ground truth: Let y be the actual observed label in the dataset

CONVENTIONAL (ALGORITHMIC) VIEW OF ML



evaluation metric: loss function e.g. $L(y, \hat{y}) = \underline{1}_{\hat{y}\neq y}$

PROBABILITY MODELLER'S VIEW



5 with prob 45%3 with prob 41%6 with prob 5%

...

evaluation metric: log likelihood i.e. $\log Pr_Y(y)$

random predicted label Y

ground truth: Let y be the actual observed temperature at time t

CONVENTIONAL (ALGORITHMIC) VIEW OF MODELLING



evaluation metric: loss function e.g. $L(y, \hat{y}) = (y - \hat{y})^2$

PROBABILITY MODELLER'S VIEW

timepoint *t*



evaluation metric: log likelihood i.e. log $Pr_Y(y; t)$

random variable for temperature Y at timepoint t Our job is to invent a probability model, specifying the **distribution** of temperature at a given timepoint.

timepoint t



random variable for temperature Y at timepoint t

Example (regression)

Given a labelled dataset consisting of pairs (x_i, y_i) of real numbers, fit the model $Y_i \sim \alpha + \beta x_i + \gamma x_i^2 + N(0, \sigma^2)$



Model for a single observation:

 $Y \sim \alpha + \beta x + \gamma x^2 + N(0, \sigma^2)$ $\sim N(\alpha + \beta x + \gamma x^2, \sigma^2)$

Likelihood of a single observation:

$$\Pr_{Y}(y; x, \alpha, \beta, \gamma, \sigma) = \frac{1}{\sqrt{2\pi\sigma^{2}}} e^{-(y - (\alpha + \beta x + \gamma x^{2}))/2\sigma^{2}}$$

Log likelihood of the dataset:

$$\log \Pr(y_1, \dots, y_n; x_1, \dots, x_n, \alpha, \beta, \gamma, \sigma) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

where $\hat{y}_i = \alpha + \beta x_i + \gamma x_i^2$

Optimize over the unknown parameters:

```
def logpr(y, x, \alpha, \beta, \gamma, \sigma):

pred = \alpha + \beta^* x + \gamma^* (x^{**2})

return - 0.5*np.log(2*\pi^* \sigma^2) - (y - pred)**2 / (2*\sigma^2)
```

```
x,y = ...
def f(θ):
    return - np.sum(logpr(y, x, θ[0], θ[1], θ[2], θ[3]))
```

scipy.optimize.fmin(f, [3,1,0.1,3])

Example (regression)

Given a labelled dataset consisting of pairs (x_i, y_i) of real numbers, fit the model $Y_i \sim \mu_{\theta}(x_i) + N(0, \sigma^2)$



The question implies that $\mu_{\theta}(\cdot)$ is some given function with unknown parameter θ .



Log likelihood of the dataset:

$$\log \Pr(y_1, \dots, y_n; x_1, \dots, x_n, \theta, \sigma) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu_{\theta}(x_i))^2$$

Optimize over the unknown parameters θ and σ :

- 1 class RWiggle(nn.Module): 2 def __init__(self): 3 super().__init__() 4 self.μ = ... 5 self.σ = nn.Parameter(torch.tensor(1.0)) # compute log Pr(y;x) 6 def forward(self, y, x): 7 return - 0.5*torch.log(2*π*σ²) - torch.pow(y - self.μ(x), 2) / (2*σ²) 8 x,y = ...
 - mymodel = RWiggle()
- 10
- 11 optimizer = optim.Adam(mymodel.parameters())
- 12 for epoch in range(10000):
- 13 optimizer.zero_grad()
- 14 loglik = torch.sum(mymodel(y, x))
- 15 (-loglik).backward()
- 16 optimizer.step()

See notes section 33 for infra to Py Torch.





edge weights θ

self.µ = nn.Sequential(
 nn.Linear(1,4), nn.LeakyReLU(),
 nn.Linear(4,20), nn.LeakyReLU(),
 nn.Linear(20,20), nn.LeakyReLU(),
 nn.Linear(20,1))

504 parameters

THIS IS YOUR MACHINE LEARNING SYSTEM?

YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.

WHAT IF THE ANSWERS ARE WRONG?

JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.



https://xkcd.com/1838 CC BY-NC 2.5

Example (regression)

Given a labelled dataset consisting of pairs (x_i, y_i) of real numbers, fit the model $Y_i \sim \mu_{\theta}(x_i) + N(0, \sigma^2)$



The question implies that $\mu_{\theta}(\cdot)$ is some given function with unknown parameter θ .

Log likelihood of the dataset:

$$\log \Pr(y_1, \dots, y_n; x_1, \dots, x_n, \theta, \sigma) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu_{\theta}(x_i))^2$$

Optimize over the unknown parameters θ and σ :

$$\max_{\theta,\sigma} \left\{ -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu_\theta(x_i))^2 \right\}$$
$$= \max_{\sigma} \left\{ \max_{\theta} \left[-\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu_\theta(x_i))^2 \right] \right\}$$
$$= \max_{\sigma} \left\{ -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \min_{\theta} \left[\sum_{i=1}^n (y_i - \mu_\theta(x_i))^2 \right] \right\}$$

"First, find θ to minimize prediction loss. Next, pick σ ."

Any useful "minimize prediction loss" problem can be restated as a maximum likelihood problem

Supervised ML is fitting a probability model

Probability modelling is a more powerful way to think about ML

The MNIST dataset consists of pairs (x_i, y_i) , where each record consists of $x_i \in \mathbb{R}^{28 \times 28}$ an image of a handwritten digit and $y_i \in \{0, 1, \dots, 9\}$ is its label.

Devise a probabilistic model to predict the label of a given input image, and fit it.







some arbitrary function, parameters θ

What sort of probability model might we use for the response *Y*?

The MNIST dataset consists of pairs (x_i, y_i) , where each record consists of $x_i \in \mathbb{R}^{28 \times 28}$ an image of a handwritten digit and $y_i \in \{0, 1, \dots, 9\}$ is its label.

Devise a probabilistic model to predict the label of a given input image, and fit it.





parameters θ



How can we make sure that \vec{p} is a valid probability vector?

(We need $p_i \in [0,1]$ for each i, and $\Sigma_i p_i = 1$.)

The MNIST dataset consists of pairs (x_i, y_i) , where each record consists of $x_i \in \mathbb{R}^{28 \times 28}$ an image of a handwritten digit and $y_i \in \{0, 1, \dots, 9\}$ is its label.

Devise a probabilistic model to predict the label of a given input image, and fit it.





How should we fit the function parameters θ ?

The MNIST dataset consists of pairs (x_i, y_i) , where each record consists of $x_i \in \mathbb{R}^{28 \times 28}$ an image of a handwritten digit and $y_i \in \{0, 1, ..., 9\}$ is its label.

Devise a probabilistic model to predict the label of a given input image, and fit it.



Model for a single datapoint:



This is called *softmax cross-entropy*, and it's the standard loss function for classification.



HOMEWORK

Jigit

- Make sure you can run this code
- For each digit {0,1,...,9}, select some images where the label is very likely, and some where it is very unlikely

class MyImageClassifier(nn.Module): def init (self): super(). init () self.f = nn.Sequential(# input shape [B*1*28*28] nn.Conv2d(1, 32, 3, 1), # -> [B*32*26*26] nn.ReLU(), nn.Conv2d(32, 64, 3, 1), # -> [B*64*24*24] nn.MaxPool2d(2), # -> [B*64*12*12] nn.Dropout2d(0.25), # -> [B*9216] nn.Flatten(1), nn.Linear(9216, 128), # -> [B*128] nn.ReLU(), nn.Dropout2d(0.5), # -> [B*10] nn.Linear(128, 10) # compute log likelihood for a batch of data def forward(self, y, x): # x.shape [B*1*28*28], y.shape [B], output.shape [B] return - nn.functional.cross entropy(self.f(x), y, reduction='none') # compute the class probabilities for a single image def classify(self, x): # input: [1*28*28] array q = self.f(torch.as tensor(x)[None,...])[0] return nn.functional.softmax(q, dim=0)



This is machine learning, too!

CONVENTIONAL VIEW OF MACHINE LEARNING

Supervised Learning

Data:

 $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$

Labels:

 y_1, y_2, \dots, y_n

Task:

Predict the label $y_i \approx f_{\theta}(x_i)$

Training goal:

Invent a loss function and learn θ to minimize the prediction loss $\sum_{i} L(y_i, f_{\theta}(x_i))$

Evaluation:

prediction loss on holdout data



Generative Modelling

Data:	$\{x_1, x_2, \dots, x_n\}$
Labels:	n/a
Task:	learn to synthesize new values similar (but not identical) to those in the dataset,
Training goal:	???
Evaluation:	???



Supervised Learning

Data:

 $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$

Labels:

- y_1, y_2, \dots, y_n
- Task:Fit a probability model $\Pr_Y(y_i; f_\theta(x_i))$

Training goal:

Learn θ to maximize the log likelihood of the dataset $\sum_{i} \log \Pr_{Y}(y_{i}; f_{\theta}(x_{i}))$

Evaluation:

log likelihood of holdout data



Generative Modelling

Data:	$\{x_1, x_2, \dots, x_n\}$
abels:	n/a
āsk:	fit the probability model $Pr_X(x; \theta)$

Training goal:

Learn θ to maximize the log likelihood of the dataset $\sum_i \log \Pr_X(x_i; \theta)$

Evaluation:

log likelihood of holdout dataset



Exercise (generative modelling).

Train a generative model for a collection of points $x^{(1)}, ..., x^{(n)} \in \mathbb{R}^2$. The model should have the form

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim f(Z) + \begin{bmatrix} N(0, \sigma^2) \\ N(0, \sigma^2) \end{bmatrix}$$

where $Z \sim U[0,1]$ and $f: [0,1] \rightarrow \mathbb{R}^2$ is a neural network to be trained.



Model for a single observation

 $Z \sim U[0,1]$ $X_1 \sim f_1(Z) + N(0,\sigma^2)$ $X_2 \sim f_2(Z) + N(0,\sigma^2)$

Likelihood for a single observation

Pr

$$(x_{1}, x_{2}) = \int_{z=0}^{1} \Pr(x_{1}, x_{2} | Z = z) \Pr_{Z}(z) dz$$

$$\Pr(x_{1} | Z = z) \Pr(x_{2} | Z = z)$$

$$\Pr(x_{i} | Z = z) = \frac{1}{\sqrt{2\pi\sigma^{2}}} e^{(x_{i} - f_{i}(z))^{2}/2\sigma^{2}}$$

 $\Pr_{Z}(z) = 1$

Log likelihood of the dataset

$$\sum_{i=1}^{n} \log \Pr(x_1^{(i)}, x_2^{(i)})$$

Maximize over unknown parameters

(We'll approximate the integral over z by a sum.)

Our job is to invent a probability model, specifying the **distribution** of the response at a given input.

input *x* (e.g. timepoint)



random variable for response Y at input x



What are we really after, when we fit a probability model?

What's a good model? How can we compare models?



dataset of (x_i, y_i) pairs



dataset of (x_i, y_i) pairs



 $Y_i \sim 1.62 + 0.49 x_i$ + Normal(0, 2.39²)



 $Y_i \sim -38.5 + 95.7 x_i - 84.8 x_i^2 + 38.3 x_i^3$ -9.5 $x_i^4 + 1.3 x_i^5 - 0.09 x_i^6 + 0.003 x_i^7$ + Normal(0, 0.31²) Question Which of these two models fits the dataset better?





dataset $\{x_1, \dots, x_n\}$

Model A: IID sample from $X \sim N(0.9, 0.03^2)$

This model is extraordinarily unlikely to generate the dataset, so it's a bad model. log lik (dataset) = -570.5

> Question Which of these two models fits the dataset better?



Model B: IID sample from $X \sim N(0.1, 0.6^2)$ This model might possibly have generated the data (but it's still not great). log lik (dataset) = -28.0





dataset of (x_i, y_i) pairs

 $Y_i \sim 1.62 + 0.49 x_i$ + Normal(0, 2.39²)

 $Y_i \sim -38.5 + 95.7 x_i - 84.8 x_i^2 + 38.3 x_i^3$ -9.5 $x_i^4 + 1.3 x_i^5 - 0.09 x_i^6 + 0.003 x_i^7$ + Normal(0, 0.31²) Question Which of these two models fits the dataset better?



10 ·

У

dataset of (x_i, y_i) pairs







$$\sim -38.5 + 95.7 x_i - 84.8 x_i^2 + 38.3 x_i^3$$

-9.5 $x_i^4 + 1.3 x_i^5 - 0.09 x_i^6 + 0.003 x_i^7$
+ Normal(0, 0.31²)
g lik (dataset) = -379.3

- The goal of modelling is to find models that fit the dataset well
- A good metric for model fit is: likelihood of the dataset, according to the model
- This applies equally to both supervised and generative modelling

In NLP, log likelihood is called "perplexity"

In sports betting, log likelihood is called "ignorance score"



Do You Understand the Variance In Your Data?

by Thomas C. Redman

August 16, 2019





Number of defective pairs of shoes each day



Monthly average temperatures in Cambridge, UK

What's a good model for this dataset?



Climate is stable? $\text{Temp}(t) \sim a + b \sin(2\pi(t + \phi)) + N(0, \sigma^2)$ The extremes are getting worse? Temperatures are increasing? Temperatures are increasing, and the increase is accelerating?

https://www.metoffice.gov.uk/research/climate/maps-and-data/historic-station-data

You've got to have models in your head. And you've got to array your experience – both vicarious and direct – on this latticework of models.

You may have noticed students who just try to remember and pound back what is remembered. Well, they fail in school and in life. You've got to hang experience on a latticework of models in your head.

Charlie Munger, A lesson on elementary, worldly wisdom as it relates to investment management & business.

Example 2.1.1

The Iris dataset has 50 records of iris measurements, from three species.

Petal. Length	Petal. Width	Sepal. Length	Sepal. Width	Species
1.0	0.2	4.6	3.6	setosa
5.0	1.9	6.3	2.5	virginica
5.8	1.6	7.2	3.0	virginica
4.2	1.2	5.7	3.0	versicolor

How does Petal.Length depend on Sepal.Length?



Let's guess that for parameters α , β , γ , σ (to be estimated), Petal.Length ~ $\alpha + \beta$ Sepal.Length + γ (Sepal.Length)² + $N(0, \sigma^2)$



Dataset collected by Edgar Anderson and popularized by Ronald Fisher in 1936

Example 2.1.1

The Iris dataset has 50 records of iris measurements, from three species.

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How does Petal.Length depend on Sepal.Length?



Let's guess that for parameters α , β , γ , σ (to be estimated), Petal.Length ~ $\alpha + \beta$ Sepal.Length + γ (Sepal.Length)² + $N(0, \sigma^2)$



2.1. LINEAR MODELS

Petal.Length $\approx \alpha + \beta$ Sepal.Length + γ (Sepal.Length)²

$$\begin{bmatrix} \mathsf{PL}_{1} \\ \mathsf{PL}_{2} \\ \vdots \\ \mathsf{PL}_{n} \end{bmatrix} \approx \alpha \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} + \beta \begin{bmatrix} \mathsf{SL}_{1} \\ \mathsf{SL}_{2} \\ \vdots \\ \mathsf{SL}_{n} \end{bmatrix} + \gamma \begin{bmatrix} (\mathsf{SL}_{1})^{2} \\ (\mathsf{SL}_{2})^{2} \\ \vdots \\ (\mathsf{SL}_{n})^{2} \end{bmatrix}$$

Models of this form are called *linear models* (because they're based on linear algebra).

They are flexible, and very fast to optimize.

We'll assume Gaussian errors. Thus, maximum likelihood estimation is the same as minimizing squared prediction loss. Linear modelling is also called "least squares model-fitting".



Petal.Length $\approx \alpha + \beta$ Sepal.Length + γ (Sepal.Length)²

$$\begin{bmatrix} \mathsf{PL}_{1} \\ \mathsf{PL}_{2} \\ \vdots \\ \mathsf{PL}_{n} \end{bmatrix} \approx \alpha \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} + \beta \begin{bmatrix} \mathsf{SL}_{1} \\ \mathsf{SL}_{2} \\ \vdots \\ \mathsf{SL}_{n} \end{bmatrix} + \gamma \begin{bmatrix} (\mathsf{SL}_{1})^{2} \\ (\mathsf{SL}_{2})^{2} \\ \vdots \\ (\mathsf{SL}_{n})^{2} \end{bmatrix}$$

iris = pandas.read_csv(...)

Fitting the model

- 2 one, SL, PL = np.ones(len(iris)), iris['Sepal.Length'], iris['Petal.Length']
- 3 model = sklearn.linear_model.LinearRegression(fit_intercept=False)
- 4 model.fit(np.column_stack([one, SL, SL**2]), PL)
- 5 $(\alpha, \beta, \gamma) = model.coef_$

Making predictions / getting fitted values from the model

- 6 newSL = np.linspace(4.2, 8.2, 20)
- 7 predPL = model.predict(np.column_stack([one, newSL, newSL**2]))

Feature design

How do we design features, so that linear models answer the questions we want answered?

ONE-HOT CODING



setosa

versicolor

virginica

e.g. first row is setosa, and linear model says $PL_1 \approx \alpha_{seto} + \beta_{seto} SL_1$ Isperios - schoo × SL -species = setosa Linear model form (linear combination of features, weighted by parameters) seto PL1 virg PL₂ virg PL_3 $+\beta_{\rm virg}$ $+\beta_{seto}$ $+\alpha_{\rm virg}$ $\approx \alpha_{seto}'$ $+\beta_{vers}$ $+\alpha_{vers}$ seto PL. vers species, SL = iris['Species'], iris['Sepal.Length'] 2 PL = iris['Petal.Length'] species_levels = ['setosa', 'versicolor', 'virginica'] 4 i1,i2,i3 = [np.where_species==k,1,2,4] for k in species_levels] 5 X = np.column_stack [[i1] i2, i3, [i1*SL, i2*SL, i3*SL]) 6 model = sklearn.linear_model.LinearRegression(fit_intercept=False) 7 model.fit(X, PL)

NON-LINEAR RESPONSE





 $\alpha + \beta$ Sepal.Length + γ (Sepal.Length)²

NON-LINEAR RESPONSE via one-hot coding



$$PL \approx \alpha_4 \mathbf{1}_{SL < 4} + \alpha_5 \mathbf{1}_{[SL]=5} + \alpha_6 \mathbf{1}_{[SL]=6} + \alpha_7 \mathbf{1}_{SL \ge 7}$$

e.g. for an observation with SL=5.3, we predict PL $pprox lpha_5$

e.g. for an observation with SL=3.1, we predict PL $\approx \alpha_4$

COMPARING GROUPS



Measurements for condition A: $a = [a_1, a_2, ..., a_m]$ Measurements for condition $B: \mathbf{b} = [\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_n]$ Can we use a linear model to compare A and B? $x \approx \alpha_A 1_{\text{and}=A} + \alpha_B 1_{\text{cond}=B}$ x x x + B 1 cond=B for an indiv. of type A: $x \propto \alpha$ for an indiv. of type B: $x = \alpha + \beta$



MODEL DIAGNOSIS

After we fit a model, how do we learn if it's a good fit?

- 1. Evaluate its log likelihood
- 2. Hypothesis testing [next week]
- 3. Eyeball it!

Find the prediction error for each datapoint, and plot it every way we can think of Find the log likelihood of each datapoint, and showcase some datapoints with very low or very high likelihood If we hadn't thought to include climate change in our temperature model ...



This suggests a revised model ...

$$temp = \alpha' + \beta' \sin(2\pi(t + \phi)) + \gamma t + \epsilon$$

Q. Should we just keep adding more and more features to our model?

A. No. If we did, we'd overfit.

