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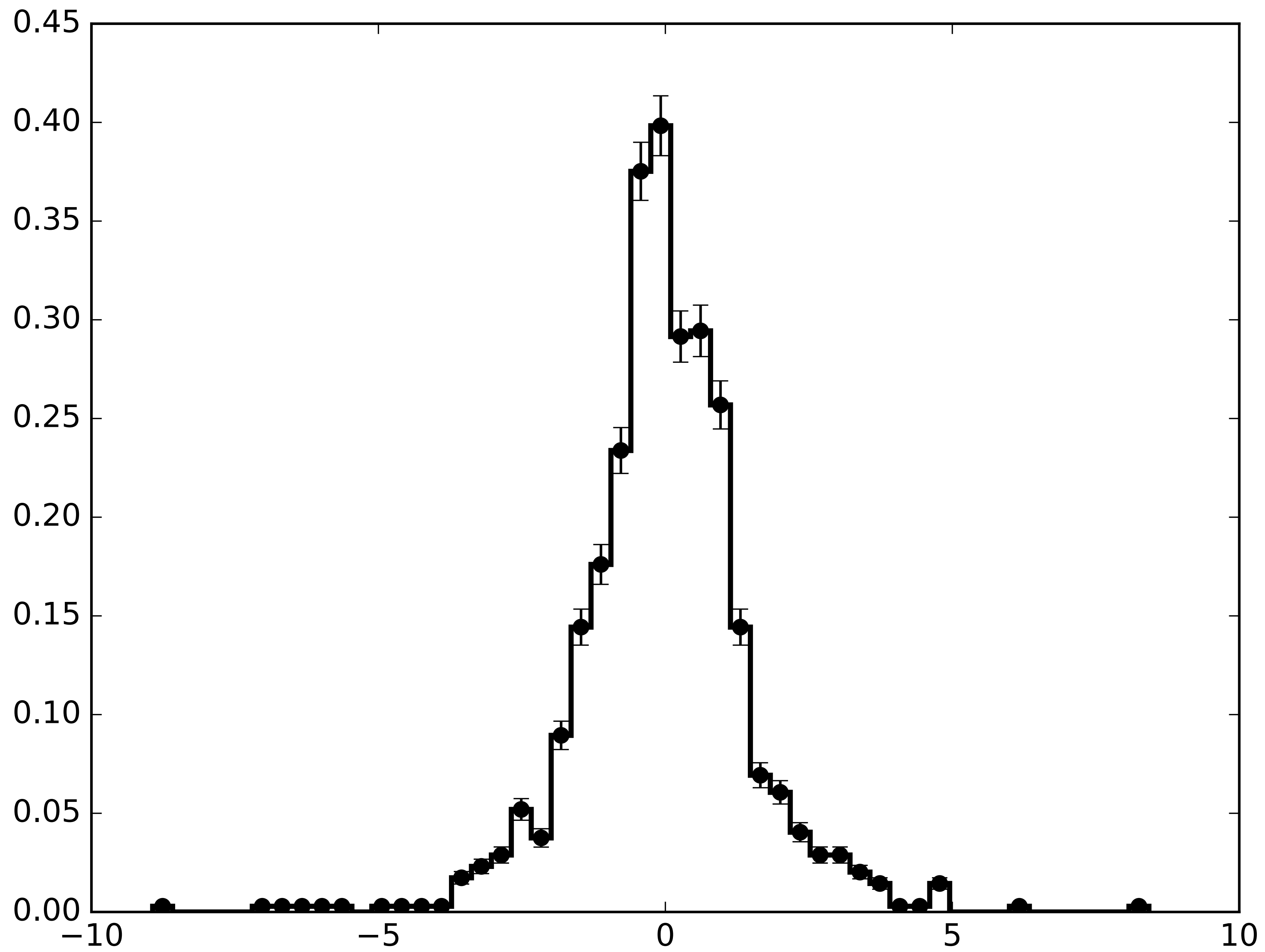
Técnicas estadísticas para el análisis de datos **astrofísicos**

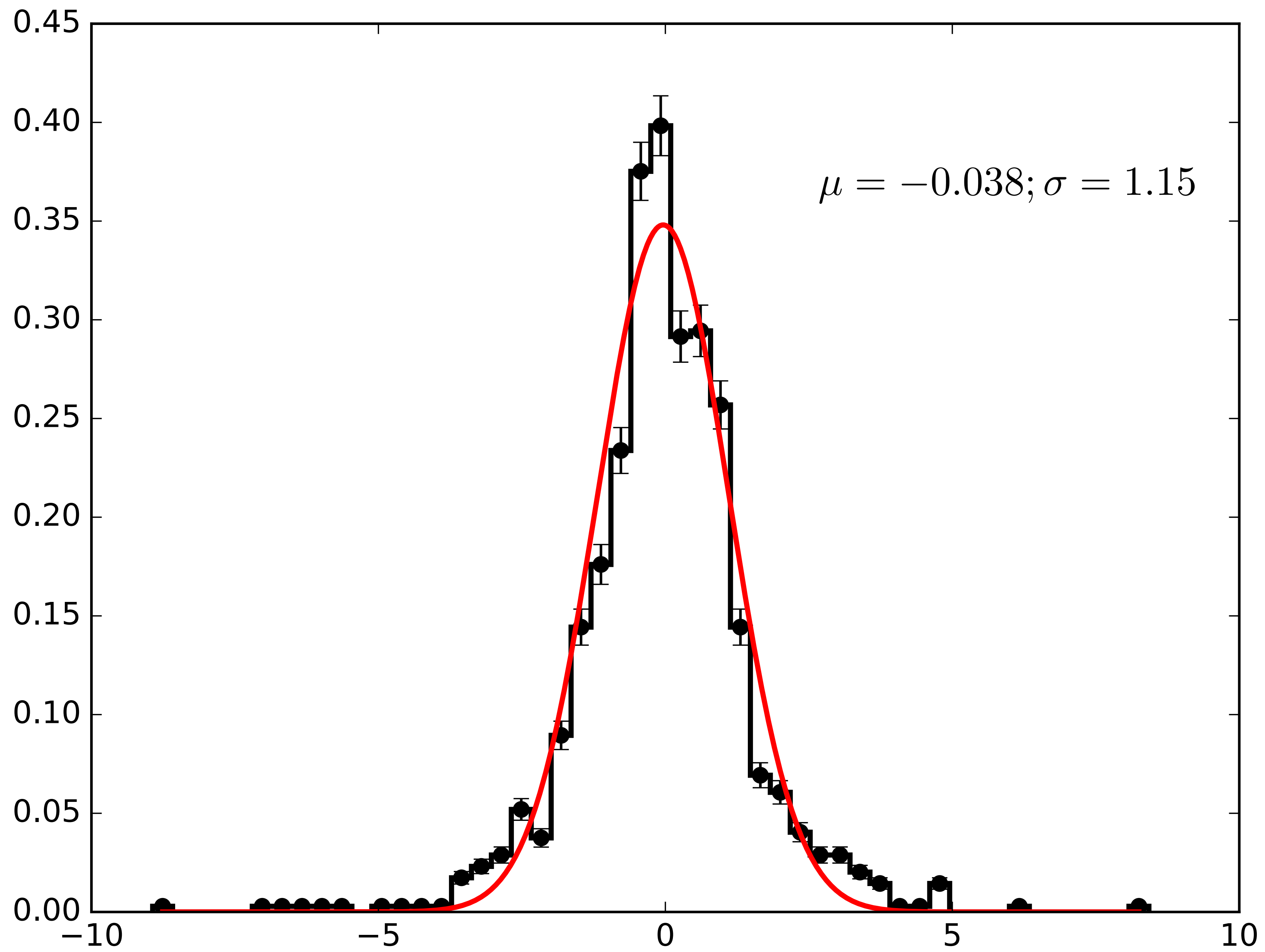
Rodrigo F. Díaz

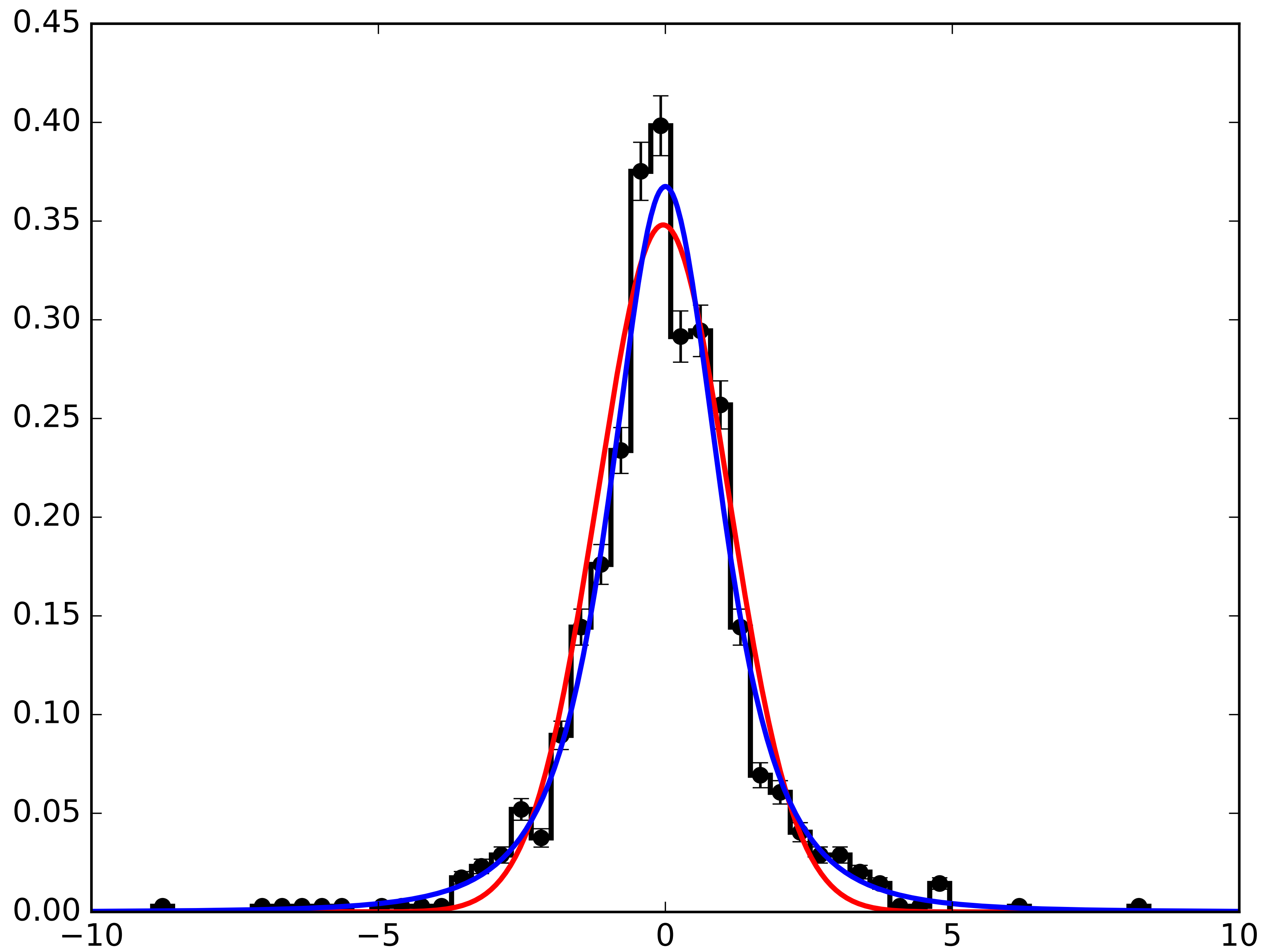
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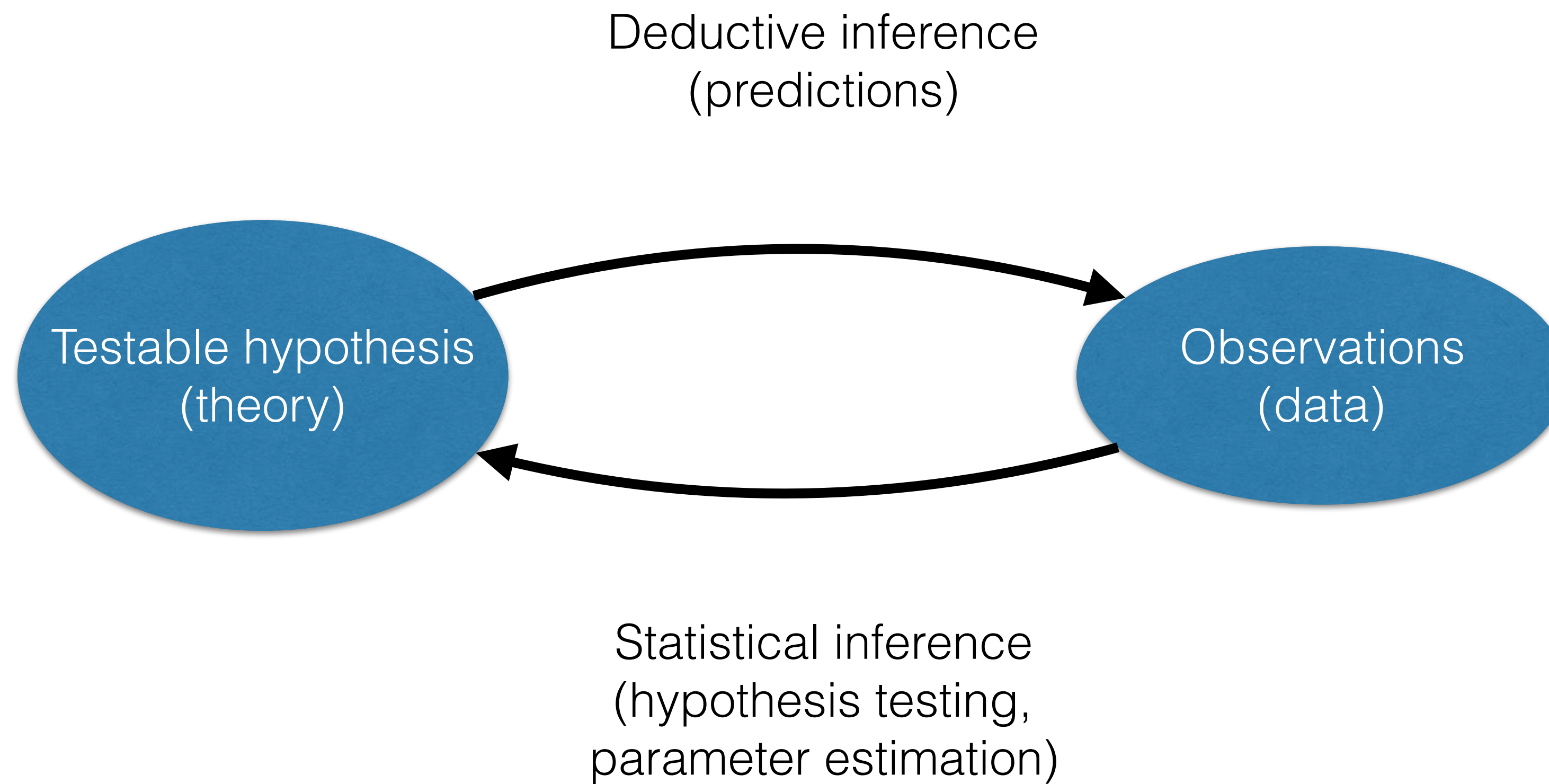






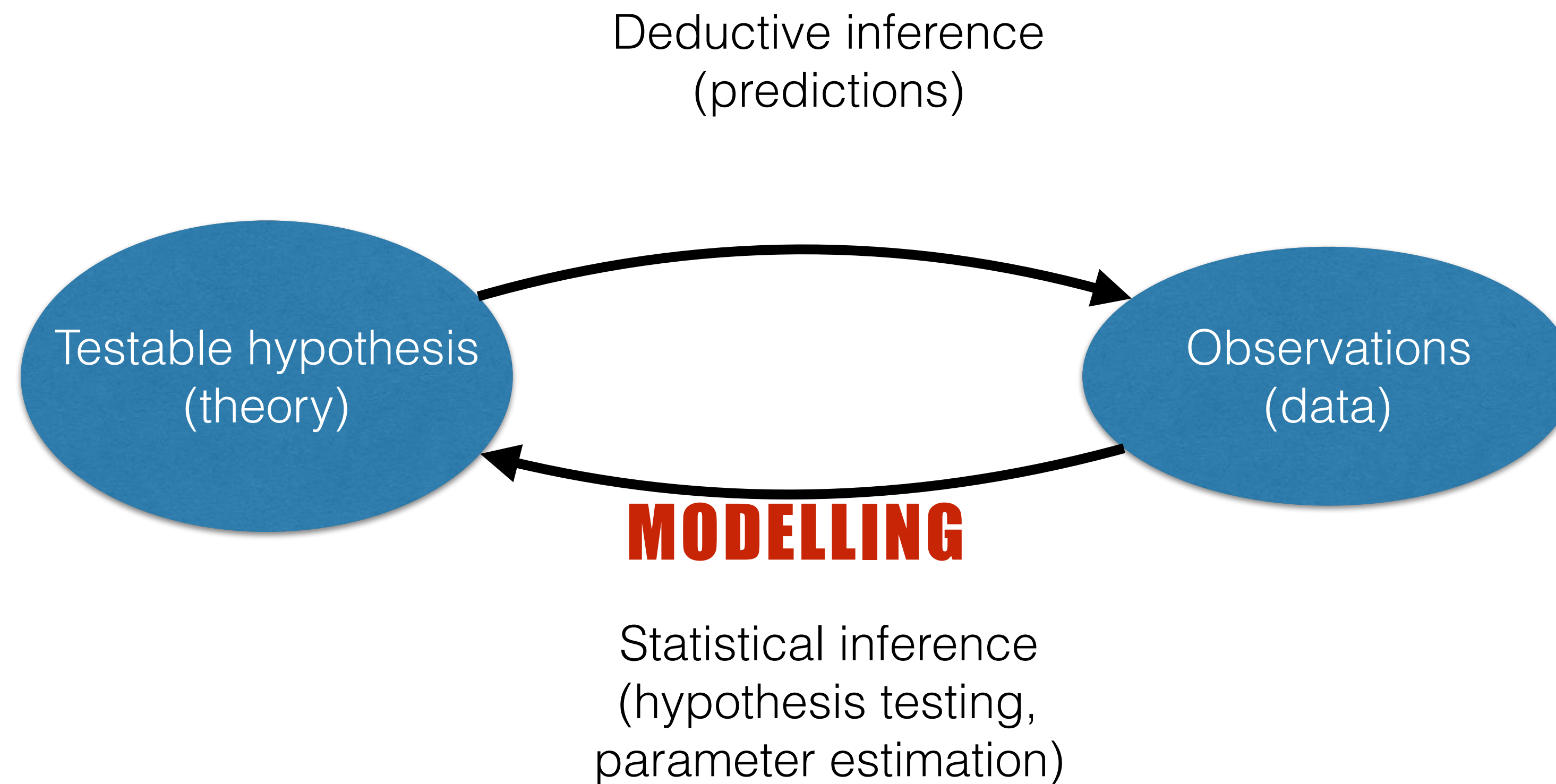
Data modelling in the scientific method

Fig. adapted from
Gregory (2005)



Data modelling in the scientific method

Fig. adapted from
Gregory (2005)



Agenda para hoy

- **Introducción a los modelos lineales para la regresión.**
 - ¿Qué son los modelos lineales?
 - ¿Qué modelan?
 - ¿Cómo encuentro los valores de los parámetros?
 - ...
- **Diagnóstico de modelos**
 - Residuos.
 - Palanca.
 - ...

Modelling

The very basic idea

$$\underset{\text{data}}{t_i} = \underset{\text{model}}{m_i} + \underset{\text{error}}{\epsilon_i} \quad i = \{1, \dots, N\}$$

$$m_i = f(X_i | \omega)$$

Modelling

The very basic idea

Target values

$$\underset{\text{data}}{t_i} = \underset{\text{model}}{m_i} + \underset{\text{error}}{\epsilon_i} \quad i = \{1, \dots, N\}$$

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Modelling

The very basic idea

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Model parameters

Modelling

The very basic idea

Target values

$$\underset{\text{data}}{t_i} = \underset{\text{model}}{m_i} + \underset{\text{error}}{\epsilon_i} \quad i = \{1, \dots, N\}$$

$$m_i = f(X_i | \omega)$$

Features

Model parameters

Modelling

The very basic idea

Target values

$$\underset{\text{data}}{t_i} = \underset{\text{model}}{m_i} + \underset{\text{error}}{\epsilon_i} \quad i = \{1, \dots, N\}$$

I'm mainly interested in the model parameters, their values and their relation with the model prediction.

$$m_i = f(X_i | \omega)$$

Features

Model parameters



Alice

Modelling

The very basic idea

Target values

$$\underset{\text{data}}{t_i} = \underset{\text{model}}{m_i} + \underset{\text{error}}{\epsilon_i} \quad i = \{1, \dots, N\}$$

I'm mainly interested in the model parameters, their values and their relation with the model prediction.



Alice

$$m_i = f(X_i | \omega)$$

Features

Model parameters

I want to create a model that gives the most accurate predictions for *unseen* values of the features x



Bob

Modelling

A probabilistic view of linear regression

$$t_i = m_i + \epsilon_i$$

Modelling

A probabilistic view of linear regression

$$t_i = m_i + \epsilon_i$$

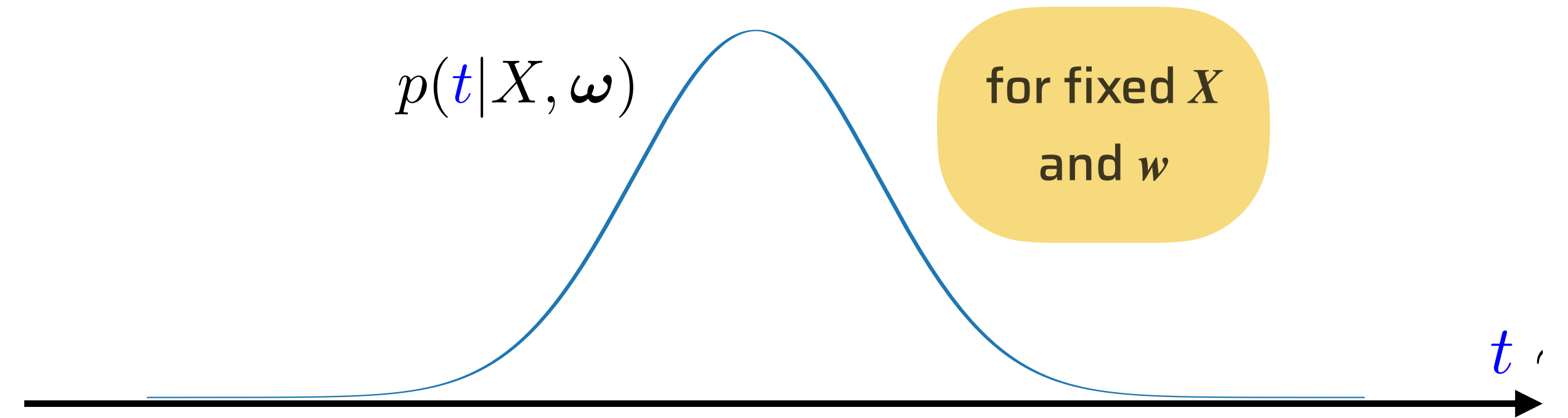
$$t \sim p(t|X, \omega)$$

Modelling

A probabilistic view of linear regression

$$t_i = m_i + \epsilon_i$$

$$t \sim p(t|X, \omega)$$



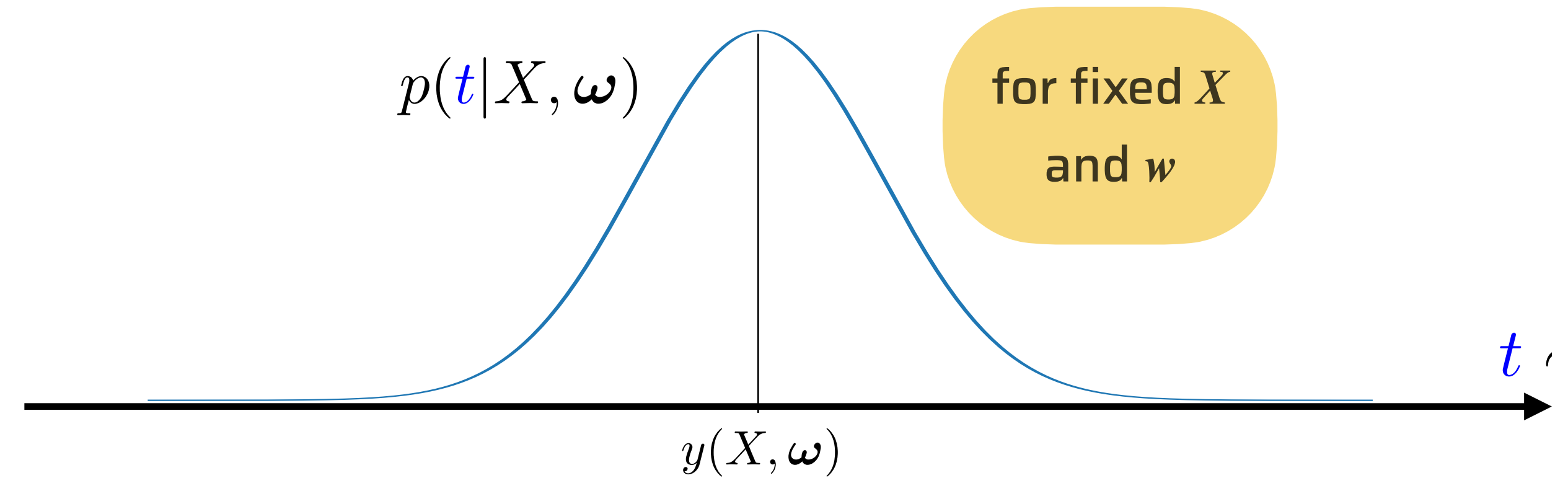
Modelling

A probabilistic view of linear regression

$$t_i = m_i + \epsilon_i$$

$$t \sim p(t|X, \omega)$$

$$\mathbb{E}(t|X) = y(X, \omega)$$

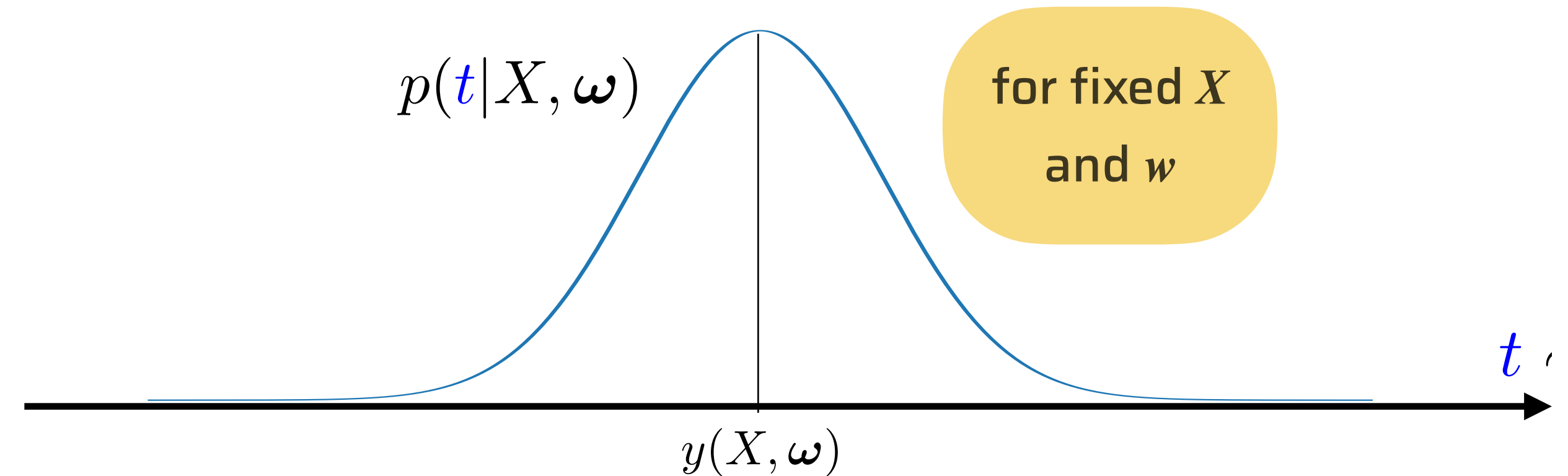


Modelling

A probabilistic view of linear regression

$$t_i = m_i + \epsilon_i$$

$$t \sim p(t|X, \omega)$$



$$\mathbb{E}(t|X) = y(X, \omega) = \omega_0 + \omega_1 \cdot X$$

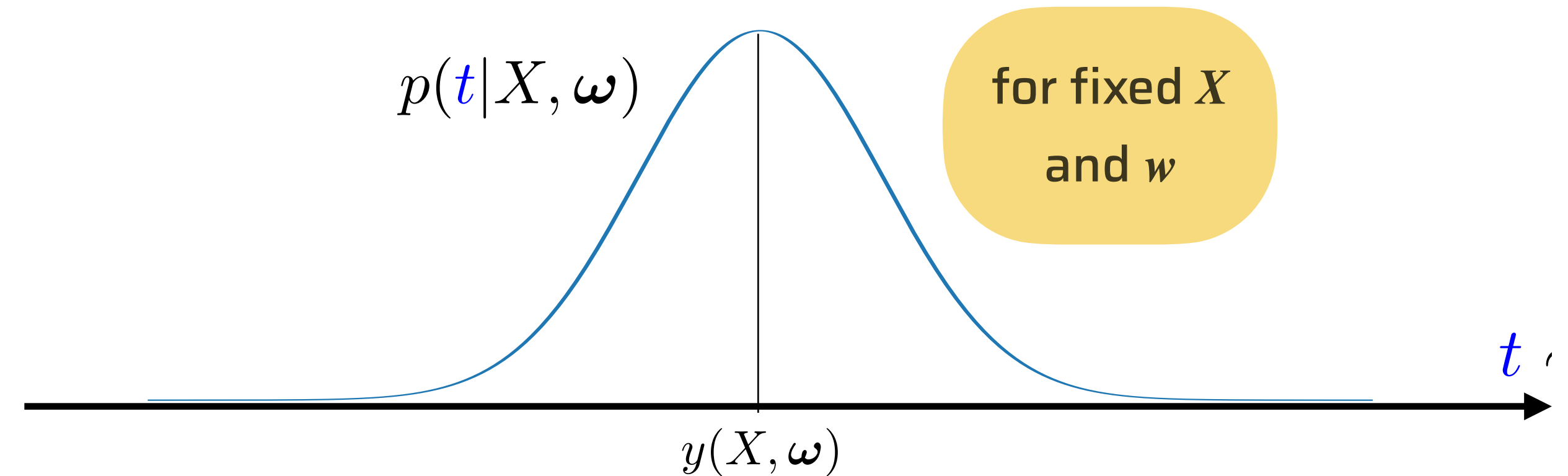
Simple Linear Regression

Modelling

A probabilistic view of linear regression

$$t_i = m_i + \epsilon_i$$

$$t \sim p(t|X, \omega)$$



$$\mathbb{E}(t|X) = y(X, \omega) = \omega_0 + \omega_1 \cdot X$$

Simple Linear Regression

$$y(\mathbf{X}, \omega) = \omega_0 + \omega_1 \cdot X_1 + \omega_2 \cdot X_2 + \dots + \omega_D \cdot X_D$$

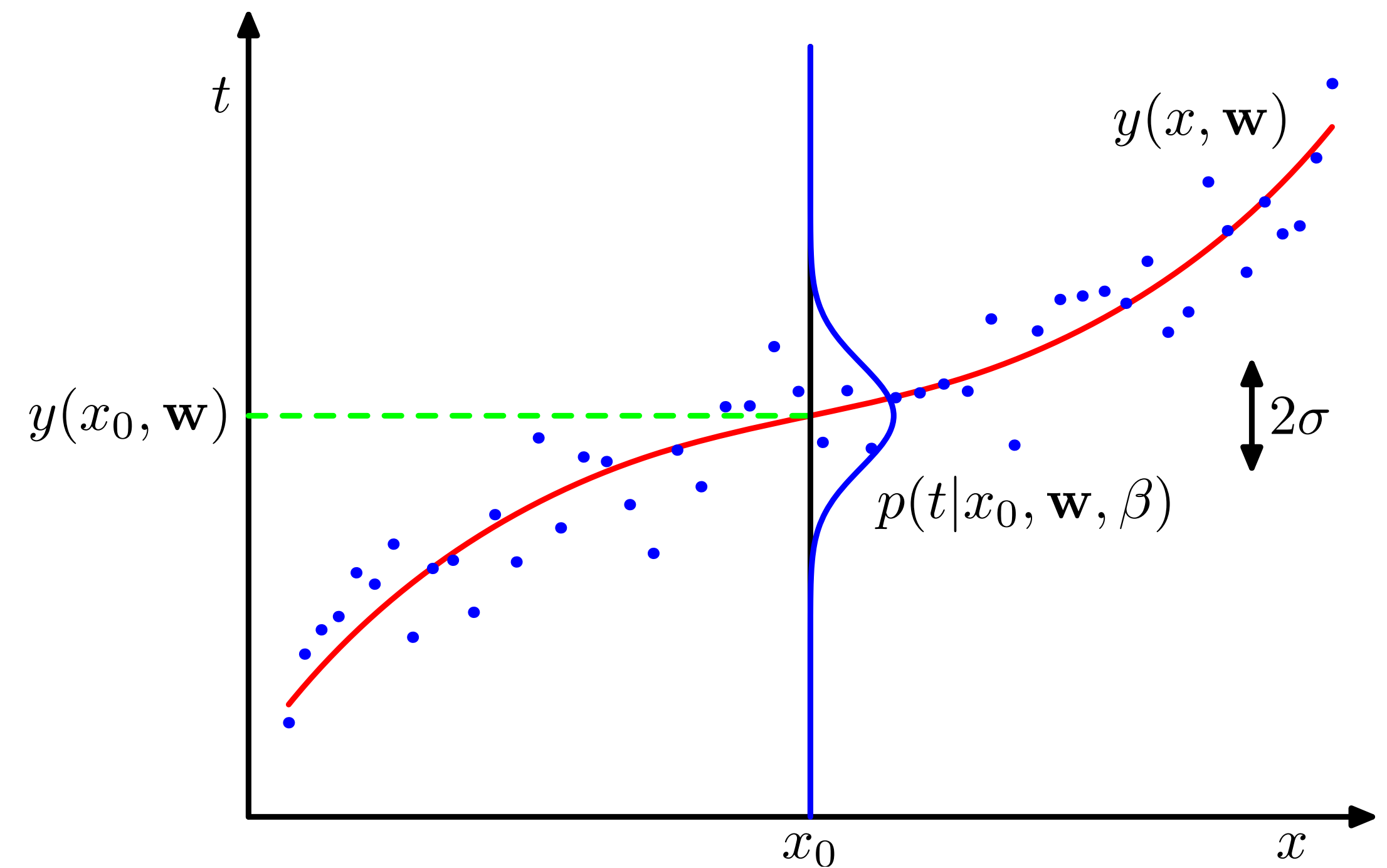
Multiple Linear Regression

Modelling

Simple linear model - what are we actually modelling?

$$t \sim N(y(X, \omega), \sigma^2)$$

$$y = \omega_0 + \omega_1 \cdot x$$



Modelling

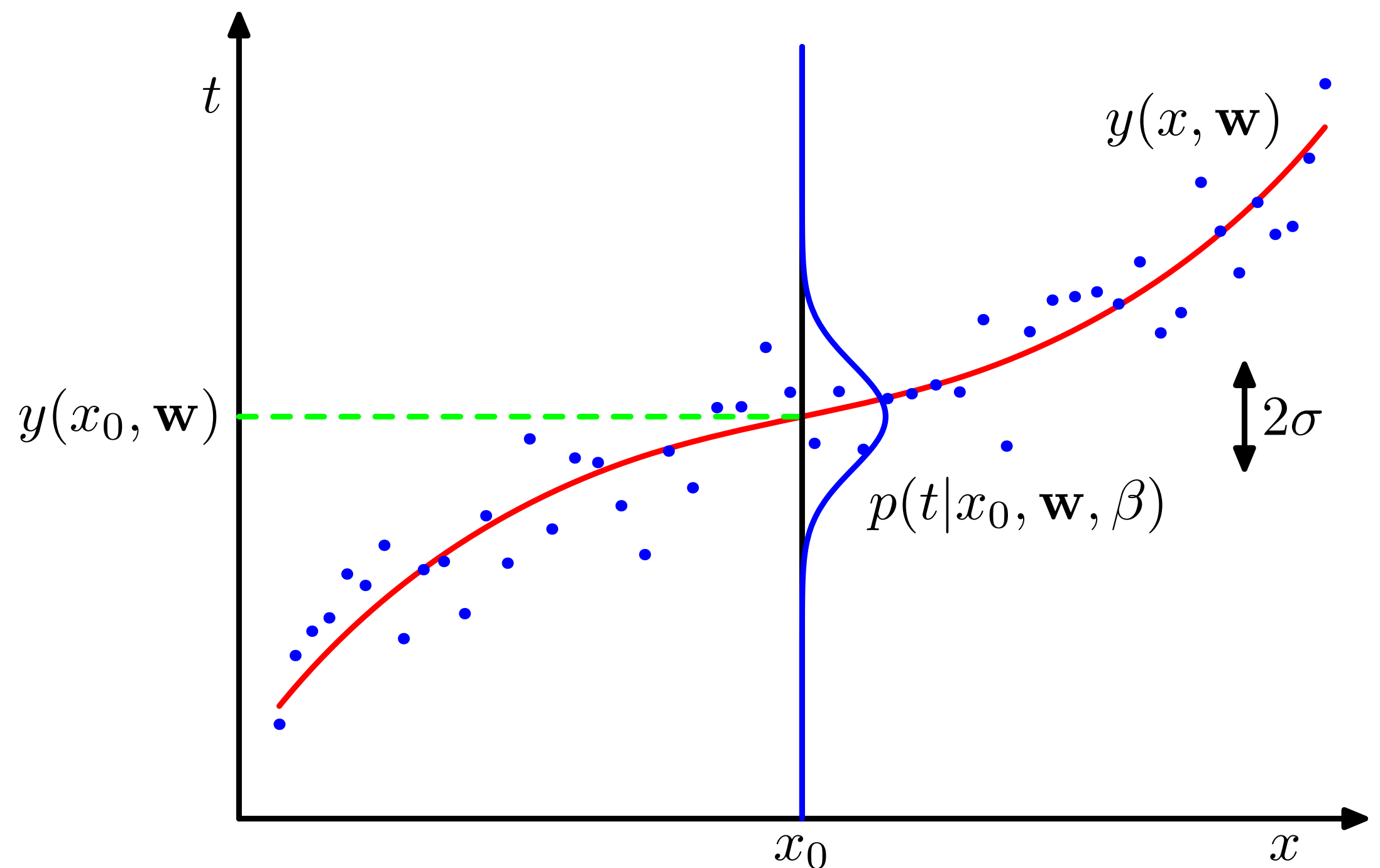
Simple linear model - what are we actually modelling?

$$t \sim N(y(X, \omega), \sigma^2)$$

$$y = \omega_0 + \omega_1 \cdot x$$

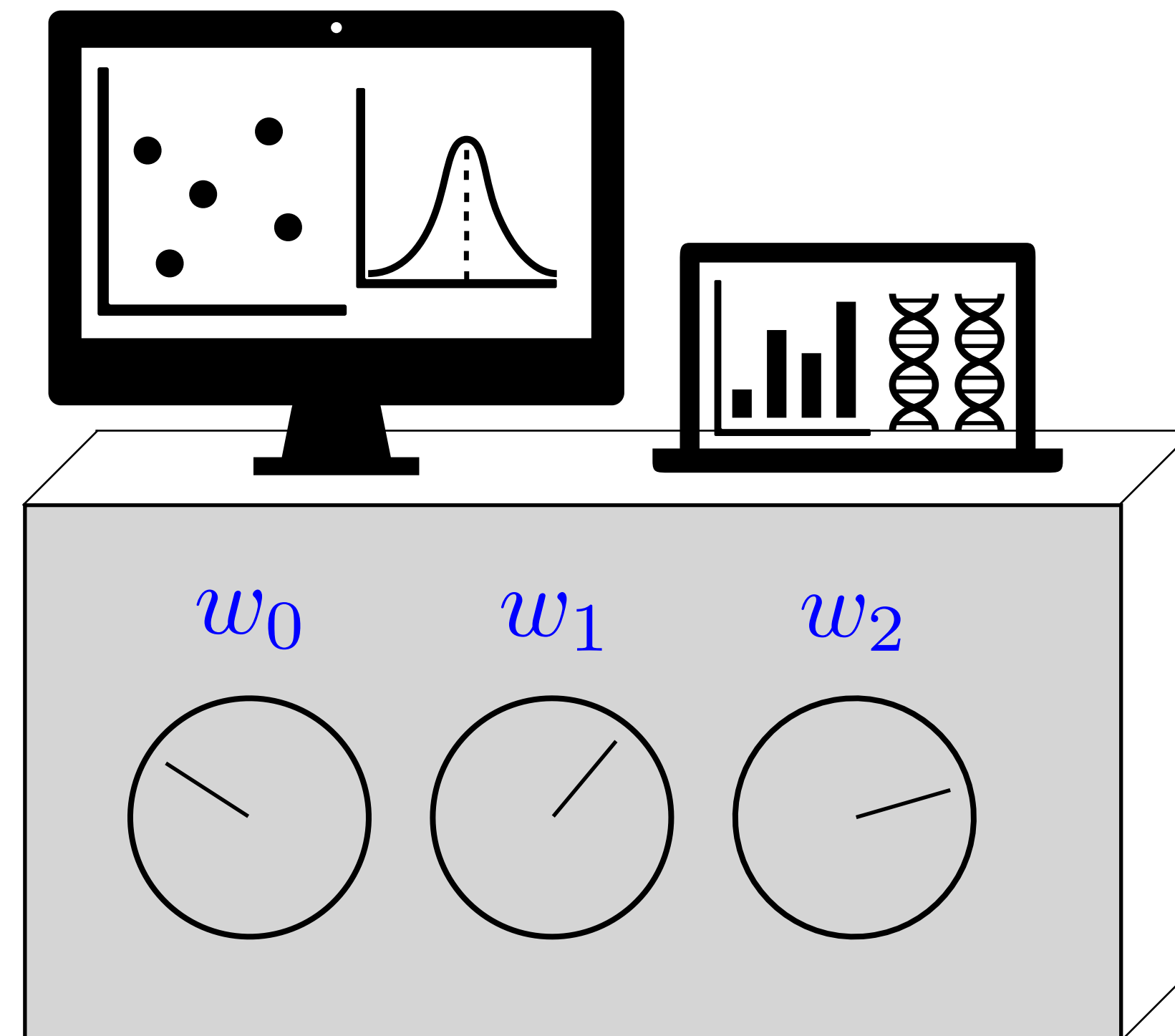
We are assuming:

- The errors have zero mean $\mathbb{E}(\epsilon) = 0$
- Their distribution is Normal.
- They share a same covariance σ^2
- Errors are independent



Model training

Adjusting the knobs



Model training

Adjusting the knobs

$$MSE = \frac{1}{N} \sum_{i=0}^{N-1} (\text{prediction}_i - \text{target}_i)^2$$

Mean Squared Error

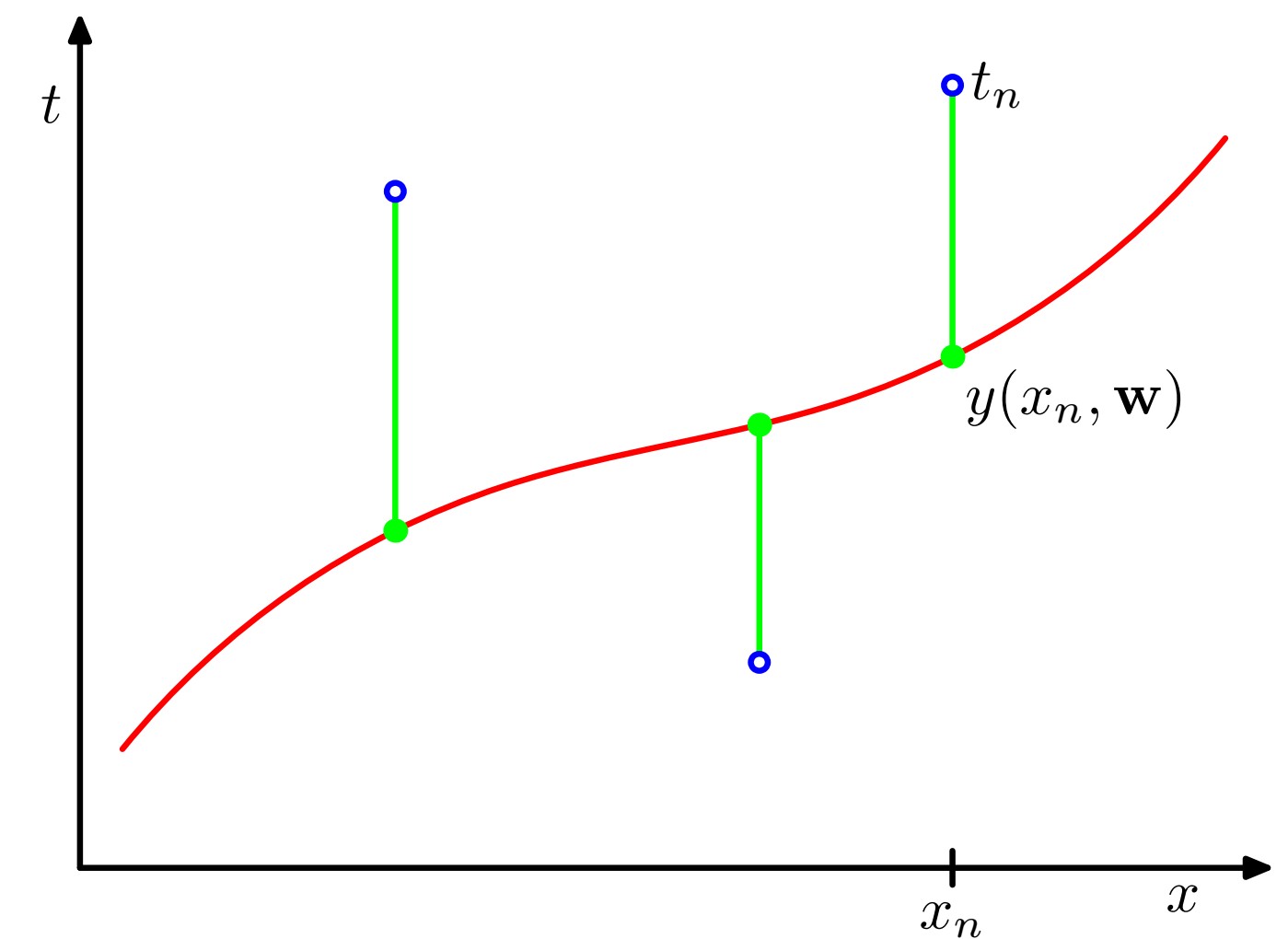
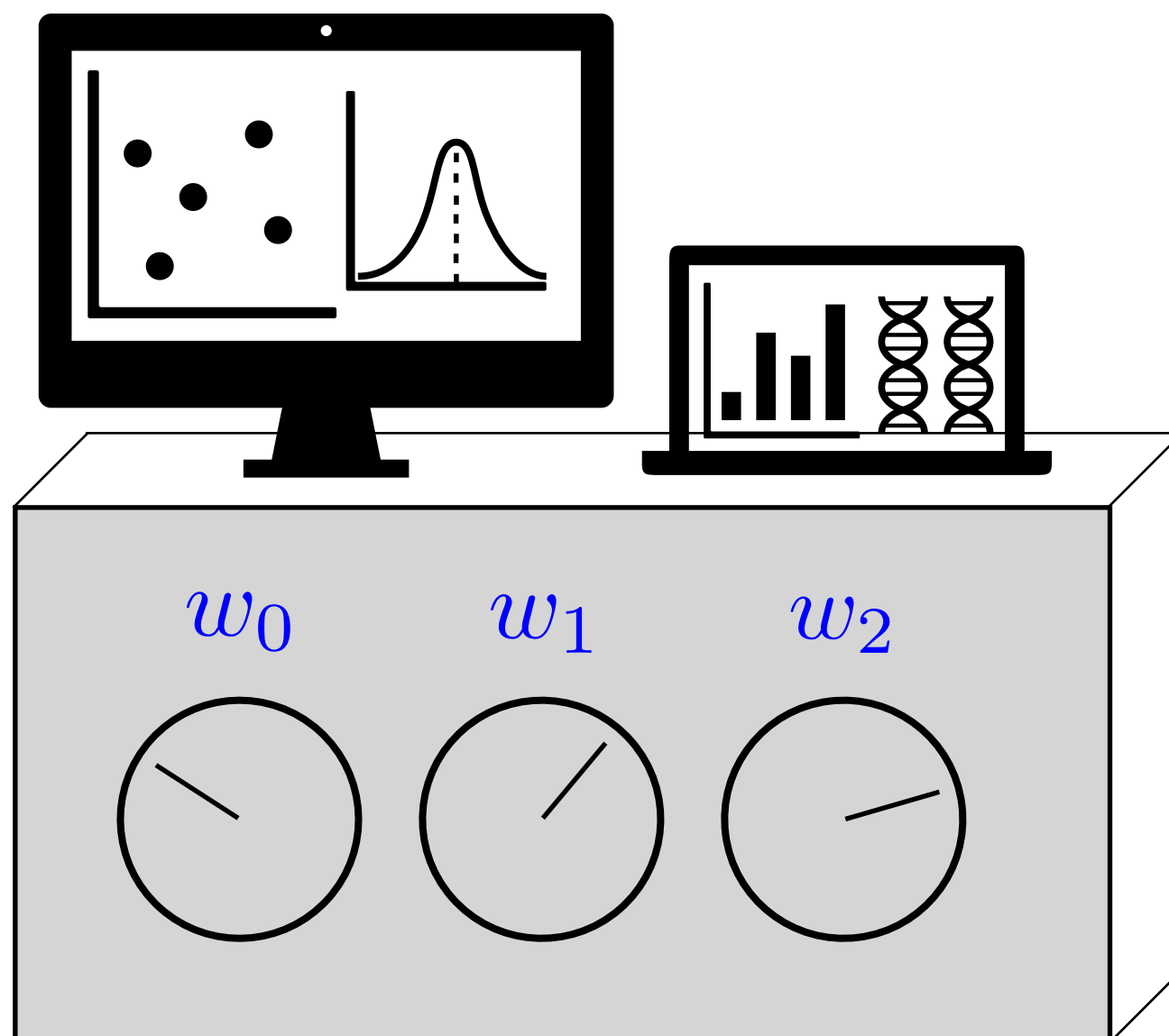


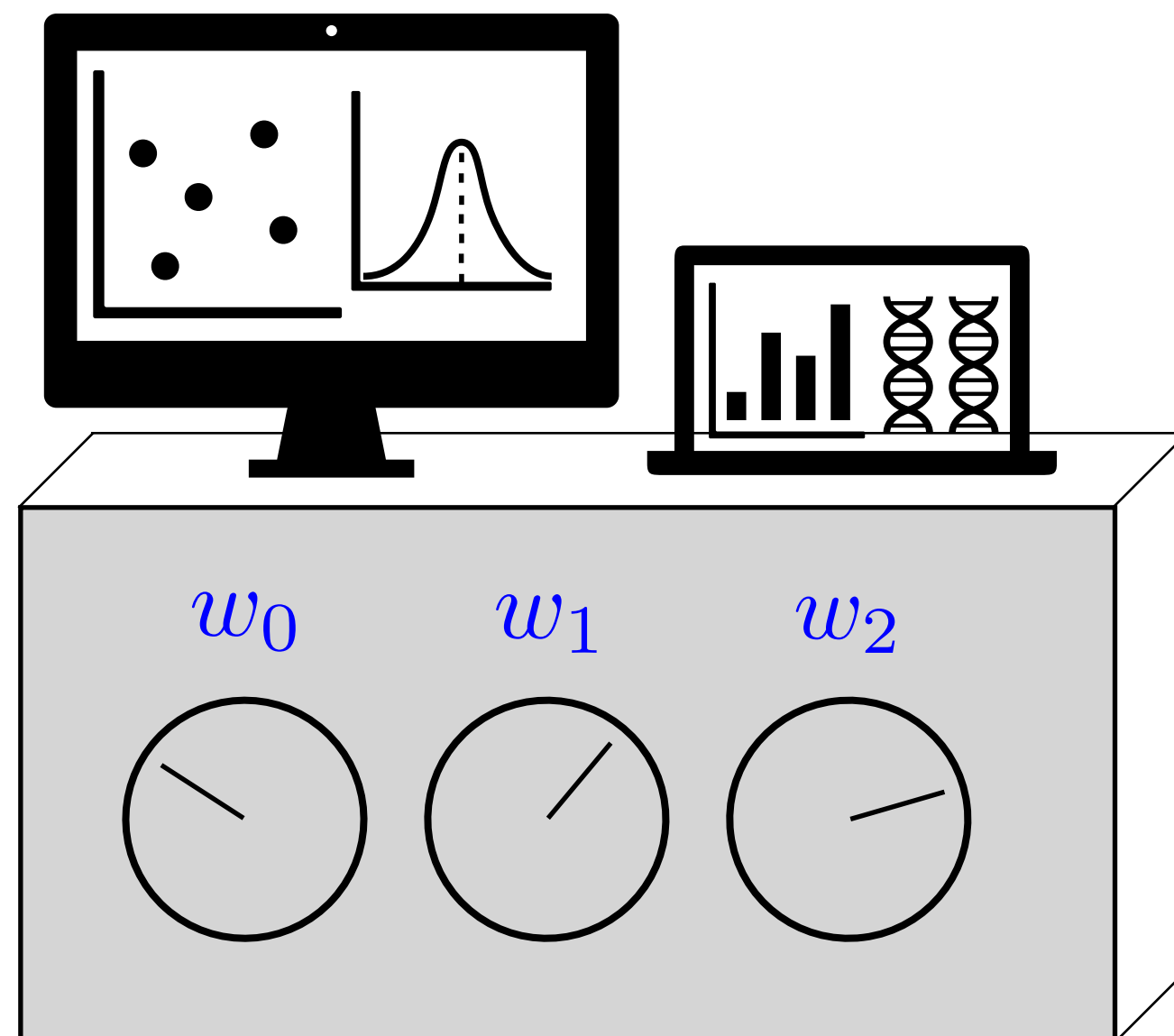
figure from Bishop

Model training

Adjusting the knobs

$$MSE = \frac{1}{N} \sum_{i=0}^{N-1} (\text{prediction}_i - \text{target}_i)^2$$

Mean Squared Error



$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - t_i)^2$$

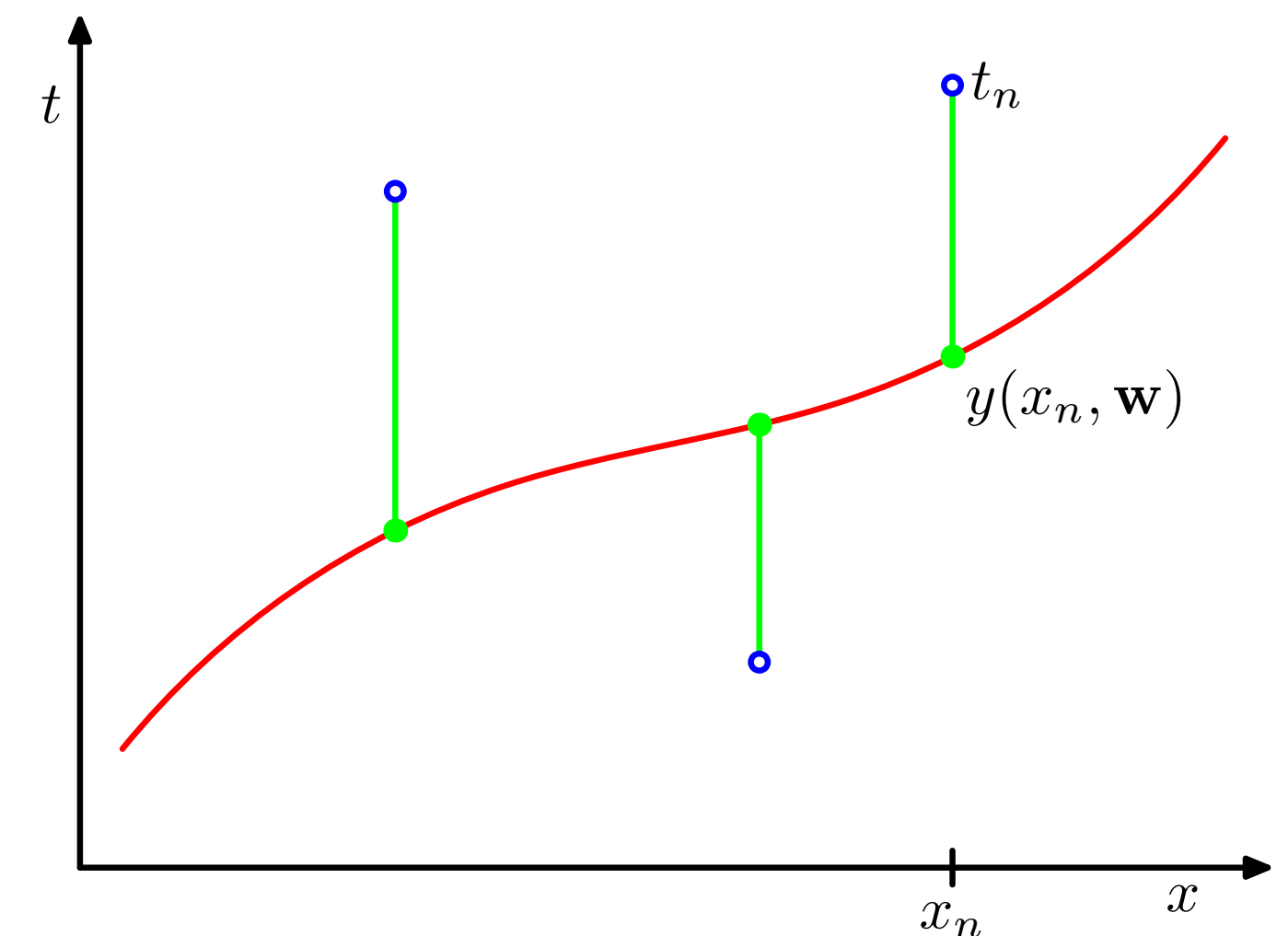
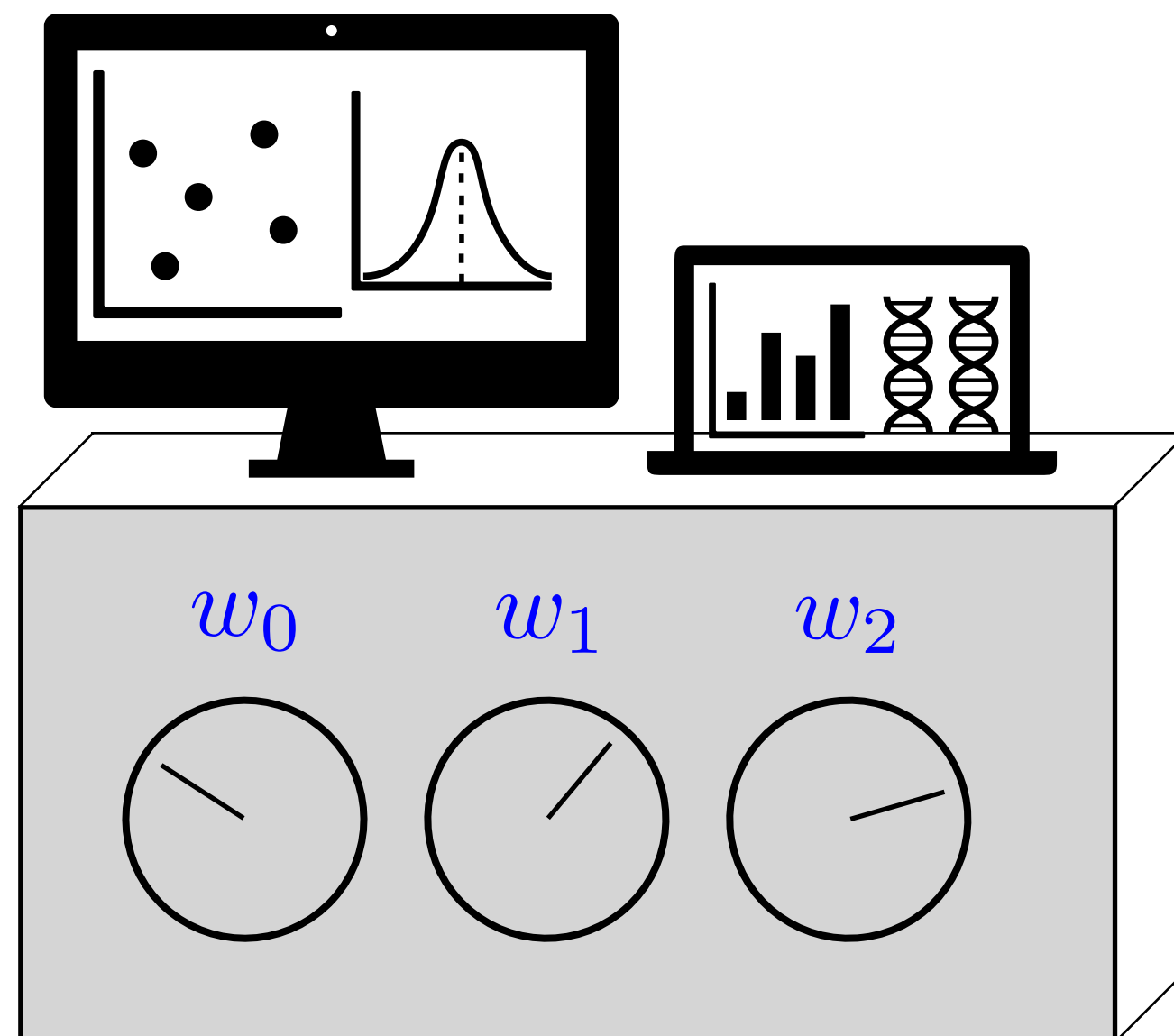


figure from Bishop

Model training

Adjusting the knobs



$$MSE = \frac{1}{N} \sum_{i=0}^{N-1} (\text{prediction}_i - \text{target}_i)^2$$

Mean Squared Error

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - t_i)^2$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - t_i)^2}$$

Root Mean Squared Error

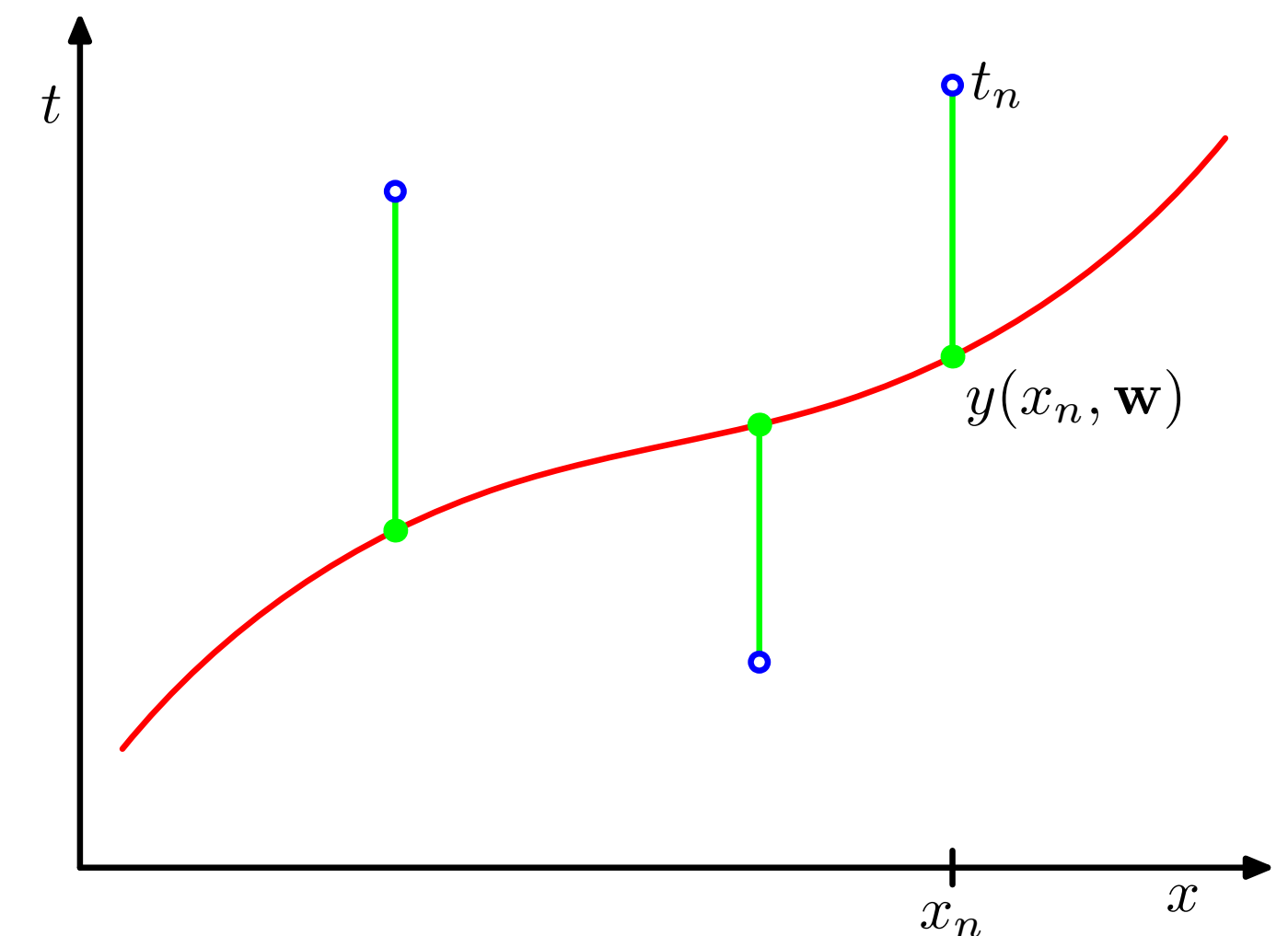


figure from Bishop

Modelling

Simple linear model - normal equations

$$y = \omega_0 + \omega_1 \cdot x \qquad MSE = \frac{1}{N} \sum_{i=1}^N (y_i - t_i)^2$$

$$\sum_{i=1}^N [t_i - (\hat{\omega}_0 + \hat{\omega}_1 \cdot x_i)] = 0$$

$$\sum_{i=1}^N [t_i - (\hat{\omega}_0 + \hat{\omega}_1 \cdot x_i)] x_i = 0$$

Modelling

Simple linear model - normal equations

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**Normal
equations**

Modelling

Simple linear model - normal equations

$$y = \omega_0 + \omega_1 \cdot x \qquad MSE = \frac{1}{N} \sum_{i=1}^N (y_i - t_i)^2$$

$$\sum_{i=1}^N [t_i - (\hat{\omega}_0 + \hat{\omega}_1 \cdot x_i)] = 0$$

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Normal
equations

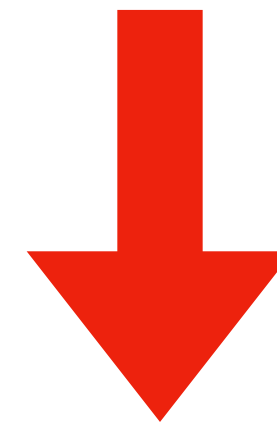
$$\begin{aligned} \hat{\omega}_1 &= \sum_{i=0}^N (x_i - \bar{X})(y_i - \bar{Y}) \left[\sum_{i=0}^N (x_i - \bar{X})^2 \right]^{-1} \\ \hat{\omega}_0 &= \bar{Y} - \hat{\omega}_1 \bar{X} \end{aligned} \qquad \bar{X} = \frac{1}{N} \sum_{i=1}^N x_i \ .$$

Model extension

Multiple linear model

Simple Linear
Regression

$$y(x, w_0, w_1) = w_0 + w_1 x \quad .$$



Multiple Linear
Regression

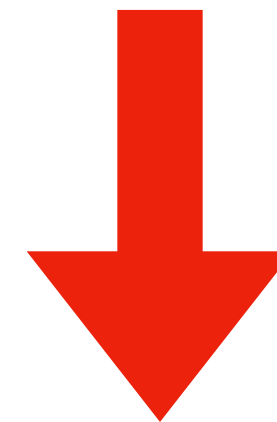
$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \cdots + w_D x_D \quad .$$

Model extension

Multiple linear model

Simple Linear
Regression

$$y(x, w_0, w_1) = w_0 + w_1 x \quad .$$



Multiple Linear
Regression

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \cdots + w_D x_D \quad .$$

More generally:

$$y_i(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^D w_j \phi_j(\mathbf{x}_i) = \sum_{j=0}^D w_j \phi_j(\mathbf{x}_i) = \mathbf{w}^T \boldsymbol{\phi}_i$$

Multiple linear model

Matrix Notation

$$y_i(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^D w_j \phi_j(\mathbf{x}_i) = \sum_{j=0}^D w_j \phi_j(\mathbf{x}_i) = \mathbf{w}^T \boldsymbol{\phi}_i$$

$$y_i(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \boldsymbol{\phi}_i \quad i = \{1, \dots, N\}$$

Multiple linear model

Matrix Notation

$$y_i(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^D w_j \phi_j(\mathbf{x}_i) = \sum_{j=0}^D w_j \phi_j(\mathbf{x}_i) = \mathbf{w}^T \boldsymbol{\phi}_i$$

$$y_i(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \boldsymbol{\phi}_i \quad i = \{1, \dots, N\}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \boldsymbol{\Phi} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_D \end{pmatrix}$$

$$(N \times 1) = (N \times D) (D \times 1)$$

Multiple linear model

Matrix Notation

$$y_i(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^D w_j \phi_j(\mathbf{x}_i) = \sum_{j=0}^D w_j \phi_j(\mathbf{x}_i) = \mathbf{w}^T \boldsymbol{\phi}_i$$

$$y_i(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \boldsymbol{\phi}_i \quad i = \{1, \dots, N\}$$

Design Matrix

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \boldsymbol{\Phi} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_D \end{pmatrix} \quad \boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

$(N \times 1) \quad = \quad (N \times D) \quad (D \times 1)$

Normal Equations

The normal equations can also be solved analytically in this case.

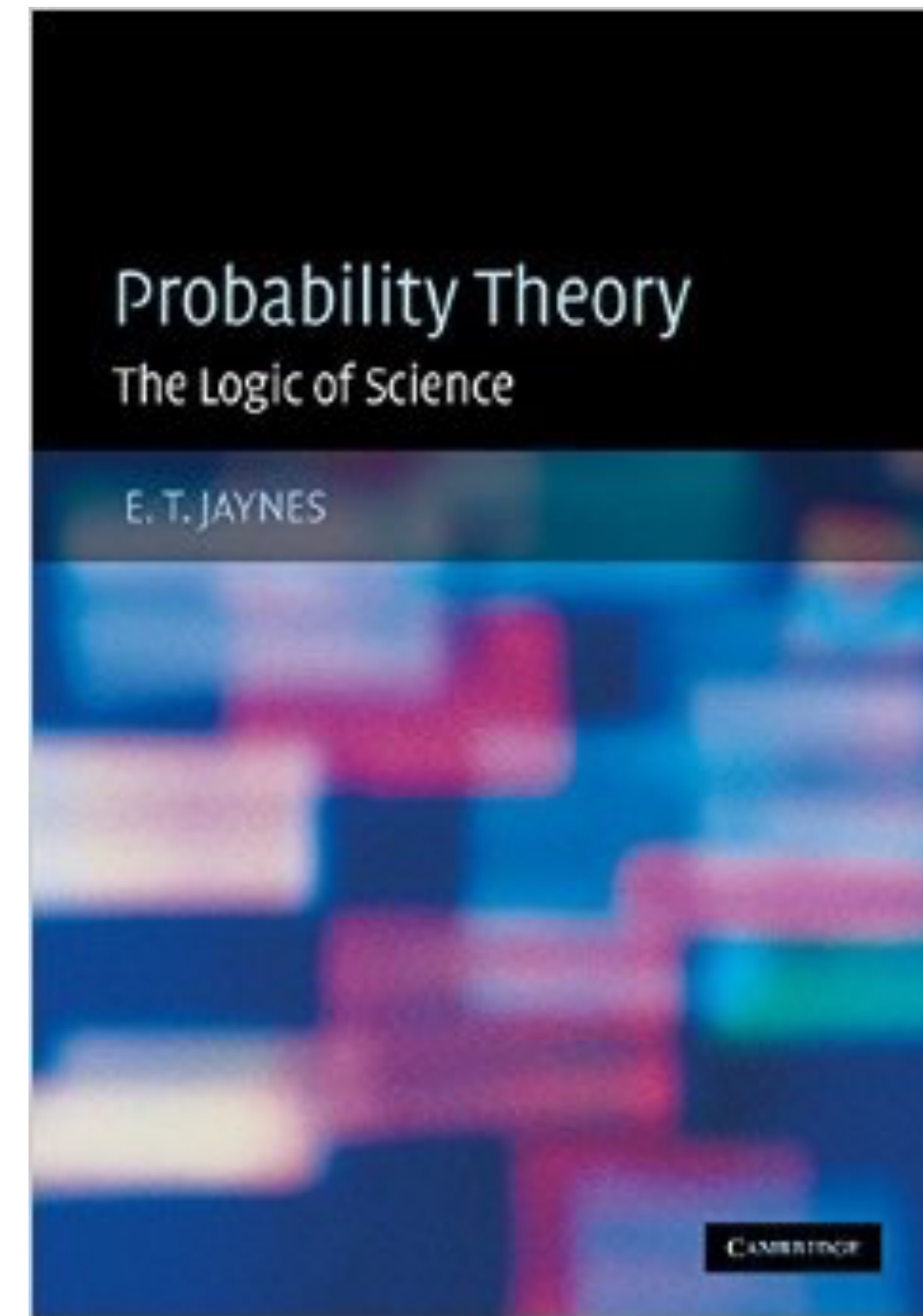
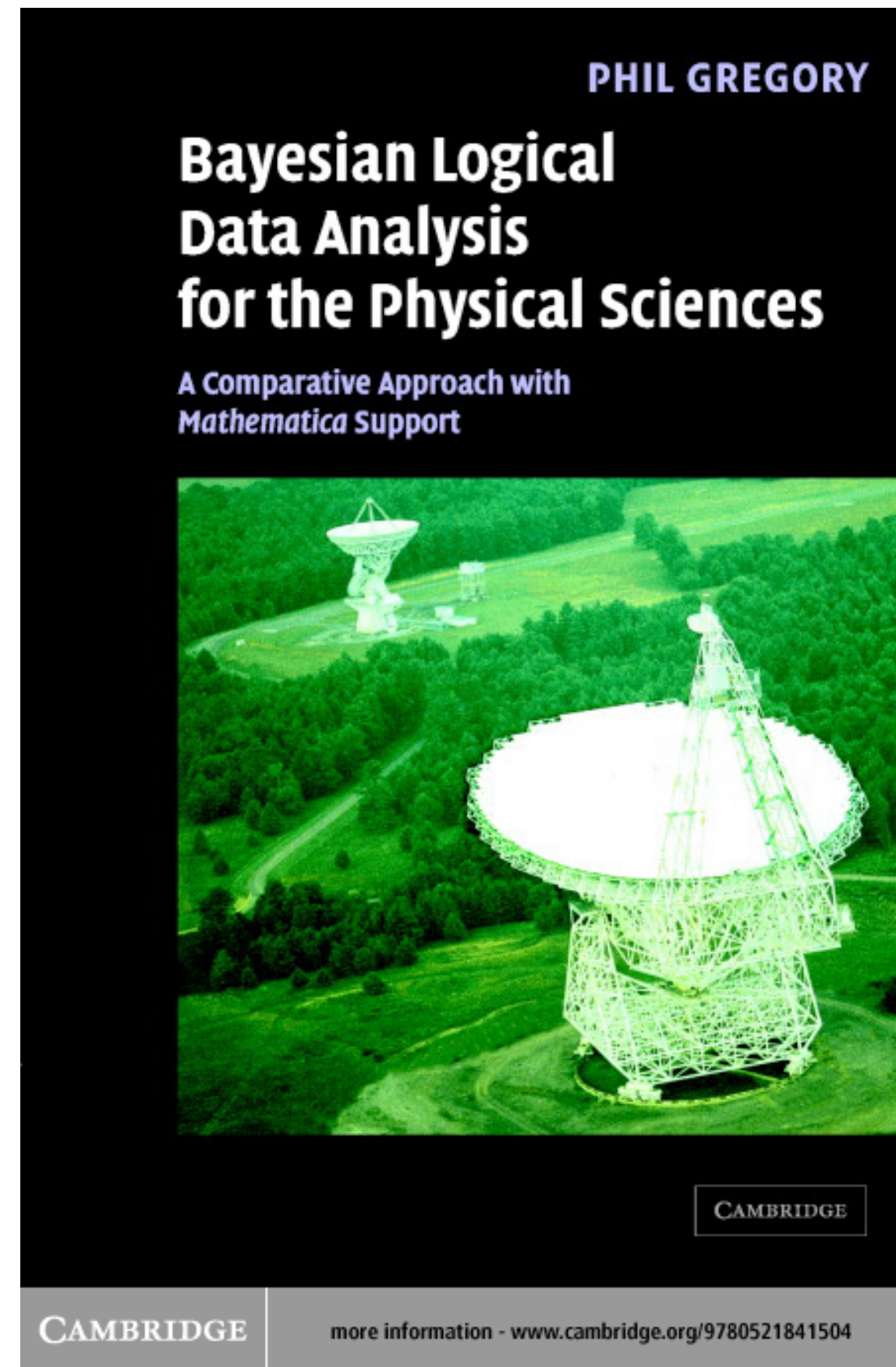
$$\mathbf{w}_{\text{ML}} = \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{t}$$

ICAS

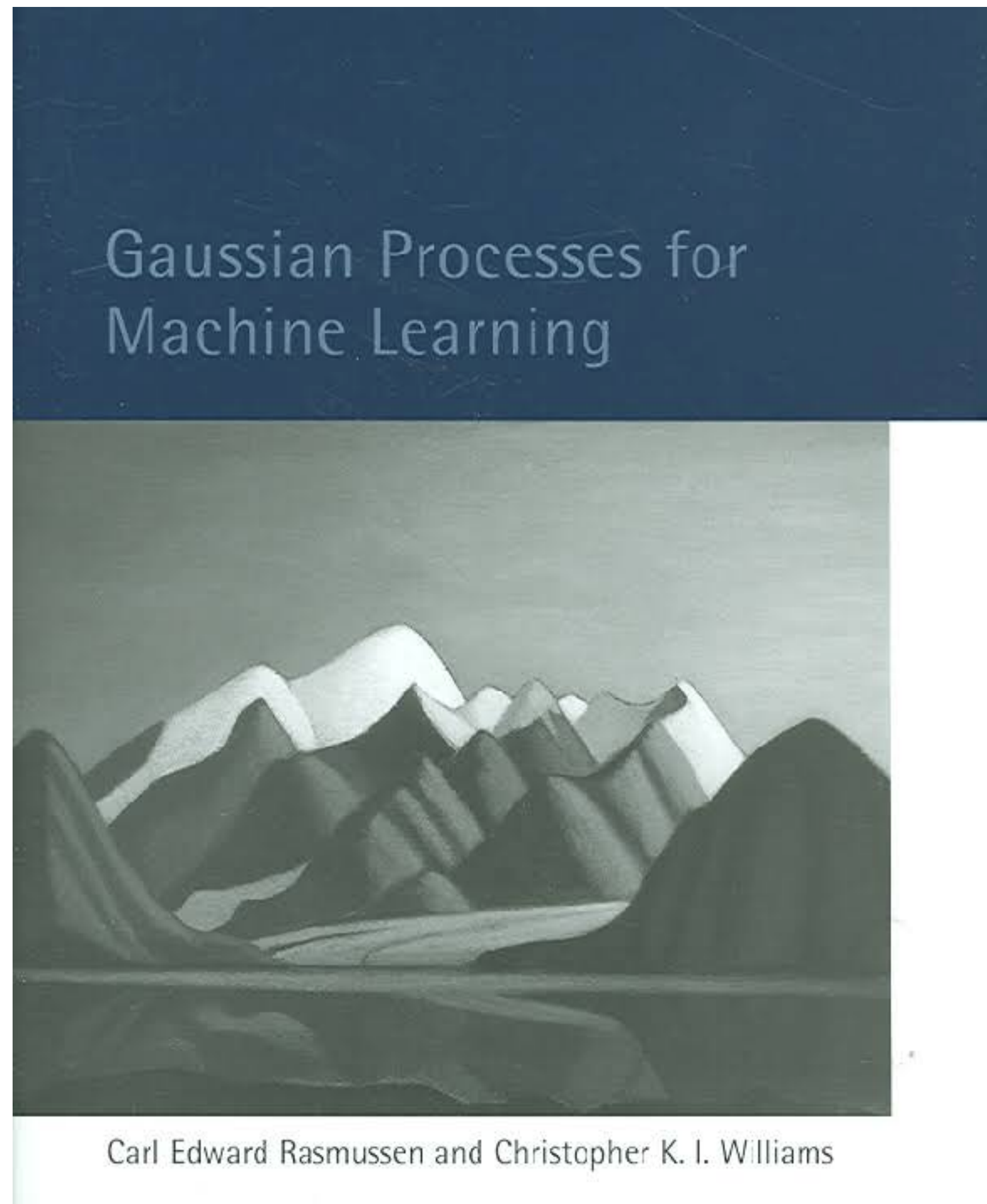


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Main references - Bayesian



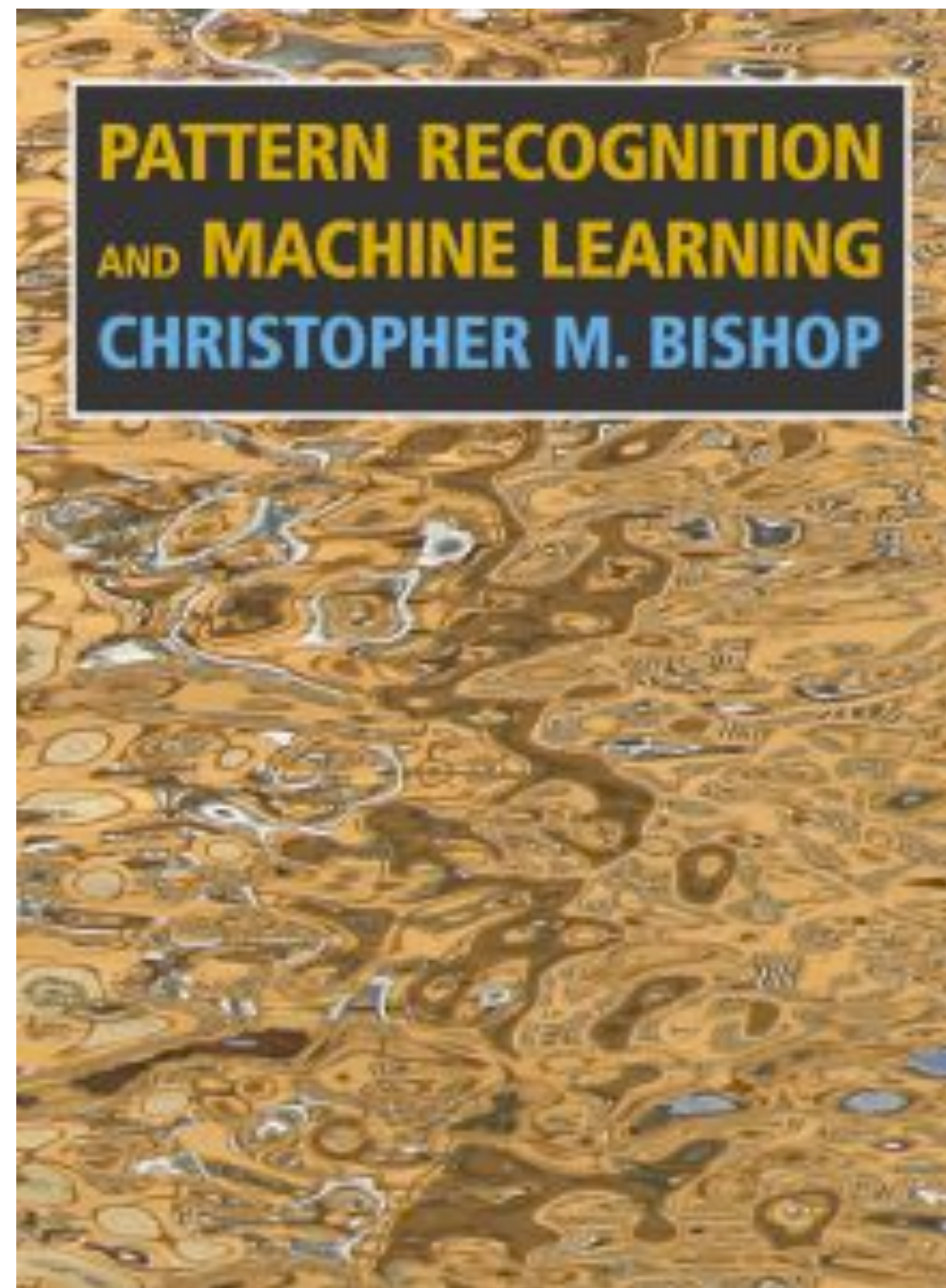
Main references - Gaussian processes



Available online

<http://www.gaussianprocess.org/gpml/>

Main references - Machine Learning



Available online

