Lecture Three
Supervised Learning: Classification

KMA Solaiman
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Adapted From
Chris Re′
Stanford ML

Supervised Learning and Classification

- Linear Regression via a Probabilistic Interpretation
- Logistic Regression
- Optimization Method: Newton's Method

> We'll learn the maximum likelihood method (a probabilistic interpretation) to generalize from linear regression to more sophisticated models.

A Justification for Least Squares?

- **Given** a training set $\{(x^{(i)}, y^{(i)})$ for $i = 1, \dots, n\}$ in which $x^{(i)} \in \mathbb{R}^{d+1}$ and $y^{(i)} \in \mathbb{R}$.
- **Do** find $\theta \in \mathbb{R}^{d+1}$ s.t. $\theta = \operatorname{argmin}_\theta \sum_{i=1}^{n} (h_\theta(x^{(i)}) - y^{(i)})^2$ in which $h_\theta(x) = \theta^T x$.

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Where did this model come from?

One way to view is via a *probabilistic interpretation (helpful throughout the course)*.

A Justification for Least Squares?

We make an assumption (common in statistics) that the data are *generated* according to some model (that may contain random choices). That is,

$$y^{(i)} = \theta^T x^{(i)} + \varepsilon^{(i)}.$$

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Please keep in mind: this is just a model! As they say, all models are wrong but some models are *useful.* This model has been *shockingly* useful.

What do we expect of the noise?

What properties should we expect from $\varepsilon^{(i)}$

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Again, it's a model and $\varepsilon^{(i)}$ is a random variable:

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- The errors for different points are *independent* and *identically distributed* (called, **iid**)

$$\mathbb{E}[\varepsilon^{(i)}\varepsilon^{(j)}] = \mathbb{E}[\varepsilon^{(i)}]\mathbb{E}[\varepsilon^{(j)}] \text{ for } i \neq j.$$

and

$$\mathbb{E}\left[\left(\varepsilon^{(i)}\right)^2\right] = \sigma^2$$

Here σ^2 is some measure of *how noisy* the data are.

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Here σ^2 is some measure of *how noisy* the data are. Turns out, this effectively defines the *Gaussian or Normal distribution.*

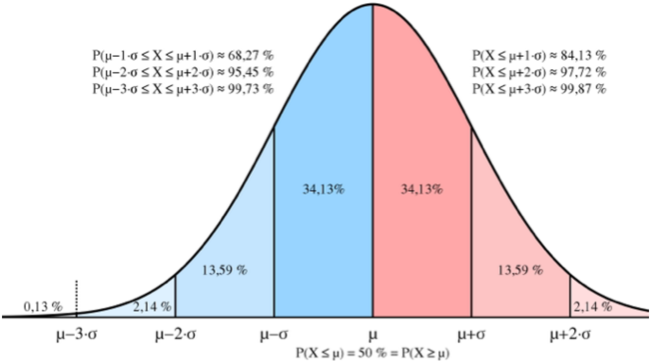
Notation for the Gaussian

We write $z \sim \mathcal{N}(\mu, \sigma^2)$ and read these symbols as

> *z is distributed as a normal with mean μ and standard deviation σ^2.*

or equivalently the probability density function -

$$P(z) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(z-\mu)^2}{2\sigma^2}\right\} \quad \text{.............} \; (10.1)$$



Notation for Guassians **in our Problem**

Recall in our model,

$$y^{(i)} = \theta^T x^{(i)} + \varepsilon^{(i)} \text{ in which } \varepsilon^{(i)} \sim \mathcal{N}(0, \sigma^2) \text{ .... } (11.1)$$

or more compactly notation:

$$y^{(i)} \mid x^{(i)}; \theta \sim \mathcal{N}(\theta^T x, \sigma^2) \text{.............. } (11.2)$$

equivalently, **Probability distribution** over $y^{(i)}$, given $x^{(i)}$ and parameterized by θ

$$P\left(y^{(i)} \mid x^{(i)}; \theta\right) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(y^{(i)} - x^{(i)}\theta)^2}{2\sigma^2}\right\} \text{ ...... } (11.3)$$

- We **condition** on $x^{(i)}$.
- In contrast, θ **parameterizes** or "picks" a distribution.

We use bar (|) versus semicolon (;) notation above.

How did we calculate Probability Distribution of $y^{(i)}$ in 11.3?

Using our $error\ term$ in place of z, we get

$$\frac{1}{\sigma\sqrt{2\pi}} exp\left\{-\frac{\left(\varepsilon^{(i)}\ - 0\right)^2}{2\sigma^2}\right\}$$

Now if we replace this with values from 11.1, we get

$$\frac{1}{\sigma\sqrt{2\pi}} exp\left\{-\frac{\left(y^{(i)}\ - x^{(i)}\theta\right)^2}{2\sigma^2}\right\}$$

This term gives us the probability distribution over $y^{(i)}$, but we must add $x^{(i)}$ as a given, since we will see it as input, so by fiat we consider this as, $P(y^{(i)}|x^{(i)};\theta)$ which is not conditioned on θ, as it isn't Random Variable

(Log) Likelihoods!

Intuition: among many distributions, pick the one that agrees with the data the most (is most "likely").

$$L(\theta) = p(y|X;\theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)};\theta) \qquad \text{iid assumption}$$

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For convenience, we use the *Log Likelihood* $\ell(\theta) = \log L(\theta)$.

$$\ell(\theta) = \sum_{i=1}^{n} \log \frac{1}{\sigma\sqrt{2\pi}} - \frac{(x^{(i)}\theta - y^{(i)})^2}{2\sigma^2}$$

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$$= n \log \frac{1}{\sigma\sqrt{2\pi}} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (x^{(i)}\theta - y^{(i)})^2 = C(\sigma, n) - \frac{1}{\sigma^2} J(\theta)$$

where $C(\sigma, n) = n \log \frac{1}{\sigma\sqrt{2\pi}}$.

(Log) Likelihoods!

So we've shown that finding a θ to maximize $L(\theta)$ is the same as *maximizing*

$$\ell(\theta) = C(\sigma, n) - \frac{1}{\sigma^2} J(\theta)$$

Or minimizing, $J(\theta)$ directly (why?)

Takeaway: "Under the hood," solving least squares *is* solving a maximum likelihood problem for a particular probabilistic model.

This view shows a path to generalize to new situations!

Summary of Least Squares

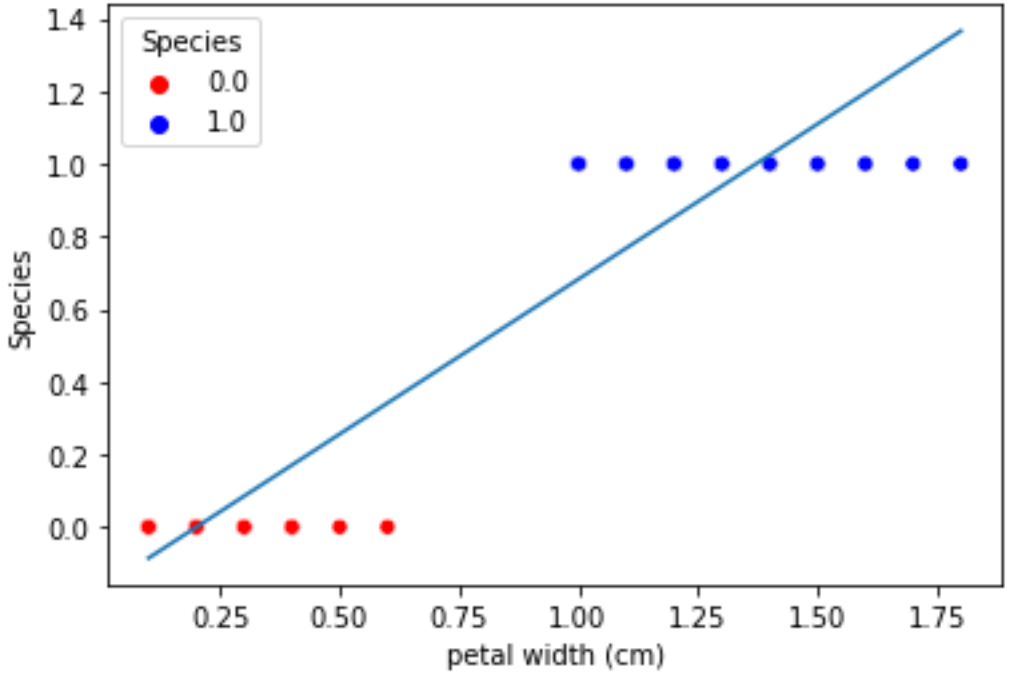
- We introduced the Maximum Likelihood framework–super powerful (next lectures)
- We showed that least squares was actually a version of maximum likelihoods.
- We learned some notation that will help us later in the course. . .

Classification

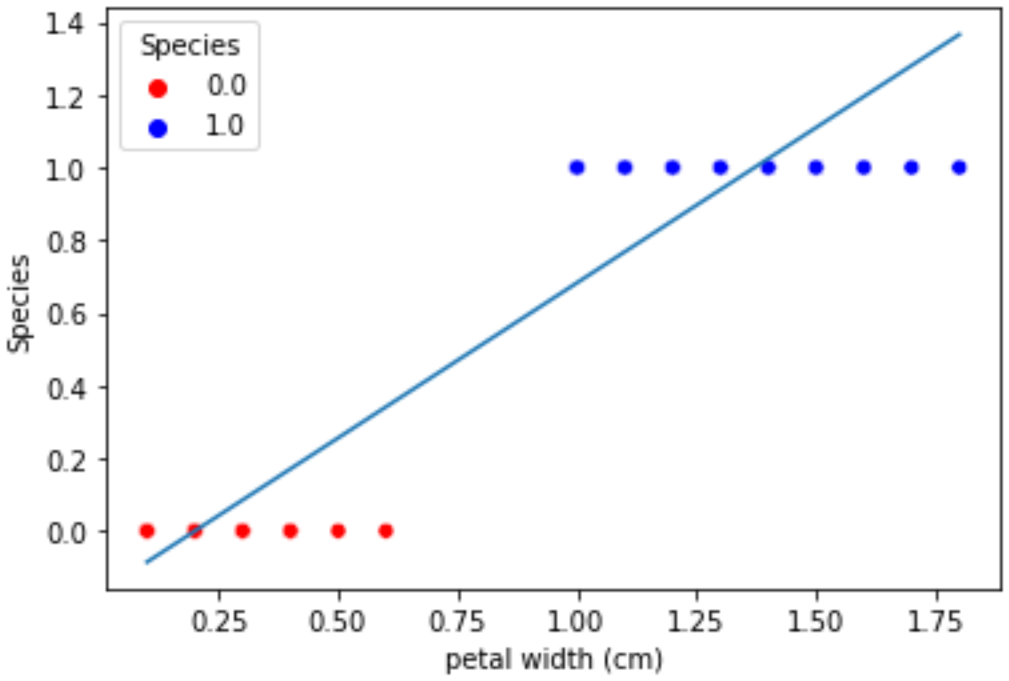
Given a training set $\{(x^{(i)}, y^{(i)})$ for $i = 1, \ldots, n\}$ let $y^{(i)} \in \{0, 1\}$.
Why not use regression, say least squares? A picture ...

	petal width (cm)	Species
0	0.2	0.0
1	0.2	0.0
2	0.2	0.0
3	0.2	0.0
4	0.2	0.0
...	...	...
95	1.2	1.0
96	1.3	1.0
97	1.3	1.0
98	1.1	1.0
99	1.3	1.0

Iris Flower Dataset



Graph of Iris Dataset with linear regression



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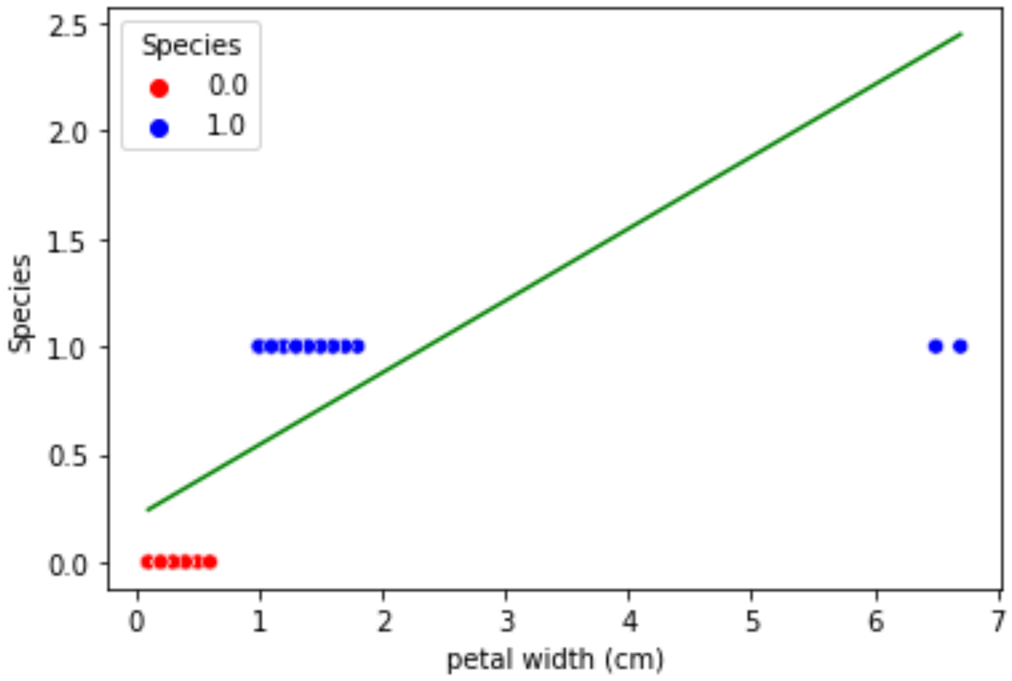
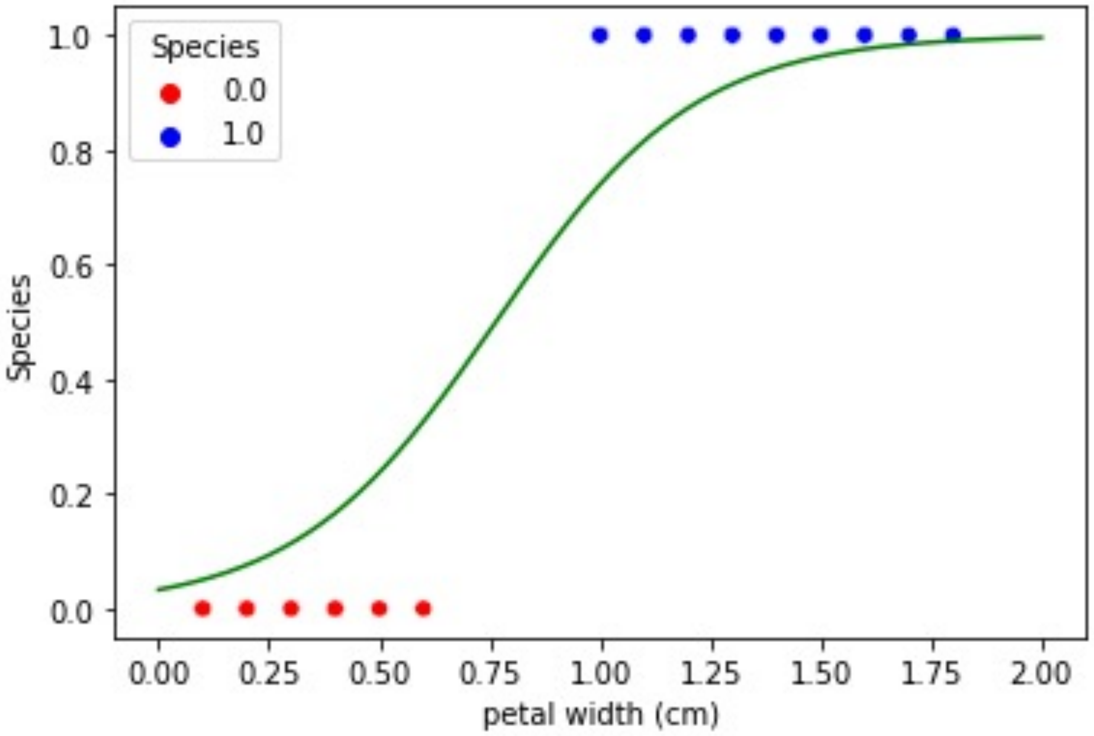


Graph of Iris Dataset(with outliers) with linear regression



Graph of Iris Dataset with logistic regression

Logistic Regression: Link Functions

Given a training set $\{(x^{(i)}, y^{(i)}) \text{ for } i = 1, \ldots, n\}$ let $y^{(i)} \in \{0, 1\}$. Want $h_\theta(x) \in [0, 1]$. Let's pick a smooth function:

$$h_\theta(x) = g(\theta^T x)$$

Here, g is a link function. There are *many*...

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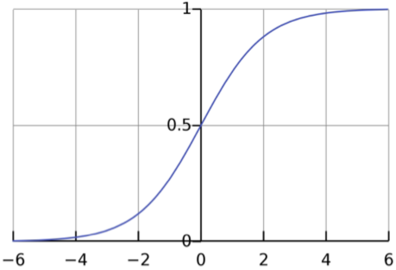
$$g(z) = \frac{1}{1 + e^{-z}}.$$



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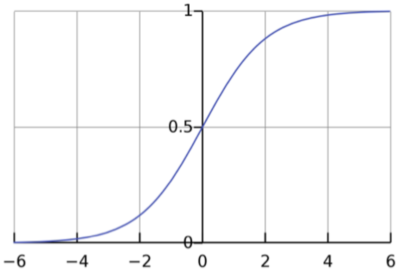
SIGMOID



How do we interpret $h_\theta(x)$?

$$P(y = 1 \mid x; \theta) = h_\theta(x)$$
$$P(y = 0 \mid x; \theta) = 1 - h_\theta(x)$$

Logistic Regression: Link Functions

Let's write the Likelihood function. Recall:

$$P(y = 1 \mid x; \theta) = h_\theta(x)$$
$$P(y = 0 \mid x; \theta) = 1 - h_\theta(x)$$

Then,

$$L(\theta) = P(y \mid X; \theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta)$$

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How do we go to a cost function from P (y I X; θ) ?

We need to go back to Maximum Likelihood Estimation that we saw before at the beginning of this lecture.

Logistic Regression: Link Functions

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$$

Taking logs to compute the log likelihood $\ell(\theta)$ we have:

$$
\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))
$$

Now to solve it...

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

We maximize for θ but we already saw how to do this! Just compute derivative, run (S)GD and you're done with it!

Takeaway: This is *another* example of the max likelihood method: we setup the likelihood, take logs, and compute derivatives.

Time Permitting: There is magic in the derivative...

Even more, the batch update can be written in a *remarkably familiar* form:

$$\theta^{(t+1)} = \theta^{(t)} + \sum_{j \in B} (y^{(j)} - h_\theta(x^{(j)}))x^{(j)}.$$

We sketch why (you can check!) We drop superscripts to simplify notation and examine a single data point:

$$\begin{aligned} & y \log h_\theta(x) + (1-y)\log(1-h_\theta(x)) \\ = & -y\log(1+e^{-\theta^T x}) + (1-y)(-\theta^T x) - (1-y)\log(1+e^{-\theta^T x}) \\ = & -\log(1+e^{-\theta^T x}) - (1-y)(\theta^T x) \end{aligned}$$

We used $1 - h_\theta(x) = \frac{e^{-\theta^T x}}{1-e^{-\theta^T x}}$. We now compute the derivative of this expression wrt θ and get:

$$\frac{e^{-\theta^T x}}{1+e^{-\theta^T x}} x - (1-y)x = (y - h_\theta(x))x$$

Perceptron Learning Algorithm

- Modify link function to output either 0 or 1.
- Make g to be a threshold function
- Then use same $h_\theta(x) = g(\theta^T x)$ using this g
- Follow the same update rule for θ

$$g(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

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- We developed logistic regression from this principle.
  - Logistic regression is *widely* used today.
- We noticed a familiar pattern: take derivatives of the likelihood, and the derivatives had this (hopefully) intuitive *"misprediction form"*

Newton's Method

Given $f : \mathbb{R}^d \to \mathbb{R}$ find x s.t. $f(x) = 0$.

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We apply this with $f(\theta) = \nabla_\theta \ell(\theta)$, the likelihood function

Newton's Method (Drawn in Class)

Given $f : \mathbb{R}^d \to \mathbb{R}$ find x s.t. $f(x) = 0$.

Newton's Method Summary

Given $f : \mathbb{R}^d \to \mathbb{R}$ find x s.t. $f(x) = 0$.

- This is the update rule in 1d

$$x^{(t+1)} = x^{(t)} - \frac{f(x^{(t)})}{f'(x^{(t)})}$$

- It may converge *very* fast (quadratic local convergence!)
- For the likelihood, i.e., $f(\theta) = \nabla_\theta \ell(\theta)$ we need to generalize to a vector-valued function which has:

$$\theta^{(t+1)} = \theta^{(t)} - \left(H(\theta^{(t)})\right)^{-1} \nabla_\theta \ell(\theta^{(t)}).$$

in which $H_{i,j}(\theta) = \frac{\partial}{\partial\theta_i \partial\theta_j} \ell(\theta)$.

Optimization Method Summary

Method	Compute per Step	Number of Steps to convergence
SGD	$\theta(d)$	$\approx \epsilon^{-2}$
Minibatch SGD		
GD	$\theta(nd)$	$\approx \epsilon^{-1}$
Newton	$\Omega(nd^2)$	$\approx \log(1/\epsilon)$

- In classical stats, d is small (< 100), n is often small, and *exact parameters matter*
- In modern ML, d is huge (billions, trillions), n is huge (trillions), and parameters used *only* for prediction
  - These are approximate number of computing steps
  - Convergence happens when loss settles to within an error range around the final value.
  - Newton would be very fast, where SGD needs a lot of step, but individual steps are fast, makes up for it
- As a result, (minibatch) SGD is the *workhorse* of ML.

Classification Lecture Summary

- We saw the differences between classification and regression.
- We learned about a principle for probabilistic interpretation for linear regression and classification: **Maximum Likelihood**.
  - We used this to derive logistic regression.
  - The Maximum Likelihood principle will be used again next lecture (and in the future)
- We saw Newton's method, which is classically used models (more statistics than ML–it's not used in most modern ML)