Deep Learning for Data Science
DS 542

Lecture 05
Loss Functions

Slides originally by Thomas Gardos.
Images from Understanding Deep Learning unless otherwise cited.

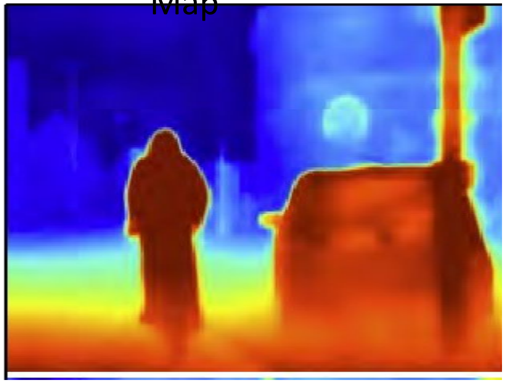
Recap

- So far, we talked about *linear regression*, *shallow neural networks* and *deep neural networks*
- Each have parameters, ϕ, that we want to choose for a *best possible mapping between input and output* training data
- A *loss function* or *cost function*, $L[\phi]$, returns a single number that describes a mismatch between $f[x_i, \phi]$and the ground truth outputs, y_i.

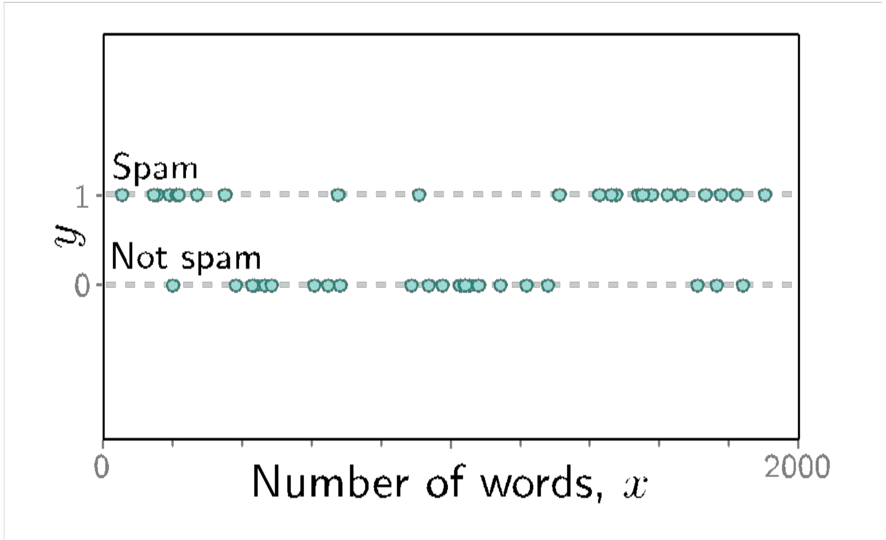
We need to find a loss function that works with…

Univariate and Multivariate Regression

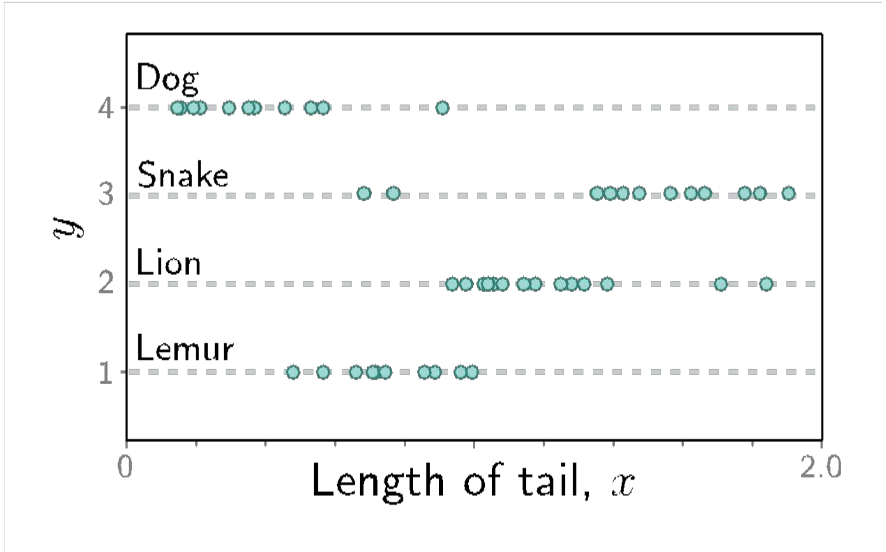
Depth Map



Binary Classification



Multiclass Classification



But First, A Digression…

- The book gives a unique, theoretically grounded approach to picking loss functions.
- Will defer that five minutes to talk about an example from my industry experience.

A long time ago in an internet far, far away…

Circa 2005

- Advertisers were starting to move beyond banner ads to monetize the Internet

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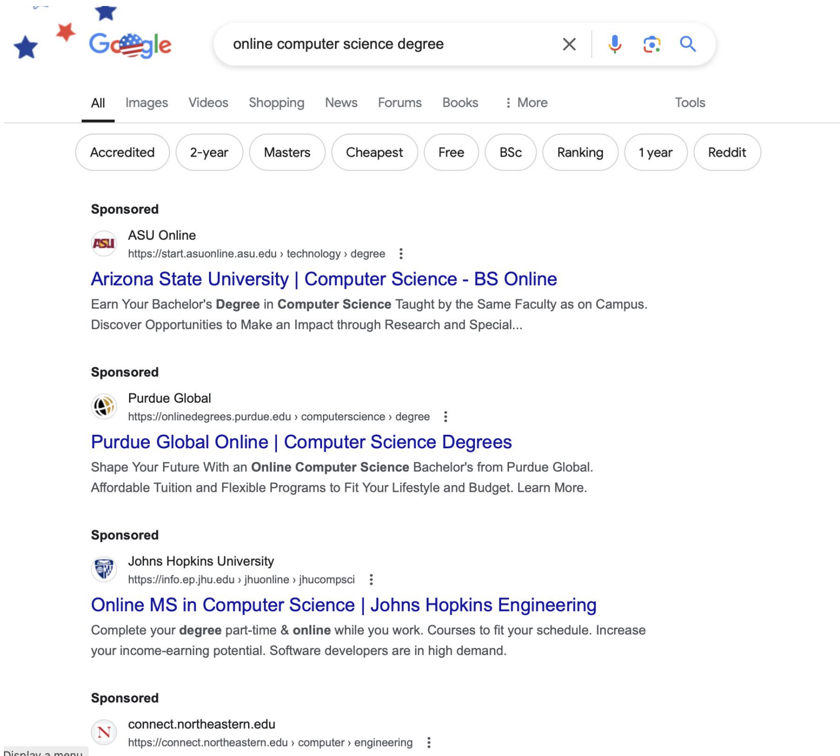
    - Not this many yet
    - Unknown dynamics
      (if you did not work at Yahoo or Google)



Circa 2005

- Advertisers were starting to move beyond banner ads to monetize the Internet
- Search engines just starting to sell ads
  - Not this many yet
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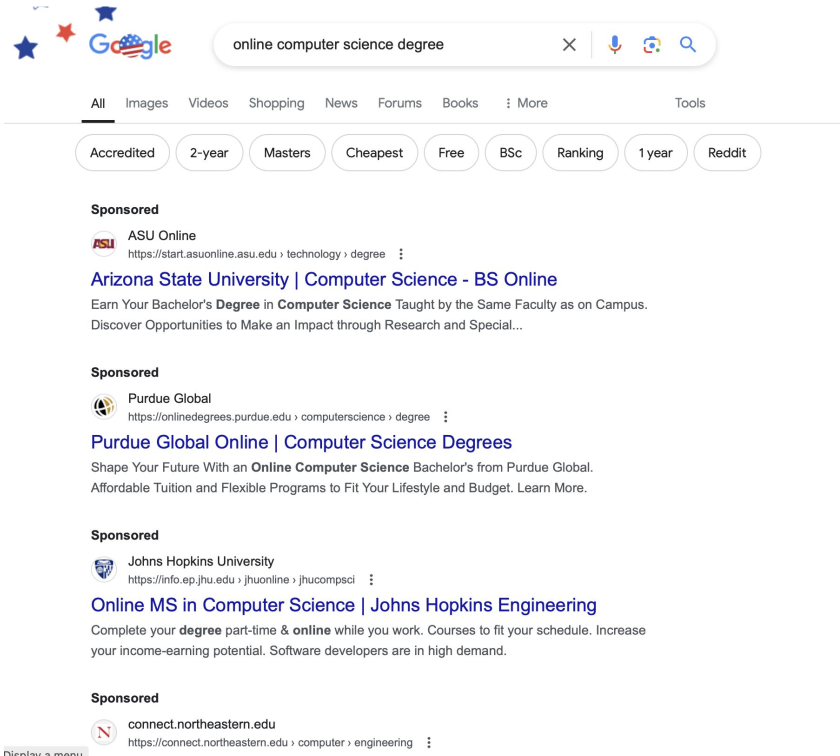
    (if you did not work at Yahoo or Google)
- Big questions
  - How to advertise effectively here?
  - What keywords to advertise on?
  - How much to bid?



My Past Life as a Research Scientist at a Tech Startup

My original task:

- Figure out how Google models ad click rates
    - Google originally sorted ads purely on expected cost per impression.
    - They said they have a model for ad click rates even with sparse data.
    - Slightly simplified sort:
        - (our bid) * (estimated ad click rate)
    - We were running a long tailed keyword campaign so ~everything controlled by their model.

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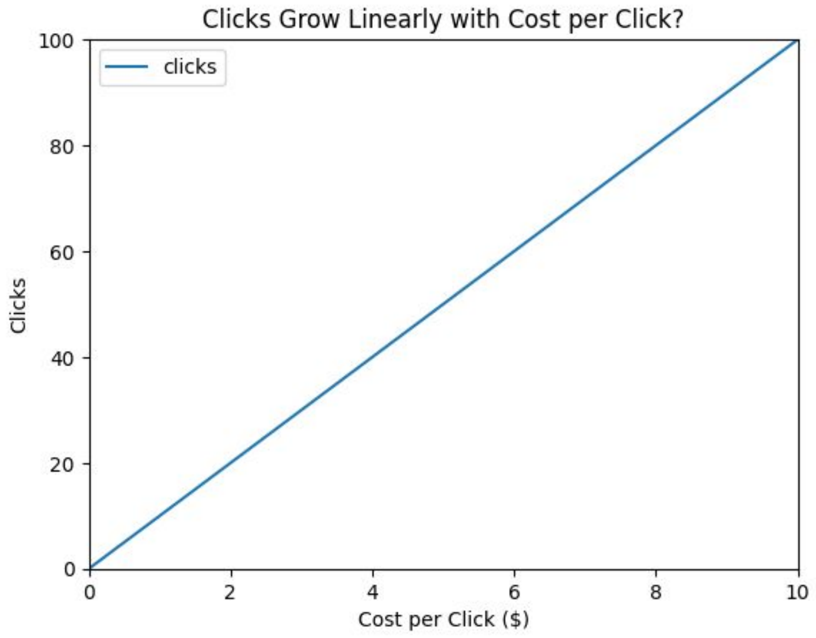
  - ~~Slightly simplified sort:~~
    - ~~our bid * estimated ad click rate~~
  - ~~We were running a long tailed keyword campaign so ~everything controlled by their model.~~
- Predict our expect revenue if someone clicks on a particular keyword
  - Use this to control our bidding.
  - We started with simple strategies like “bid 50% of our expected revenue”
  - BTW we have 100K keywords, only 1K have clicks

The Linear Traffic Curve Model (RIP 2009)

One of my coworkers observed the following…

- The clicks that we get on our ads are surprisingly linear in our cost per click.



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  - Clicks $\propto$ cost per click
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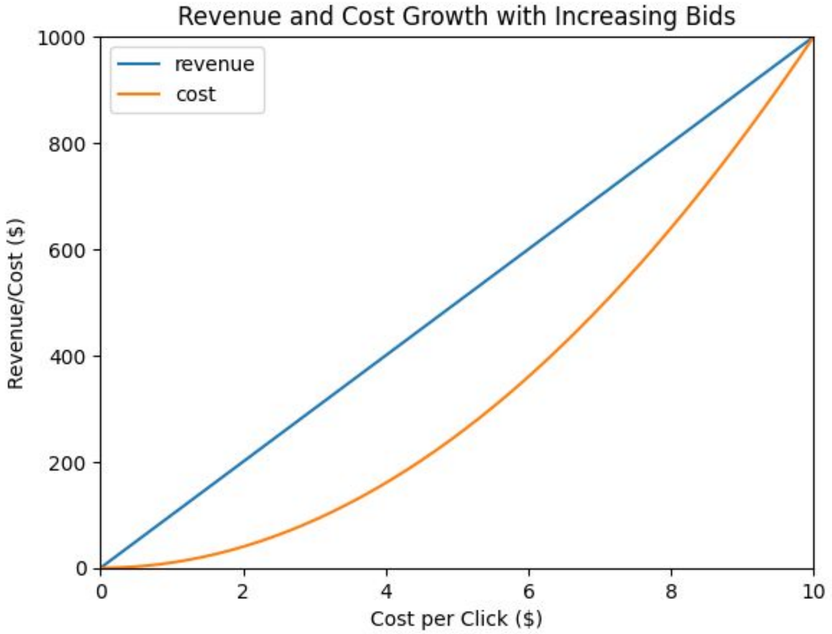
  - Cost $\propto$ (cost per click)^2



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  - Clicks ∝ cost per click
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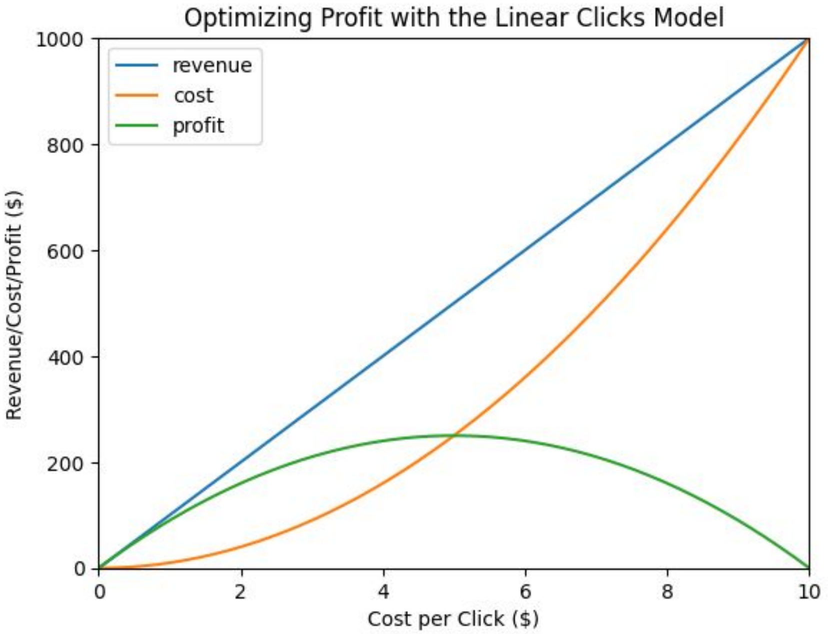
- We can solve for max profit!
  - Simple analytical solution
  - Bid up to 50% margins
  - So (cost per click) = ½ (revenue per click)



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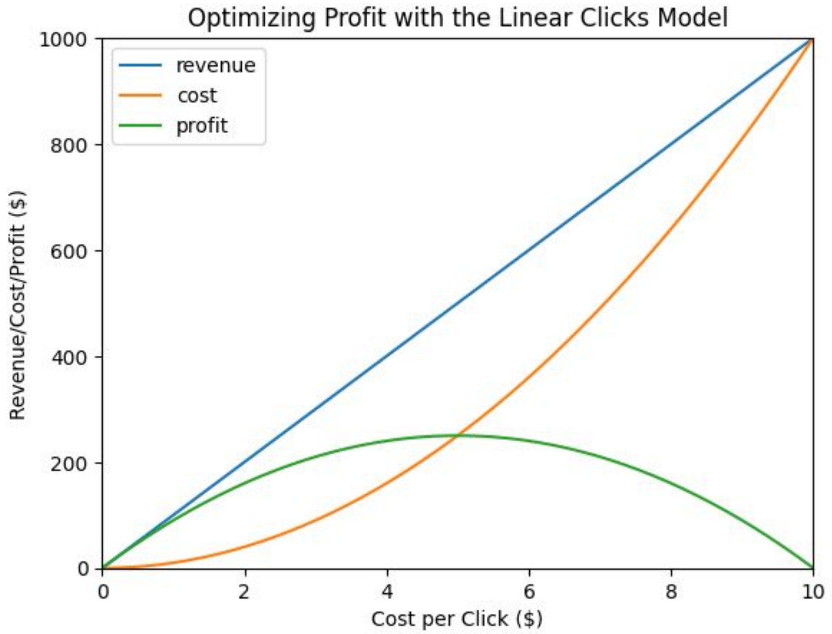
  - Profit drops quadratically from optimal point.



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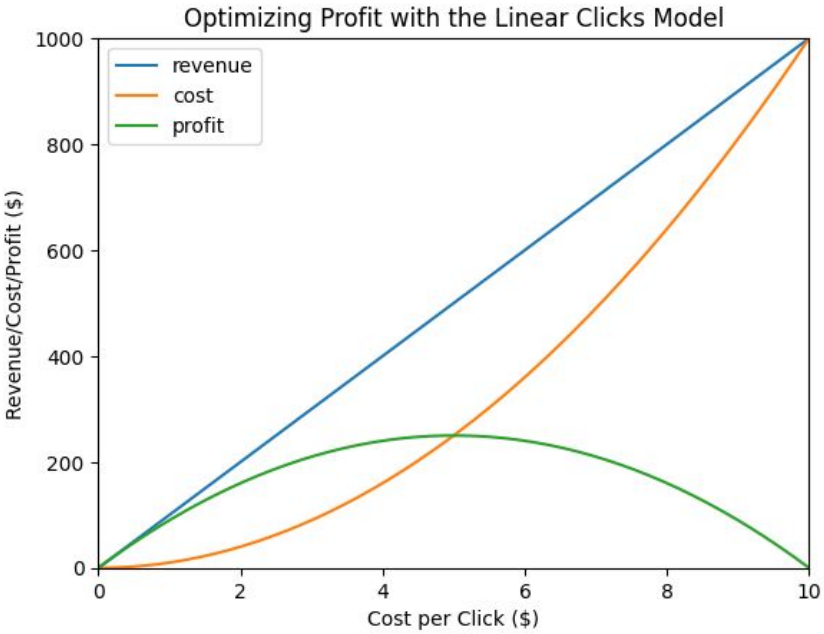
  - This is an L_2 loss!



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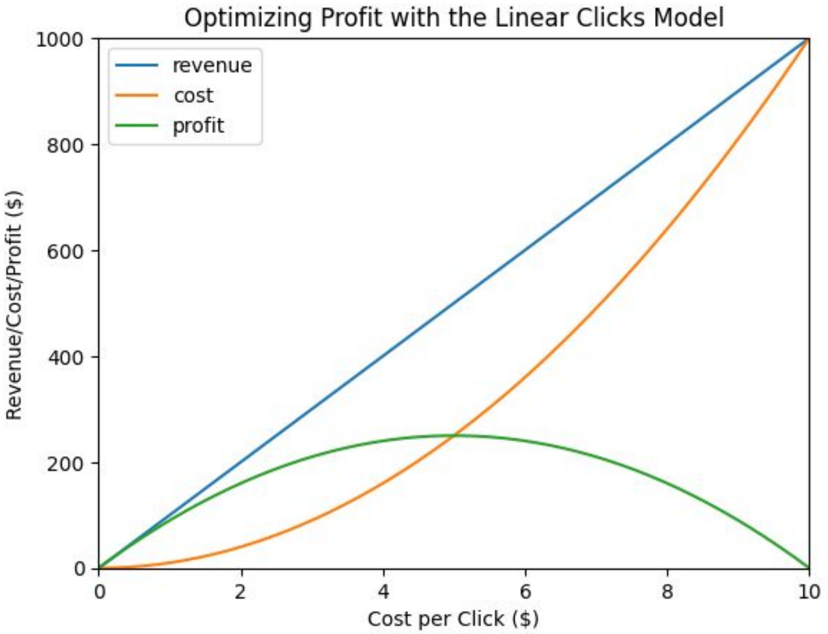
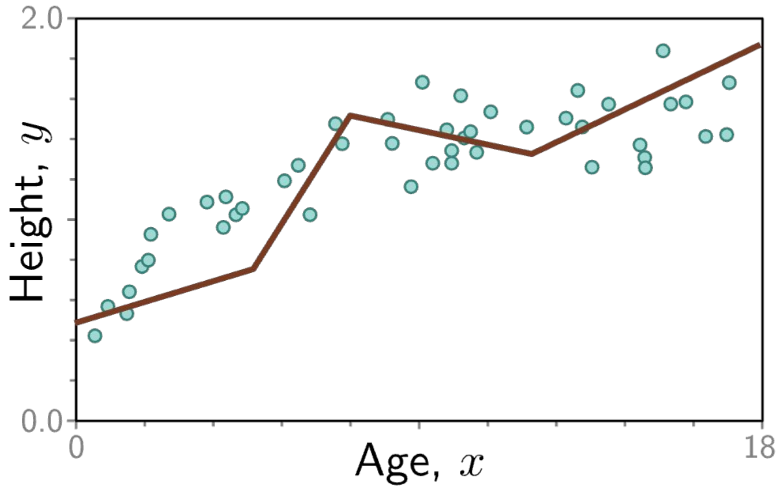
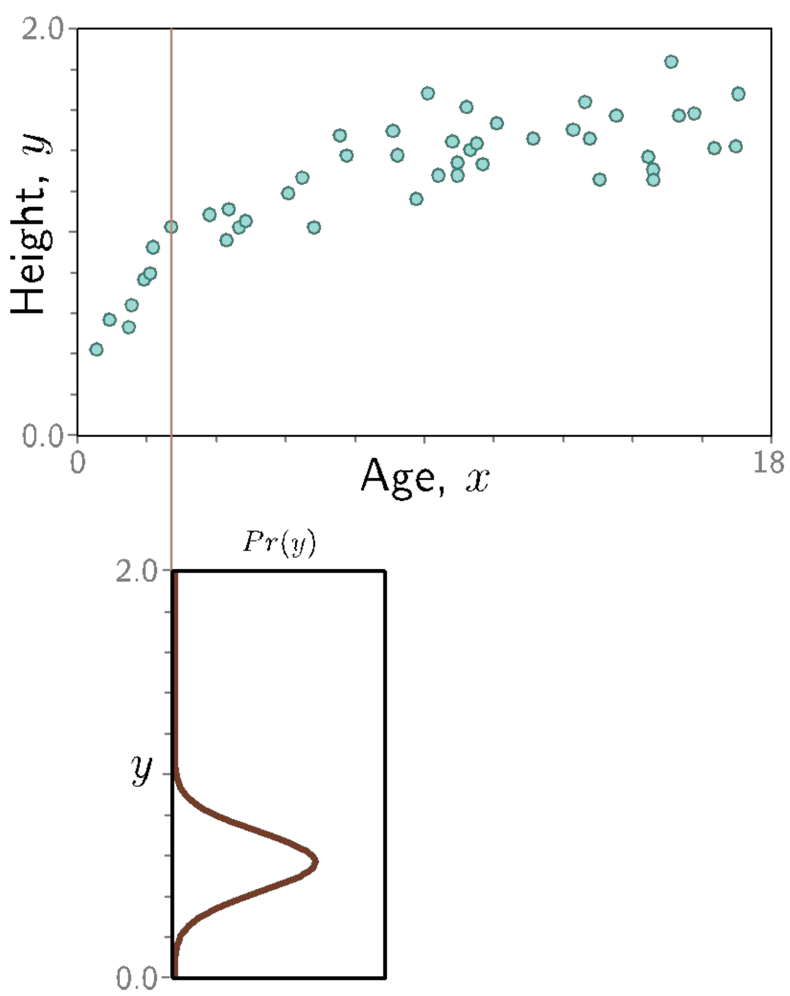
  - So (cost per click) = ½ (revenue per click)
- If we bid differently,
  - Profit drops quadratically from optimal point.
  - This is an L_2 loss!
- In practice, we bid to 40% margins.
  - 96% of optimal profit
  - 20% more data (improve per-keyword bids)



Returning to the modern day…



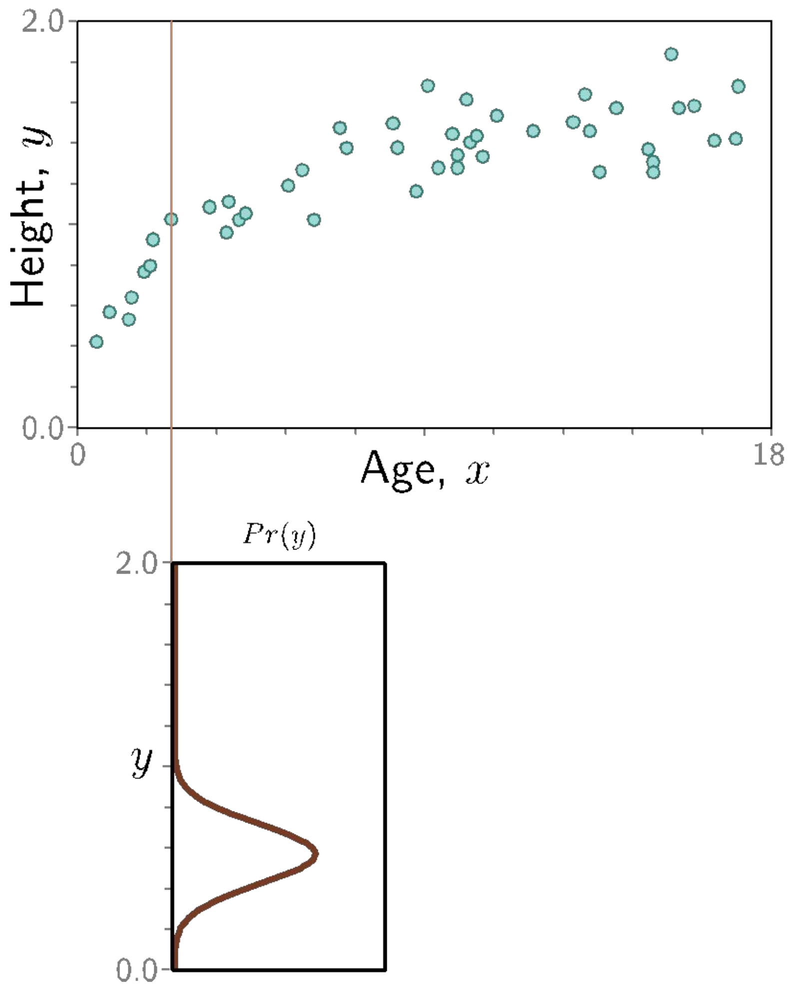
So far, we thought about fitting a model to the data…



Alternatively, we can think about fitting a *probability model* to the data.

$$\Pr(y|x)$$

Why?



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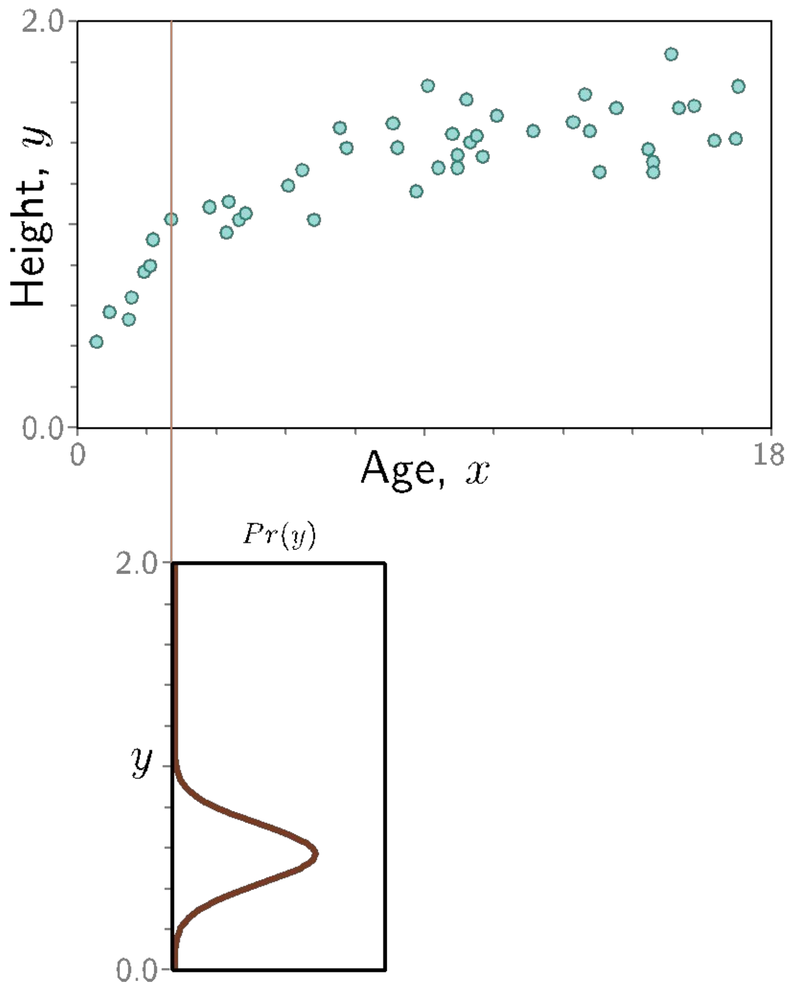
Why?

Because this provides a *framework* to build loss functions for other prediction types…



Alternatively, we can think about fitting a *probability model* to the data.

$$\Pr(y|x)$$

Why?

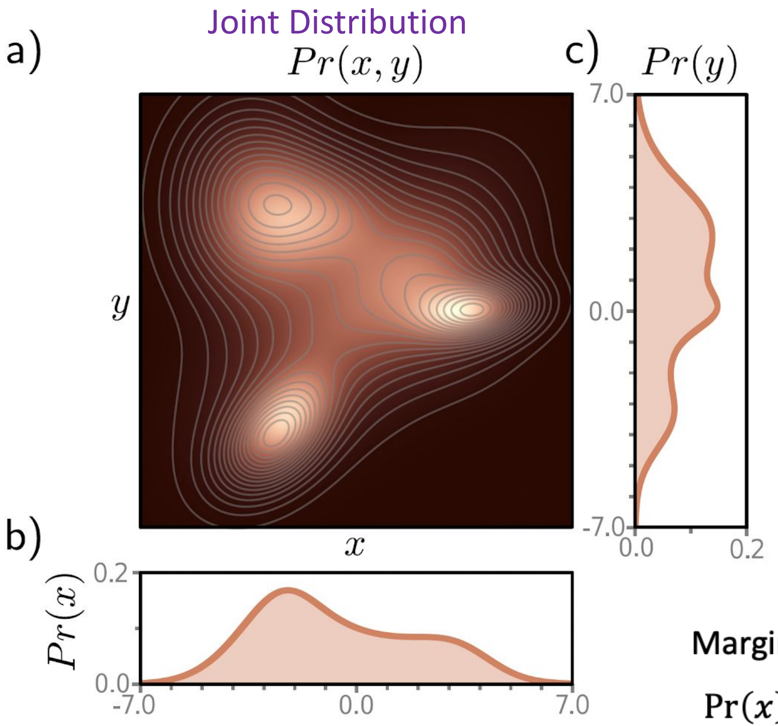
Because this provides a *framework* to build loss functions for other prediction types…

… and justifies least squares for real-valued regression models.

Brief Probability Review

- Random variables, e.g. x and y
- $\Pr(x)$ is a probability distribution over x
- $0 \leq \Pr(x) \leq 1$
- $\int_x \Pr(x)\,dx = 1$ or $\sum_i \Pr(x_i) = 1$
- $\Pr(x, y) = \Pr(x) \cdot \Pr(y)$ when x and y are independent
- $\Pr(x \mid y)\Pr(y) = \Pr(x, y) = \Pr(y \mid x)\Pr(x)$
- And…

Joint and Marginal Probability Distributions



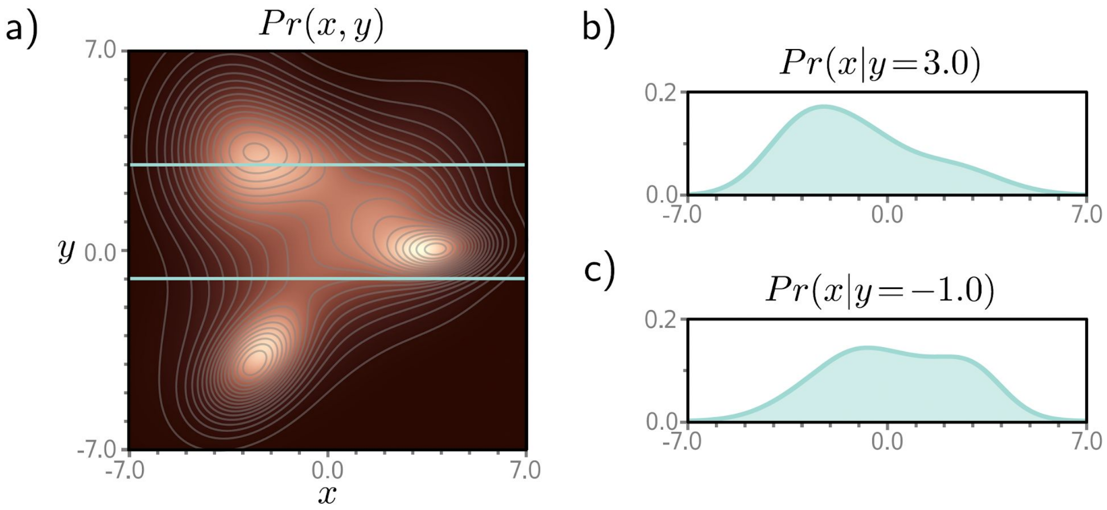
Marginal distribution

$$\Pr(y) = \int_x \Pr(x,y)\,dx$$

Marginal distribution

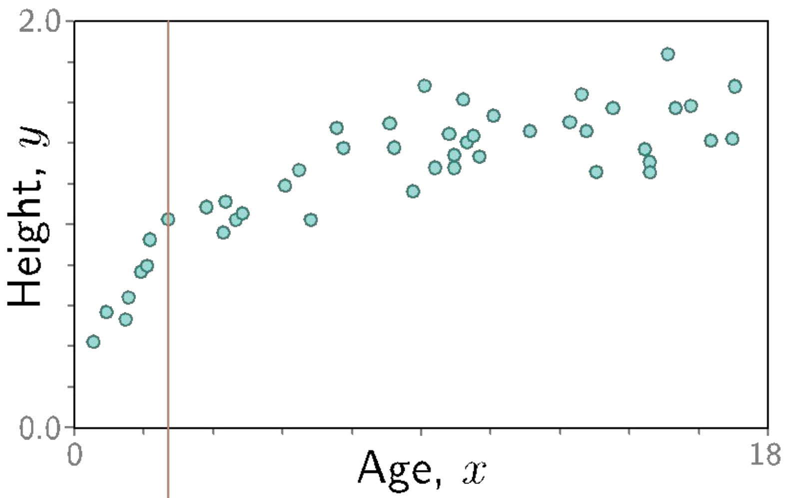
$$\Pr(x) = \int_y \Pr(x,y)\,dy$$

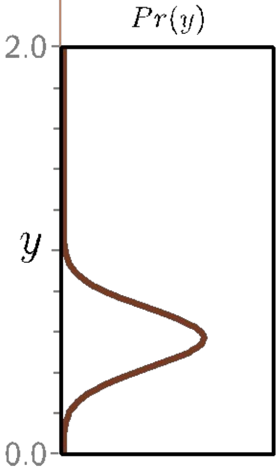
Conditional Probabilities



$$\int_x \Pr(x \mid y = 3.0)\, dx = 1$$

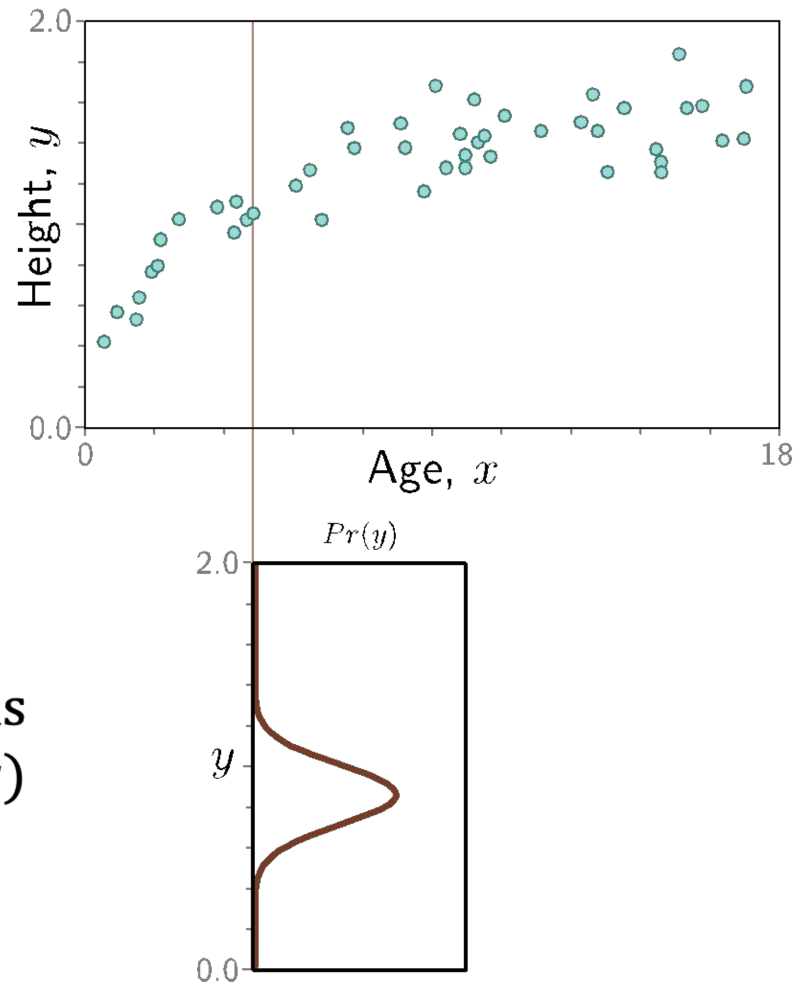
$$\int_x \Pr(x \mid y = -1.0)\, dx = 1$$

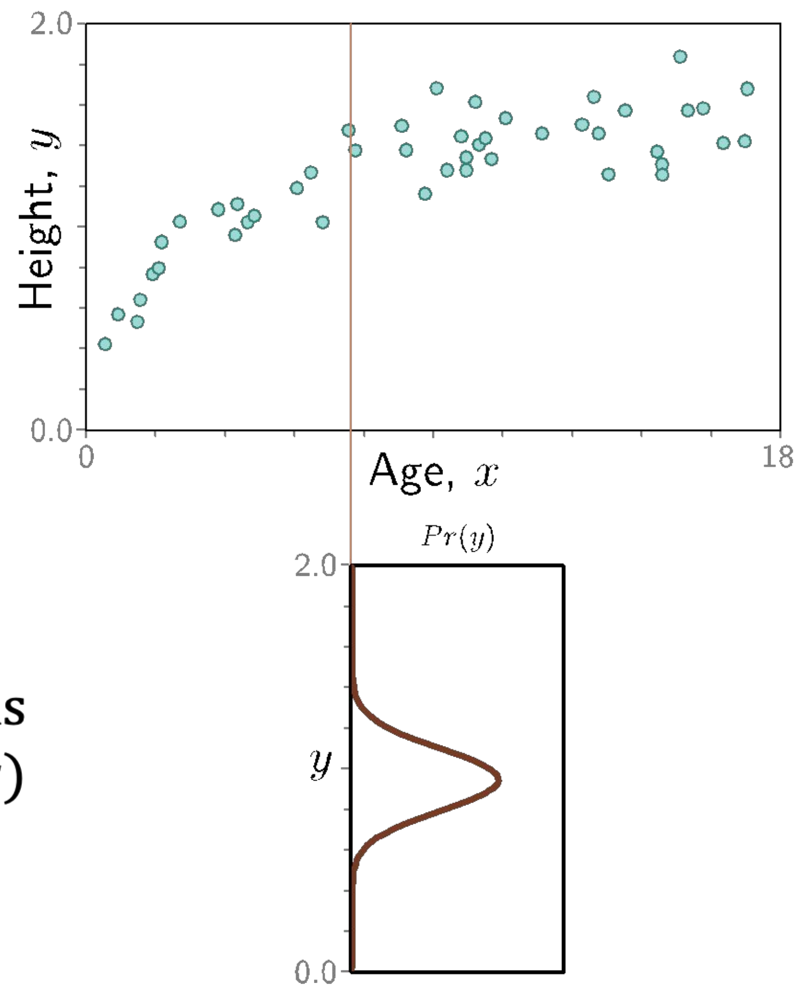




Continuous
$Pr(y|x)$

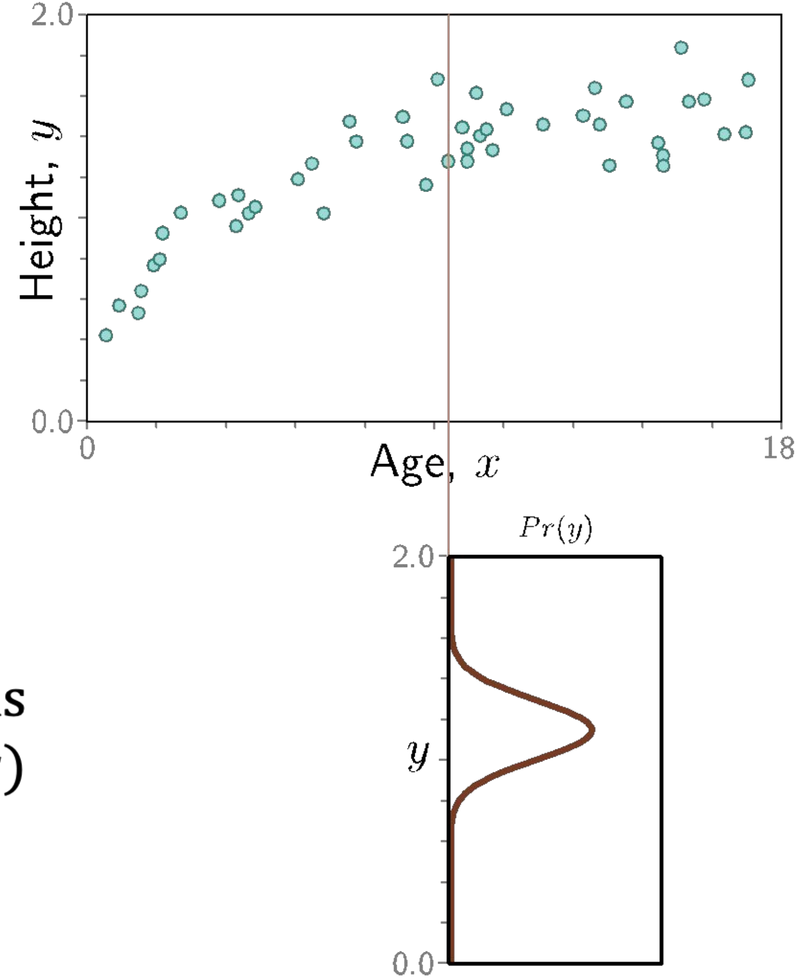
Continuous
$\Pr(y|x)$

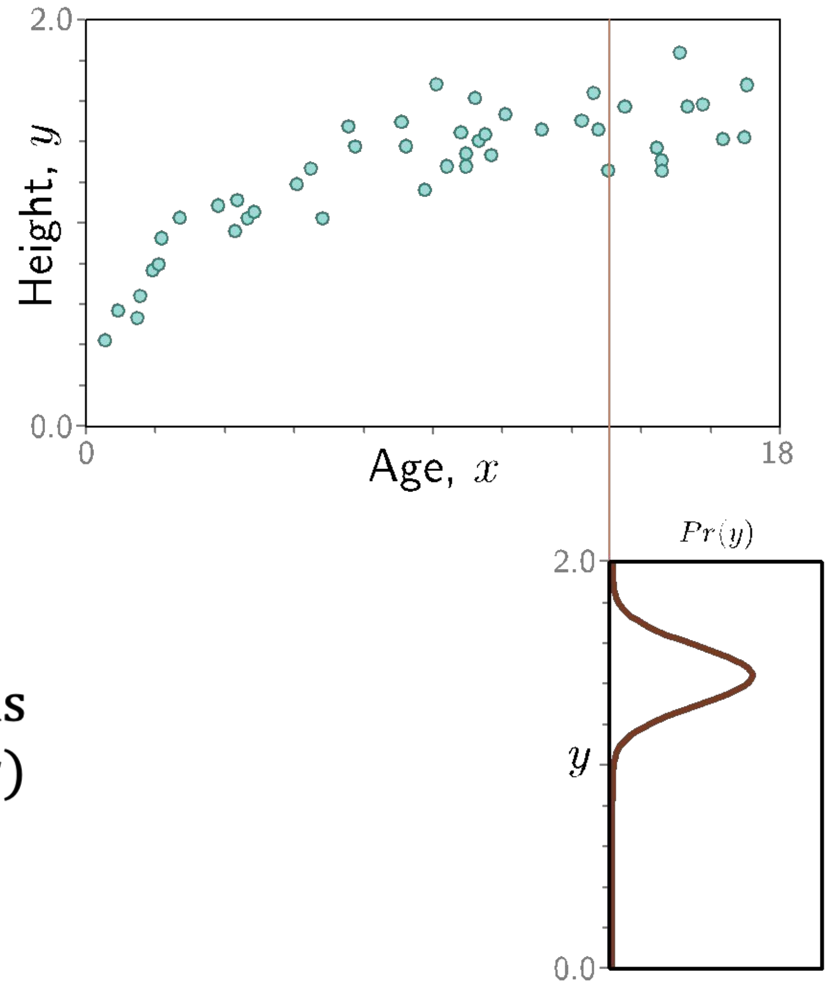




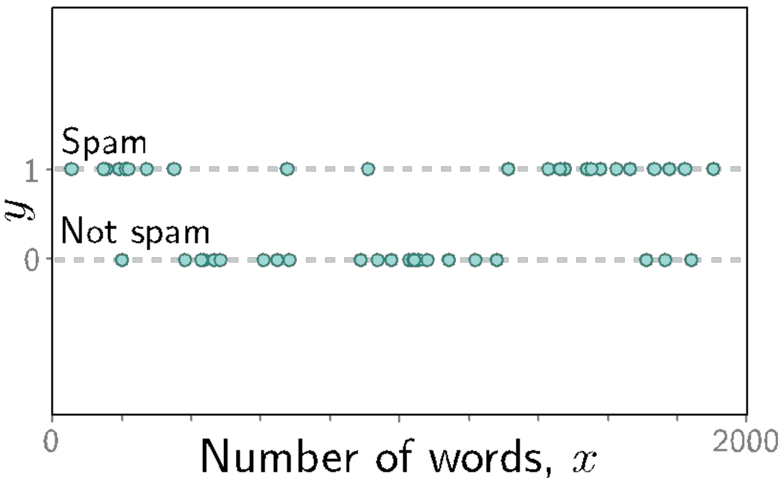
Continuous
$\Pr(y|x)$

Continuous
Pr($y|x$)

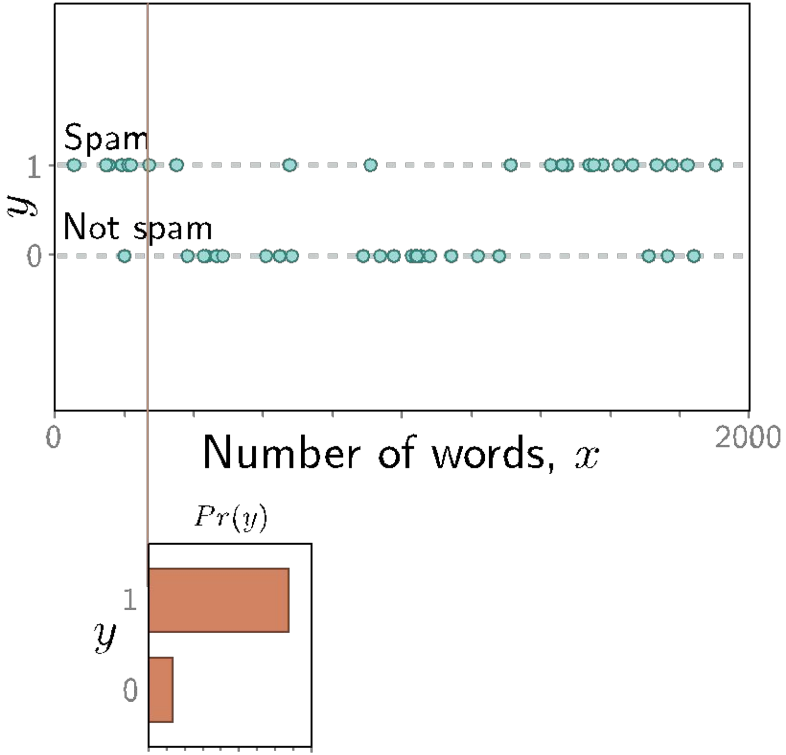




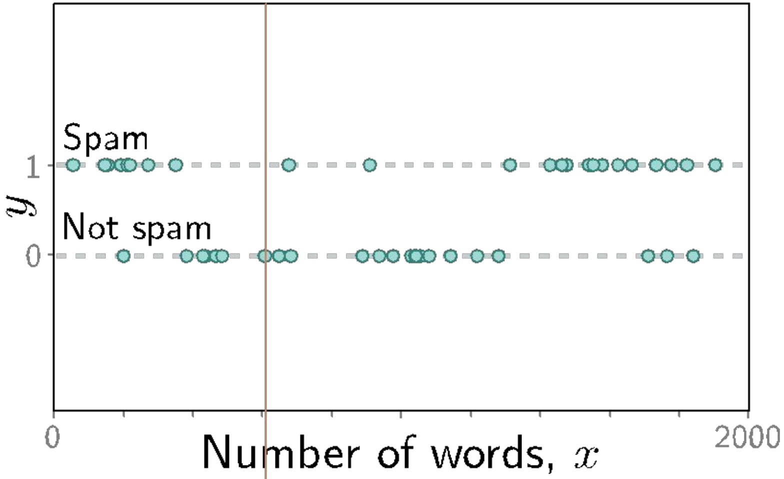
Continuous
$\Pr(y|x)$

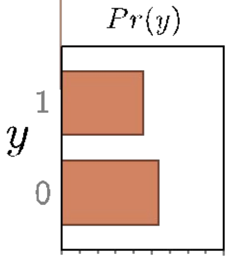


Spam
Not spam
1
0
y
0
2000
Number of words, x



Discrete
$\Pr(y|x)$





Discrete
$\Pr(y|x)$

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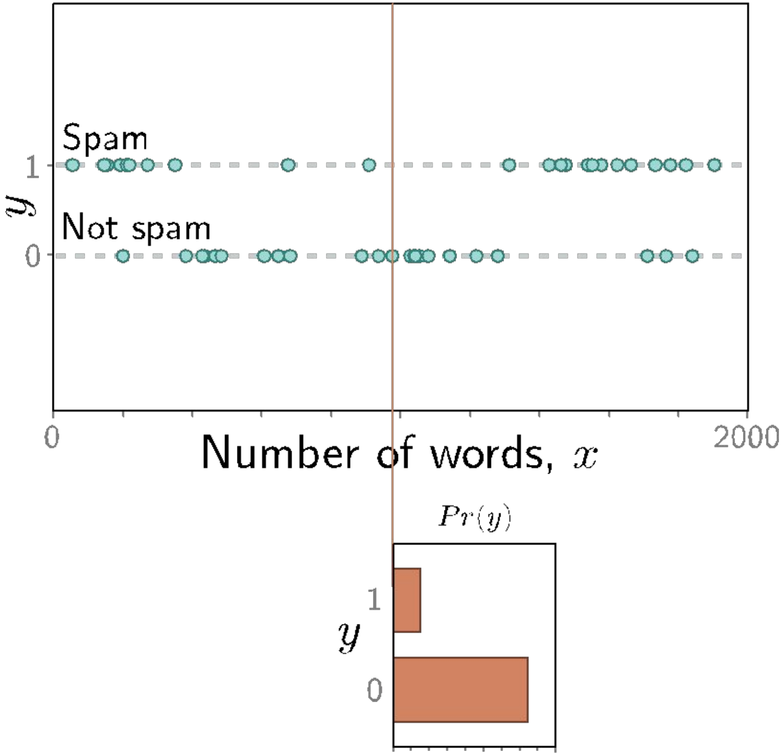
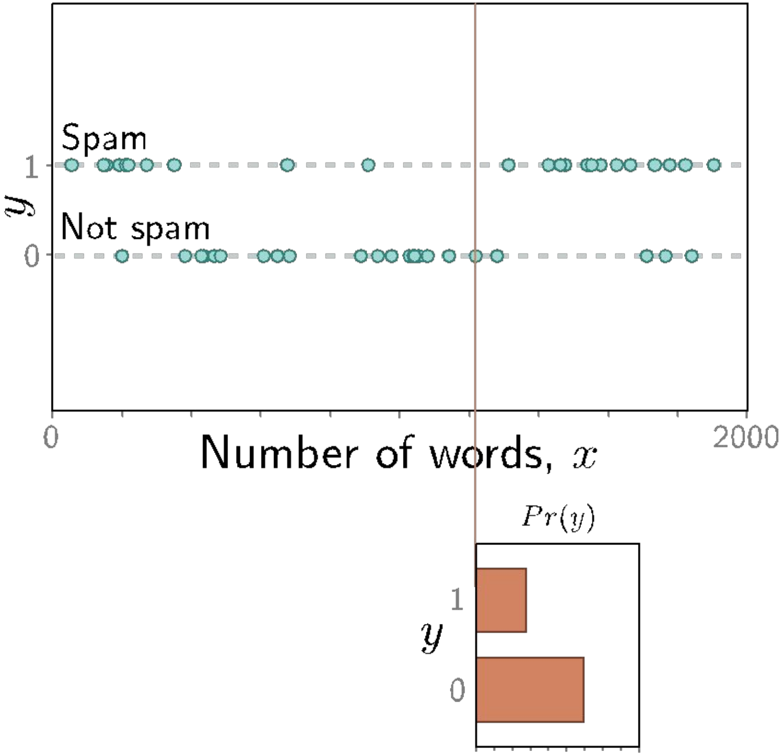
$\Pr(y|x)$





Discrete
$\Pr(y|x)$

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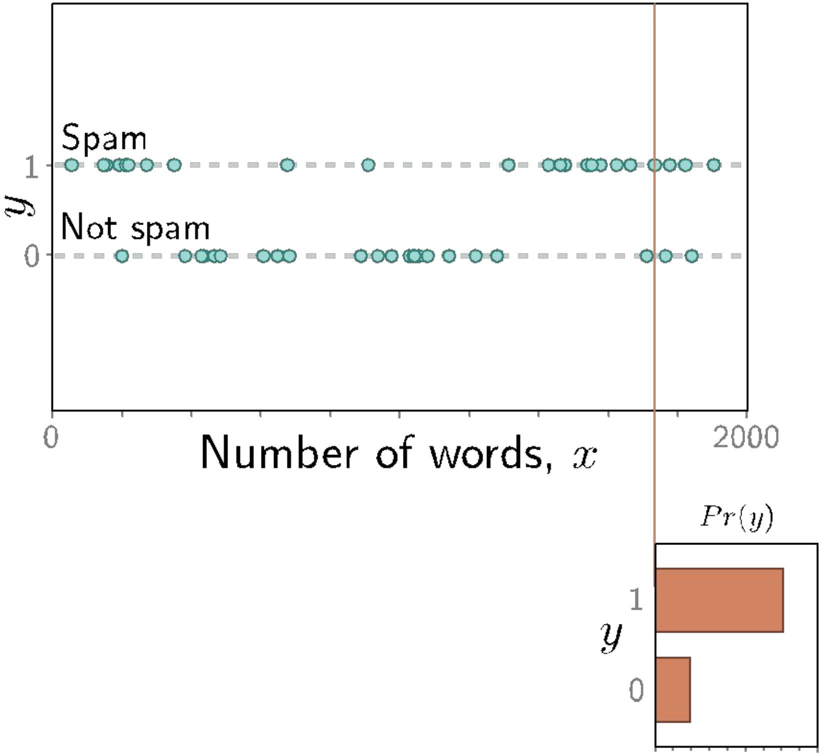
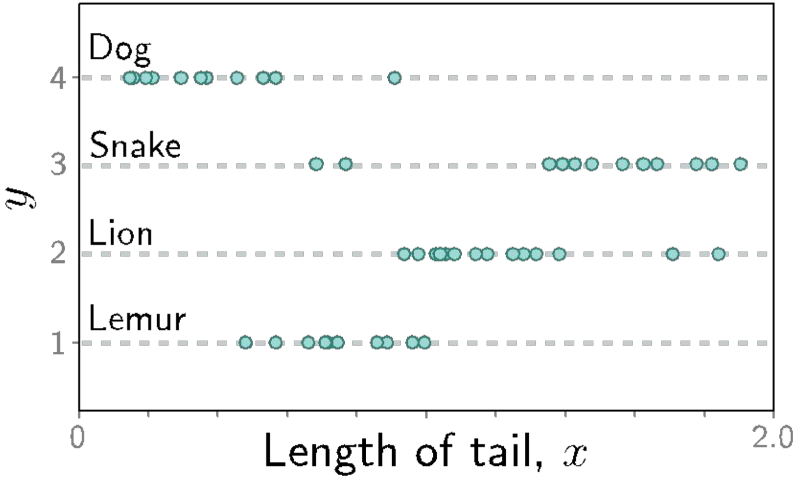
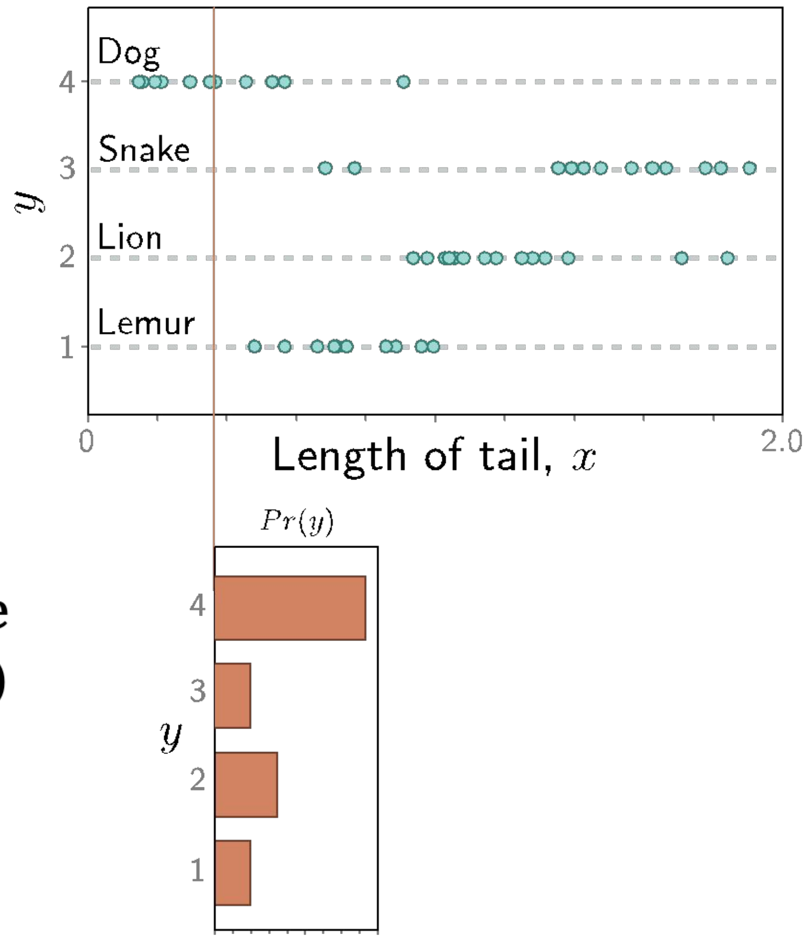
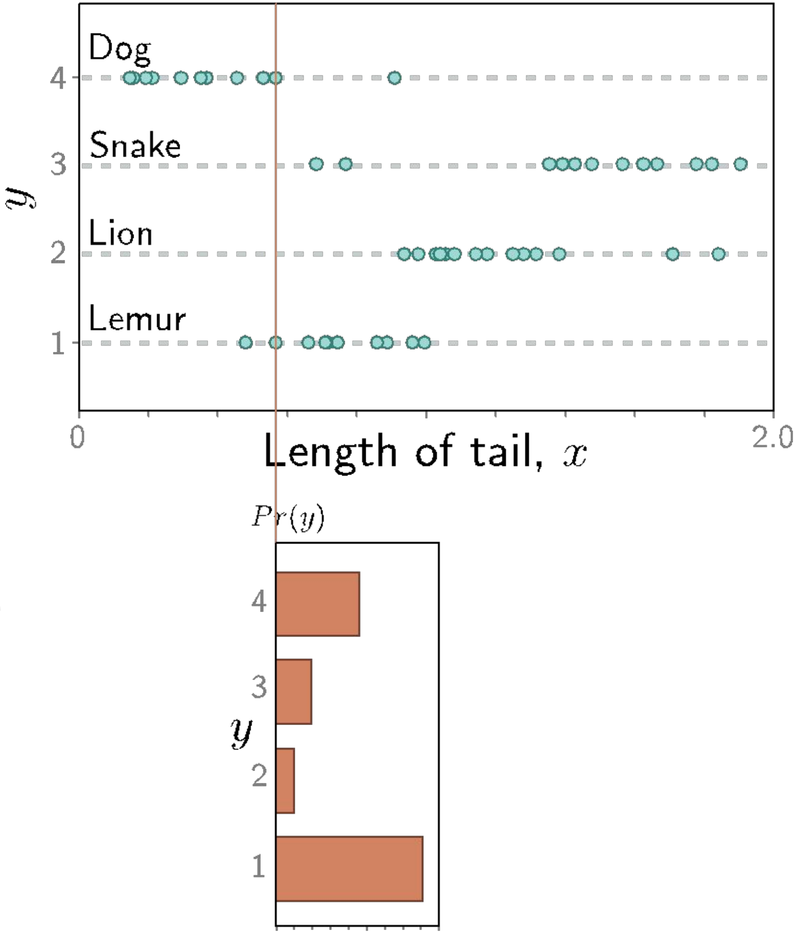



Dog
Snake
Lion
Lemur
4
3
2
1
y
0
2.0
Length of tail, x

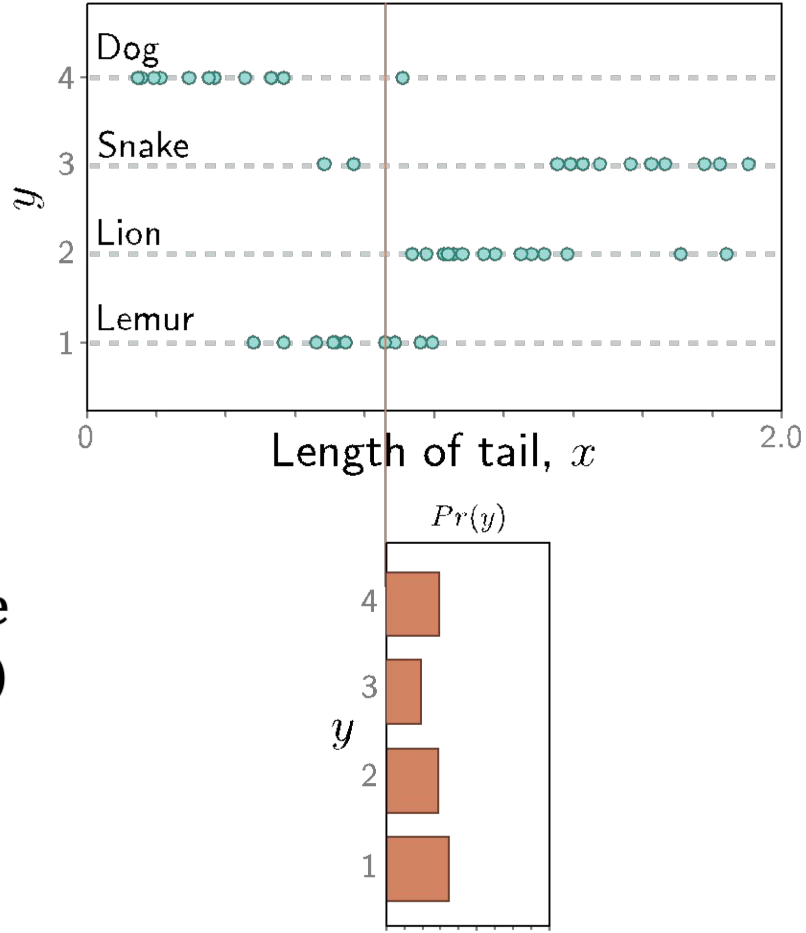
Discrete
Pr(y|x)



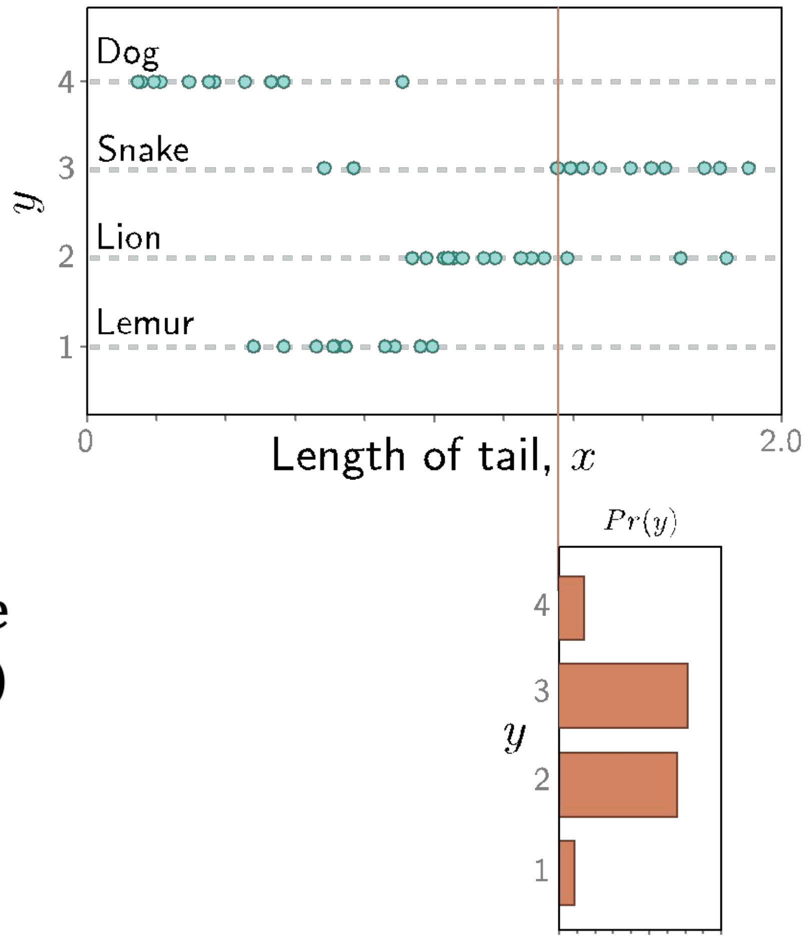
Discrete
$\Pr(y|x)$

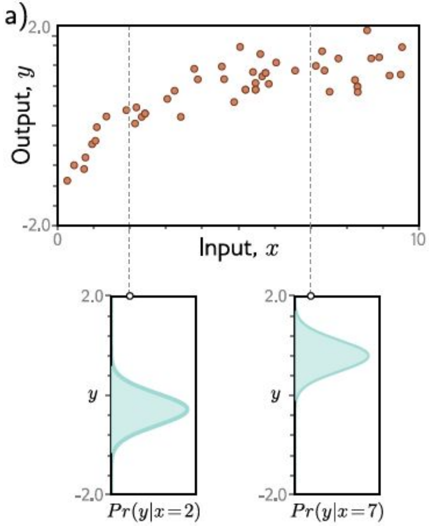


Discrete Pr($y|x$)

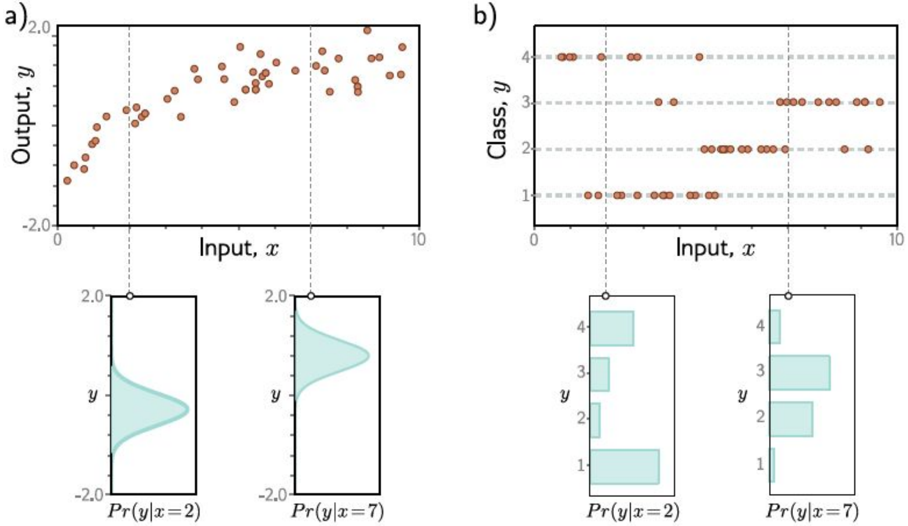


Discrete $\Pr(y|x)$

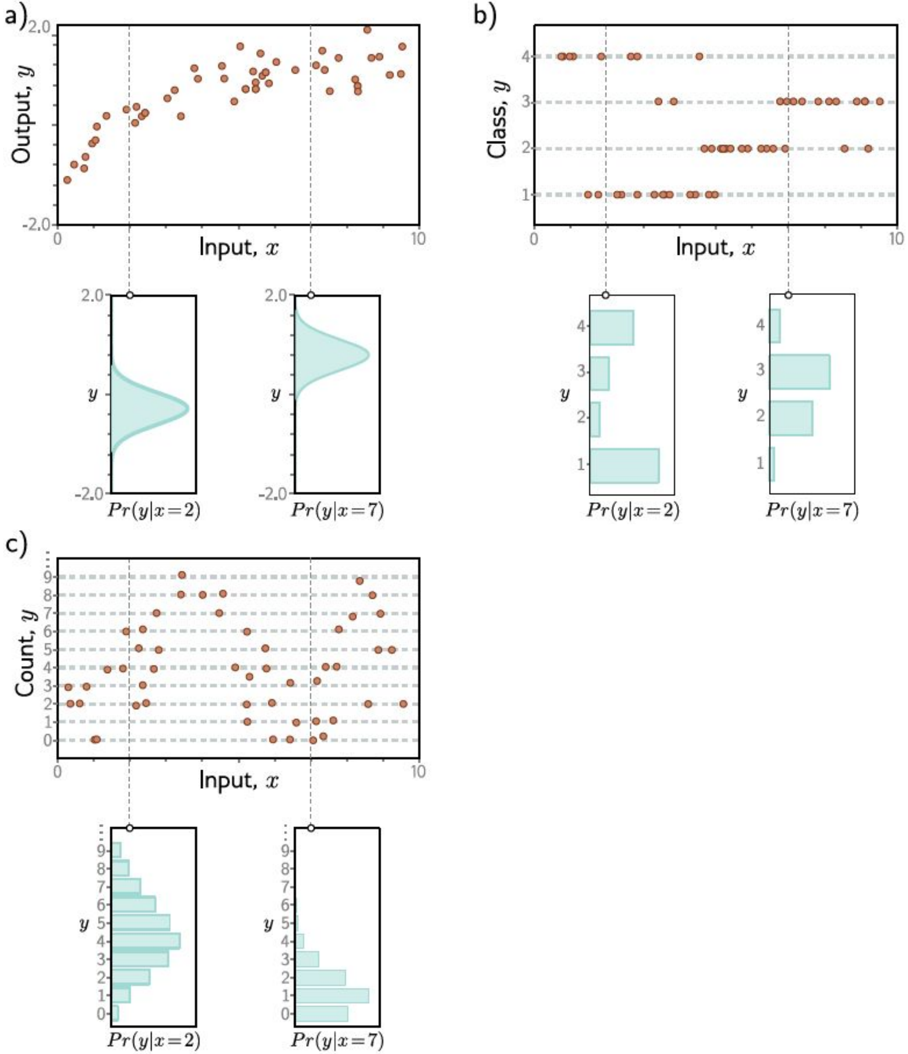




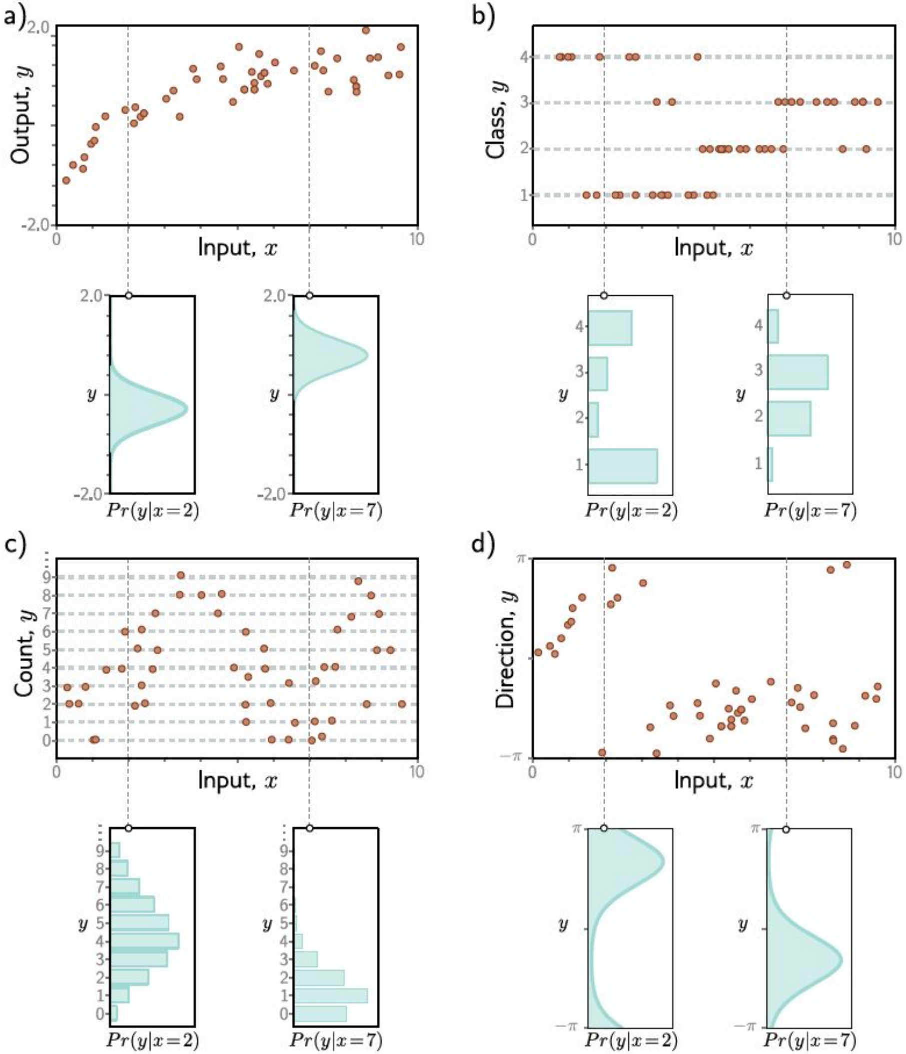
a)
2.0
-2.0
Output, y
0
10
Input, x
2.0
-2.0
y
$Pr(y|x=2)$
2.0
-2.0
y
$Pr(y|x=7)$



a)
2.0
-2.0
Output, y
0
10
Input, x
2.0
-2.0
y
$Pr(y|x=2)$
2.0
-2.0
y
$Pr(y|x=7)$
b)
4
3
2
1
Class, y
0
10
Input, x
4
3
2
1
y
$Pr(y|x=2)$
4
3
2
1
y
$Pr(y|x=7)$



a)
b)
c)
Output, y
Input, x
Class, y
Count, y
2.0
-2.0
0
10
$Pr(y|x=2)$
$Pr(y|x=7)$



a)
2.0
-2.0
Output, y
Input, x
0
10
y
$Pr(y|x=2)$
$Pr(y|x=7)$
b)
Class, y
1
2
3
4
Input, x
$Pr(y|x=2)$
$Pr(y|x=7)$
c)
Count, y
0
1
2
3
4
5
6
7
8
9
Input, x
$Pr(y|x=2)$
$Pr(y|x=7)$
d)
Direction, y
π
$-\pi$
Input, x
$Pr(y|x=2)$
$Pr(y|x=7)$

Loss function

- Training dataset of I pairs of input/output examples:

$$\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{I}$$

- Loss function or cost function measures how bad model is:

$$L\Big[\phi, \underbrace{\mathrm{f}[\mathbf{x}, \phi]}_{\text{model}}, \underbrace{\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{I}}_{\text{train data}}\Big]$$

Loss function

- Training dataset of I pairs of input/output examples:

$$\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{I}$$

- Loss function or cost function measures how bad model is:

  or for short:

$$L[\phi]$$

Returns a scalar that is smaller when model maps inputs to outputs better

Training

- Loss function:

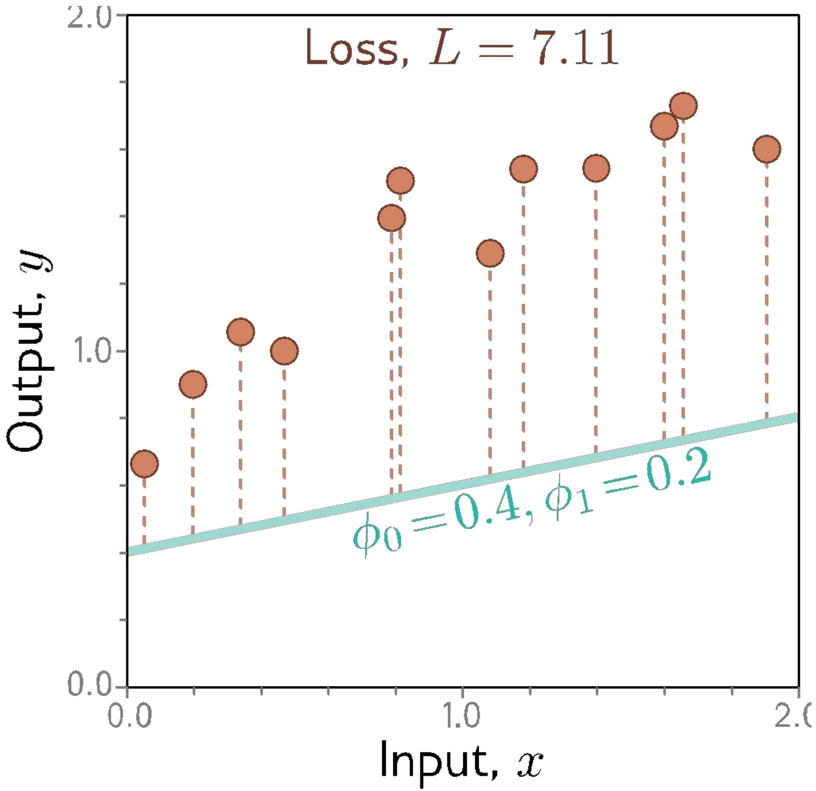
$$L[\phi]$$

Returns a scalar that is smaller when model maps inputs to outputs better

- Find the parameters that minimize the loss:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}}\Big[\mathrm{L}[\phi]\Big]$$

Example: 1D Linear regression loss function



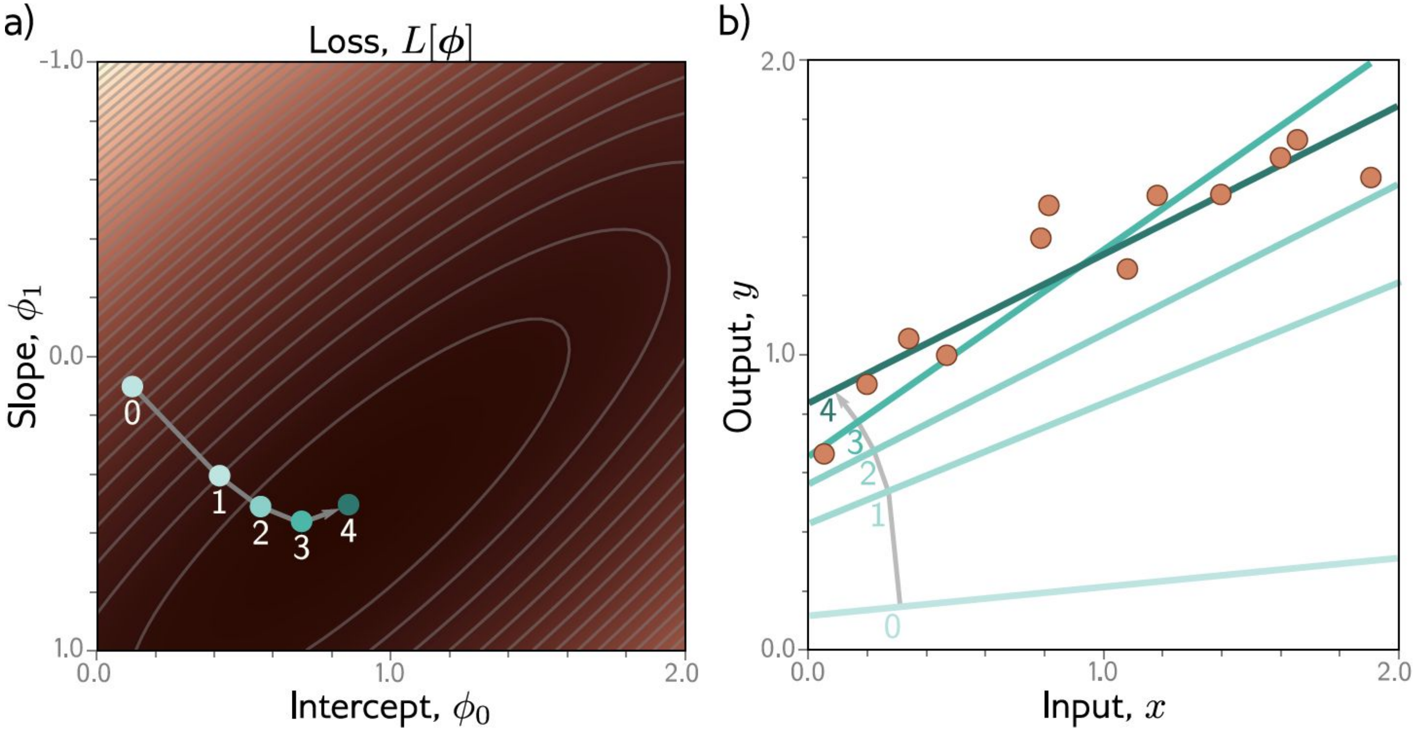
Loss function:

$$L[\phi] = \sum_{i=1}^{I} (\mathrm{f}[x_i, \phi] - y_i)^2$$

$$= \sum_{i=1}^{I} (\phi_0 + \phi_1 x_i - y_i)^2$$

"Least squares loss function"

Example: 1D Linear regression training



This technique is known as gradient descent

Loss functions

- Maximum likelihood
- Recipe for loss functions
- Example 1: univariate regression
- Example 2: binary classification
- Example 3: multiclass classification
- Other types of data
- Multiple outputs
- Cross entropy

Maximum Likelihood Estimation

- In statistics, maximum likelihood estimation (MLE) is a method of estimating the parameters of an assumed probability distribution, given some observed data.
- This is achieved by maximizing a likelihood function so that, under the assumed statistical model, the observed data is most probable.

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- This is achieved by maximizing a likelihood function so that, under the assumed statistical model, the observed data is most probable.

- Does not take into account prior beliefs or likelihoods of particular parameter settings.
- Won’t talk (much) about Bayesian improvements.

How do we do this?

- Model predicts output y given input x

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- ~~Model predicts output y given input x~~

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- ~~Model predicts output y given input x~~
- Model predicts a conditional probability distribution:

$$Pr(\mathbf{y}|\mathbf{x})$$

over outputs y given inputs x.

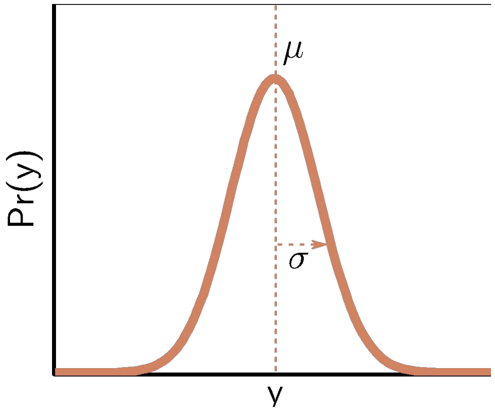
- Define and minimize a loss function that makes the outputs have high probability

How can a model predict a probability distribution? Parametric Models

1. Pick a known distribution (e.g., normal distribution) to model output y with parameters $\boldsymbol{\theta}$

   e.g., the normal distribution

$$\boldsymbol{\theta} = \{\mu, \sigma^2\}$$



2. Use model to predict parameters $\boldsymbol{\theta}$ of probability distribution

Maximize the joint, conditional probability

- We know we picked a good model and the right parameters when the joint conditional probability is high for the observed (e.g. training) data.

$$\Pr(y_1, y_2, \dots, y_I \mid x_1, x_2, \dots, x_I)$$

Two simplifying assumptions

Identically distributed (the form of the probably distribution is the same for each input/output pair)

$$\Pr(y_1, y_2, \ldots, y_I | x_1, x_2, \ldots, x_I) = \prod_{i=1}^{I} \Pr(y_i | x_i)$$

Independent

Independent and identically distributed (i.i.d)

Maximum likelihood criterion

$$\hat{\phi} = \underset{\phi}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\mathbf{x}_i) \right]$$

$$= \underset{\phi}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\boldsymbol{\theta}_i) \right]$$

$$= \underset{\phi}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\mathbf{f}[\mathbf{x}_i, \boldsymbol{\phi}]) \right]$$

θ_i are the parameters of the probability distribution

ϕ are the parameters of the neural network, e.g.

$$\theta_i = \mathrm{f}[\mathrm{x}_i, \phi]$$

When we consider this probability as a function of the parameters ϕ, we call it a likelihood.

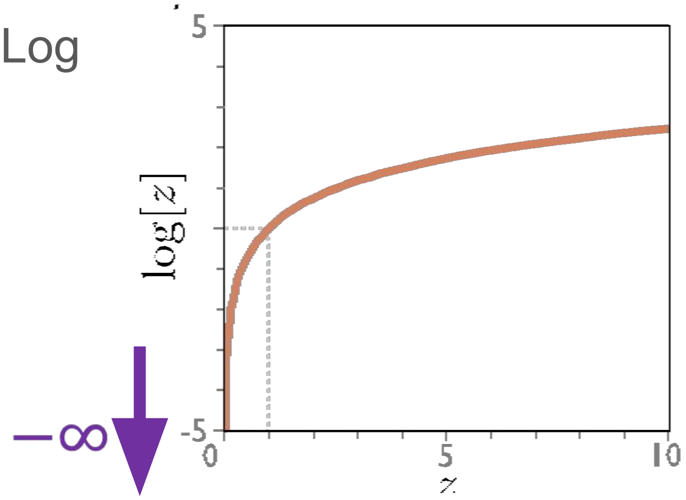
Problem:

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmax}} \left[\prod_{i=1}^{I} Pr(\mathbf{y}_i | \mathbf{f}[\mathbf{x}_i, \boldsymbol{\phi}]) \right]$$

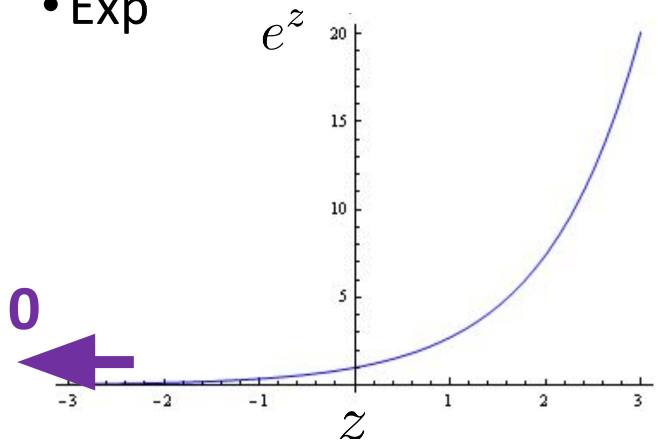
- The terms in this product might all be small
- The product might get so small that we *can't* easily represent it in fixed precision arithmetic

Log and exp functions

- Log



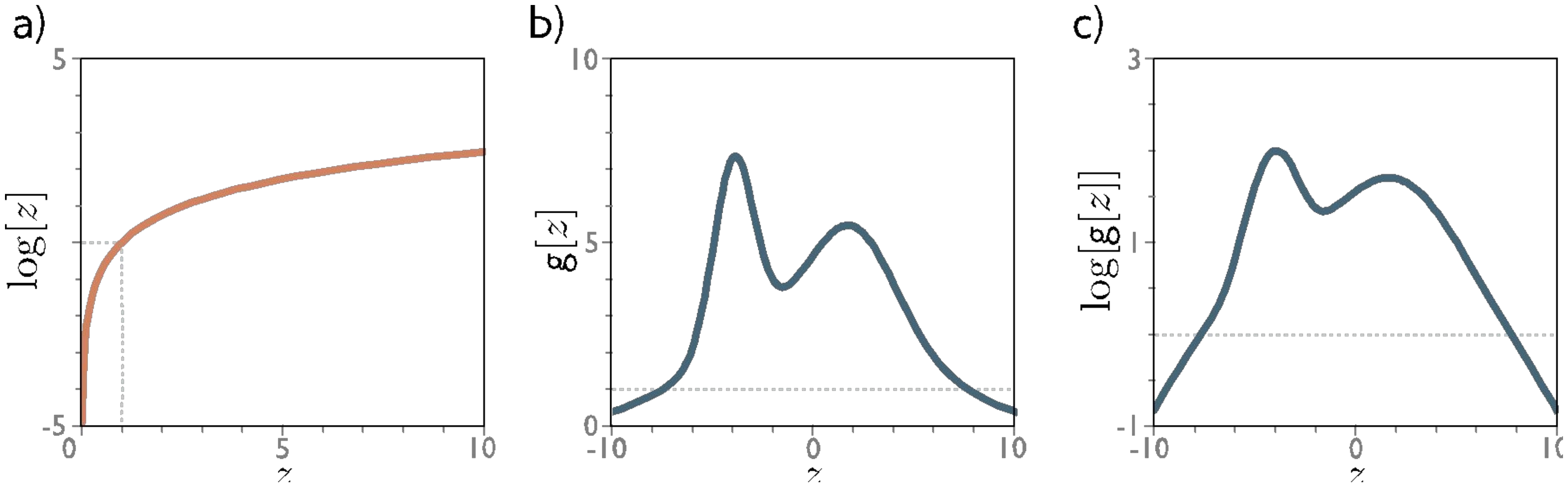
- Exp



- Two rules:

$$\log[\exp[z]] = z \qquad\qquad \log[a \cdot b] = \log[a] + \log[b]$$

The log function is monotonic



Maximum of the logarithm of a function is in the same place as maximum of function

Maximum log likelihood

$$\begin{aligned}\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmax}}\left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\mathbf{f}[\mathbf{x}_i,\boldsymbol{\phi}])\right] \\ &= \underset{\boldsymbol{\phi}}{\operatorname{argmax}}\left[\log\left[\prod_{i=1}^{I} Pr(\mathbf{y}_i|\mathbf{f}[\mathbf{x}_i,\boldsymbol{\phi}])\right]\right] \\ &= \underset{\boldsymbol{\phi}}{\operatorname{argmax}}\left[\sum_{i=1}^{I}\log\Bigl[Pr(\mathbf{y}_i|\mathbf{f}[\mathbf{x}_i,\boldsymbol{\phi}])\Bigr]\right]\end{aligned}$$

Now it’s a sum of terms, so doesn’t matter so much if the terms are small

Minimizing negative log likelihood

- By convention, we minimize things (i.e., a loss)

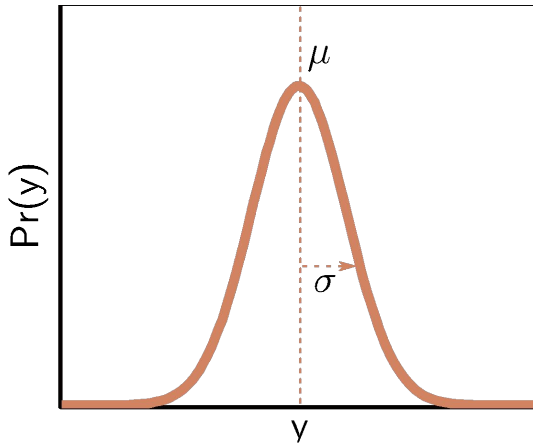
$$
\begin{aligned}
\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmax}} \left[\sum_{i=1}^{I} \log\Big[Pr(\mathbf{y}_i | \mathbf{f}[\mathbf{x}_i, \boldsymbol{\phi}]) \Big] \right] \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log\Big[Pr(\mathbf{y}_i | \mathbf{f}[\mathbf{x}_i, \boldsymbol{\phi}]) \Big] \right] \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \Big[\mathrm{L}[\boldsymbol{\phi}] \Big]
\end{aligned}
$$

Inference

But now we predict a probability distribution

- We need an actual prediction (point estimate)
- Find the peak of the probability distribution (i.e., mean for normal)

$$\hat{y} = \hat{\mu} = \underset{y}{\operatorname{argmax}}[\Pr(y|\mathbf{f}[\mathbf{x}, \phi])]]$$



Why Peak Probability?

- We started from maximum likelihood…
  - Picked parameters maximizing likelihood of training data
  - Now pick maximum likelihood output given our input data.
- Aligns with mean and median for normal distributions.

Not always the right answer if we are not starting from maximum likelihood.

- If you start from your own loss function…
- And particularly if that loss function is asymmetric…

Loss functions

- Maximum likelihood
- Recipe for loss functions
- Example 1: univariate regression
- Example 2: binary classification
- Example 3: multiclass classification
- Other types of data
- Multiple outputs
- Cross entropy

Recipe for loss functions

1. Choose a suitable probability distribution $Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.

Recipe for loss functions

1. Choose a suitable probability distribution $Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.
2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \phi]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \phi]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \phi])$.

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3. To train the model, find the network parameters $\hat{\boldsymbol{\phi}}$ that minimize the negative log-likelihood loss function over the training dataset pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$:

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[L[\boldsymbol{\phi}] \right] = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[Pr(\mathbf{y}_i|\mathbf{f}[\mathbf{x}_i, \boldsymbol{\phi}]) \right] \right]. \qquad (5.7)$$

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4. To perform inference for a new test example $\mathbf{x}$, return either the full distribution $Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \hat{\boldsymbol{\phi}}])$ or the maximum of this distribution.

Let’s apply this recipe to

- Example 1: Real valued univariate regression
- Example 2: Binary Classification
- Example 3: Multiclass Classification

Loss functions

- Maximum likelihood
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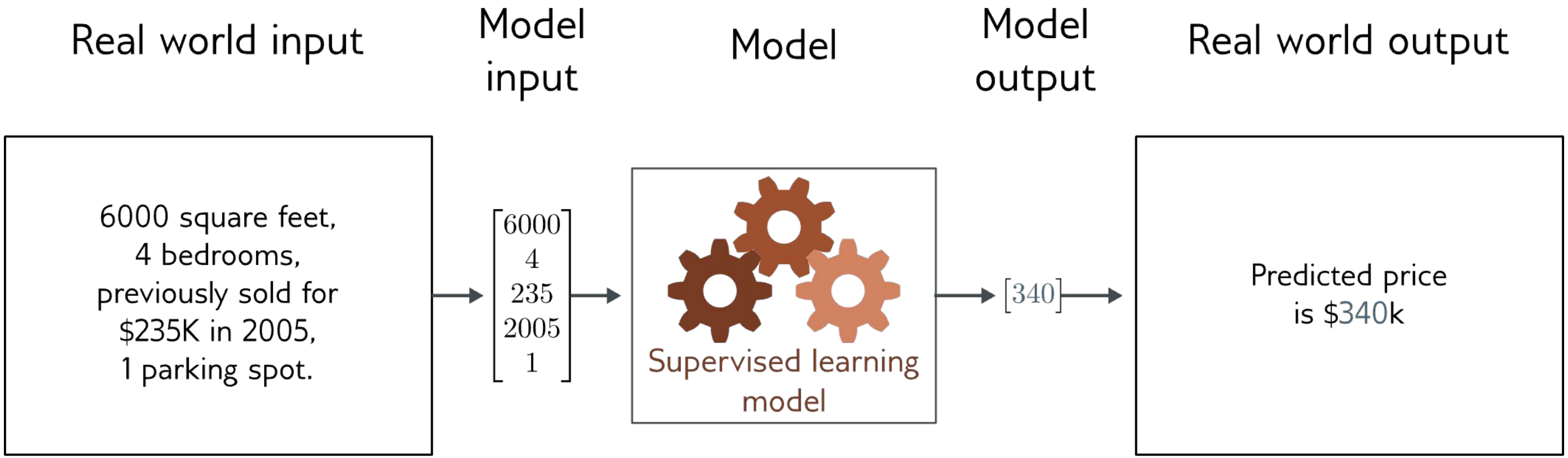
Example 1: univariate regression

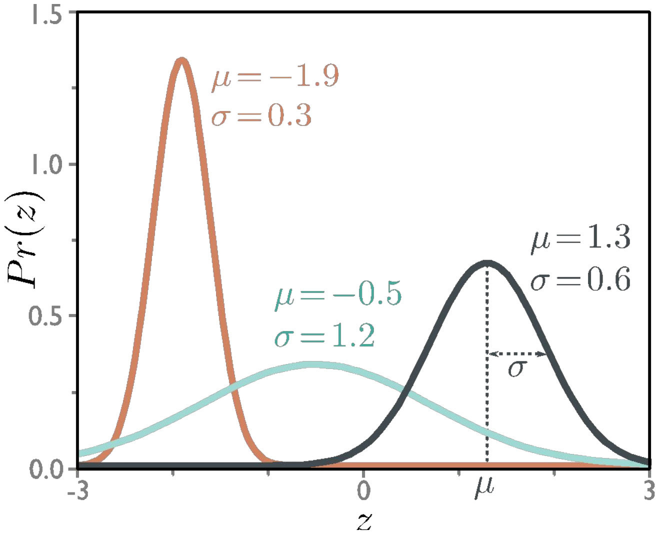


Example 1: univariate regression

1. Choose a suitable probability distribution $Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.

- Predict scalar output: $y \in \mathbb{R}$
- Sensible probability distribution:
  - Normal distribution

$$Pr(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\mu)^2}{2\sigma^2}\right]$$



Example 1: univariate regression

2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \phi]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \phi]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \phi])$.

$$Pr(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\mu)^2}{2\sigma^2}\right]$$

In this case, just the mean

$$Pr(y|\mathrm{f}[\mathbf{x}, \phi], \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\mathrm{f}[\mathbf{x}, \phi])^2}{2\sigma^2}\right]$$

Just learn the mean, μ, and assume the variance is fixed,.

Example 1: univariate regression

3. To train the model, find the network parameters $\hat{\phi}$ that minimize the negative log-likelihood loss function over the training dataset pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$:

$$
\begin{aligned}
L[\phi] &= -\sum_{i=1}^{I} \log\left[Pr(y_i|\mathrm{f}[\mathbf{x}_i, \phi], \sigma^2)\right] \\
&= -\sum_{i=1}^{I} \log\left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \phi])^2}{2\sigma^2}\right]\right]
\end{aligned}
$$

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \boldsymbol{\phi}])^2}{2\sigma^2} \right] \right] \right]$$

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \boldsymbol{\phi}])^2}{2\sigma^2} \right] \right] \right]$$

$$= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} \right] + \log \left[\exp \left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \boldsymbol{\phi}])^2}{2\sigma^2} \right] \right] \right]$$

$$\log[a \cdot b] = \log[a] + \log[b]$$

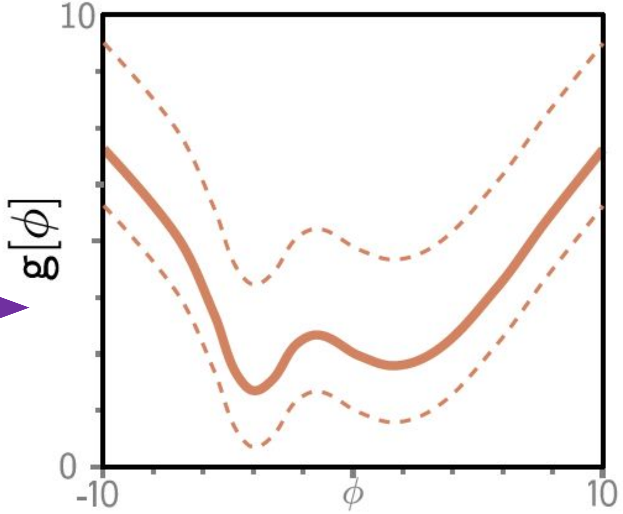
$$
\begin{aligned}
\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]+\log\left[\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]
\end{aligned}
$$

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]$$

$$= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]+\log\left[\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]$$

$$= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]$$

Just a constant offset



$$
\begin{aligned}
\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]+\log\left[\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]
\end{aligned}
$$

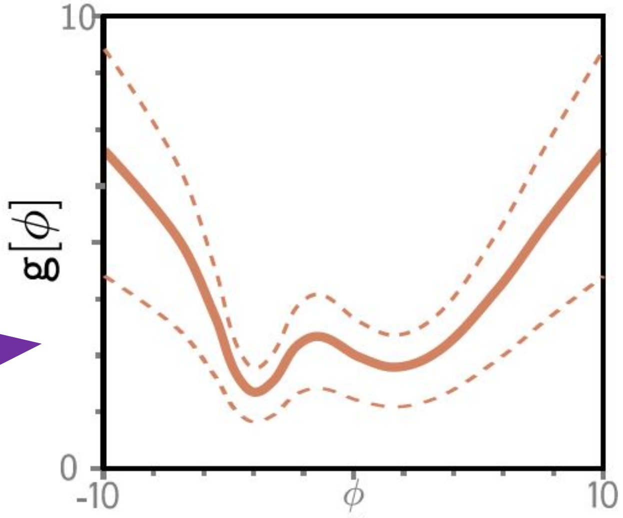
$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]$$

$$= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right] + \log\left[\exp\left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]$$

$$= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right] - \frac{(y_i - \mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]$$

$$= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I} -\frac{(y_i - \mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]$$

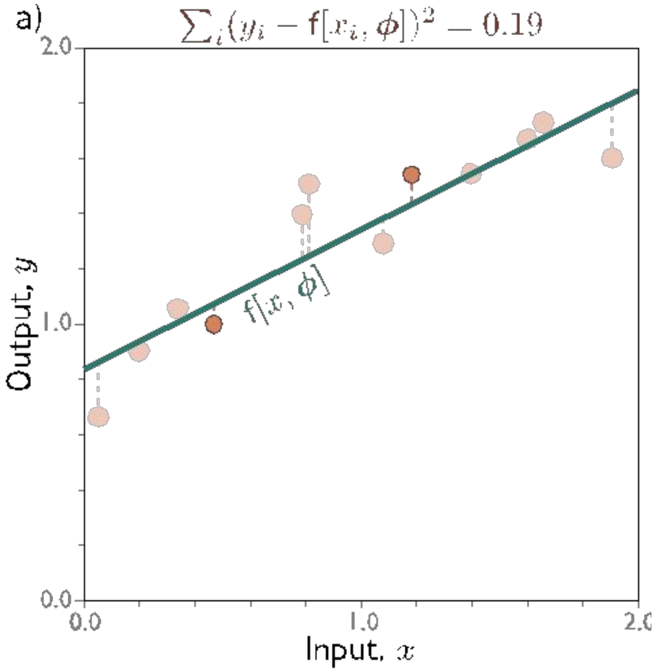
Just dividing by a positive constant



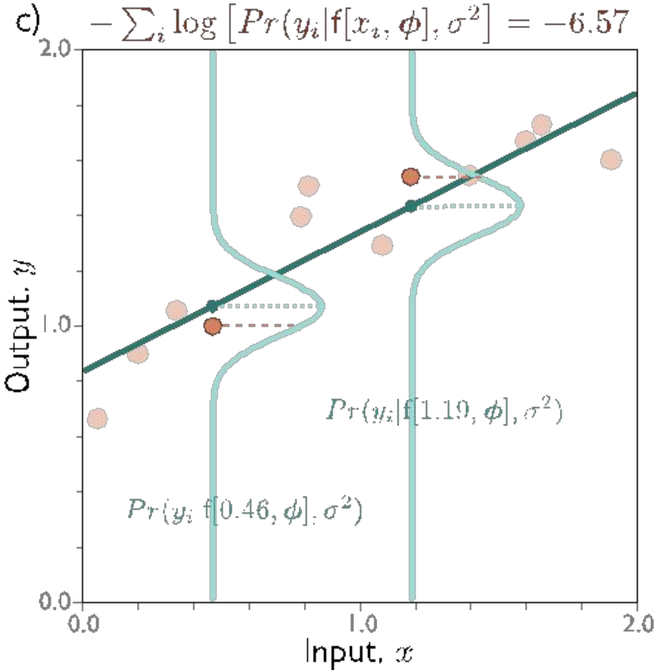
$$
\begin{aligned}
\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]+\log\left[\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[\sum_{i=1}^{I}(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2\right],
\end{aligned}
$$

← Least squares!

Least squares

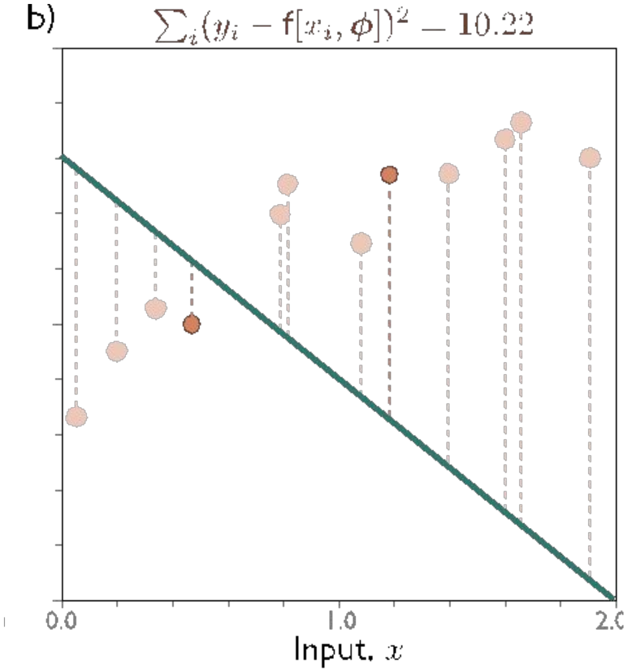


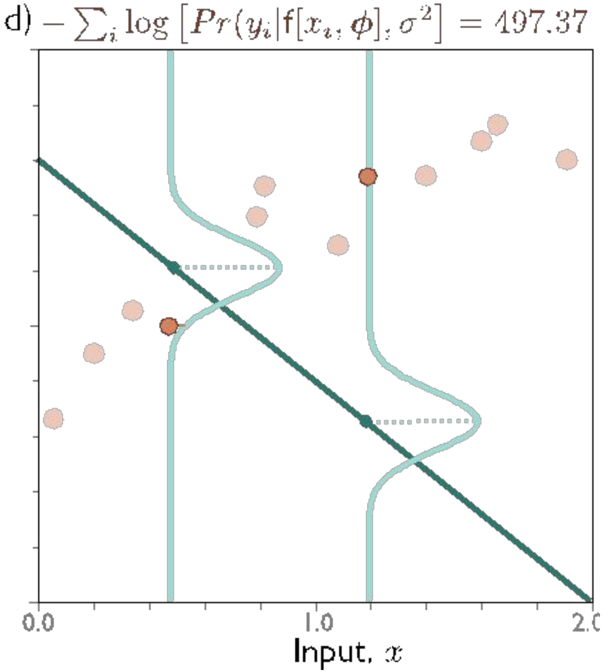
Negative log likelihood



Least squares

Maximum likelihood





Example 1: univariate regression

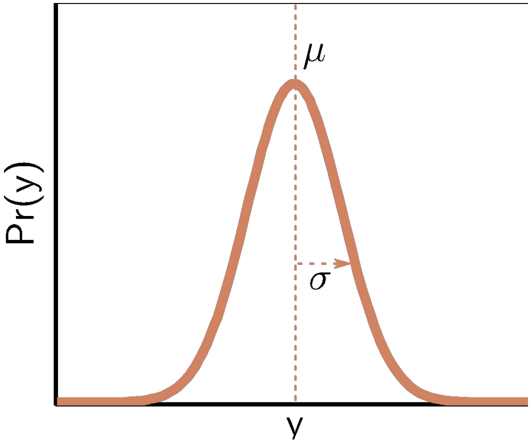
4. To perform inference for a new test example $\mathbf{x}$, return either the full distribution $Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \hat{\phi}])$ or the maximum of this distribution.

Full distribution:

$$Pr(y|\mathrm{f}[\mathbf{x}, \phi], \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y - \mathrm{f}[\mathbf{x}, \phi])^2}{2\sigma^2}\right]$$

Max probability:

$$\hat{y} = \hat{\mu} = \mathrm{f}[\mathrm{x}\,|\phi]$$



Estimating variance

- Perhaps surprisingly, the variance term disappeared:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \phi])^2}{2\sigma^2} \right] \right] \right]$$

$$= \underset{\phi}{\operatorname{argmin}} \left[\sum_{i=1}^{I} (y_i - \mathrm{f}[\mathbf{x}_i, \phi])^2 \right]$$

Estimating variance

- But we could learn it during training:

$$\hat{\boldsymbol{\phi}}, \hat{\sigma}^2 = \underset{\boldsymbol{\phi}, \sigma^2}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \mathrm{f}[\mathbf{x}_i, \boldsymbol{\phi}])^2}{2\sigma^2} \right] \right] \right]$$

- Do gradient descent on both model parameters, ϕ, and the variance, σ^2

$$\frac{\partial L}{\partial \phi} \text{ and } \frac{\partial L}{\partial \sigma^2}$$

Heteroscedastic regression

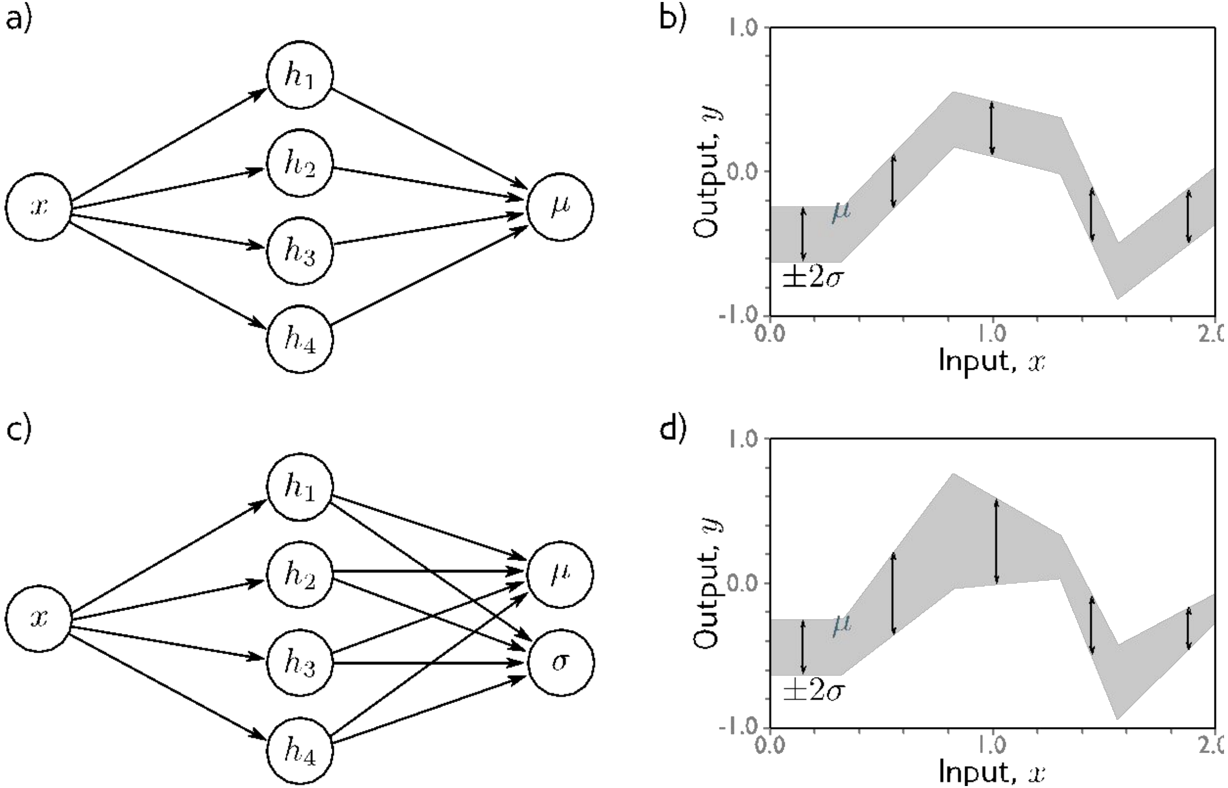
- We were assuming that the noise σ^2 is the same everywhere (homoscedastic).
- But we could make the noise a function of the data *x*.
- Build a model with two outputs:

$$\mu = \mathrm{f}_1[\mathbf{x}, \boldsymbol{\phi}]$$

$$\sigma^2 = \mathrm{f}_2[\mathbf{x}, \boldsymbol{\phi}]^2$$

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\mathrm{argmin}} \left[-\sum_{i=1}^{I} \log \left[\frac{1}{\sqrt{2\pi \mathrm{f}_2[\mathbf{x}_i, \boldsymbol{\phi}]^2}} \right] - \frac{(y_i - \mathrm{f}_1[\mathbf{x}_i, \boldsymbol{\phi}])^2}{2\mathrm{f}_2[\mathbf{x}_i, \boldsymbol{\phi}]^2} \right]$$

Heteroscedastic regression



Example 1: Univariate Regression Takeaways

- Least squares loss is a good choice assuming normal distribution
- The best prediction is the predicted mean
- We can also estimate global or local variance

Example 1: Univariate Regression Takeaways

- Least squares loss is a good choice assuming normal distribution
- The best prediction is the predicted mean
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BTW the Central Limit Theorem suggests we will see lots of normal distributions…

Loss functions

- Maximum likelihood
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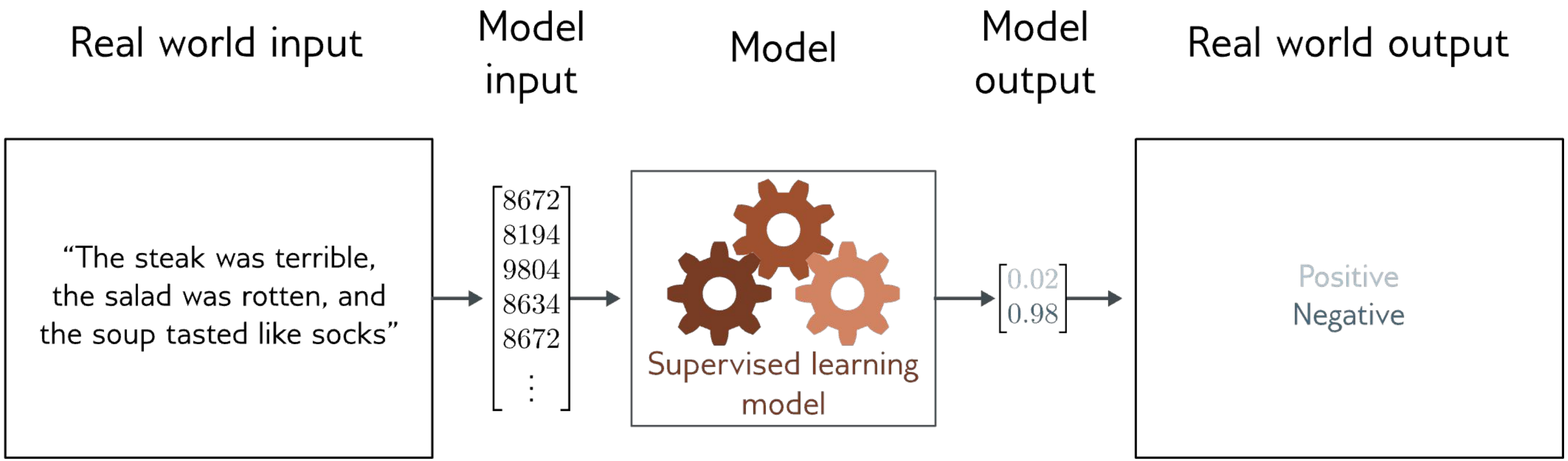
Example 2: binary classification



- Goal: predict which of two classes $y \in \{0, 1\}$ the input *x* belongs to

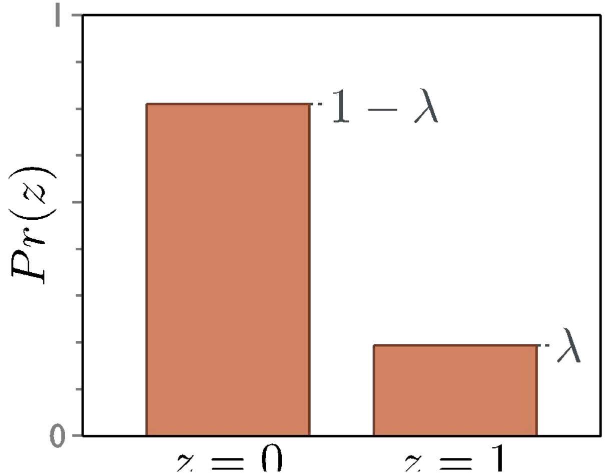
Example 2: binary classification

1. Choose a suitable probability distribution $Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.

- **Domain:** $y \in \{0, 1\}$
- **Bernoulli distribution**
- **One parameter $\lambda \in [0,1]$**

$$Pr(y|\lambda) = \begin{cases} 1-\lambda & y=0 \\ \lambda & y=1 \end{cases}$$

$$Pr(y|\lambda) = (1-\lambda)^{1-y} \cdot \lambda^{y}$$



Example 2: binary classification

2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \phi]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \phi]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \phi])$.

Problem:

- Output of neural network can be anything
- Parameter $\lambda \in [0,1]$

Solution:

- Pass through function that maps "anything" to [0,1]

Example 2: binary classification

2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}])$.

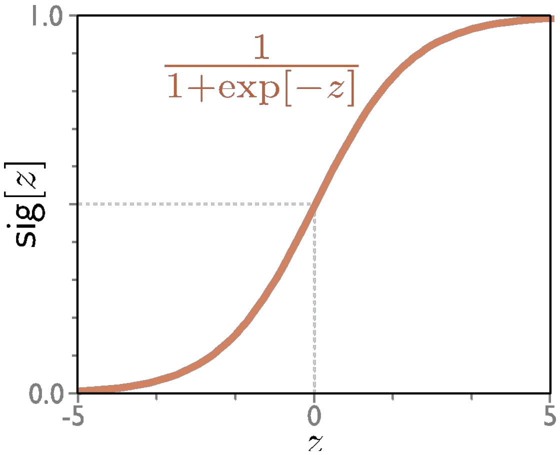
Problem:

- Output of neural network can be anything
- Parameter $\lambda \in [0,1]$

Solution:

- Pass through logistic sigmoid function that maps "anything to [0,1]:

$$\text{sig}[z] = \frac{1}{1 + \exp[-z]}$$



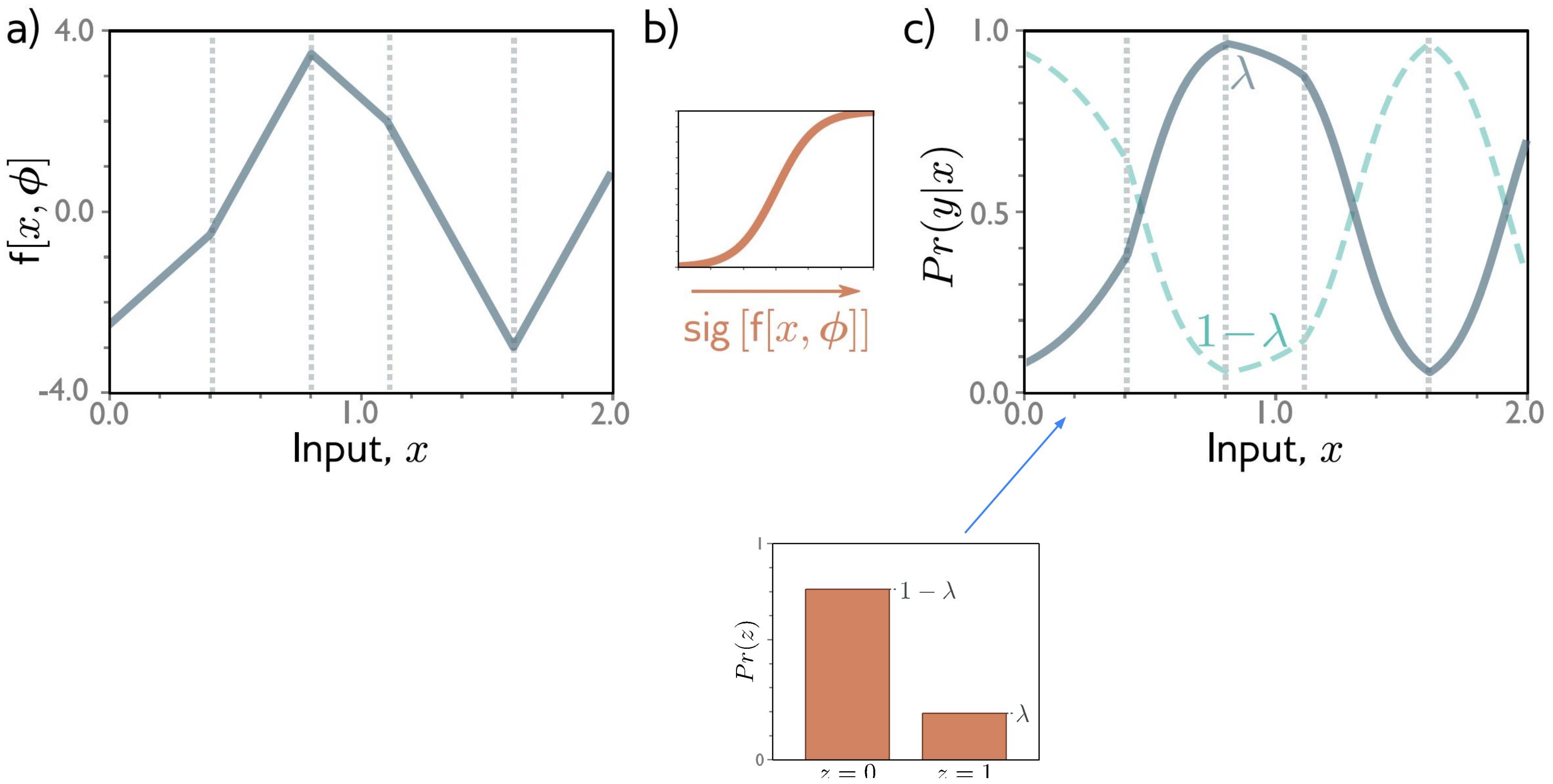
Example 2: binary classification

2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \phi]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \phi]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \phi])$.

$$Pr(y|\lambda) = (1-\lambda)^{1-y} \cdot \lambda^{y}$$

$$Pr(y|\mathbf{x}) = (1 - \text{sig}[\text{f}[\mathbf{x}|\phi]])^{1-y} \cdot \text{sig}[\text{f}[\mathbf{x}|\phi]]^{y}$$

Example 2: binary classification



Example 2: binary classification

3. To train the model, find the network parameters $\hat{\phi}$ that minimize the negative log-likelihood loss function over the training dataset pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}}\left[L[\phi]\right] = \underset{\phi}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[Pr(\mathbf{y}_i|\mathbf{f}[\mathbf{x}_i,\phi])\right]\right]. \tag{5.7}$$

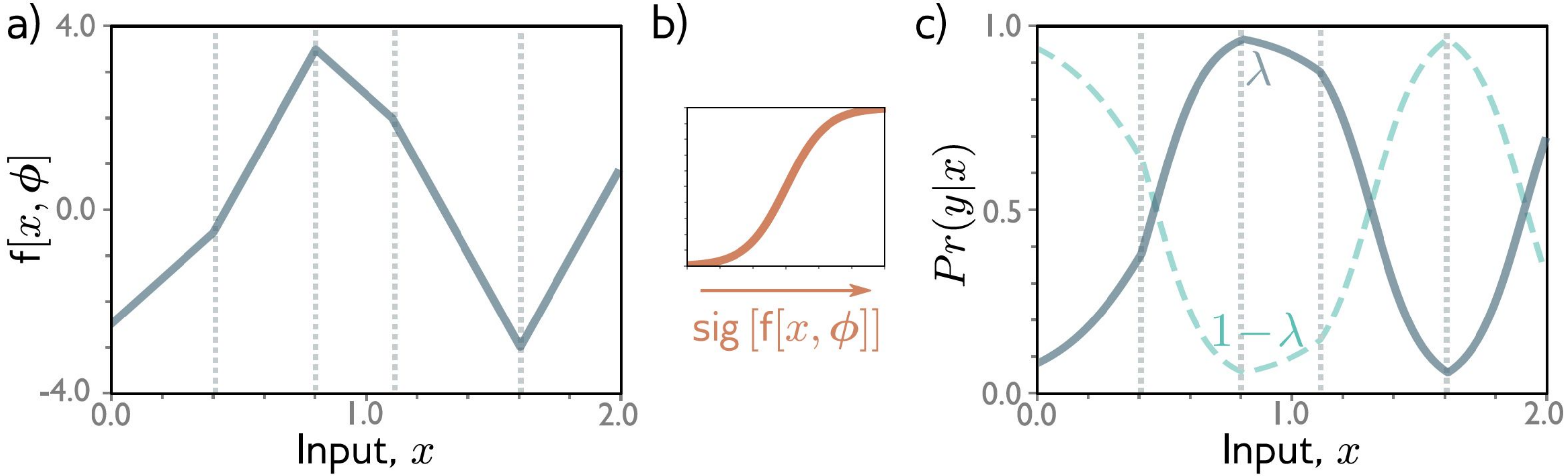
$$Pr(y|\mathbf{x}) = (1-\text{sig}[\text{f}[\mathbf{x}|\phi]])^{1-y}\cdot\text{sig}[\text{f}[\mathbf{x}|\phi]]^{y}$$

$$L[\phi] = \sum_{i=1}^{I} -(1-y_i)\log\left[1-\text{sig}[\text{f}[\mathbf{x}_i|\phi]]\right] - y_i\log\left[\text{sig}[\text{f}[\mathbf{x}_i|\phi]]\right]$$

Binary cross-entropy loss

Example 2: binary classification

4. To perform inference for a new test example $\mathbf{x}$, return either the full distribution $Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \hat{\phi}])$ or the maximum of this distribution.



Choose y=1 where λ is greater than 0.5, otherwise 0

And we get a probability estimate!

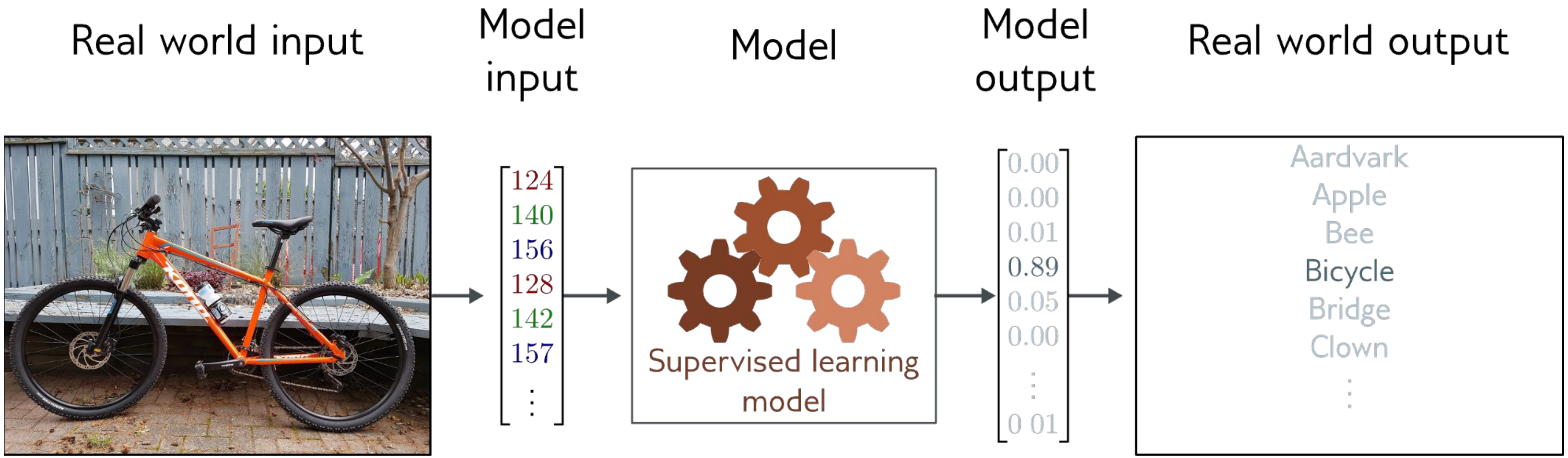
Example 2: Binary Classification Takeaways

- Binary cross entropy loss as the loss function
- Threshold to get prediction
- We also get a probability or “confidence value”

Loss functions

- Maximum likelihood
- Recipe for loss functions
- Example 1: univariate regression
- Example 2: binary classification
- Example 3: multiclass classification
- Other types of data
- Multiple outputs
- Cross entropy

Example 3: multiclass classification



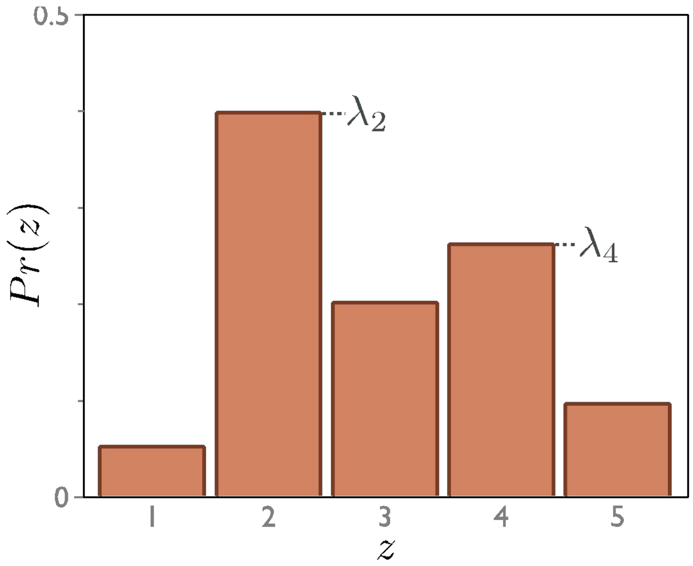
Goal: predict which of K classes $y \in \{1, 2, \ldots, K\}$ the input *x* belongs to

Example 3: multiclass classification

1. Choose a suitable probability distribution $Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.

- Domain: $y \in \{1, 2, \ldots, K\}$
- Categorical distribution
- K parameters $\lambda_k \in [0,1]$
- Sum of all parameters = 1

$$Pr(y = k) = \lambda_k$$



Example 3: multiclass classification

2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \phi]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \phi]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \phi])$.

Problem:

- Output of neural network can be anything
- Parameters $\lambda_k \in [0,1]$, sum to one

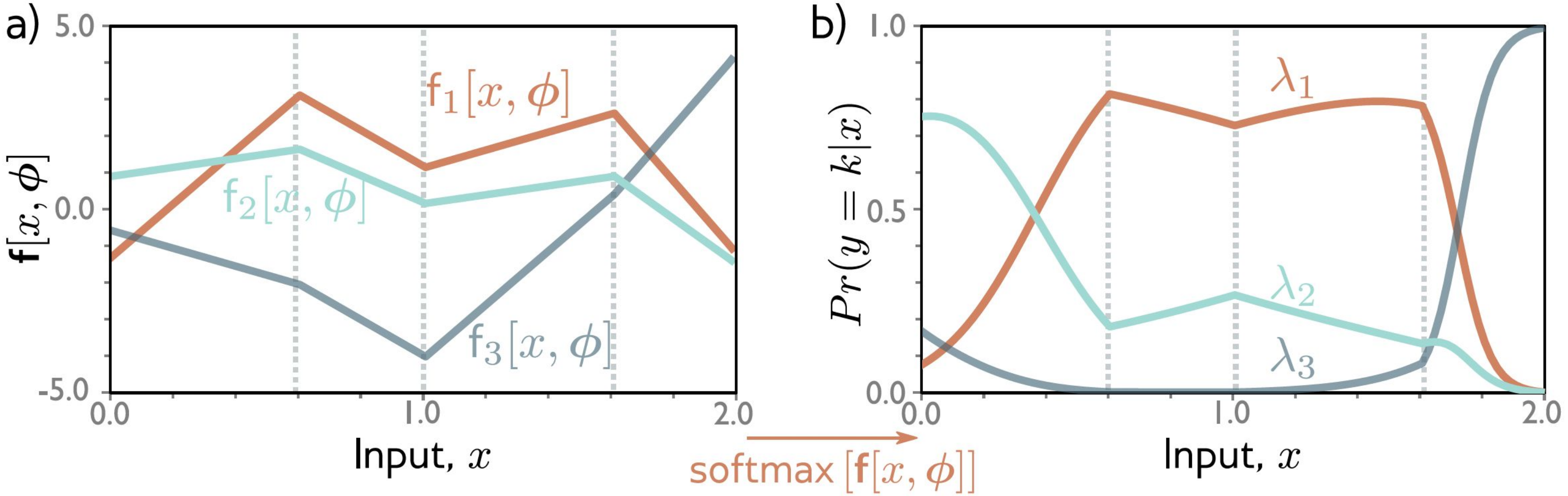
$$\text{softmax}_k[\mathbf{z}] = \frac{\exp[z_k]}{\sum_{k'=1}^{K} \exp[z_{k'}]}$$

Solution:

- Pass through function that maps "anything" to [0,1], sum to one

$$Pr(y = k|\mathbf{x}) = \text{softmax}_k[\mathbf{f}[\mathbf{x}, \phi]]$$

Example 3: multiclass classification



$$Pr(y = k|\mathbf{x}) = \text{softmax}_k[\mathbf{f}[\mathbf{x}, \phi]]$$

Example 3: multiclass classification

3. To train the model, find the network parameters $\hat{\boldsymbol{\phi}}$ that minimize the negative log-likelihood loss function over the training dataset pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$:

$$\hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[L[\boldsymbol{\phi}] \right] = \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left[-\sum_{i=1}^{I} \log \left[Pr(\mathbf{y}_i | \mathbf{f}[\mathbf{x}_i, \boldsymbol{\phi}]) \right] \right]. \qquad (5.7)$$

$$L[\boldsymbol{\phi}] = -\sum_{i=1}^{I} \log \left[\text{softmax}_{y_i} \left[\mathbf{f}\left[\mathbf{x}_i, \boldsymbol{\phi}\right] \right] \right]$$

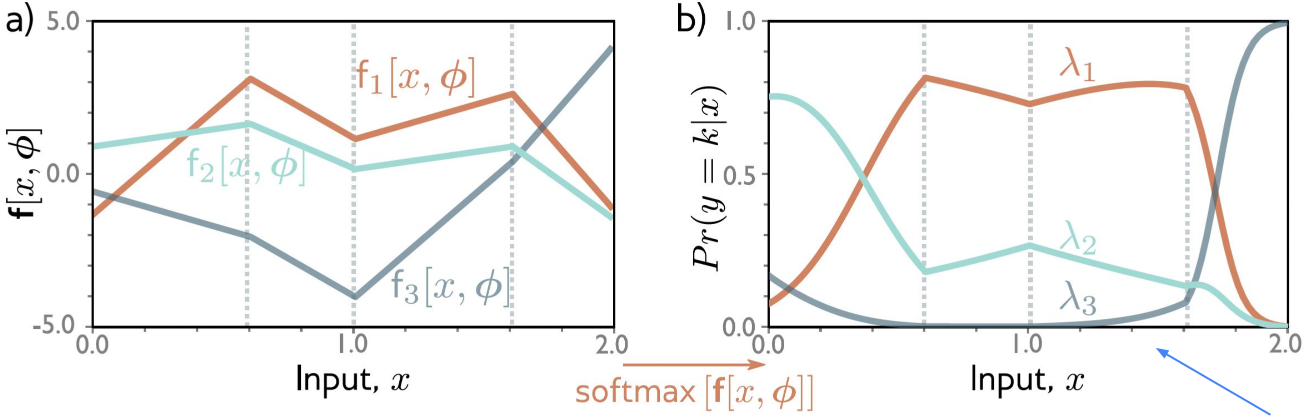
$$= -\sum_{i=1}^{I} \text{f}_{y_i} \left[\mathbf{x}_i, \boldsymbol{\phi}\right] - \log \left[\sum_{k=1}^{K} \exp\left[\text{ f}_k \left[\mathbf{x}_i, \boldsymbol{\phi}\right] \right] \right]$$

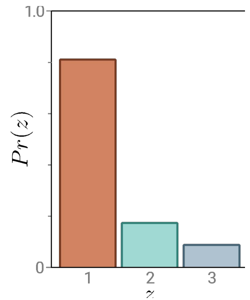
$$\text{softmax}_k[\mathbf{z}] = \frac{\exp[z_k]}{\sum_{k'=1}^{K} \exp[z_{k'}]}$$

Multiclass cross-entropy loss

Example 3: multiclass classification

4. To perform inference for a new test example $\mathbf{x}$, return either the full distribution $Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \hat{\phi}])$ or the maximum of this distribution.





Choose the class with the largest probability

We also get probability or “confidence”

Loss functions

- Maximum likelihood
- Recipe for loss functions
- Example 1: univariate regression
- Example 2: binary classification
- Example 3: multiclass classification
- Other types of data
- Multiple outputs
- Cross entropy

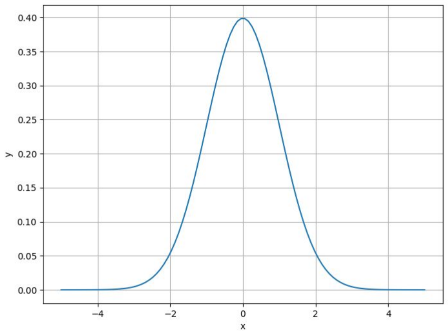
Other data types

Data Type	Domain	Distribution	Use
univariate, continuous, unbounded	$y \in \mathbb{R}$	univariate normal	regression
univariate, continuous, unbounded	$y \in \mathbb{R}$	Laplace or t-distribution	robust regression
univariate, continuous, unbounded	$y \in \mathbb{R}$	mixture of Gaussians	multimodal regression
univariate, continuous, bounded below	$y \in \mathbb{R}^+$	exponential or gamma	predicting magnitude
univariate, continuous, bounded	$y \in [0, 1]$	beta	predicting proportions
multivariate, continuous, unbounded	$\mathbf{y} \in \mathbb{R}^K$	multivariate normal	multivariate regression
univariate, continuous, circular	$y \in (-\pi, \pi]$	von Mises	predicting direction
univariate, discrete, binary	$y \in \{0, 1\}$	Bernoulli	binary classification
univariate, discrete, bounded	$y \in \{1, 2, \ldots, K\}$	categorical	multiclass classification
univariate, discrete, bounded below	$y \in [0, 1, 2, 3, \ldots]$	Poisson	predicting event counts
multivariate, discrete, permutation	$\mathbf{y} \in \text{Perm}[1, 2, \ldots, K]$	Plackett-Luce	ranking

Figure 5.11 Distributions for loss functions for different prediction types.

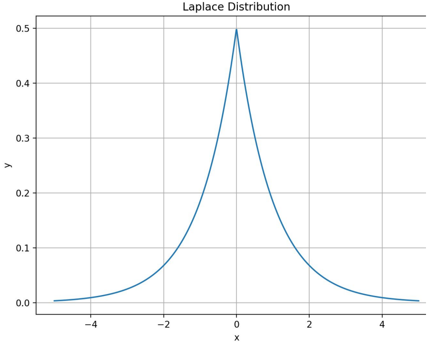
Other Distributions

Gaussian



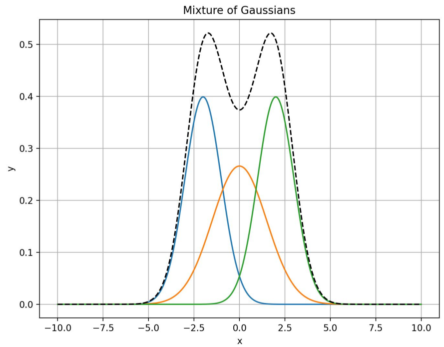
$y \in \mathbb{R}$ Regression

Laplace



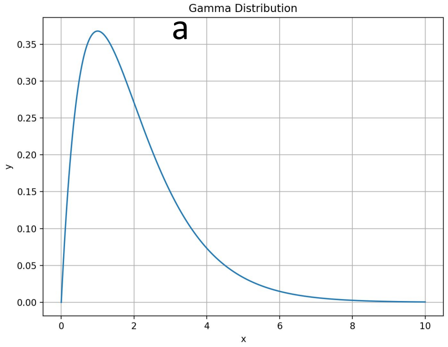
$y \in \mathbb{R}$ Robust Regression

Mixture of Gaussians



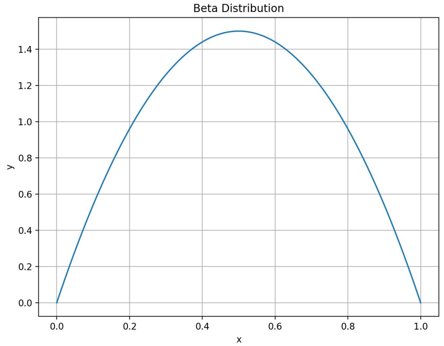
$y \in \mathbb{R}$ Multimodal Regression

Gamma



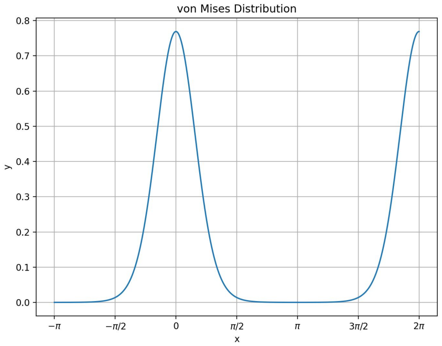
$y \in \mathbb{R}^+$ Predict Magnitude

Beta



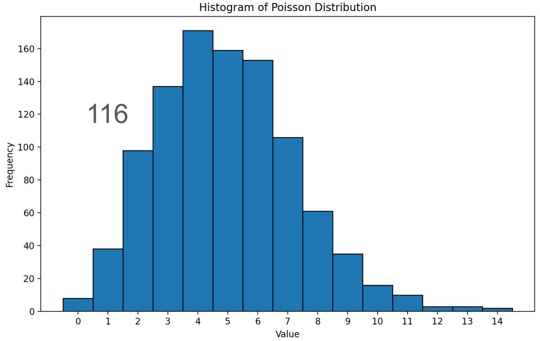
$y \in [0,1]$ Predict Proportions

Von Mises



$y \in (-\pi, \pi]$ Predict Directions

Poisson



$y \in [0,1,2,\ldots]$ Predict Event Counts

Loss functions

- Maximum likelihood
- Recipe for loss functions
- Example 1: univariate regression
- Example 2: binary classification
- Example 3: multiclass classification
- Other types of data
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- Cross entropy

Multiple outputs

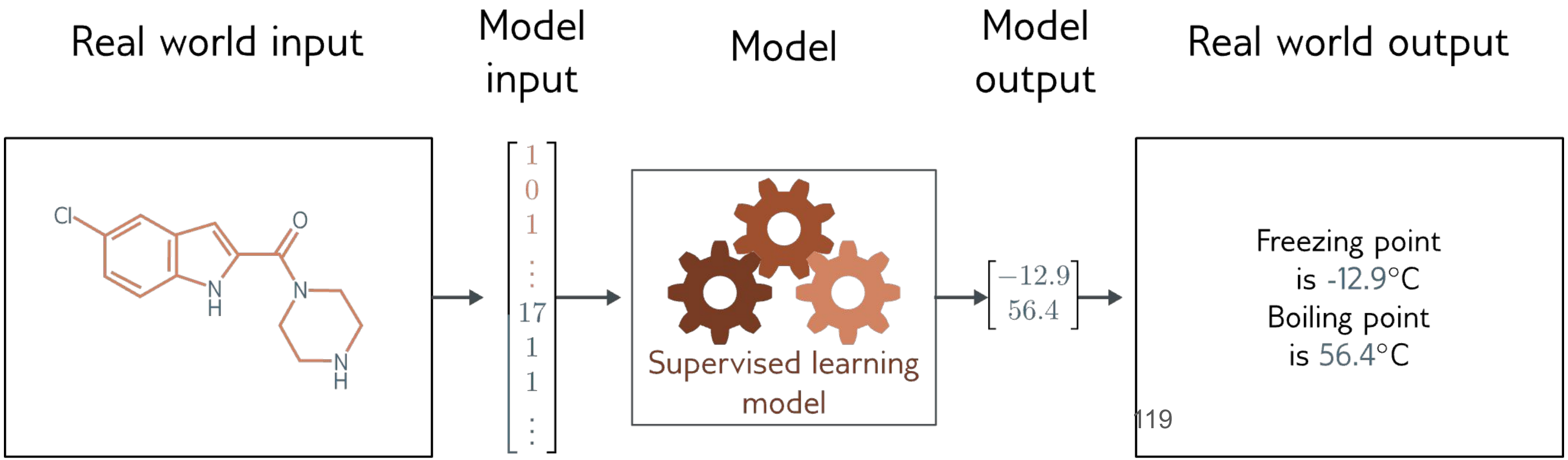
- Treat each output y_d as independent:

$$Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}_i, \phi]) = \prod_d Pr(y_d|\mathbf{f}_d[\mathbf{x}_i, \phi])$$

- Negative log likelihood becomes sum of terms:

$$L[\phi] = -\sum_{i=1}^{I} \log\Big[Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}_i, \phi])\Big] = -\sum_{i=1}^{I}\sum_d \log\Big[Pr(y_{id}|\mathbf{f}_d[\mathbf{x}_i, \phi])\Big]$$

Example 4: multivariate regression



Example 4: multivariate regression

- Goal: to predict a multivariate target $\mathbf{y} \in \mathbb{R}^{D_o}$
- Solution treat each dimension independently

$$
\begin{aligned}
Pr(\mathbf{y}|\boldsymbol{\mu}, \sigma^2) &= \prod_{d=1}^{D_o} Pr(y_d|\mu_d, \sigma^2) \\
&= \prod_{d=1}^{D_o} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y_d - \mu_d)^2}{2\sigma^2}\right]
\end{aligned}
$$

- Make network with D_o outputs to predict means

$$
Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}], \sigma^2) = \prod_{d=1}^{D_o} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y_d - \mathrm{f}_d[\mathbf{x}, \boldsymbol{\phi}])^2}{2\sigma^2}\right]
$$

Example 4: multivariate regression

- What if the outputs vary in magnitude
  - E.g., predict weight in kilos and height in meters
  - One dimension has much bigger numbers than others
- Could learn a separate variance for each…
- …or rescale before training, and then rescale output in opposite way

Loss functions

- Maximum likelihood
- Recipe for loss functions
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- Example 2: binary classification
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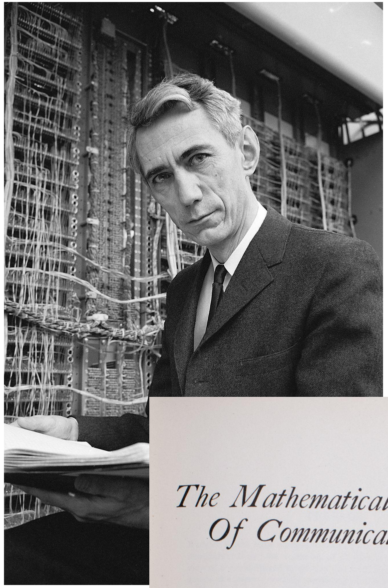
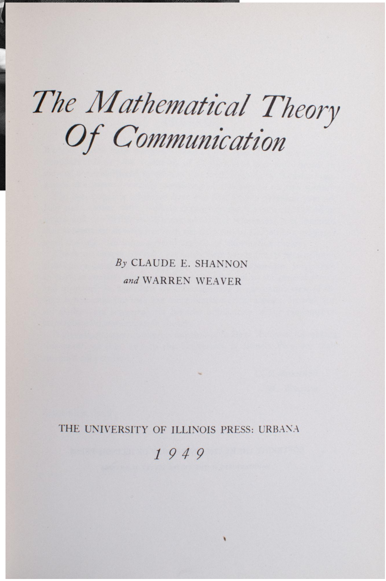
- Other types of data
- Multiple outputs
- Cross entropy

Information Theory and Entropy

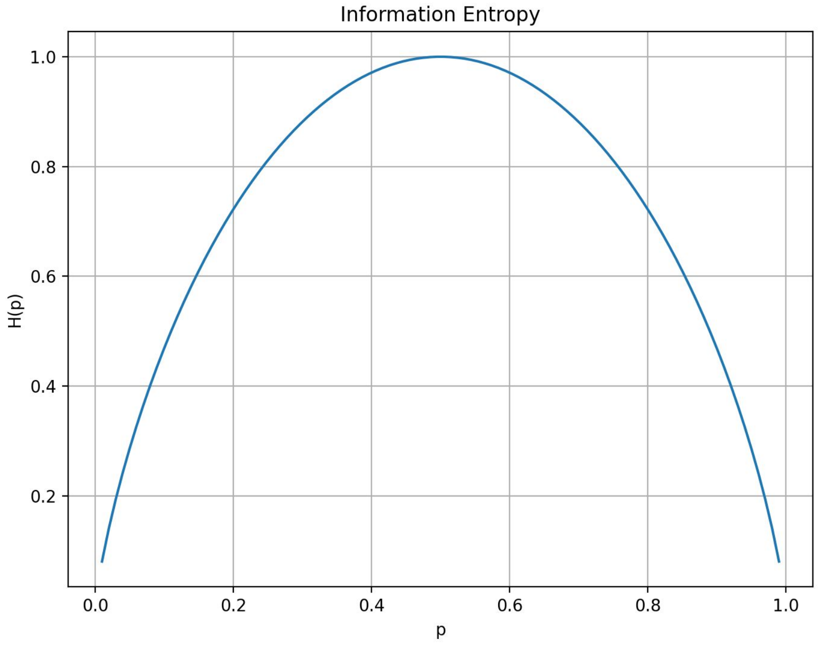
- **Claude Shannon:** the "father of information theory," was an American mathematician, electrical engineer, and cryptographer
- **Theory of Communication:** In his landmark 1948 paper, "A Mathematical Theory of Communication," Shannon introduced a formal framework for the transmission, processing, and storage of information.
- **Information Theory:** Quantified information, allowing for the measurement of information content in messages, which is crucial for data compression, error detection and correction, and more.
- **Concept of Information Entropy:** introduced entropy as a measure of the uncertainty or randomness in a set of possible messages, providing a limit on the best possible lossless compression of any communication.

$$H(x) = -\sum_{x} P(x) \log_2(P(x))$$





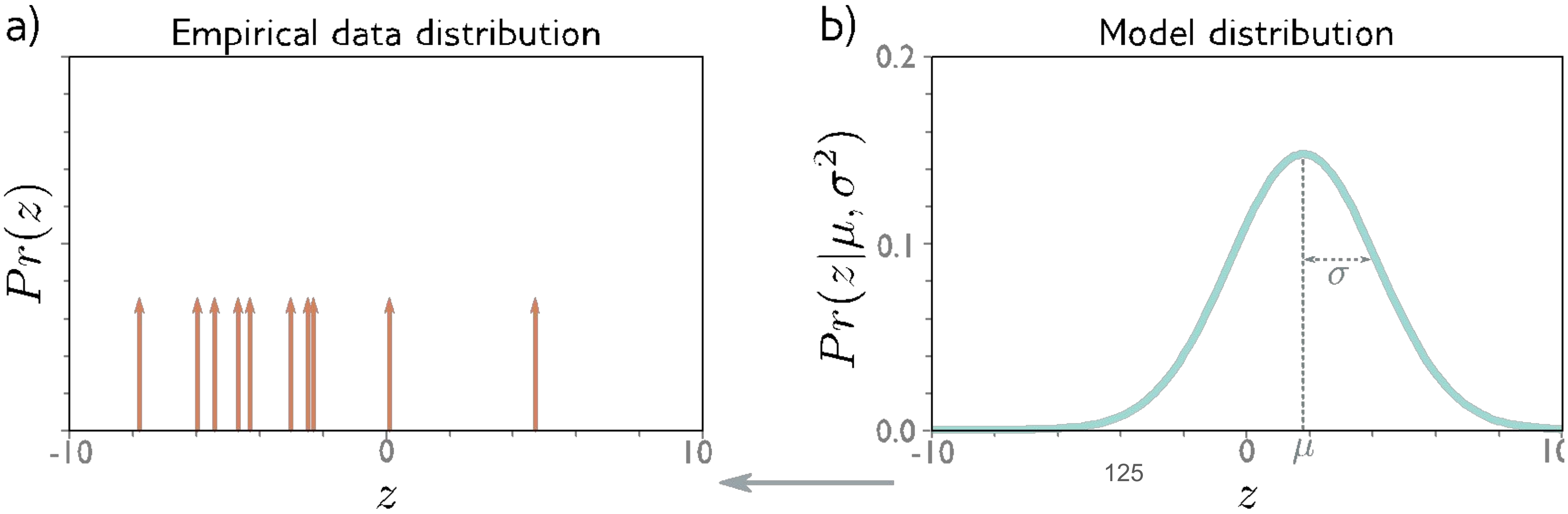
Entropy for a Binary Event $x \in \{0,1\}$



$$H(x) = -\sum_{x} P(x)\ \log_2\big(P(x)\big) = -p\log_2(p) - (1-p)\log_2(1-p)$$

Cross Entropy – Concept from Information Theory

Measures the difference between two probability distributions: the true distribution of the labels and the predicted distribution of the labels by a model.



$$\mathrm{KL}[q||p] = \int_{-\infty}^{\infty} q(z)\log[q(z)]dz - \int_{-\infty}^{\infty} q(z)\log[p(z)]dz$$

Kullback-Leibler Divergence -- a measure between probability distributions

Cross Entropy – Concept from Information Theory

- For discrete distributions, the cross-entropy between two distributions p and q over the same underlying set of events is defined as:

$$H(p,q) = -\sum p(x)\ log\ q(x)$$

Here, $p(x)$ is the true probability of an event x, and $q(x)$ is the estimated probability of the same event according to the model.

For instance, in binary classification:

$$H(p,q) = -[y\log(\hat{y}) + (1-y)\log(1-\hat{y})$$

Here, y is the true label (0 or 1), and $\hat{y}$ is the predicted probability of the class being 1.

Recap

- Reconsidered loss functions as fitting a parametric probability model
- Introduced Maximum Likelihood criterion for finding parameters to making the training data most probably under that model
- Introduced a 4-step recipe for (1) picking a suitable parametric probability distribution, (2) defining the model to pick one or more of the parameters, (3) training the model and (4) doing inference
- Derived loss functions for univariate regression, binary and multiclass classification
- Briefly reviewed parametric probability models for other types of data
- Discussed how this is the same as Cross Entropy from Information Theory

Minimizing Negative Log Likelihood

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\Pr(\mathrm{y}_i \mid \mathrm{f}[\mathrm{x}_i, \phi])\right]\right]$$

$$= \underset{\phi}{\operatorname{argmin}}\left[L[\phi]\right]$$

Recipe for loss functions

1. Choose a suitable probability distribution $\Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.
2. Set the machine learning model $\mathbf{f}[\mathbf{x}, \phi]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \phi]$ and $\Pr(\mathbf{y} \mid \mathbf{f}[\mathbf{x}, \phi])$.
3. To train the model, find the network parameters $\hat{\phi}$ that minimize the negative log-likelihood loss function over the training dataset pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}}\big[L[\phi]\big] = \underset{\phi}{\operatorname{argmin}}\left[-\sum_{i=1}^{I} \log[\Pr(\mathrm{y}_i \mid \mathrm{f}[\mathrm{x}_i, \phi])]\right]$$

4. To perform inference for a new test example x, return either the full distribution $\Pr(\mathbf{y} \mid \mathbf{f}[\mathbf{x}, \phi])$ or the maximum of this distribution.

Next up

- Now let's find the parameters that give the smallest loss
  - Training the model

Feedback?