# CS60020: Foundations of Algorithm Design and Machine Learning

### Sourangshu Bhattacharya

Some slides are taken from Christopher Bishop and Geoffrey Hinton's courses

# **OVERVIEW**

# What is Machine Learning?

- It is very hard to write programs that solve problems like recognizing a face.
  - We don't know what program to write because we don't know how our brain does it.
  - Even if we had a good idea about how to do it, the program might be horrendously complicated.
- Instead of writing a program by hand, we collect lots of examples that specify the correct output for a given input.
- A machine learning algorithm then takes these examples and produces a program that does the job.
  - The program produced by the learning algorithm may look very different from a typical hand-written program. It may contain millions of numbers.
  - If we do it right, the program works for new cases as well as the ones we trained it on.

A classic example of a task that requires machine learning: It is very hard to say what makes a 2

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# Some more examples of tasks that are best solved by using a learning algorithm

Recognizing patterns:

Facial identities or facial expressions

Handwritten or spoken words

Medical images

Generating patterns:

Generating images or motion sequences

Recognizing anomalies:

Unusual sequences of credit card transactions

Unusual patterns of sensor readings in a nuclear power plant or unusual sound in your car engine.

Prediction:

Future stock prices or currency exchange rates

#### Some web-based examples of machine learning

The web contains a lot of data. Tasks with very big datasets often use machine learning

especially if the data is noisy or non-stationary.

Spam filtering, fraud detection:

The enemy adapts so we must adapt too.

**Recommendation systems:** 

Lots of noisy data. Million dollar prize!

Information retrieval:

Find documents or images with similar content.

Data Visualization:

Display a huge database in a revealing way

# Displaying the structure of a set of documents using Latent Semantic Analysis (a form of PCA)



Each document is converted to a vector of word counts. This vector is then mapped to two coordinates and displayed as a colored dot. The colors represent the hand-labeled classes.

When the documents are laid out in 2-D, the classes are not used. So we can judge how good the algorithm is by seeing if the classes are separated.

### **Machine Learning & Symbolic Al**

Knowledge Representation works with facts/assertions and develops rules of logical inference. The rules can handle quantifiers. Learning and uncertainty are usually ignored.

- Expert Systems used logical rules or conditional probabilities provided by "experts" for specific domains.
- Graphical Models treat uncertainty properly and allow learning (but they often ignore quantifiers and use a fixed set of variables)
  - Set of logical assertions → values of a subset of the variables and local models of the probabilistic interactions between variables.
  - Logical inference → probability distributions over subsets of the unobserved variables (or individual ones)
  - Learning = refining the local models of the interactions.

#### **Machine Learning & Statistics**

A lot of machine learning is just a rediscovery of things that statisticians already knew.

But the emphasis is very different:

- A good piece of statistics: Clever proof that a relatively simple estimation procedure is asymptotically unbiased.
- A good piece of machine learning: Demonstration that a complicated algorithm produces impressive results on a specific task.

Data-mining: Using very simple machine learning techniques on very large databases because computers are too slow to do anything more interesting with ten billion examples.

### A spectrum of machine learning tasks

#### Statistics-----Artificial Intelligence

Low-dimensional data (e.g. less than 100 dimensions)

Lots of noise in the data

There is not much structure in the data, and what structure there is, can be represented by a fairly simple model.

The main problem is distinguishing true structure from noise.

#### High-dimensional data (e.g. mo

High-dimensional data (e.g. more than 100 dimensions)

The noise is not sufficient to obscure the structure in the data if we process it right.

There is a huge amount of structure in the data, but the structure is too complicated to be represented by a simple model.

The main problem is figuring out a way to represent the complicated structure that allows it to be learned.

# REGRESSION

# Linear Basis Function Models (1)

#### **Example: Polynomial Curve Fitting**



# Linear Basis Function Models (2)

#### Generally

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

where  $\phi_j(\mathbf{x})$  are known as *basis functions*. Typically,  $\phi_0(\mathbf{x}) = 1$ , so that  $w_0$  acts as a bias. In the simplest case, we use linear basis functions :  $\phi_d(\mathbf{x}) = x_d$ .

# Linear Basis Function Models (3)

Polynomial basis functions:

$$\phi_j(x) = x^j.$$

These are global; a small change in x affect all basis functions.



# Linear Basis Function Models (4)

Gaussian basis functions:

$$\phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$

These are local; a small change in x only affect nearby basis functions.  $\mu_j$  and s control location and scale (width).



# Linear Basis Function Models (5)

Sigmoidal basis functions:

$$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

Also these are local; a small change in x only affect nearby basis functions.  $\mu_j$  and scontrol location and scale (slope).



# Least Squares Estimation

A a polynomial curve is represented by the parameters *w*.

 $f(x) = x - x^2$  $f(x) = x + x^2$ 

Error (loss) function for a given parameter:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

Estimate  $w^* = \min_w E(w)$ 

### Maximum Likelihood and Least Squares (1)

Assume observations from a deterministic function with added Gaussian noise:

 $t = y(\mathbf{x}, \mathbf{w}) + \epsilon$  where  $p(\epsilon|\beta) = \mathcal{N}(\epsilon|0, \beta^{-1})$ 

which is the same as saying,

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}).$$

Given observed inputs,  $\mathbf{X} = {\{\mathbf{x}_1, \dots, \mathbf{x}_N\}}$ , and targets,  $\mathbf{t} = [t_1, \dots, t_N]^T$ , we obtain the likelihood function  $p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^N \mathcal{N}(t_n | \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}).$ 

### Maximum Likelihood and Least Squares (2)

Taking the logarithm, we get

$$\ln p(\mathbf{t}|\mathbf{w},\beta) = \sum_{n=1}^{N} \ln \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n),\beta^{-1})$$
$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w})$$

where

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\}^2$$

is the sum-of-squares error.

### Maximum Likelihood and Least Squares (3)

Computing the gradient and setting it to zero yields

$$\nabla_{\mathbf{w}} \ln p(\mathbf{t}|\mathbf{w},\beta) = \beta \sum_{n=1}^{N} \left\{ t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) \right\} \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}} = \mathbf{0}.$$



$$\boldsymbol{\Phi} = \left(\begin{array}{ccccc} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{array}\right)$$

# **Geometry of Least Squares**

Consider

 $\mathbf{y} = \mathbf{\Phi} \mathbf{w}_{\mathrm{ML}} = [\mathbf{\varphi}_1, \dots, \mathbf{\varphi}_M] \mathbf{w}_{\mathrm{ML}}.$  $\mathbf{y} \in \mathcal{S} \subseteq \mathcal{T} \qquad \mathbf{t} \in \mathcal{T}$  $\bigwedge_{N\text{-dimensional}}^{N\text{-dimensional}}$ 

S is spanned by  $\varphi_1, \ldots, \varphi_M$ .  $\mathbf{w}_{ML}$  minimizes the distance between  $\mathbf{t}$  and its orthogonal projection on S, i.e.  $\mathbf{y}$ .

![](_page_20_Figure_4.jpeg)

# **Normal Equations**

$$(\mathbf{A}^T \mathbf{A})\widehat{\boldsymbol{\beta}} = \mathbf{A}^T \mathbf{Y}$$

If  $(\mathbf{A}^T \mathbf{A})$  is invertible,

$$\widehat{\beta} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{Y} \qquad \widehat{f}_n^L(X) = X \widehat{\beta}$$

When is  $(\mathbf{A}^T \mathbf{A})$  invertible ? Recall: Full rank matrices are invertible.

What if  $(\mathbf{A}^T \mathbf{A})$  is not invertible ?

# **Gradient Descent**

Even when  $(\mathbf{A}^T \mathbf{A})$  is invertible, might be computationally expensive if **A** is huge.

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n} (\mathbf{A}\beta - \mathbf{Y})^T (\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

Treat as optimization problem

![](_page_22_Figure_4.jpeg)

### **Gradient Descent**

Even when  $(\mathbf{A}^T \mathbf{A})$  is invertible, might be computationally expensive if **A** is huge.

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n} (\mathbf{A}\beta - \mathbf{Y})^T (\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

#### Since $J(\beta)$ is convex, move along negative of gradient

![](_page_23_Figure_4.jpeg)

![](_page_23_Figure_5.jpeg)

< 8.

Stop: when some criterion met e.g. fixed # iterations, or  $\frac{\partial J(\beta)}{\partial \beta}$ 

# Effect of step--size α

![](_page_24_Figure_1.jpeg)

Large  $\alpha \Rightarrow$  Fast convergence but larger residual error Also possible oscillations

Small  $\alpha \Rightarrow$  Slow convergence but small residual error

# 0<sup>th</sup> Order Polynomial

![](_page_25_Figure_1.jpeg)

# 1<sup>st</sup> Order Polynomial

![](_page_26_Figure_1.jpeg)

# 3<sup>rd</sup> Order Polynomial

![](_page_27_Figure_1.jpeg)

# 9<sup>th</sup> Order Polynomial

![](_page_28_Figure_1.jpeg)

# **Over-fitting**

![](_page_29_Figure_1.jpeg)

Root-Mean-Square (RMS) Error

# Polynomial Coefficients

	M = 0	M = 1	M=3	M = 9
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^{\star}$		-1.27	7.99	232.37
$w_2^{\star}$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^{\star}$				-231639.30
$w_5^{\star}$				640042.26
$w_6^\star$				-1061800.52
$w_7^{\star}$				1042400.18
$w_8^{\star}$				-557682.99
$w_9^{\star}$				125201.43

# Regularization

Penalize large coefficient values

$$J_{\mathbf{X},\mathbf{y}}(\mathbf{w}) = \frac{1}{2} \sum_{i} \left( y^{i} - \sum_{j} w_{j} \phi_{j}(\mathbf{x}^{i}) \right)^{2} + \frac{\lambda}{2} \|\mathbf{w}\|^{2}$$

# **Regularization:**

$$\ln \lambda = -18$$

![](_page_32_Figure_2.jpeg)

# **Over Regularization**

![](_page_33_Figure_1.jpeg)

# Regularization

#### 9<sup>th</sup> Order Polynomial

![](_page_34_Figure_2.jpeg)

# Regularized Least Squares (1)

Consider the error function:

 $E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$ 

Data term + Regularization term

With the sum-of-squares error function and a quadratic regularizer, we get

$$\frac{1}{2}\sum_{n=1}^{N} \{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

 $\lambda$  is called the regularization coefficient.

which is minimized by

$$\mathbf{w} = \left(\lambda \mathbf{I} + \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}.$$

# Regularized Least Squares (2)

With a more general regularizer, we have

![](_page_36_Figure_2.jpeg)

# Regularized Least Squares (3)

Lasso tends to generate sparser solutions than a quadratic regularizer.  $w_2 \uparrow w_2 \uparrow w_2$ 

![](_page_37_Figure_2.jpeg)

Analogously to the single output case we have:

$$p(\mathbf{t}|\mathbf{x}, \mathbf{W}, \beta) = \mathcal{N}(\mathbf{t}|\mathbf{y}(\mathbf{W}, \mathbf{x}), \beta^{-1}\mathbf{I})$$
$$= \mathcal{N}(\mathbf{t}|\mathbf{W}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\mathbf{I}).$$

Given observed inputs,  $\mathbf{X} = {\mathbf{x}_1, \dots, \mathbf{x}_N}$ , and targets,  $\mathbf{T} = [\mathbf{t}_1, \dots, \mathbf{t}_N]^T$ , we obtain the log likelihood function

$$\ln p(\mathbf{T}|\mathbf{X}, \mathbf{W}, \beta) = \sum_{n=1}^{N} \ln \mathcal{N}(\mathbf{t}_n | \mathbf{W}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1} \mathbf{I})$$
$$= \frac{NK}{2} \ln \left(\frac{\beta}{2\pi}\right) - \frac{\beta}{2} \sum_{n=1}^{N} \left\|\mathbf{t}_n - \mathbf{W}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n)\right\|^2.$$

Maximizing with respect to  $\mathbf{W}$ , we obtain

$$\mathbf{W}_{\mathrm{ML}} = \left( \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi} 
ight)^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{T}.$$

If we consider a single target variable,  $t_k$ , we see that

$$\mathbf{w}_k = \left( \mathbf{\Phi}^{\mathrm{T}} \mathbf{\Phi} 
ight)^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{t}_k = \mathbf{\Phi}^{\dagger} \mathbf{t}_k$$

where  $\mathbf{t}_k = [t_{1k}, \dots, t_{Nk}]^T$ , which is identical with the single output case.

# **CLASSIFICATION**

# **Discrete and Continuous Labels**

![](_page_41_Figure_1.jpeg)

![](_page_41_Figure_2.jpeg)

An emergency room in a hospital measures 17 variables (e.g., blood pressure, age, etc) of newly admitted patients.

- A decision is needed: whether to put a new patient in an intensive-care unit.
- Due to the high cost of ICU, those patients who may survive less than a month are given higher priority.
- Problem: to predict high-risk patients and discriminate them from low-risk patients.

# Another application

A credit card company receives thousands of applications for new cards. Each application contains information about an applicant,

age

Marital status

annual salary

outstanding debts

credit rating

etc.

Problem: to decide whether an application should approved, or to classify applications into two categories, approved and not approved. The data and the goal

Data: A set of data records (also called examples, instances or cases) described by

*k* attributes:  $A_1, A_2, \ldots A_k$ .

a class: Each example is labelled with a predefined class.

Goal: To learn a classification model from the data that can be used to predict the classes of new (future, or test) cases/instances.

## Supervised learning process: two steps

- Learning (training): Learn a model using the training data
- Testing: Test the model using unseen test data to assess the model accuracy

![](_page_45_Figure_3.jpeg)

# Least squares classification

Binary classification.

Each class is described by it's own linear model:  $y(x) = w^T x + w_0$ 

Compactly written as:

$$\mathbf{y}(\boldsymbol{x}) = \boldsymbol{W}^T \boldsymbol{x}$$

W is  $[w w_0]$ .  $E_D(W) = \frac{1}{2} (XW - t)^T (XW - t)$   $n^{th}$  row of X is  $x_n$ , the  $n^{th}$  datapoint. t is vector of +1, -1.

### Least squares classification

# Least squares W is: $W = (X^T X)^{-1} X^T t$ Problem is affected by outliers.

### Least squares classification

![](_page_48_Figure_1.jpeg)

### From Linear to Logistic Regression

Assumes the following functional form for P(Y|X):

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

![](_page_49_Figure_3.jpeg)

# Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

Decision boundary:

$$P(Y=0|X) \stackrel{0}{\underset{1}{\gtrless}} P(Y=1|X)$$

$$w_0 + \sum_i w_i X_i \stackrel{0}{\gtrless} 0$$

(Linear Decision Boundary)

![](_page_50_Figure_7.jpeg)

### Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow P(Y=0|X) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow \frac{P(Y=0|X)}{P(Y=1|X)} = \exp(w_0 + \sum_i w_i X_i) \quad \stackrel{0}{\gtrless} 1$$
$$\Rightarrow w_0 + \sum_i w_i X_i \quad \stackrel{0}{\gtrless} 0$$

Label t 
$$\in \{+1, -1\}$$
 modeled as:  
 $P(t = 1 | x, w) = \sigma(w^T x)$   
 $P(y | x, w) = \sigma(yw^T x), y \in \{+1, -1\}$   
Given a set of parameters w, the probability or

likelihood of a datapoint (x,t):

$$P(t|x,w) = \sigma(tw^T x)$$

Given a training dataset  $\{(x_1, t_1), \dots, (x_N, t_N)\}$ , log likelihood of a model w is given by:

$$L(w) = \sum_{n} \ln(P(t_n | x_n, w))$$

Using principle of maximum likelihood, the best w is given by:

$$w^* = \arg \max_w L(w)$$

# Logistic Regression

**Final Problem:** 

$$\max_{w} \sum_{i=1}^{n} -\log(1 + \exp(-t_n w^T x_n))$$

Or, 
$$\min_{w} \sum_{i=1}^{n} \log(1 + \exp(-t_n w^T x_n))$$

Error function:

$$E(w) = \sum_{i=1}^{n} \log(1 + \exp(-t_n w^T x_n))$$

E(w) is convex.

# Logistic Regression

Final Problem:  

$$\max_{w} \sum_{i=1}^{n} -\log(1 + \exp(-t_{n}w^{T}x_{n}))$$
Regularized Version:  

$$\max_{i=1}^{n} -\log(1 + \exp(-t_{n}w^{T}x_{n})) - \lambda w^{T}w$$
Or, 
$$\min_{i=1}^{n} \log(1 + \exp(-t_{n}w^{T}x_{n})) + \lambda ||w||^{2}$$

 $\min_{w} \sum_{i=1}^{n} \log(1 + \exp(-t_n w^T x_n)) + \lambda ||w||^{\epsilon}$ 

### **Properties of Error function**

Derivatives:

$$\nabla E(w) = \sum_{i=1}^{n} -(1 - \sigma(t_i w^T x_i))(t_i x_i)$$

$$\nabla E(w) = \sum_{i=1}^{n} (\sigma(w^{T} x_{i}) - t_{i}) x_{i}$$

$$\nabla^2 E(w) = \sum_{i=1}^n \sigma(t_i w^T x_i) \left(1 - \sigma(t_i w^T x_i)\right) x_i x_i^T$$

# **Gradient Descent**

Problem: min f(x)
f(x): differentiable
g(x): gradient of f(x)
Negative gradient is
 steepest descent
 direction.

At each step move in the gradient directic so that there is "sufficient decrease"

![](_page_57_Figure_3.jpeg)

**input** : Function f, Gradient  $\nabla f$ **output**: Optimal solution  $w^*$ Initialize  $w_0 \leftarrow 0, k \leftarrow 0$ while  $|\nabla f_k| > \epsilon$  do Compute  $\alpha_k \leftarrow \text{linesearch}(f, -\nabla f_k, w_k)$ Set  $w_{k+1} \leftarrow w_k - \alpha_k \nabla f_k$ Evaluate  $\nabla f_{k+1}$  $k \leftarrow k+1$ end  $w^* \leftarrow w_k$ 

### Logistic Regression is a Linear Classifier!

Assumes the following functional form for P(Y|X):

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow P(Y = 0|X) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow \frac{P(Y=0|X)}{P(Y=1|X)} = \exp(w_0 + \sum_i w_i X_i) \quad \stackrel{0}{\gtrless} 1$$
$$\Rightarrow w_0 + \sum_i w_i X_i \quad \stackrel{0}{\gtrless} 0$$

#### Logistic Regression for more than 2 classes

Logistic regression in more general case, where
 Y {y<sub>1</sub>,...,y<sub>k</sub>}

for kP(Y = y\_k | X) = \frac{\exp(w\_{k0} + \sum\_{i=1}^{d} w\_{ki} X\_i)}{1 + \sum\_{j=1}^{K-1} \exp(w\_{j0} + \sum\_{i=1}^{d} w\_{ji} X\_i)}

for *k*=*K* (normalization, so no weights for this class)

$$P(Y = y_K | X) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{d} w_{ji} X_i)}$$

One-vs-all: K - 1 hyperplanes each separating  $C_1, \ldots, C_{K-1}$  classes from rest. Otherwise  $C_K$ Low number of classifiers.

 $\mathcal{C}_1$ 

 $\mathcal{R}_3$ 

not  $C_2$ 

 $\bullet$  not  $\mathcal{C}_1$ 

 $\mathcal{C}_2$ 

One-vs-one: Every pair  $C_i - C_j$  get a boundary. Final by majority vote. High number of classifiers.

![](_page_62_Figure_2.jpeg)

K-linear discriminant functions:

$$y_k(x) = w_k^T x + w_{k0}$$
  
Assign x to  $C_k$  if  $y_k(x) \ge y_j(x)$  for all  $j \ne k$ 

Decision boundary:

$$\left(w_k - w_j\right)^T \boldsymbol{x} + \left(w_{k0} - w_{j0}\right) = 0$$

Decision region is singly connected:

$$x = \lambda x_A + (1 - \lambda) x_B$$

If  $x_A$  and  $x_B$  have same label, so does x.

# **Multiple Classes**

![](_page_64_Figure_1.jpeg)