

# Lecture 2: Supervised Learning

**Tao LIN**

March 1, 2023



# Feedback on the Questionnaire

- Course Project evaluation protocol
  - CS student: either (by-team) or (by-team-and-supervisor)
  - non-CS student: (by-team-and-supervisor)

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- Theoretical foundation for DL
  - We will explain the mathematical intuitions and insights behind DL methods.

## **This lecture:**

- Basic concept of regression and classification
- Linear regression
  - Definition
  - Gradient Descent (GD) optimization
  - Least Square
  - The probabilistic interpretation of linear regression

## **Next lecture:**

- Over-fitting and under-fitting
- Polynomial regression and Ridge regression
- Model selection
- Bias-Variance Decomposition



# Reading materials

- Chapter 1, Stanford CS 229 Lecture Notes,  
[https://cs229.stanford.edu/notes2022fall/main\\_notes.pdf](https://cs229.stanford.edu/notes2022fall/main_notes.pdf)
- Chapter 3.1, Bishop, Pattern Recognition and Machine Learning

# Reference

- EPFL, CS-433 Machine Learning, [https://github.com/epfml/ML\\_course](https://github.com/epfml/ML_course)

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## 1 Regression and Classification

- Regression
- Classification

## 2 Linear Regression

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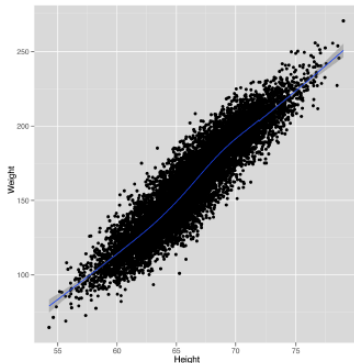
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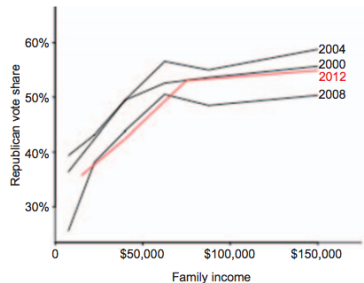
## 2 Linear Regression

- Definition of Linear Regression
- Optimization and Gradient Descent (GD)
- Normal Equations and Least Squares
- Probabilistic Interpretation of Linear Regression

# What is regression?



(a) Height is correlated with weight. Taken from "Machine Learning for Hackers"



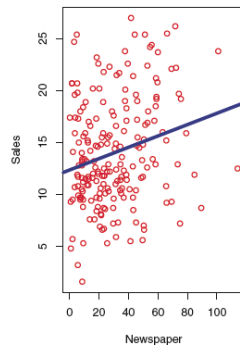
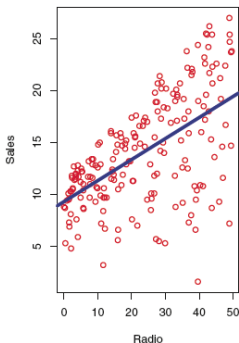
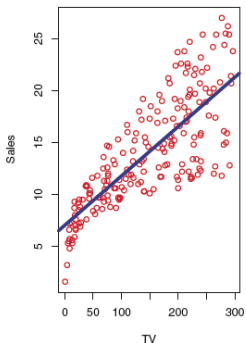
(b) Do rich people vote for republicans? Taken from Avi Feller et. al. 2013, Red state/blue state in 2012 elections.

**Regression** is to relate input variables to the output variable.

# Dataset for regression

$$\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N \in \mathcal{X} \times \mathcal{Y} \quad (1)$$

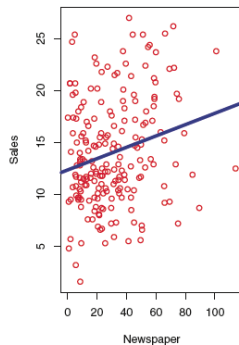
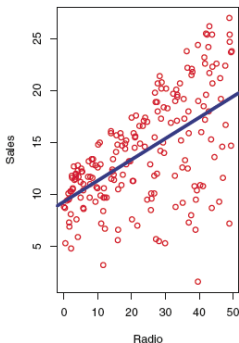
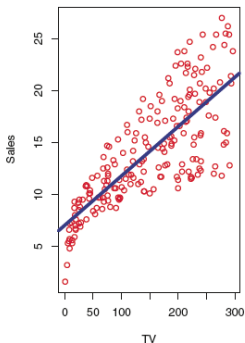
- **data** consists of pairs  $(\mathbf{x}_n, y_n)$ , where  $y_n$  is the  $n$ 'th **output** and  $\mathbf{x}_n$  is a vector of  $D$  **inputs**.



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- The number of pairs  $N$  is the **data-size** and  $D$  is the **dimensionality**.



## Two goals of regression

**The regression function** approximates the output  $y_n$  “well enough” given inputs  $\mathbf{x}_n$ .

$$y_n \approx f(\mathbf{x}_n), \text{ for all } n \quad (2)$$



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*Regression finds a correlation not a causal relationship, so interpret your results with caution.*

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## Remark 2 (Shortcut learning in Deep Learning)

*Models may only learn spurious correlation (and thus sensitive to distribution shifts).*

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We observe some data

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## Remark 3

*no ordering between classes.*

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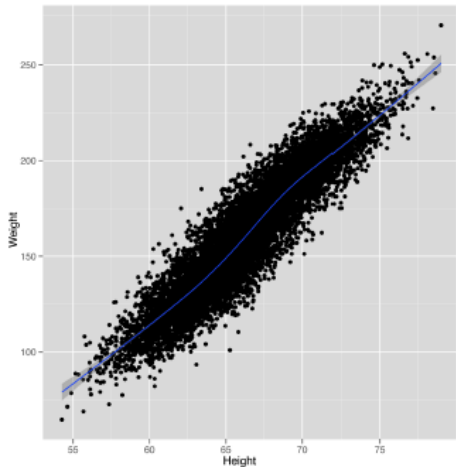
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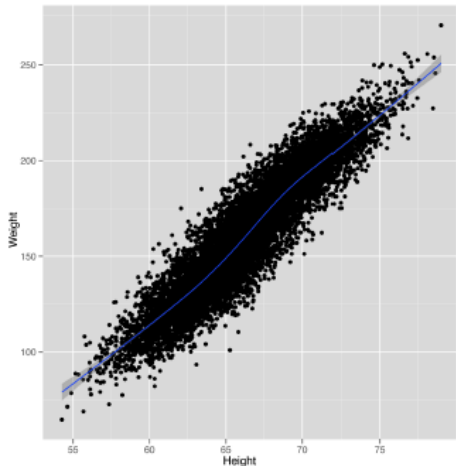
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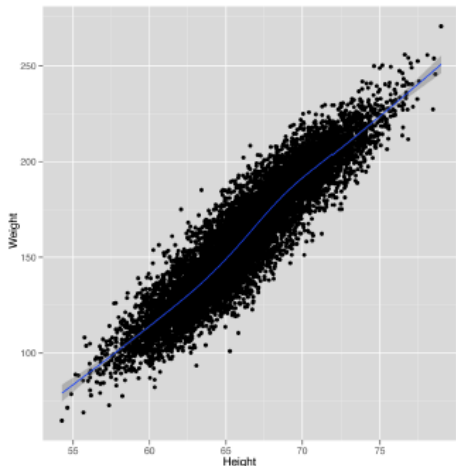
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# Definition

Linear regression is a **model**:

- $y_n \approx f(\mathbf{x}_n)$  for all  $n$  and  $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N \in \mathcal{X} \times \mathcal{Y}$
- a linear relationship is assumed for  $f$





# Detailed definition

**Simple linear regression** (w/ only one input dimension):

$$y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1}$$

Here,  $\mathbf{w} = (w_0, w_1)$  are the two **parameters** of the model. They describe  $f$ .

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Given data  $\mathcal{D}$ , we would like to find  $\tilde{\mathbf{w}} = [w_0, w_1, \dots, w_D]$ .

**We need an optimization algorithm!**

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- easily generalized to non-linear models
- we can learn almost all fundamental concepts of ML with regression alone

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Consider the following models.

1-parameter model:  $y_n \approx w_0$

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- the cost penalizes “large” mistakes and “very-large” mistakes similarly

# Mean Squared Error (MSE) and Outliers

$$\text{MSE}(\mathbf{w}) := \frac{1}{N} \sum_{n=1}^N [y_n - f_{\mathbf{w}}(\mathbf{x}_n)]^2 \quad (7)$$

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- + MAE is more robust to outliers.
- MAE is not differentiable at zero.

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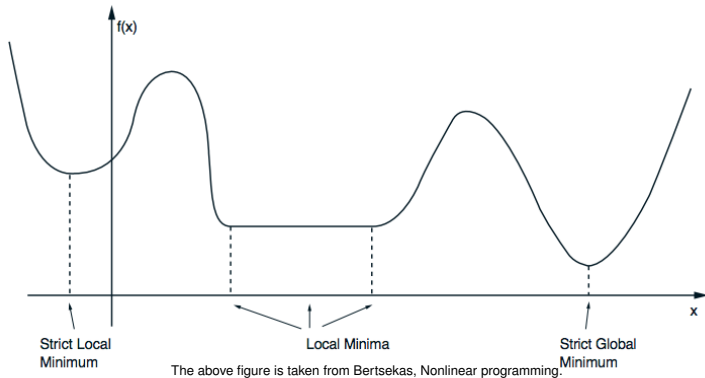
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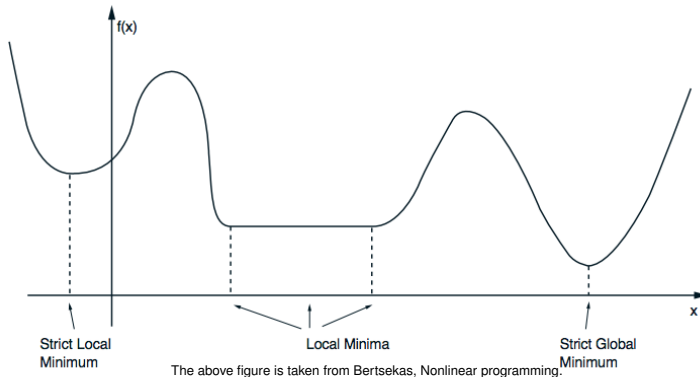
We will use an **optimization algorithm** to solve the problem (to find a good  $\mathbf{w}$ ).

# Optimization Landscapes





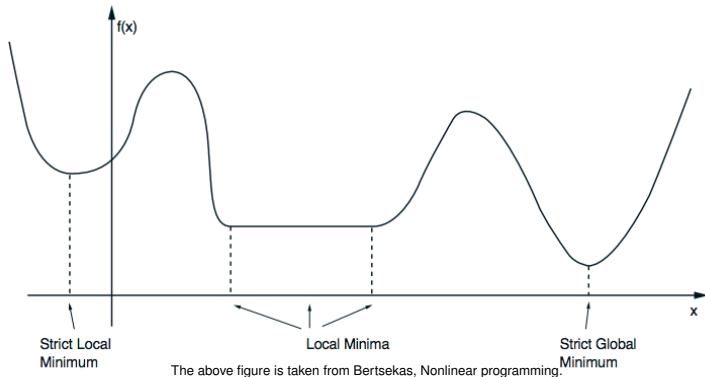
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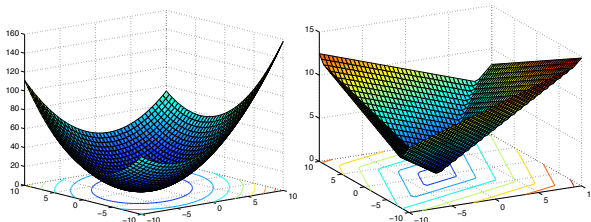
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For a 2-parameter model,  $\text{MSE}(\mathbf{w})$  and  $\text{MAE}(\mathbf{w})$  are shown below.

(We used  $y_n \approx w_0 + w_1 x_{n1}$  with  $\mathbf{y}^\top = [2, -1, 1.5]$  and  $\mathbf{x}^\top = [-1, 1, -1]$ ).



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where  $\gamma > 0$  is the **step-size** (or **learning rate**). Then repeat with the next  $t$ .

# Gradient Descent for Linear Regression with MSE

Considering a dataset  $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$  and learnable weights  $\mathbf{w} \in \mathbb{R}^D$  for  $f(\mathbf{w}, \mathbf{X}) = \mathbf{X}\mathbf{w}$ .

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \quad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N \times D} \quad (12)$$

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and then the gradient is given by

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- Classification

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- Definition of Linear Regression
- Optimization and Gradient Descent (GD)
- **Normal Equations and Least Squares**
- Probabilistic Interpretation of Linear Regression

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- Here its solution can be obtained explicitly, by solving a linear system of equations.
  - ⇒ These equations are sometimes called the **normal equations**.
  - ⇒ Solving the normal equations is called the **least squares**.

Recall that the cost function for linear regression with MSE is given by

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^N (y_n - \mathbf{x}_n^\top \mathbf{w})^2 = \frac{1}{2N} (\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w}), \quad (16)$$

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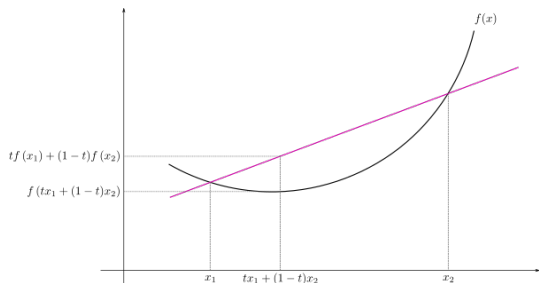
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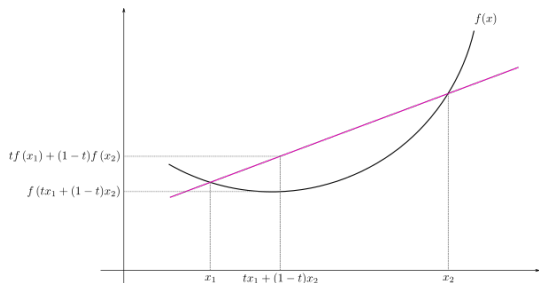
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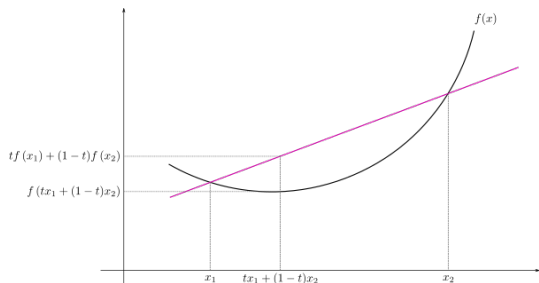
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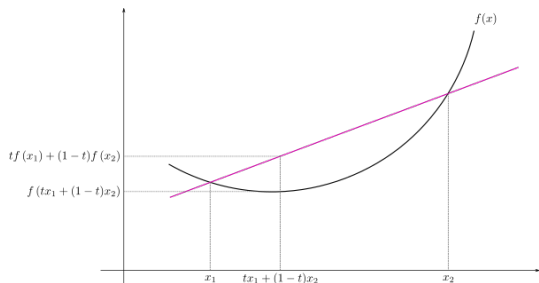
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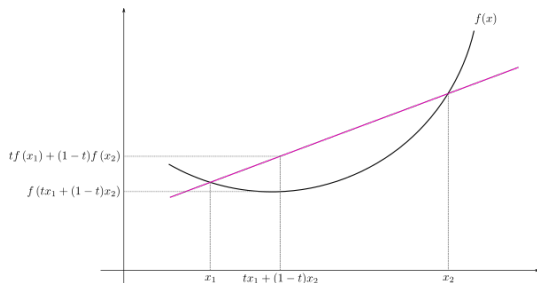
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$$\nabla \mathcal{L}(\mathbf{w}^*) = \mathbf{0}, \quad (19)$$

where  $\mathbf{w}^*$  corresponds to the parameter at the optimum point.



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Given the property of convexity  $\nabla \mathcal{L}(\mathbf{w}^*) = \mathbf{0}$ , we can get the [normal equations for linear regression](#):

$$\mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}, \quad (23)$$

where the error  $\mathbf{e} := \mathbf{y} - \mathbf{X}\mathbf{w}$  is orthogonal to all columns of  $\mathbf{X}$ .

# Geometric Interpretation

## Definition 9 (Span of a set of vectors)

The **span** of a set of vectors,  $\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ , is the set of all possible **linear combinations** of these vectors; i.e.  $\text{span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\} = \{\alpha_1 \mathbf{x}_1 + \dots + \alpha_k \mathbf{x}_k \mid \alpha_1, \dots, \alpha_k \in \mathbb{R}\}$ .



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Which element  $\mathbf{u}$  of  $\text{span}(\mathbf{X})$  shall we take? (for the normal equation  $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$ )

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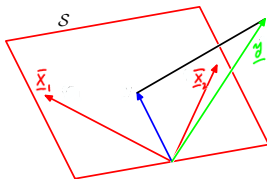
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(taken from Bishop's book)

# Geometric Interpretation

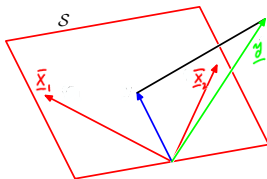
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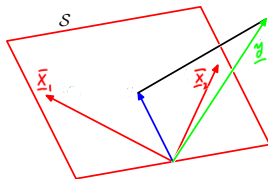
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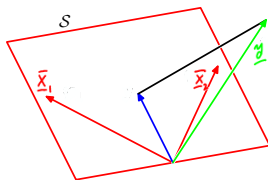
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- $\mathbf{u}^*$  should be equal to *the projection of  $\mathbf{y}$  onto  $\text{span}(\mathbf{X})$* .

# Least Squares

We need to solve the linear system of the normal equation  $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$ , where

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## Remark 10

*The Gram matrix  $\mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{D \times D}$  is invertible if and only if  $\mathbf{X}$  has **full column rank**, or in other words  $\text{rank}(\mathbf{X}) = D$ .*

# Rank Deficiency and Ill-Conditioning

Unfortunately, in practice,  $\mathbf{X} \in \mathbb{R}^{N \times D}$  is often **rank deficient**.

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Can we solve least squares if  $\mathbf{X}$  is **rank deficient**?

Yes, using a linear system solver, e.g., `np.linalg.solve( $\mathbf{X}$ ,  $\mathbf{y}$ )`.

# Table of Contents

## 1 Regression and Classification

- Regression
- Classification

## 2 Linear Regression

- Definition of Linear Regression
- Optimization and Gradient Descent (GD)
- Normal Equations and Least Squares
- Probabilistic Interpretation of Linear Regression

# Recall: Gaussian distribution and independence

## Definition 11 (A Gaussian random variable)

The definition of a Gaussian random variable in  $\mathbb{R}$  with mean  $\mu$  and variance  $\sigma^2$ . It has a density of

$$p(y | \mu, \sigma^2) = \mathcal{N}(y | \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ -\frac{(y - \mu)^2}{2\sigma^2} \right\}. \quad (27)$$

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Two random variables  $X$  and  $Y$  are called *independent* when  $p(x, y) = p(x)p(y)$ .



# A probabilistic model for linear regression

## Definition 13 (Data generation process)

We assume that the data is generated by the model,

$$y_n = \mathbf{x}_n^\top \mathbf{w} + \epsilon_n, \quad (29)$$

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**The probabilistic view point:** maximize this likelihood over the choice of model  $\mathbf{w}$ .

# Maximum-likelihood estimator (MLE)

Instead of maximizing the likelihood, we can maximize take the logarithm of the likelihood, i.e., **log-likelihood** (LL):

$$\mathcal{L}_{\text{LL}}(\mathbf{w}) := \log p(\mathbf{y} | \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^N (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst.} \quad (31)$$

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Maximizing the LL is equivalent to minimizing the MSE:

$$\arg \min_{\mathbf{w}} \mathcal{L}_{\text{MSE}}(\mathbf{w}) = \arg \max_{\mathbf{w}} \mathcal{L}_{\text{LL}}(\mathbf{w}). \quad (34)$$

# Properties of MLE

MLE is a *sample* approximation to the *expected log-likelihood*:

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- 4 MLE is **efficient**, i.e. it achieves the Cramer-Rao lower bound.

$$\text{Covariance}(\mathbf{w}_{MLE}) = \mathbf{F}^{-1}(\mathbf{w}_{true}) \quad (38)$$

## Another example

What if we replace the Gaussian distribution with a Laplace distribution?

$$p(y_n | \mathbf{x}_n, \mathbf{w}) = \frac{1}{2b} e^{-\frac{1}{b} |y_n - \mathbf{x}_n^\top \mathbf{w}|} \quad (39)$$



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we can recover the MAE cost function!

## **This lecture:**

- Basic concept of regression and classification
- Linear regression
  - Definition
  - Gradient Descent (GD) optimization
  - Least Square
  - The probabilistic interpretation of Linear Regression

## **Next lecture:**

- Over-fitting and under-fitting
- Polynomial regression and Ridge regression
- Model selection
- Bias-Variance Decomposition