Decision Making: An Introduction

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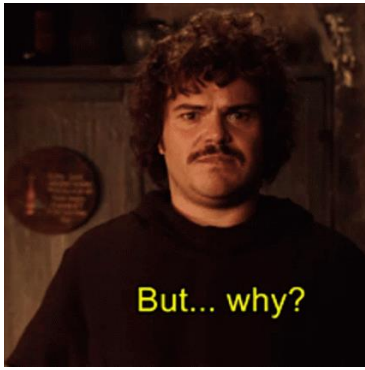
How to be a PhD student?

- Things to do with your supervisor:
  - Decide core working hours (e.g., 10am - 3pm), so you and your supervisor can easily reach each other via email or IM and start discussions during this time.
  - Schedule a fixed meeting time slot. The frequency depends on you and your supervisor's preference. Most common period is weekly or biweekly.
- Things to keep in mind:
  - Stick to your meeting schedule. Even if there is not much to report, it is still nice to update him/her regularly on your research.
  - Get up early! Working at night constantly causes mental health issues.
  - Go to seminars (in particular, statistics seminars.)

Prologue

- Unit Director: Dr. Song Liu (Office GA 18)
- Who am I?
  - A former MSc student in the University of Bristol, 14 years ago.
  - Went to Japan for my PhD and Postdoc.
  - Came back to work as a lecturer in Statistical Science
    - Why?
  - Homepage: http://allmodelsarewrong.net



- What do I do?
  - *intractable model inference, estimating statistical discrepancies, and their applications (such as Score Matching and GAN).*

Prologue

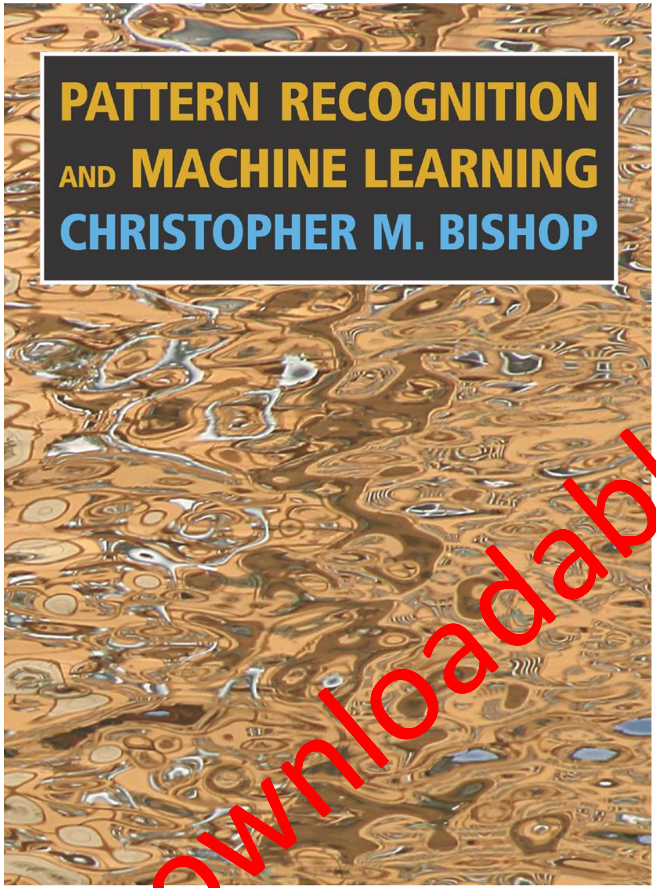
- **Two Classes** (Lectures) + **One Computing Lab**. (Practice)
  - Classes: Monday 12-1pm and Wednesday, 9-10am
  - Lab: Friday, 10am-12, 2 hours.

- **Assessment Plan (Read online document):**
  - 5 Personal portfolio (30%)
    - Summary of lectures, in your own words
    - Answers to Homework.
  - 2 Assessed coursework (40%)
    - Announcement: Wednesday after lecture, Week 5 and Week 9
    - Deadline: Friday 5pm, Week 5 and Week 9
  - 1 SM1 + SC1 Group project (30%)

Prologue

- **Syllabus:**
  - Introduction of Statistical Decision Making/Learning Week 1-2
    - 4 lectures
  - Probability Theory Week 3
    - 2 lectures
  - Linear Methods for Regression Week 4-5
    - 3 lectures
  - Linear Methods for Classification Week 6-7
    - 3 lectures
  - Probabilistic Graphical Model Week 8
    - 2 lectures
  - Advanced Topics in Machine Learning (2 guest lectures) Week 9

Reference



Downloadable!

This unit **roughly** follows Chapter 1,2,3 and 4 of

Pattern Recognition and Machine Learning

Christopher Bishop, 2006

Decision Making

- Many modern-day computational tasks are about making decisions or predictions.



- Decision making has been a great challenge of human society for a long time.

◀◀ A Look back … in China

"Oracle Bones"

- Emperor has a **question**.
- **Write it down** on the bones of large animals and **toss** it to **flame**.
- **Cracks on bones** reveal "Gods' will".
- **Priest deciphers** the patterns of cracks and provides an answer.

◀◀ A Look back … in Greece

Pythia

- Supplicant has a **question**.
- He/she travels to Delphi **asks Pythia**.
- **Pythia** inhales vapors at Temples of Apollo, speaks gibberish.
- Priest deciphers her gibberish and provides supplicant an answer.

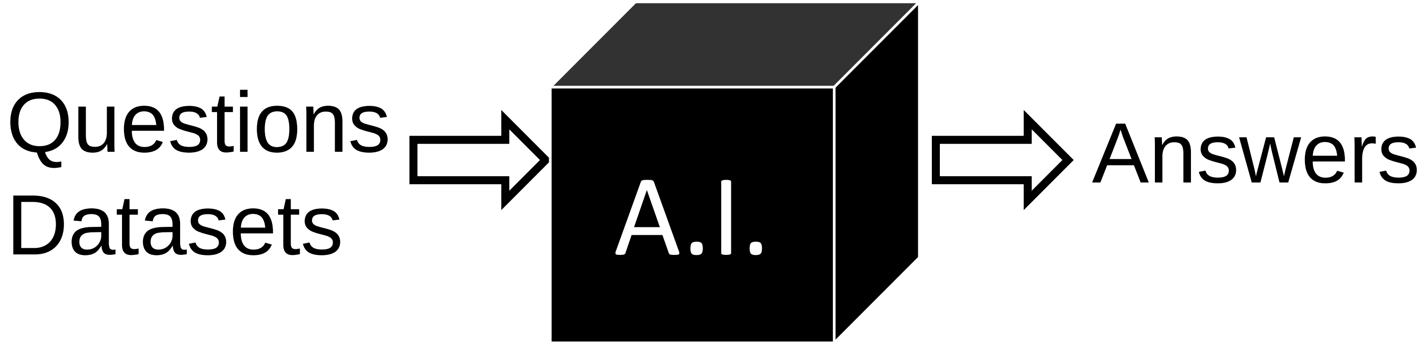
Fast forward ▶▶ … Modern Era

- No one believes in Pythia or Oracle bones anymore.
- However, the modern-day society faces another great challenge on decision making.

- Human cannot digest information fast enough and make rationalized decisions.

Fast forward ▶▶ … Modern Era

- Therefore, computer algorithms are utilized to answer **complex questions** (often via blackbox procedures).



- If we do not understand how A.I. makes decisions, we are not different from our ancestors.

Rational Decision Making

- Predictions should be Precise (no gibberish).
  - Need to study decision making under a math framework.
- Prediction should be Data-driven.
  - e.g. "sun rises up from west tomorrow" is not backed up by historical data.
- Takes Cost into consideration.
  - Cost of making a wrong decision may be different in tasks.
- Takes Random nature of Data into consideration!
  - Data generation/collection maybe noisy.

Statistical Decision Making

- We will see how **statistical** decision making exemplifies these guidelines.

- **Fun fact**: They way of taking randomness into account in decision making defines two distinct groups of statisticians: Frequentists and Bayesians.

Formal Notations

- x, y, z, scalars, $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$, vectors.
- $\boldsymbol{x} \in R^d$, vector $\boldsymbol{x}$ in d dimensional real-space.
- $x^{(i)}$, the i-th dimension of $\boldsymbol{x}$.
- X, a set
- $\boldsymbol{x}_i \in X$, the i-th member in X.
- $\boldsymbol{f}(\boldsymbol{x}) \in R^m$, function takes input vector $\boldsymbol{x}$ and maps it into m dimensional real space.
- $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z} \in R^{b \times d}$, **matrices,** with b rows and d columns.
- "=" is equality, ":=" is definition.
  - $X \coloneqq \{x_1, x_2\}$
  - $\sum_i \sum_j x_i y_j = \sum_j \sum_i x_i y_j$

Least Squares Regression

Regression Problem

- Regression is a common decision task.
- Predict outcome given some known inputs.

- For example,
  - Predict blood pressure given a patient's physical conditions.
  - Predict final year grade given a student's first-year scores.
  - etc.

Regression Problem

- **Input:** $\boldsymbol{x} \in R^d$
  - d-dimensional real-input,
  - e.g. weight, height, age, etc.
- **Output:** $y \in R$**,**
  - one dimensional real-output,
  - e.g. blood-pressure
- **The Problem**:
  - Given an input $\boldsymbol{x}$, predict its output.
- **Dataset** $D \coloneqq \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$
  - Observed **pairs of inputs** and **outputs**.

Least Squares (LS)

$$\min_{f} \sum_{i \in D_0} [y_i - f(\boldsymbol{x}_i)]^2$$

- $f(\boldsymbol{x})$: **prediction function given $\boldsymbol{x}$**.
  - return a real-valued prediction
- $[\cdot]^2$: **square cost function**.
  - cost on difference between prediction and observed output
- $D_0 \subseteq D$: **training dataset**.
  - contains paired observations for tuning prediction f

Linear LS

$$\boxed{\begin{gathered}\boldsymbol{w}_{\mathrm{LS}} := \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D_0} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2 \\ f(\boldsymbol{x}; \boldsymbol{w}) := \langle \boldsymbol{w}_1, \boldsymbol{x} \rangle + w_0, \boldsymbol{w} := \begin{bmatrix} \boldsymbol{w}_1 \\ w_0 \end{bmatrix}\end{gathered}}$$

- Solution: $\boxed{\boldsymbol{w}_{\mathrm{LS}} = (\boldsymbol{X}\boldsymbol{X}^\top)^{-1}\boldsymbol{X}\boldsymbol{y}^\top}$.
  - Suppose $\boldsymbol{x}$ is a column vector.
  - $\boldsymbol{X} := \begin{bmatrix} \boldsymbol{x}_1, \cdots, \boldsymbol{x}_n \\ 1, \cdots, 1 \end{bmatrix} \in R^{(d+1)\times n}, \boldsymbol{y} = [y_1, \cdots, y_n] \quad \in R^n$.
  - **Proof: Homework**
- LS Prediction: $f(\boldsymbol{x}; \boldsymbol{w}_{\mathrm{LS}})$.

Linear Least Squares (LS)

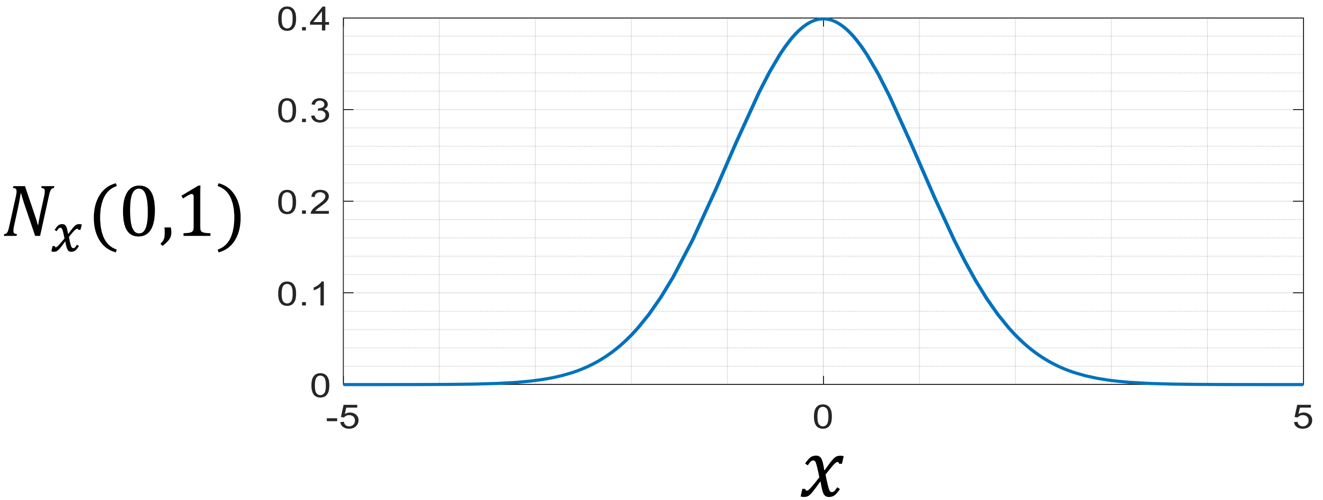
$$\boldsymbol{w}_{\mathrm{LS}} := \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D_0} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2$$

$$f(\boldsymbol{x}; \boldsymbol{w}) := \langle \boldsymbol{w}_1, \boldsymbol{x} \rangle + w_0, \boldsymbol{w} := [\boldsymbol{w}_1, w_0]^\top$$

- LS is data-driven and uses squared function as its cost.
- **How does LS take randomness of dataset into account?**
- To answer this, we see LS from a probabilistic perspective.

Normal Distribution

- Random events of a Normal dist. happen on real domain.
- Normal dist. has a probability density function (PDF):
- $p(x|\mu,\sigma) \coloneqq \frac{1}{Z(\sigma)} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \mathrm{Z}(\sigma) = \sigma\sqrt{2\pi}, x \in R.$
- We use $N_x(\mu, \sigma^2)$ denote a Normal PDF. w.r.t. x.

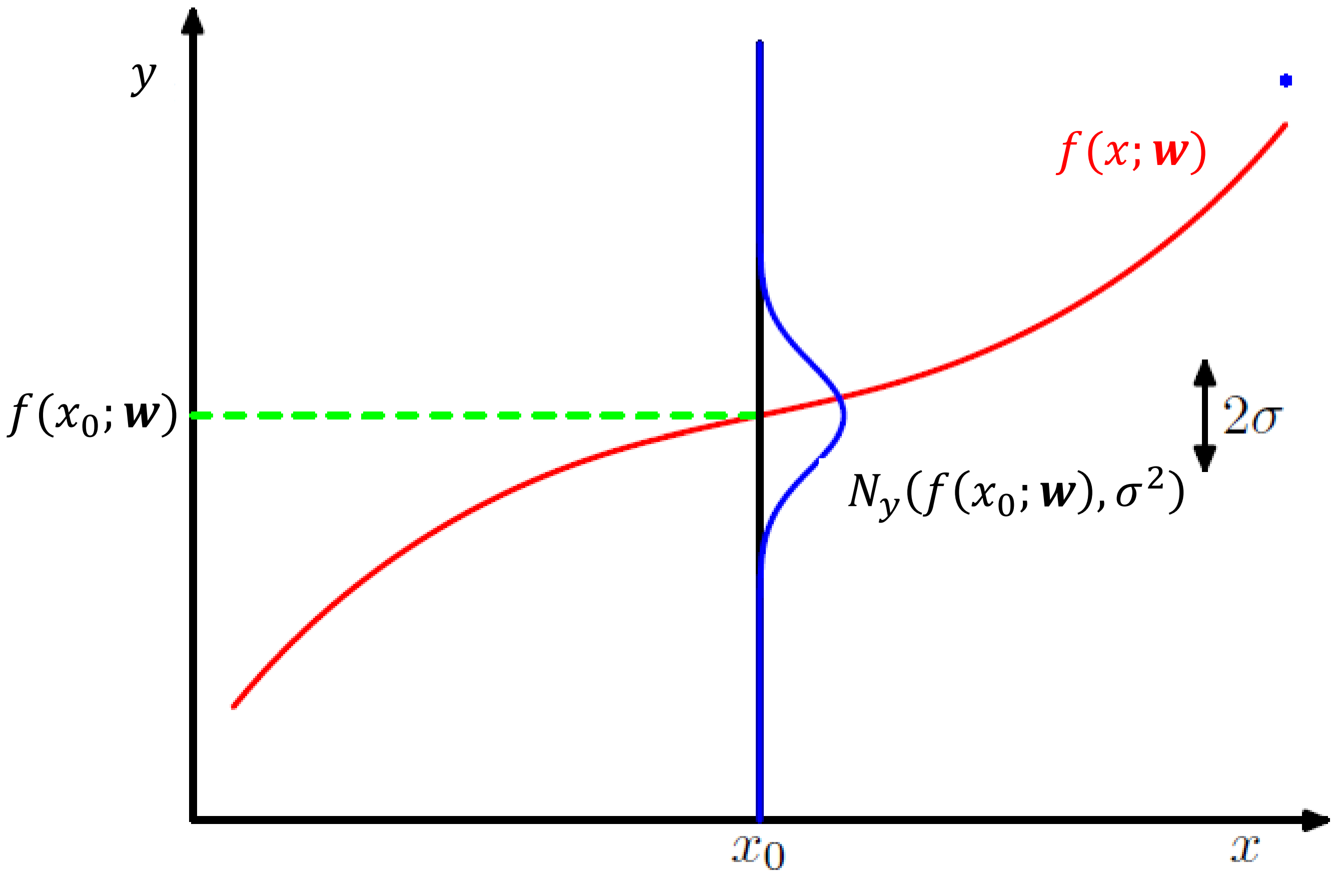


Probabilistic Modelling PRML 1.2.5

- We express randomness of y using a prob. distribution.
- Given $\boldsymbol{x}$, we assume $p(y|\boldsymbol{x}, \boldsymbol{w}, \sigma) = N_y(f(\boldsymbol{x}; \boldsymbol{w}), \sigma^2)$.
  - y follows a Normal dist. with mean $f(\boldsymbol{x}; \boldsymbol{w})$ and var. σ^2.
- This is only the model for a single y and $\boldsymbol{x}$ pair.
  - We have a dataset of n $(\boldsymbol{x}, y)$ pairs!
- By assuming $(y_i, \boldsymbol{x}_i)$ are independent and identically distributed (IID), we can model
  - $p(y_1 \dots y_n|\boldsymbol{x}_1 \dots \boldsymbol{x}_n, w, \sigma) = \prod_{i=1}^{n} N_{y_i}(f(\boldsymbol{x}_i; \boldsymbol{w}), \sigma^2)$.
  - Why?

LS from a probabilistic view

PRML Figure 1.16



Q: How to determine $\boldsymbol{w}$ and σ in a data-driven approach?

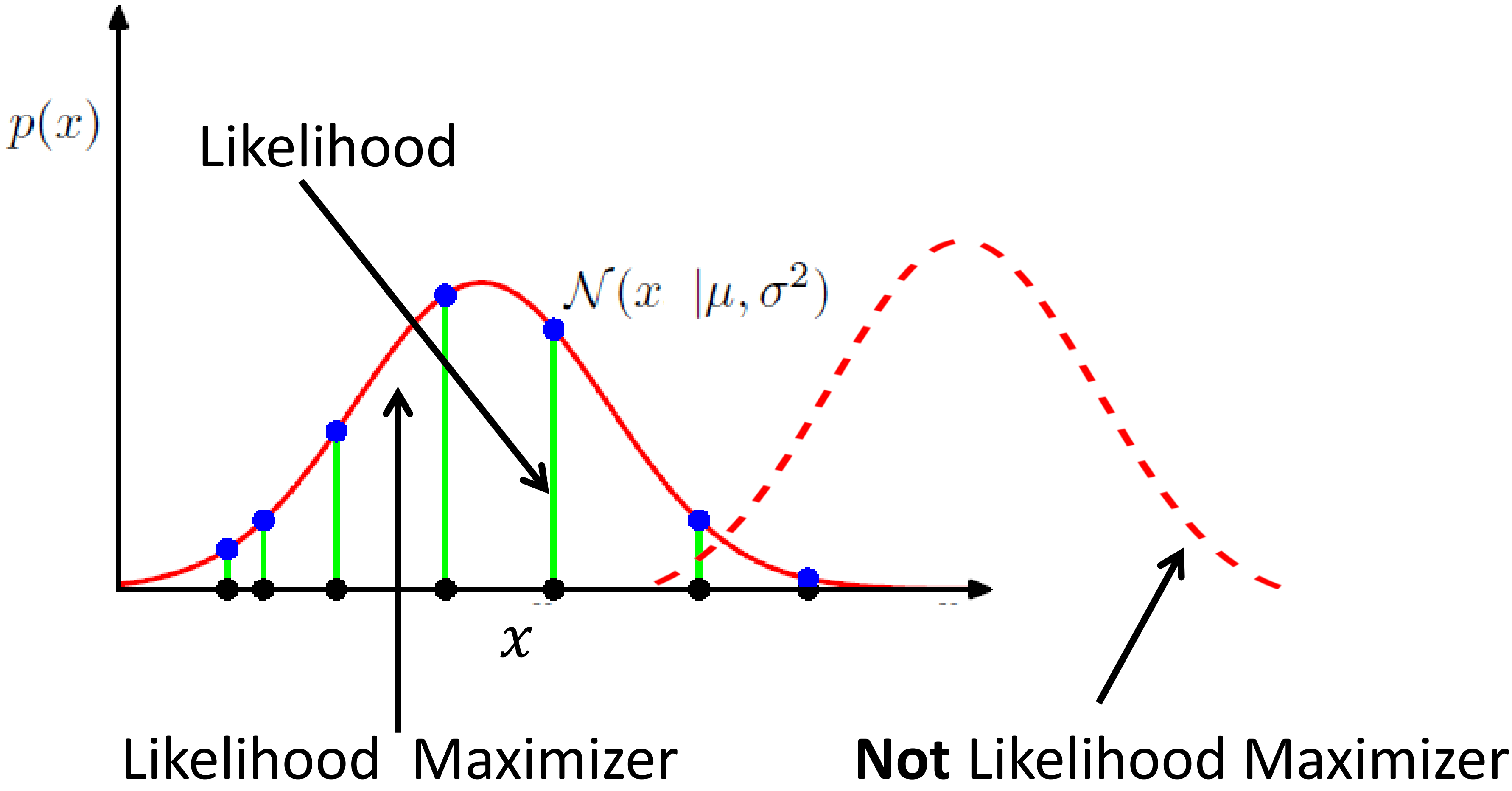
Maximum Likelihood Estimation (MLE)

PRML Figure 1.14

- PDF evaluated at observations are called **likelihood**.
- Given a dataset D, MLE maximizes (log) likelihood with respect to the unknown parameter θ.
- To determine parameter θ in $p(x|\theta)$:
- $\boxed{\theta_{\mathrm{ML}} \coloneqq \operatorname*{argmax}_{\theta} \log p(D|\theta) = \operatorname*{argmax}_{\theta} \log p(x_1 \dots x_n|\theta)}$

- Assuming $D \coloneqq \{x_1 \dots x_n\}$ is IID
- $\theta_{\mathrm{ML}} = \operatorname*{argmax}_{\theta} \sum_i \log p(x_i|\theta)$

Likelihood and Maximizing Likelihood



LS from a probabilistic view

- We have
  - a probabilistic model of y given $\boldsymbol{x}$ with unknown parameters
  - a dataset D_0
- We can perform MLE to find $\boldsymbol{w}_{\mathrm{ML}}$!
- $\boldsymbol{w}_{\mathrm{ML}} \coloneqq \mathrm{argmax}_{\boldsymbol{w}} \log \prod_i^n N_{y_i}(f(\boldsymbol{x}_i; \boldsymbol{w}), \sigma^2)$

$$= \mathrm{argmax}_{\boldsymbol{w}} \left[\sum_{i=1}^{n} - \frac{\left(y_i - f(\boldsymbol{x}_i; \boldsymbol{w})\right)^2}{2\sigma^2} \right] - n \log \sigma \sqrt{2\pi}$$

$$= \mathrm{arg}\mathrm{min}_{\boldsymbol{w}} \left[\sum_{i=1}^{n} \left(y_i - f(\boldsymbol{x}_i; \boldsymbol{w})\right)^2 \right]$$

- We can see $\boldsymbol{w}_{\mathrm{ML}} = \boldsymbol{w}_{\mathrm{LS}}$.

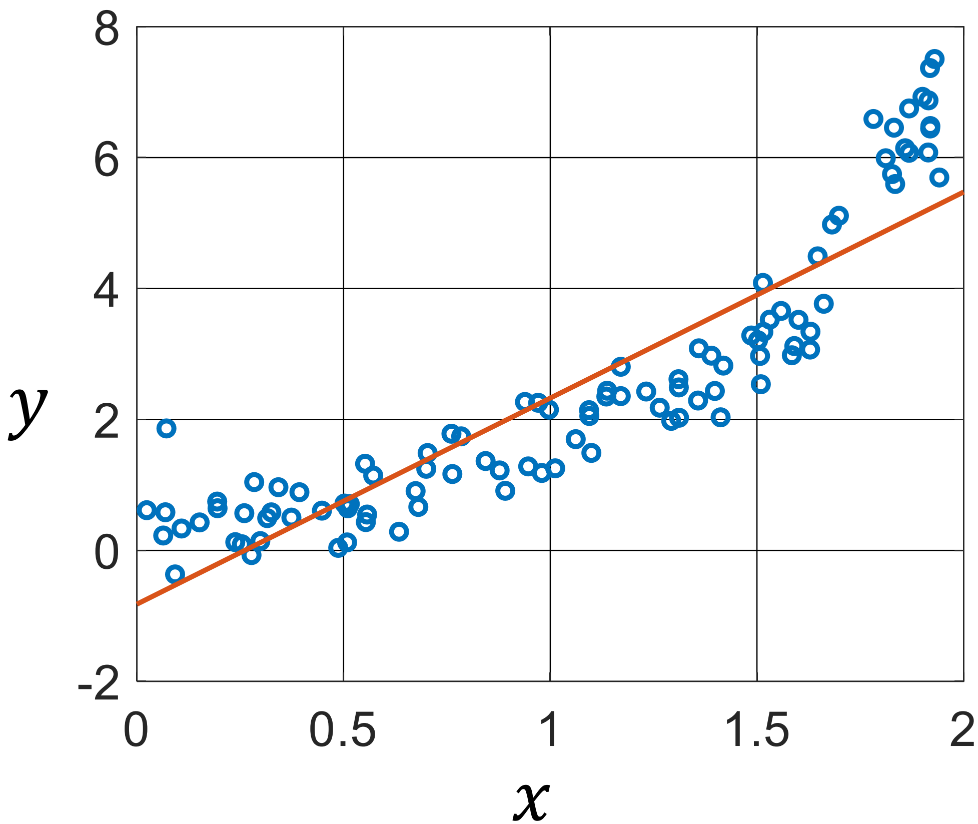
LS from a probabilistic view

- $\sigma_{\mathrm{ML}} := \operatorname{argmax}_{\sigma>0} \left[\sum_{i=1}^{n} -\frac{\left(y_i - f(x;\boldsymbol{w})\right)^2}{2\sigma^2} \right] - n \log \sigma\sqrt{2\pi}$
- $\sigma_{\mathrm{ML}}^2 = \frac{1}{n}\left[y - f(\boldsymbol{x};\boldsymbol{w}_{\mathrm{ML}})\right]^2$
- This probabilistic view not only allows us to fit a prediction function $\boldsymbol{f}$, but also the uncertainty of our prediction σ.

- This probabilistic view enables us to develop powerful regression tools on top of LS, which we will see in later.

LS with Feature Transform

- Linear LS only fits straight lines, which can be a problem if the relationship between y and x is non-linear.



LS with Feature Transform

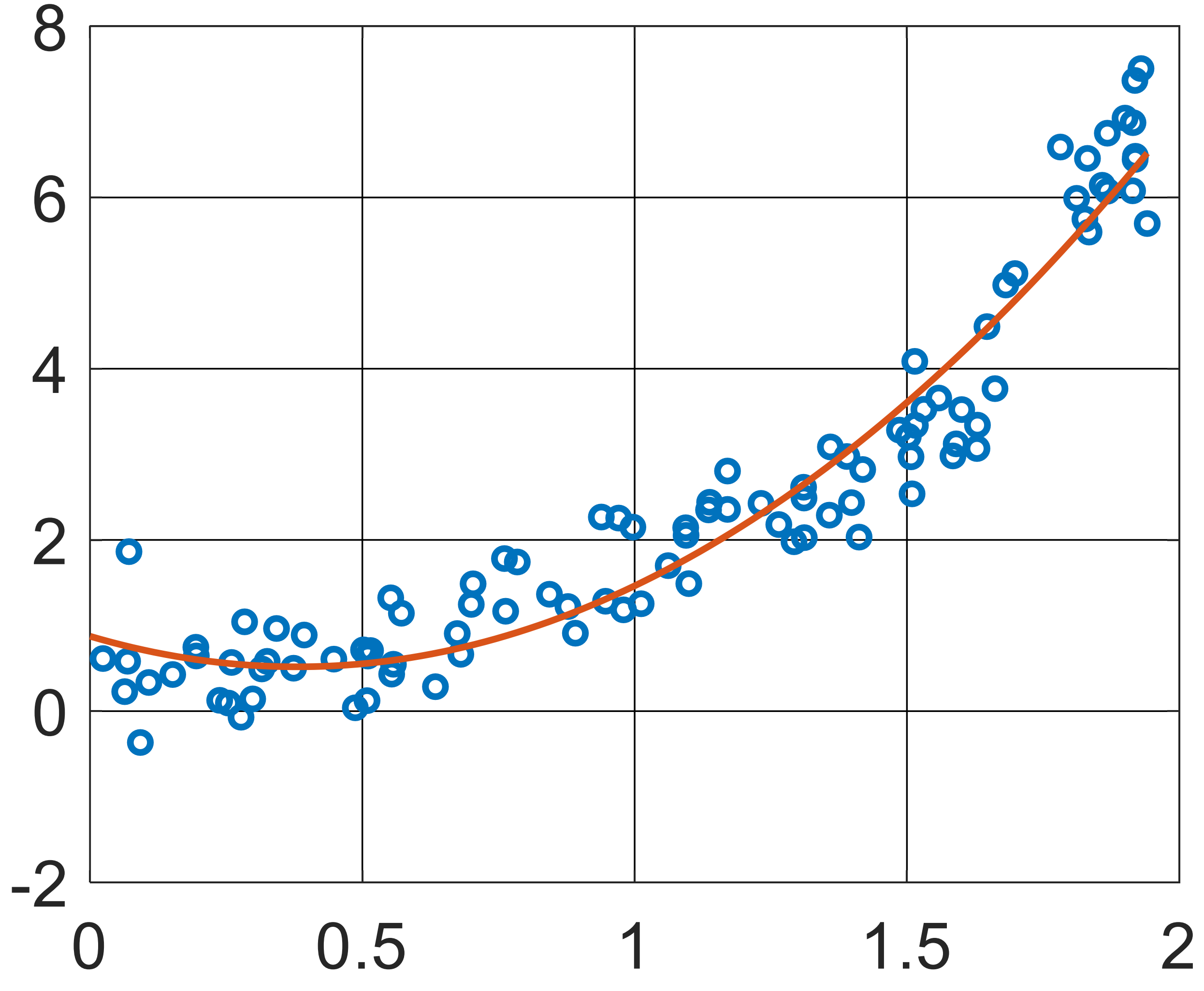
- It is easy to fit a nonlinear curve to our dataset, while maintaining the simple solution of linear LS.

$$\boldsymbol{w}_{\mathrm{LS}} := \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i \in D_0} [y_i - f'(\boldsymbol{x}_i; \boldsymbol{w})]^2$$

$$f'(\boldsymbol{x}; \boldsymbol{w}) := \langle \boldsymbol{w}_1, \boldsymbol{\phi}(\boldsymbol{x}) \rangle + w_0, \boldsymbol{w} := \begin{bmatrix} \boldsymbol{w}_1 \\ w_0 \end{bmatrix}$$

- $\boldsymbol{\phi}(\boldsymbol{x})$: $R^d \to R^b$, is called a feature transform.
  - $\boldsymbol{\phi}(\boldsymbol{x}) := \boldsymbol{x}$, Linear transform.
  - $\boldsymbol{\phi}(x) := [x, x^2, x^3, \dots, x^b]^\top$, Polynomial transform
- Solution: $\boldsymbol{w}_{\mathrm{LS}} = (\boldsymbol{\phi}(\boldsymbol{X})\boldsymbol{\phi}(\boldsymbol{X})^\top)^{-1}\boldsymbol{\phi}(\boldsymbol{X})\boldsymbol{y}^\top$
- $\boldsymbol{\phi}(\boldsymbol{X}) := \begin{bmatrix} \boldsymbol{\phi}(\boldsymbol{x}_1), \cdots, \boldsymbol{\phi}(\boldsymbol{x}_n) \\ 1, \cdots, 1 \end{bmatrix} \in R^{(b+1)\times n}$,

LS with Polynomial Transform ($b = 2$)



LS with Feature Transform

$$\boxed{\begin{aligned} &\boldsymbol{w}_{\mathrm{LS}} \coloneqq \operatorname*{argmin}_{\boldsymbol{w}} \sum_{i \in D_0} [y_i - f'(\boldsymbol{x}_i; \boldsymbol{w})]^2 \\ &f'(\boldsymbol{x}; \boldsymbol{w}) \coloneqq \langle \boldsymbol{w}_1, \boldsymbol{\phi}(\boldsymbol{x}) \rangle + w_0, \boldsymbol{w} \coloneqq [\boldsymbol{w}_1, w_0]^\top \end{aligned}}$$

- However, introducing complex feature transform in regression also opens cans of worms.
    - Overfitting
    - Curse of dimensionality
- Next lecture, we are going to see what are these problems and how to handle them using probabilistic methods.

Homework

- Prove $\boldsymbol{w}_{\mathrm{LS}} = (\boldsymbol{X}\boldsymbol{X}^\top)^{-1}\boldsymbol{X}\boldsymbol{y}^\top$
- The solution of $\boldsymbol{w}_{\mathrm{LS}}$ on page 15 is useless if $n < d$.
  - Why?
  - Can you find a solution to this problem?
- In what scenarios, the use of Normal distribution to model $p(y|\boldsymbol{x}, \boldsymbol{w}, \sigma)$ on page 21 is a bad idea?
  - Find at least 2 scenarios and explain why.
- Prove $\boldsymbol{w}_{\mathrm{LS}} = [\boldsymbol{\phi}(\boldsymbol{X})]^{-1}\, \boldsymbol{y}^\top$ if $\boldsymbol{\phi}(\boldsymbol{X})$ is symmetric and invertible.
- If we increase b of $\boldsymbol{\phi}(\boldsymbol{x})$ by 2-fold, by how many folds will the computation time of w_{LS} increase?

Homework (Challenge)

- LS principle can be seen in many other machine learning problems outside of regression. Given a dataset $D := \{\boldsymbol{x}_i\}_{i=1}^{n}$, where $\boldsymbol{x} \in R^d$. Consider the following objective:
- $\boldsymbol{w}' := \operatorname{argmin}_{\boldsymbol{w} \in R^d, \langle \boldsymbol{w}, \boldsymbol{w} \rangle = 1} \sum_i \left|\left| \boldsymbol{w}\boldsymbol{w}^\top \boldsymbol{x}_i - \boldsymbol{x}_i \right|\right|^2$.
  - $||\boldsymbol{a} - \boldsymbol{b}||$: the Euclidean distance between two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$.
- Express $\boldsymbol{w}'$ in terms of $\boldsymbol{x}_i$.
- What is the geometric interpretation of the obj. above?

Homework (Challenge)

- Kullback-Leibler (KL) divergence is a measure of dissimilarity between distributions and is expressed as:
- $KL[q,p] \coloneqq \int q(x) \log \frac{q(x)}{p(x)} \mathrm{d}x$
- If you have a probabilistic model $p(\boldsymbol{x}|\boldsymbol{\theta})$ and you know your data is drawn from a probability distribution with density q, it makes sense to select your model parameter $\boldsymbol{\theta}$ by $\min_{\theta} KL[q, p_\theta]$, **so that the fitted model is closest to the actual data distribution in terms of KL.**
- Q: What is the relationship between this model fitting objective and MLE? Under what assumptions, they are closely related?