Deep Learning for Data Science
DS 542

https://dl4ds.github.io/sp2026/

Loss Functions

Gardos and Considine,
other content from Understanding Deep Learning unless otherwise cited

Recap

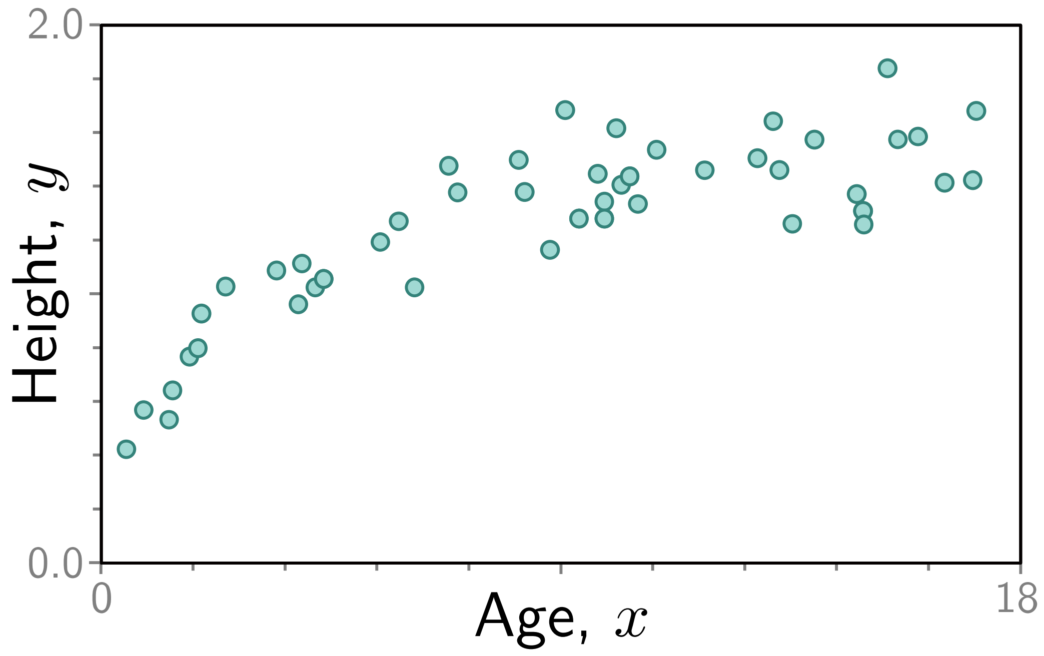
- Last time we talked about supervised learning with the example of linear regression.
- Models have parameters, ϕ, that we want to choose for a best possible mapping between input and output training data
- A loss function or cost function, $L[\phi]$, returns a single number that describes a mismatch between $f[x_i, \phi]$ and the ground truth outputs, y_i.

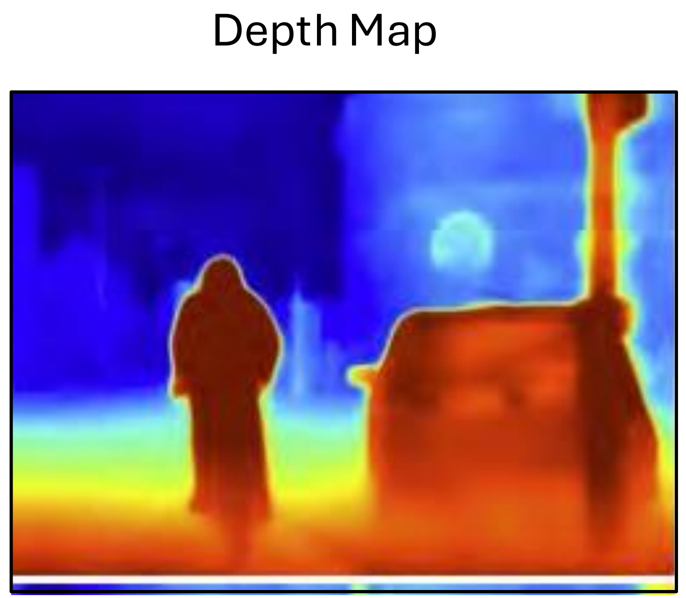
Plan for Today

- Use cases for loss functions
- Maximum likelihood approach
- Deriving common loss functions
  - Real-valued univariate regression
  - Binary classification
  - Multiclass classification
  - Multiple outputs (if extra time)
- Connections to cross entropy (if extra time)

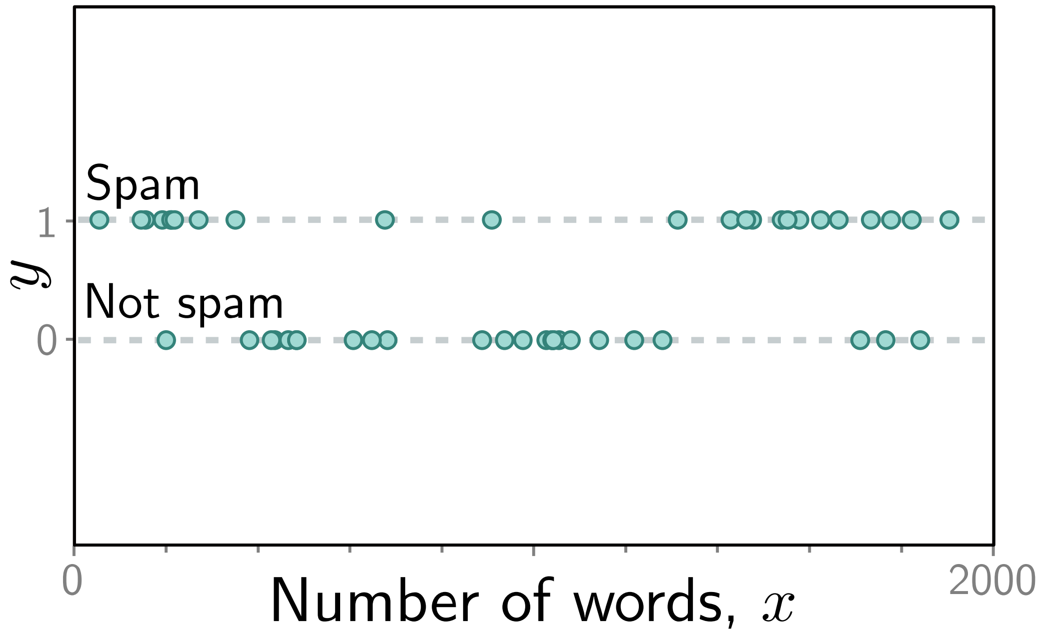
How do we choose a loss function?

Univariate and Multivariate Regression

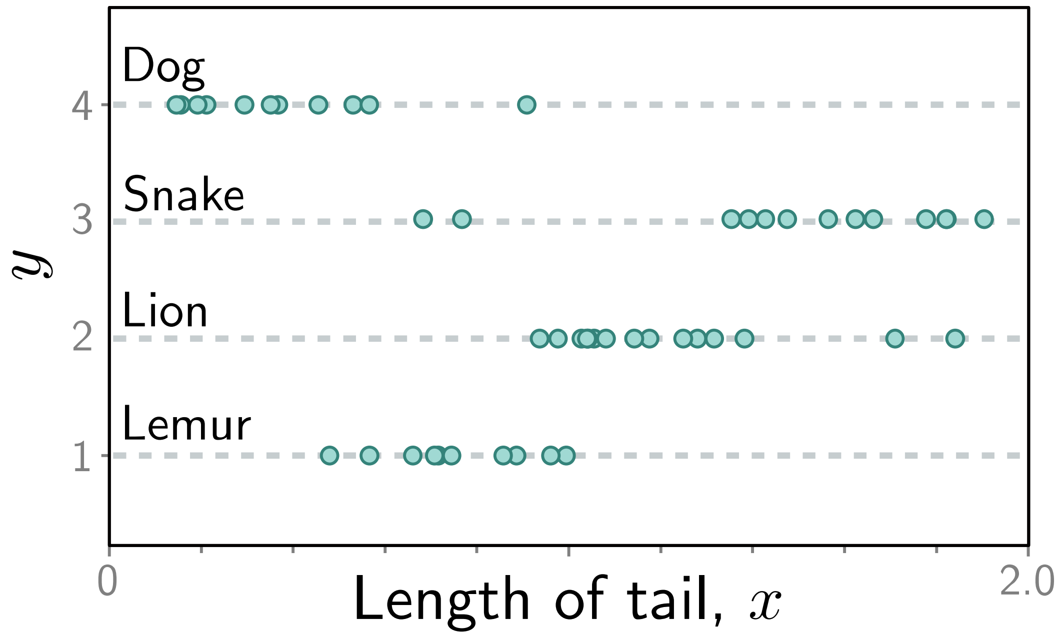


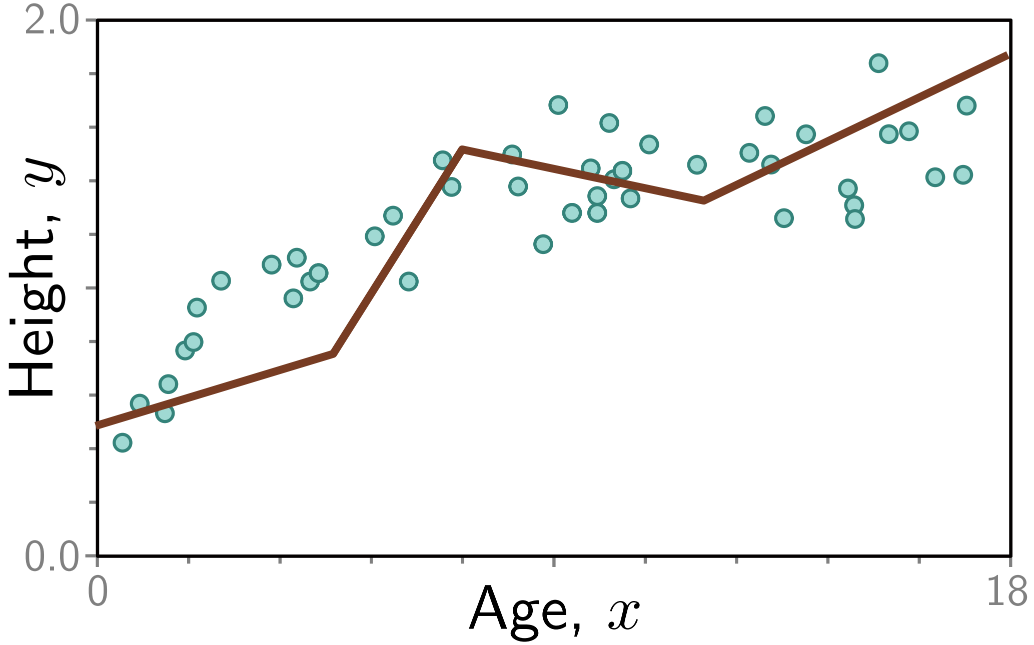


Binary Classification



Multiclass Classification





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

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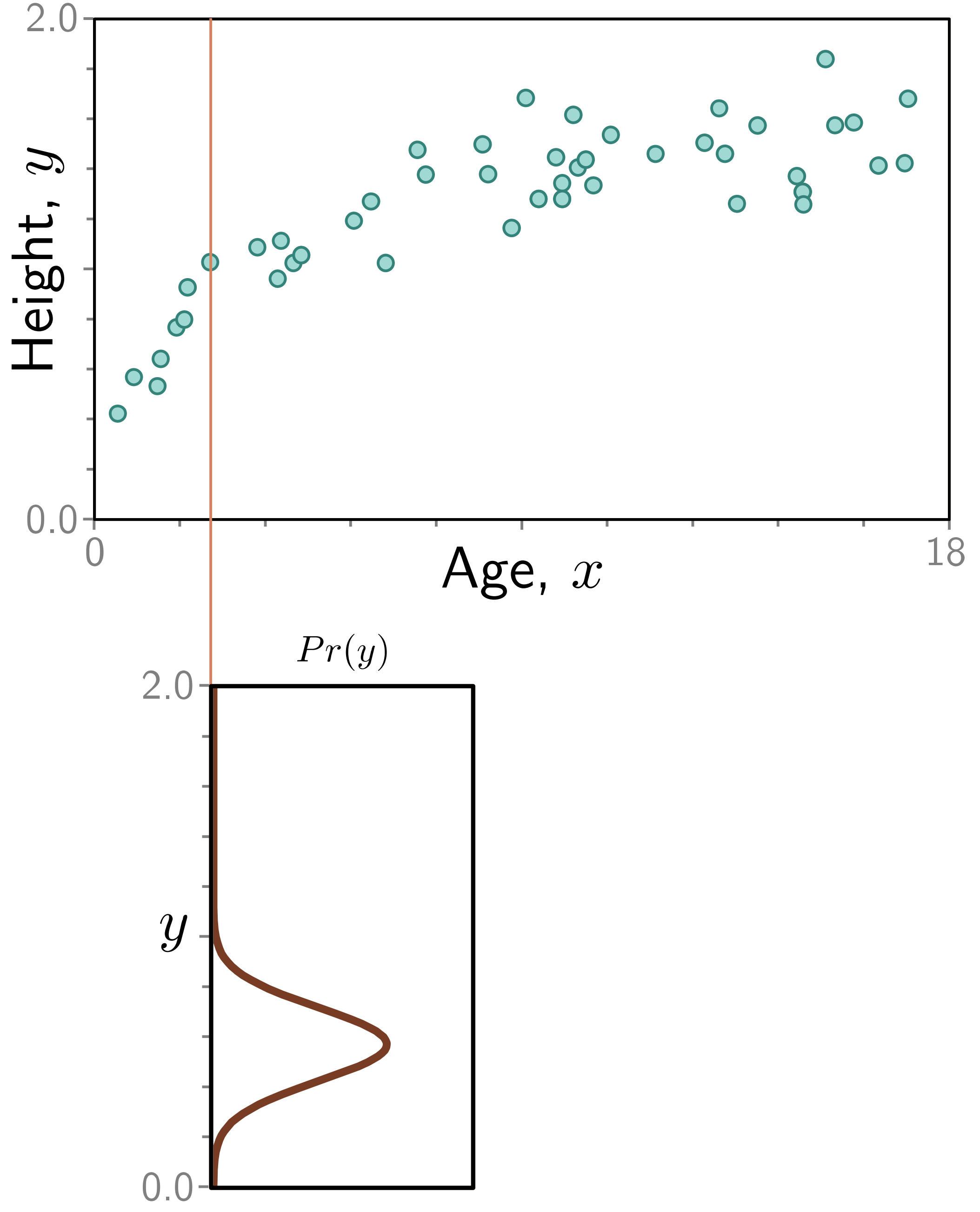
Competing Takes on Loss Functions

1. How bad are my model estimates on average?
   - Model predicts a specific value.
   - Loss function compares that value to the ground truth.

2. How likely did my model think the actual result was?
   - Model predicts a probability distribution.
   - Loss function checks likelihood of ground truth from that distribution.



Suppose we fit a *probability model* to this data, and outputs conditional probability distribution

$$\Pr(y|x = 2.8)$$

Isn't this a better fit for the reality?

Probability Approach Suggests 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*.

- This will directly suggest choices of loss functions.

How do we do this?

- Model predicts a conditional probability distribution:

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

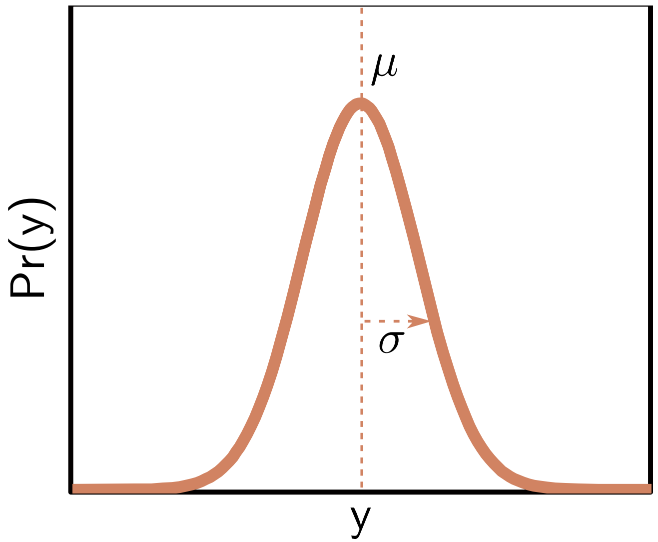
  over outputs $\boldsymbol{y}$ given inputs $\boldsymbol{x}$.

- 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 θ.

   e.g., the normal distribution $\theta = \{\mu, \sigma^2\}$



2. Use model to predict parameters θ 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.

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

Two simplifying assumptions

$$\Pr(y_1, y_2, \ldots, y_I | x_1, x_2, \ldots, x_I) = \underbrace{\prod_{i=1}^{I} \overbrace{\Pr(y_i | x_i)}^{\text{Identically distributed (the form of the probably distribution is the same for each input/output pair)}}}_{\text{Independent}}$$

Independent and identically distributed (i.i.d)

Maximum likelihood criterion

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

θ_i are the parameters of the probability distribution

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

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

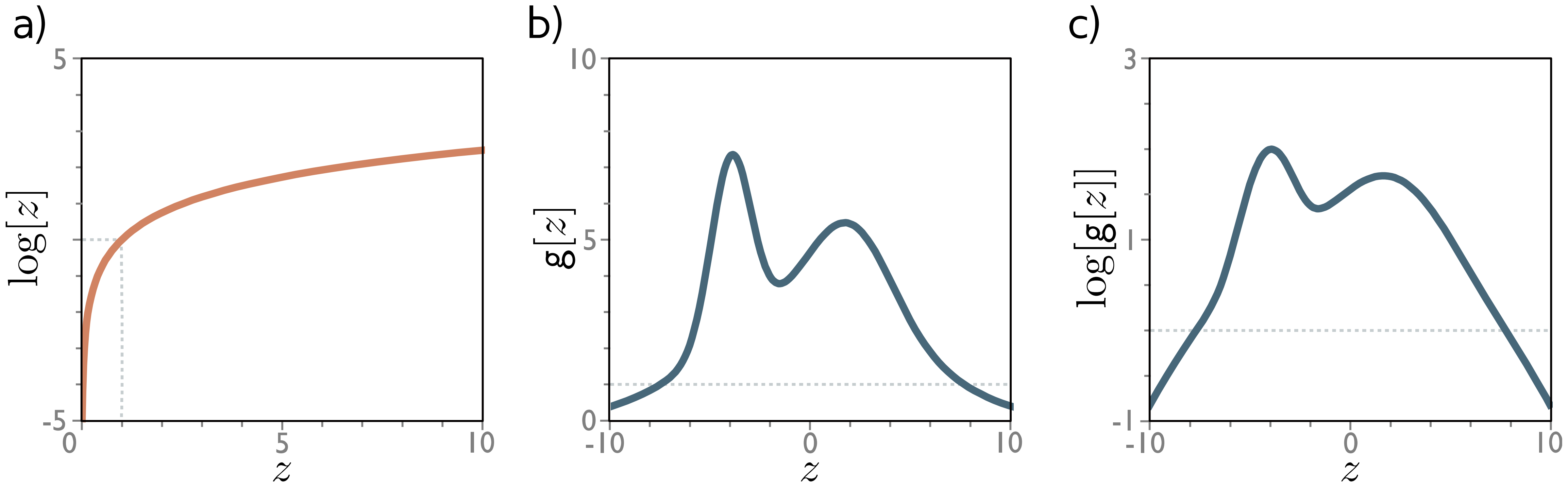
When we consider this probability as a function of the parameters ϕ, we call it a likelihood.

Practical 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, $0 \leq \Pr(\cdot) \leq 1$
- The product might get so small that we *can't* easily represent it in fixed precision arithmetic

The log function is monotonic



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

Maximum log likelihood

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

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

Minimizing negative log likelihood

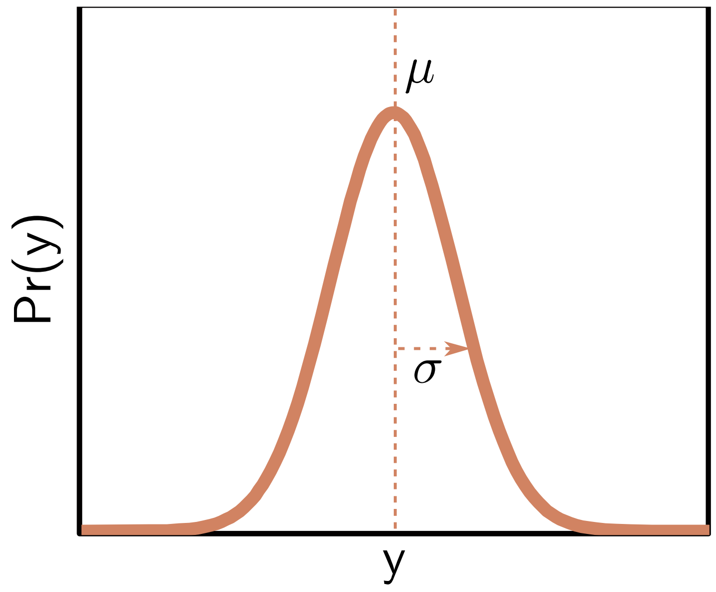
- By convention, we minimize things (i.e., a loss)

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

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)

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



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 $\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$ to predict one or more of these parameters so $\boldsymbol{\theta} = \mathbf{f}[\mathbf{x}, \boldsymbol{\phi}]$ and $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}])$.
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 $\{\mathbf{x}_i, \mathbf{y}_i\}$:

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

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.

Plan for Today

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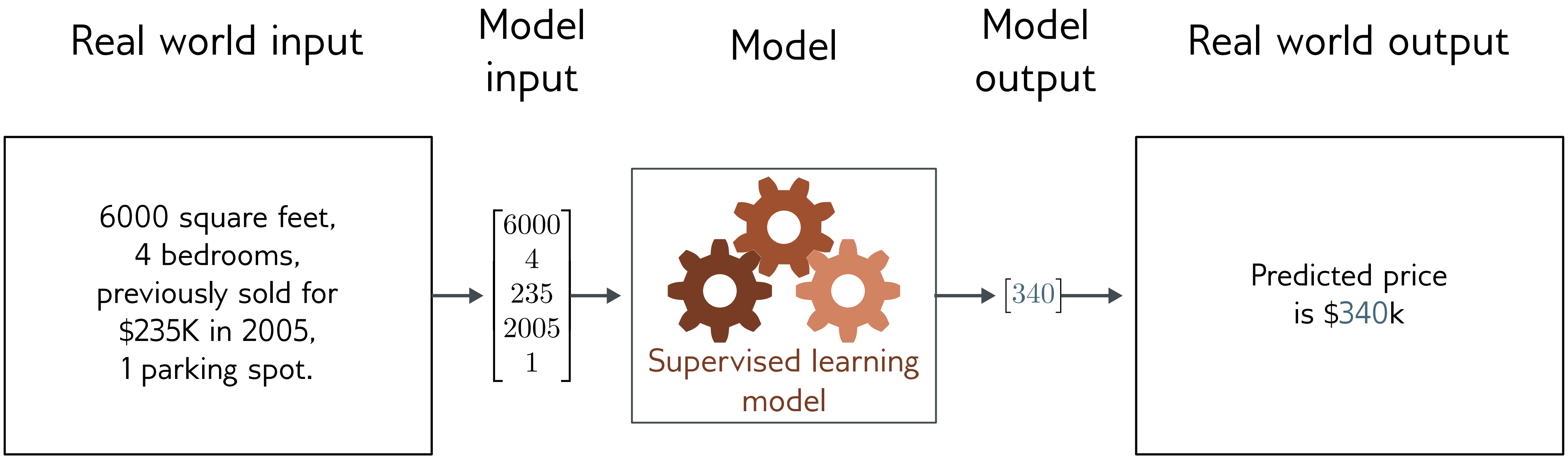
Example 1: univariate regression

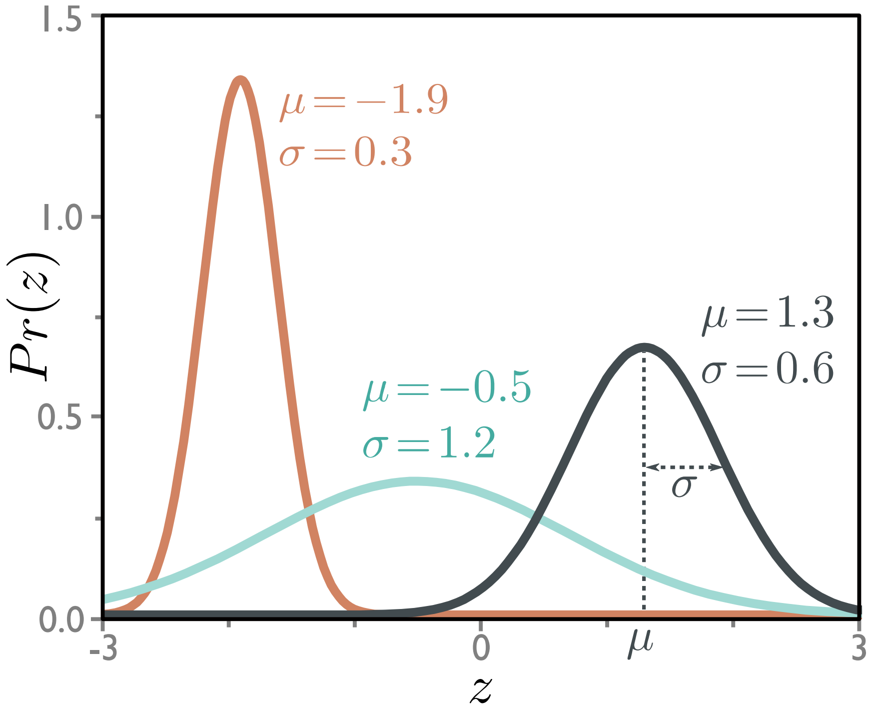


Example 1: univariate regression

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

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

In this case, just the mean

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

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

Example 1: univariate regression

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

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

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

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

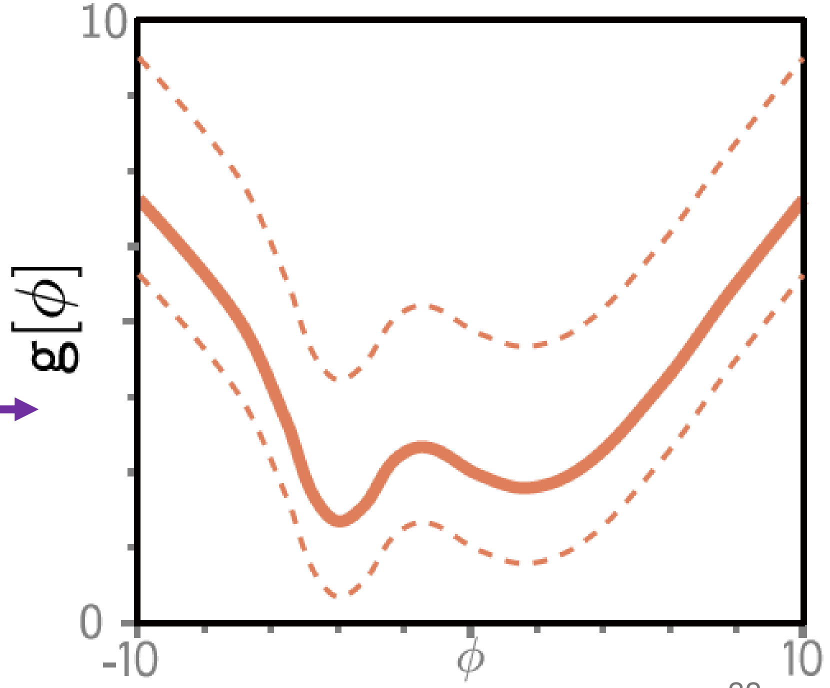
$$
\log[a\cdot b] = \log[a] + \log[b]
$$

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

$\log[\exp[x]] = x$

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

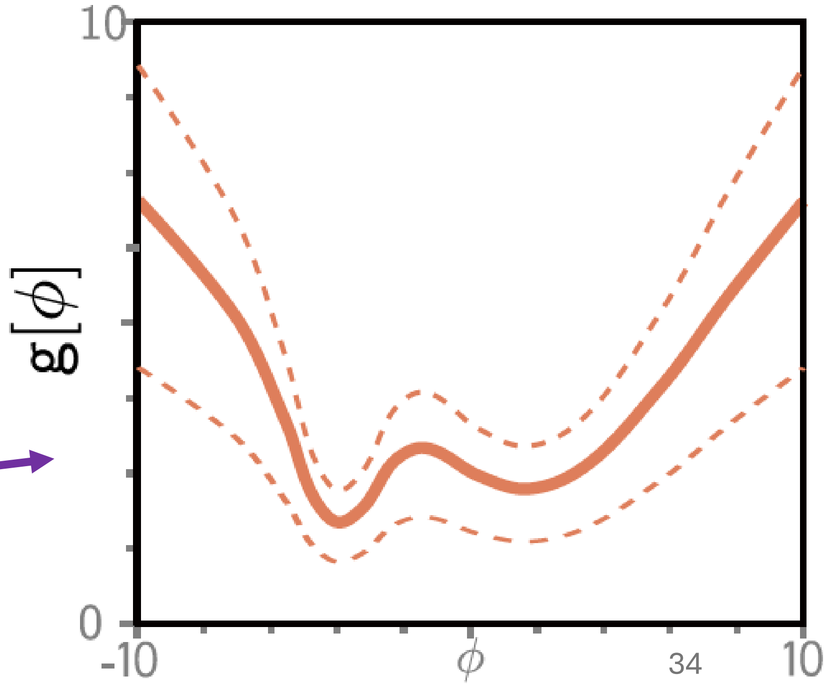
Just a constant offset



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

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

Just dividing by a positive constant

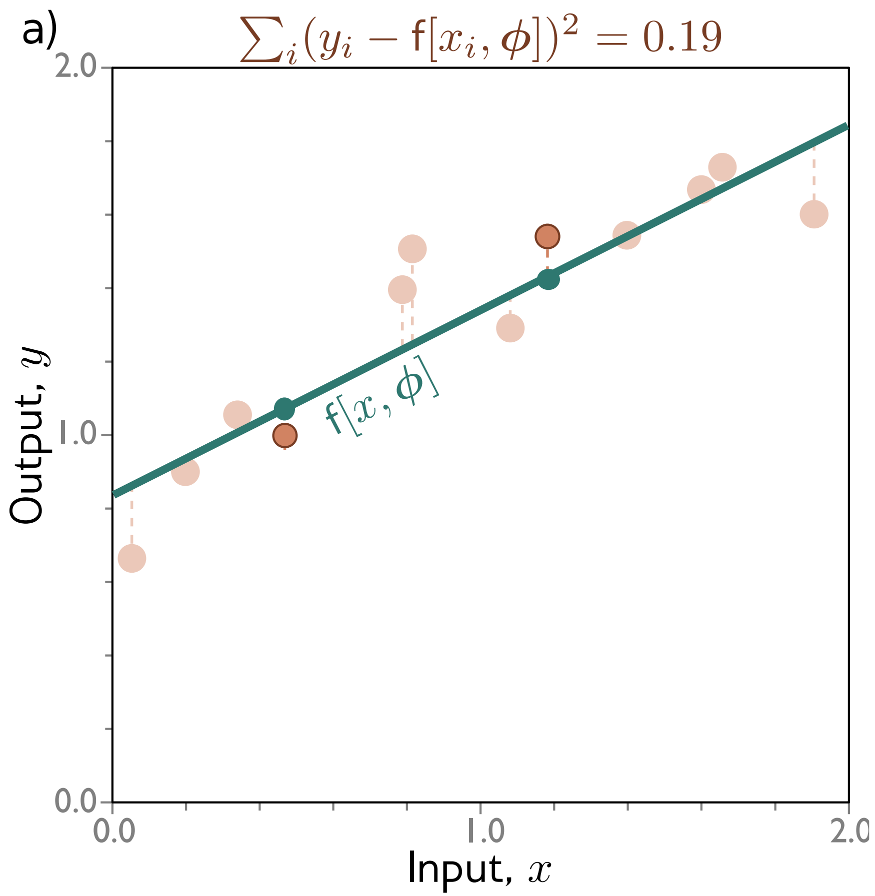


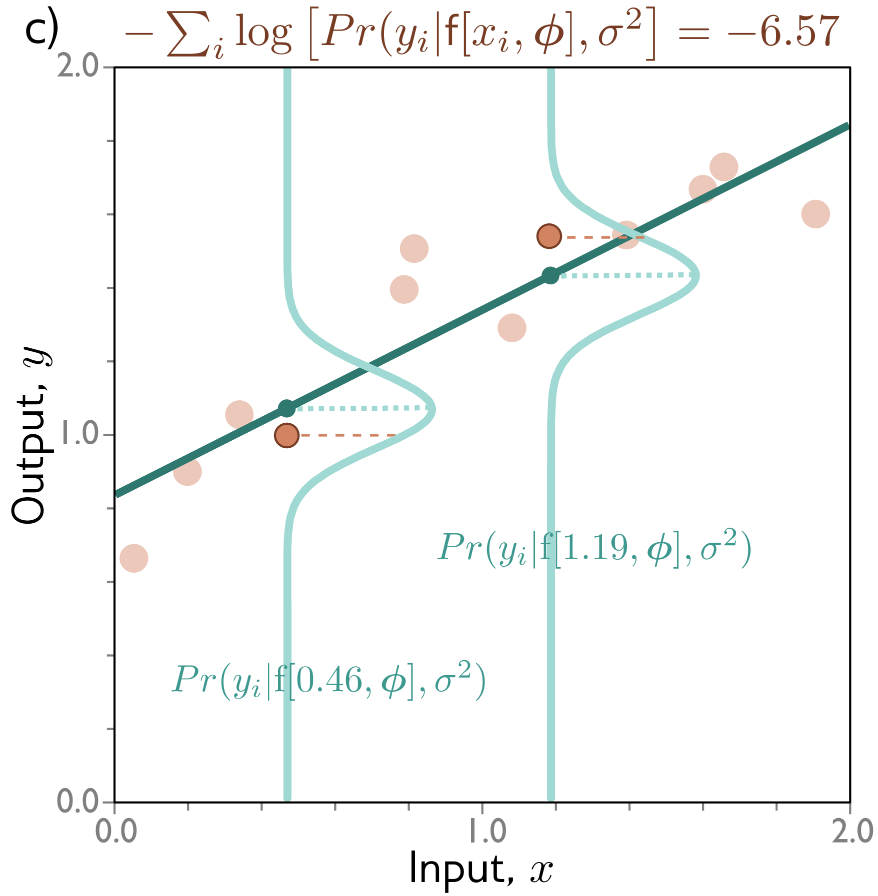
$$
\begin{aligned}
\hat{\boldsymbol{\phi}} &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y_i-\mathrm{f}[\mathbf{x}_i,\boldsymbol{\phi}])^2}{2\sigma^2}\right]\right]\right]\\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\left[-\sum_{i=1}^{I}\log\left[\frac{1}{\sqrt{2\pi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

Least squares!

Least squares

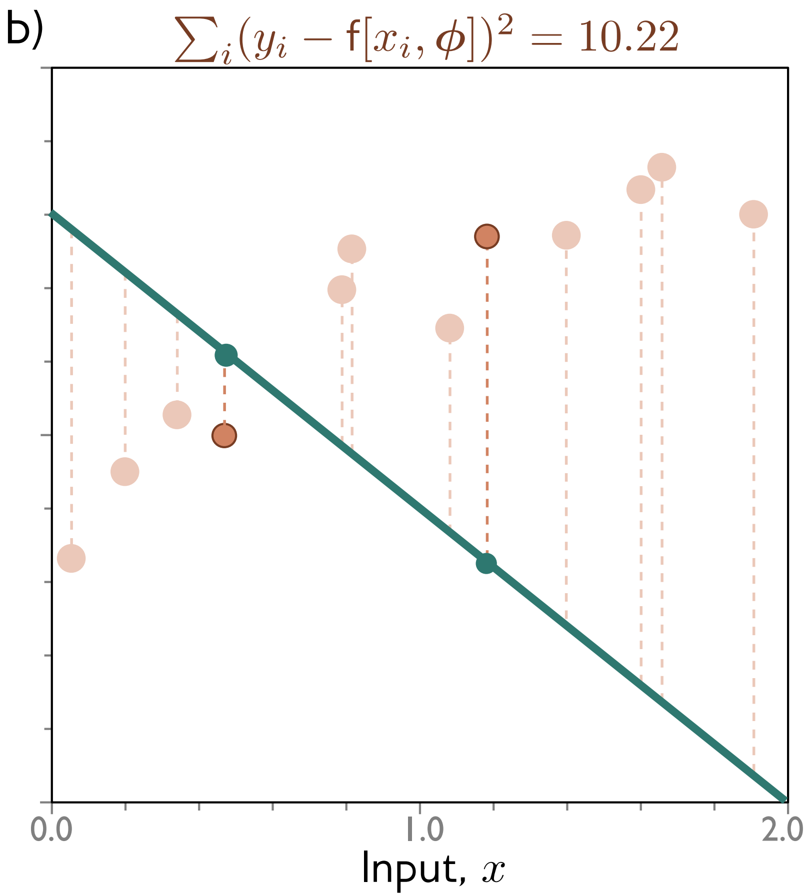
Negative log likelihood

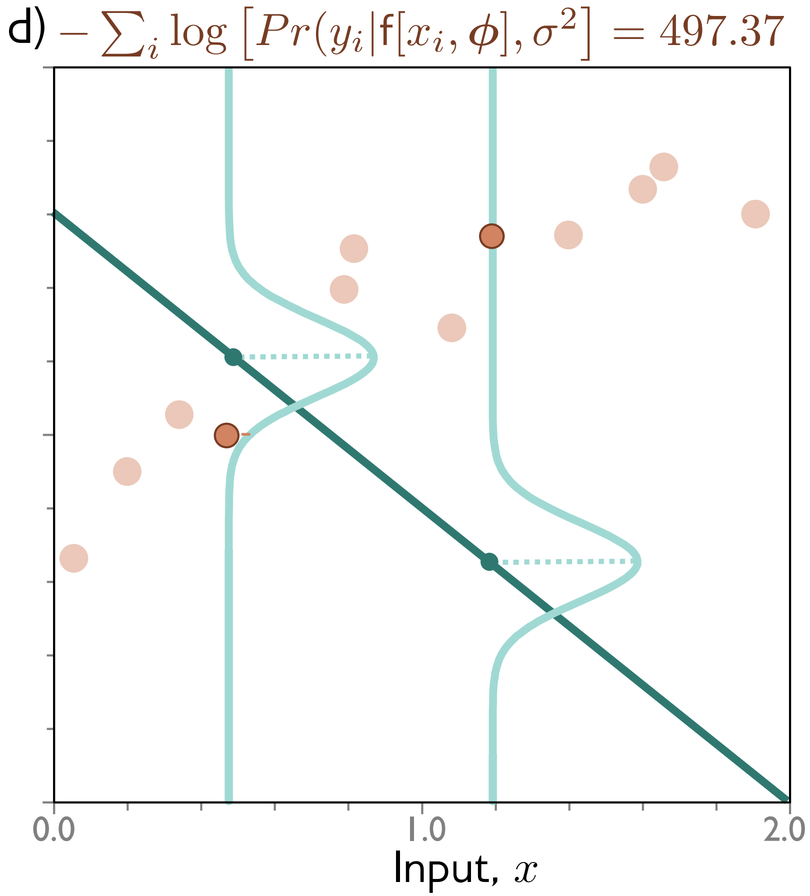




Least squares

Maximum likelihood





Example 1: univariate regression

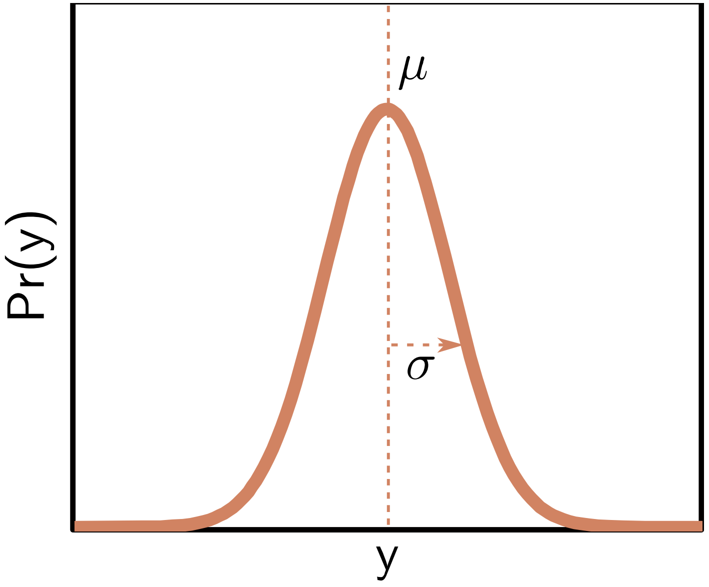
4. To perform inference for a new test example $\mathbf{x}$, return either the full distribution $Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \hat{\phi}])$ or the maximum of this distribution.

Full distribution:

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

Max probability:

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



Estimating variance

- Perhaps surprisingly, the variance term disappeared:

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

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

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

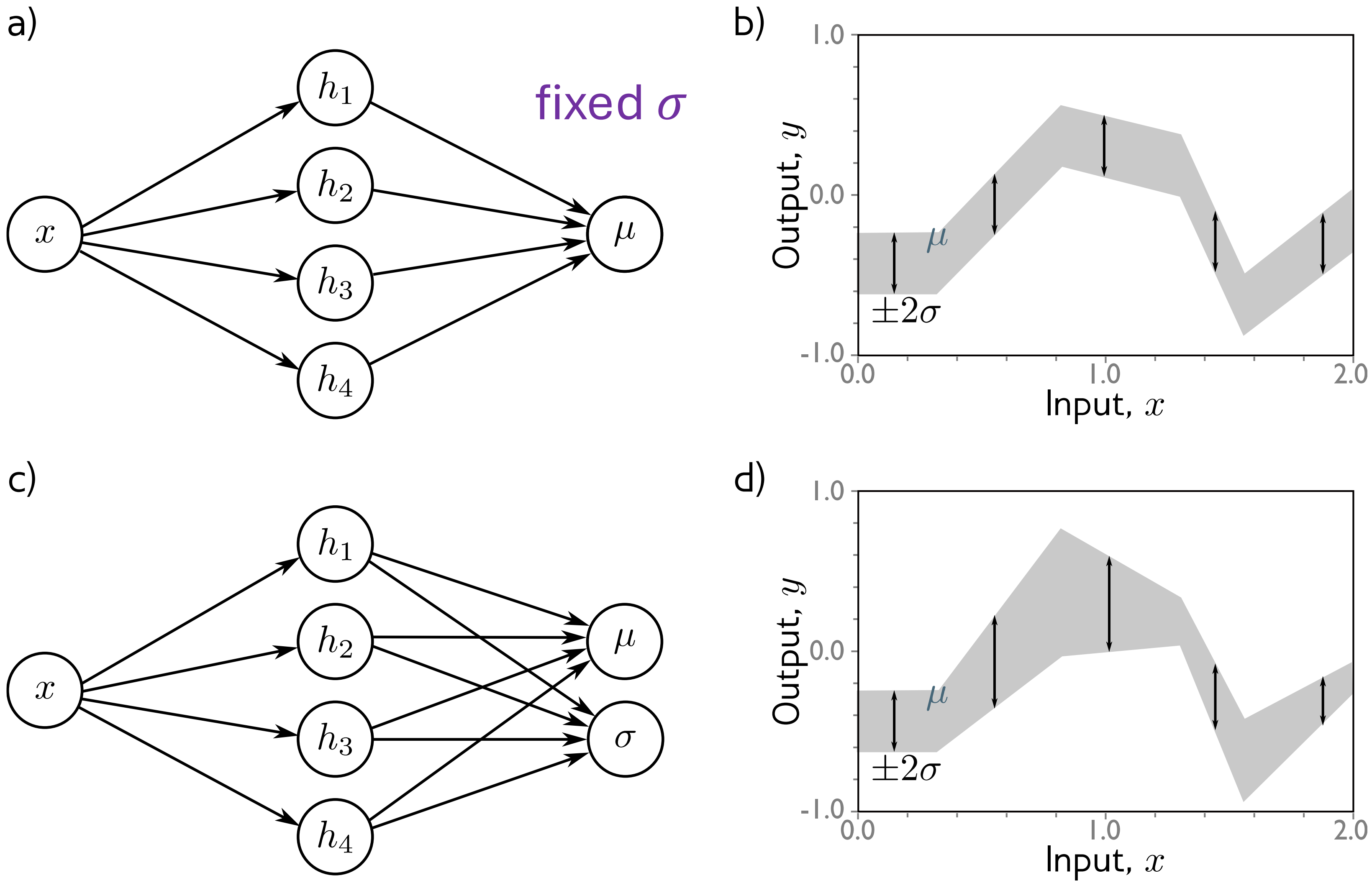
- We were assuming that the noise σ^2 is the same everywhere (homoscedastic).
- But we could make the noise a function of the data *x*.
- Build a model with two outputs:

$$\mu = \mathrm{f}_1[\mathbf{x}, \phi]$$
$$\sigma^2 = \mathrm{f}_2[\mathbf{x}, \phi]^2$$

Squared to ensure it is positive

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

Heteroscedastic regression



Example 1: Univariate Regression Takeaways

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

Plan for Today

- Use cases for loss functions
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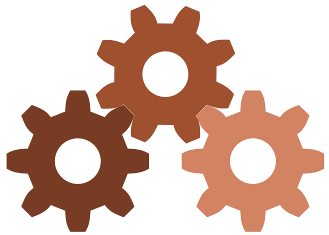
- Deriving common loss functions
  - Real-valued univariate regression
  - Binary classification
  - Multiclass classification
  - Multiple outputs (if extra time)
- Connections to cross entropy (if extra time)

Example 2: binary classification

Real world input	Model input	Model	Model output	Real world output
"The steak was terrible, the salad was rotten, and the soup tasted like socks"	$\begin{bmatrix} 8672 \\ 8194 \\ 9804 \\ 8634 \\ 8672 \\ \vdots \end{bmatrix}$	 Supervised learning model	$\begin{bmatrix} 0.02 \\ 0.98 \end{bmatrix}$	Positive Negative

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

Example 2: binary classification

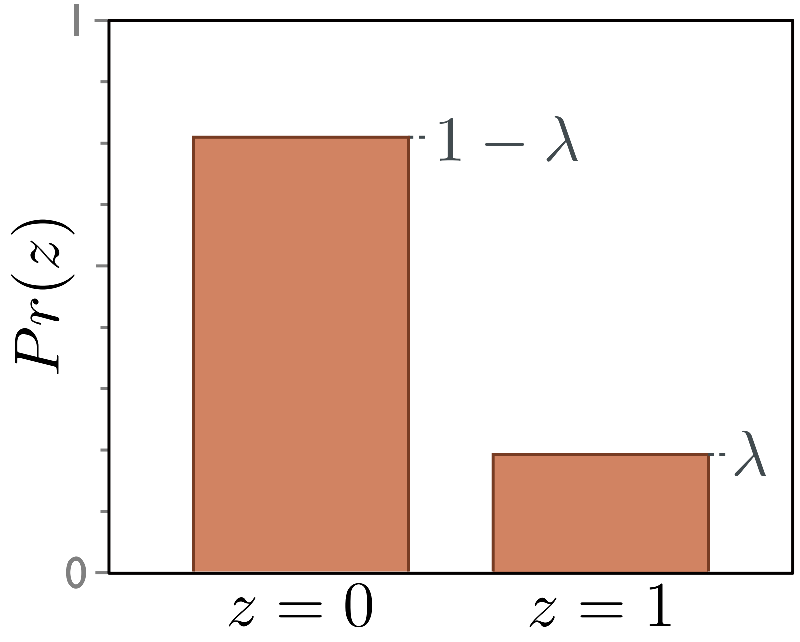
1. Choose a suitable probability distribution $Pr(\mathbf{y}|\boldsymbol{\theta})$ that is defined over the domain of the predictions $\mathbf{y}$ and has distribution parameters $\boldsymbol{\theta}$.

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

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

or

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



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 most models 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 $Pr(\mathbf{y}|\boldsymbol{\theta}) = Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}])$.

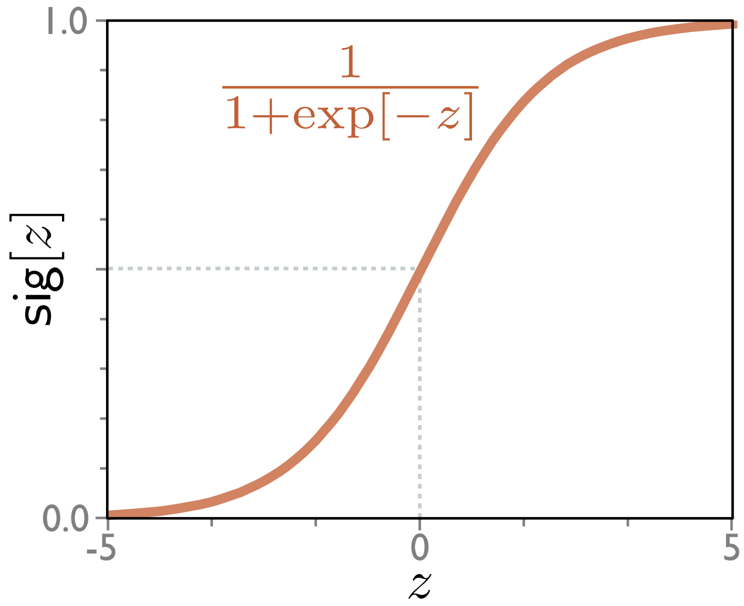
Problem:

- 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

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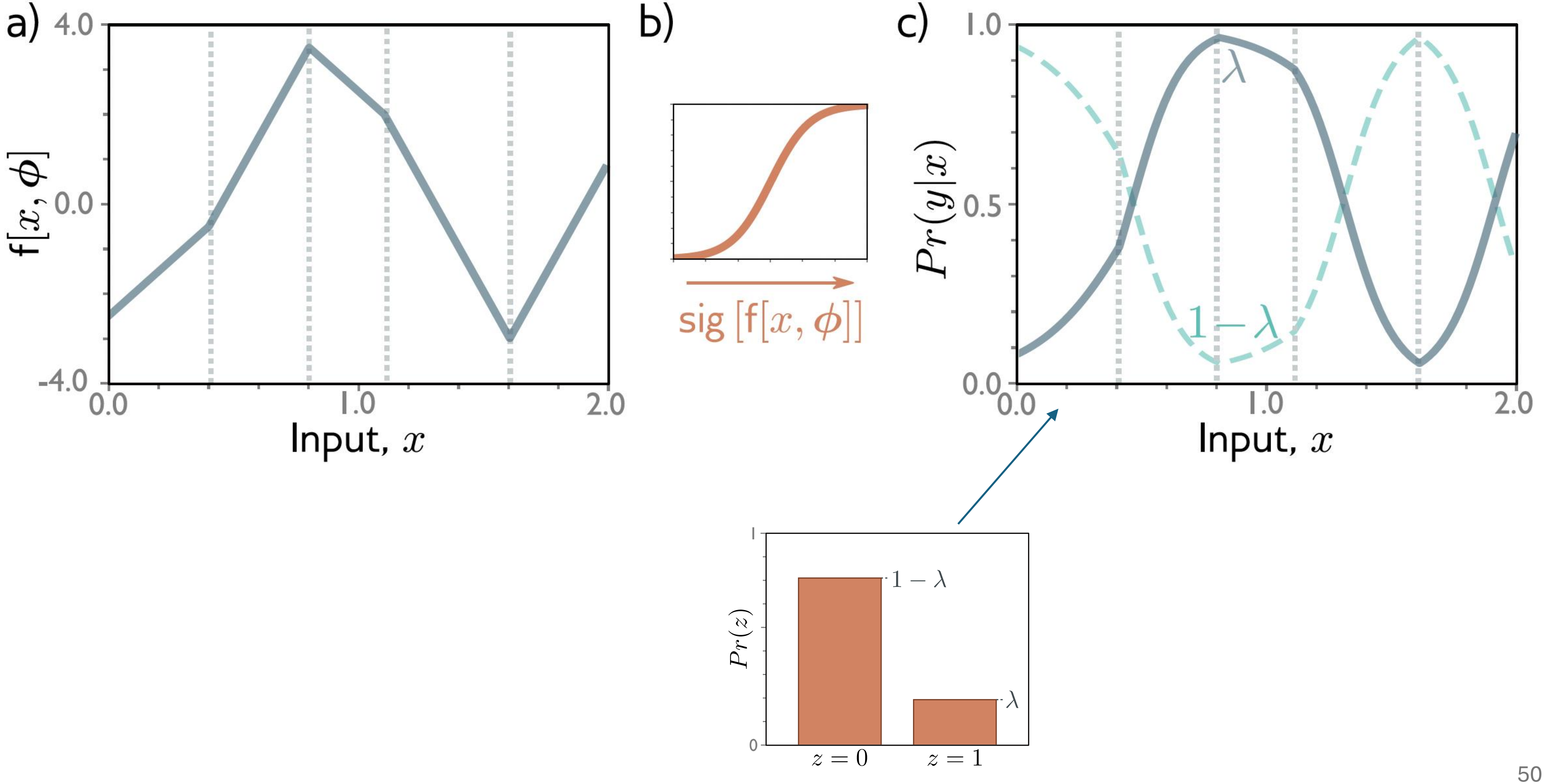
$$Pr(y|\lambda) = (1-\lambda)^{1-y} \cdot \lambda^{y}$$

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

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 $\{\mathbf{x}_i, \mathbf{y}_i\}$:

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

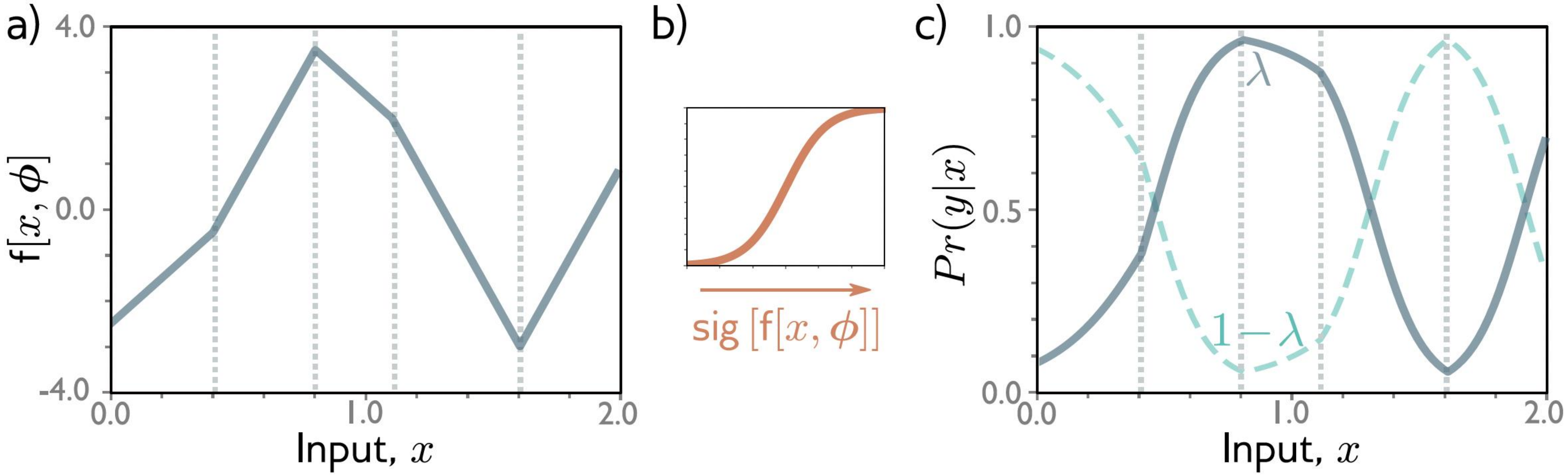
$$Pr(y|\mathbf{x}) = (1 - \text{sig}[\text{f}[\mathbf{x}|\boldsymbol{\phi}]])^{1-y} \cdot \text{sig}[\text{f}[\mathbf{x}|\boldsymbol{\phi}]]^{y}$$

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

Also called binary cross-entropy loss as it is result from cross-entropy loss calculation – discussed later.

Example 2: binary classification

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



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

And we get a probability estimate!

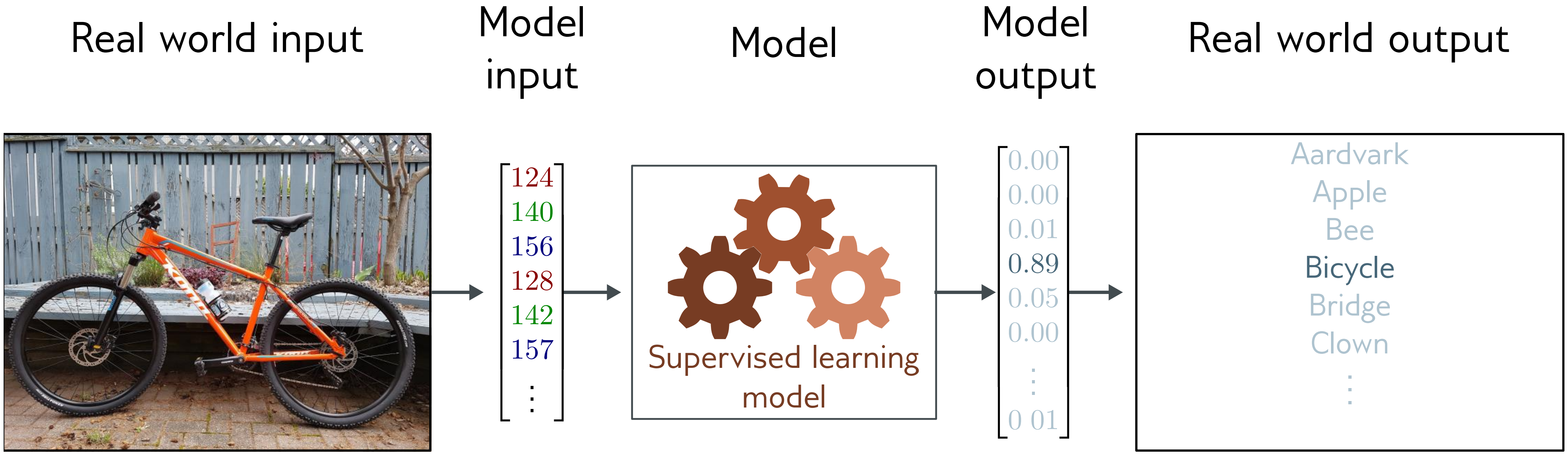
Example 2: Binary Classification Takeaways

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

Plan for Today

- Use cases for loss functions
- Maximum likelihood approach
- Deriving common loss functions
  - Real-valued univariate regression
  - Binary classification
  - Multiclass classification
  - Multiple outputs (if extra time)
- Connections to cross entropy (if extra time)

Example 3: multiclass classification



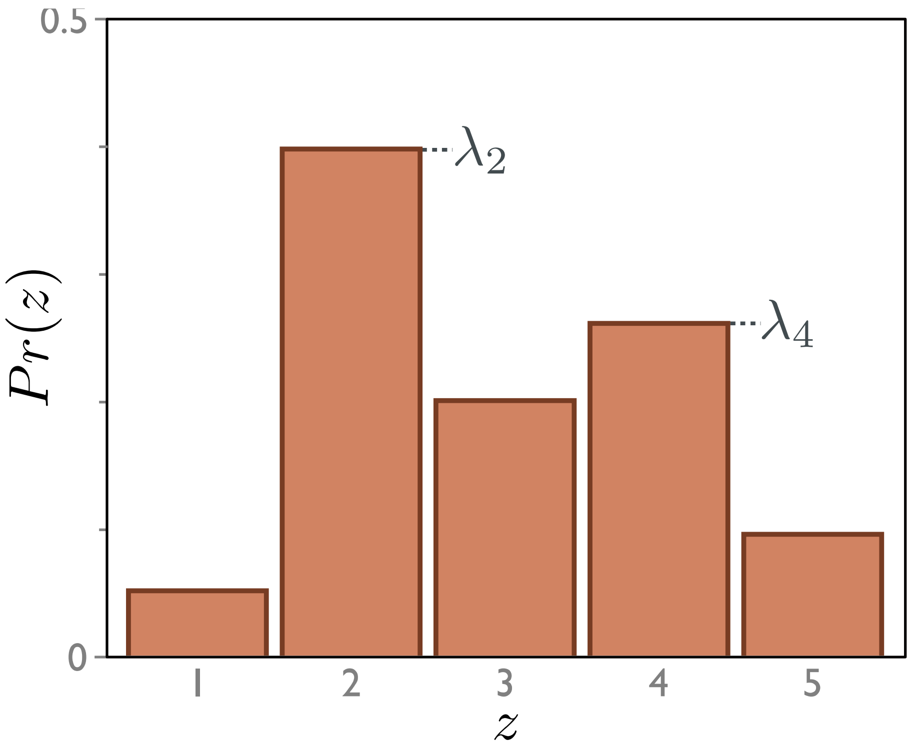
Goal: predict which of K classes $y \in \{1, 2, \ldots, K\}$ the input x belongs to.

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 $\lambda_k \in [0, 1]$
- $\sum_k \lambda_k = 1$

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



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Problem:

- Output of neural network can be anything
- Parameters λ_k ∈[0,1], sum to one

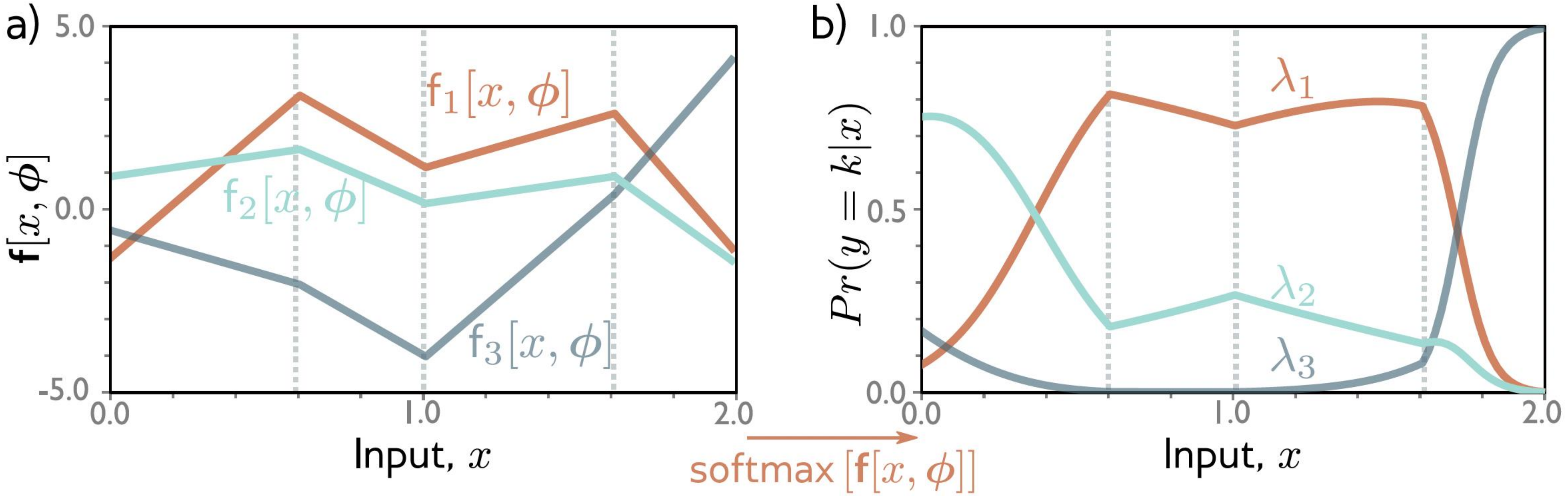
$$\text{softmax}_k[\mathbf{z}] = \frac{\exp[z_k]}{\sum_{k'=1}^{K} \exp[z_{k'}]}$$

Solution:

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

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

Example 3: multiclass classification



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$$\begin{aligned} L[\phi] &= -\sum_{i=1}^{I} \log \left[\operatorname{softmax}_{y_i} \left[\mathbf{f}\left[\mathbf{x}_i, \phi\right] \right] \right] \\ &= -\sum_{i=1}^{I} \mathrm{f}_{y_i}\left[\mathbf{x}_i, \phi\right] - \log \left[\sum_{k=1}^{K} \exp\left[\, \mathrm{f}_k\left[\mathbf{x}_i, \phi\right] \right] \right] \end{aligned}$$

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

Multiclass cross-entropy loss

Example 3: multiclass classification

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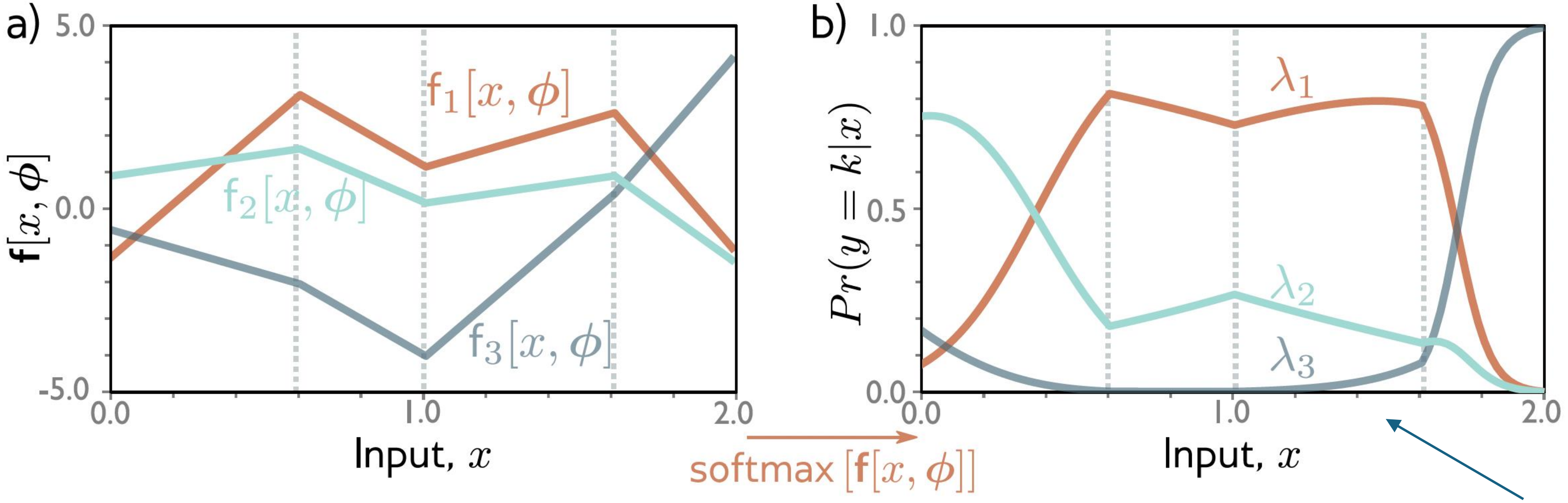

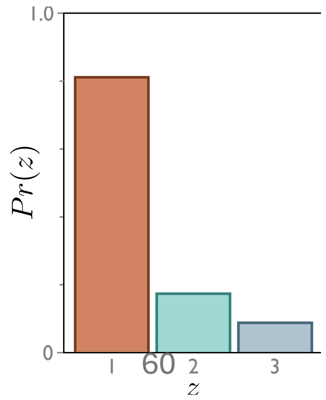

Choose the class with the largest probability
We also get probability or "confidence"

Plan for Today

- Use cases for loss functions
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- Connections to cross entropy (if extra time)

Multiple outputs

- Treat each output y_d as *independent*:

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

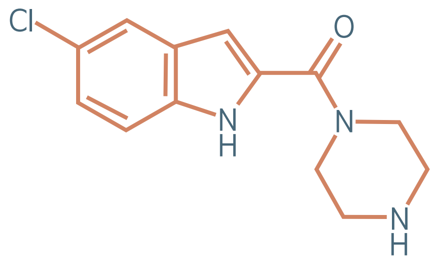
where $\mathbf{f}_d[\mathbf{x},\phi]$ is the d^{th} set of network outputs

- Negative log likelihood becomes sum of terms:

$$L[\boldsymbol{\phi}] = -\sum_{i=1}^{I}\log\Big[Pr(\mathbf{y}|\mathbf{f}[\mathbf{x}_i,\boldsymbol{\phi}])\Big] = -\sum_{i=1}^{I}\sum_{d}\log\Big[Pr(\underbrace{y_{id}}_{d^{th}\text{output of the } i^{th} \text{ training example}}|\mathbf{f}_d[\mathbf{x}_i,\boldsymbol{\phi}])\Big]$$

Example 4: multivariate regression

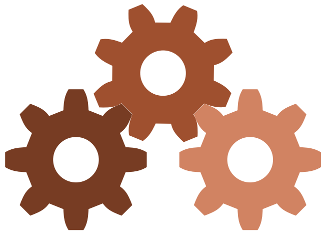
Real world input



Model input

$$\begin{bmatrix} 1 \\ 0 \\ 1 \\ \vdots \\ 17 \\ 1 \\ 1 \\ \vdots \end{bmatrix}$$

Model



Supervised learning model

Model output

$$\begin{bmatrix} -12.9 \\ 56.4 \end{bmatrix}$$

Real world output

Freezing point is -12.9°C
Boiling point is 56.4°C

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

Plan for Today

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- Connections to cross entropy (if extra time)

Cross-entropy loss

- So far we defined loss functions that minimize negative log-likelihood.

- Cross-entropy loss is common in neural network training.

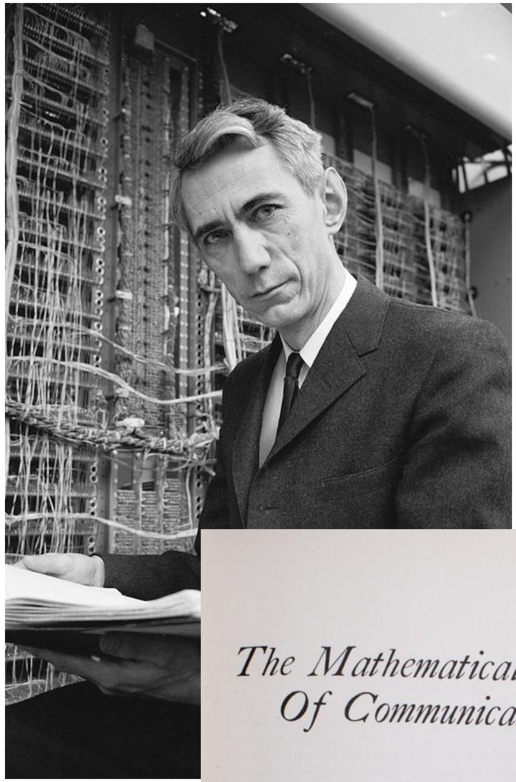
- We can show that it is equivalent to negative log-likelihood

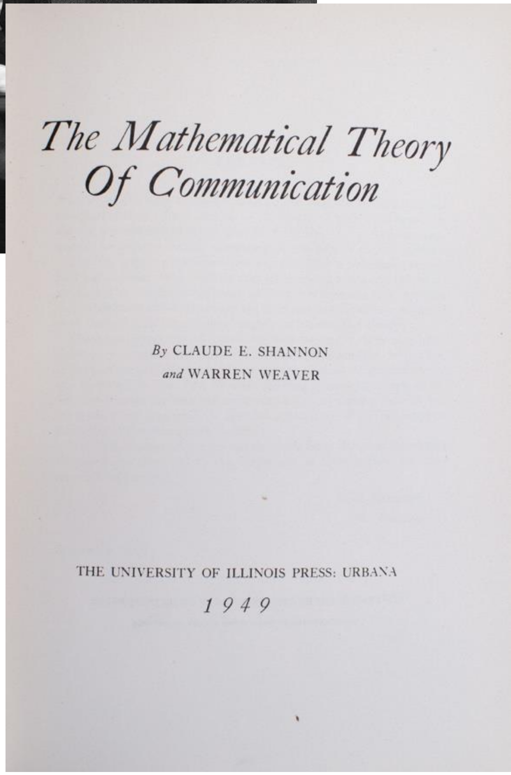
One can approach problems from different mathematical formulations.

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.

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





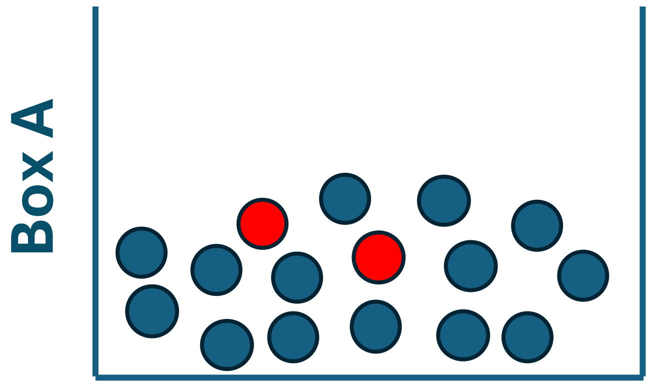
The Mathematical Theory Of Communication

By CLAUDE E. SHANNON
and WARREN WEAVER

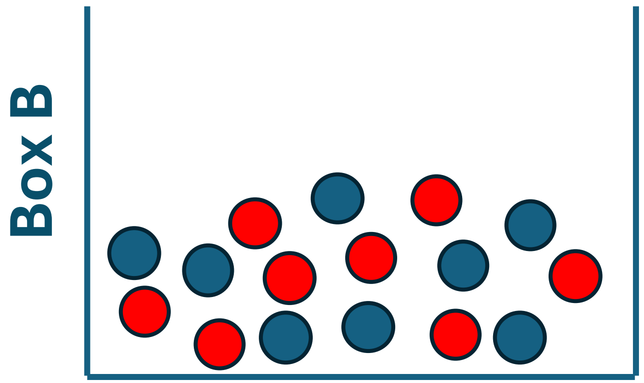
THE UNIVERSITY OF ILLINOIS PRESS: URBANA
1949

Entropy is a measure of *surprise* or *uncertainty*

Randomly pick a ball from the box



Low or High
Entropy?



Low or High
Entropy?

In class poll: https://piazza.com/class/m5v834h9pcatx/post/27

Connection to Deep Learning

Cross-Entropy Loss

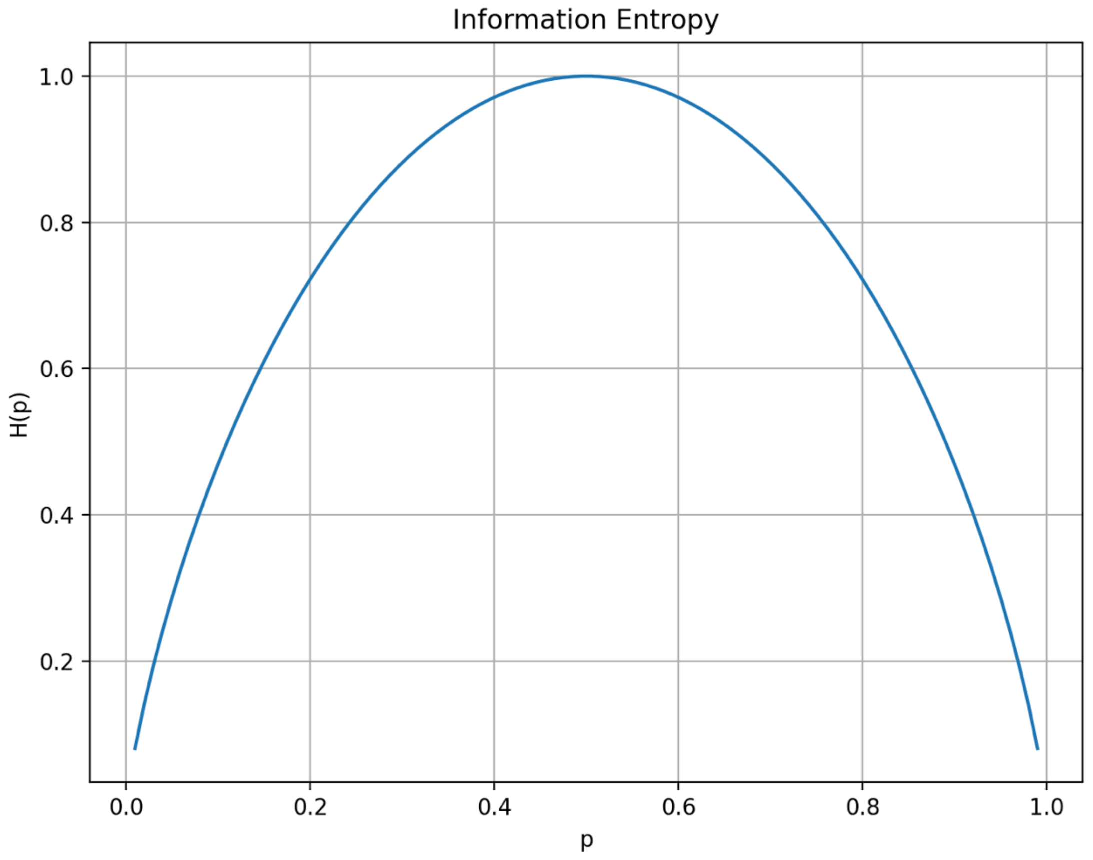
- If a neural network predicts **(0.25, 0.25, 0.25, 0.25)** for four possible classes, **high entropy** → uncertain.
- If it predicts **(0.99, 0.01, 0, 0)**, **low entropy** → confident.

Regularization & Overfitting

- A **high-entropy** model makes diverse predictions → good for exploration.
- A **low-entropy** model could be overconfident → might overfit.

"Raise the temperature in LLMs."

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

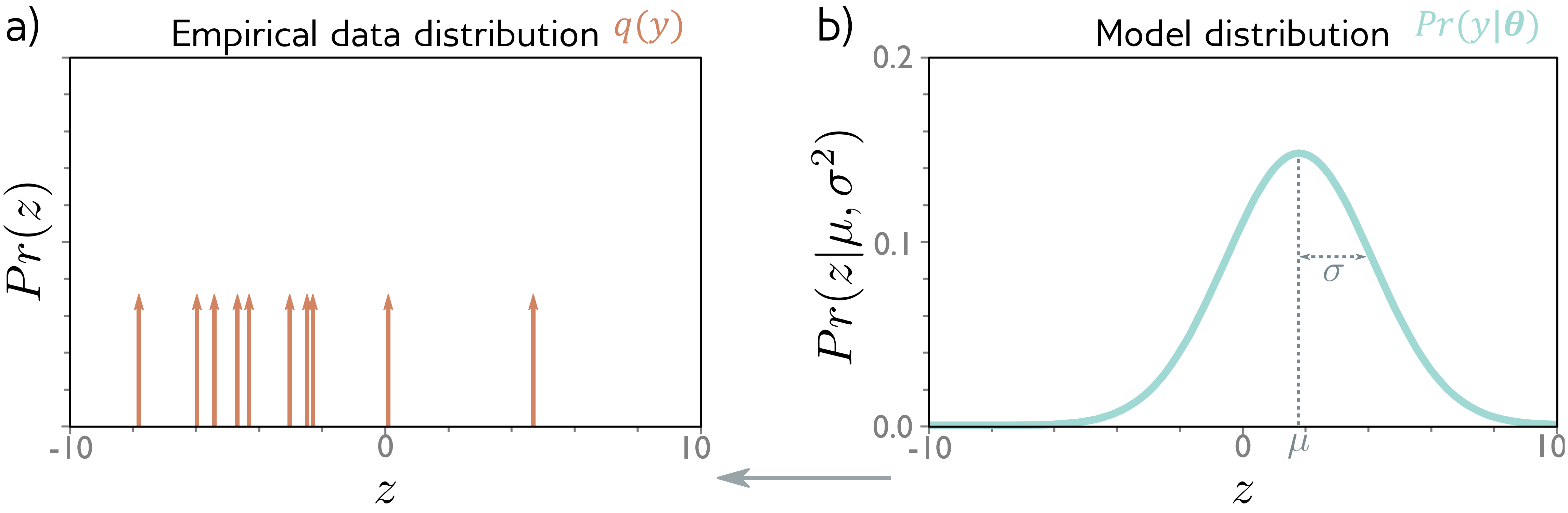


Peaks at 50/50.

$$H(x) = -\sum_x P(x)\ \log_2\big(P(x)\big) = -p\log_2(p) - (1-p)\log_2(1-p)$$

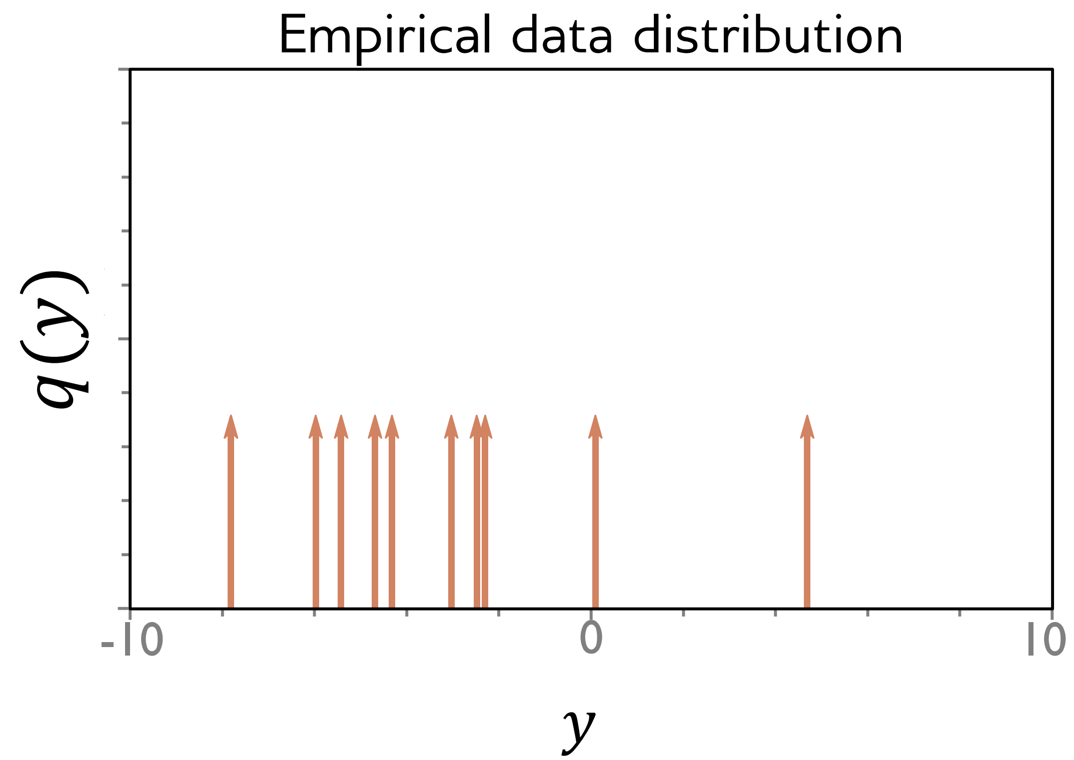
Cross Entropy – Concept from Information Theory

Measures the difference between the empirical distribution, $q(y)$, and a model distribution, $\Pr(y|\theta)$.



Kullback-Leibler Divergence -- a measure between probability distributions

Empirical Distribution – Collection of samples



Each sample represented by a shifted Dirac delta function.

$$\int \delta[x - x_0]dx = 1$$

$$\int f[x]\,\delta[x - x_0]\,dx = f[x_0]$$

So, we say empirical distribution is

$$q(y) = \frac{1}{I}\sum_{i=1}^{I} \delta[\,y - y_i]$$

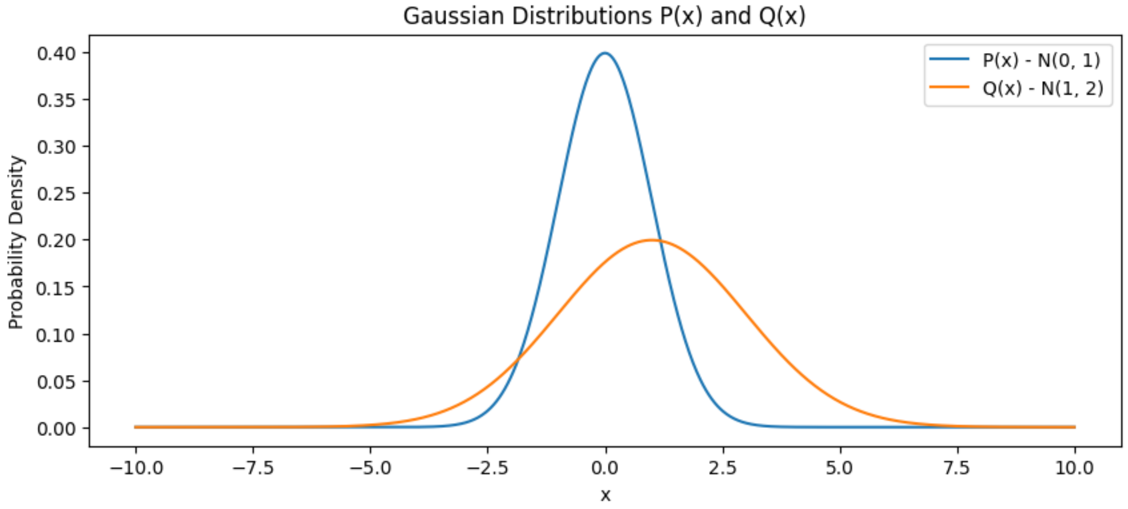
which will be helpful formulation in a moment.

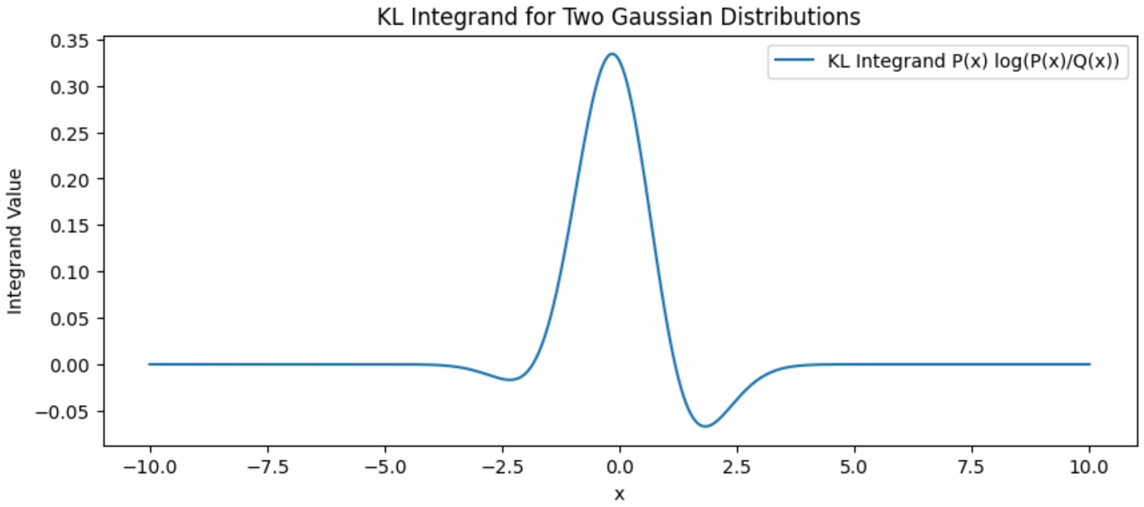
Kullback-Leibler (KL) divergence

How much a model distribution, Q, is different from a true probability distribution, P.

$$D_{KL}[q(z) \parallel p(z)] = \int q(z) \log \frac{q(z)}{p(z)} dz$$

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



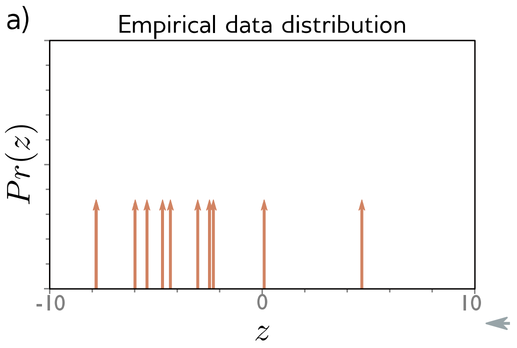


[Interactive Colab Notebook]

KL Divergence: 0.4431

Derivation

$$q(y) = \frac{1}{I}\sum_{i=1}^{I}\delta[y - y_i],$$



Training dataset as collection of Dirac delta functions.

Derivation

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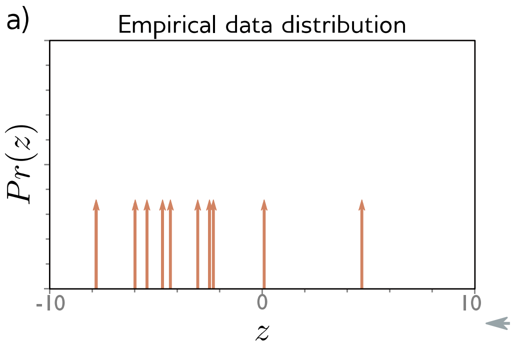

Training dataset as collection of Dirac delta functions.

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\text{argmin}}\left[\int_{-\infty}^{\infty} q(y)\log\big[q(y)\big]dy - \int_{-\infty}^{\infty} q(y)\log\big[Pr(y|\boldsymbol{\theta})\big]dy\right]$$

Minimize KL divergence.

Derivation

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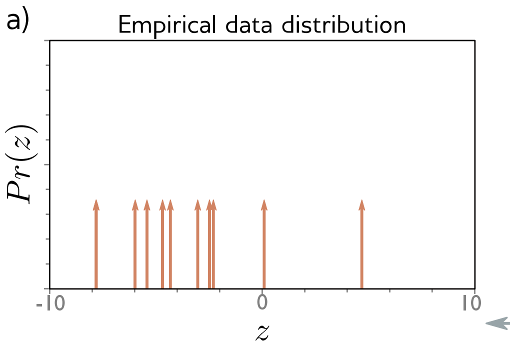

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Minimize KL divergence.

1st term not dependent on θ.

Derivation

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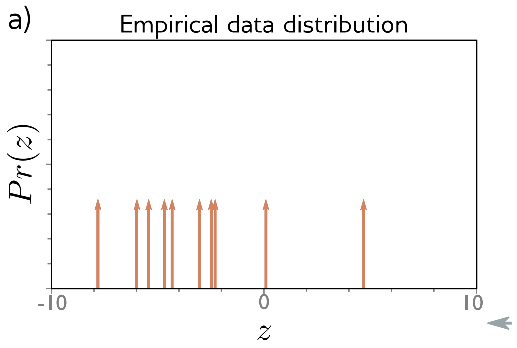

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Substituting for $q(y)$.

Derivation

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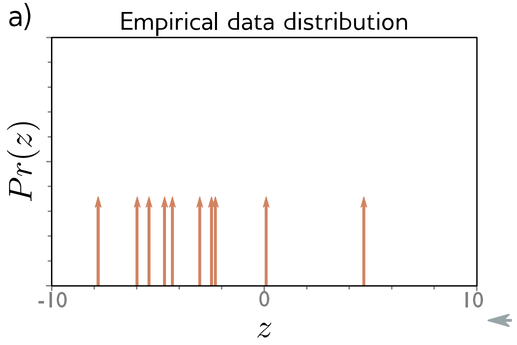

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$$= \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\left[-\frac{1}{I}\sum_{i=1}^{I}\log\bigl[Pr(y_i|\boldsymbol{\theta})\bigr]\right]$$

Property of the Dirac delta function.

Derivation

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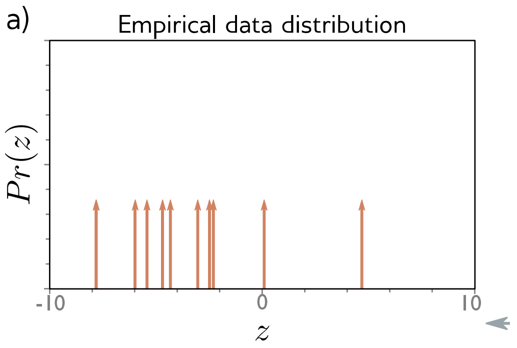

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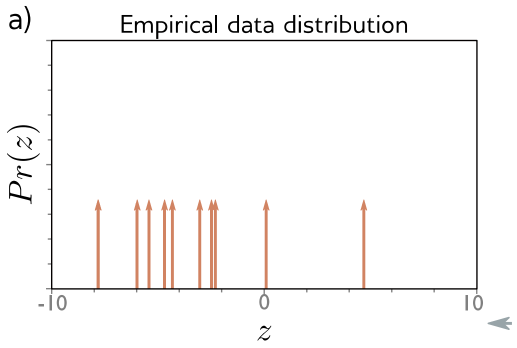
Substituting for $q(y)$.

Property of the Dirac delta function.

$^1/_I$ is just a constant, so ignore.

Derivation

$$q(y) = \frac{1}{I}\sum_{i=1}^{I} \delta[y - y_i],$$



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Minimize KL divergence.

$$= \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\left[-\int_{-\infty}^{\infty} q(y)\log\big[Pr(y|\boldsymbol{\theta})\big]dy\right],$$

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Substituting for $q(y)$.

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$^1/_I$ is just a constant, so ignore.

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

Model is predicting θ ➔ **Negative Log Likelihood!!**

Minimizing Negative Log Likelihood (or equivalently KL Divergence)

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

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