# Lecture 2: Supervised Learning

**Tao LIN**

February 23, 2023

WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

# Feedback on the Questionnaire

- Course Project evaluation protocol
  - CS student: either (by-team) or (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`
- Chapter 3.1, Bishop, Pattern Recognition and Machine Learning

# Reference

- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

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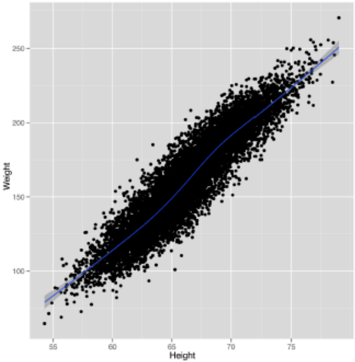
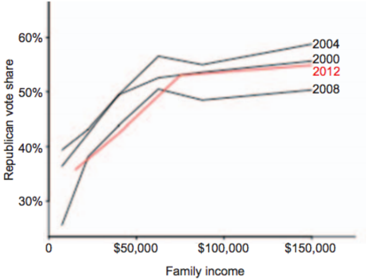
# What is regression?




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



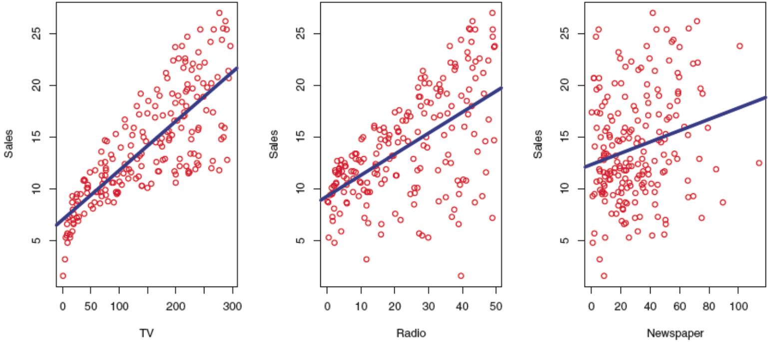

(b) Do rich people vote for republicans? Taken from Avi Feller et. al. 2013, Red state/blue state in 2012 elections.

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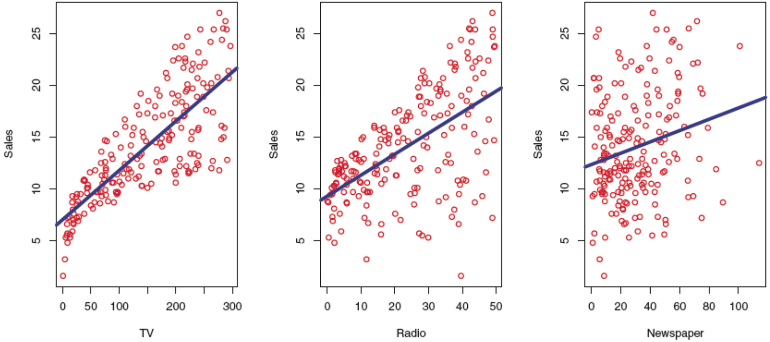
- The number of pairs $N$ is the data-size and $D$ is the dimensionality.



# Two goals of regression

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

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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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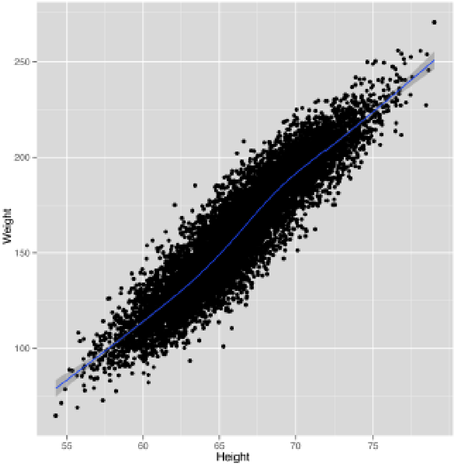

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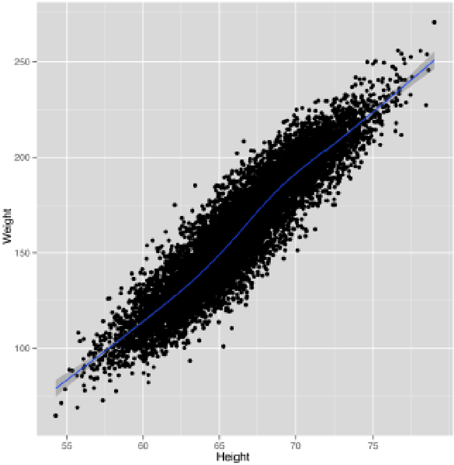

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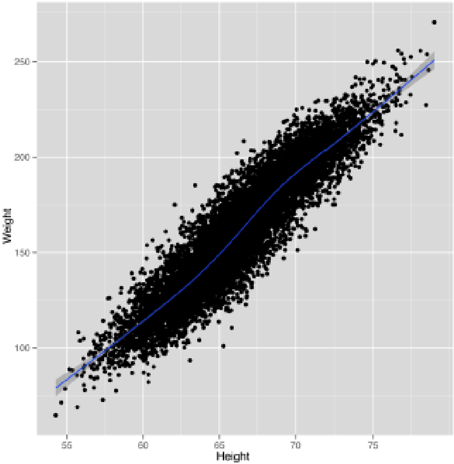
- $y_n \approx f(\mathbf{x}_n)$ for all $n$ and $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N \in \mathcal{X} \times \mathcal{Y}$
- a linear relationship is assumed for $f$



# 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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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.

$$\text{1-parameter model: } y_n \approx w_0$$
$$\text{2-parameter model: } y_n \approx w_0 + w_1 x_{n1}$$

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- the cost penalizes "large" mistakes and "very-large" mistakes similarly

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- **Cons:** It is very sensitive to outliers.

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

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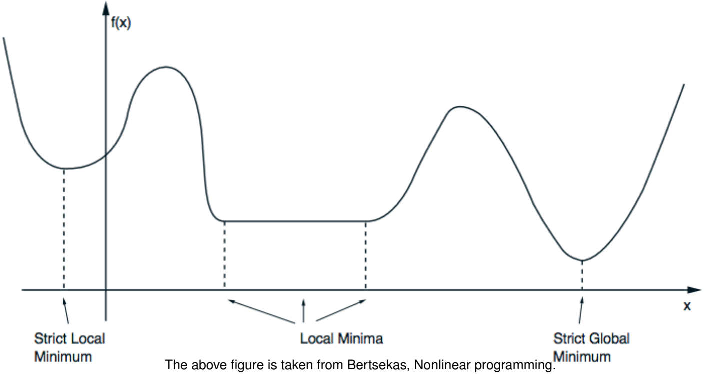
We will use an optimization algorithm to solve the problem (to find a good $\mathbf{w}$).

# Optimization Landscapes

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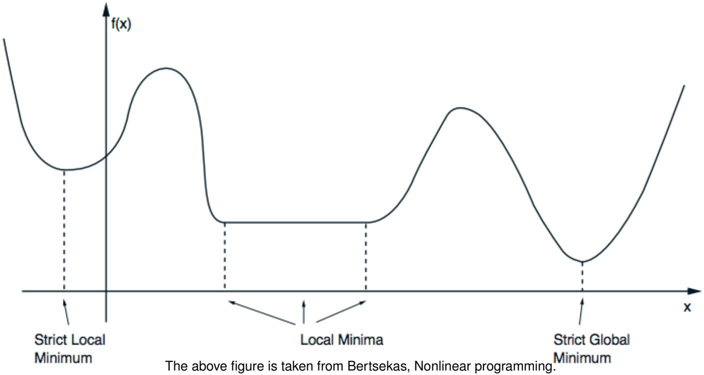


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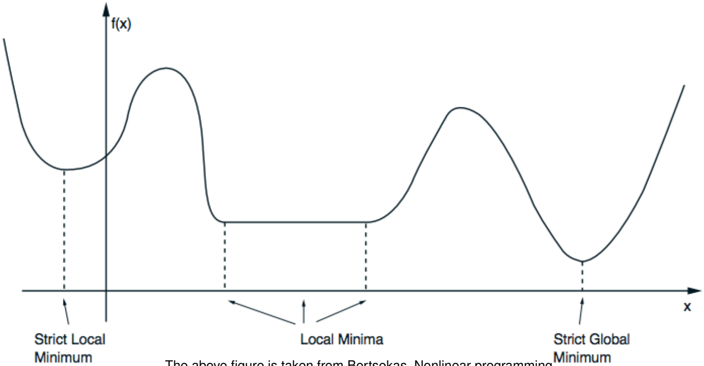


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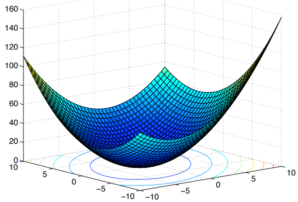
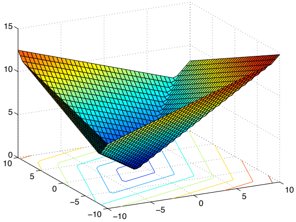
For a 2-parameter model, $\text{MSE}(\mathbf{w})$ and $\text{MAE}(\mathbf{w})$ are shown below.

(We used $\mathbf{y}_n \approx w_0 + w_1 x_{n1}$ 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 $f(\mathbf{w}, \mathbf{X}) = \mathbf{X}\mathbf{w}$.

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$\Rightarrow$ These equations are sometimes called the normal equations.

$\Rightarrow$ Solving the normal equations is called the least squares.

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

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

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A function $h(\mathbf{u})$ with $\mathbf{u} \in \mathbb{R}^D$ is convex, if for any $\mathbf{u}, \mathbf{v} \in \mathbb{R}^D$ and for any $0 \leq \lambda \leq 1$, we have:

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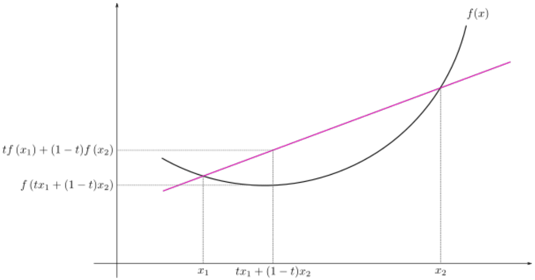

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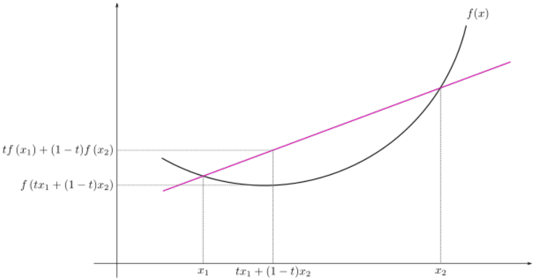


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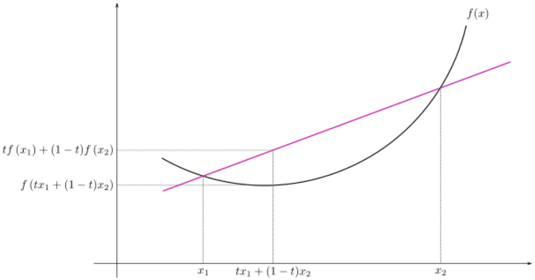


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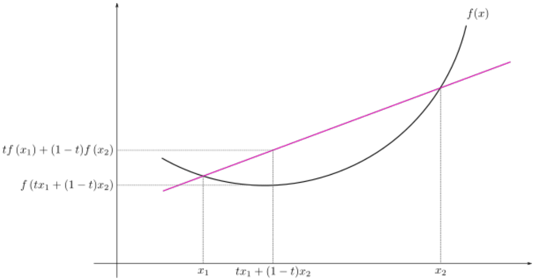


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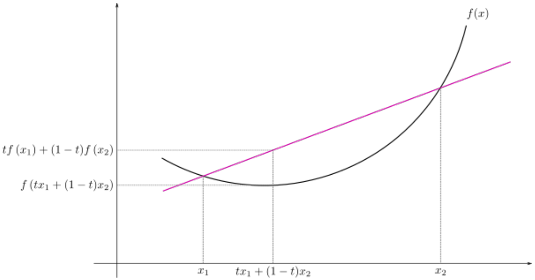


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$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}\,, \tag{19}$$

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

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

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

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, $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$, is the set of all possible linear combinations of these vectors; i.e. span$\{\mathbf{x}_1, \ldots, \mathbf{x}_k\} = \{\alpha_1 \mathbf{x}_1 + \ldots + \alpha_k \mathbf{x}_k \,|\, \alpha_1, \ldots, \alpha_k \in \mathbb{R}\}$.

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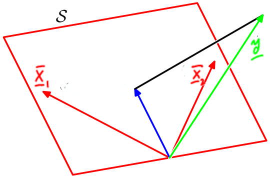


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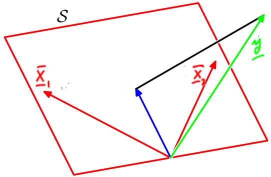


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From $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, we have:

# Geometric Interpretation

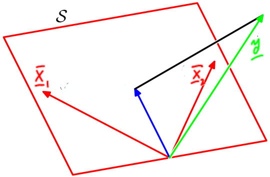
## Definition 9 (Span of a set of vectors)

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

- The span of $\mathbf{X} \in \mathbb{R}^{N \times D}$ is the space spanned by the columns of $\mathbf{X}$

$$\mathcal{S} := span(\mathbf{X}) = \{\mathbf{u} := \mathbf{X}\mathbf{w} | \mathbf{w} \in \mathbb{R}^D\}$$

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

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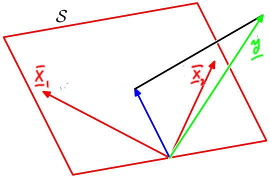


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- the optimum choice for $\mathbf{u}$, i.e. $\mathbf{u}^\star$, requires $\mathbf{y} - \mathbf{u}^\star$ to be orthogonal to $span(\mathbf{X})$.
- $\mathbf{u}^\star$ should be equal to *the projection of* $\mathbf{y}$ *onto* $span(\mathbf{X})$.

# 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

$$\mathbf{X}^\top y = \underbrace{\mathbf{X}^\top\mathbf{X}}_{\text{Gram matrix}} \mathbf{w} \tag{24}$$

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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* $rank(\mathbf{X}) = D$.

# Rank Deficiency and Ill-Conditioning

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Can we solve least squares if $\mathbf{X}$ is rank deficient?
Yes, using a linear system solver, e.g., $\text{np.linalg.solve}(\mathbf{X}, \mathbf{y})$.

# Table of Contents

# 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

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

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## Definition 13 (Data generation process)

We assume that the data is generated by the model,

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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):

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

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Maximizing the LL is equivalent to minimizing the MSE:

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

# Properties of MLE

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

$$\mathcal{L}_{\mathsf{LL}}(\mathbf{w}) \approx \mathbb{E}_{p(y,\mathbf{x})}\left[\log p(y \mid \mathbf{x}, \mathbf{w})\right] \tag{35}$$

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$$(\mathbf{w}_{\text{MLE}} - \mathbf{w}_{\text{true}}) \quad \longrightarrow^{d} \quad \frac{1}{\sqrt{N}}\mathcal{N}(\mathbf{w}_{\text{MLE}} \mid \mathbf{0}, \mathbf{F}^{-1}(\mathbf{w}_{\text{true}}))\,, \tag{37}$$

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

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

# Another example

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

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

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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