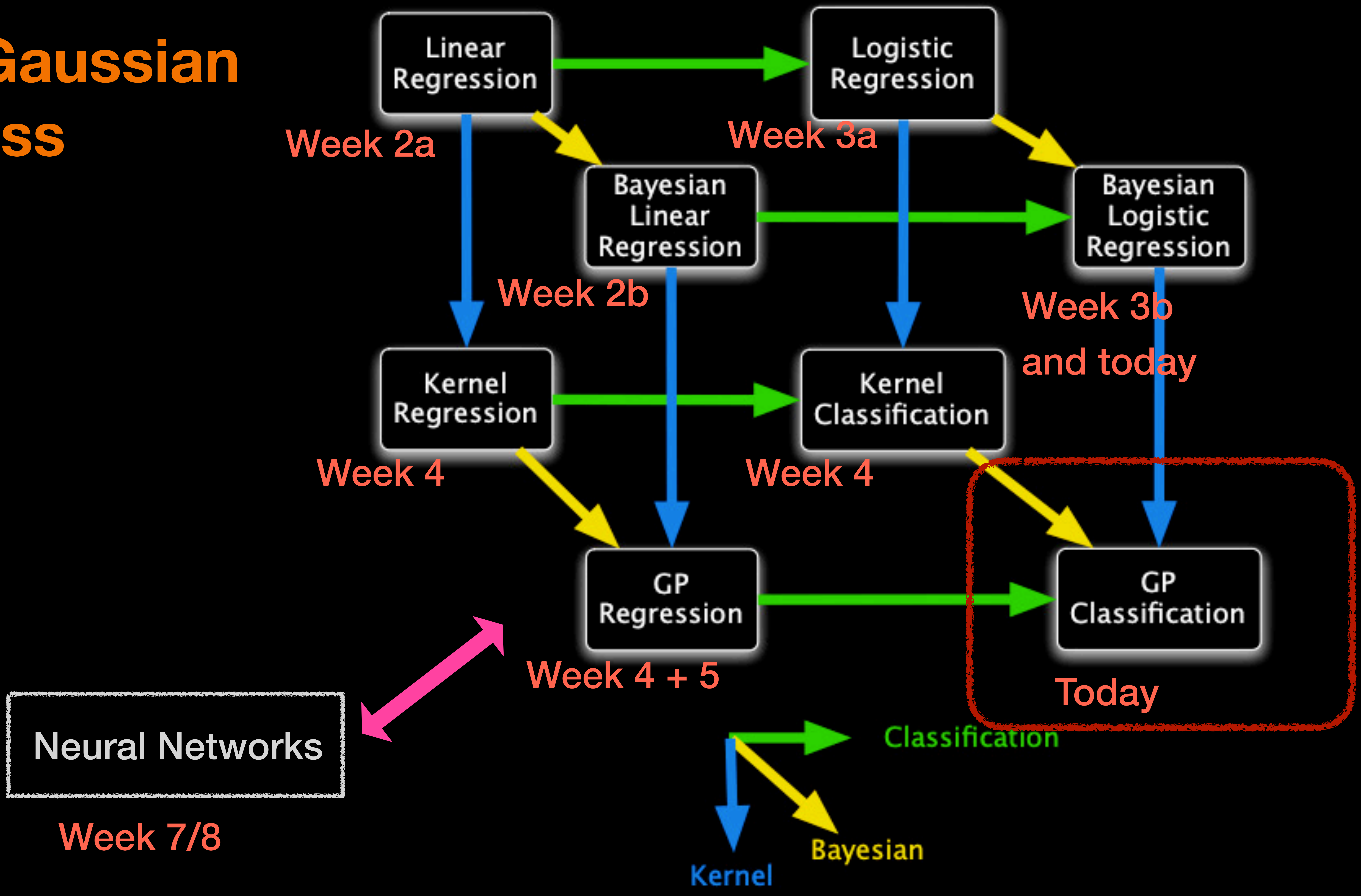
- Laplace Approximation for Bayesian Logistic Regression
- Gaussian Process Classification
- Laplace Approximation for Gaussian Process Classification

# Why Gaussian Process



# Why Gaussian Process



# Last Time on Bayesian Linear Regression

Predictive distribution

$$p(y^* \,|\, \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int \underbrace{\mathbf{p}(\mathbf{y}^* \,|\, \mathbf{x}^*, \theta)}_{\text{Gaussian}} \, \underbrace{\mathbf{p}(\theta \,|\, \mathbf{y}, \mathbf{X})}_{\text{Gaussian}} \, \mathrm{d}\theta$$

Recall in Bayesian linear regression

$$p(\theta \,|\, \mathbf{X}, \mathbf{y}) = \mathcal{N}(\theta; \mathbf{m}, \mathbf{S})$$

# Recap : Logistic Regression

$$p(y = 1 \mid \theta, x) = g_\theta(\mathbf{x}) = \underbrace{\sigma}_{\text{Sigmoid}}\left(\theta^T \phi(\mathbf{x})\right)$$

Bishop eq 4.87

Given training data $\{\mathbf{x_n}, \mathbf{y_n}\}, y_n \in \{0,1\}$

Likelihood

$$p(\mathbf{Y} \mid \theta, \mathbf{X}) = \prod_{n=1}^{N} g_n^{y_n} (1 - g_n)^{(1-y_n)}$$

Bishop eq 4.89

# Recap : Logistic Regression

## Likelihood

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

# Recap : Logistic Regression

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

Prior

$$p(\theta) = \mathcal{N}(\theta; \mathbf{m_0}, \mathbf{S_0})$$

Bishop eq 4.140

# Recap : Logistic Regression

Likelihood

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

Prior

$$p(\theta) = \mathcal{N}(\theta; \mathbf{m_0}, \mathbf{S_0})$$

Bishop eq 4.140

Posterior

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

# Bayesian Logistic Regression

Predictive distribution

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

# Bayesian Logistic Regression

Predictive distribution

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

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

# Bayesian Logistic Regression

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Not analytically tractable

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

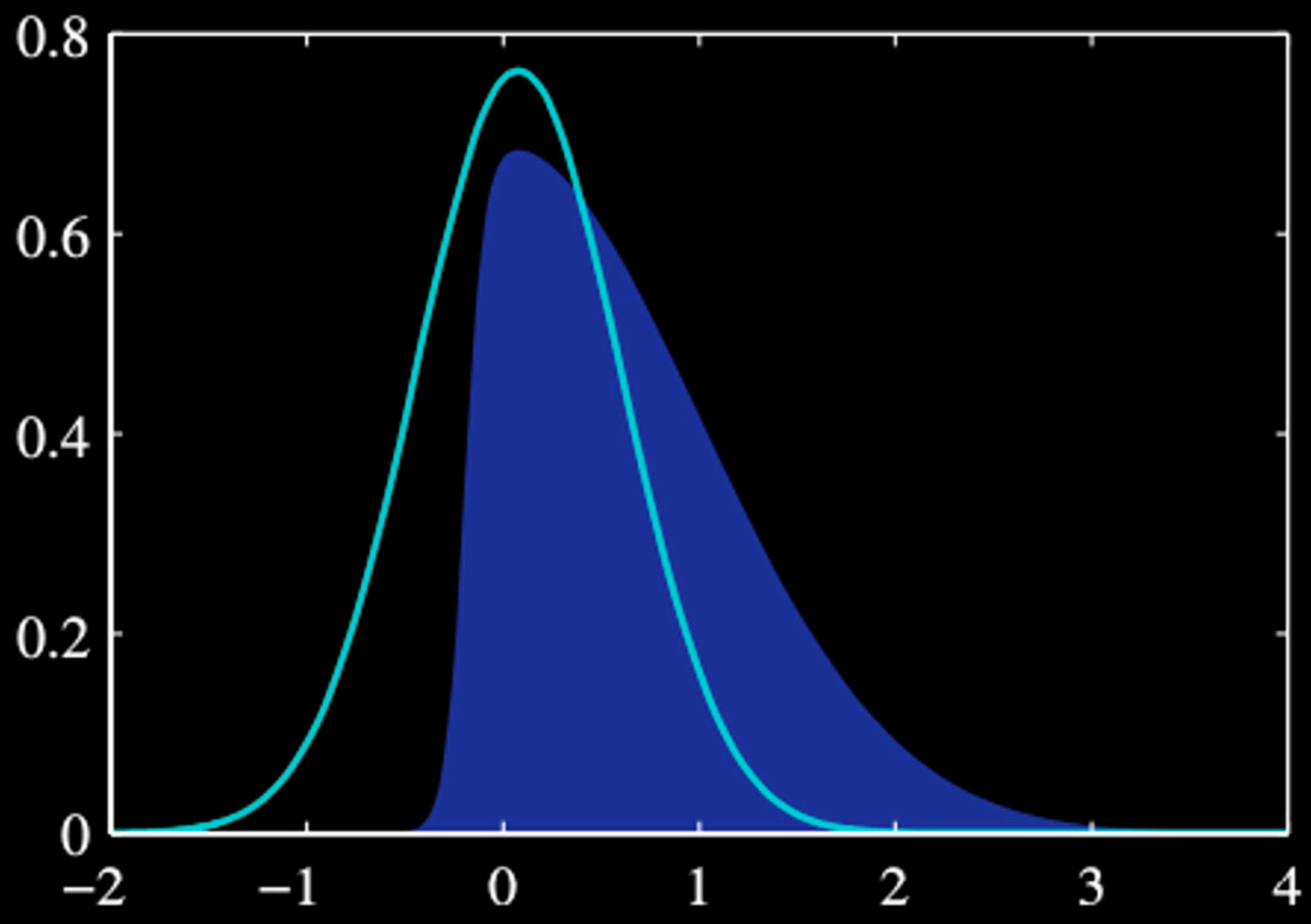
$$\propto \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0) \cdot \prod_{n=1}^{N} g_n^{y_n} \{1 - g_n\}^{1-y_n}$$

Let's first "Gaussianise" this part
using Laplace Approximation

# Laplace Approximation in 1D

- Goal: find a Gaussian distribution $q(z)$ that approximates the PDF $p(z)$

- Idea: find out $q(z)$ which centers at the mode of $p(z)$ with the same "curvature" at that maximum point



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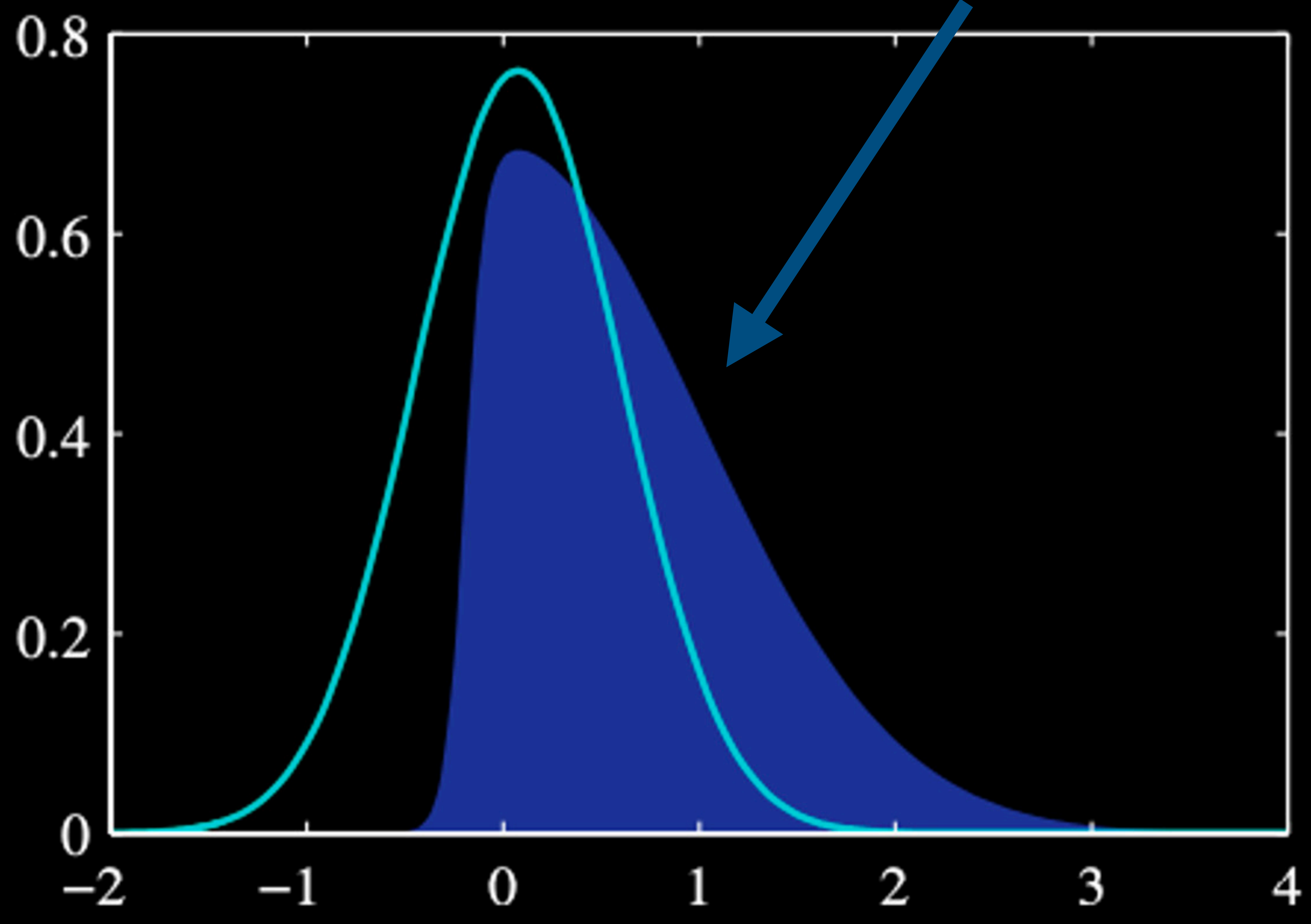
$$p(z) \propto \exp(-z^2/2)\,\overbrace{\sigma}^{\text{Sigmoid}}(20z+4)$$



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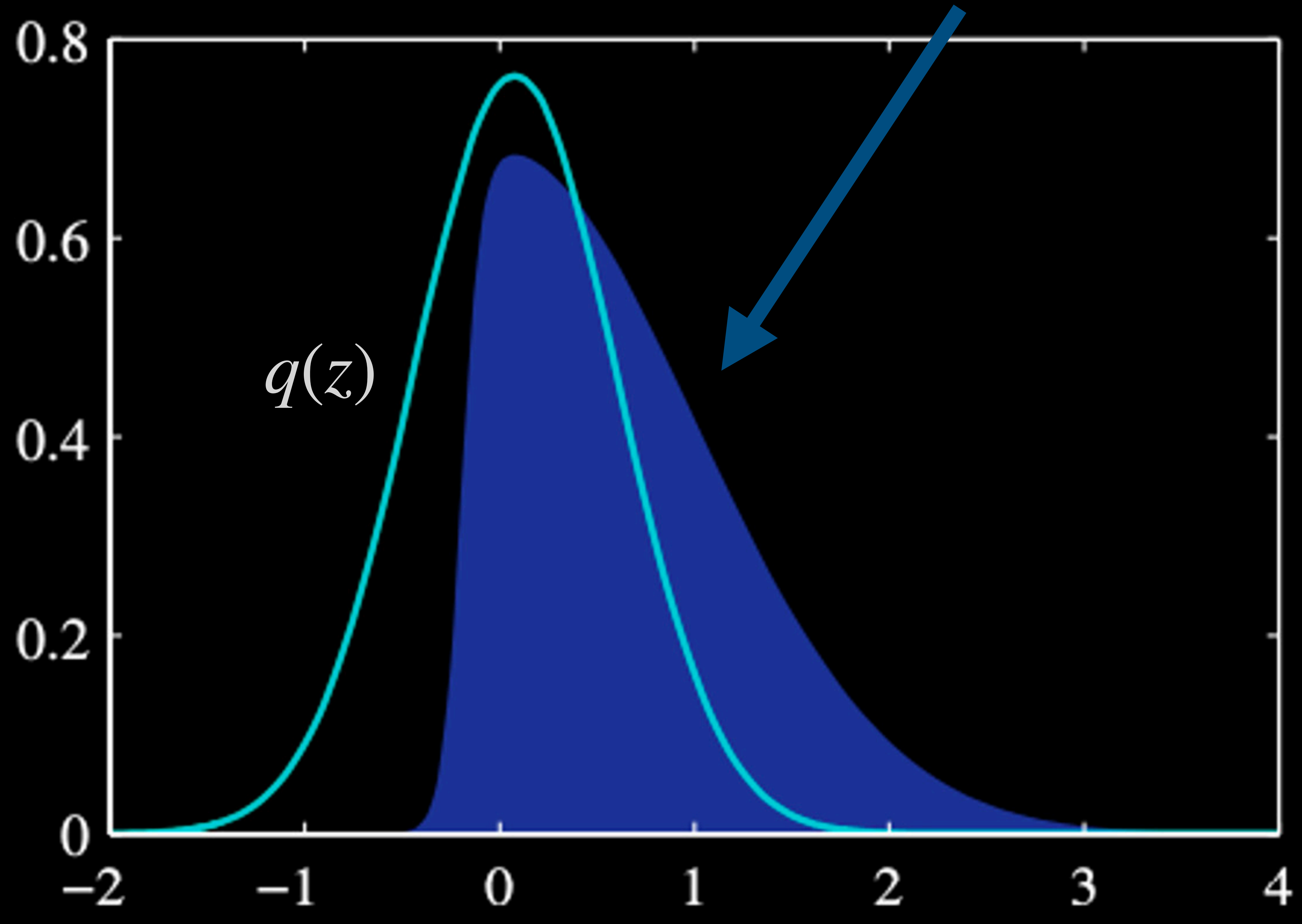
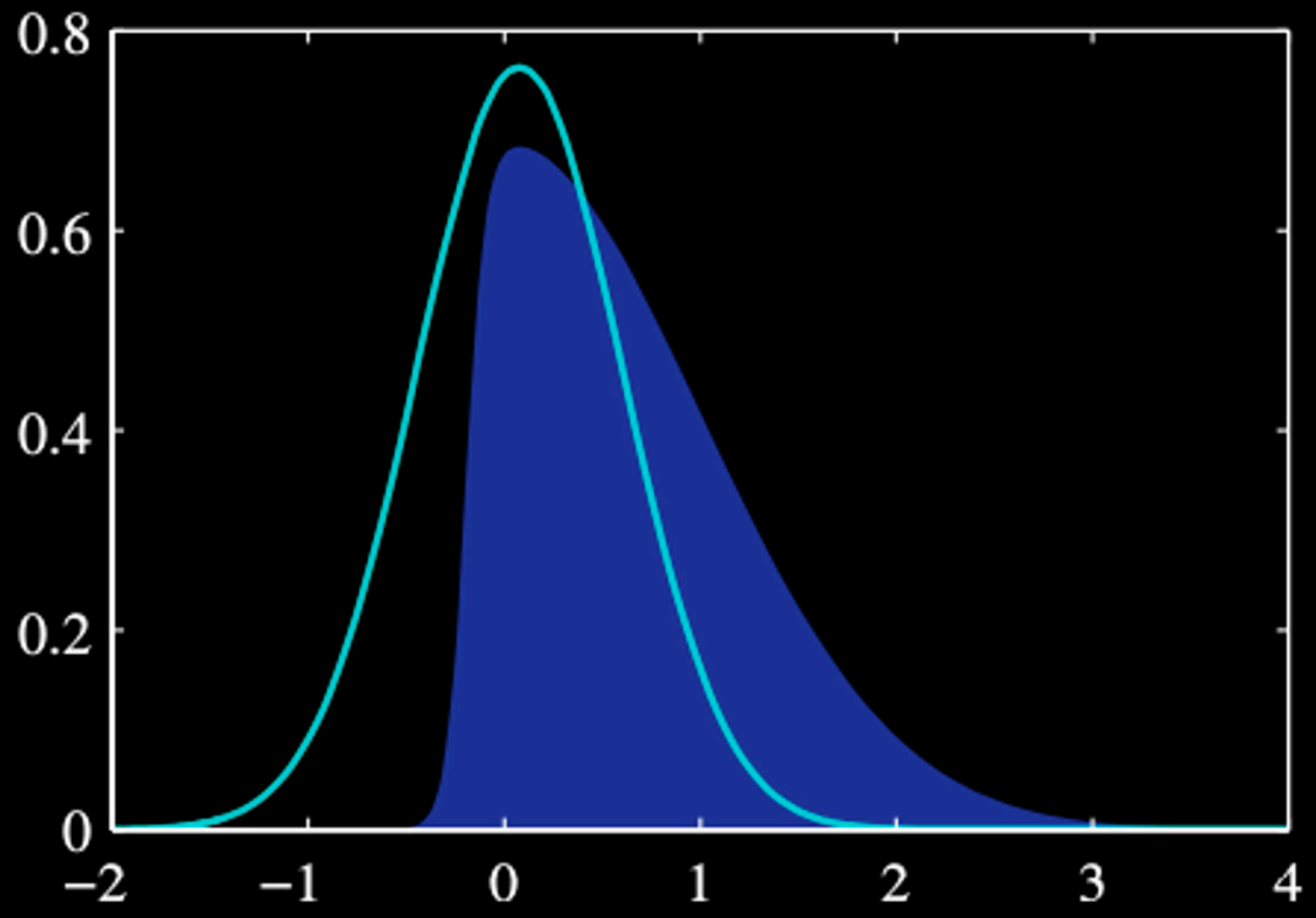


# Laplace Approximation in 1D

Let $p(z) = \frac{1}{Z} f(z)$ where $Z = \int f(z)\,\mathrm{d}z$

Bishop eq 4.125



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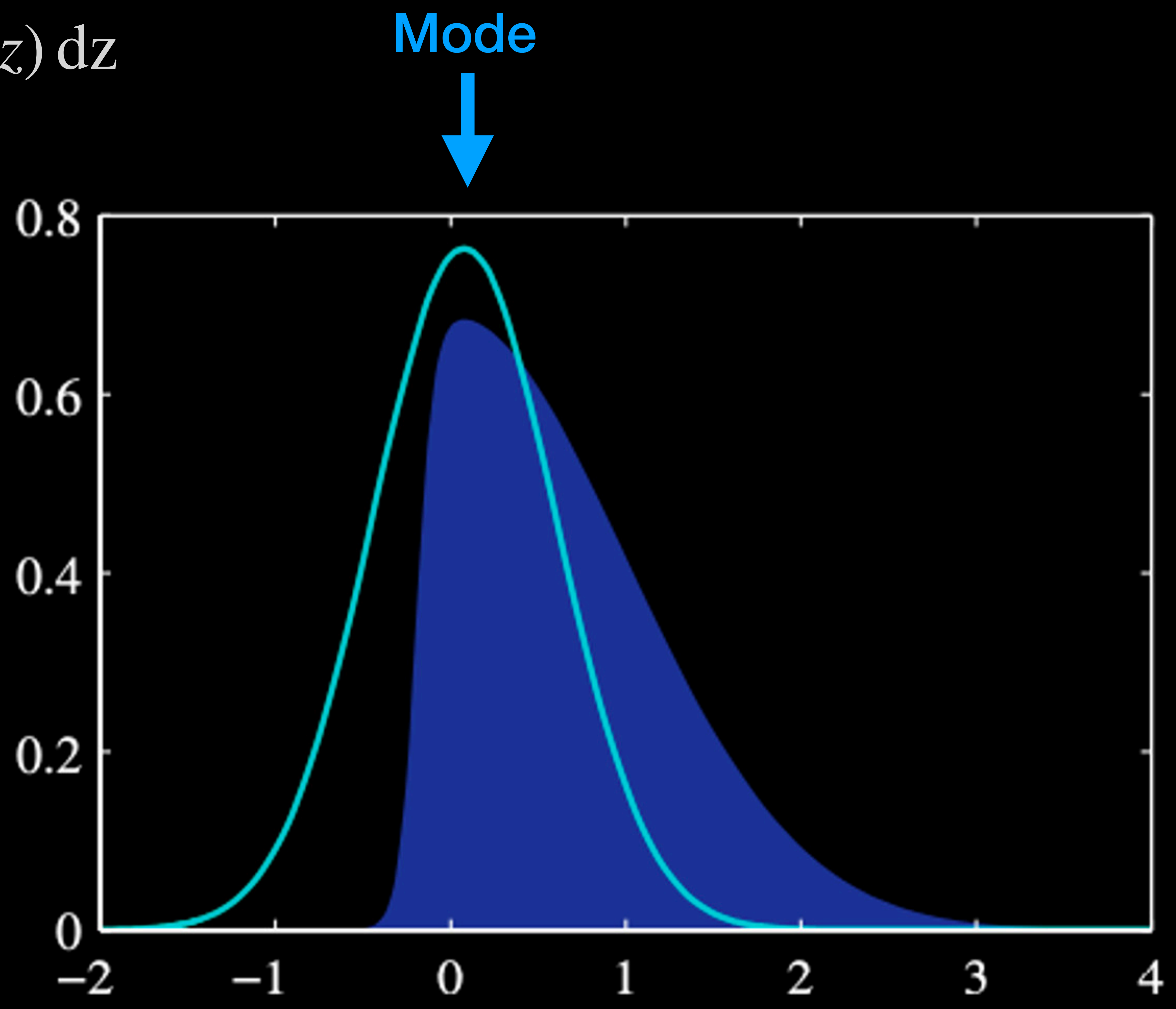
Find the mode



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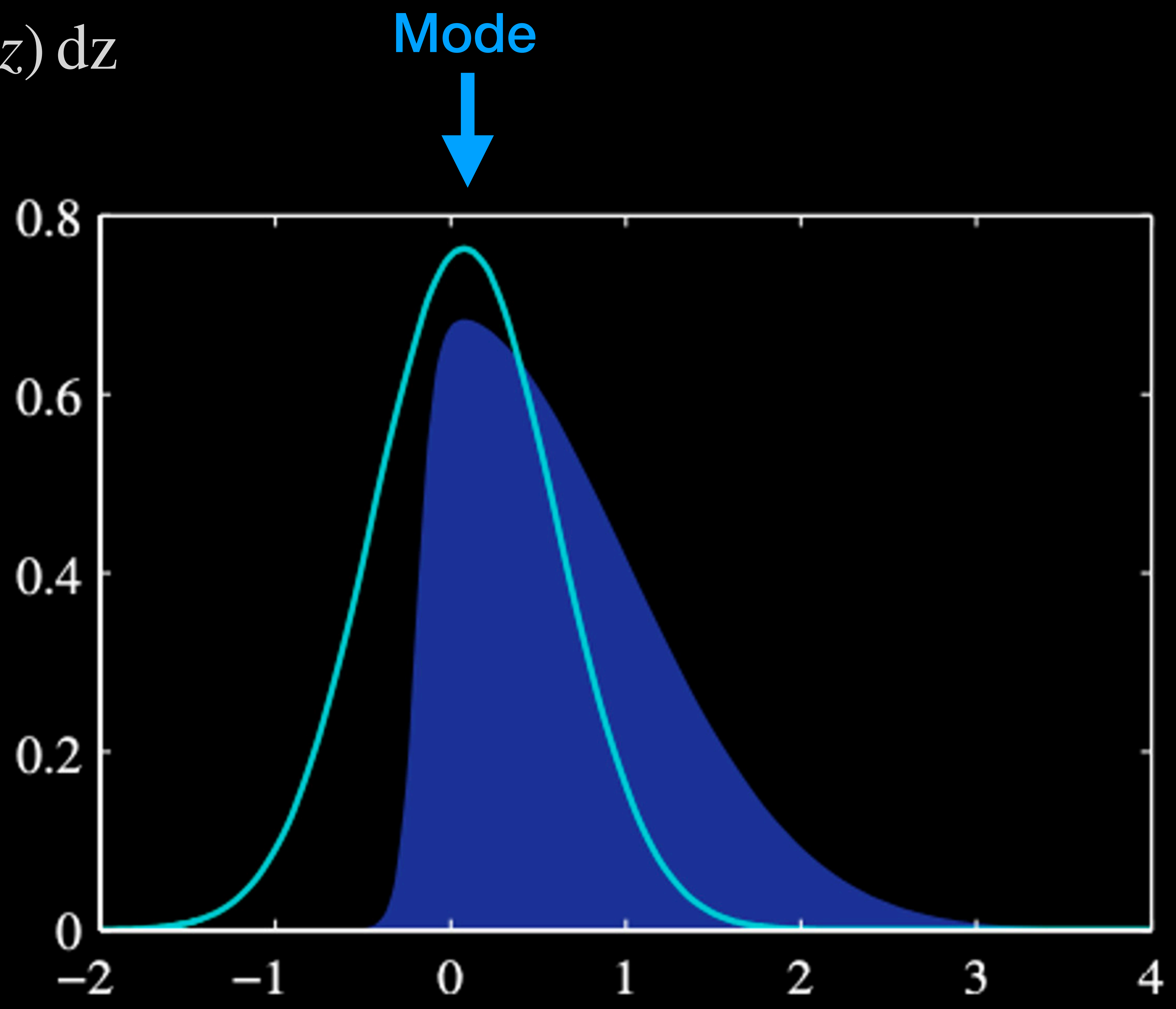
Find the mode

$$\left. \frac{\mathrm{d}f(z)}{\mathrm{d}z} \right|_{z=z_0} = 0$$

Bishop eq 4.126



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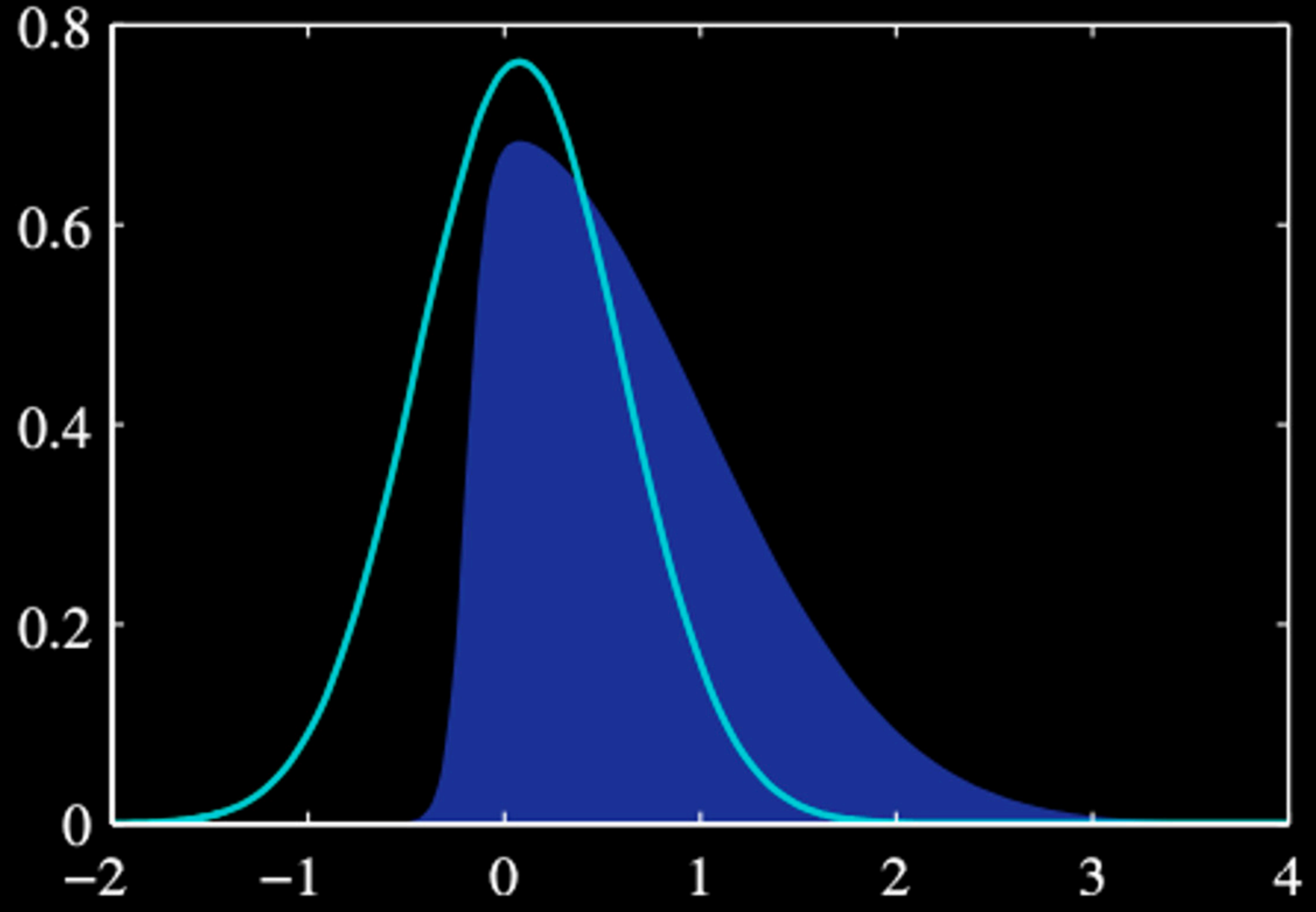
Taylor expansion at $z_0$



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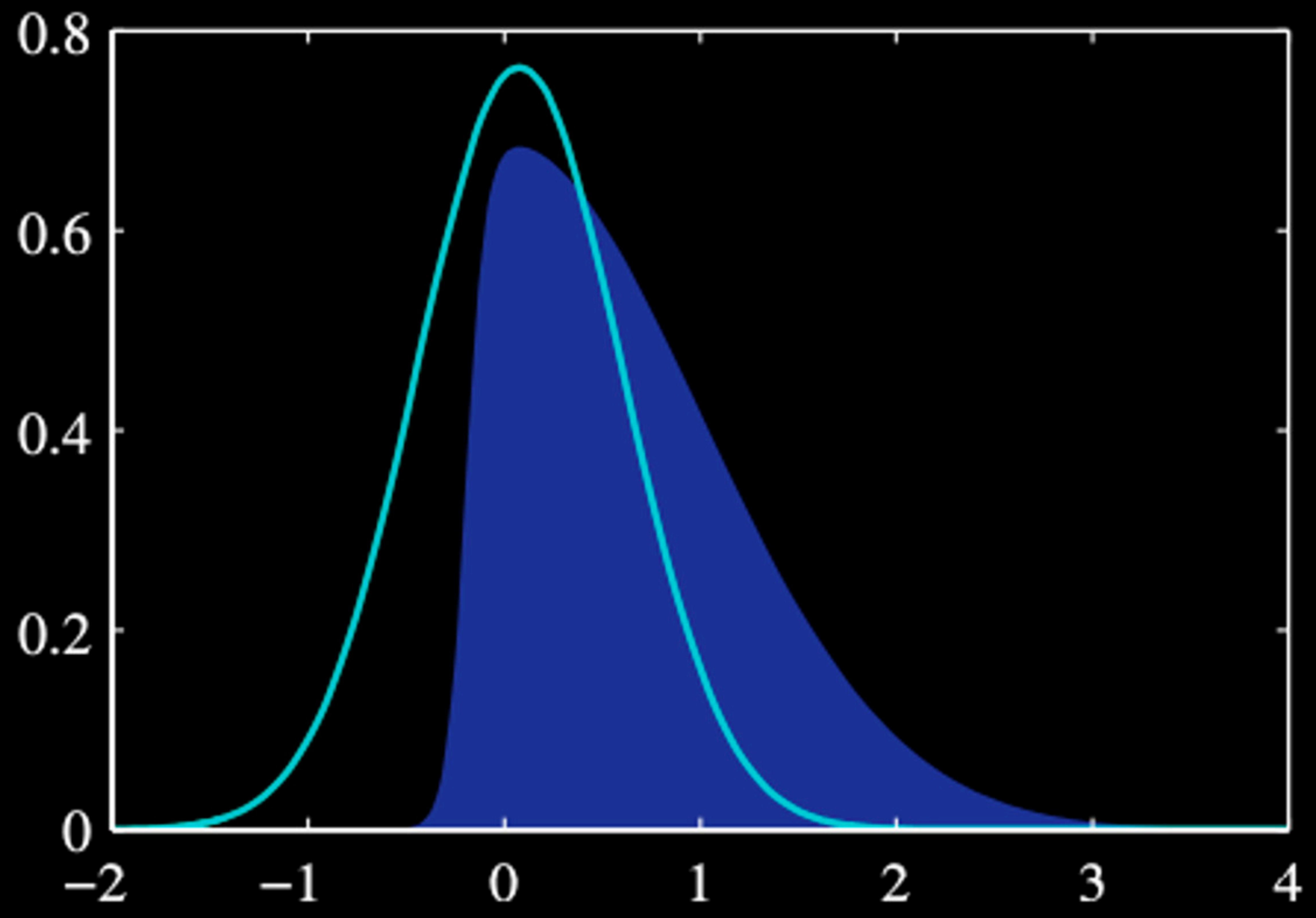
$$\ln f(z) \simeq \ln f(z_0) - \frac{1}{2} A (z - z_0)^2$$

Bishop eq 4.127



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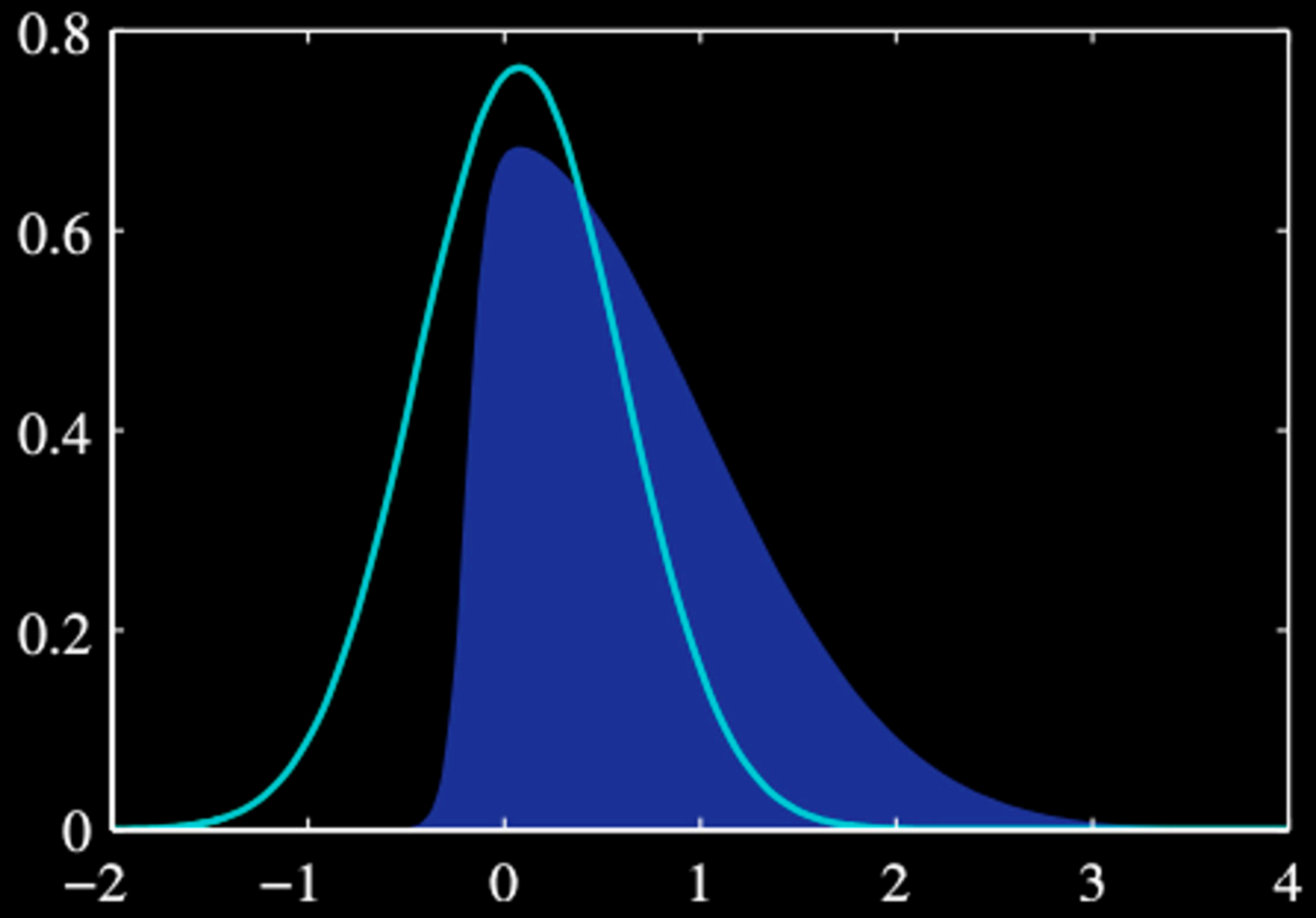
$$A = -\frac{\mathrm{d}^2}{\mathrm{d}z^2} \ln f(z) \bigg|_{z=z_0}$$

Bishop eq 4.128



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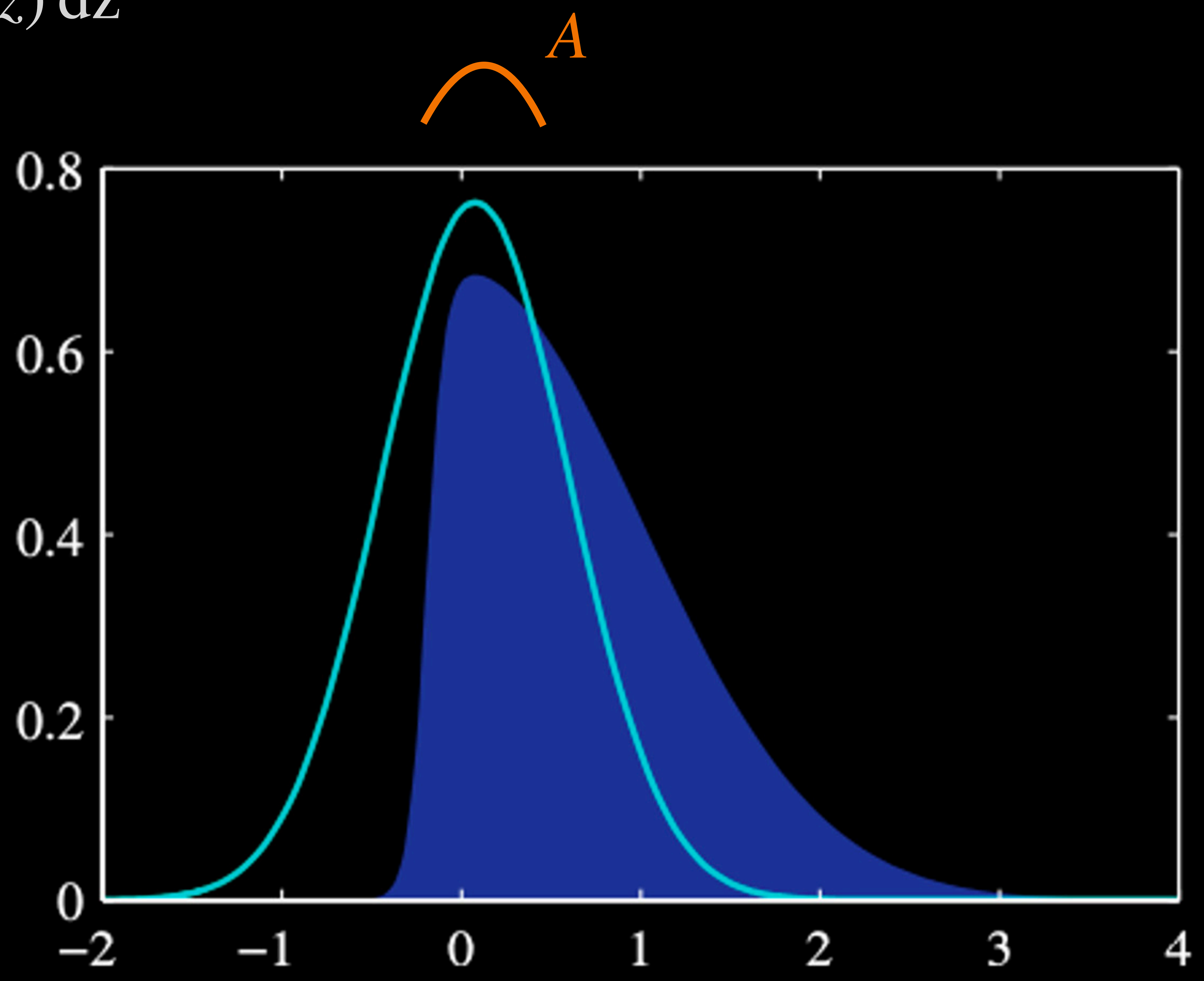

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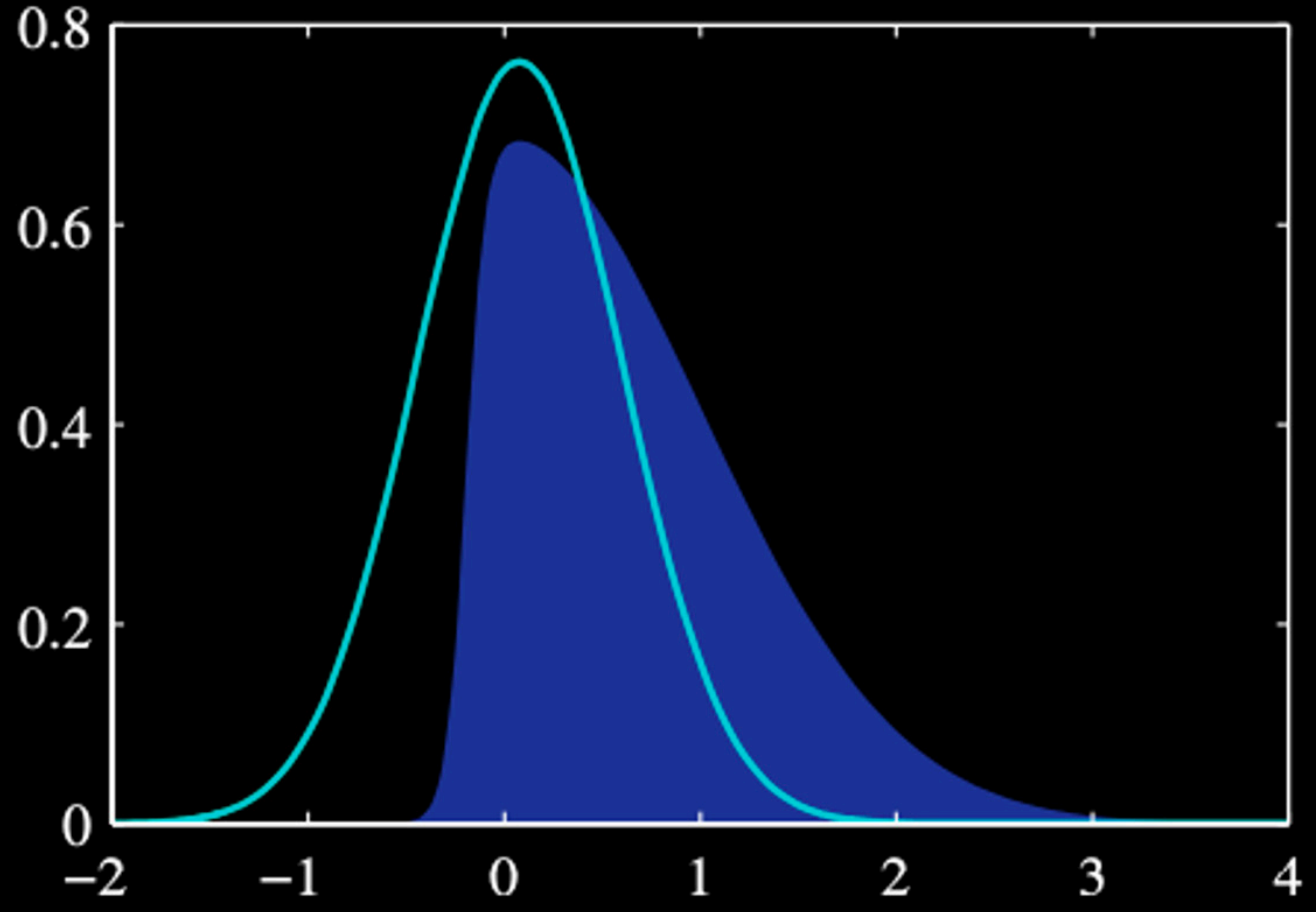

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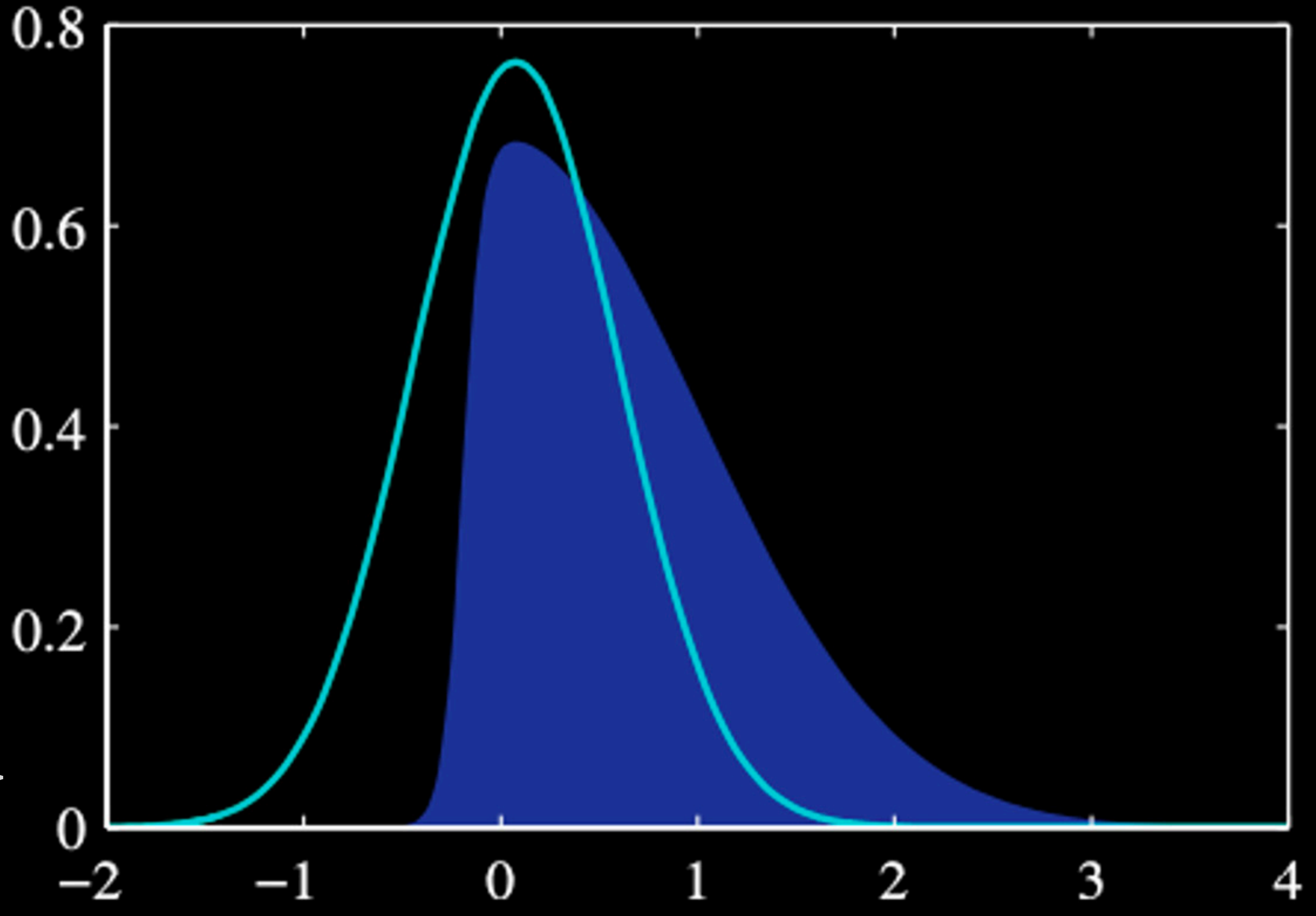
Normalize

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

Bishop eq 4.130



# Laplace Approximation in 1D

Mode $\left.\frac{\mathrm{d}f(z)}{\mathrm{d}z}\right|_{z=z_0} = 0$

$$A = -\left.\frac{\mathrm{d}^2}{\mathrm{d}z^2}\ln f(z)\right|_{z=z_0}$$

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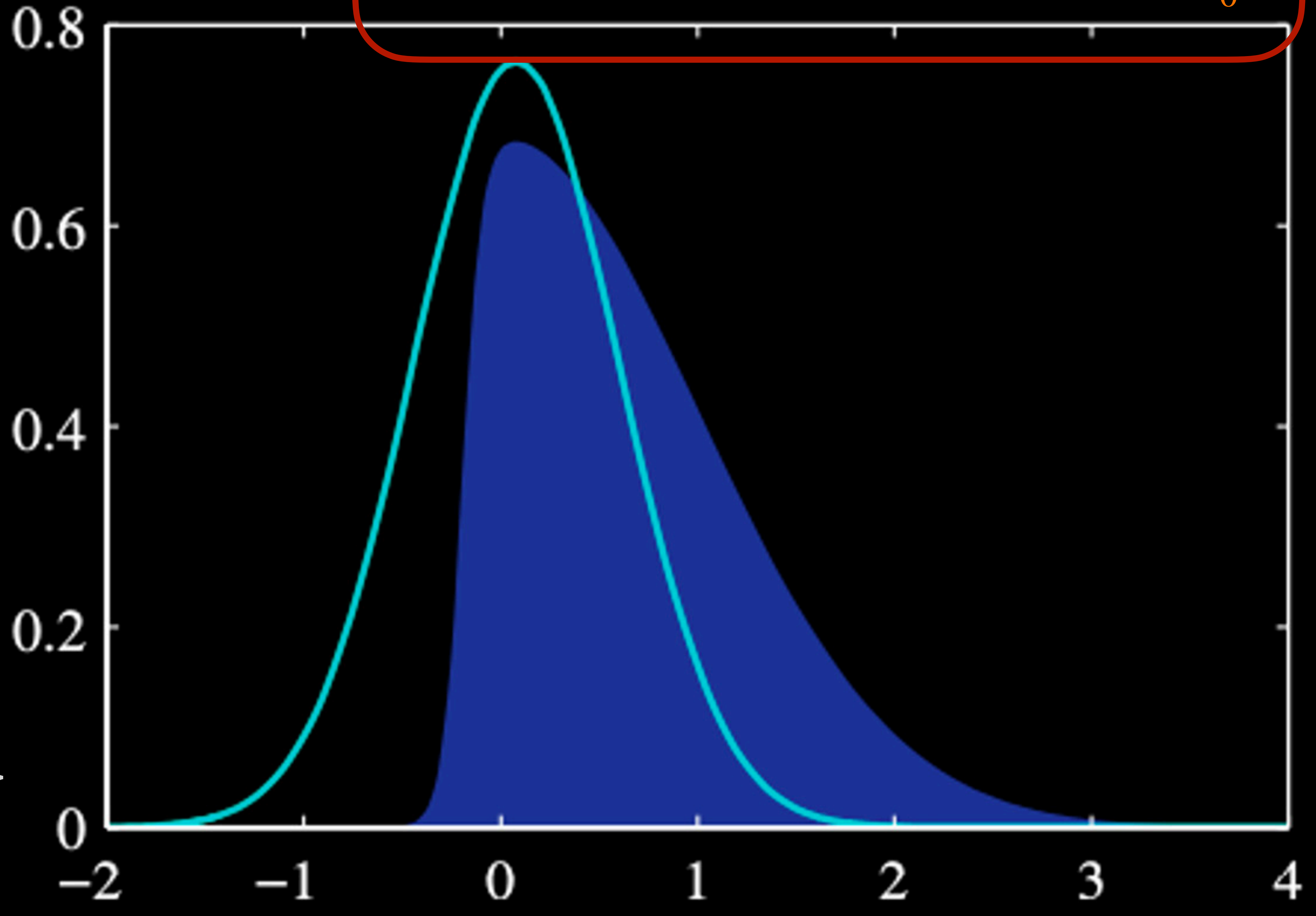
Bishop eq 4.130



Pros:

Cons:

Pros: ✓

Cons: ✗

- Assume that $\mathbf{z}$ spans the entire support of $\mathbb{R}^d$, might need to perform a change of variable if, e.g., $\mathbf{z} \in \mathbb{R}^{+d}$

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- Normalization constant $Z$ for $p(\mathbf{z})$ is not needed

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Pros: ✓

- Normalization constant $Z$ for $p(\mathbf{z})$ is not needed

- Central Limit Theorem ensures that the posterior is better approximated by a Gaussian as the number of observed data increases

---

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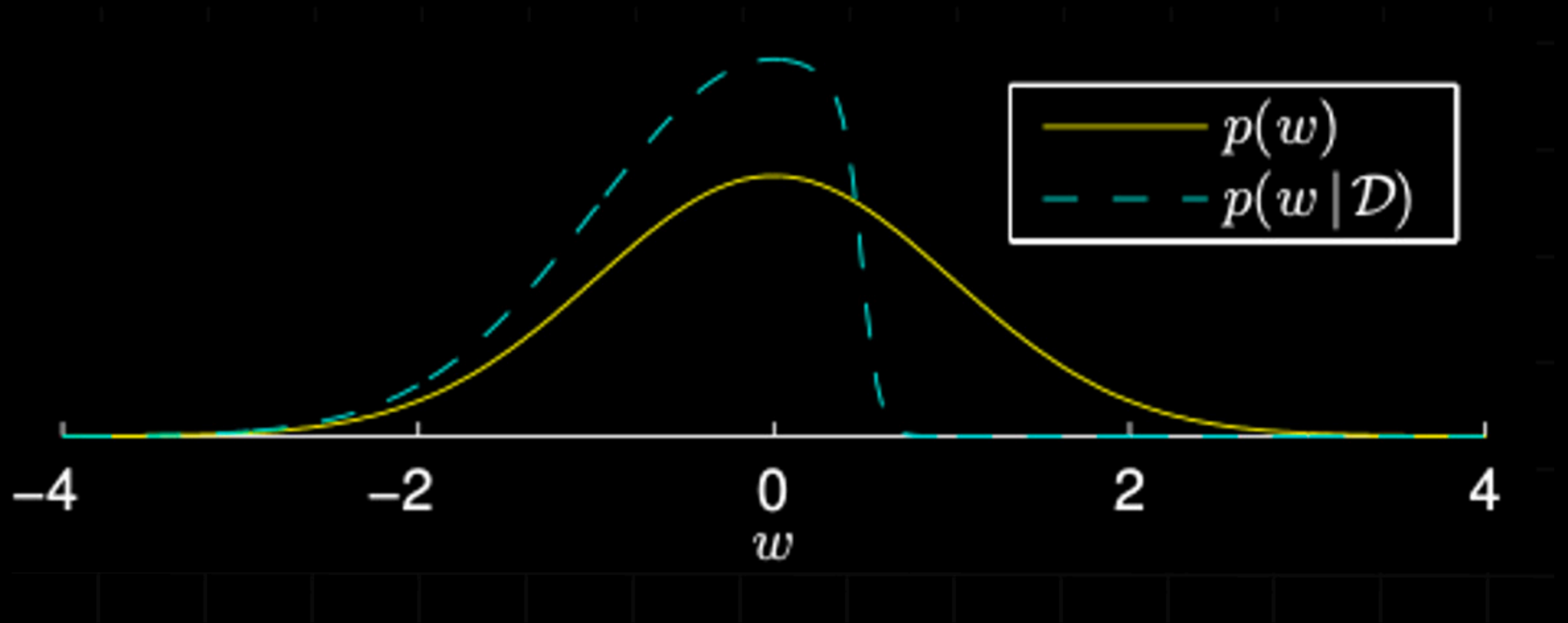
# Why Laplacian Approximation Works Well

Recall

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




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

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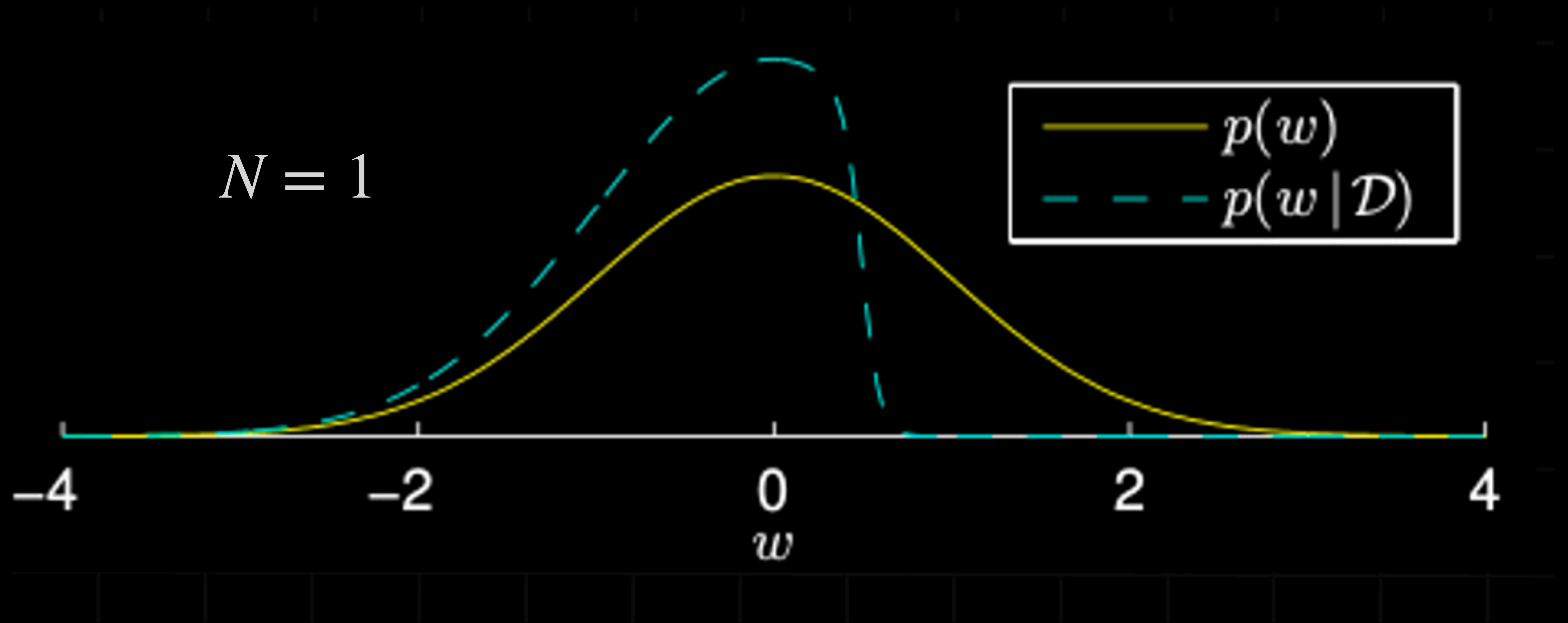


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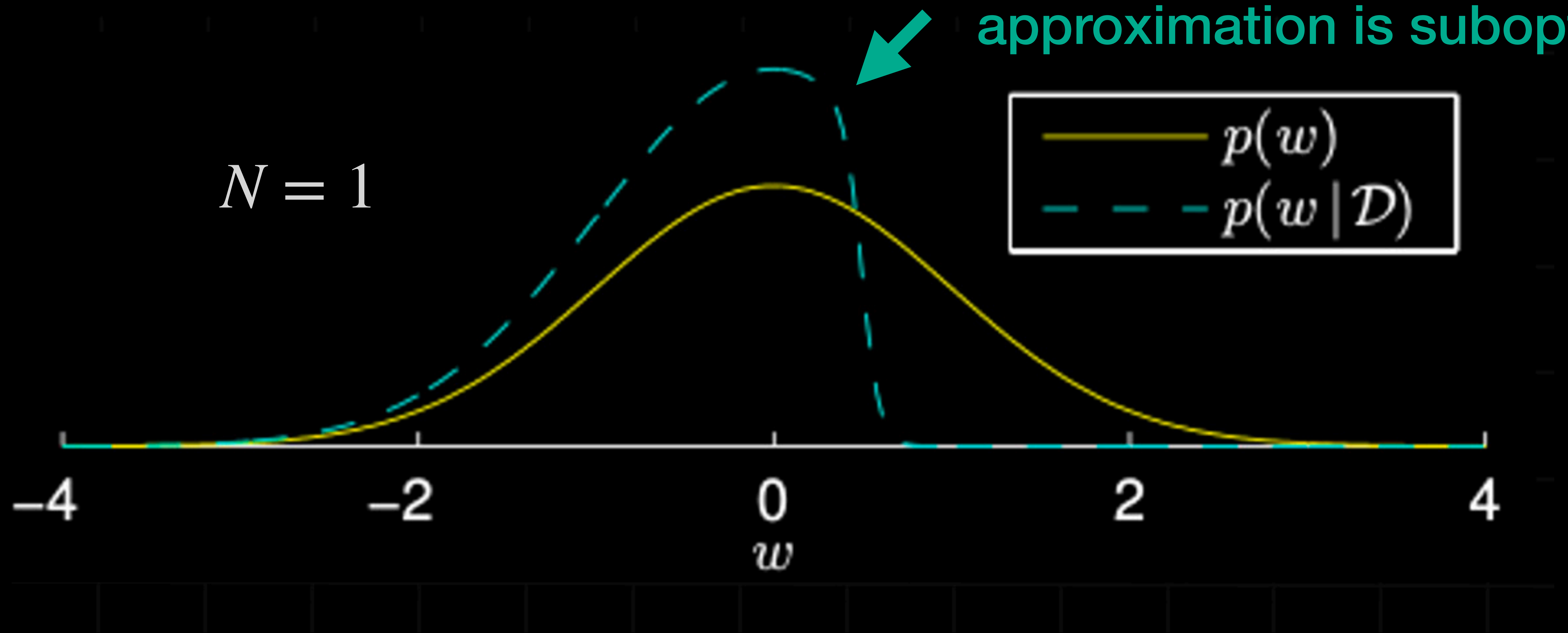
Posterior : Gaussian approximation is suboptimal

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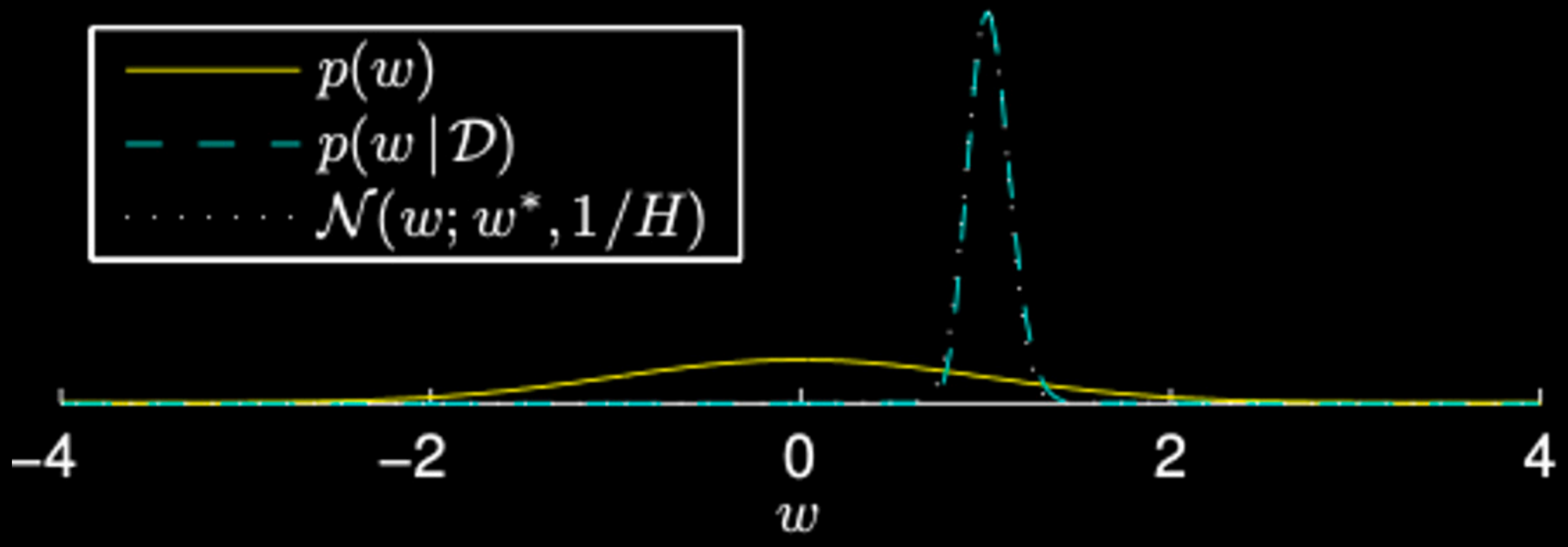
$N = 500$

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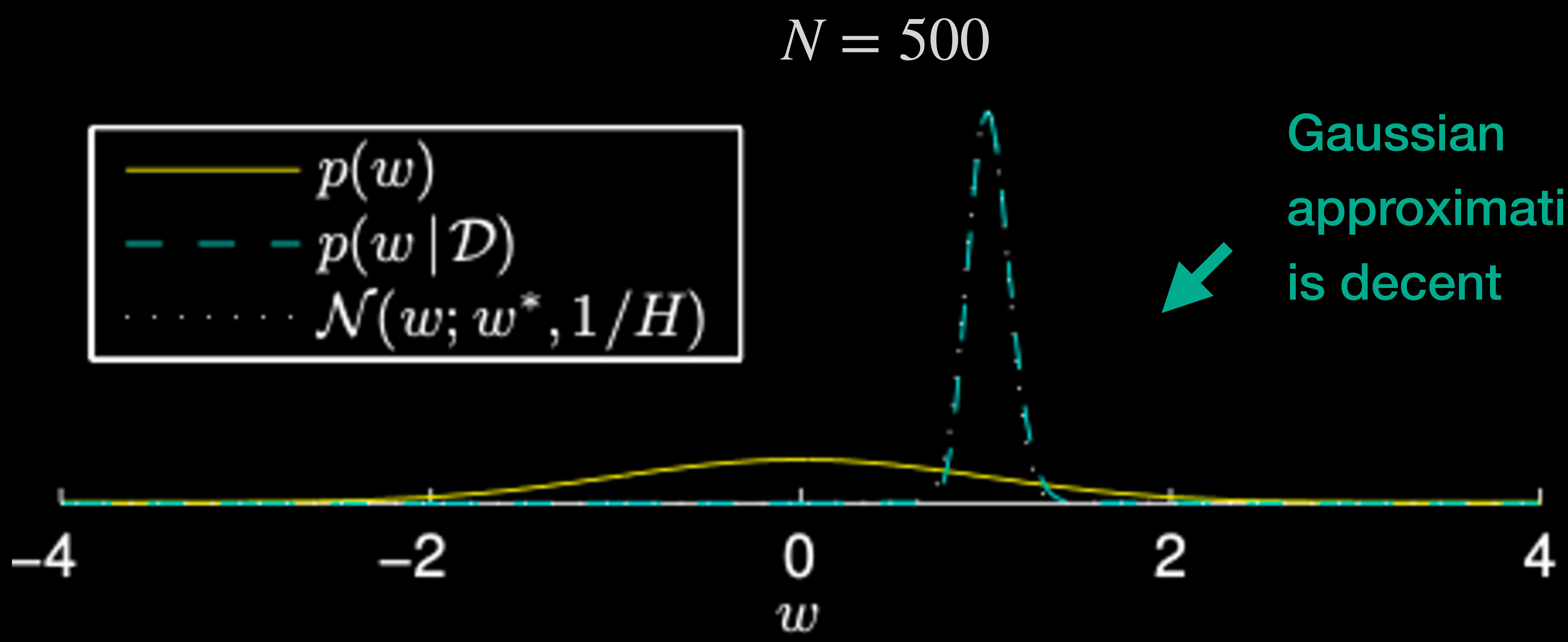


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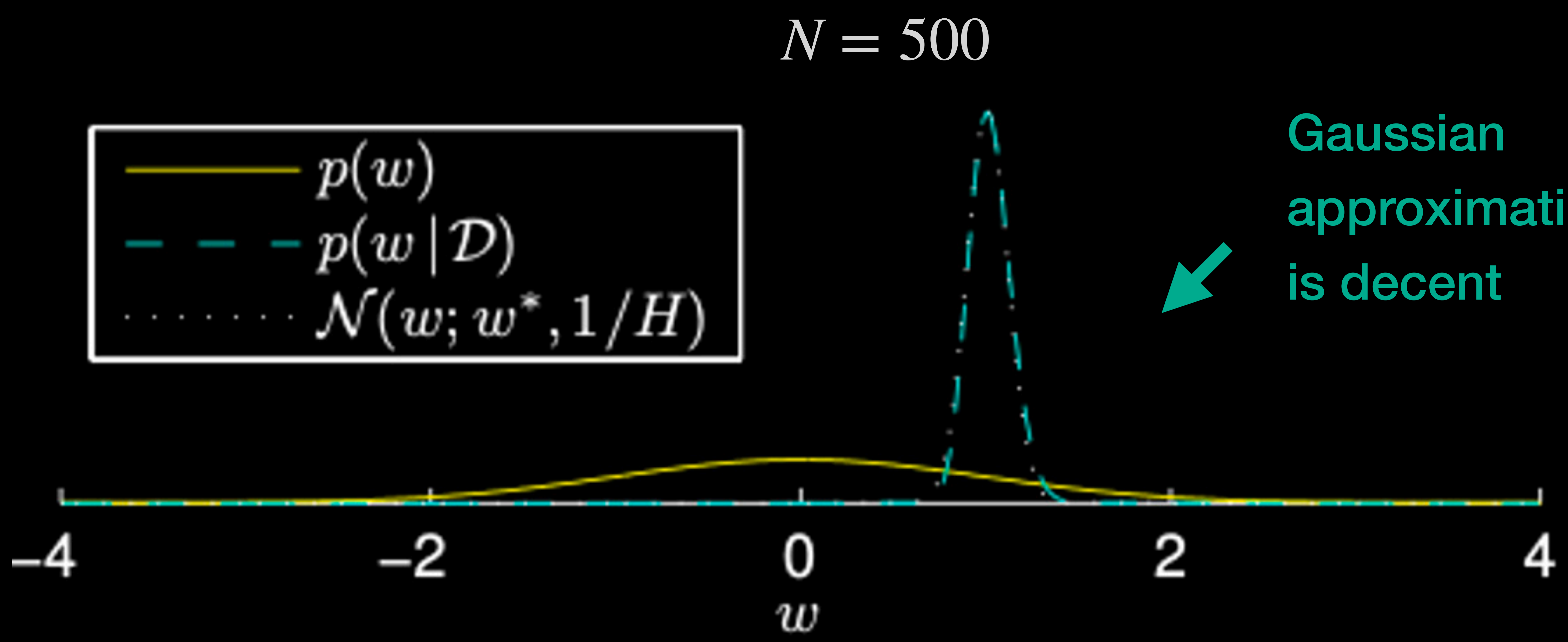
This function is concave and have a unique maximum (exercise)

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# 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

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

Bishop eq 4.144

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

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Bishop eq 4.144

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

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

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Bishop eq 4.142

$$\downarrow \nabla_\theta$$

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

$$\downarrow \nabla_\theta$$

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

Bishop eq 4.143

# Predictive Distribution for Bayesian Logistic Regression

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

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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

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Probit function (closely related to the erf function)

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

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

**Proof :** $\lambda = 1/\omega$

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

**Proof :** $\lambda = 1/\omega$

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

Let

$$X \sim \mathcal{N}(0,\omega^2), \quad Y \sim \mathcal{N}(\mu, \sigma^2)$$

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On the one hand

$$P(X \leq Y) = P(Z \leq 0) = \Phi\left(\frac{\mu}{\sqrt{\omega^2 + \sigma^2}}\right)$$

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$$P(X \leq Y) = P(Z \leq 0) = \Phi\left(\frac{\mu}{\sqrt{\omega^2 + \sigma^2}}\right)$$

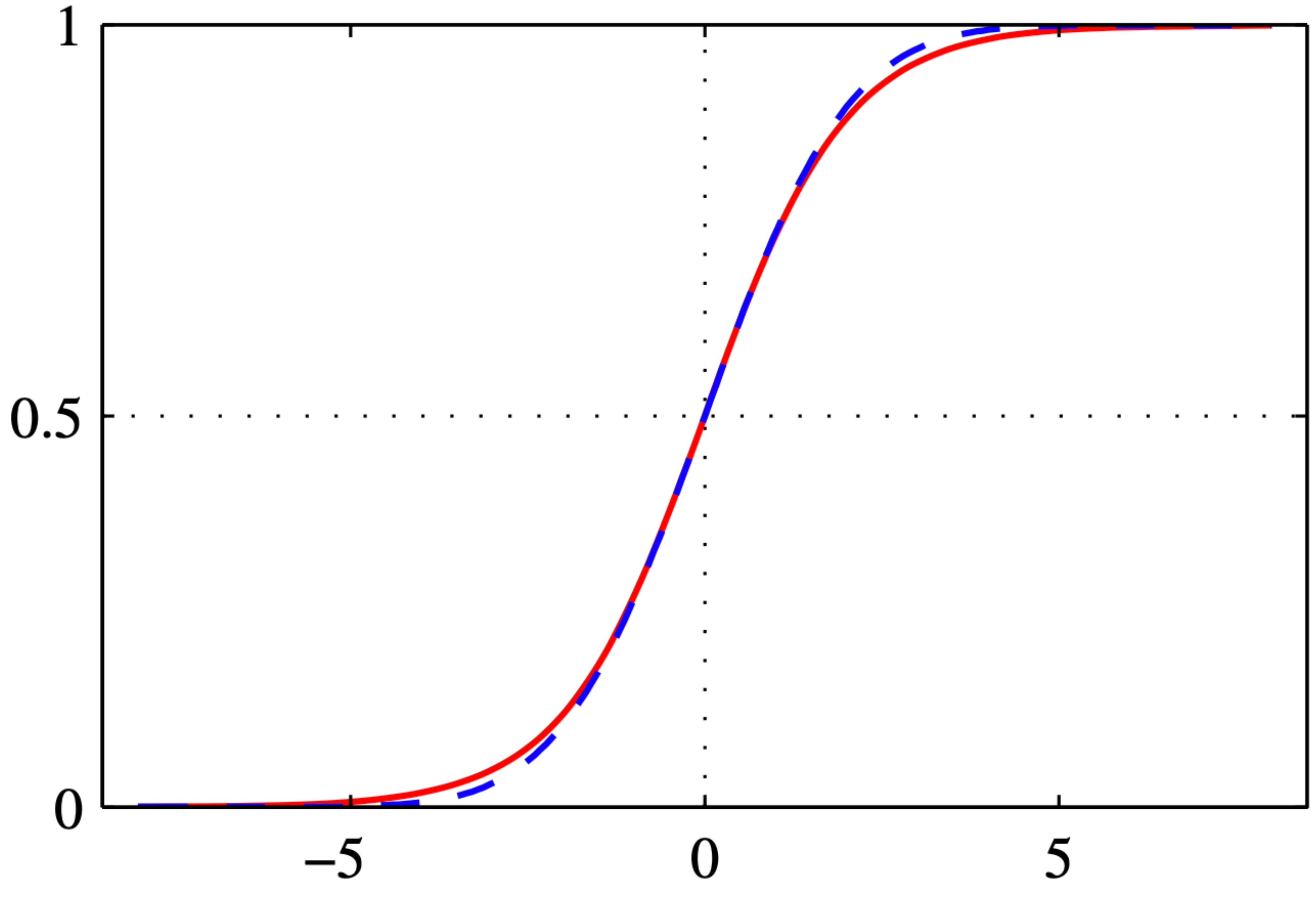
On the other hand, integrating all possible $Y$

$$P(X \leq Y) = \int_{-\infty}^{\infty} P(X \leq a) \mathcal{N}(a \,|\, \mu, \sigma^2)\,\mathrm{d}a = \int_{-\infty}^{\infty} \Phi\left(\frac{a}{\omega}\right) \mathcal{N}(a \,|\, \mu, \sigma^2)\,\mathrm{d}a$$

# 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 $a = 0$.



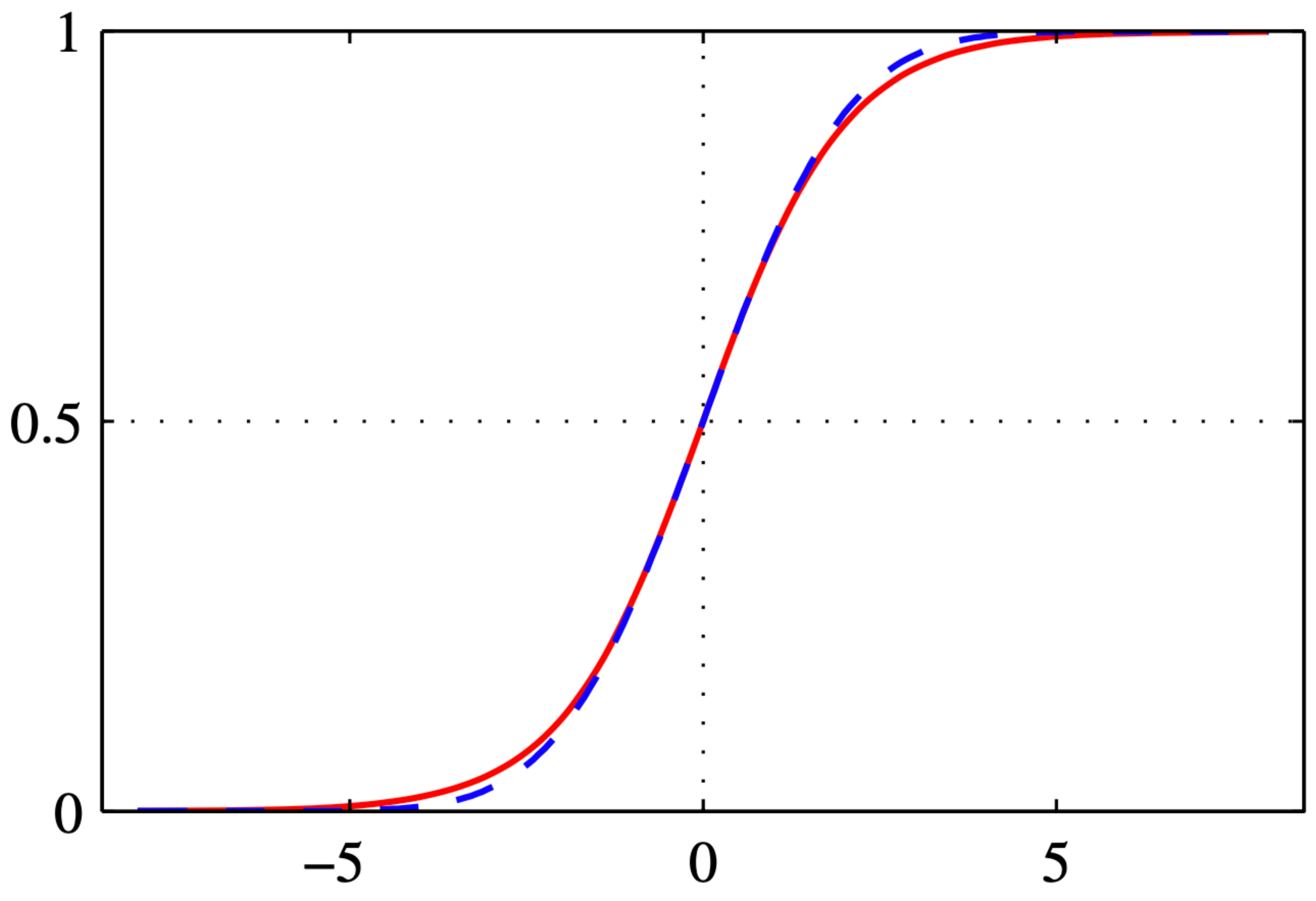
# Approximating Sigmoid Function with Probit Function

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

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

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

Bishop eq 4.153

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# 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

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$$\mathcal{N}(a \mid \mu_a, \sigma_a^2)$$

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

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

Bishop eq 4.147, 4.151

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

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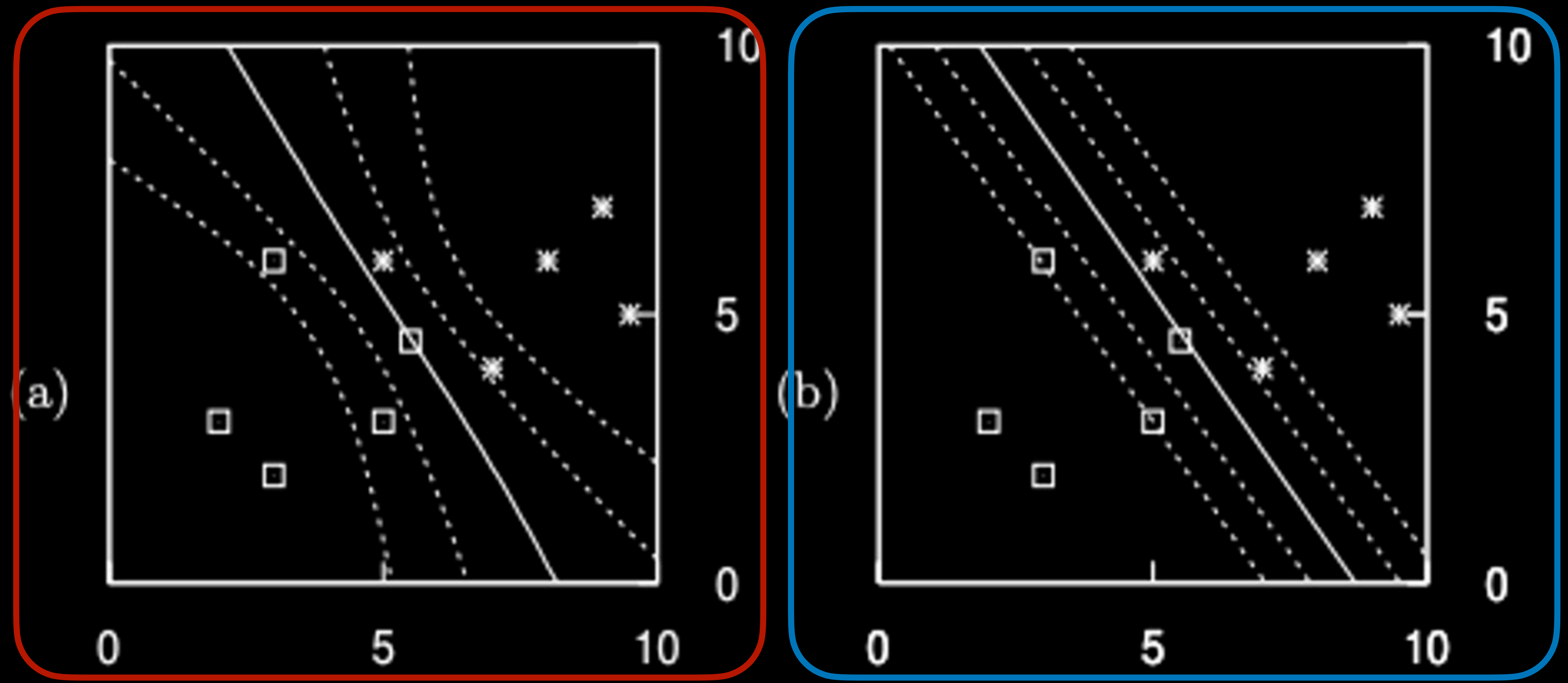
Bishop eq 4.147, 4.151

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

Bishop eq 4.153

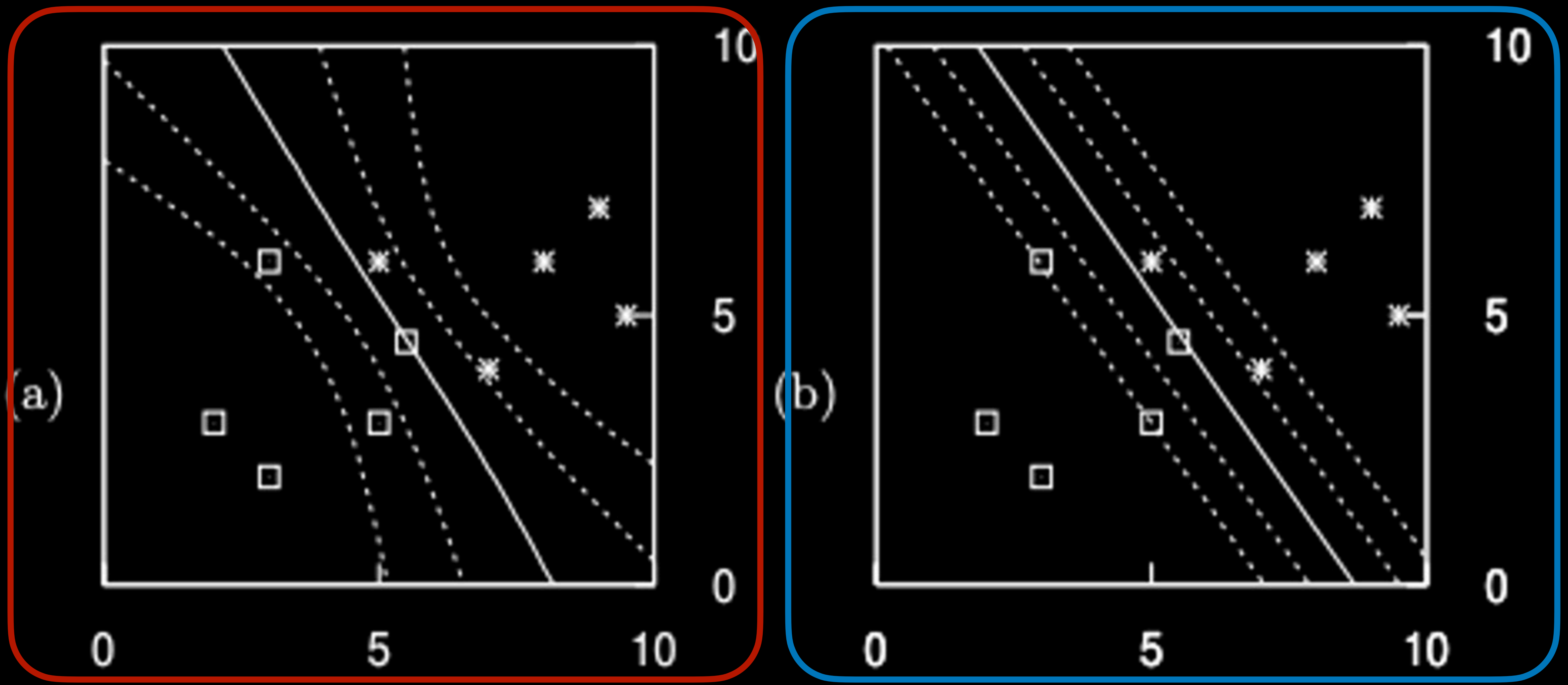
# Predictive Distribution with Laplace Approximation




Again, the axes are the input features $x_1$ and $x_2$. The right hand figure shows $P(y=1 \mid \mathbf{x}, \mathbf{w}^*)$ for some fitted weights $\mathbf{w}^*$. No matter how these fitted weights are chosen, the contours have to be linear. The parallel contours mean that the uncertainty of predictions falls at the same rate when moving away from the decision boundary, no matter how far we are from the training inputs.

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 with Laplace Approximation




$p(\mathbf{y}^* \,|\, \mathbf{x}^*, \theta_{\text{MAP}})$

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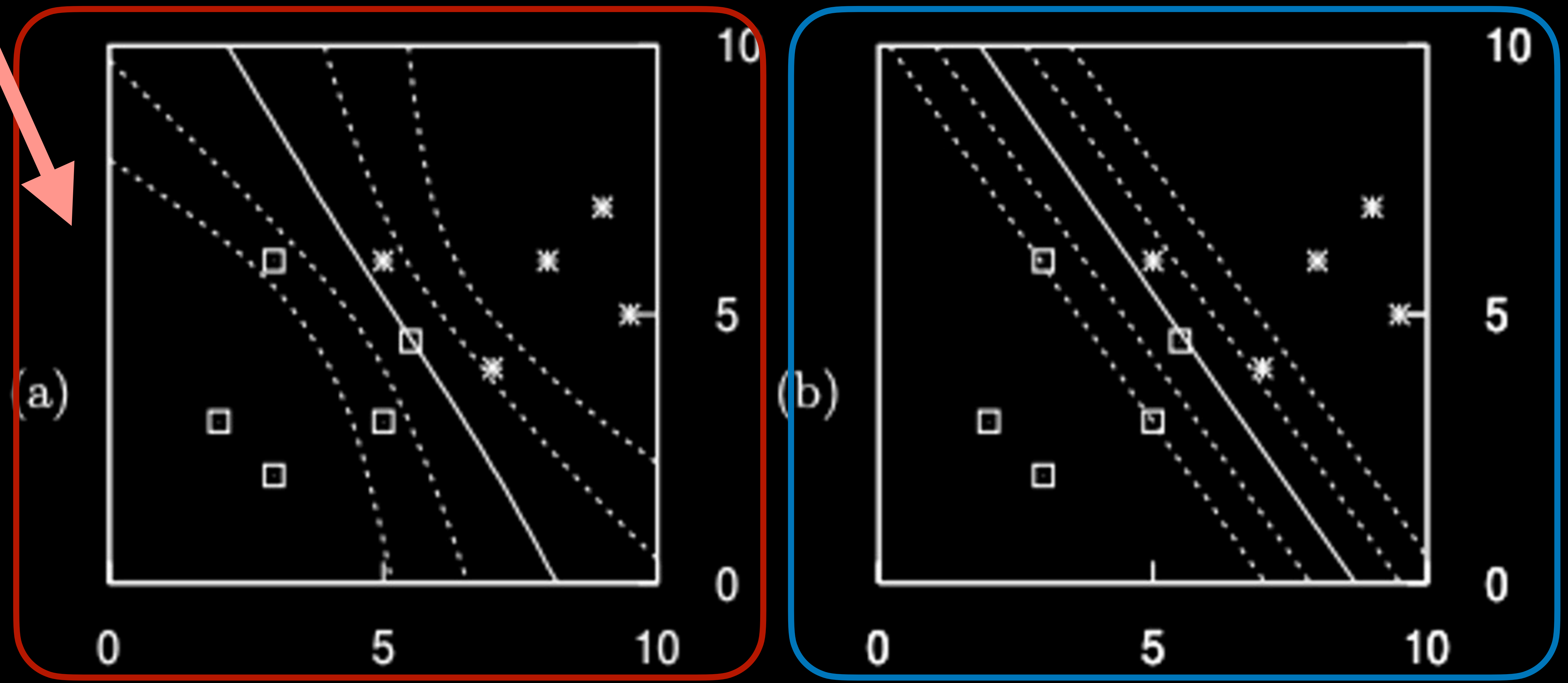
$p(y^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y})$

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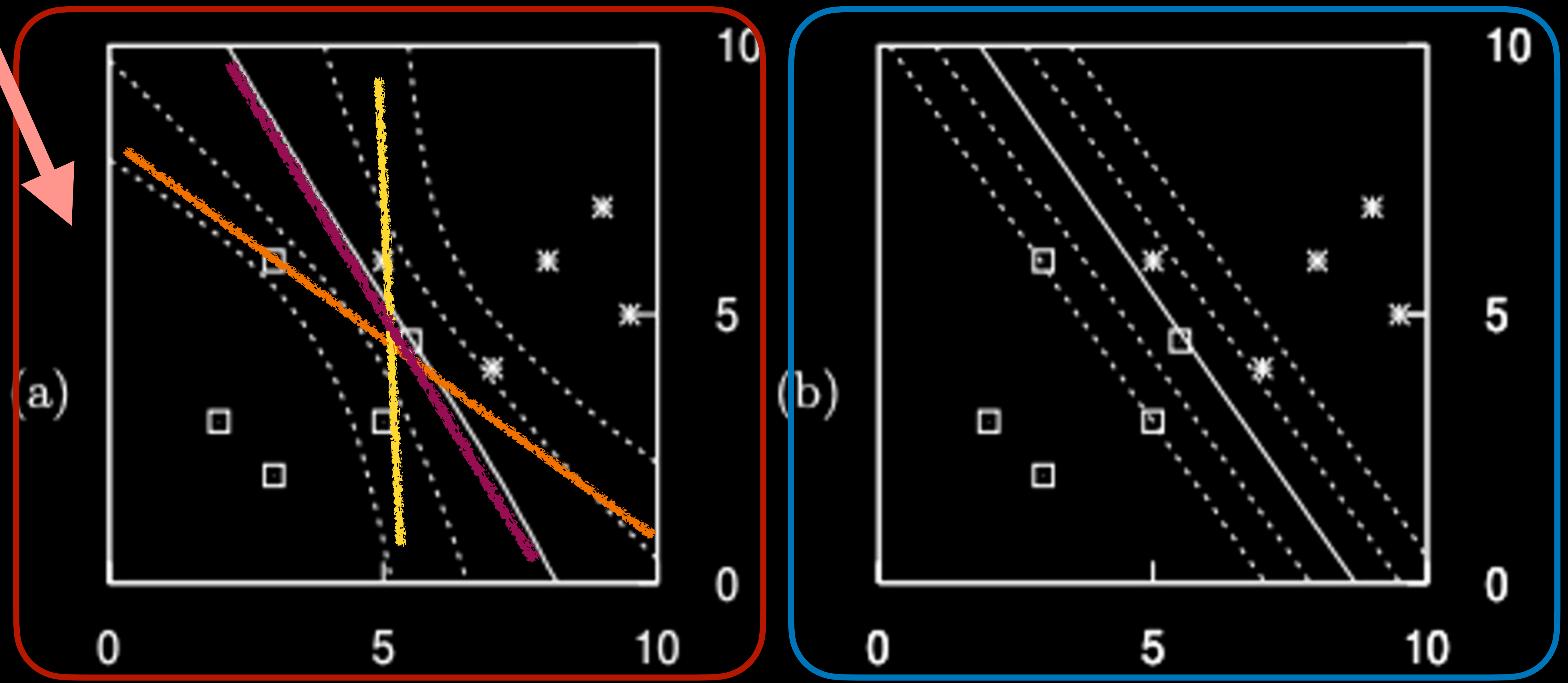


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# Gaussian Process for Classification

Recall in Gaussian Process Regression

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

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

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Key idea — using GP as a intermediate step

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Key idea — using GP as a intermediate step

Recall in logistic regression

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

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Key idea — using GP as a intermediate step

And the "squash" it with a sigmoid function

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

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

Bishop eq 6.73

Recall in logistic regression

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

# Gaussian Process for Classification

Recall in Gaussian Process Regression

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Key idea — using GP as a intermediate step

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

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

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

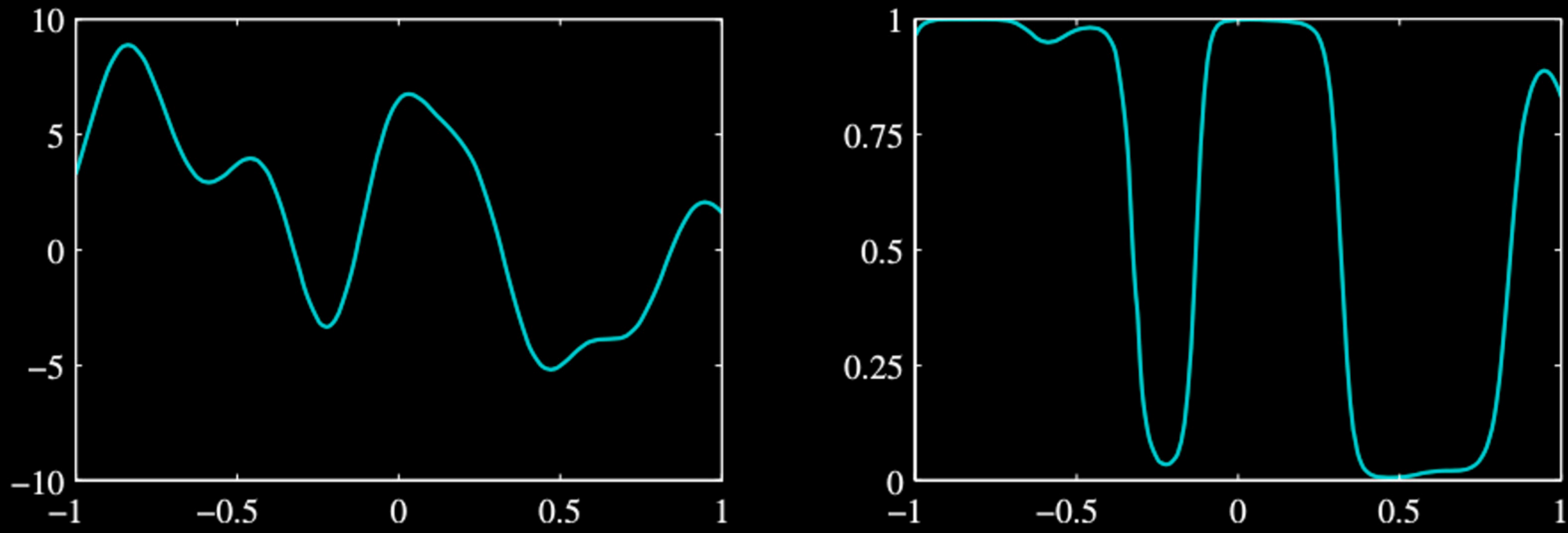


**Figure 6.11** The left plot shows a sample from a Gaussian process prior over functions $a(\mathbf{x})$, and the right plot shows the result of transforming this sample using a logistic sigmoid function.

# Gaussian Process for Classification

Input Variable

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

# Gaussian Process for Classification

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

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

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

Bishop eq 6.75

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

# Gaussian Process for the Intermediate Variable

Bishop eq 6.74

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Recall from Gaussian Process Regression that

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

# Gaussian Process for the Intermediate Variable

Bishop eq 6.74

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

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

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

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

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

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

Bishop eq 6.79

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

Bishop eq 6.80, GP Book eq 3.12

# Laplace Approximation for Gaussian Process Classification

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

$$\boxed{\mathbf{y}^T\mathbf{f}} - \boxed{\sum_{n=1}^{N}\ln(1+e^{f_n})} \qquad -\boxed{\frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f}} - \frac{N}{2}\ln(2\pi) - \frac{1}{2}\ln|\mathbf{K}|$$

Bishop eq 6.80, GP Book eq 3.12

Bishop eq 6.79

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

Bishop eq 6.81, GP Book eq 3.13, 3.15

# Laplace Approximation for Gaussian Process Classification

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

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

Bishop eq 6.79

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

Bishop eq 6.80, GP Book eq 3.12

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

Bishop eq 6.81, GP Book eq 3.13, 3.15

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

Bishop eq 6.84, GP Book eq 3.17

# Laplace Approximation for Gaussian Process Classification

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

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

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Bishop eq 6.80, GP Book eq 3.12

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

Bishop eq 6.81, GP Book eq 3.13, 3.15

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

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

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

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

# Laplace Approximation for Gaussian Process Classification

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

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

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

Bishop eq 6.82, GP Book eq 3.14, 3.15

# Laplace Approximation for Gaussian Process Classification

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

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

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

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

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

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

Bishop eq 6.82, GP Book eq 3.14, 3.15

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

Bishop eq 6.86

# One More Layer Up …

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

# One More Layer Up …

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

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

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

# One More Layer Up …

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

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

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

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

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

# One More Layer Up …

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

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

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

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

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# One More Layer Up …

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

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

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

Bishop eq 2.115

# One More Layer Up …

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

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

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

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

Bishop eq 2.115

# One More Layer Up …

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

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

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

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

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

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# One More Layer Up ...

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

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

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

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

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

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

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

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

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 …

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

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

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

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

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

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

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

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

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 ...

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

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

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

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

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

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

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

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

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

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

Bishop eq 6.88,
GP Book eq 3.22

# Predictive Distribution for Gaussian Process Classification

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

GP Book eq 3.10

# Predictive Distribution for Gaussian Process Classification

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

GP Book eq 3.10

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

# Predictive Distribution for Gaussian Process Classification

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

GP Book eq 3.10

# Predictive Distribution for Gaussian Process Classification

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

GP Book eq 3.10

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

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

GP Book eq 3.10

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

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

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

Bishop eq 6.87, GP Book eq 3.21

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

Bishop eq 6.88, GP Book eq 3.22

**Recall with Probit approximation**

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

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

Bishop eq 4.153

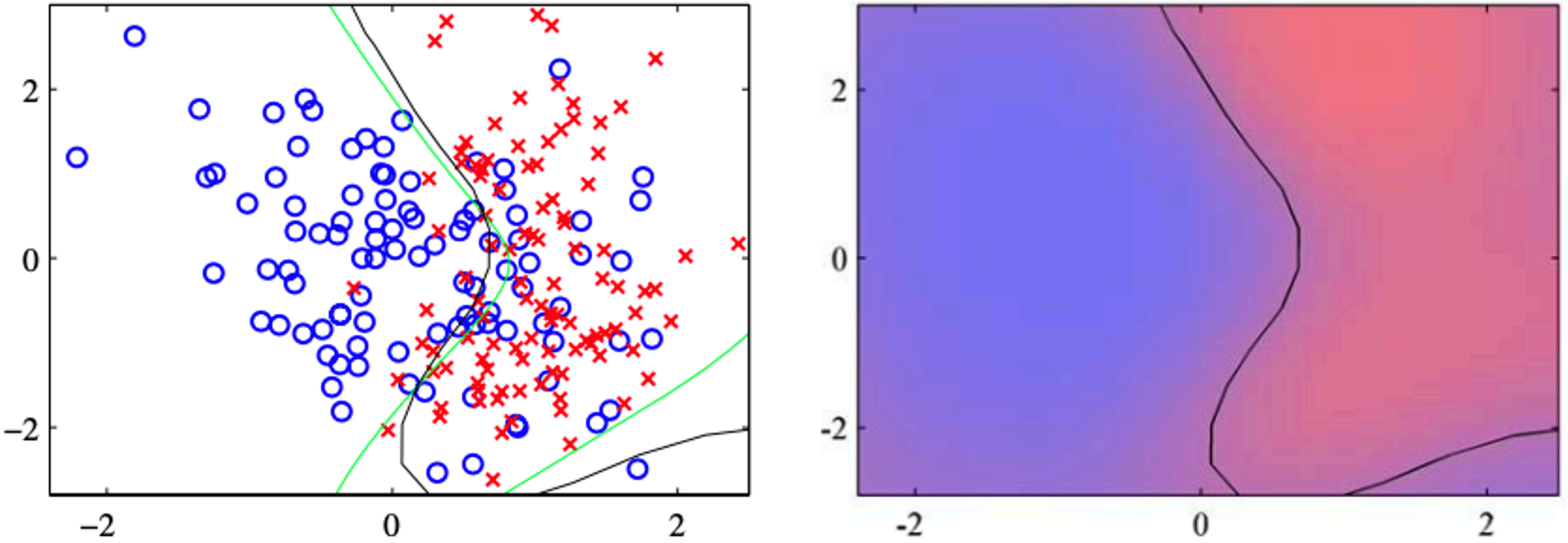


**Figure 6.12** Illustration of the use of a Gaussian process for classification, showing the data on the left together with the optimal decision boundary from the true distribution in green, and the decision boundary from the Gaussian process classifier in black. On the right is the predicted posterior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

# Recap: Learning Hyperparameters in GP Regression

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

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

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

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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)

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Learning through gradient descent

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

(Bishop eq 6.70)

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# 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

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For a scaled Gaussian, the “normalising” constant

Bishop eq 4.135, 4.137, GP Book eq 3.31

$$p(\mathbf{y}\,|\,\mathbf{X},\theta) =$$

$$\int -\frac{1}{2}(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})^T\,\mathbf{H}\,(\mathbf{f}-\mathbf{f}_{\mathrm{MAP}})\,\mathrm{d}\mathbf{f}$$

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Goodness of fit at the optimal parameter

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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

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# What we have learned

- Bayesian Logistic Regression

  - the challenge to computing a non-Gaussian predictive distribution

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